1ST Annual CASL Round Table Meeting
North Carolina State University
Centennial Campus
Building EBIII, Room 2124
Raleigh, NC
August 9-11, 2011

Welcome to the 1st Annual CASL Round Table Meeting!

Travel Arrangements:
All travel arrangements will be made by each individual through their own institution.

Parking:
North Carolina State University parking is $2.00 per day. Centennial Campus requires visitors to purchase a parking permit at the Information Booth located on Varsity Drive. For your convenience please advise the attendant that you will require multiple days for your permit. Please pay for the parking permit and include this in your expenses for the trip. The attached map indicates where parking is available.

Registration:
There will be tables set up in the foyer of the EBIII building. Please allow enough time to stop by these tables to pick up your badge and register your attendance.

Meals:
All meals will be provided each day. There will be a variety of items to ensure your dietary needs are met.

Posters:
If you will be presenting a poster during the Wed poster session please deliver them to the registration desk at the time of your registration. All posters must be turned in for review by noon on Tuesday, August 9.

Directions:
Attached is a map of how to get from the RDU airport to NCSU. Once you are there please enter the NW corner of the building (signage will guide the way).

If you have any questions please contact Ronaldo Szilard (208) 757-3030, ronaldo.szilard@inl.gov or Linda Weltman (865) 574-9970, weltmanlk@ornl.gov/Hermine Kabbendjean (919) 513-2275.

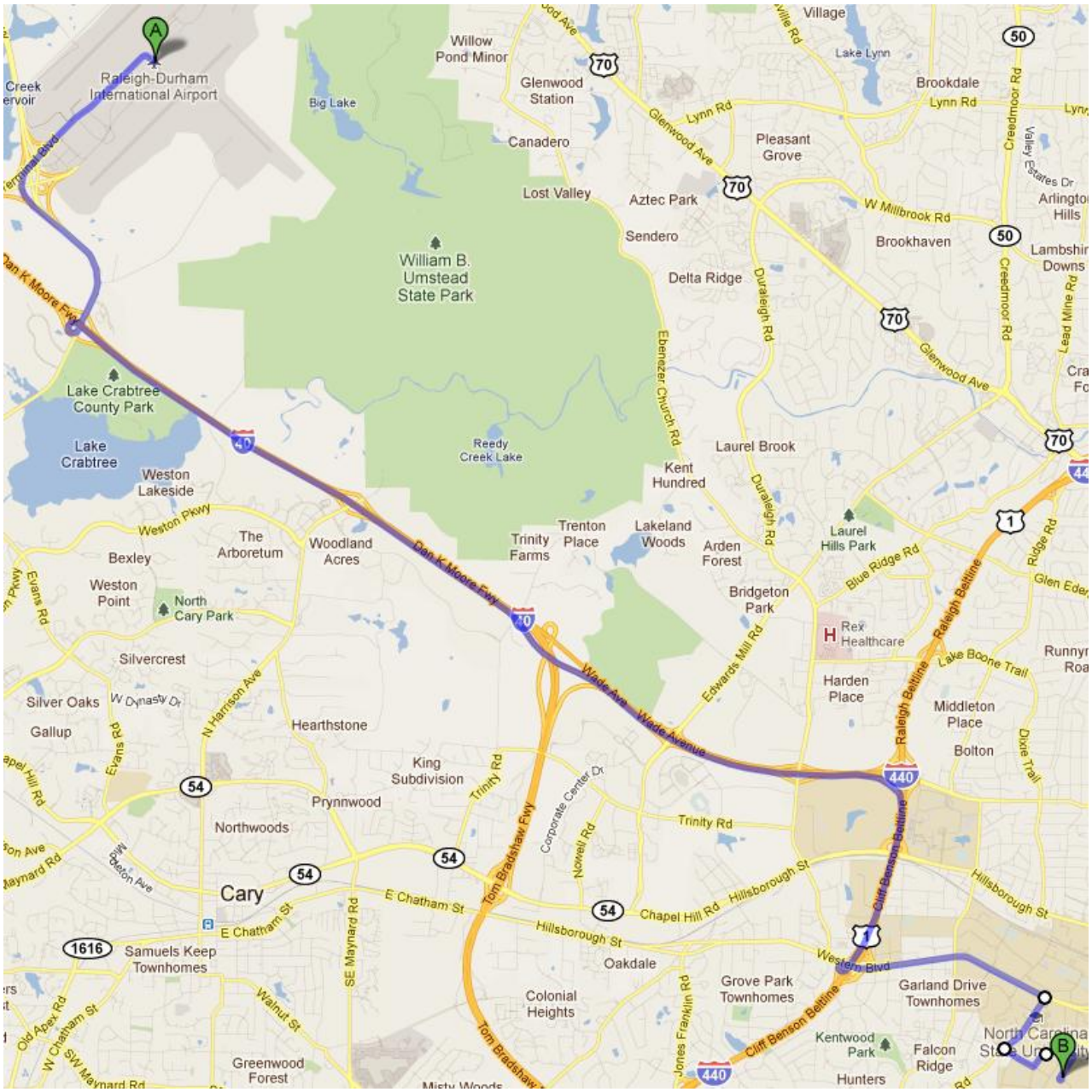
Consortium for Advanced Simulation of LWRs

CASL ROUND TABLE MEETING -- AGENDA

North Carolina State University
Centennial Campus, Building EBIII, Room 2124
Raleigh, NC
August 9-11, 2011

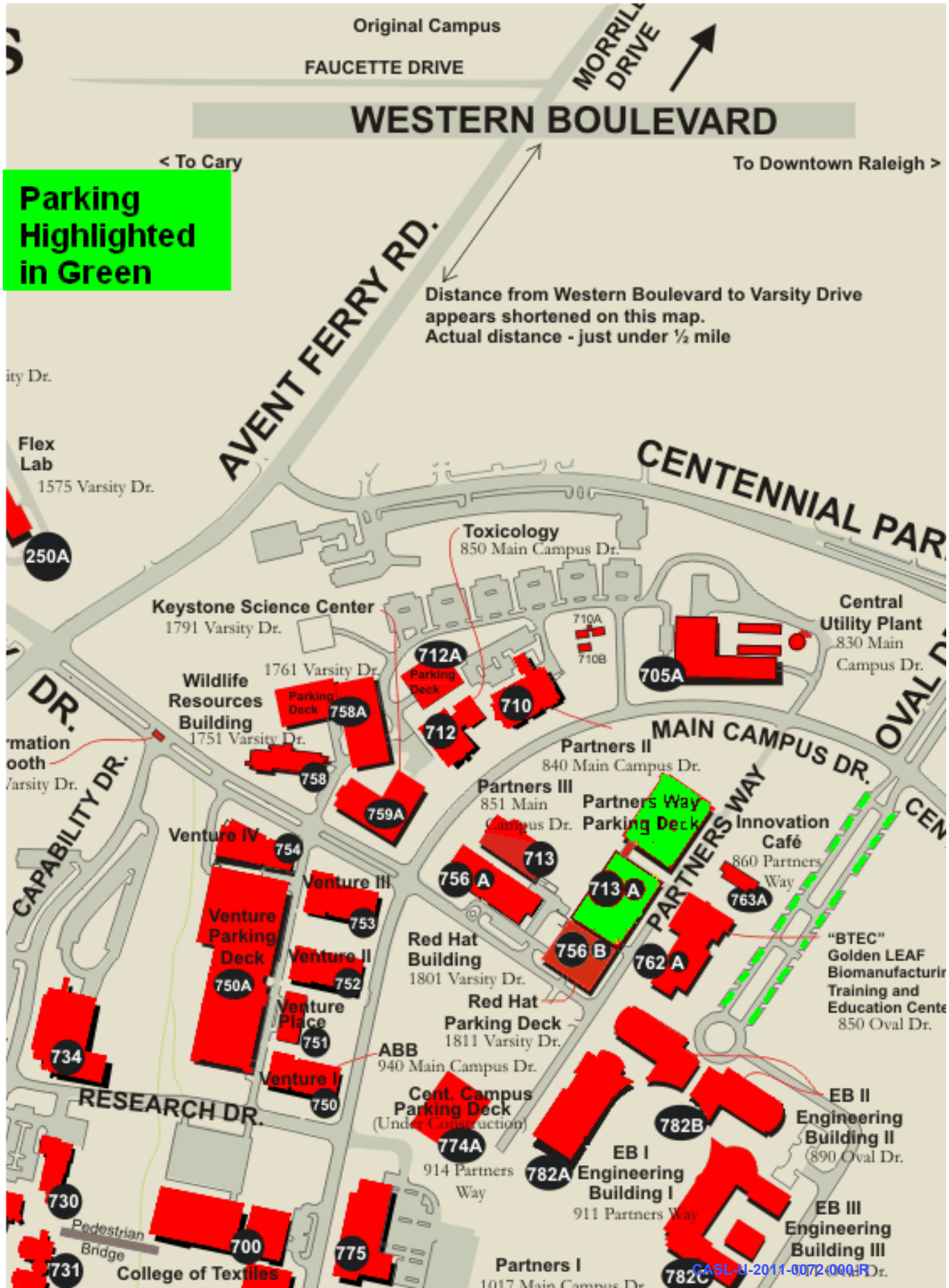
Tuesday, August 9, 2011		Speaker	Master of Ceremony
7:30 am – 8:00 am	Registration		Linda Weltman/ Hermine Kabbendjian
8:00 am – 8:30 am	Introduction and Welcome	Louis Martin-Vega, NCSU Terri Lomax, NCSU Doug Kothe Ronaldo Szilard	Doug Kothe
8:30 am – 9:15 am	Opening - Motivation, EPRI	David Modeen	
9:15 am – 10:00 am	Industry Needs, WEC	Sumit Ray	
10:00 am – 10:30 am	Break		
10:30 am – 11:30 am	Charge, Vision	Doug Kothe	
11:30 am – 12:15 pm	Industry Council	John Gaertner	
12:15 pm – 1:00 pm	Working Lunch, Fuel Challenges, *Room 2402*	Rose Montgomery	
1:00 pm – 1:30 pm	CASL Goals	Paul Turinsky	Paul Turinsky
1:30 pm – 2:15 pm	CRUD	Zeses Karoutas	
2:15 pm – 3:00 pm	GTRF, FAD	Zeses Karoutas/ Jeff Secker/ Yixing Sung/Jin Yan	
3:00 pm – 3:30 pm	Break		
3:30 pm – 4:00 pm	PCI	Chris Stanek / Rich Martineau	
4:00 pm – 4:30 pm	Strategic Plan	Mario Carelli	
4:30 pm – 5:00 pm	Life Extension	Ronaldo Szilard	
5:00 pm – 5:30 pm	Advanced Fuels	Kurt Edsinger	
6:00 pm – 8:00 pm	Banquet – Invited Talk: Effective Public Communication of the Fukushima Event, *Room 2402*	Margaret Harding, 4 Factor Consulting	
Wednesday, August 10, 2011			
8:00 am – 10:15 am **VRI**	- Overview (process & testing infrastructure) - ANC/VIPRE/BOA evolution - DeCART/Star (software challenges, numeric, etc.) - SCALE reactor and neutronics status/plans - Panel/Q&A	John Turner/ Randy Summers Rod Schmidt/Jeff Secker Ben Collins Jay Billings (remote)/ Greg Davidson All VRI	John Turner
10:15 am – 10:45 am	Break		
10:45 am – 12:15 pm **MPO**	- Overview - PCI - Peregrine - CRUD formation and growth - Mamba	Chris Stanek	Chris Stanek

	- GTRF - Crosscutting activities		
12:15 pm – 1:15 pm	Working Lunch, Facilities (VOCC), *Room 2402*	April Lewis (remote)/ Doug Kothe	
1:15 pm – 3:00 pm **RTM**	- RTM Overview including status of current projects - RTM activities for FY12 and long term strategy - Panel discussion	Bill Martin John Wagner All RTM	Bill Martin
3:00 pm – 3:30 pm	Break		
3:30 pm – 5:45 pm **THM**	- THM overview - Overview of ITM and experiments - Drekar CFD code and GTRF results - The latest on DEM and 7-equation model - Sensitivity study results - Industry perspective - Specific ITM results - Panel discussion	Rob Lowrie Jacopo Buongiorno John Shadid Ray Berry Chris Fidkowski Jin Yan Gretar Tryggvason All THM	Rob Lowie
6:00 pm – 8:00 pm	Reception, *EBIII Lobby*	Student Poster Session	Paul Turinsky
Thursday, August 11, 2011			
8:00 am – 10:00 am **AMA**	- Overview, Issues, and Challenges - Assessment of the Status of Integrated Virtual Reactor Simulation - Physical Reactor Data Measurements and Needs - Development and Implementation of a Predictive Capability Maturity Model (PCMM)	Jess Gehin Scott Palmtag Rose Montgomery Steve Hess	Jess Gehin
10:00 am – 10:30 am	Break		
10:30 am – 12:30 pm **VUQ**	- Overview - VUQ activities for Crud - VUQ activities for GTRF - CASL Validation Data - VUQ Issues, Risks, and Challenges	Jim Stewart Brian Adams Bill Rider Nam Dinh Jim Stewart/Dana Kelly	Jim Stewart
12:30 am – 1:30 pm	Working Lunch, Education Mission, *Room 2402*	John Gilligan	
1:30 am – 2:00 pm	Product Description Rollout	Rose Montgomery	
2:00 pm – 3:00 pm	Closing Ceremony: - Discussion of problems - Award Ceremony	CASL SLT	Ronaldo Szilard
3:00 pm – 6:00 pm	Closed Session – CASL ELT	By Invitation Only	CASL ELT
Friday, August 12, 2011			
8:00 pm – 12:00 pm	Closed Session – CASL ELT	By Invitation Only	CASL ELT



Head northwest on Terminal Blvd toward W International Dr	go 220 ft
Keep left at the fork	go 1.2 mi
Take the Aviation Pkwy S ramp on the left to I-40 E/Raleigh	go 0.6 mi
Merge onto Aviation Pkwy	go 0.8 mi
Take the Interstate 40 E/Dan K Moore Freeway ramp	go 0.2 mi
Merge onto I-40 E	go 3.7 mi
Slight right onto Wade Ave/Wade Avenue (signs for I-440/US-1 N)	go 2.9 mi
Take the I-440 S/US-1 S exit toward I-40 E/Hillsborough St/Sanford	go 0.4 mi
Merge onto I-440 W/US-1 S	go 1.2 mi
Exit onto Western Blvd toward N C State Univ/Downtown	go 1.7 mi
Turn right onto Avent Ferry Rd	go 0.5 mi
Turn left onto Varsity Dr	go 0.3 mi
Turn left onto Main Campus Dr	go 0.3 mi
Turn right onto Oval Dr	go 0.2 mi

911 Oval Dr, Raleigh, NC 27606


Original Campus
FAUCETTE DRIVE
MORRILL DRIVE
WESTERN BOULEVARD
< To Cary
To Downtown Raleigh >
Parking Highlighted in Green
Distance from Western Boulevard to Varsity Drive appears shortened on this map.
Actual distance - just under ½ mile
AVENT FERRY RD.
CENTENNIAL PAR
Flex Lab
1575 Varsity Dr.
250A
Toxicology
850 Main Campus Dr.
Keystone Science Center
1791 Varsity Dr.
Central Utility Plant
830 Main Campus Dr.
710A
710B
705A
712A
Parking Deck
710
712
Wildlife Resources Building
1751 Varsity Dr.
1761 Varsity Dr.
Parking Deck
758A
758
759A
MAIN CAMPUS DR.
Partners II
840 Main Campus Dr.
Partners III
851 Main Campus Dr.
Partners Way Parking Deck
PARTNERS WAY
Innovation Café
860 Partners Way
763A
CAPABILITY DR.
Venture IV
754
Venture III
753
Venture Parking Deck
750A
Venture II
752
Venture Place
751
Venture I
750
713
713 A
756 A
756 B
762 A
Red Hat Building
1801 Varsity Dr.
Red Hat Parking Deck
1811 Varsity Dr.
"BTEC" Golden LEAF Biomanufacturing Training and Education Center
850 Oval Dr.
734
ABB
940 Main Campus Dr.
RESEARCH DR.
Cent. Campus Parking Deck
(Under Construction)
774A
914 Partners Way
782B
782A
EB I Engineering Building I
911 Partners Way
EB II Engineering Building II
890 Oval Dr.
EB III Engineering Building III
730
Pedestrian Bridge
700
775
731
College of Textiles
Partners I
782C

Industry Needs Presentation

CASL Roundtable Meeting
August 9 to 11, 2011

Sumit Ray, Director

New Reactor Fuel Engineering

Westinghouse Electric Company

CASL-U-2011-0072-000-R

Outline

- Key Industry benefits of current challenge problems
- Connecting the Dots Between CASL, the Vendors, Utilities and the Ratepayers
  - Using Uprating programs as an example
- Some post Fukushima considerations consistent with the CASL core mission

Key Challenge Problems Limiting Reactor Performance

	Power uprate	High burnup	Life extension
Operational			
CRUD-induced power shift (CIPS)	✕	✕	
CRUD-induced localized corrosion (CILC)	✕	✕	
Grid-to-rod fretting failure (GTRF)		✕	
Pellet-clad interaction (PCI)	✕	✕	
Fuel assembly distortion (FAD)	✕	✕	
Safety			
Departure from nucleate boiling (DNB)	✕		
Cladding integrity during loss of coolant accidents (LOCA)	✕	✕	
Cladding integrity during reactivity insertion accidents (RIA)	✕	✕	
Reactor vessel integrity	✕		✕
Reactor internals integrity	✕		✕

As Identified, the Challenge Problems do Address Many Key Industry Needs

- CIPS & CILC
  - In-depth phenomenological understanding is sorely needed as reactors move to higher power densities, or change chemistry programs
- Grid- to- Rod Fretting
  - Key understanding will enable faster prototype fuel development and enable more advanced fuel designs
    - Modelling of the complex area around the baffle would be a plus
      - These are the areas most susceptible to GTRF
- Pellet Clad Interaction
  - Accurate models will provide a much better understanding of margins
    - Can provide operator guidance, and reduce overly conservative restrictions that currently exist for power maneuvers
    - Can provide insights into better pellet designs

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As Identified, the Challenge Problems do Address Many Key Industry Needs

- Fuel Assembly Distortion
  - Better understanding would remove semi empirical methods that are in use today
  - Overly conservative assumptions in place today limit burnup
    - Better knowledge of key phenomenon will allow more reactor operating margins and potentially better fuel designs
- Departure From Nucleate Boiling
  - Current empirical correlations do not allow for any extrapolation
  - New fuel designs cannot be developed without a DNB test
  - Phenomenological understanding will open up many new possibilities for higher reactor operating margins
- Cladding integrity during LOCA
  - NRC about to impose restrictions based on research done to date
  - These restrictions impact fuel cycle economics and reduce allowable burnup
  - Better understanding would potentially allow some of these restrictions to be lifted

As Identified, the Challenge Problems do Address Many Key Industry Needs

- Cladding Integrity During RIA
  - It will be difficult to model the complex interactions that are involved
  - But demonstrating margins based on fundamental understanding will help programs such as mega upratings
- Reactor Vessel Integrity & Reactor Internals Integrity
  - Understandings will help life extension programs, and will clearly be need for life beyond 60 years
  - Will also help in understanding margins during upratings

Connecting the Dots Between CASL, the Vendors, Utilities and the Ratepayers

Two Questions Come to mind:

- " Assuming the CASL project is successful in solving the challenge problems, so that the simulation of the PWR core is much more advanced than today, how can we leverage this knowledge to benefit the utility and the ratepayer?"

- In light of Fukushima, what contribution can CASL make that is consistent with its core mission?

POWER UPRATE

Types of Power Uprates - Terms

Measurement Uncertainty Recapture (MUR) Power Uprate: $1\% \leq X \leq 2\%$

Taking credit for a way to reduce inaccuracy in feed water flow measurement hence more accurate calculation of power calorimetric

Stretch Power Uprate (SPU): $2\% \leq X \leq 7\%$

Within the design capacity of the plant; Usually involves changes to instrumentation setpoints but NOT major plant modifications

Extended Power Uprate (EPU): $X > 7\%$

EPUs require significant modifications to major BOP equipment (e.g., high-pressure turbines, condensate pumps & motors, main generators and/or transformers)

CASL Efforts would be most useful in enabling the Extended Power Uprate Scenario

Typical Uprate Work Scope

NSSS Scope
- Fuel
- Safety Analyses
- Systems & Components

BOP Scope
- Systems & Components
- Design Change Packages
- Installation

Turbine/Generator Scope
- HP Turbine upgrade/modifications
- Generator Rewind/Replacement

Licensing Scope
- License Amendment Request
- FSAR, Tech Spec, etc

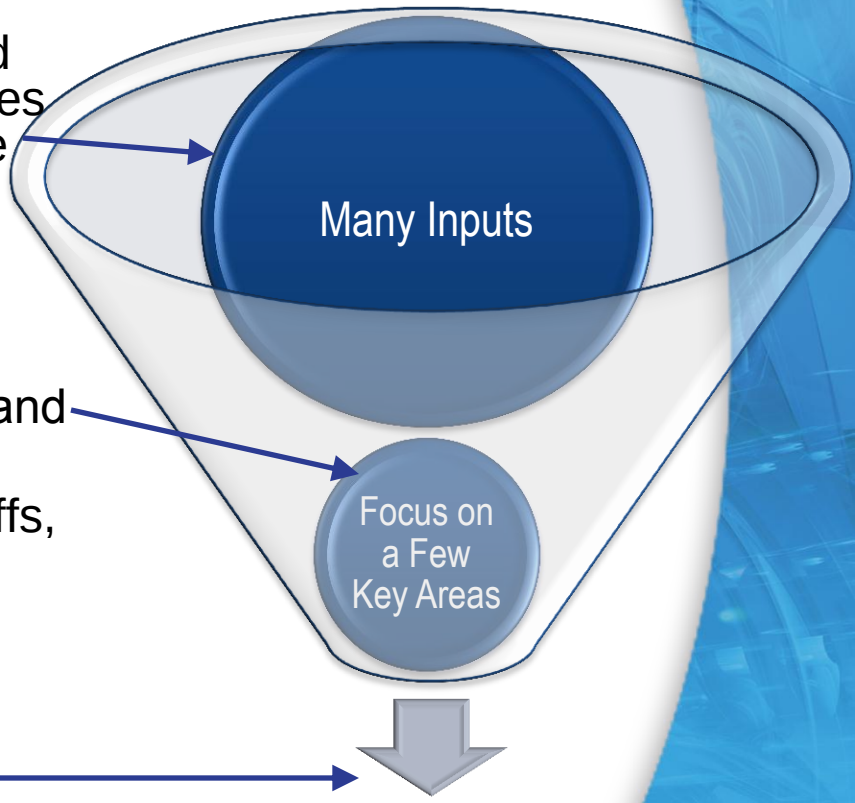
Environmental Impact
- State, Federal, Local

Grid Impact Studies

Outage Planning
- Training, simulator, procedures, etc

Typical 3 Step Process for Uprates

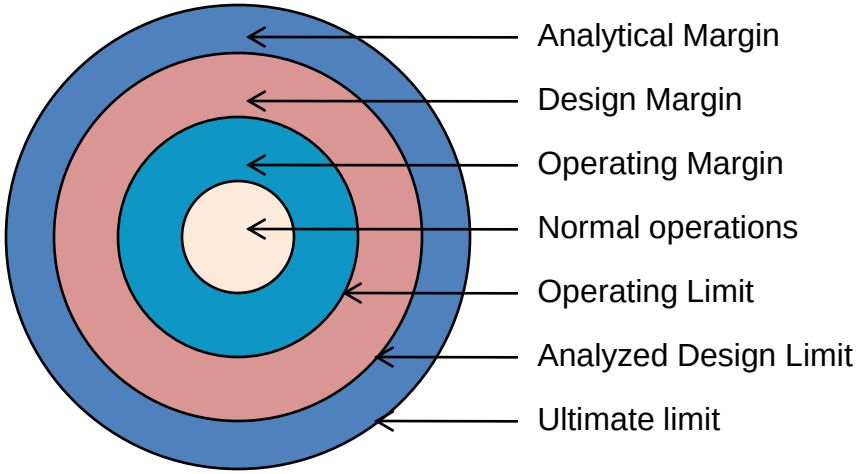
- Step 1: Joint Expert Panel
  - Determine recommended target uprated power level, identify limiting plant features and regulatory approval issues, provide preliminary schedule and budgetary estimates
- Step 2: Feasibility Study
  - Using Expert Panel results, perform "scoping" calculations to better identify and understand selected pinch points
  - Recommend margin usage and trade-offs, fuel design, operating parameters, and regulatory approach
  - Refine work scope and cost required to implement uprate
- Step 3: Technical Work Scope
  - Perform uprate program and obtain regulatory approval to operate at uprated thermal power



This 3 step phased uprating process follows the concepts identified in NEI-08-10 and has resulted in a 100% success rate for achieving upratings at plants throughout the world

Margin Management Overview

- Establishing or maintaining a margin management program is the best way to make sure that the reactor will operate efficiently and safely



The CASL toolbox is ideally suited to provide enhanced insights in the area of critical reactor margins

Margin Management

- Effective Margin Management requires a Strategic approach rather than tactical decisions.
  - How much is needed? How to allocate?
  - How can margin be transferred from one bucket to another?
- Key considerations:
  - Plant operating parameters & assumptions (plant optimization & flexibility, load follow)
  - Fuel hardware (advanced product features & materials)
  - Design software and methodology (advanced technologies)
  - Core monitoring
  - In-core fuel management
  - Margins for the unknown or uncertain
  - Reload flexibility
  - Regulatory changes

Margin trade-offs and evaluation of risks require involvement of many stakeholders within the Utility (Fuels and Plant Operations) and Suppliers (BOP, NSSS, T/G, etc.)

Key Margin Recovery Areas listed in NEI- 08-10 and Areas of CASL Relevance

- There are a variety of ways to recover margin, including:
  - Change in design or operation or testing
  - Reduced safety factor
  - Reduced calculational conservatism (possibly employing advanced analytic tools)
  - Changes to design characteristics of a limiting variable
  - Decrease in the margin of one parameter to increase the margin in another
  - Modification of system or component

What can CASL do to Connect the Dots?

Some thoughts:

1. Develop the linkage between the CASL tools and key industry needs (e.g. upratings, burnup, life extension) and use these linkages to guide future development

   - This will also enable the ability to demonstrate what benefit CASL tools can provide under different scenarios

2. After completing item 1, perform an assessment to determine if there are any key gaps that should be addressed that are within CASL's core mission

3. Develop an application process for the CASL tools that could become the standard for risk management assessments as the industry continues to look to squeeze more power from reactor cores

Post Fukushima Considerations (consistent with CASL strategic objectives)

- CASL white paper does a very good job in defining the strategy for post Fukushima response:
  - Partner with another organization (e.g.,Sandia) that will carry the major responsibility for modelling severe accidents
  - Provide a linkage between VERA , or bring the analysis of severe accidents into the VERA framework, utilizing the LIME software structure
- Additionally, Fukushima has raised the issue of what can be done to develop revolutionary fuel designs that have significantly higher margins to severe accidents:
  - CASL could take a central role in developing the modeling capability of fuels such as Silicon Carbide

Summary

- CASL Objectives as defined do address key industry needs
- Drawing a direct line of sight to how CASL tools will be used by the industry, and maintaining this throughout the program, is important to ensure industry adoption
- While CASL's key mission may not (and should not) address all the issues for upratings, increased burnups or life extension, CASL tools should be developed so that they can become an essential element of the activities that are required for these programs

CASL Year One

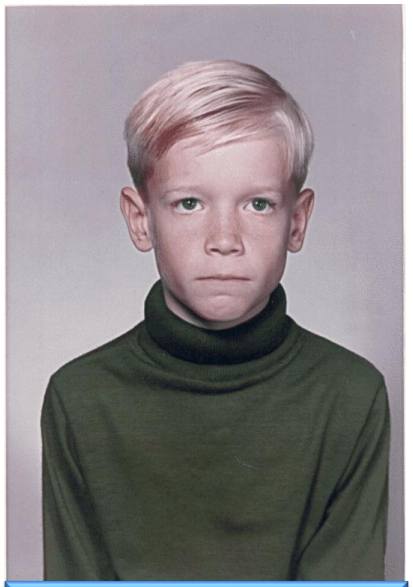
Doug Kothe

Inaugural CASL Roundtable
North Carolina State University
August 9, 2011

CASL-U-2011-0072-000-R

Outline

- How did we get here?
  - Retrospective: DOE Hub FOA and what we said in the proposal
- Year 1: how did we do?
- Bumps along the way
- Path forward (Year 2 …)
- End game



Pre-CASL

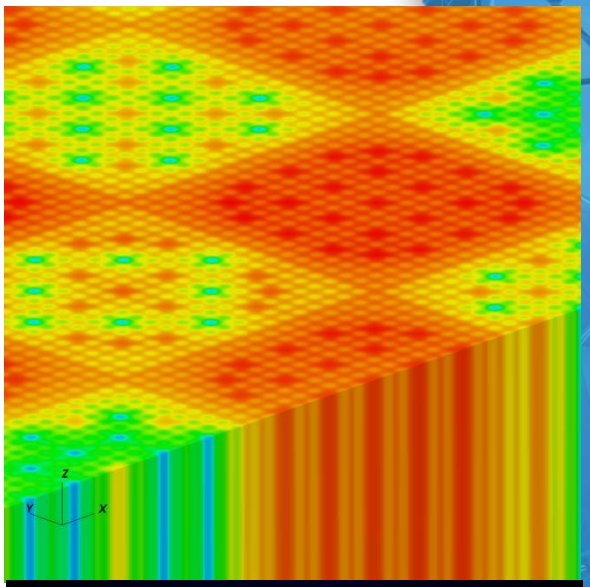
CASL years are like dog years

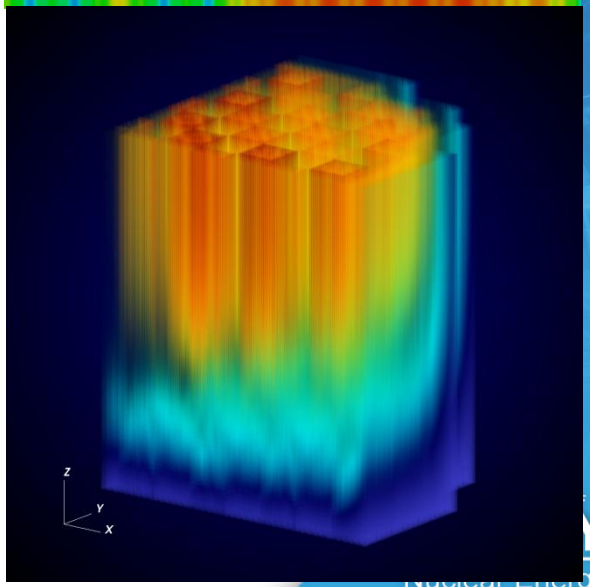
What is a DOE Energy Innovation Hub?

- Target problems in areas presenting the most critical barriers to achieving national climate and energy goals that have heretofore proven the most resistant to solution via the normal R&D enterprise
- Represent a new structure, modeled after research entities likes
  - the Manhattan Project (nuclear weapons), Lincoln Lab at MIT (radar), and AT&T Bell Labs (transistor)
- Consistent with Brookings Institution's recommendations for "Energy Discovery-Innovation Institutes" (early 2009)
  - "…new research paradigms are necessary, we believe, that better leverage the unique capacity of America's research" - Dr. Jim Duderstadt, President Emeritus, University of Michigan
- Focus on a single topic, with work spanning the gamut, from basic research through engineering development to partnering with industry in commercialization
- Large, highly integrated and collaborative creative teams working to solve priority technology challenges
  - Bring together the top talent across the R&D enterprise (gov, academia, industry, non-profits) to become a world-leading R&D center in its topical area

Attributes Sought by DOE for the Energy Innovation Hub for Modeling & Simulation of Nuclear Reactors

- **Utilize existing** advanced modeling and simulation capabilities developed in other programs within DOE and other agencies
- **Apply them** through a new multi-physics environment **and develop capabilities *as appropriate***
- **Adapt the new tools** into the current and future culture of nuclear engineers and produce a multi-physics environment to be used by a wide range of practitioners **to conduct predictive simulations**
- Have a **clear mission that focuses and drives R&D**
- Use **data from real physical operation reactors to validate** the virtual reactor
- Lead organization with **strong scientific leadership** and a clearly defined central location ("one roof" plan)





Timeline from inception to award (>1 year)

- 04/06/2009: Secretary Chu proposes 8 Energy Innovation Hubs
  - "mini-Bell Labs" focused on tough problems relevant to energy
  - $25M per yr for 5 years, with possible 5-yr extension
- 06/25/2009: House bill does not approve any of the 8 proposed Hubs
  - provides $35M in Basic Energy Sciences for the Secretary to select one Hub
- 07/09/2009: Senate approves 3 of the 8 proposed hubs, but at $22M
  - Fuels from sunlight (in BES)
  - Energy efficient building systems (in EERE)
  - Modeling and simulation (in NE)
- 07/22/2009: Johnson memo providing more detail on Hubs
- 10/01/2009: Final bill out of conference matches Senate bill
- 12/07/2009: Informational workshop
- 01/20/2010: FOA released
- 03/08/2010: proposals due ~~(originally 3/1/10)~~
- 04/23/2010: CASL site visit at ORNL
- 05/28/2010: CASL selected

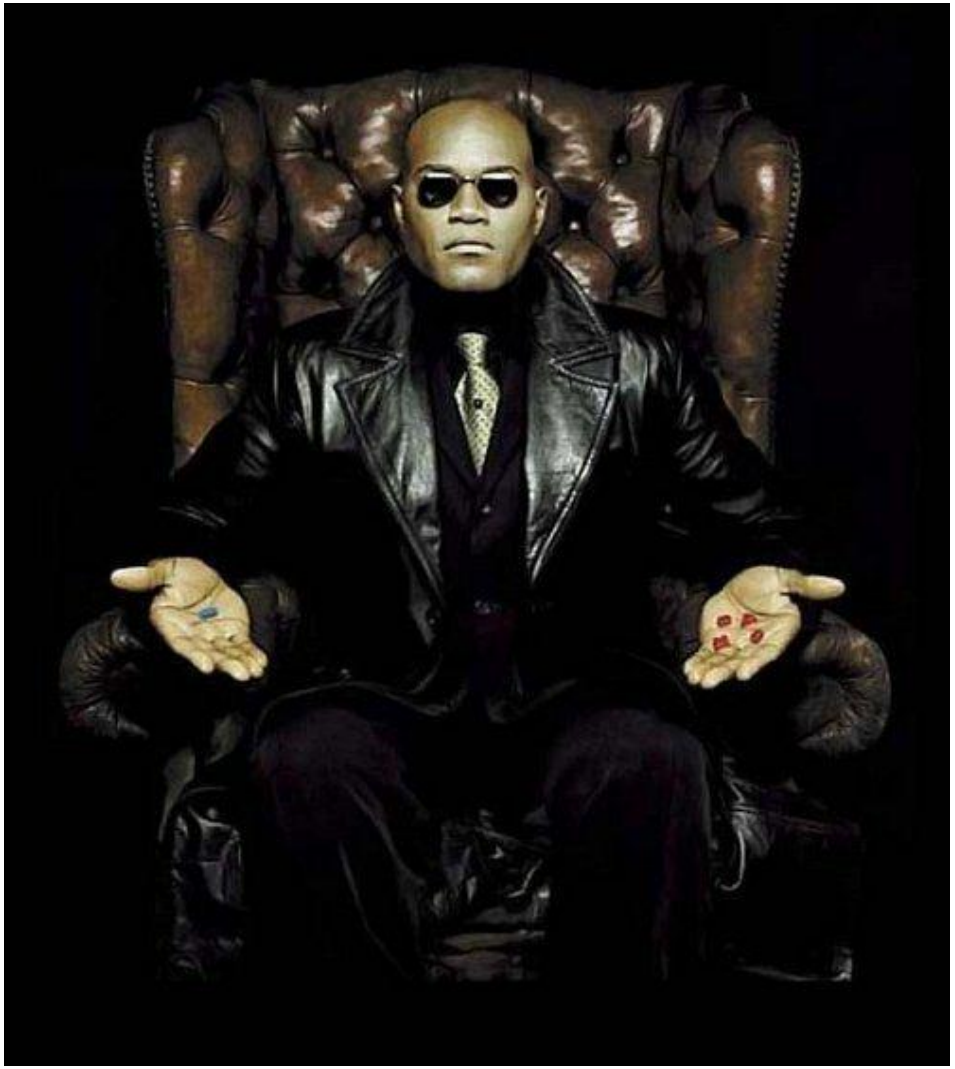
~45 days!!

Merit Review Criteria Used to Judge Proposals for the Energy Innovation Hub for M&S of Nuclear Reactors

- Criterion 1: Technical Quality (30%)
  - Physical nuclear and its relevance/impact
  - M&S environment and the existing and advanced physics capabilities within that environment; proposed middleware to be used within that environment
  - Support of education and training
  - Adequacy and appropriateness of schedule, including sequencing of tasks and milestones
  - Acceptability of assignment of responsibilities and level of resources
- Criterion 2: Potential for Successful Hub Execution (40%)
  - Requirements and risk management and SQA
  - Quality and credibility of schedule; cost effectiveness and efficiency of design
  - V&V and UQ approach
  - ES&H and security
  - One-roof approach and management
- Criterion 3: Applicant Team Capabilities (30%)
  - Team's ability to provide expertise and experience
  - Team's ability to deliver
  - Involvement, communication, and collaboration of team

In retrospect 70% on "non technical" was about right

I think we took (or were given) the red pill when CASL won the award ….



This is your last chance. After this, there is no turning back. You take the blue pill - the story ends, you wake up in your bed and believe whatever you want to believe. You take the red pill - you stay in Wonderland and I show you how deep the rabbit-hole goes.

We "sprinted a marathon" to get here

- You can't be too organized or too prepared or start too early
  - First planning meeting: Jul 09
  - 11 large group meetings total (Dallas!); many more smaller meetings
- Assemble a proposal team that mirrors the eventual hub team
  - Leadership, operations (project management, IP, contracts, finances, facilities, quality, etc.), support (IT, writing/editing, graphics, etc.)
- Communicate, communicate, communicate
- Conduct many "red team" reviews of the proposal and site visit briefings
  - Way upstream of when you think you're ready
- Liberally allocate resources to support the proposal activity
- Try to implement and use the virtual collaboration technologies during the planning that you plan to use upon execution
- Industry partners are keys to success

Unsolicited advice received upon award…

- Be nimble and fast-moving
- Manage and lead with engaged SMEs
- Your research should contain a high-risk, high-reward component
- This is longer term (not your normal FY funding cycles)
- Have a fierce sense of urgency
- Cover understanding *and* use with the R&D activities
- You'll get what you ask for if you act like a normal DOE program
- Should be a career opportunity for technical staff
- Don't over manage
- Don't $*&% this up

CASL targets key limiting phenomena that are barriers to improved reactor performance

	Power uprate	High burnup	Life extension
Operational "Challenge Problems"			
CRUD-Induced Power Shift (CIPS)	✖	✖	
CRUD-Induced Localized Corrosion (CILC)	✖	✖	
Grid-to-Rod Fretting Failure (GTRF)		✖	
Pellet Clad Interaction (PCI)	✖	✖	
Fuel Assembly Distortion (FAD)	✖	✖	
Safety "Challenge Problems"			
Departure from Nucleate Boiling (DNB)	✖		
Cladding Integrity during Loss of Coolant Accidents (LOCA)	✖	✖	
Cladding Integrity during Reactivity Insertion Accidents (RIA)	✖	✖	
Reactor Vessel Integrity	✖		✖
Reactor Internals Integrity	✖		✖

CASL Challenge Problems Drive the Virtual Reactor Development and Application

Challenge Problem	Description	Relevance
CRUD	CIPS: Deviation in axial power shape caused by CRUD deposition in high power density regions with subcooled boiling. CILC: Clad corrosion and failure due to CRUD deposition	Power uprates require higher power density with increased potential for CRUD growth, axial power offsets, and clad failures
GTRF	Clad failure due to flow vibration-induced rod-spring interactions amplified by irradiation-induced grid spacer growth and spring relaxation	Currently the leading cause of fuel failures in PWRs; power uprates and burnup can further increase potential for fretting failures
RPV Internals Lifetime (Life Extension)	Damage to RPV internal components caused by thermal fatigue, mechanical fatigue, radiation damage, and stress corrosion cracking.	Replacement cost of internals is high, making lifetime extension less economically attractive
DNB (Safety)	Local clad surface dryout causing dramatic reduction in heat transfer capability during certain accident transients (e.g., overpower and low coolant flow)	Power uprates require improved quantification of margins for DNB limits
FAD	Distortion or component structural failure due to excessive axial forces caused by radiation-induced swelling	Power uprates and increased burnups may increase fuel distortions and alter core power distributions and fuel handling scenarios
Advanced Fuel Forms (AF, Safety, GTRF)	Examination of new cladding material, fuel material, and fuel pin geometries.	New fuel forms will enable extended power uprates, higher fuel burnups, and lower fuel cycle costs than can be achieved by incremental modifications of current fuel forms

CASL Challenge Problems Drive the Virtual Reactor Development and Application

Challenge Problem	Description	Relevance
LOCA (Safety)	Numerous fuel failure modes resulting in fission product release and coolable geometry degradation	Realistic LOCA analyses (10 CFR 50.46) can enable power uprates that would not have been achievable with previously licensed evaluation models
RIA (Safety)	Clad failure due to rapid heating of the pellet, leading to pellet disintegration caused by the rim effect	Higher fuel burnup increases rim effect; power uprates may lead to increased energy release during RIA; currently not limiting but may change with further test data (e.g., CABRI)
PCI (Safety, AF)	Clad failure due to radiation-induced fuel rod/cladding contact from stress corrosion cracking and fuel defects	Power uprates and increased burnups increase fuel/clad contact and the likelihood for fuel failures; currently only limits power ramp rates during normal operation
Reactor Vessel Lifetime (Life Extension)	Radiation damage resulting in increased temperature for onset of brittle failure, making failure more likely due to thermal shock stresses during Safety Injection System (SIS) operation	Increased power rating and lifetime both increase radiation damage to the vessel; low leakage loading patterns and proposed revised NRC rule indicate that expected vessel lifetime exceeds 80 years for most PWRs

CASL scope: Develop and apply the VR to assess fuel design, operation, and safety criteria

CASL
Consortium for Advanced Simulation of LWRs

Near-term priorities (years 1–5)

- Deliver improved predictive simulation of PWR core, internals, and vessel
  - Couple VR to evolving out-of-vessel simulation capability
  - Maintain applicability to other NPP types
- Execute work in 5 technical focus areas to:
  - Equip the VR with necessary physical models and multiphysics integrators
  - Build the VR with a comprehensive, usable, and extensible software system
  - Validate and assess the VR models with self-consistent quantified uncertainties

Longer-term priorities (years 6–10)

- Expand activities to include structures, systems, and components beyond the reactor vessel
- Established a focused effort on BWRs and SMRs
- Continue focus on delivering a useful VR to:
  - Reactor designers
  - NPP operators
  - Nuclear regulators
  - New generation of nuclear energy professionals

Focus on challenge problem solutions

U.S. DEPARTMENT OF ENERGY
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A comprehensive set of milestones is defined to drive solution of the challenge problems

Industry challenges and needs

Challenge problems

L1 Milestones in 6 challenge categories

- CRUD
- Grid-to-rod fretting (GTRF)/ fuel assembly distortion (FAD)
- Operational reactor
- Safety
- Lifetime extension
- Advanced fuels

17 milestones, ~$5M each

L2 Milestones
Discipline-oriented focus areas

36 milestones, ~$2M each

L3 Milestones
Projects

90 milestones, ~$1M each

Year	VR Capability	L1 Milestone Category	L1 Milestone
1	Initial core simulation using coupled tools and models	CRUD	Apply 3D transport with T-H feedback and CFD with neutronics to isolate CRUD-vulnerable assembly and pin in PWR full-core configuration; generate quantities relevant to CRUD initiation and growth
		GTRF/FAD	Apply full-core CFD model to calculate 3D localized flow distributions to identify transverse flow that could result in grid-rod fretting
2	Detailed phenomena modeling in fully coupled VR	CRUD	Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness
		GTRF/FAD	Model interaction of fluid flow distribution with fuel rods to calculate dynamic forces that may lead to fuel rod vibration
3	Assembly simulation with rod fretting and upscaled materials models	CRUD	Model boron uptake from reactor coolant into CRUD on fuel rods
		GTRF/FAD	Model changes in spacer grid geometry and relaxation of grid springs; calculate gaps between grid springs and fuel rods
		Safety	Initial modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients
4	Initial predictive reactor modeling in coupled VR	OR	Initial modeling of reactor operation; qualify with operational data
		CRUD	Predict CIPS by calculating CRUD formation, boron uptake, and resulting axial power shape
		GTRF/FAD	Calculate fuel rod material wear resulting from GTRF
		LE	Model reactor vessel fluence and material property changes that result in material degradation and limit vessel performance
5	Predictive reactor simulation coupled to physical plant	CRUD	Analyses to mitigate CRUD formation and minimize CIPS
		GTRF/FAD	Analyze grid geometry and spring materials to mitigate materials changes and wear
		Safety	Improved modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients
		LE	Model mechanical and thermal stresses and fatigue that result in material failures of core internals
		AF	Demonstrate the impact of new fuel forms (clad materials, fuel materials, and fuel geometries) for use in current reactor core configurations
		OR	Improved simulation of reactor operation; qualify with operational data

The CASL challenge problems drive VR requirements and define L1 milestones

- Each challenge problem carries a unique set of functional science and engineering requirements
- CASL activities have been prioritized to meet these requirements
  - Priority placed on 6 problems
  - Selected aspects of 4 problems to be addressed

Challenge Problem	Description	Relevance
CRUD	CIPS: Deviation in axial power shape caused by CRUD deposition in high power density regions with subcooled boiling. CIL/C: Clad corrosion and failure due to CRUD deposition	Power uprates yield higher power density and an increased potential for CRUD growth, axial power offsets, and clad failures
GTRF	Clad failure due to flow vibration-induced rod-spring interactions amplified by irradiation-induced grid spacer growth and spring relaxation	Power uprates and burnup increase potential for fretting failures, the leading cause of fuel failures in PWRs
Internals Lifetime (LE)	Damage to internals packages caused by thermal fatigue, mechanical fatigue, radiation damage, and stress corrosion cracking.	Replacement cost of internals is high, making lifetime extension less economically attractive
DNB (Safety)	Local clad surface dryout causing dramatic reduction in heat transfer capability during certain accident transients (e.g., overpower and low coolant flow)	Power uprates require improved quantification of margins for DNB limits
FAD	Distortion or component structural failure due to excessive axial forces caused by radiation-induced swelling	Power uprates and increased burnups may increase fuel distortions and alter core power distributions and fuel handling scenarios
Advanced Fuel Forms (AF, Safety, GTRF)	Examination of new cladding material, fuel material, and fuel pin geometries.	New fuel forms will enable power uprates, higher fuel burnups, and lower fuel cycle costs than can be achieved by incremental modifications of current fuel forms, i.e., zirconium alloy cladding, UO_2 fuel pellet, and cylindrical geometry
LOCA (Safety)	Numerous fuel failure modes resulting in fission product release and coolable geometry degradation	Realistic LOCA analyses (10 CFR 50.46) can enable power uprates that would not have been achievable with previously licensed evaluation models
RIA (Safety)	Clad failure due to rapid heating of the pellet, leading to pellet disintegration caused by the rim effect	Higher fuel burnup increases rim effect; power uprates may lead to increased energy during RIA. Currently not limiting but may change with further test data (e.g., CABRI)
PCI (Safety, AF)	Clad failure due to radiation-induced fuel rod/cladding contact from stress corrosion cracking and fuel defects	Power uprates and increased burnups increase fuel/clad contact and the likelihood for fuel failures. Currently only limits power ramp rates during normal operation, which are infrequent
Reactor Vessel Lifetime (LE)	Radiation damage resulting in increased temperature for onset of brittle failure, making failure more likely due to thermal shock stresses with Safety Injection System (SIS)	Increased power rating and lifetime both increase radiation damage to the vessel. Low leakage loading patterns and proposed revised NRC rule indicate that expected vessel lifetime exceeds 80 years for most PWRs

Challenge problem

- Tackles key limiting reactor phenomena
- Is beyond the ability of existing M&S tools to deliver acceptable and reliable results

CASL milestones provide an aggressive yet attainable path to success

CRUD formation: A significant barrier to increasing power output in existing reactors

Approach to each challenge problem

Milestone category	CRUD
Limiting phenomena	CRUD-induced Power Shift (CIPS), CRUD-induced Localized Corrosion (CILC)

Level 1 milestone map

Year 1	Apply 3D transport with T-H feedback and CFD with neutronics to isolate CRUD-vulnerable assembly and pin in PWR full-core configuration; generate boundary conditions relevant to CRUD initiation and growth
Year 2	Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness
Year 3	Model boron uptake from reactor coolant into CRUD on fuel rods
Year 4	Predict CIPS by calculating CRUD formation, boron uptake, and resulting axial power shape
Year 5	Simulation insight into CRUD formation and CIPS mitigation: Where and how will CRUD form and how can we anticipate and mitigate it?

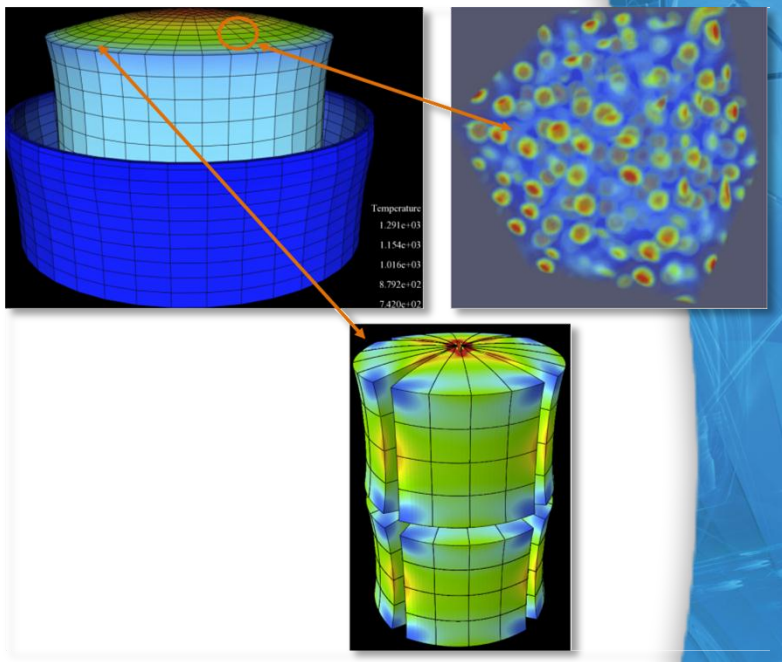
The CASL milestone plan focuses the VR development

CASL will apply a remarkable set of assets

- A U.S. team focused on U.S. leadership in nuclear energy
  - Carefully picked to leverage and pair partner strengths
  - A distinguished record of LWR regulatory and design accomplishments
- Industry partners are embedded to assure relevance and focus
  - Representing the entire U.S. nuclear industry landscape: Vendors, owner-operators, R&D for nuclear utilities
- Implements a new paradigm: University-industry-lab leadership balance
- Unparalleled collective institutional knowledge and nuclear science and engineering talent
  - The lead DOE laboratories in science, nuclear energy, and national security
  - Preeminent university nuclear engineering programs (Core + contributing partners: 7 of top 10 nuclear engineering programs)
  - Intimately connecting key science challenges to the nuclear energy enterprise: Unmatched expertise in materials science, chemistry, nuclear engineering, and multi-scale/multi-physics computational science
- Leaders in HPC (top 3 systems) and computational science (production code)

Executing a clear, milestone-driven technical strategy for real-world NPP solutions

CASL legacy:
A preeminent computational science institute for nuclear energy



- CASL VR: Advanced M&S environment for predictive simulation of LWRs
  - Operating on current and future leadership-class computers
  - Deployed by industry (software "test stands" at EPRI and Westinghouse)
- Advanced M&S capabilities:
  - Advances in HPC algorithms and methods
  - Validated tools for advancing reactor design
- Fundamental science advances documented in peer-reviewed publications
- Innovations that contribute to U.S. economic competitiveness
- Highly skilled work force with education and training needed:
  - To sustain and enhance today's nuclear power plants
  - To deliver next-generation systems

Now back to reality….

The CASL Organization (is complicated)

Oak Ridge National Laboratory
Thom Mason, Laboratory Director
Nuclear Science and Engineering Directorate
Kelly Beierschmitt, Associate Laboratory Director

COUNCILS

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VOCC Project Manager
John Shaw Jr.
VOCC IT & Cyber Security
Teresa Robison
Web & Database Design
Lara James
IT Project Manager
Brian Beal
Export Control
Rolf Migun / Sam Howard

Technical Focus Areas

MPO
Materials Performance & Optimization
Chris Stanek
Sid Yip
Brian Wirth

VUQ
Validation & Uncertainty Quantification
Jim Stewart
Dana Kelly

AMA
Advanced Modeling Applications
Jess Gehin
Zeses Karoutas
Stephen Hess

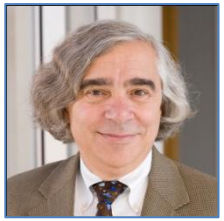
RTM
Radiation Transport Methods
Bill Martin
John Wagner

THM
Thermal Hydraulics Methods
Rob Lowrie
Rich Martineau

VRI
Virtual Reactor Integration
John Turner
Randy Summers

The CASL Board of Directors

has kept the leadership moving in the right direction



Ernest Moniz (MIT)
Chair

Dale Klein
At-large member

J Bennett Johnston,
At-large member

Charles Curtis
At-large member

Dennis Assanis
(Michigan)

Jack Bailey
(TVA)

Tom Geer
(Westinghouse)

Dave Hill
(INL)

David Modeen
(EPRI)

Mujid Kazimi
(MIT)

Terri Lomax
(NCSU)

Steve Rottler
(SNL)

Terry Wallace
(LANL)

Thomas Zacharia
(ORNL)

Feb 17 2011 Board Meeting Actions

Category	Action	Status
Board	New At-Large Board Member	Candidates available for nomination & selection
Board	Combine DOE CASL Dedication ceremony with Board Meeting	May 3-4 @ ORNL
Consortium	Construct & document CASL fundamental operating principles, how core & contributing partners can change & why, process for allocation decisions, etc.	Draft memo available for review & approval
Strategy	Capture thinking about SMRs in a white paper for review and feedback; present options for Board consideration	SMR White Paper available for review, including proposed responses
Strategy	Capture post-Fukushima considerations in a white paper for review and feedback; present options for Board consideration	Fukushima White Paper available for review, including proposed responses
Management	Revise Management Plan to reflect current operating status	Draft available for Board review & feedback
Quality	Understand and document NRC M&S requirements (e.g,. NQA-1, etc.) for tools that can ultimately be used for licensing	Draft Quality Plan available for review & feedback
Communication	Provide detail and update on the scope, plan, need, uniqueness, and status of the CASL Communication, Policy, and Economic Development Council	Briefing on inaugural meeting outcomes this meeting
DOE Integration	Formulate and document a plan by which CASL and the DOE NE NEAMs Program should co-exist, be synergistic and complement one another; report back on plans for interaction/coordination with ANL exascale project	Integration Plan still being formulated; briefing on status for Board feedback this meeting
Technology Control	Distribute CASL's initial draft Technology Control Plan (TCP)	Distributed to Board in March; updated & more comprehensive TCP available for review & feedback

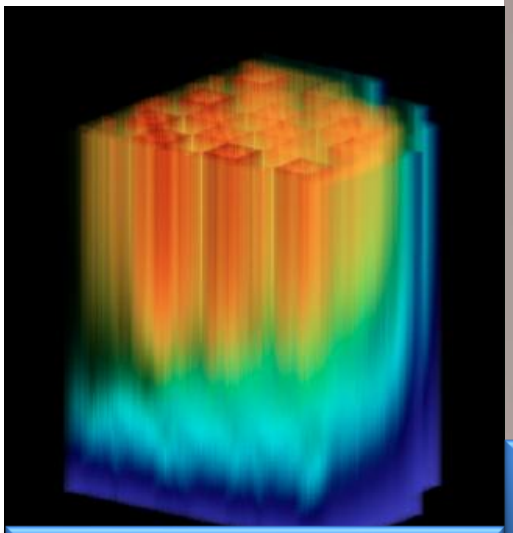
Overall CASL Cadence

- CASL is executing per 6-month *Plan of Record (PoR)* tasks, deliverables, and milestones
  - Imposes more agility and flexibility in our plan and actions
- We plan to release our virtual reactor (VERA) regularly and follow an evolutionary delivery life cycle
  - Place our M&S products into hands of users early and often
  - Follow quarterly "treadmills": science delivery, release, assessment, solution
- We encourage & need collaborations and partnerships to succeed
  - This is too hard of a problem; our partnerships (formal and informal) will likely change as we encounter new problems and solve old ones

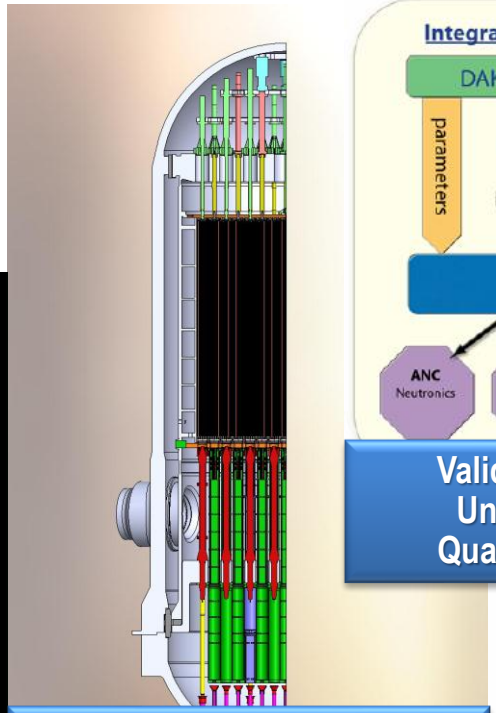
CASL will need industry interaction and collaboration and the leveraging of other DOE Programs to succeed

S&T Outcomes / Accomplishments

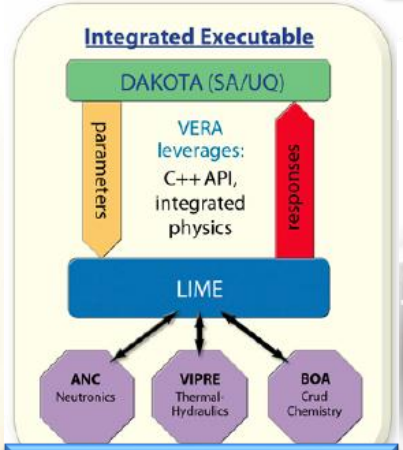
Consortium for Advanced Simulation of LWRs



Models and Numerical Methods

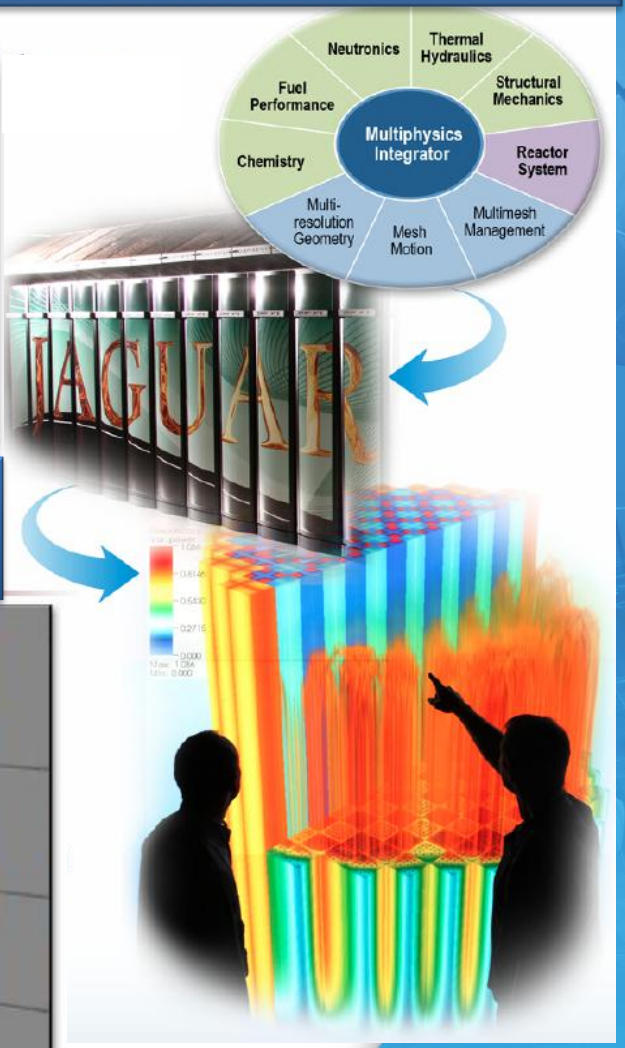


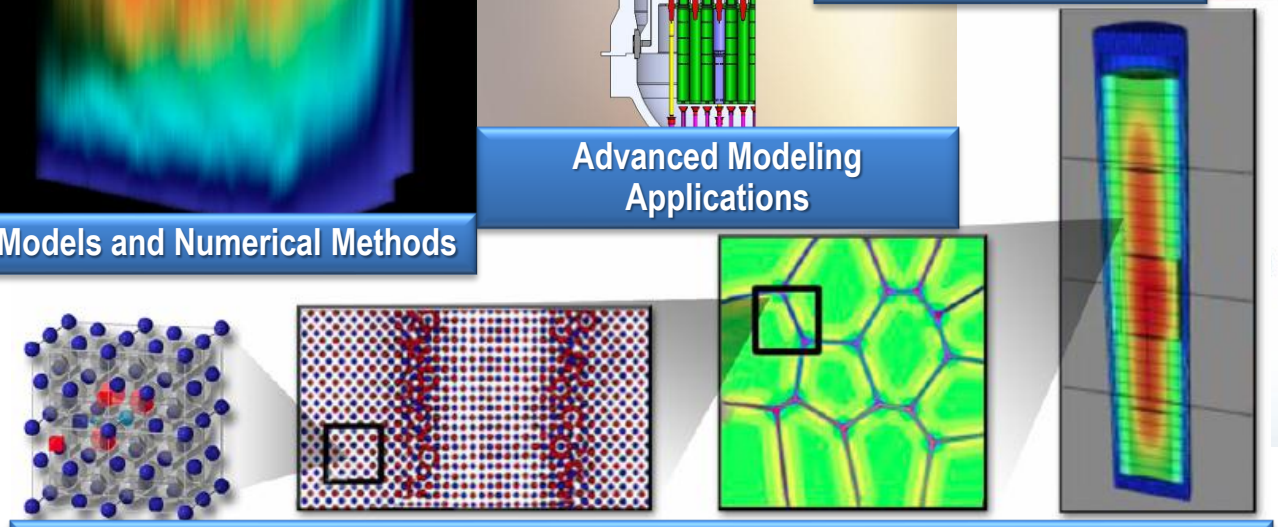
Advanced Modeling Applications



Validation and Uncertainty Quantification

Virtual Reactor Integration





Materials Performance and Optimization

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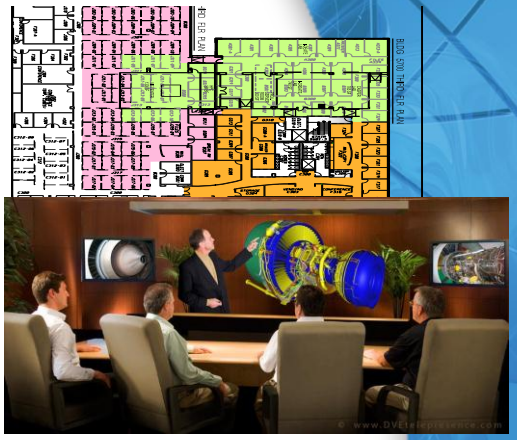
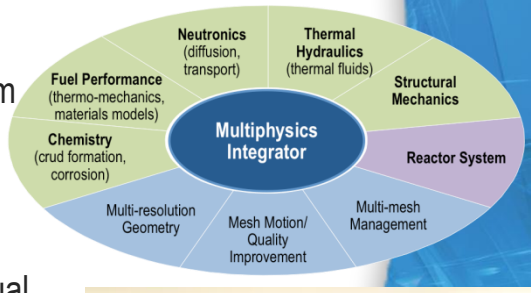
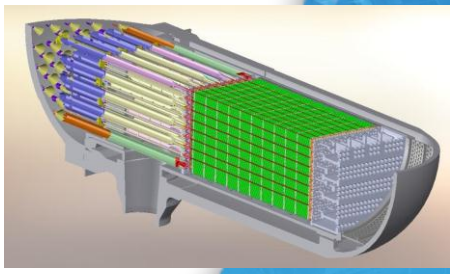
Achievements the First 6 Months

Period 1 Plan of Record (PoR-1): Jul – Dec 2010



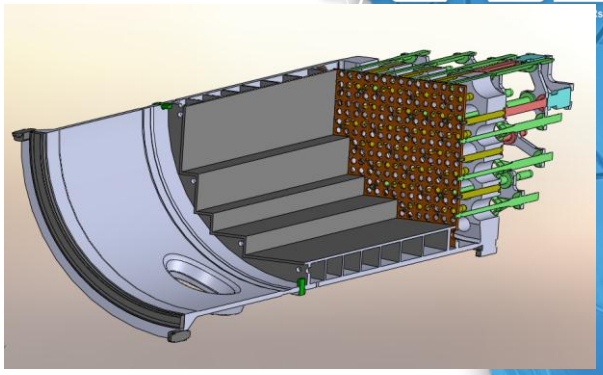
- Operational Achievements
  - Building out HQ Facility: 5600/5700 redesign with HQ & partner virtual collaboration (I-DEATE/I-CREATE) & design (IVAC) centers
  - Bringing up operations and operational team
  - Stood up Board of Directors, Councils, best-practice program management processes
- Technical Achievements
  - Delivered on technical milestones: 2 L1s, 5 L2s, 14 L3s
    - 3 L3s slipped by 1-3 months due to staff availability and delays in IP/NDA negotiations
  - Established the CASL virtual reactor "software repository" known as VERA (Virtual Environment for Reactor Analysis) and integrated 8 different computational capabilities from CASL partners (including 2 WEC codes and 1 commercial code) into the common VERA software environment
  - First release of Version 0.5 of VERA to CASL partners
  - Application of advanced radiation transport and computational fluid dynamics in VERA virtual reactor to a operational PWR sub-core scenario to demonstrate feedback coupling and contrast predictions with Westinghouse coupled tool predictions.
  - State-of-the-art sensitivity and optimization capability integrated within VERA to support uncertainty analysis of nuclear reactor operational and safety scenarios
  - Development of requirements and validation plan to support and guide CASL virtual reactor development
  - Comprehensive plan developed for upscaling fundamental and improved fuel, materials science, and coolant chemistry research efforts into operational reactor analysis and design workflows with VERA



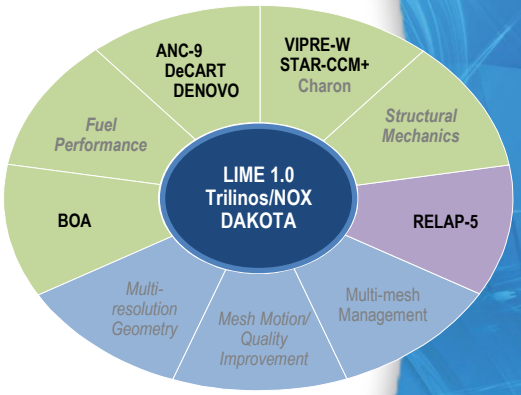


S&T Outcomes / Accomplishments

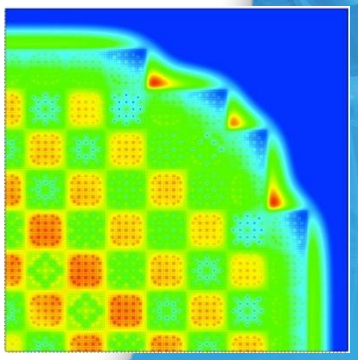
First 9 months

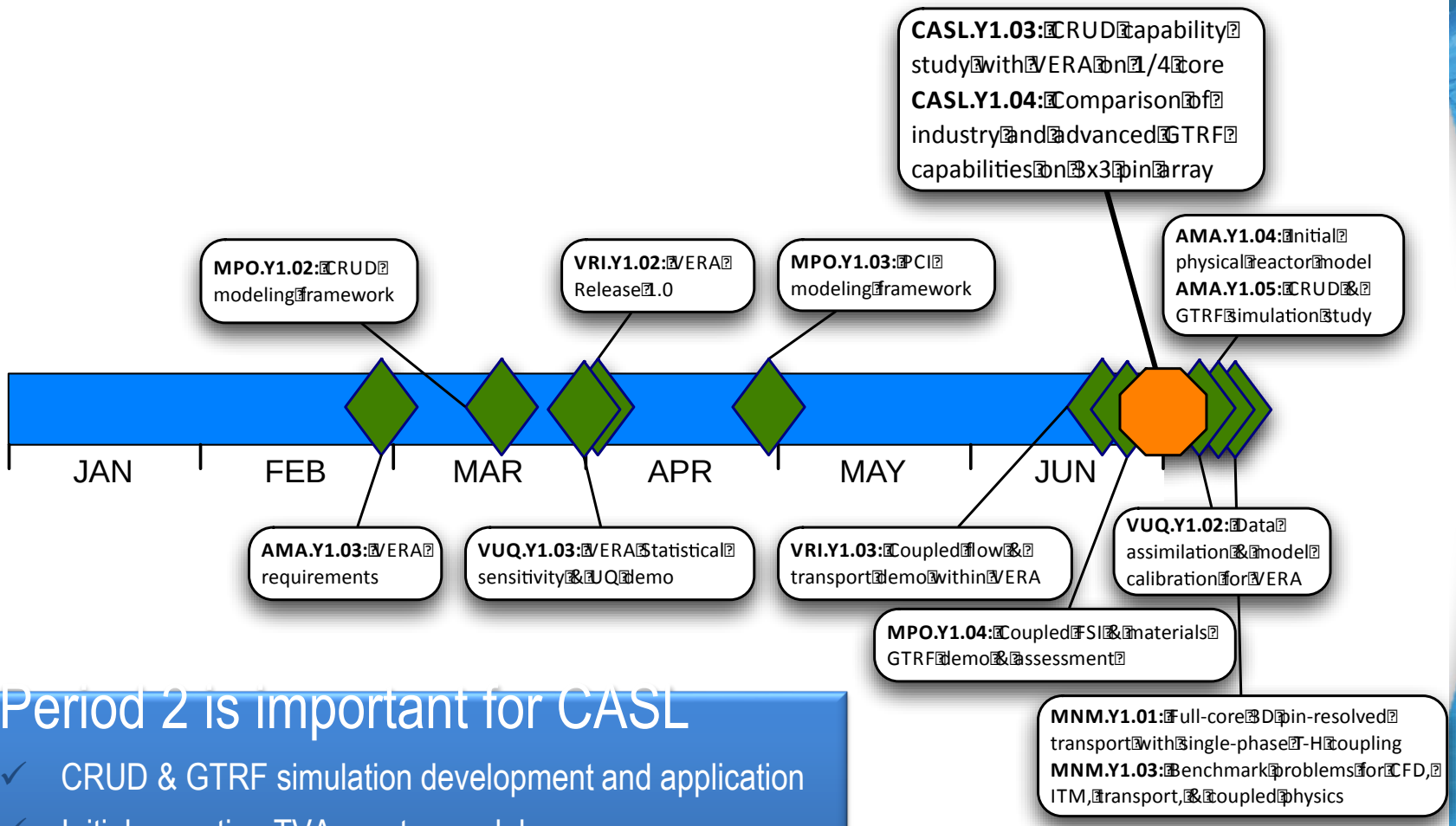


- Advanced Modeling Applications (AMA) Focus Area
  - ✓ Developed QA Plan, Virtual Reactor Validation Plan and Requirements Document and Challenge Problem specifications and model development, initial core model for TVA Watts Bar Plant
- Virtual Reactor Integration (VRI) Focus Area
  - ✓ Released Version 1.0 of the CASL Virtual Reactor
    - software framework for physics capability integration
    - Optimization, sensitivity analysis, and uncertainty quantification capability
    - Baseline industry capability for neutronics, thermal hydraulics, and corrosion chemistry
    - Initial advanced capability coupling neutronics with CFD-based thermal hydraulics
    - Initial coupling to reactor system capability



- Validation and Uncertainty Quantification (VUQ) Focus Area
  - ✓ Initial sensitivity and uncertainty quantification capability in the CASL Virtual Reactor
- Models and Numerical Methods (MNM) Focus Area
  - ✓ Delivered a state-of-the-art full-core pin-homogenized Sn transport capability (Denovo) into the CASL Virtual Reactor
- Materials Performance and Optimization (MPO) Focus Area
  - ✓ Delivered a modeling framework for selected aspects of the CRUD Challenge Problem





Period 2 is important for CASL

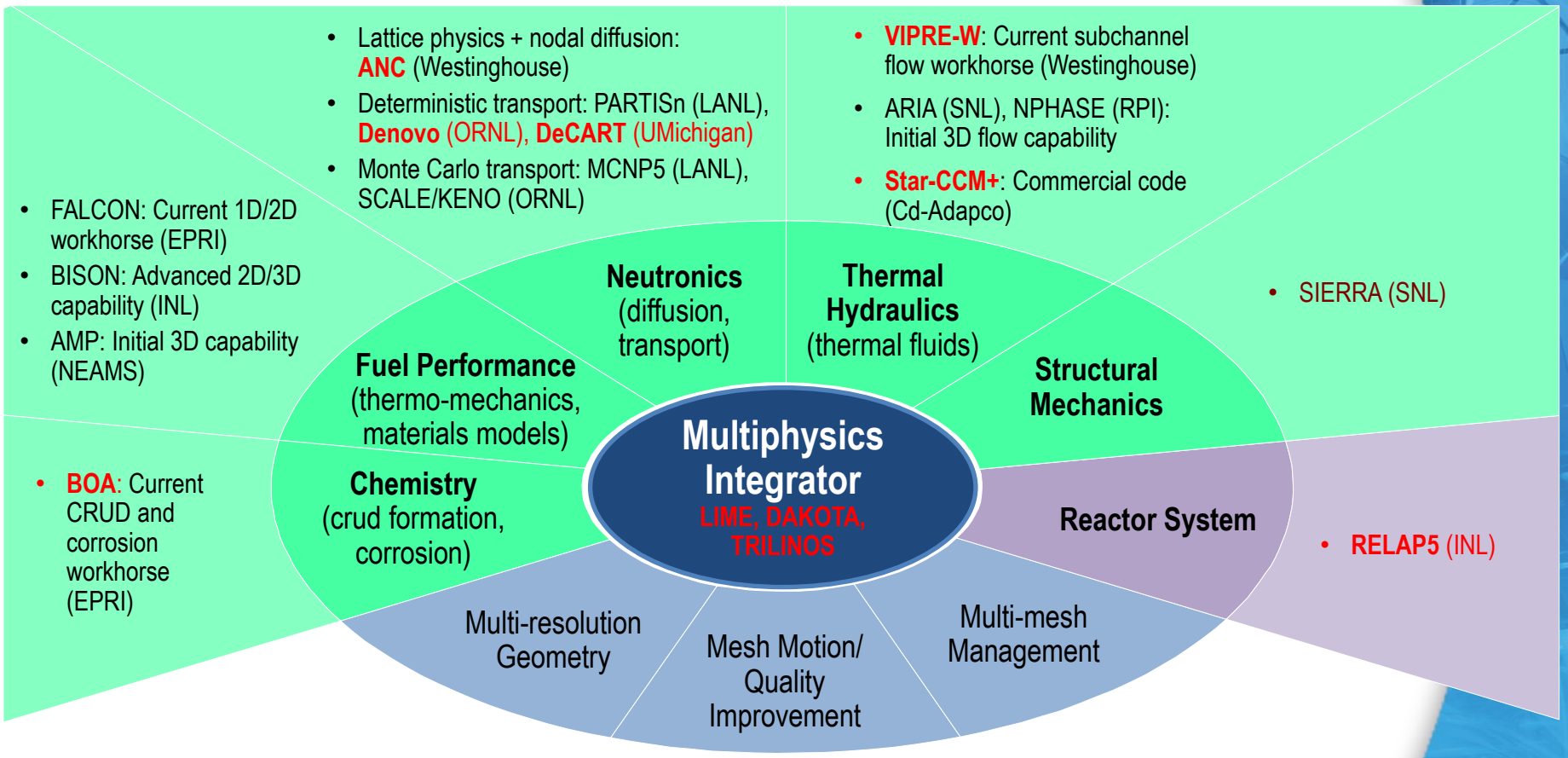
- ✓ CRUD & GTRF simulation development and application
- ✓ Initial operating TVA reactor model
- ✓ VERA release and baseline UQ capability demo
- ✓ Transport and T-H evolution and benchmarking

PoR-2 Milestone Timeline

Milestone	Jan 2011	Feb 2011	Mar 2011	Apr 2011	May 2011	Jun 2011	
L1* Owner: CASL Number: 2						CASL.Y1.03 CASL.Y1.04	
L2* Owner: FAs Number: 12		MPO.Y1.02 AMA.Y1.03	VUQ.Y1.03	MPO.Y1.03 VRI.Y1.02		MNM.Y1.01 VRI.Y1.03 AMA.Y1.04 MPO.Y1.04	MNM.Y1.03 VUQ.Y1.02 AMA.Y1.05
L3* Owner: Projects Number: 51	MNM.TH.Y1-1.04 VUQ.VVDA.Y1-1.02	AMA.RX.Y1.05 AMA.REQ.Y1.02 AMA.CHALNG.Y1.07 AMA.NRC.Y1.02 MPO.CRUD.Y1.03 VRI.PSS.Y1.02	VRI.CPI.Y1.01 MNM.TH.Y1-2.05 MNM.RAD.Y1-2.01 MNM.RAD.Y1-2.02 VUQ.VVDA.Y1-2.03 VUQ.VVDA.Y1-2.06 VUQ.SAUQ.Y1-2.01 VUQ.SAUQ.Y1-2.02 AMA.CHALNG.Y1.02 AMA.CHALNG.Y1.03 AMA.RX.Y1.02	MPO.PCI.Y1.02 MPO.GTRF.Y1.03 VRI.PSS.Y1.03 AMA.RX.Y1.03 AMA.RX.Y1.06	MPO.GTRF.Y1.04 MPO.PCI.Y1.03 MPO.CRUD.Y1.04 MPO.CRUD.Y1.05 VRI.VERA.Y1.02	MPO.GTRF.Y1.05 MNM.RAD.Y1-2.03 MNM.RAD.Y1-2.05 MNM.TH.Y1-2.02 MNM.TH.Y1-2.04 VUQ.VVDA.Y1-2.02 VUQ.VVDA.Y1-2.05 AMA.RX.Y1.04 AMA.CHALNG.Y1.06 AMA.CHALNG.Y1.05 AMA.REQ.Y1.04	MPO.PCI.Y1.04 MNM.RAD.Y1-2.04 MNM.TH.Y1-2.01 MNM.TH.Y1-2.03 VRI.VERA.Y1.03 VUQ.VVDA.Y1-2.01 VUQ.VVDA.Y1-2.04 AMA.VAL.Y1.03 AMA.CHALNG.Y1.04 AMA.REQ.Y1.03 VRI.CPI.Y1.02

*red, green, and blue font denote milestones directly supporting PCI, CRUD, and GTRF challenge problems, respectively. Black font denotes milestones supporting more than one class of challenge problems.

VERA builds on a foundation of mature, validated, and widely used software

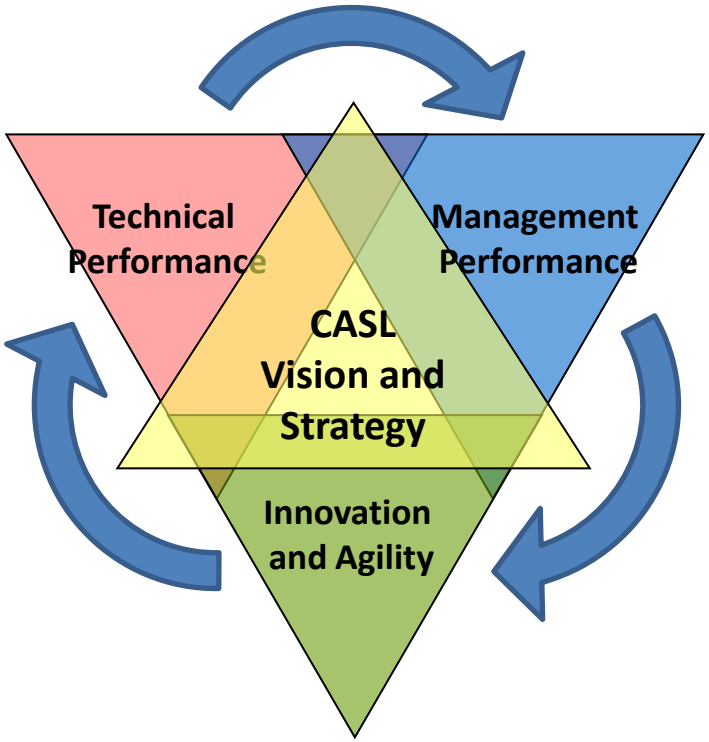


CASL needs a strategic roadmap for VERA capabilities and products

Virtual Reactor (VERA) Capability Roadmap

Capability	Year 1	Year 2	Year 3	Year 4	Year 5
Neutron Transport	• Full core 3D homogeneous pin cell Sn transport • Full core 2D/1D resolved pin cell MOC transport with T-H coupling	• Full-core 3D homogeneous pin cell Sn transport with T-H coupling	• Full-core 3D pin-resolved (Sn, MOC) transport • Initial transient 3D (Sn, MOC) transport capability	• Full-core 3D pin-resolved (Sn, MOC) transport with T-H coupling • Initial 3D hybrid MC transport	• Transient full-core 3D pin-resolved (Sn, MOC) transport with T-H coupling • Full-core 3D hybrid MC transport with T-H coupling
Thermal Fluids with Conjugate Heat Transfer	• Subchannel legacy and commercial CFD • Continuum & ITM multiphase benchmarks	• Next-generation sub-cooled boiling capability • Subgrid single-phase models informed by ITM	• Next-generation multiphase flow capability • Subgrid multiphase models informed by ITM	• Evaluate multiphase flow capability • Improved numerical methods & coupling	• Refined multiphase flow capability • Targeted methods & coupling advances
Fuel & Clad Performance	• 1.5D legacy capability • Phenomenological models & properties	• Initial fuel mesoscale models for FG release, swelling, μ-structural evolution • Initial corrosion models	• Clad mesoscale μ-structural evolution • Fuel chemistry evolution	• Clad corrosion & refined μ-structural evolution • SCC & fatigue crack propagation	• Full upscale model for fuel performance and life extension predictions
Coolant Chemistry	• Legacy capability	• CRUD source terms & growth model	• Boron uptake in CRUD	• CRUD formation	• CRUD formation & induced corrosion
Structural Thermo Mechanics	• Assess and integrate existing capability	• Loosely coupled structural vibrations • Initial radiation creep & hardening models	• Fully coupled structural vibration for fretting	• Implicit nonlinear fretting • Improved radiation damage models	• Formally assessed structural vibration capability
Physics Coupling	• Legacy coupled via LIME • Subchannel transport & single-phase CFD	• Homogeneous cell transport & CFD • Initial FSI	• Improved FSI • Homogeneous cell transport, CFD, fuel, & chemistry	• Pin-resolved transport & CFD	• Full-core transport, CFD, fuel, chemistry, mechanics • Core + physical plant
Validation and Uncertainty Quantification	• DAKOTA for scoping UQ	• Time-dependent DA for parameters and responses • Model V&V procedures and initial databases	• Sensitivity and UQ for coupled components • Model V&V tools for selected modules	• DA with reduced-order modeling • Model V&V tools for selected coupled modules	• High-order DA including errors and uncertainties • Model V&V tools for coupled VERA system

Performance Metrics



CASL strives to deliver on 3 basic themes

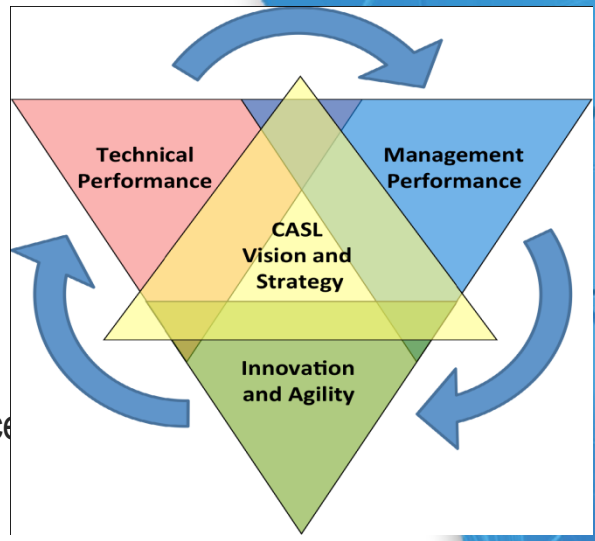
- Solutions to selected industry Challenge Problems
- Provide advanced, value-added M&S technology (VERA)
- A unique and better Industry-DOE-University approach to solving nuclear energy problems ("hubification")

Performance Metrics: Period 2 Plan of Record

Jan-Jul 2011

Category	Activity	Metric/Target
Innovation & Agility	• Demonstrate the effectiveness of using advanced M&S capabilities versus the current practice for GTRF • Demonstrate the application and associated benefits of stronger coupling of the relevant physics for CRUD • Demonstrate the benefit of coupled neutron transport & CFD • Generate meaningful near-term SA and UQ results • Ability to recognize that an L1 or L2 milestone cannot be completed due to scientific, technical, resource or staffing issue	• Demonstrate the effectiveness of using advanced M&S • Positive review by the Science Council • Submission of peer reviewed, full-length manuscript to either an archived journal or topical meeting • Months delayed in completing milestone • Percentage overrun in budget • Months prior to milestone schedule that problem is recognized.
Technology	• Integrate key outstanding industry and DOE simulation capabilities (BOA, FALCON, Sierra) into VERA • Define, document, and deploy a CASL test stand at WEC • Release VERA Version 1.0 to the CASL community	• Execute L2 Milestone VRI.Y1.02 • Execute L3 Milestone OPS.Y1.02 • Engage one or more IC members in substantive technical (FA) exchange, leading to a formal and mutually beneficial collaboration
Management	• CASL HQ facility and operations • DOE ribbon cutting and annual review • DOE FY11 Milestones • FY10-FY11 execution and FY12 planning • DOE integration • Collocation and partner cohesion	• Facility build-out and timely move-in • Reach operational steady state • Execute successful ribbon cutting and Annual Review for DOE • Meet all 3 DOE FY11 milestones and implement aggressive FY12 plan • Detailed coordination plan in place for DOE Program interactions

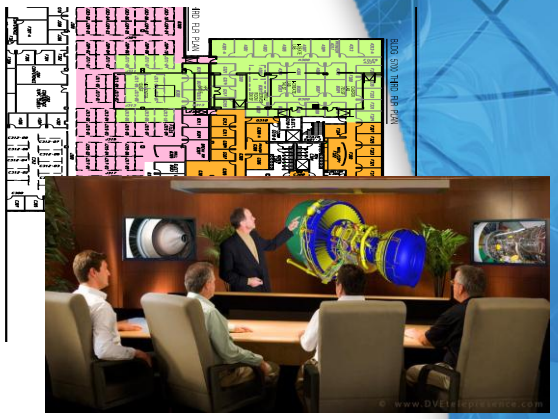
Performance



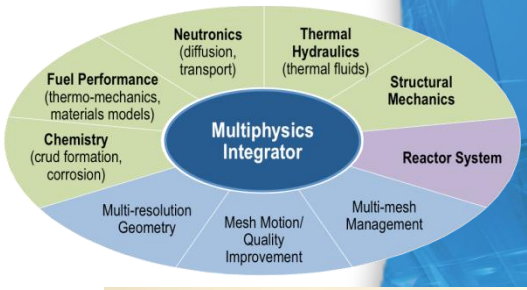
- Management Performance
  - ✓ Chartered and engaged Board of Directors (3 face-to-face meetings)
  - ✓ Weekly update reports to DOE and monthly dashboard reports to Board
  - ✓ Chartered and executed 5 advisory, review, and functional Councils: Science, Education, Industry, Commercialization, and Communication
  - ✓ Hit all DOE FY11 Milestones
  - ✓ Formulated and documented Management Plan, Plan-of-Record, Quality Plan, Technology Control Plan
  - ✓ Design and buildout of CASL HQ Facility; dedication on May 3, 2011
- Technology Delivery
  - ✓ Integrate key outstanding industry and DOE simulation capabilities (BOA, FALCON, Sierra) into VERA
  - ✓ Define, document, and deploy a CASL test stand at WEC
  - ✓ Release VERA Version 1.0 to the CASL community
  - ✓ NRC engagement
- Innovation and Agility
  - ✓ Demonstrate the effectiveness of using advanced M&S capabilities versus the current practice for a grid-to-rod fretting relevant application and for prediction of the impact of CRUD on reactor operational performance
  - ✓ Demonstrate the benefit of coupled neutron transport & CFD versus neutron diffusion-subchannel
  - ✓ Generate meaningful near-term SA and UQ results for a CP to help inform research and development needs

Outstanding Challenges

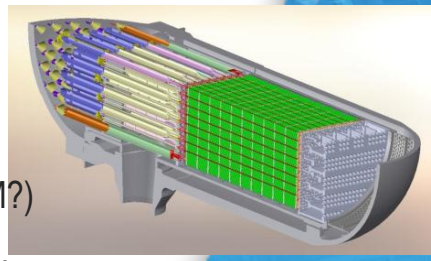
- **Outcome:** Develop and apply a "virtual reactor" to proactively address critical performance goals for operating PWRs
  - Power uprates, higher burnup, lifetime extension
  - Build in predictability by validating and quantifying uncertainties against WEC designs at TVA (Watts Bar I/II, Sequoyah)



- **Strategic Actions:**
  - ☐ Build out HQ Facility: 5600/5700 redesign
  - ☐ Deploy HQ & partner virtual collaboration & design centers
  - ☐ Staff a lean-and-mean operational team
  - ☐ Award all partner subcontracts & minimize ORNL prime overhead (TN state tax)
  - ☐ Define and implement Technology Control & IP Management Plan
  - ☐ Deploy mission-specific compute & networking infrastructure while leveraging OLCF
  - ☐ Deliver on aggressive milestones for 2nd 6-month "PoR" (Plan of Record)
  - ☐ Execute successful DOE ribbon cutting event (May 2011) & 1st annual review (Aug 2011)



- **Key Decisions:**
  - Scope & schedule in a 30% FY10-FY11 funding reduction reality (FY10 - $21.1M; FY11 - $12-16M?)
  - Defining the coordination of CASL & DOE NE Programs, a coherent and doable plan for validation, a plan for NRC interactions, and a strategic plan for scope augmentation into SMRs and BWRs
  - Maintaining consortium cohesion without managing to lowest common denominator



FY12 Expected Accomplishments

- VERA Release 2.0*
  - Neutron transport
    - Full core transport: pin-homogenized 3D Sn and pin-resolved 2D/1D MOC with conjugate heat transfer T-H feedback
  - Thermal fluids with conjugate heat transfer
    - Initial single phase capability with subgrid models informed by ITM
  - Fuel & clad performance
    - Initial mesoscale models for FG release, swelling, and microstructural evolution
  - Coolant chemistry
    - CRUD source terms (from industry models) with initial formation/growth model; upscaling plan in place
  - Structural thermo-mechanics
    - Initial structural mechanics code framework; loosely coupled vibrations
  - Physics coupling
    - Pin-resolved 2D/1D transport & CFD with conjugate heat transfer; initial fluid-structure interaction
  - Validation and uncertainty quantification
    - Data assimilation of parameters using time-dependent responses

*Selected components will be released broadly through ORNL's RSICC S/W distribution center

FY12 Expected Accomplishments

- CRUD Challenge Problem
  - Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness based on best available industry and CASL capabilities
- GTRF/FAD Challenge Problem
  - Model interaction of fluid flow distribution with fuel rods to calculate dynamic forces that may lead to fuel rod vibration

FY13 and beyond?

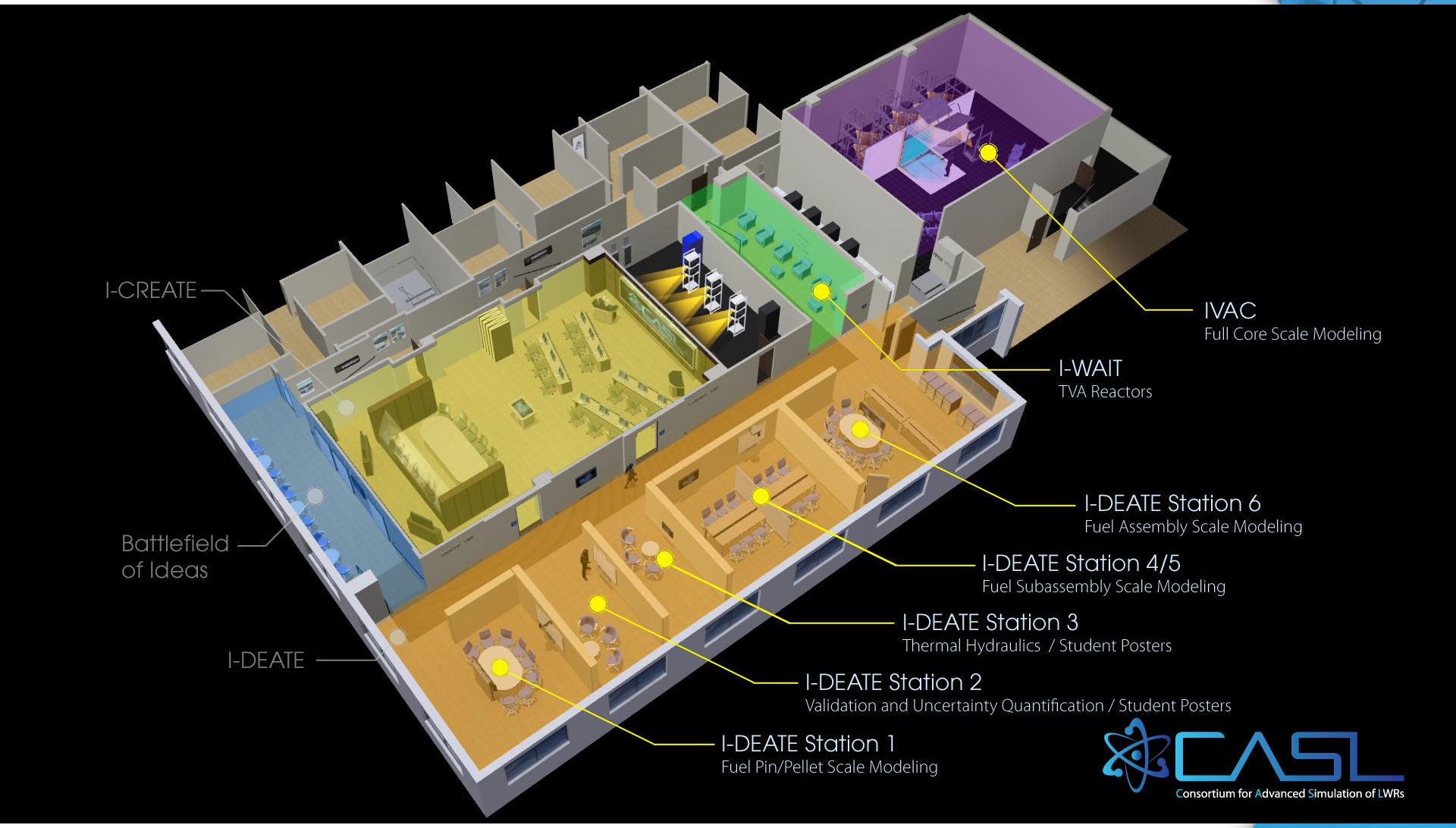
FY16 Expected Accomplishments

- 2nd 5-year plan of execution submitted and approved by DOE, including 10-year success/completion metrics
  - Plan to incorporate expansion of 5-year scope considerations such as LWR-based SMRs, BWRs, and severe accident analysis support
- VERA Release 6.0
- At least 5 formally-deployed CASL PWR Test Stands to industry
- Rigorous assessment of VERA's ability to predictively model BWRs and LWR-based SMRs
- Influence analysis activities and decisions supporting core reload and new core design for one or more vendors and owners/operators with VERA & CASL staff expertise.

Strategic Goals?

- 2015
  - The CASL Virtual Reactor (VR) is released to the nuclear energy industry and demonstrates - through industry adaption – that its technology is a useful advance for the industry
  - Influence analysis activities and decisions supporting core reload and new core design for one or more vendors and owners/operators through use of the CASL VR and CASL staff expertise.
  - Demonstrably address, through new insights afforded by the CASL VR, key nuclear energy industry challenges to furthering power uprates, higher burnup, and/or lifetime extension while providing higher confidence in assuring nuclear safety.
- 2018
  - The CASL VR (or portions thereof) becomes the leading nuclear energy industry modeling and simulation capability for supporting and furthering advanced nuclear steam supply system (NSSS) and nuclear fuel research, development, and deployment
- 2020
  - Facilitate one or more nuclear energy industry licensing activities related to power uprates and/or lifetime extension through direct involvement of one or more CASL VR components.
  - The CASL VR (or portions thereof) becomes one of the standard, reliant technologies in licensing by one or more nuclear energy vendors and/or owners/operators.
  - Demonstrably expand the applicability of CASL VR to LWR-based SMRs and/or BWRs.

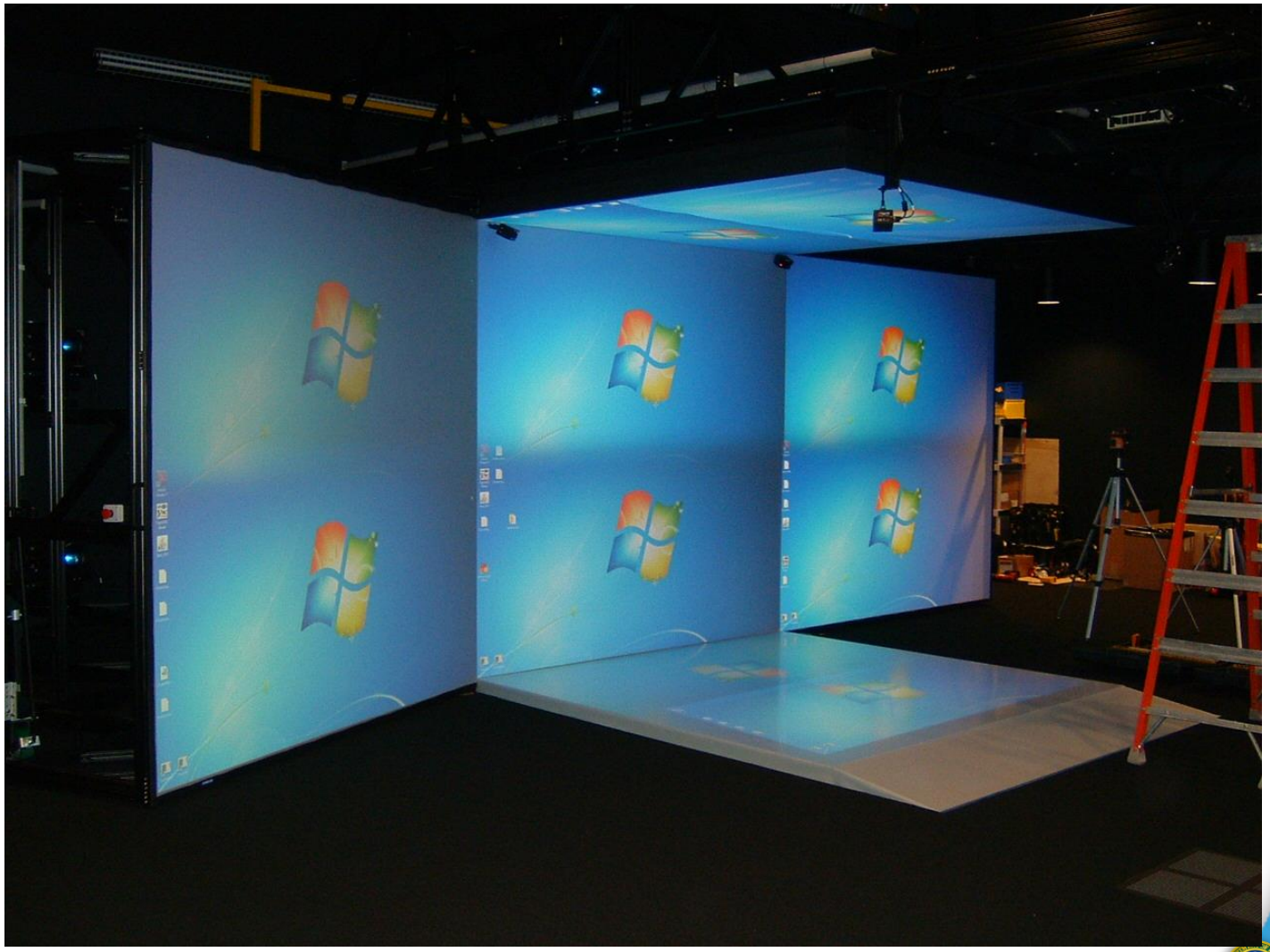
CASL HQ Facility: Floorplan



CASL HQ Facility at ORNL
Augmented Reality Podium

CASL HQ Facility at ORNL

"C5" Immersive Visualization and Analysis Center



CASL HQ Facility

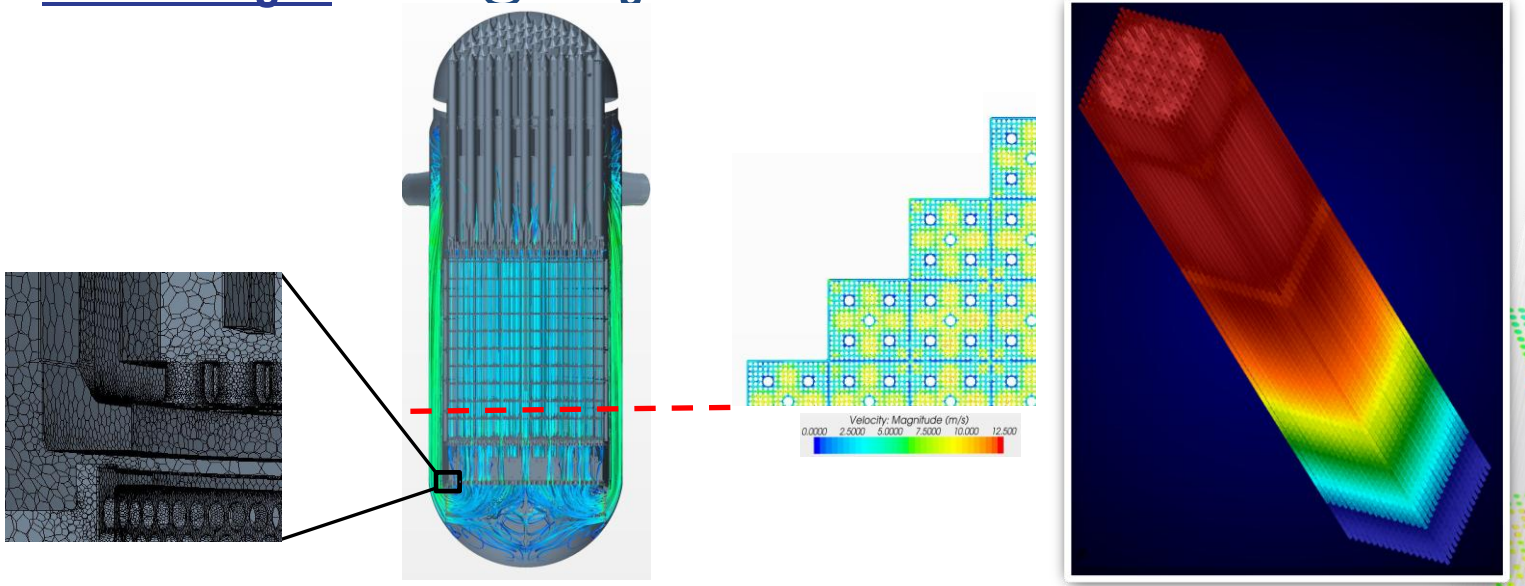
Roundtable Comments

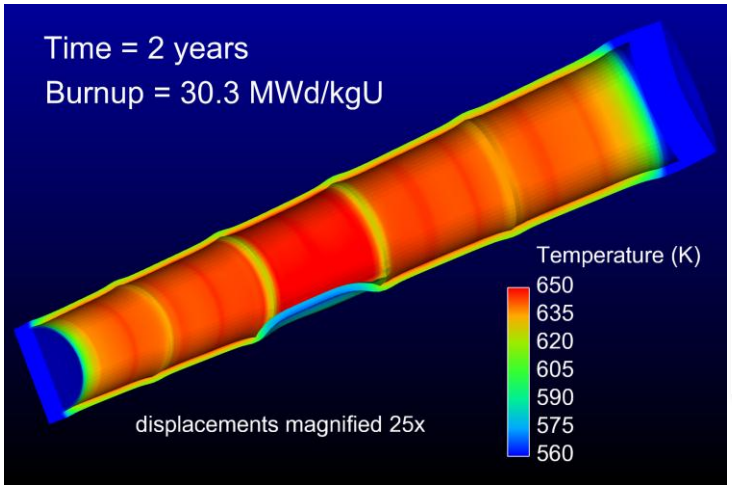
- For our first one we wanted to keep it "internal"
  - We need to first get our own house in order before we invite guests over
- Need to better understand ourselves and each other's roles, strengths, weaknesses
- A chance to communicate highlights, but, even more important: challenges, issues, and areas of disagreement
  - Silence is compliance
- We need to hear your problems and roadblocks to productivity and success
  - Contracts, contracts, contracts, …
  - NDAs
  - Increased communication

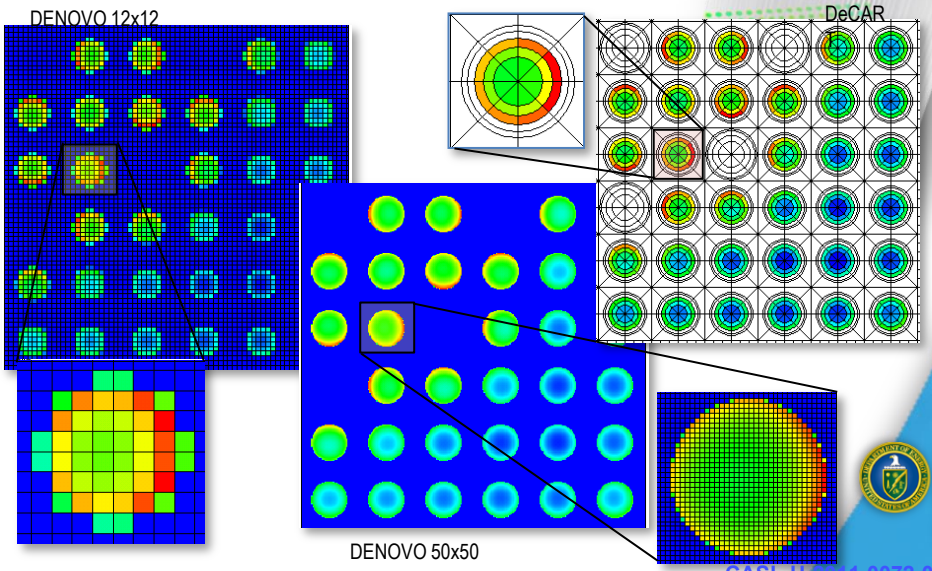
This is a great chance to listen and learn

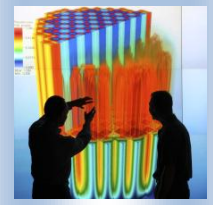
Questions?

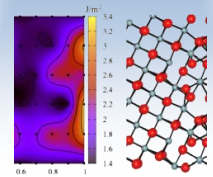
www.casl.gov or *info@casl.gov*











CASL Industry Council:

Purpose, Status, and Path Forward

Consortium for Advanced Simulation of LWRs

John Gaertner, EPRI

August 3, 2011

Vision

The Industry Council (IC) is one of 5 councils designed for continual communication with non-project stakeholders. The IC supports that:

CASL will deliver solutions that are "used and useful" by industry, and industry will recognize CASL leadership for advancing the M&S state-of-the-art.

Charter accepted by IC and by BOD addresses purpose, membership, meetings, process, and expenses

Purpose

- IC provides critical two-way communications and information exchange between the CASL Project and those who should benefit from CASL products
  - CASL receives
    - advice on industry technology gaps, critical needs
    - candid review of plans, specifications, preliminary products
  - IC members can
    - influence CASL development
    - prepare their business and technical processes for early use of CASL products
  - Both CASL and members can
    - exchange data and technical results
    - participate in testing, regulatory interface, and other collaboration

Meetings

- IC kickoff was September 2010 at EPRI Charlotte
- 3 Meetings in 2011:
  - January 11 at Oak Ridge (ORNL)

    (and February 9 in EPRI Charlotte due to inclement weather on 1/11)
  - May 12 Webcast
  - August 23-24 at Oak Ridge (ORNL)

Membership

- The Industry Council is chaired by a CASL team member from the Electric Power Research Institute (EPRI) approved by the CASL Director.
  - John Gaertner of EPRI is the first Industry Council Chairman.
- Members represent a spectrum of organization types including
  - Fuel vendors
  - design engineering companies
  - engineering service providers
  - computer technology companies
  - owner/operators of nuclear plants
  - Simulator hardware/software vendors
  - DOE and the CASL Board of Directors are ex-officio members.

Membership

Current membership:

EPRI
Battelle

AREVA
Westinghouse
GE Nuclear Fuels

Rolls Royce
Bettis
Boeing
Studsvik Scandpower

Dominion
Duke Energy
EDF
TVA

ANSYS
GSE Simulators

IBM
Cray Computing
DOE and BOD (ex-officio)

New members can be nominated and approved as needed

Themes and CASL Interfaces Selected by IC

- **Intellectual Property**, Licensing and Distribution of VERA and Other CASL Products
- **Technical Content and Configuration of VERA** to balance technology and practicality
- Specifying **Functional Requirements** to assure VERA is used and useful
- Appropriate **Computer Platforms** for Development, Testing, and Release
- **Scope of Applications** to beyond Westinghouse-4 loop: new plants, BWRs, ex-vessel applications, advanced fuel designs, next fuel performance problem
- **CASL as Center of Excellence** – delivering methods vs tools, problem solving vs code development, publishing results and papers
- **Quality Assurance, Verification, Documentation** – including eventual NRC acceptance
- **Communications Plan** – dynamic two way interface at all times

Highlights to Date

- Detailed review of VERA Requirements Document by IC
- Other IC activities are commencing now:
  - provide “Use Cases” and “Work Flow” definitions to ensure VERA is useful
  - assist CASL to define attributes of first (and subsequent) VERA release
  - critical review to ensure that CASL technology is accessible, modular and expandable from challenge problems to their problems of interest
- Individual members are identifying collaborative activities with CASL
  - Supplying data and code modules
  - Preparing to test and apply early VERA releases
  - Defining advanced instrumentation to supply validation data
- IC members attend willingly and participate enthusiastically

Draft Agenda
CASL Industry Council Meeting
Location: The Cabin at Oak Ridge National Laboratory
Tuesday, August 23

8:00	Registration and Coffee	
8:30	Introductions and IC Business	*John Gaertner*
9:00	Update CASL Activities/Plans since May	*CASL Team*
10:30	Use Cases and Workflow Project	*John Turner*
12:00	Lunch	
12:30	CASL management of IP	*Jeff Cornett*
1:15	VERA Release Plan – Milestones and Schedule	*Ronaldo Szilard*
1:45	VERA Open release attributes	*John Turner*
	•Platform, Functionality, User interface, etc.	
3:30	CASL Quality Assurance	*Matt Sieger*
4:00	Tour of CASL facilities	*John Shaw*
	•IVAC - Cave, CASPER, Ideate Station, Huddle	
5:30	Adjourn	
6:30	Dinner	*TBD*

Wednesday, August 24

8:00	Coffee	
8:30	Applications of VERA Beyond Challenge Problems	*Steve Hess*
10:15	Round Table: What's good, bad, missing?	*John Gaertner*
11:30	Action Items and Wrap up	
12:00	Adjourn	

Discussion

Questions, suggestions, complaints, …?

VERA: *a product-based description*

CASL Roundtable

August 10, 2011

CASL-U-2011-0072-000-R

CASL's Objectives (from the proposal)

- Produce a usable tool for addressing practical problems for the nuclear energy industry
  - maximize the value of the U.S. investment in its existing NPPs
  - enable the development and deployment of transformational nuclear energy systems
  - improve the ability of the U.S. industry to compete in worldwide market
- Capable of simulating (as a minimum)
  - Steady state and transient neutronics
  - Steady state and transient thermal/hydraulics,
  - fuel rod thermal-mechanics, and
  - fluid-structural interaction, including the analysis of systems events such as a loss of coolant or seismic event.

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We must "Institutionalize" our Product!

Capability-based VERA description

- Applies existing modeling and simulation (M&S) capabilities
- Develops advanced capabilities
- Equipped with the necessary physical and analytical models and multiphysics integrators
- Functions as a comprehensive, usable, and extensible system
- Driven by challenge problems that address essential issues for NPP design and operation
- Incorporates the validation and UQ needed for credible predictive M&S.

Provides direction, but not specific goals

Other Guiding Documents

- Challenge Problems
  - Describes in depth the capabilities of VERA to be demonstrated
  - Not intended to provide detailed requirements of the necessary physics and coupling
- Requirements Documents
  - Imposes conditions or capability needed to solve a problem or achieve an objective
  - Primarily addresses the Functional ("what") and Quality ("how well") requirements imposed
  - Targets the highest level of VERA performance and functionality (wish list)
  - Doesn't address intermediate development milestones

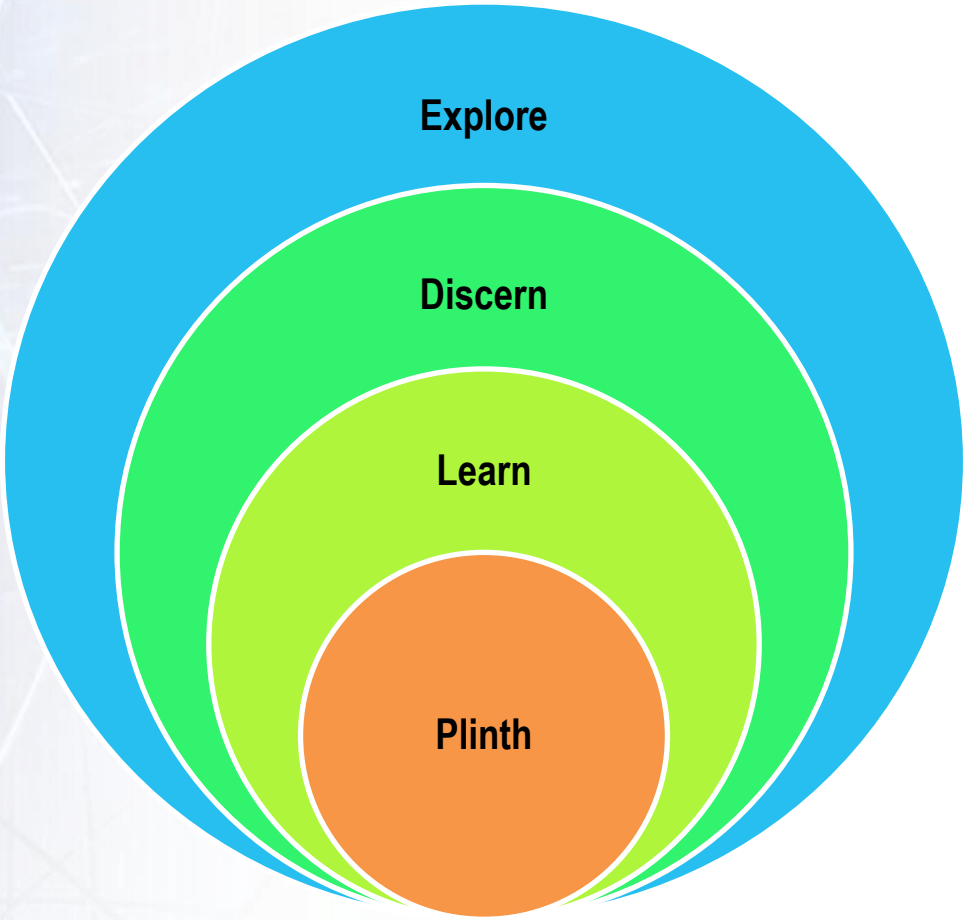
Provides goals, but without a concrete development path

Proposal: a product-based VERA description

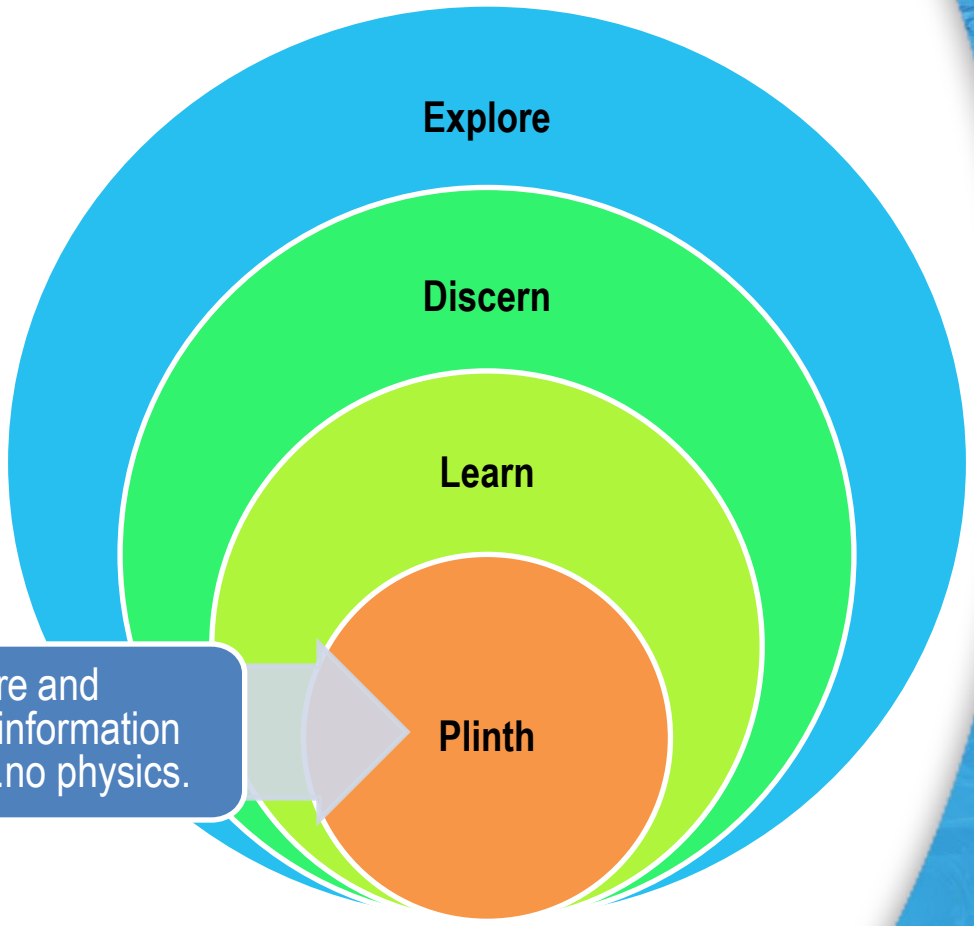
- Links capabilities, requirements and challenge problems to produce relevant and usable products
- Targeted towards specific User groups
- Modular approach ensures the code is upgradable as the project evolves
- Each level of product has potential for HPC and lesser platform deployment
- Allows long term research while producing industry usable packages in the short term

Provides insurance that CASL's objectives will be successfully met

VERA
Virtual Environment for Reactor Applications



Full Core Virtual Reactor, Targeted towards User groups, evolving with time, allowing for Institutionalization



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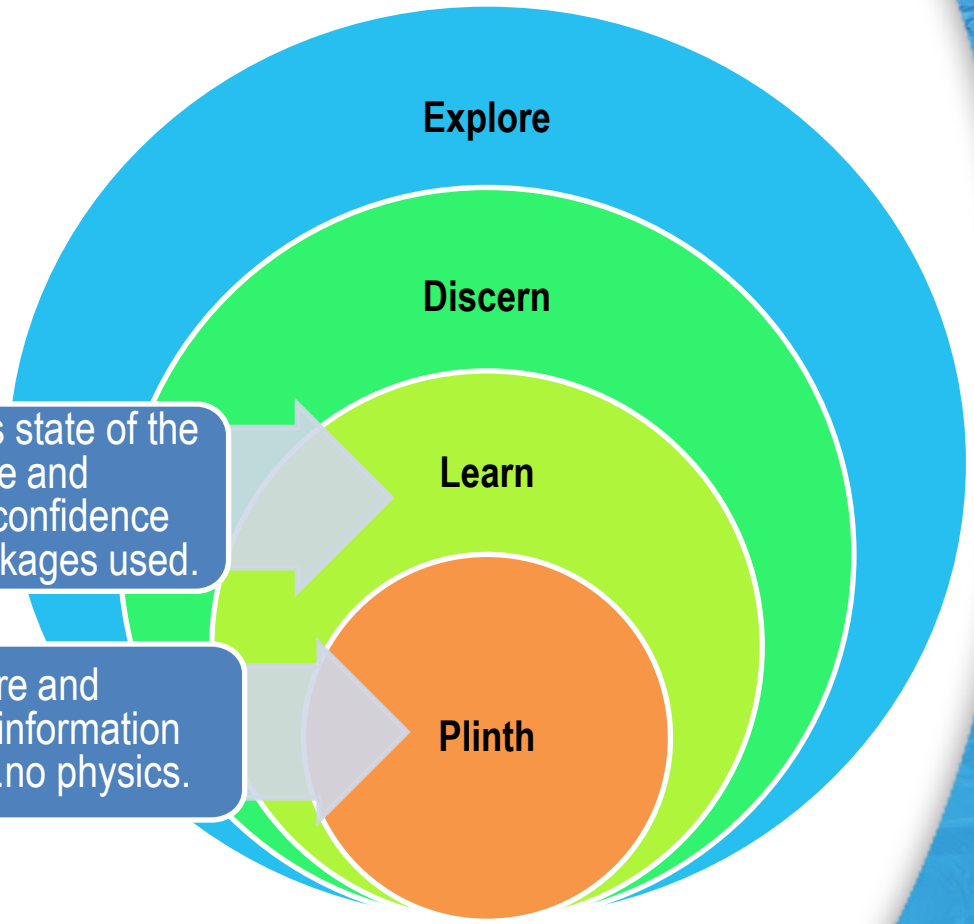

The basic collection of physics, at today's state of the art, required to describe core performance and distributable to a wide User base. High confidence in product success based on physics packages used.

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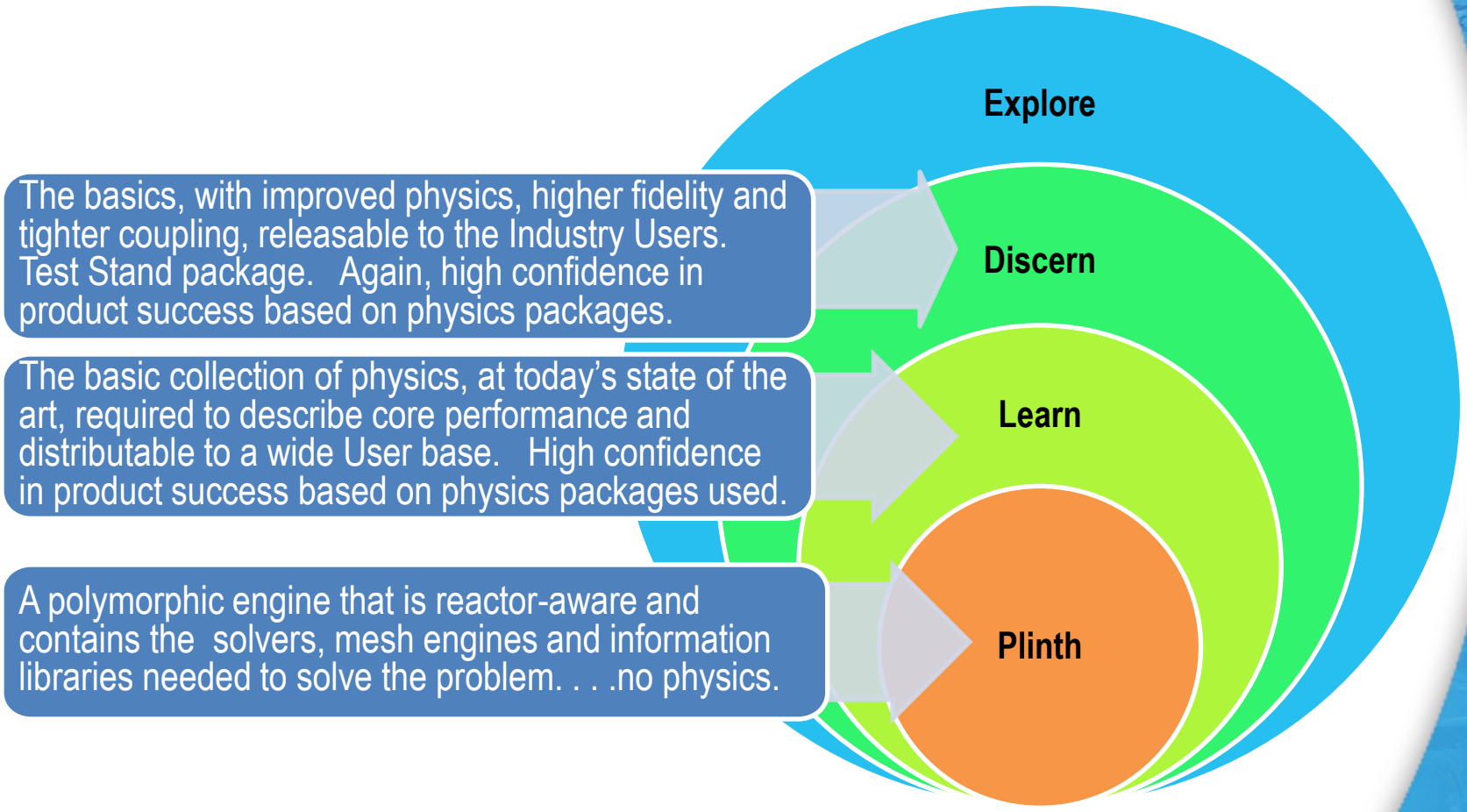

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The basics, with improved physics, higher fidelity and tighter coupling, releasable to the Industry Users. Test Stand package. Again, high confidence in product success based on physics packages.

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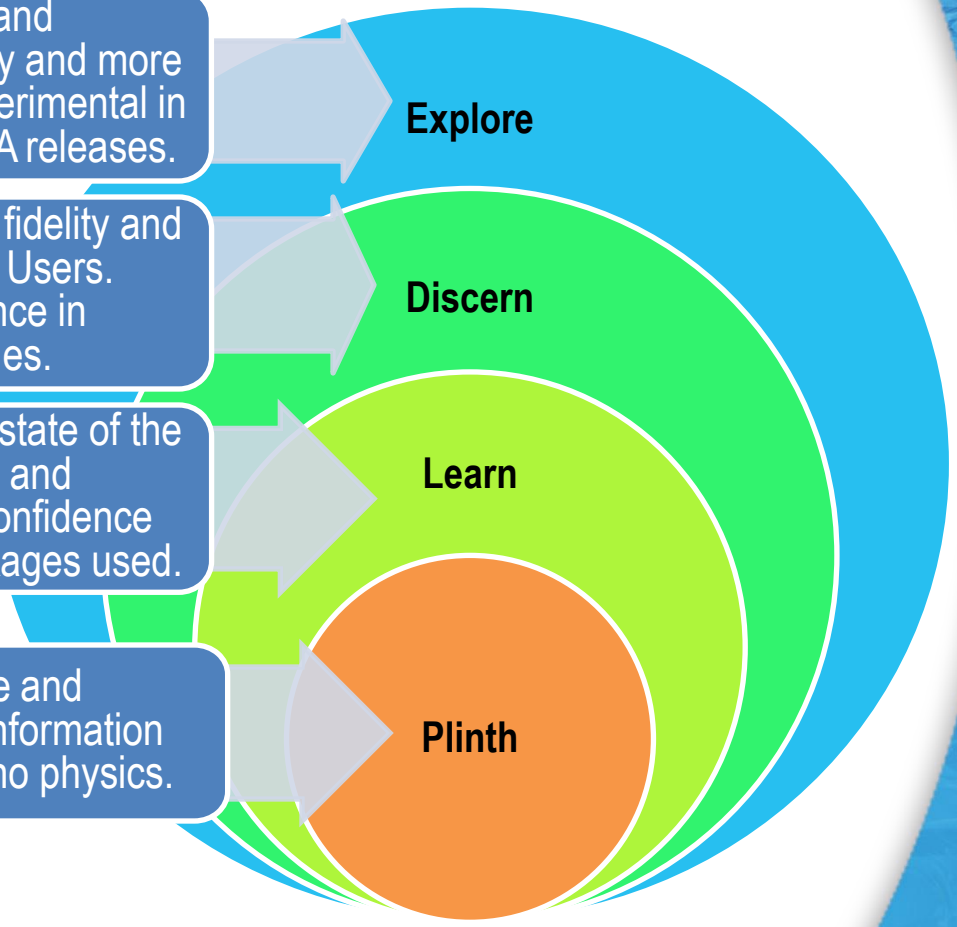

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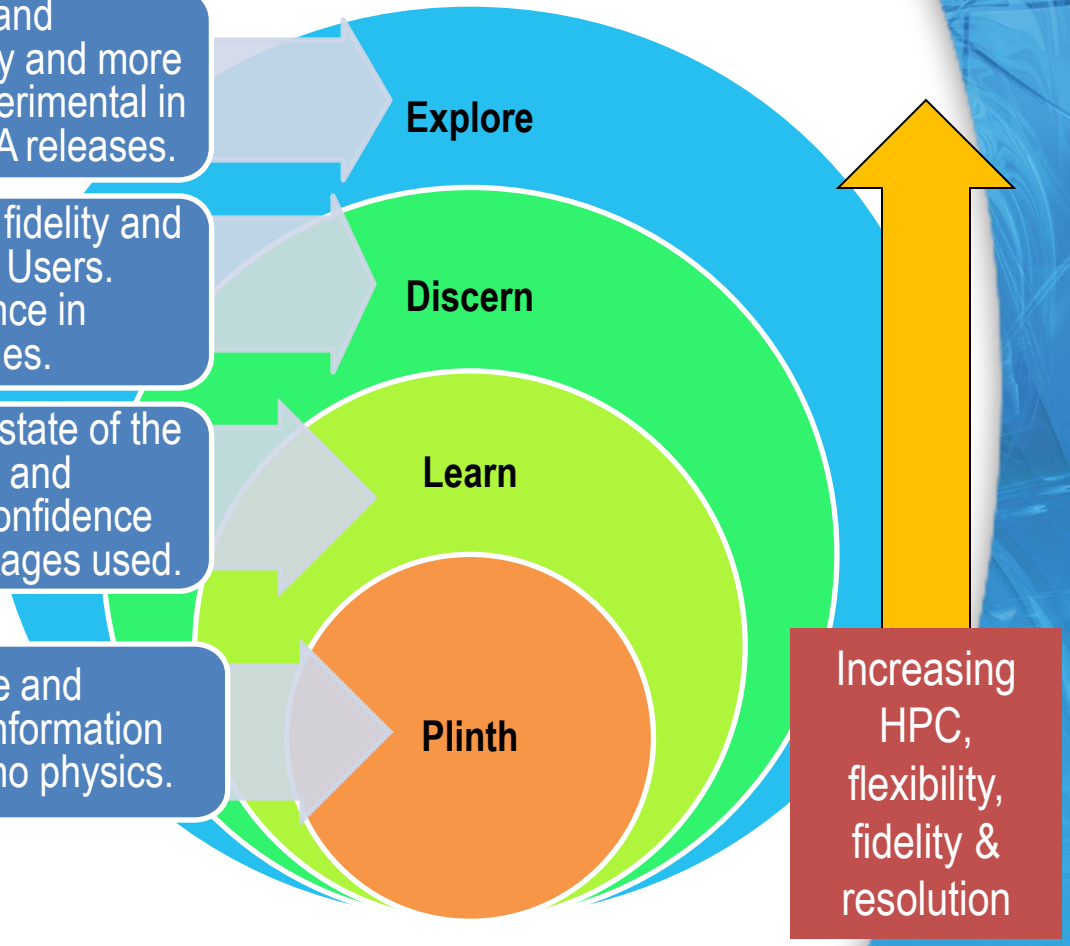

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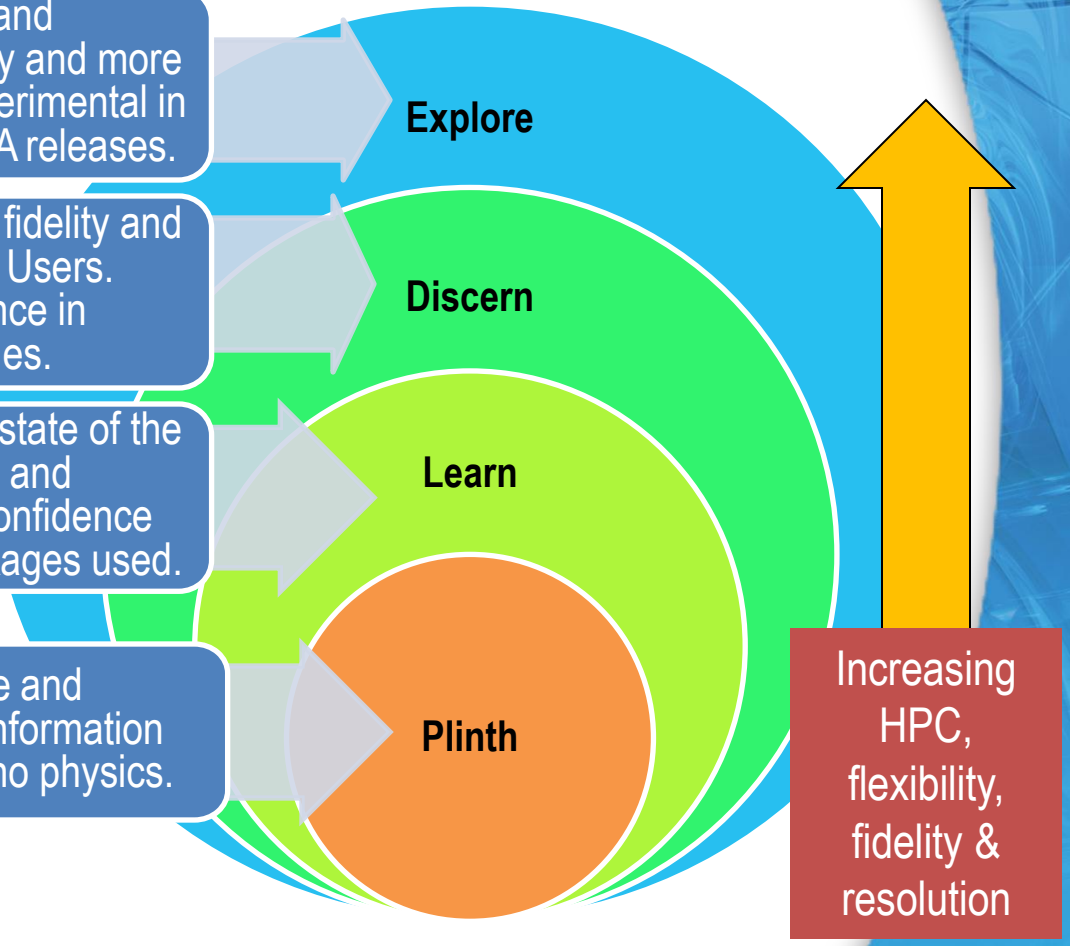

Specific releasable CASL Products

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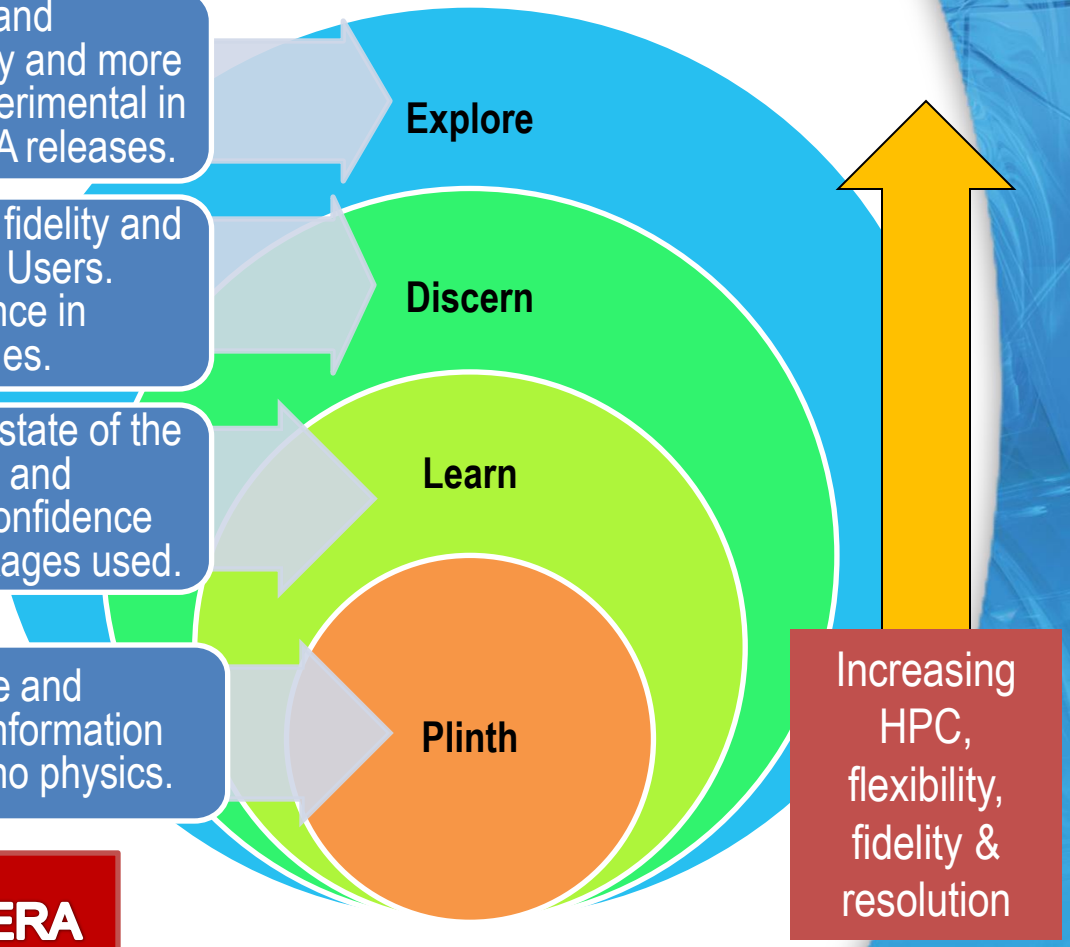

Agile, iterative approach to VERA

Specific releasable CASL Products

VERA
Virtual Environment for Reactor Applications

Plinth

VERA
Virtual Environment for Reactor Applications

Polymorphic Engine to couple codes/physics

- A vehicle for addition of physics predictors such as neutronics, rod mechanics, and thermal-hydraulics
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Pre & Post processing

- Consolidate the necessary inputs such that the user only need enter them once
- Provide visualization of the outputs

Plinth

VERA
Virtual Environment for Reactor Applications

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- Provide visualization of the outputs

Solvers

Plinth

VERA
Virtual Environment for Reactor Applications

Polymorphic Engine to couple codes/physics
- A vehicle for addition of physics predictors such as neutronics, rod mechanics, and thermal-hydraulics
- Allows fuel vendor codes to be used in VERA

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Official Use Only
Protected under CASL Master NDA

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- Zircaloy alloys
- Inconel alloys
- Uranium dioxide
- Helium & fission gases
- Water/Steam
- Corrosion products
- CRUD

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Evolves in capability as the project progresses

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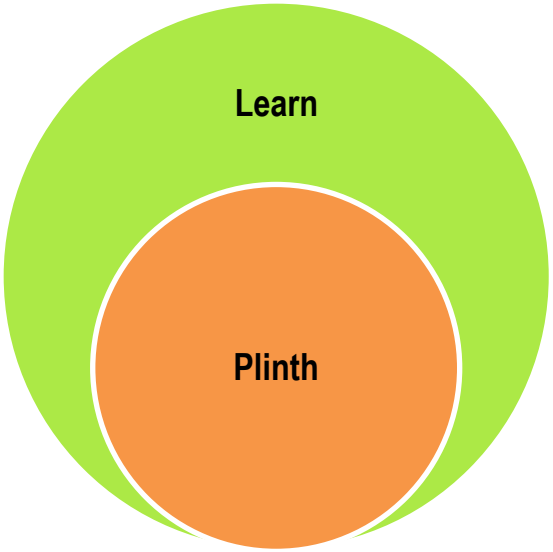
Virtual Environment for Reactor Applications



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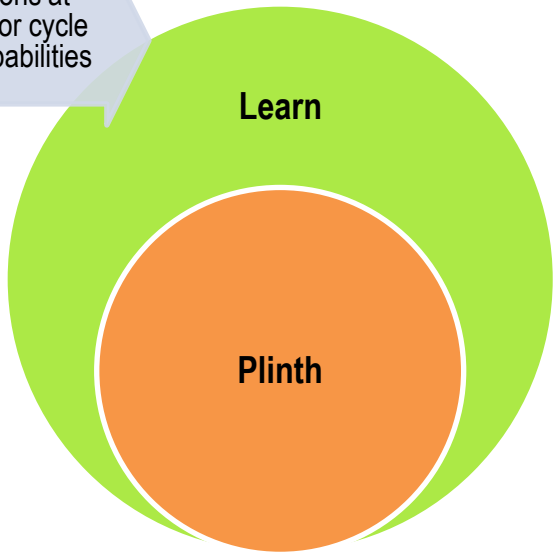
Provides the basic physics

- Steady state single phase evaluations at specific time steps within the reactor cycle
- Transient effects to the current capabilities of the codes



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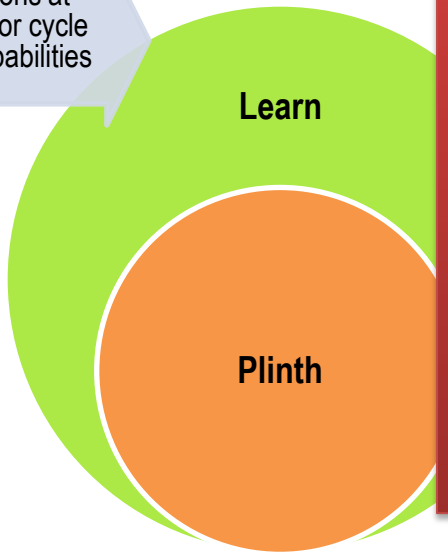

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Rod mechanics

CRUD deposition

Neutronics & x-sect processing

UQ

CFD??

Suggest EPRI codes as basis

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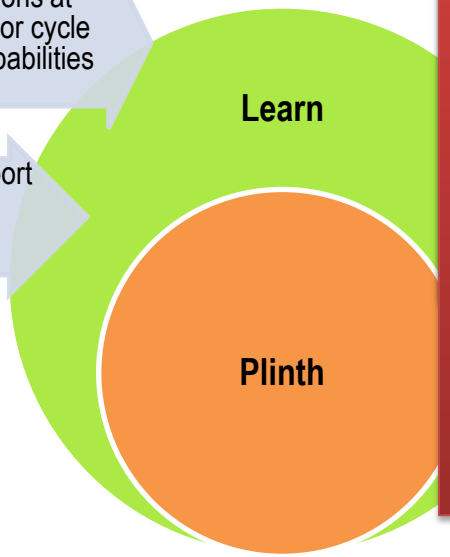

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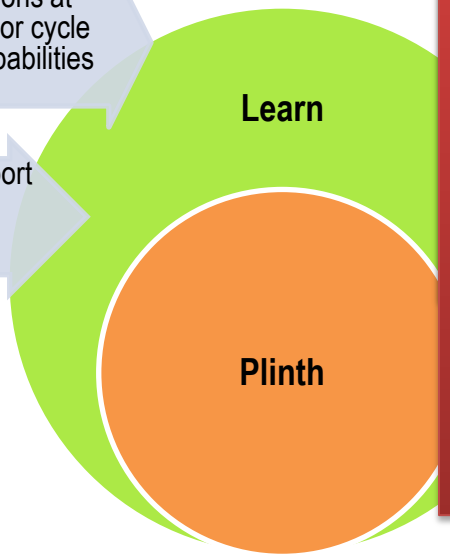

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Suggest EPRI codes as basis

- Shows solid progress
- Provides new capabilities in the coupling and use of HPC for large challenge problem solutions
- Demonstrates future development advantages
- Suggest use of EPRI codes as a basis supplemented by DOE/University codes to provide very strong assurance that industry will affirm it.
  - Inclusion of CFD capability at a later date
  - Includes a specific version of LEARN proprietary to Westinghouse.
- Multi-platform usable

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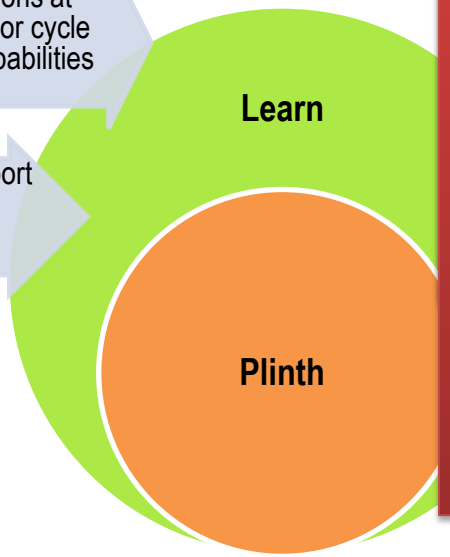

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- Multi-platform usable, but advertised as a "lite" version for laptop/workstation

Early demonstration of return on investment and benefit to industry

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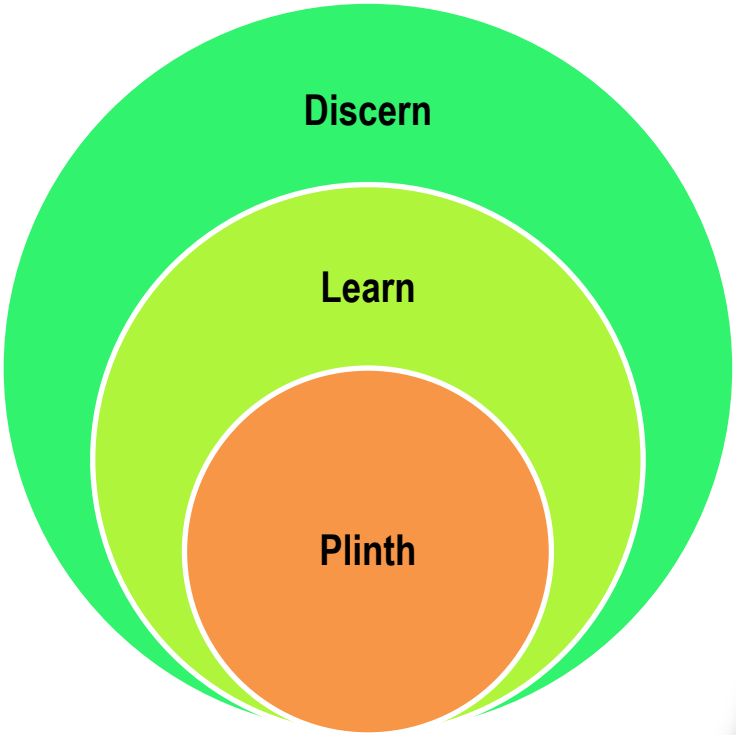

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Provides enhanced physics

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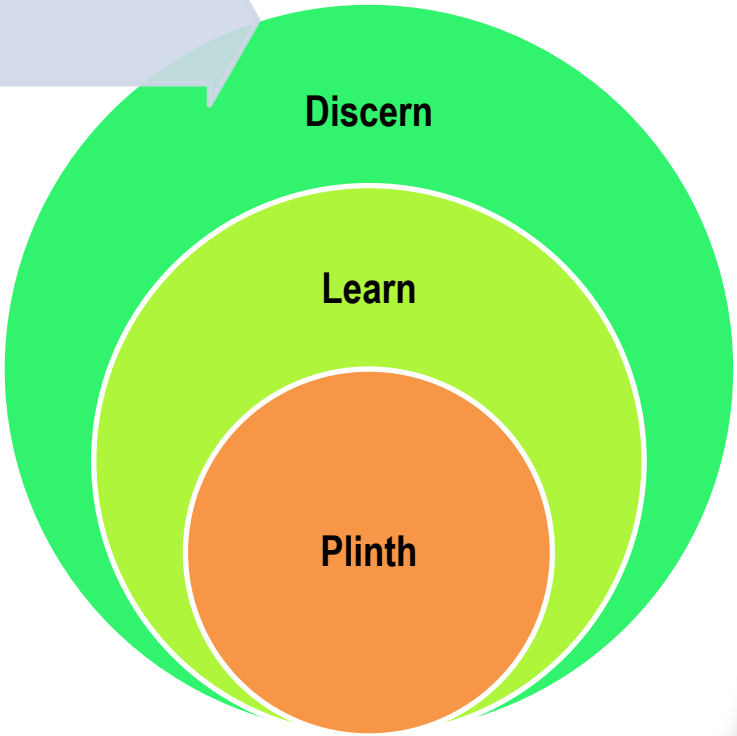

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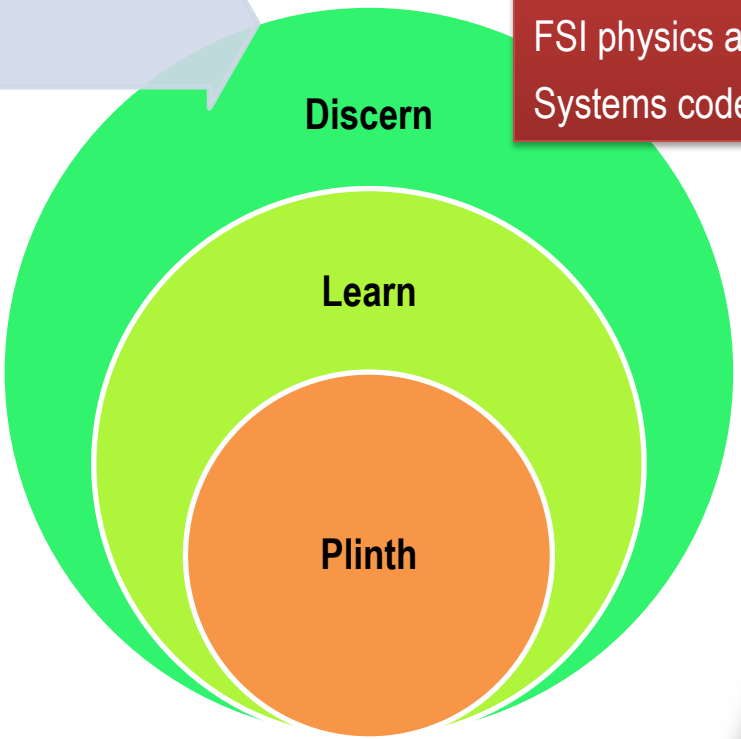

Enhance LEARN codes or substitute more capable codes

CFD

FSI physics added

Systems codes?

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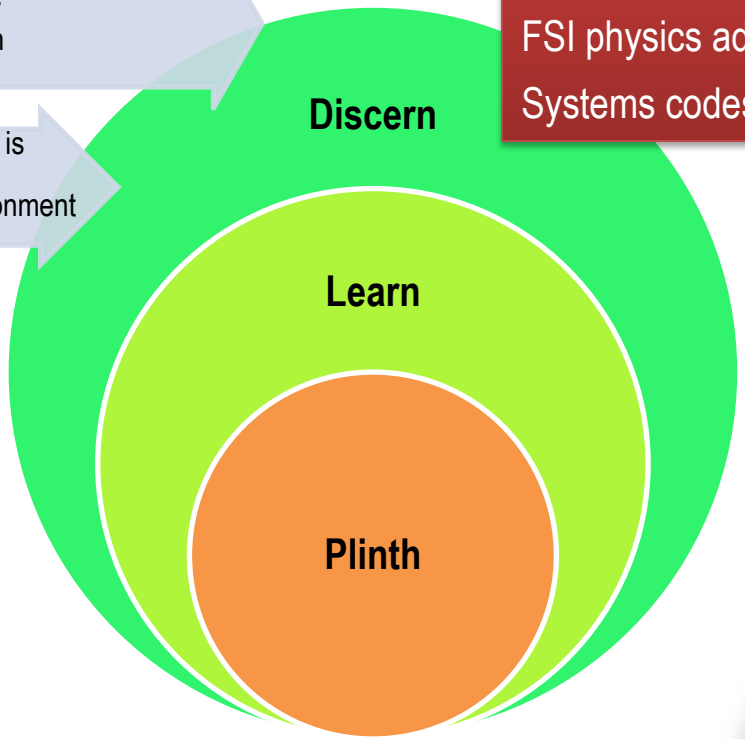
Includes enhancements to Plinth

- Integrates new information as it is published by CASL Staff
- Takes advantage of HPC environment
- Full plant or just a single rod



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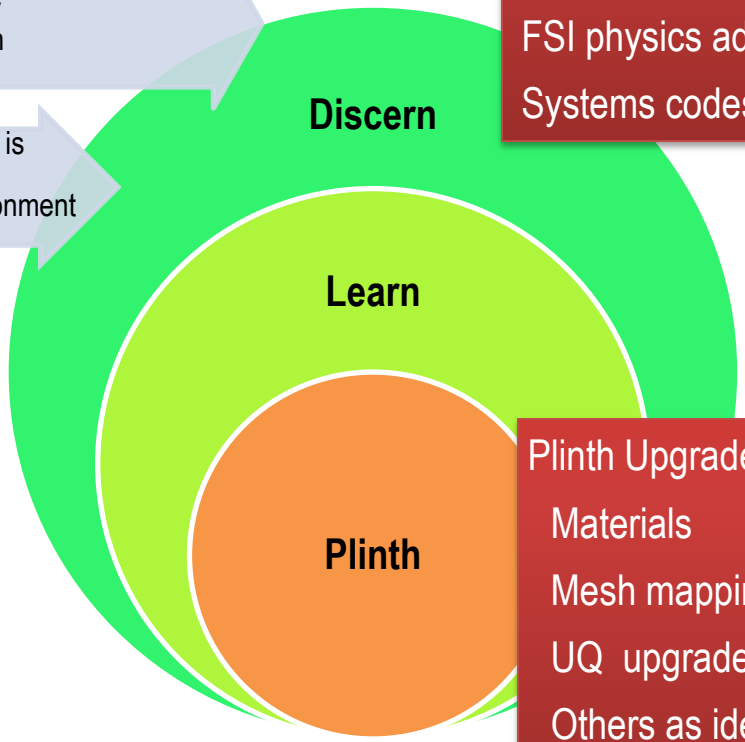

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Plinth Upgrades:

- Materials
- Mesh mapping
- UQ upgrades?
- Others as identified in the review process

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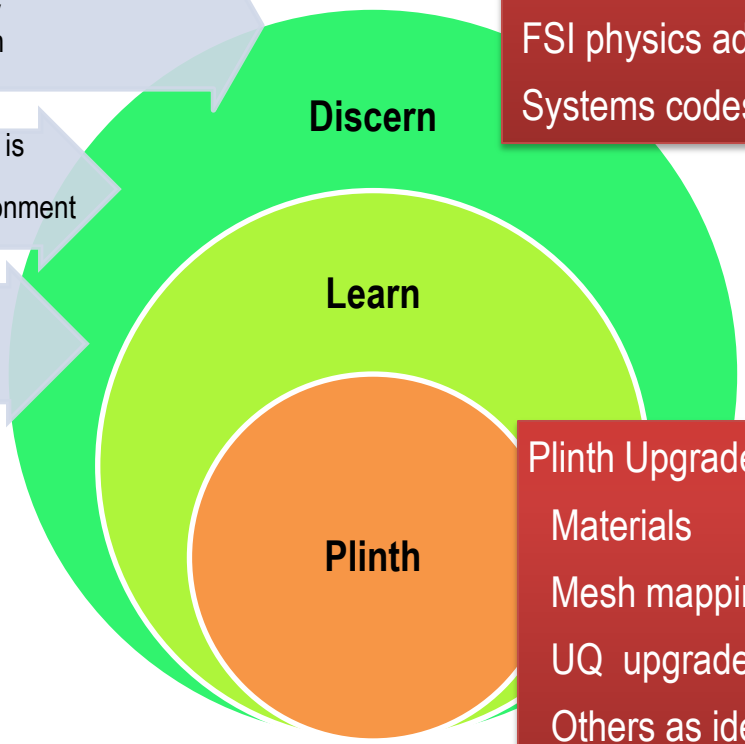

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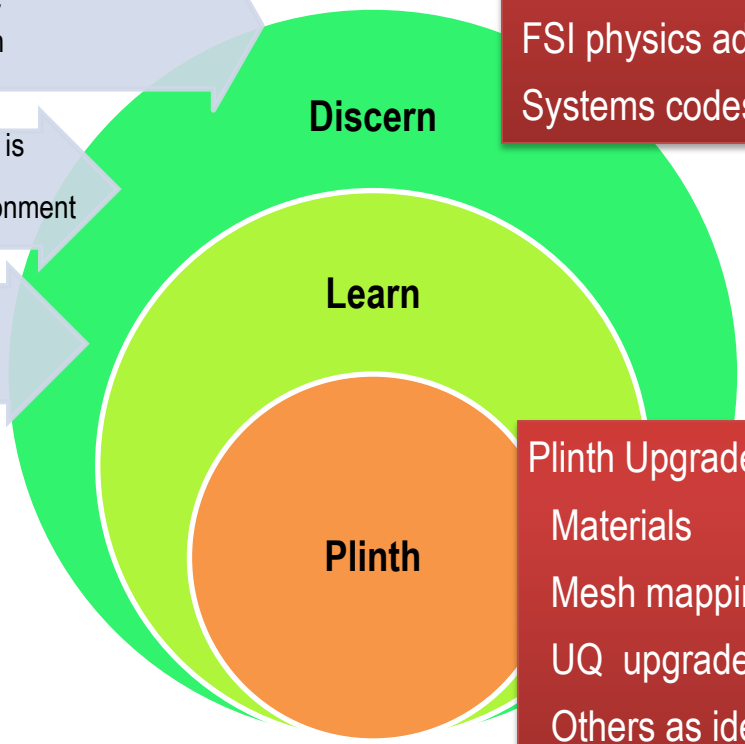

- Comes with the advertised codes, but allows Users to substitute other codes when they are configured per the Plinth requirements
- Provides enhanced and new capabilities in VRI, MPO, T/H, RT, VUQ
- HPC or large cluster platform for large challenge problem solutions
- Retain ability to license

Enhance LEARN codes or substitute more capable codes

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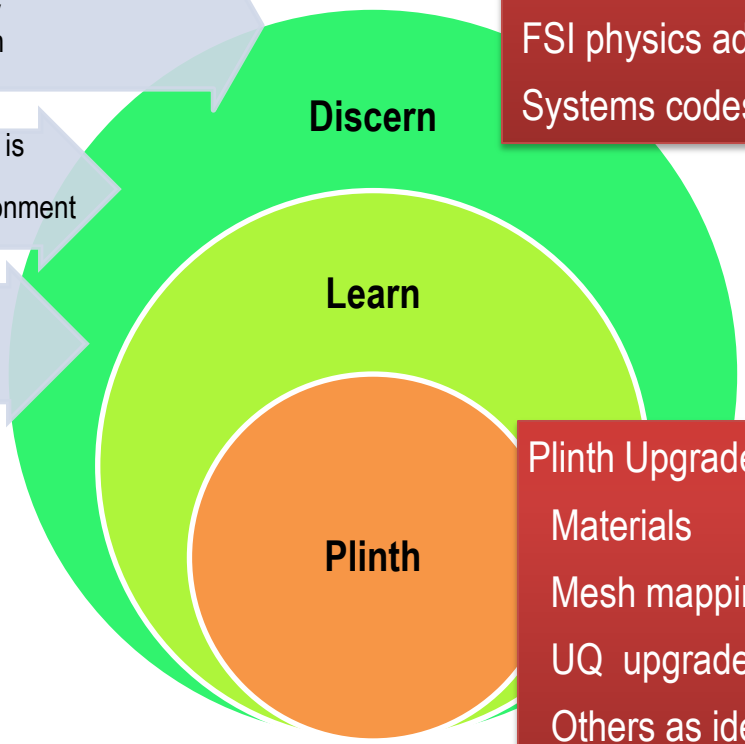

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Workhorse product for industry

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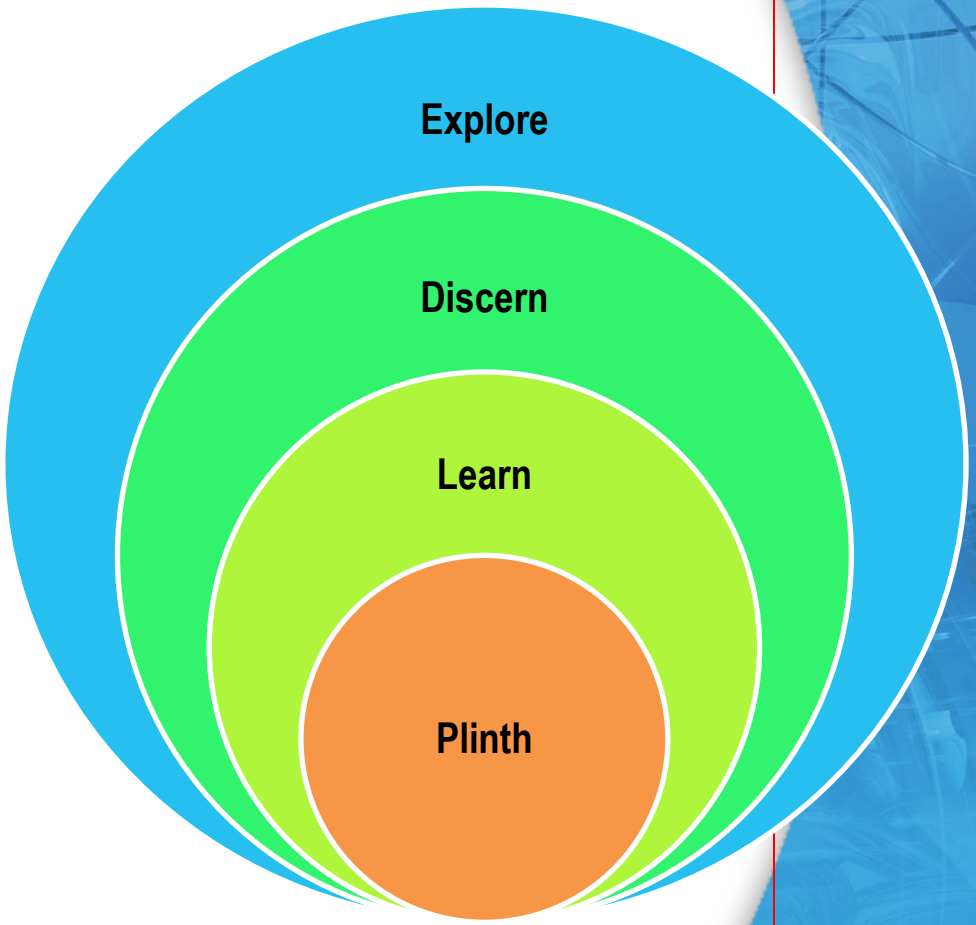

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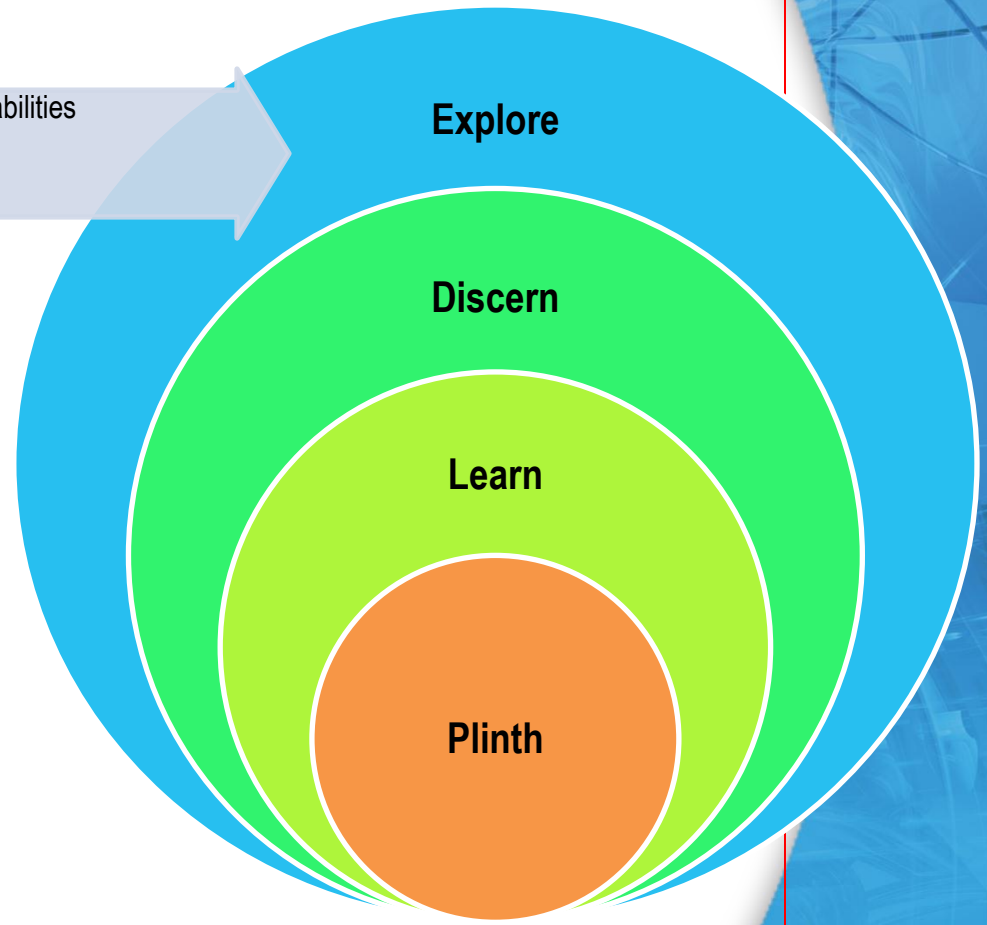
Virtual Environment for Reactor Applications

Allows research of individual physics

- Multi-scale and multi-platform capabilities
- Code and Executable
- Allows line by line editing



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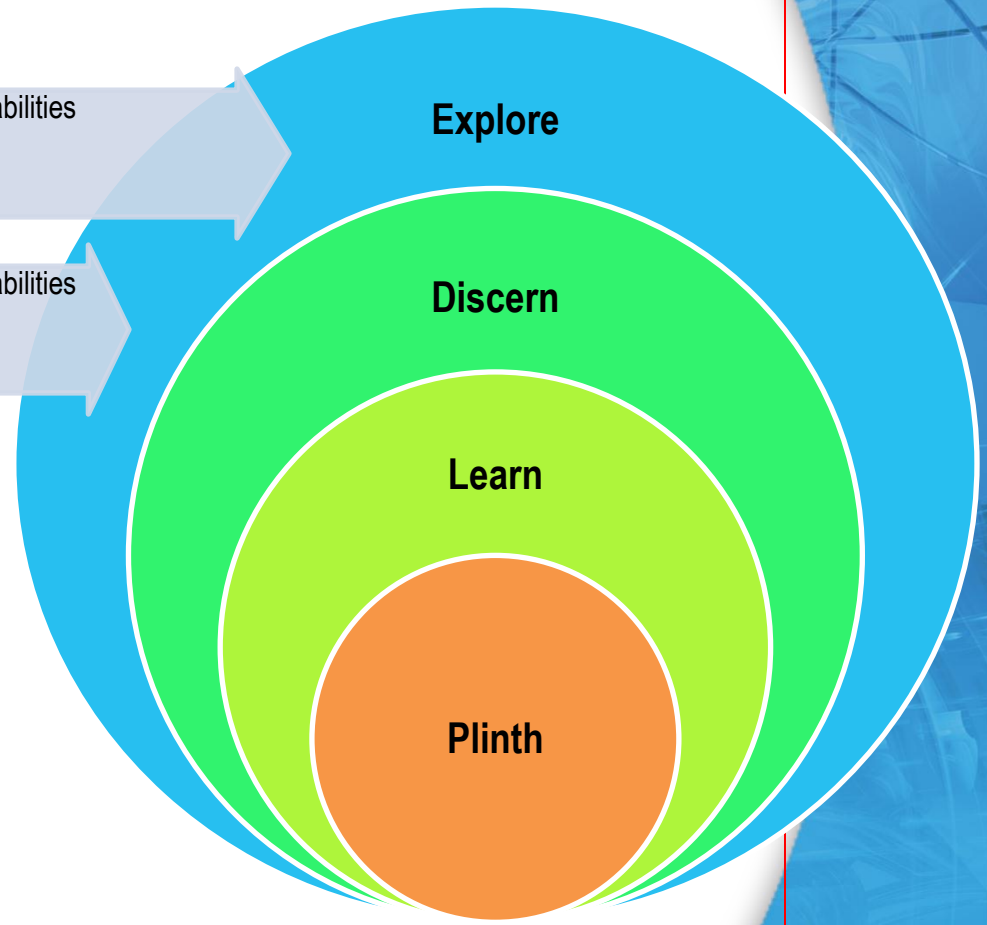

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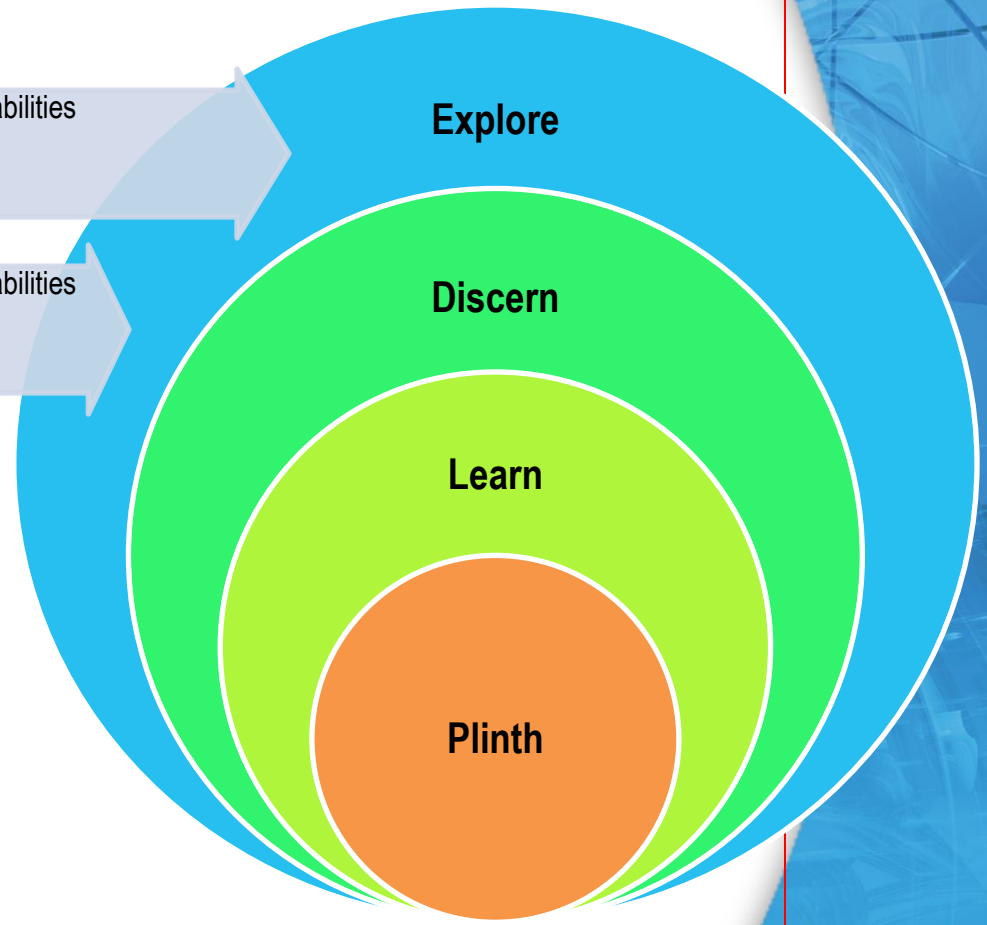

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- Efficient, numerically stable, and scalable
- Provides freedom to fully evaluate reactor response to large changes such as new reactor designs, advanced fuel configurations and materials and additions of control or instrumentation components.

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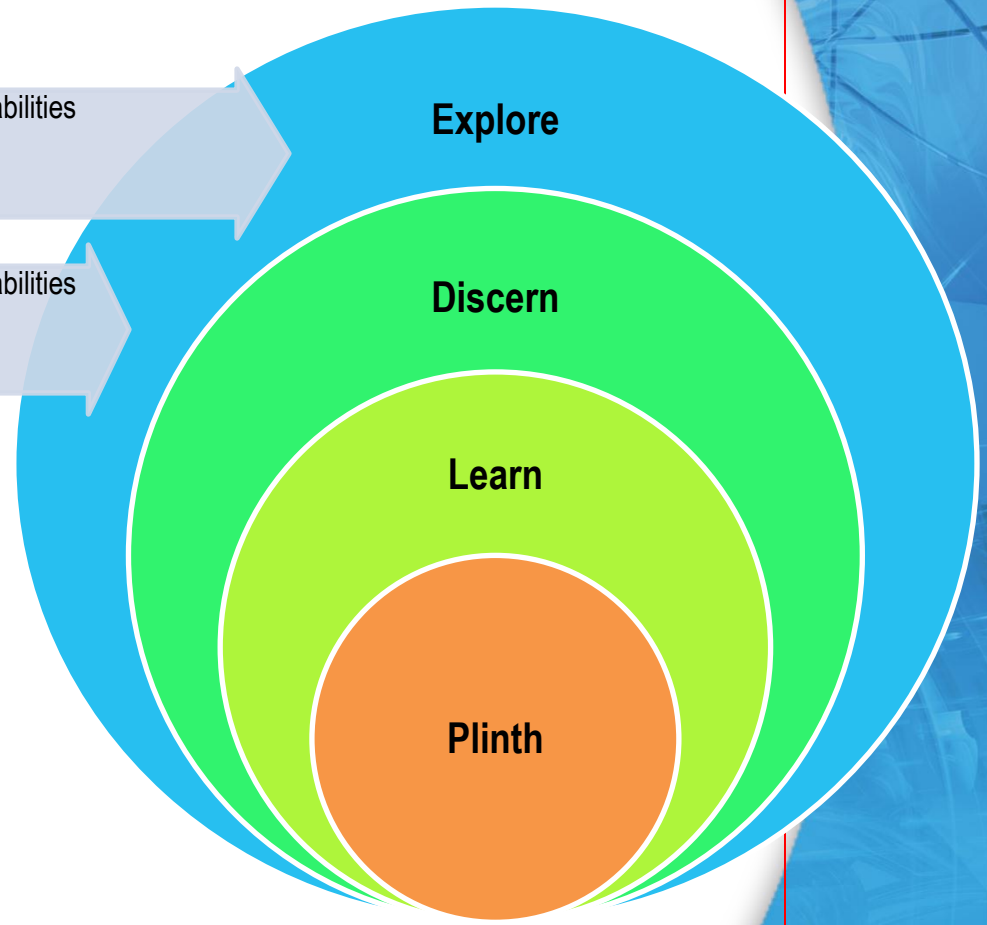

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Freedom to research all scales of response

Good correspondence of the product description with Level 1 Milestones

- Plinth
- LEARN
- DISCERN
- EXPLORE

Table 1-3: CASL Level 1 Milestones

Year	VR Capability	L1 Milestone Category	L1 Milestone
1	Initial core simulation using coupled tools and models	CRUD	Apply 3D transport with T-H feedback and CFD with neutronics to isolate CRUD-vulnerable assembly and pin in PWR full-core configuration; generate quantities relevant to CRUD initiation and growth
		GTRF/FAD	Apply full-core CFD model to calculate 3D localized flow distributions to identify transverse flow that could result in grid-rod fretting
2	Detailed phenomena modeling in fully coupled VR	CRUD	Model CRUD source terms, localized pin subcooled boiling, initiation of CRUD deposition, and CRUD thickness
		GTRF/FAD	Model interaction of fluid flow distribution with fuel rods to calculate dynamic forces that may lead to fuel rod vibration
3	Assembly simulation with rod fretting and upscaled materials models	CRUD	Model boron uptake from reactor coolant into CRUD on fuel rods
		GTRF/FAD	Model changes in spacer grid geometry and relaxation of grid springs; calculate gaps between grid springs and fuel rods
		Safety	Initial modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients
		OR	Initial modeling of reactor operation; qualify with operational data
4	Initial predictive reactor modeling in coupled VR	CRUD	Predict CIPS by calculating CRUD formation, boron uptake, and resulting axial power shape
		GTRF/FAD	Calculate fuel rod material wear resulting from GTRF
		LE	Model reactor vessel fluence and material property changes that result in material degradation and limit vessel performance
5	Predictive reactor simulation coupled to physical plant	CRUD	Analyses to mitigate CRUD formation and minimize CIPS
		GTRF/FAD	Analyze grid geometry and spring materials to mitigate materials changes and wear
		Safety	Improved modeling of peak clad temperature, oxidation, DNB, and fuel performance parameters during transients
		LE	Model mechanical and thermal stresses and fatigue that result in material failures of core internals
		AF	Demonstrate the impact of new fuel forms (clad materials, fuel materials, and fuel geometries) for use in current reactor core configurations
		OR	Improved simulation of reactor operation; qualify with operational data

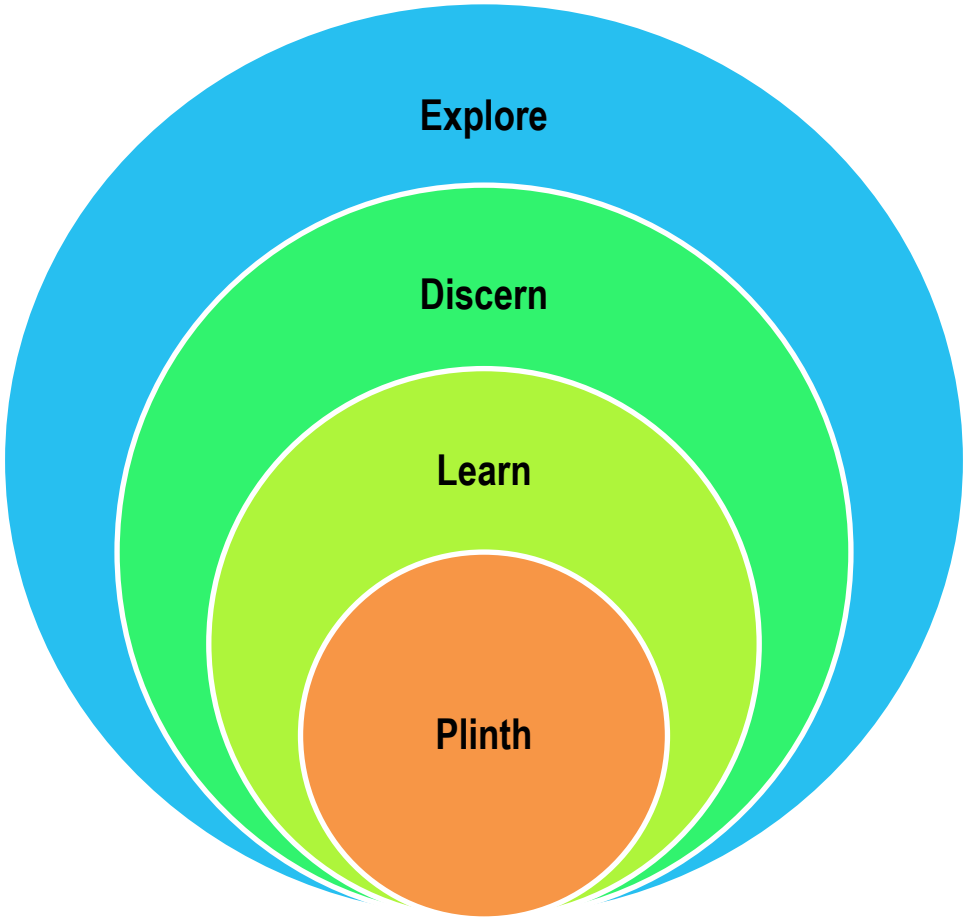
The product description identifies new areas for development

- Plinth
  - Reactor-aware structure
  - Adapt and Apply configuration
  - Standard material, geometry and mesh libraries
  - Add control components
  - Common input deck
- LEARN
  - control rod insertion model
  - Fluid-structure interaction models for seismic
  - Reactor CRUD inventory libraries
- Others??

Deployment of an industry-usable product requires more infrastructure

Product-based Metrics and Programmed Releases

VERA
Virtual Environment for Reactor Applications



Provides a high probability success path for CASL

CASL Goals

{along with some random thoughts}

Paul Turinsky

CASL Roundtable

August 9-11, 2011

NC State University

CASL-U-2011-0072-000-R

Where Have We Been?

Topic	Half Century Ago	Today
Radiation Transport		
Lattice Physics	Fine-mesh transport corrected diffusion theory using Strawbridge Correlation	MOC using Equivalence Theory + Multi-band Method
Core Wide	Few-group diffusion theory using FDM	Few-group diffusion theory using Nodal Method + pin-power reconstruction
Fuel Performance	Macro-scale coupled physics + closure relationships	Macro-scale coupled enhanced physics + some microphysics + closure relationships

Where Have We Been?

Topic	Half Century Ago	Today
Thermal-Hydraulics		
Core	Linked sub-channel analysis + closure relationships	Linked sub-channel analysis or porous media flow model + closure relationships
System	3 or 4 equation set for transverse integrated N-S equations + closure relationships	6 equation set for transverse integrated N-S equations + non-condensable + closure relationships + limited CFD
Uncertainty Quantification	Stack Uncertainties + Statistical DNB	Best Estimate + Uncertainty (CSAU Method)

Why Appearance of Lethargic Advancements?

- Licensing hurdle
- Expensive and lack of market to recover investment
- Little to be gained in technical advancement
- Really hard technical problems to model
- Lack of computational power required
- Inability to validate due to lack of experimental data

Unlikely Reason Moderate Reason Likely Reason

How Does CASL Address These Impediments to Advancement?

- Licensing hurdle: No magic bullet beyond frequent communications.
- Expensive and lack of market to recover expense: DOE is subsidizing and reliant on industry partners regarding satisfying market needs.
- Little to be gained in technical advancement: Really don't know answers yet, e.g. larger margins achieved allowing Q increase.
- Really hard technical problems to model: Diverse, talented team.
- Lack of computational power required: Unused capabilities in past, so need to demonstrate value in investing in computational power.
- Inability to validate due to lack of experimental data: Not going to change this situation very much.

Addressed Moderate Addressed Not Addressed

High Level Goals

- Economics: Power uprates & lifetime extension
  - Near-term focus is on increasing margins
  - Longer-term focus is on product improvements, e.g. fuel
- Waste Minimization: Higher fuel burnup
  - Addressing volume but not heat load/radioactive burden
  - Fuel cycle cost can be fairly flat vs burnup at these burnups
- Assuring Safety: Enhanced understanding
  - Key to regulatory acceptance of first two goals
  - In real world, by using margins to achieve first two goals places plant closer to vulnerabilities onset

Addressing Moderate Addressing Not Addressing

Working Goals

- Develop M&S capabilities to understand challenge problems and deviates from them
- Provide tools that support the work environment, e.g. V&V, portable, robust, flexible, ease of usage, insightful presentation of results, spanning designers, operators, researchers and educators
- Develop the human resources capable of developing and utilizing M&S capabilities developed, e.g. multiscale and multiphysics
- Successfully demonstrate (**market**) capabilities developed to a wide audience
- Lay the foundations to expand capabilities to other LWR systems, e.g. BWRs and LWR-SMRs, in 2nd 5 years

Focus Moderate Focus Lack Focus

Ultimate Success Metrics

- Nuclear industry employs VERA in whole or in part as part of standard business practices in support of achieving high level goals
- Funding is secured (DOE, EPRI, membership) to institutionalize CASL for the long haul

Risks to Achieving Goals

- Solving the wrong problems
- Not addressing effects of unknowns
- Lack of validation data
- Allocating resources improperly
- Missing required expertise on the team
- Inadequate or disruptive budgets
- Parochial interests, e.g. *use my code*, dominate
- Not knowing who the customers are
- Ignoring customer feedback
- Paying too much attention to customer feedback

Unlikely Moderate Likely Likely

CASL Challenge Problems CRUD, GTRF, FAD, etc

CASL Roundtable Meeting
August 9 to 11, 2011

Zeses Karoutas

Yixing Sung

Jeff Secker

Jin Yan

CASL-U-2011-0072-000-R

Outline

- Challenge Problems
- Process for Addressing Challenge Problems
- Summary of Work Performed for CRUD & GTRF – Documented in NURETH14 Papers
  - "Advanced Thermal Hydraulic Method Using 3x3 Pin Modeling", NURETH 14-338
  - "Flow Induced Vibration Forces on a Fuel Rod by LES CFD Analysis", NURETH 14-365
  - "A Multi-physics Code System Based on ANC9, VIPRE-W and BOA for CIPS Evaluation", NURETH 14-399
  - "Coupled Computational Fluid Dynamics and MOC Neutronic Simulations of Westinghouse PWR Fuel Assemblies with Grid Spacers", NURETH 14-254
- Fuel Assembly Distortion (FAD)

CASL Challenge Problems

- Industry goals will challenge fuel and plant performance:
  - Power uprates
  - Higher burnup
  - Life extension
- CASL evaluated detailed safety, operating, and design criteria to determine key phenomena that limit reactor performance
- Challenge problems tackle these key phenomena
- Better understanding of safety margins

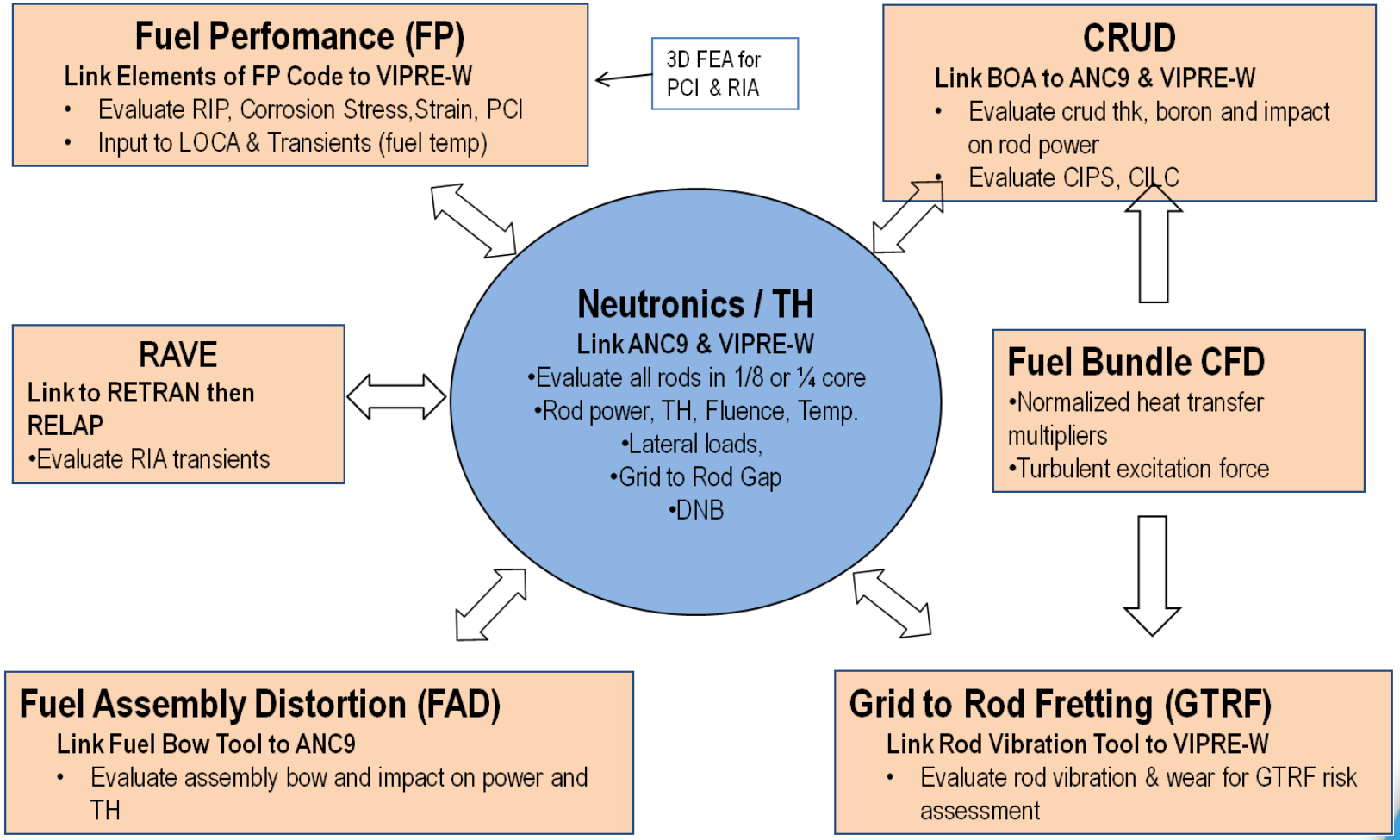
	Power uprate	High burnup	Life extension
Operational			
CRUD-induced power shift (CIPS)	×	×	
CRUD-induced localized corrosion (CILC)	×	×	
Grid-to-rod fretting failure (GTRF)		×	
Pellet-clad interaction (PCI)	×	×	
Fuel assembly distortion (FAD)	×	×	
Safety			
Departure from nucleate boiling (DNB)	×		
Cladding integrity during loss of coolant accidents (LOCA)	×	×	
Cladding integrity during reactivity insertion accidents (RIA)	×	×	
Reactor vessel integrity	×		×
Reactor internals integrity	×		×

Core CASL objective:
Develop advanced Modeling & Simulation methods and investigate new fuel designs to address challenge problems

Process for Addressing Challenge Problems

- Perform analysis of challenge problems using current tools (REF)
- Couple existing tools
- Utilize coupled existing tools to help developed advanced ones
- Start development of advanced tools with 3x3 multi-physics pin modeling then scale up to larger geometries (e.g. 17x17 & Vessel)
- Develop test problems/data packages to validate tools used for challenge problems
- Apply coupled existing and advanced tools to challenge problems for Watts Bar 1 reactor
- Utilize PCMM to summarize benefits of coupled and advanced tools and better understand safety margins

1st Step - Coupling Existing Tools to confirm benefits and help develop Advanced Tools



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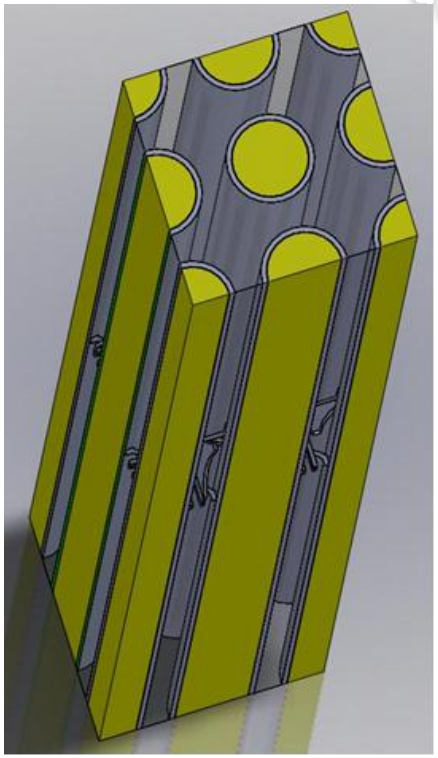
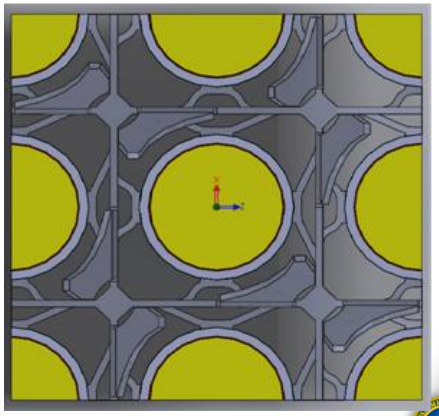
Use 3x3 Benchmark Model to Help Develop Advanced Tools

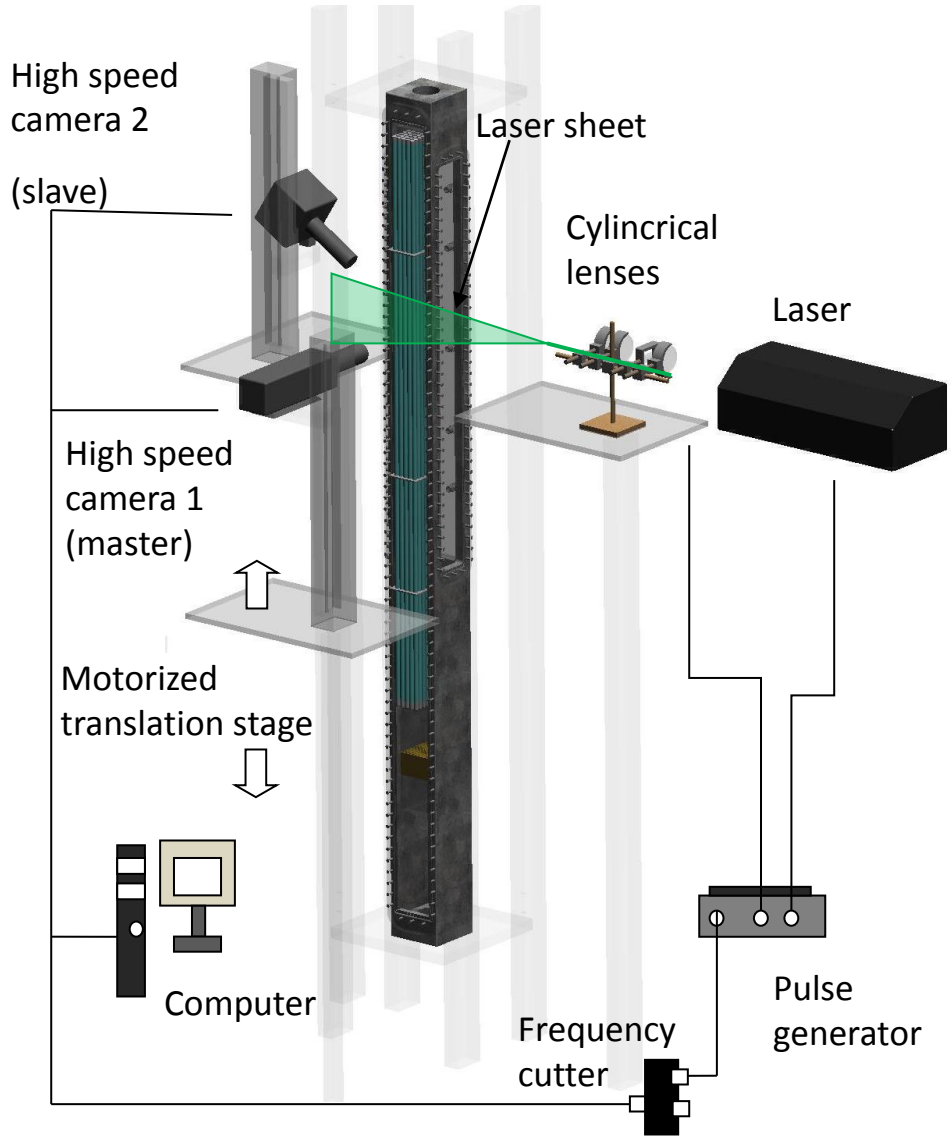
- Define a 3x3 pin bench CFD/Neutronics model with 3D fuel rod where different multi-physics models can be developed and compared to available test data and validation problems
  - Crud, Corrosion,
  - PCI
  - GTRF, Rod Vibration & FSI
  - Hydrogen, Primary Hydriding,
  - DNB, LOCA, RIA
  - Axial/Radial Growth





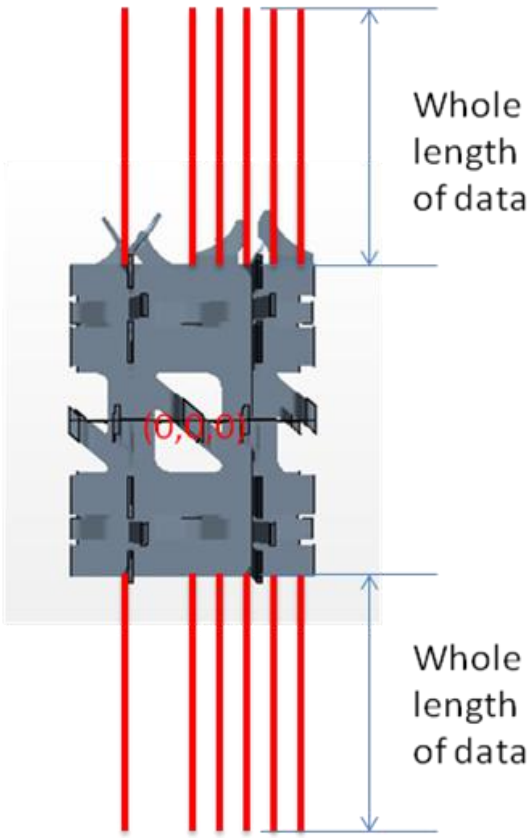
Initially Build Model for one Grid Span

Use Data from Texas A&M 5x5 Rod Bundle PIV Test Facility for Validation*

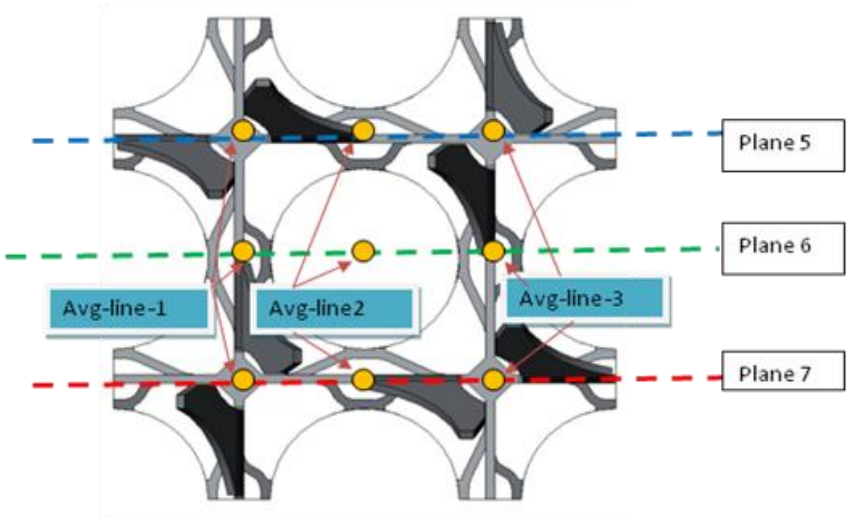


* Courtesy of Dr. Y. Hassan

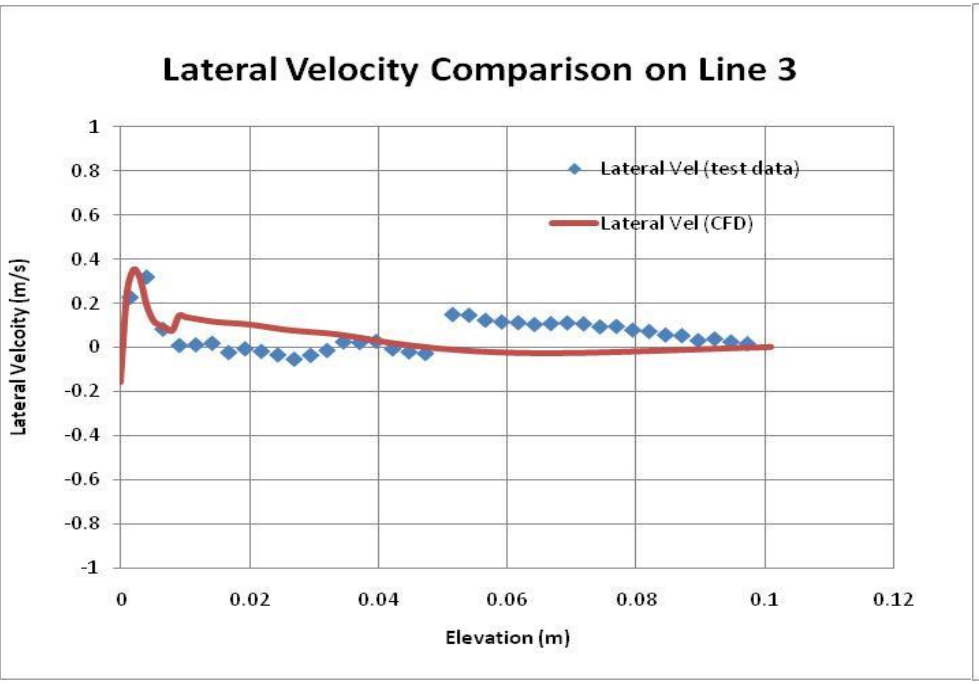
Locations for Axial and Lateral Velocity Measurements

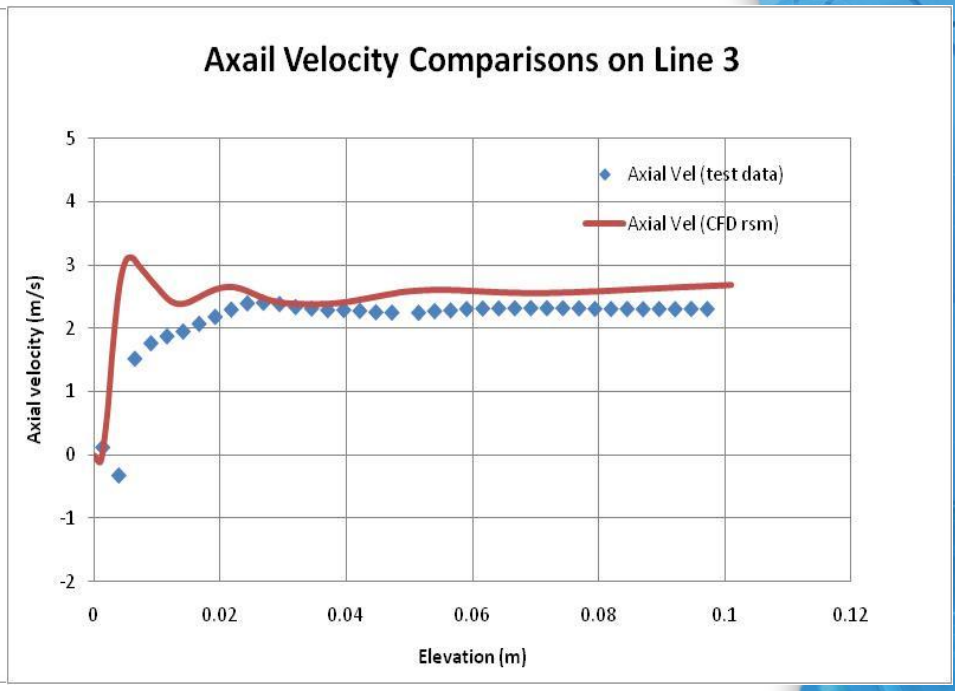


- Comparing locations
  - Axial and Lateral velocity on Line 1, 2, 3 on plane 5 will be compared



Comparison of CFD Predictions to Measurements

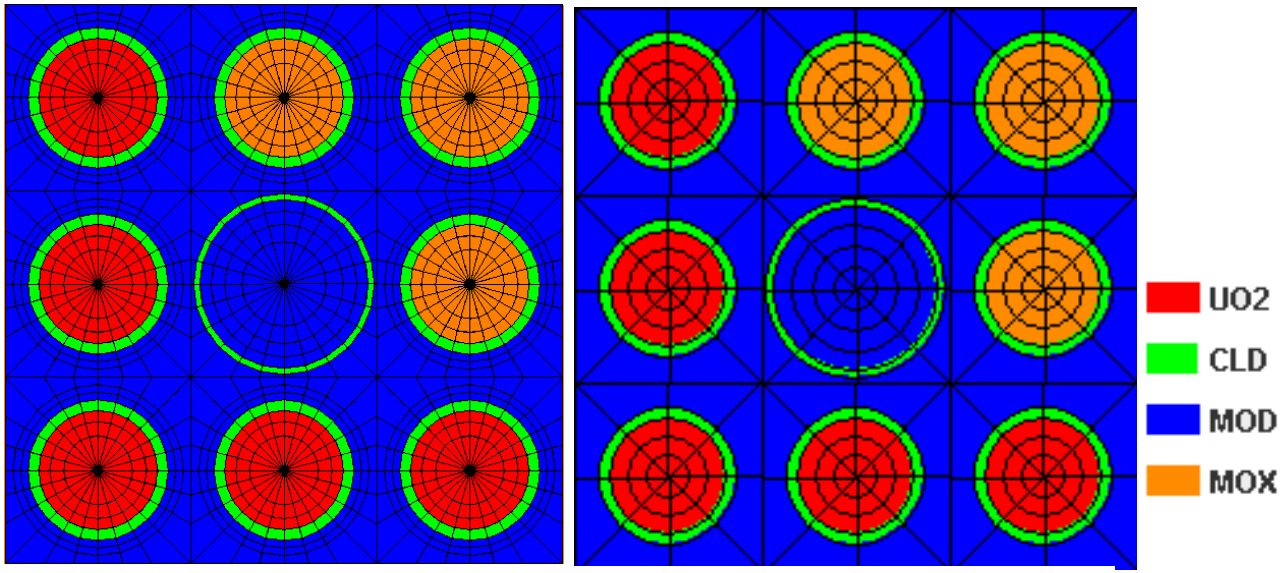


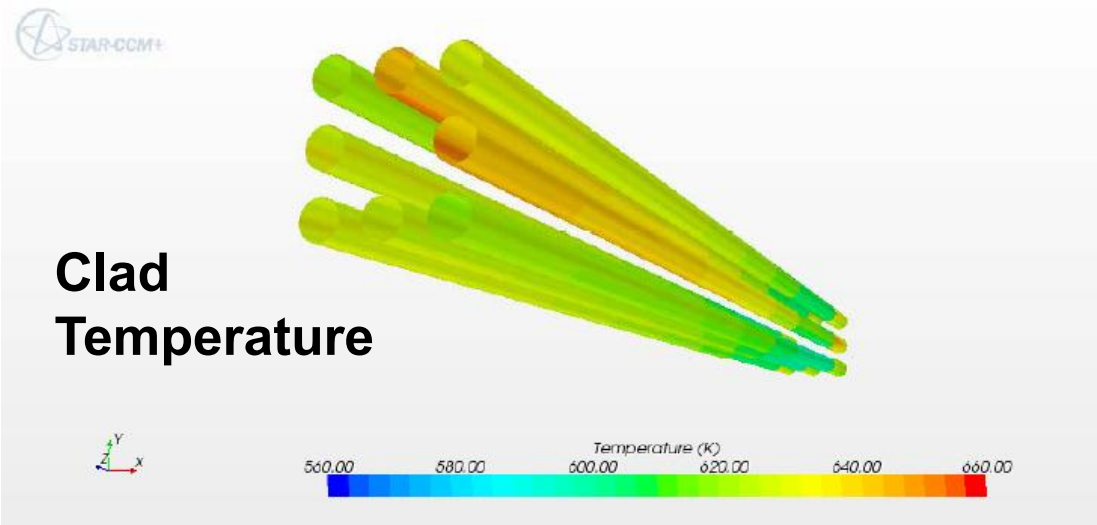


Reasonable Agreement

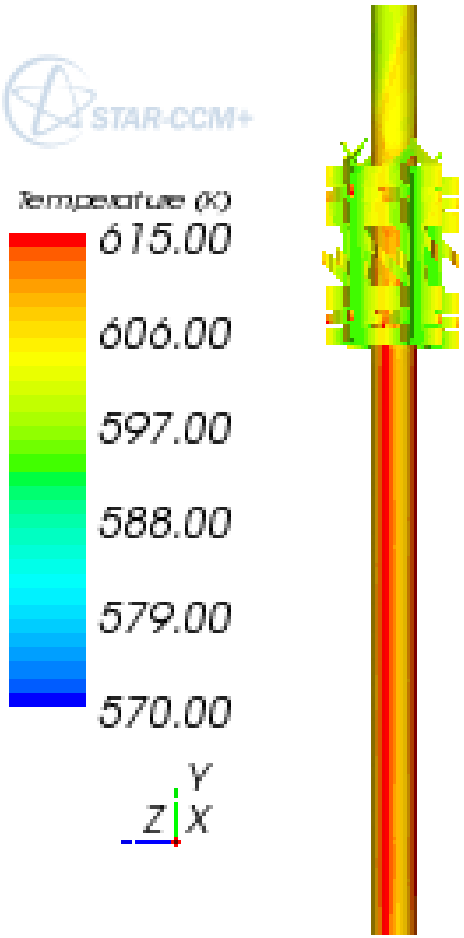
CFD / Neutronics Coupling: Star-CCM+ / DeCart

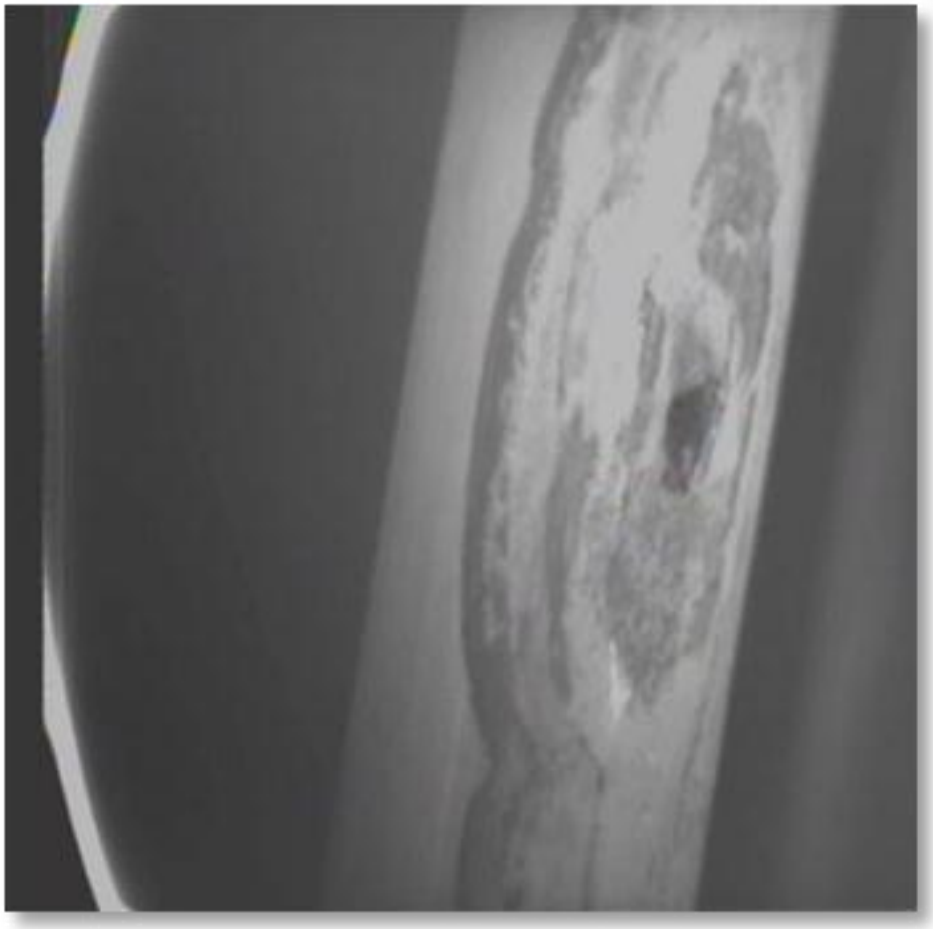
Star-CCM+ **DeCart**





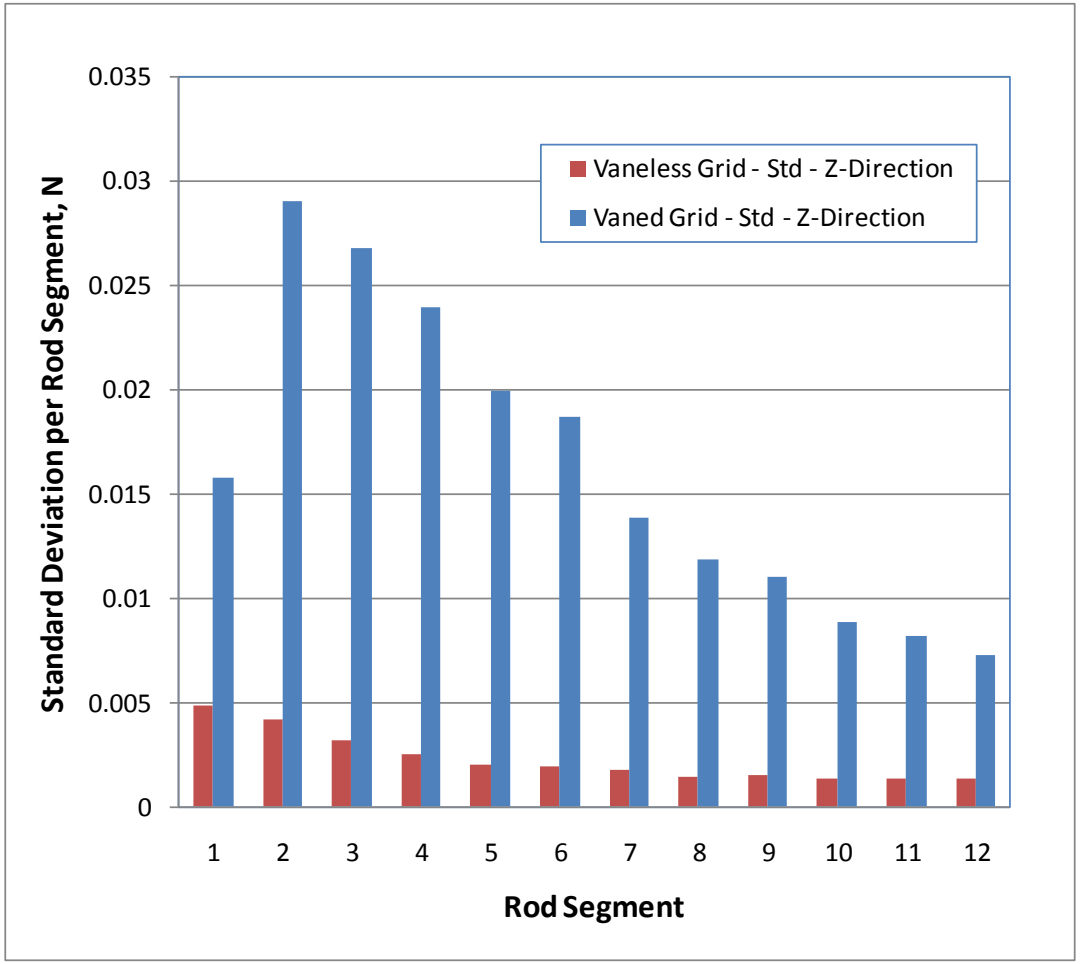
Fuel Rod Heat Transfer Modeling





Hotspots can Lead to Localized Crud Deposits

3x3 Pin LES Turbulence Modeling



Turbulence Excitation Force with and without Mixing Vanes

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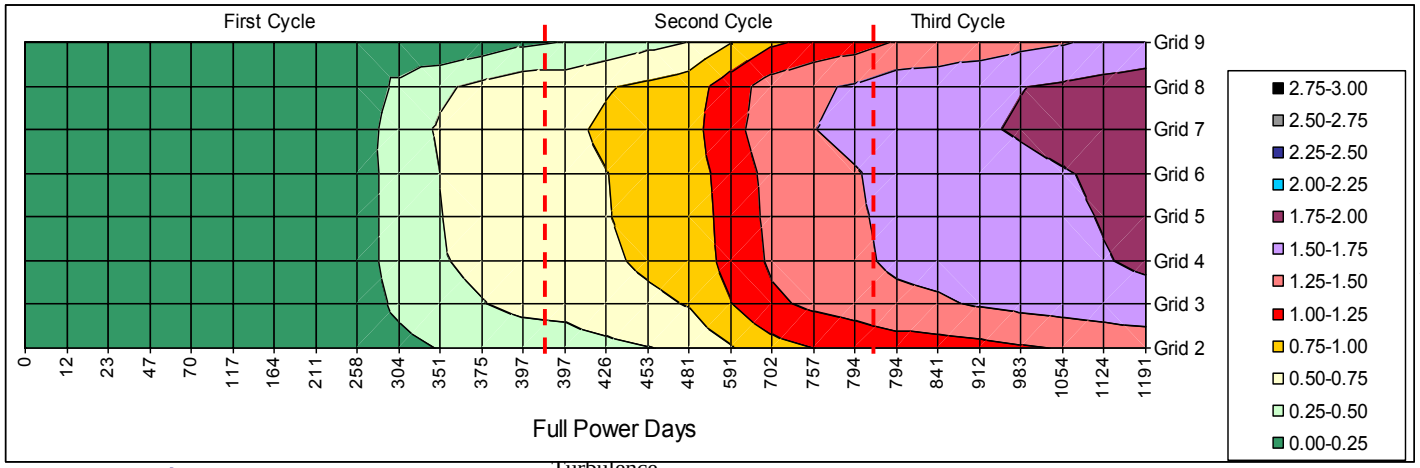
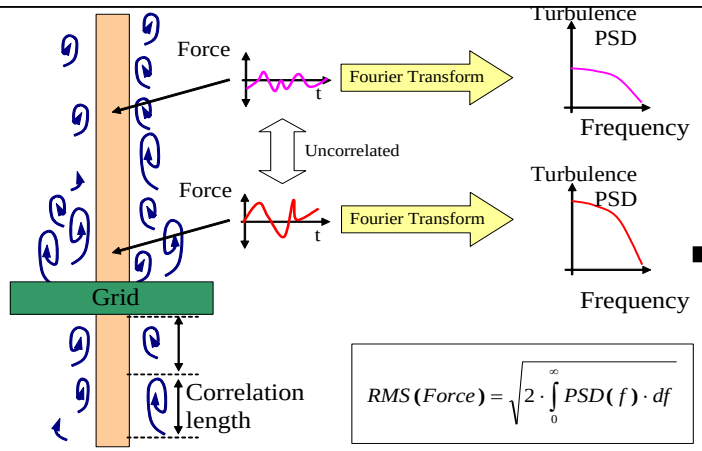
Predict Grid to Rod Gap / CFD Turbulent Excitation forces / Rod Vibration & Wear

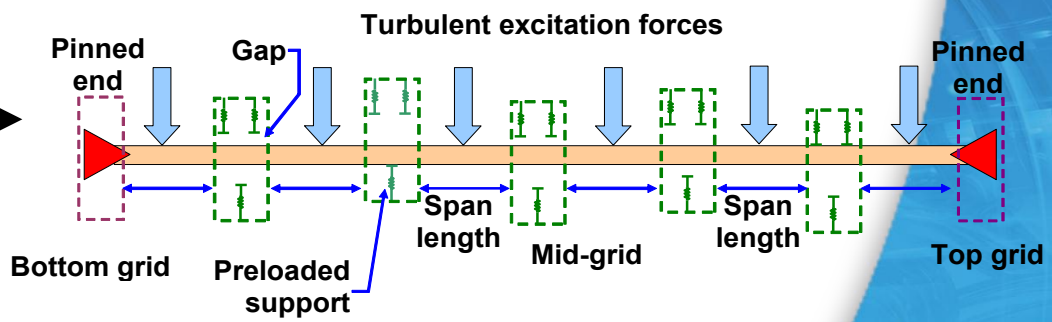


Predict grid to rod gap for all cells in core



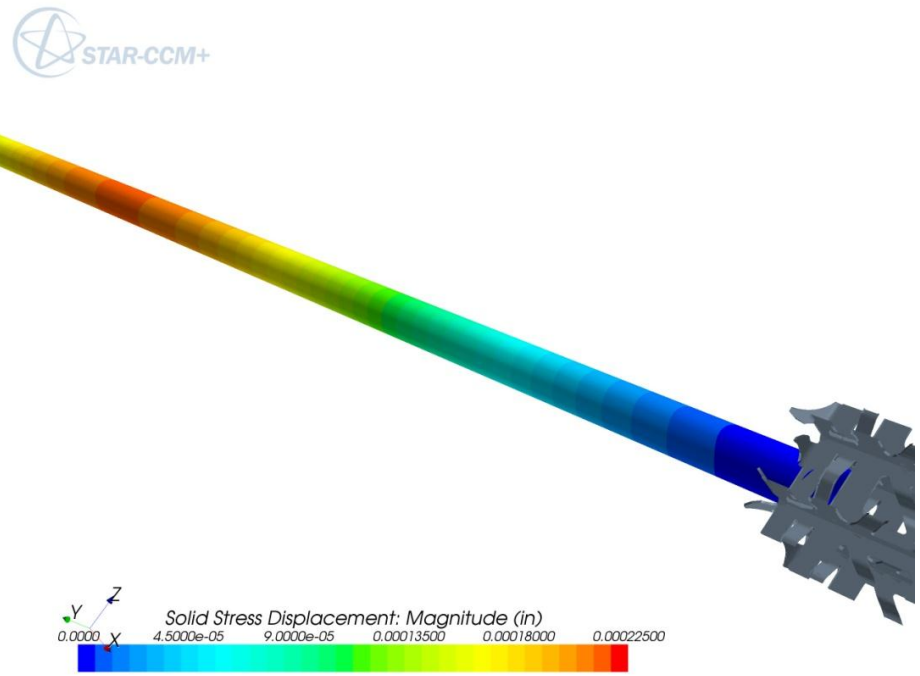
$$RMS(Force) = \sqrt{2 \cdot \int_0^{\infty} PSD(f) \cdot df}$$

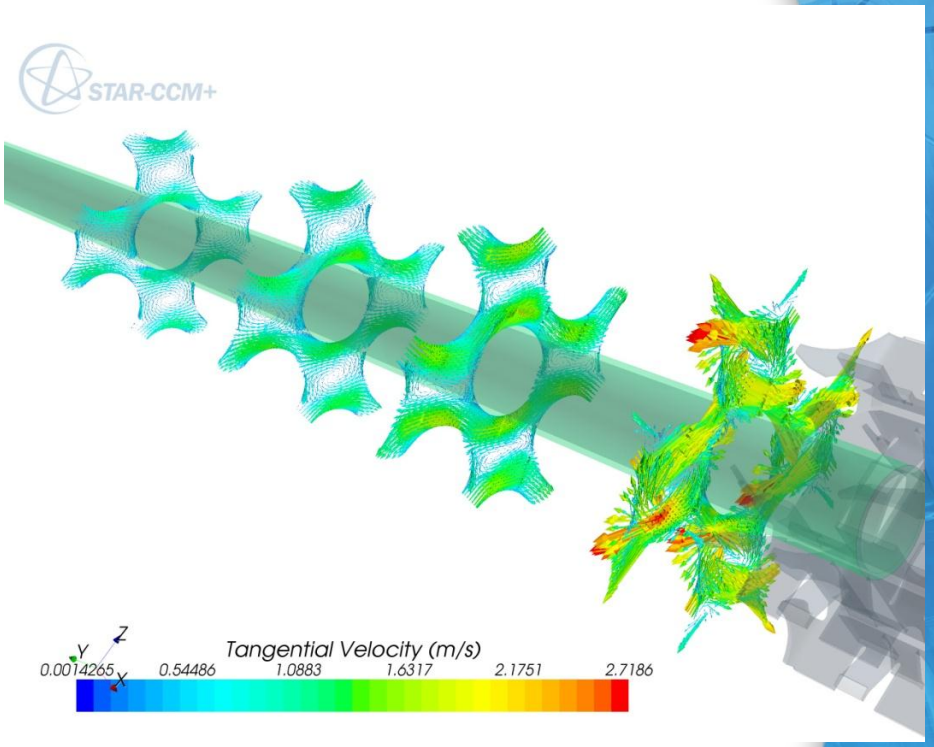
*Use **CFD** to determine turbulent excitation force*



*Use **VITRAN** code to predict rod vibration and wear*

Fluid Structural Interaction for Rod Vibration in 3x3





Maximum Vibration in Mid Span

3x3 Advanced Pin Modeling

Fuel Perfomance (FP)

Link 3D FEA Fuel Rod to Neutronic/CFD

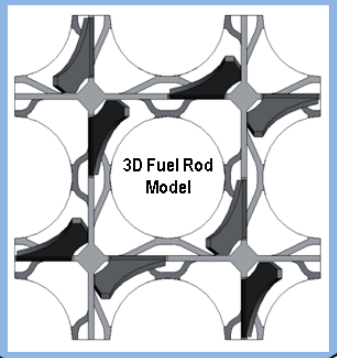
- Evaluate fuel temp, RIP, Corrosion Stress,Strain, Hydrogen, Growth, PCI
- Hot Cell, PIE, Halden, Stiudsvik data

CRUD / Corrosion

Link BOA to Neutronic/CFD

- Evaluate crud thk, boron uptake, clad corroion, CIPS, CILC
- WALT loop, PIE, Halden PIV, LDV, Nester , PSBT, MIT, Data

Neutronics /CFD



Transient Eval.

Link to RELAP, RETRAN

- Evaluate DNB, RIA , LOCA
- CHF, CABRI, FLECHT, APEX, NSRR, Halden Data

Advanced Materials

Link to 3D FEA Fuel Rod

- Evaluate fuel temp, RIP, Corrosion Stress,Strain, Hydrogen,Growth, PCI
- HFIR, Data

Fuel Assembly Distortion (FAD)

Link 3D FEA of Fuel in Core to Neutroic/CFD

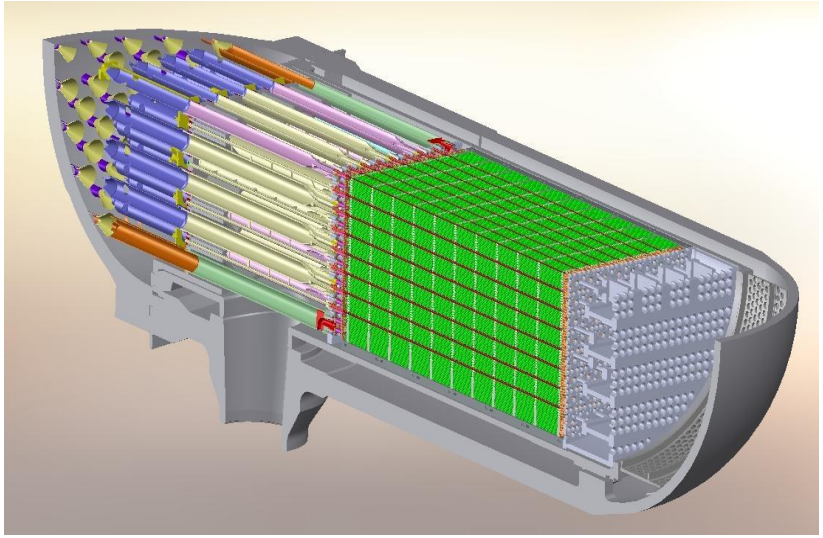
- Evaluate assembly bow and impact on power and TH
- PIE Data

Grid to Rod Fretting (GTRF)

Link Single Rod FSI to Neutronic/CFD

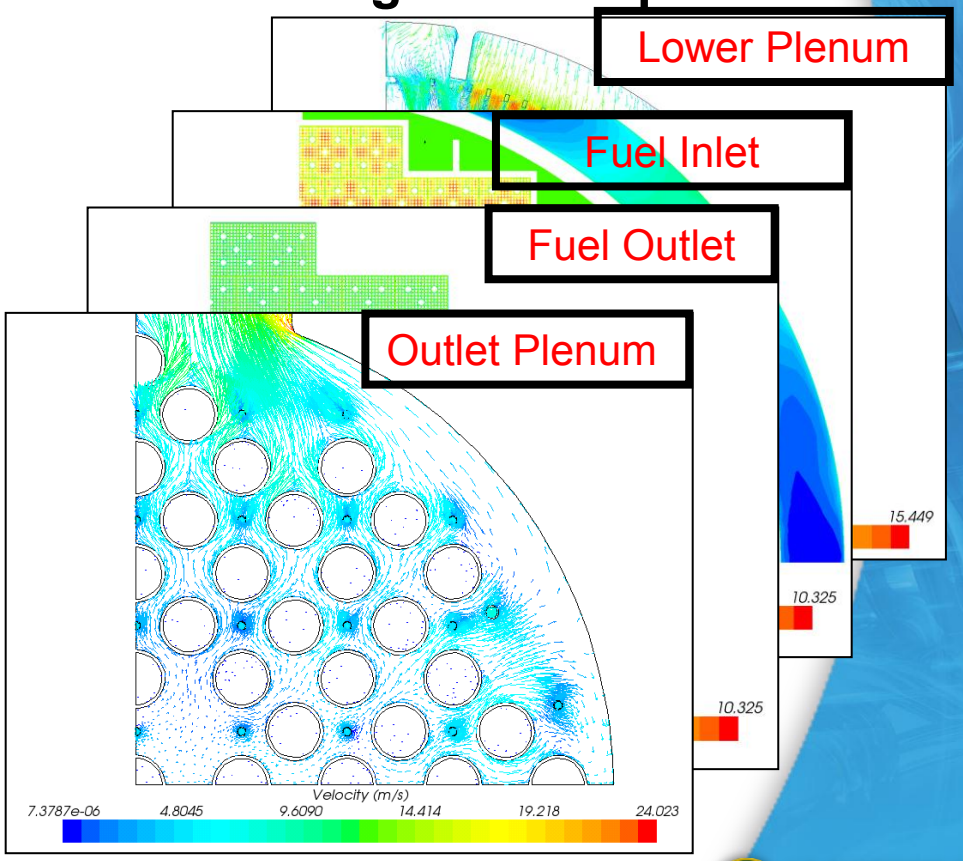
- Evaluate grid to rod gap, rod vibration & wear
- Westinghouse Labs, PIE

Expand from 3x3 to a CE Vessel Model with coupled CFD and Neutronics



3D CAD Models for Vessel, Internals and Fuel

Perform detailed pin CFD modeling and two-phase flow



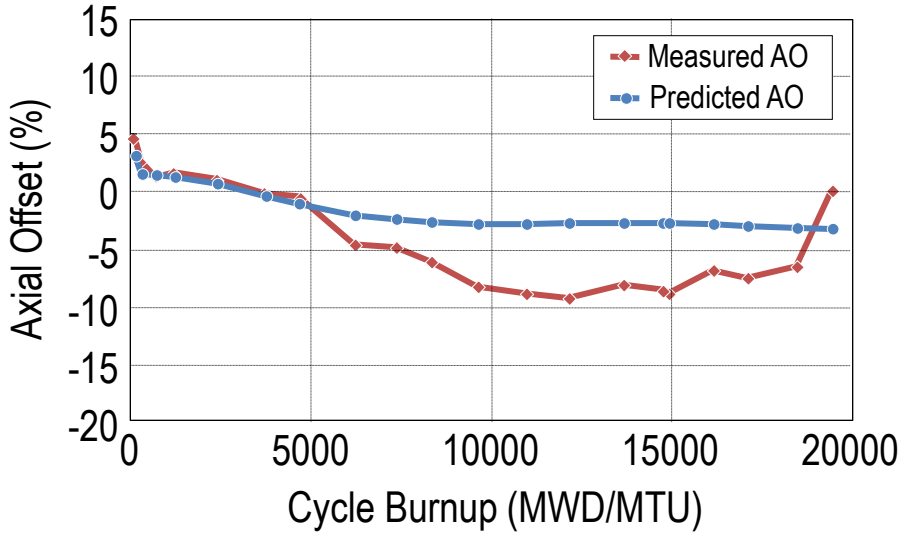
"A Multi-physics Code System Based on ANC9, VIPRE-W and BOA for CIPS Evaluation", NURETH 14-399

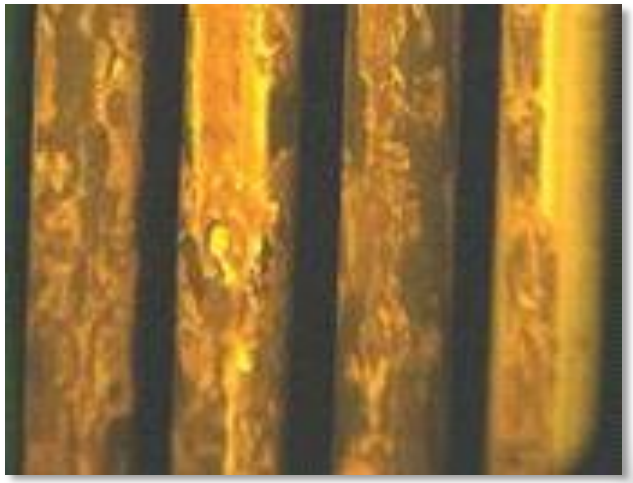
- As the 1st step, current design codes used in the industry are coupled for a PWR crud-related issue evaluation
  - ANC9 – Westinghouse neutronic nodal code
  - VIPRE-W – Westinghouse version of EPRI VIPRE-01 reactor core thermal-hydraulic code
  - BOA – EPRI crud and boron deposition risk assessment code
- CIPS – Crud Induced Power Shift
- A prototype ANC9/VIPRE-W/BOA code system was developed based on existing ANC9/VIPRE-W
  - Initial setup of data interface between ANC9 and BOA
  - Initial codes for further development of VERA software

ANC9/VIPREW/BOA

Crud Induced Power Shift (CIPS)

- Deviation in axial power shape
  - Cause: Boron uptake in crud deposits in high power regions with subcooled boiling
  - Affects fuel management and thermal margin in many plants
- Power uprates will increase potential for crud growth

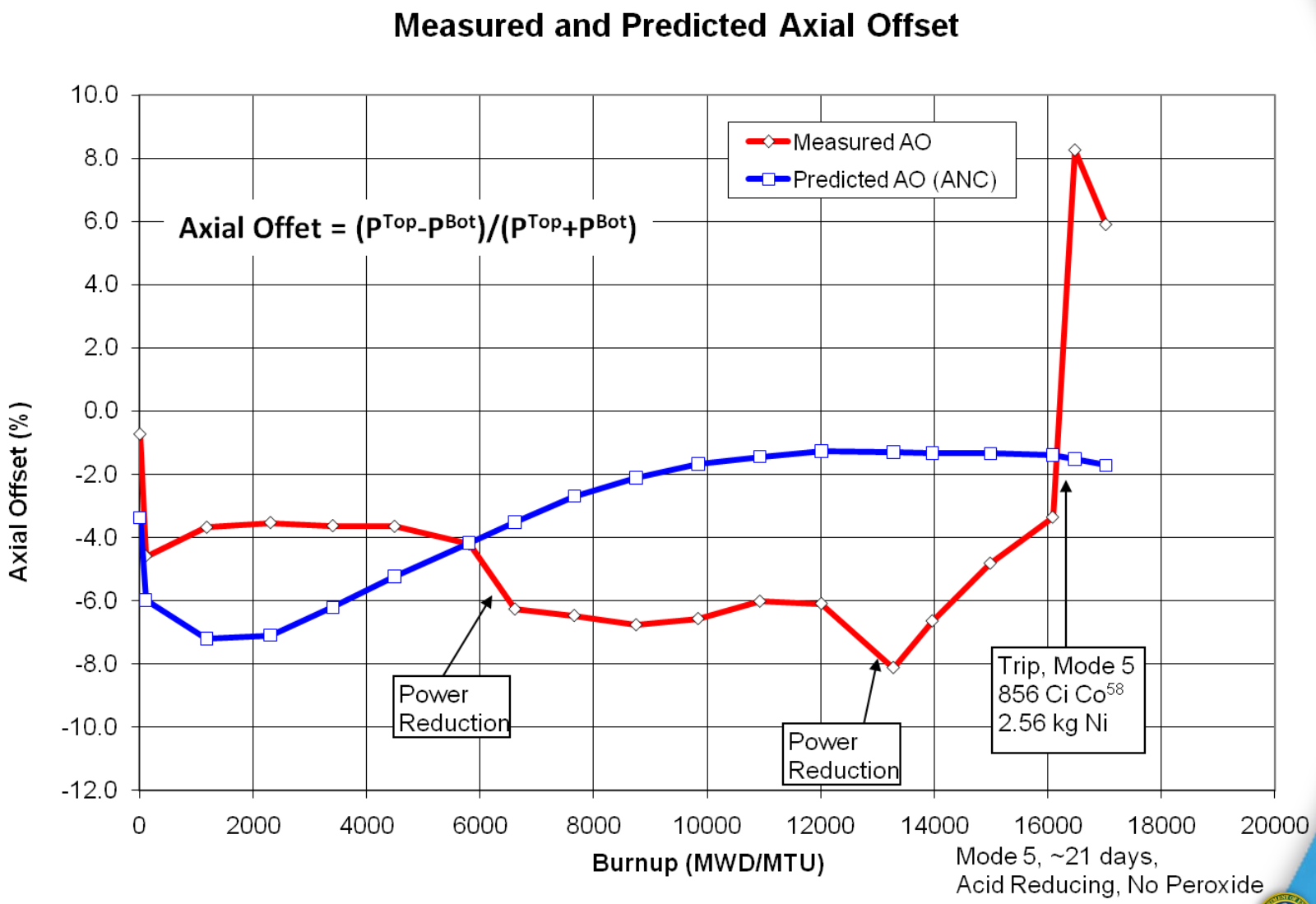




CRUD deposits

Need: Multi-physics chemistry, T-H, and neutronics model to predict crud growth

CIPS Axial Power Distribution Behavior



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ANC9 Neutronics

- New version of Westinghouse neutronic nodal steady state and kinetic code
- 3D semi-analytical nodal expansion method
- Construct node cross-sections based on nodal history and local conditions
- Code capabilities for PWR design applications include:
  - Fuel burnup predictions
  - Rod power predictions
  - Control rod model
  - Coolant boron concentration changes

ANC9

VIPREW Thermal-Hydraulics

- Westinghouse version of EPRI VIPRE-01 code
  - Developed from COBRA
  - Steady state and transient reactor core thermal-hydraulic calculations
- VIPRE-W contains enhancements for PWR applications
  - Grid heat transfer model
  - Fuel boiling rate model
- Core model consistent with ANC9
  - Quarter fuel assembly per channel
  - More detailed axial nodes in VIPRE-W as needed

VIPRE-W

BOA Crud Deposition and Chemistry

- EPRI code for predicting crud deposition and boron accumulation on fuel cladding surface
  - Corrosion product mass transfer and balance
  - Coolant chemistry effects
  - Corrosion product release in coolant system
  - Fuel sub-cooled boiling rates and distribution
  - Porous deposit modeling
  - Boron deposition modeling

BOA

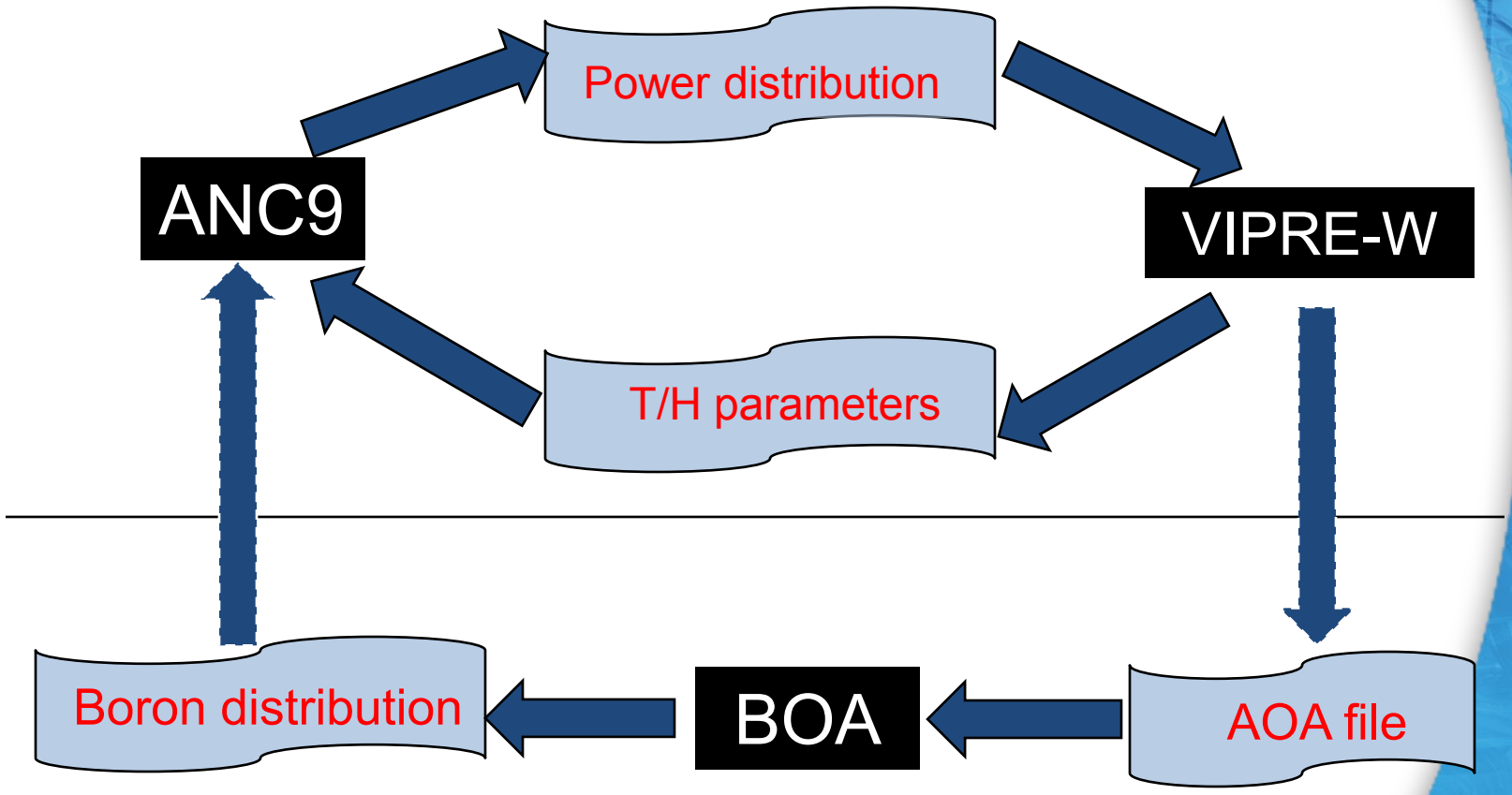
Code Coupling Approach

- Initial code linkage is to address CIPS – core wide phenomenon
- Focused on interactions on boron accumulation and effect of B-10 absorption on power distribution change
  - Impact on fuel temperature feedback not yet considered
  - Assumed slow deposition and accumulation (~days)
- Adjustment to ANC9 feedback model

$$\Sigma_{a,g}^{Correct} = \Sigma_{a,g}^{NoCrud} + N_{B10}^{Crud} \cdot \sigma_{a,g}^{B10}$$

ANC9/VIPREW/BOA

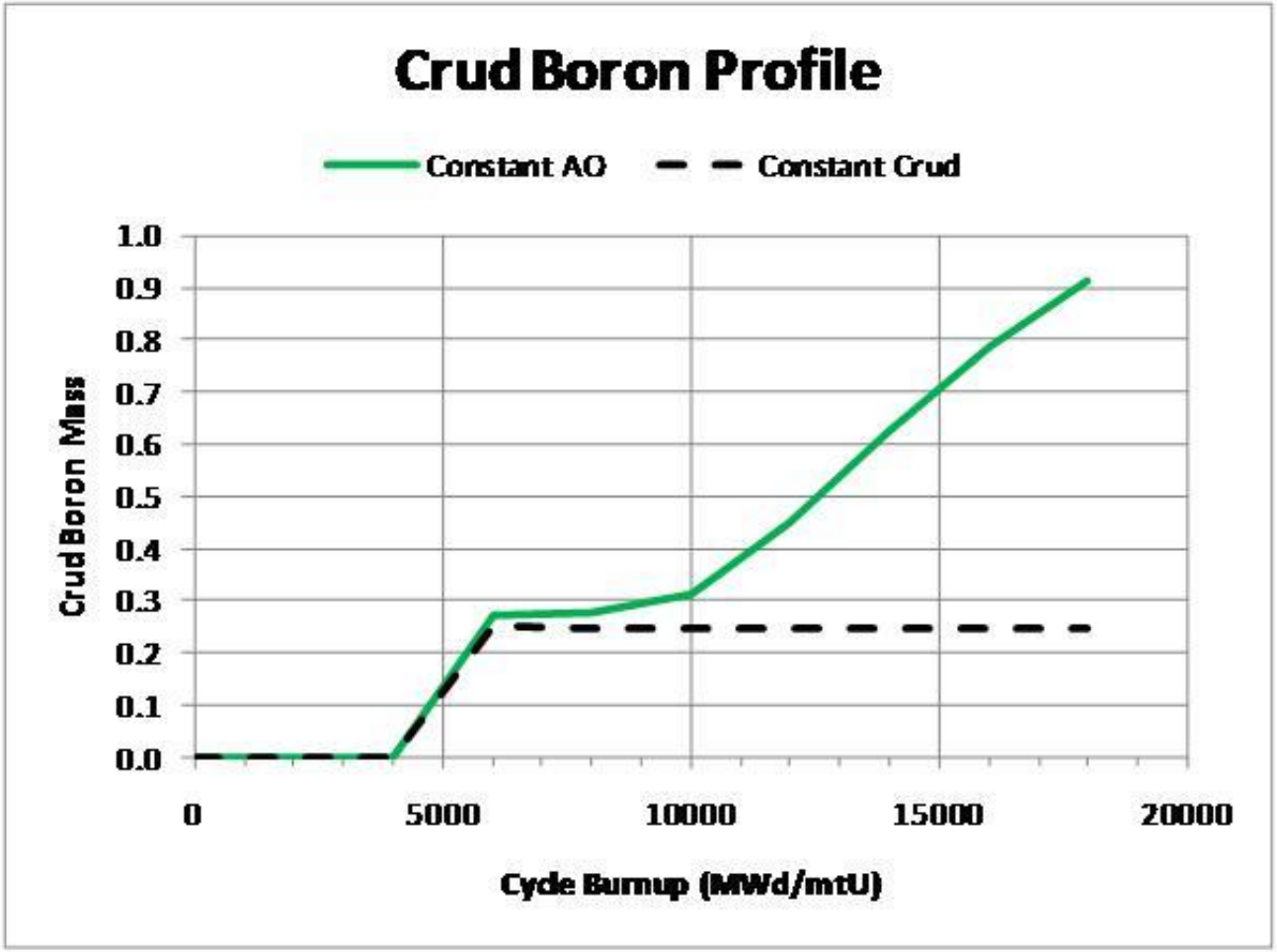
ANC9/VIPRE-W/BOA Linkage



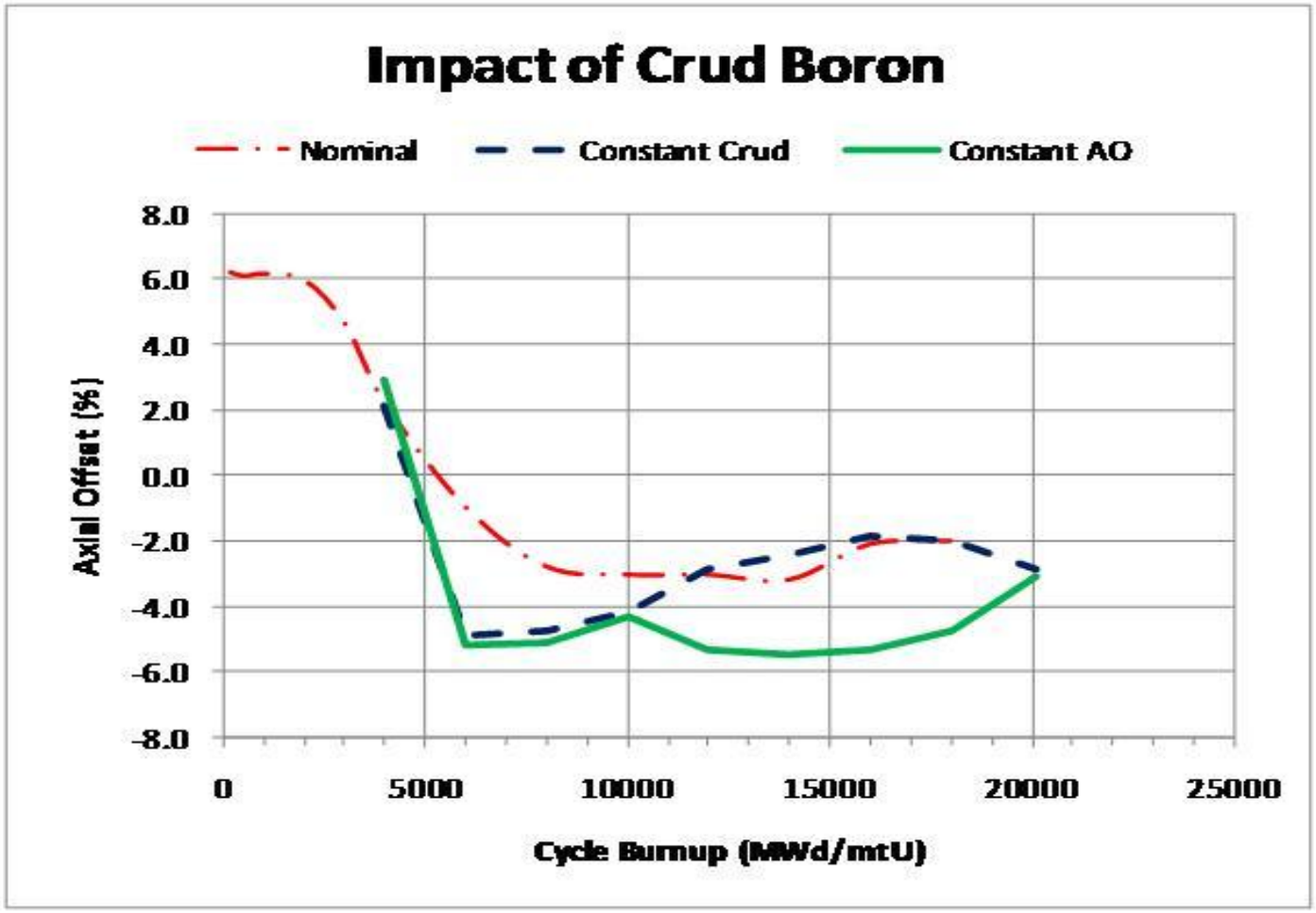
Boron/Crud Effect Evaluation

- Case description
  - Case 1: HFP depletion without crud deposition (standard calculation)
  - Case 2: Assumed a boron distribution to slightly reduce the core axial offset at 6000 MWd/mtU and the boron distribution held uniform for the remainder of the cycle
  - Case 3: Started as the second case, but varied the amount of boron to keep the core-wise axial offset at a constant value
- Effect of boron mass is evaluated

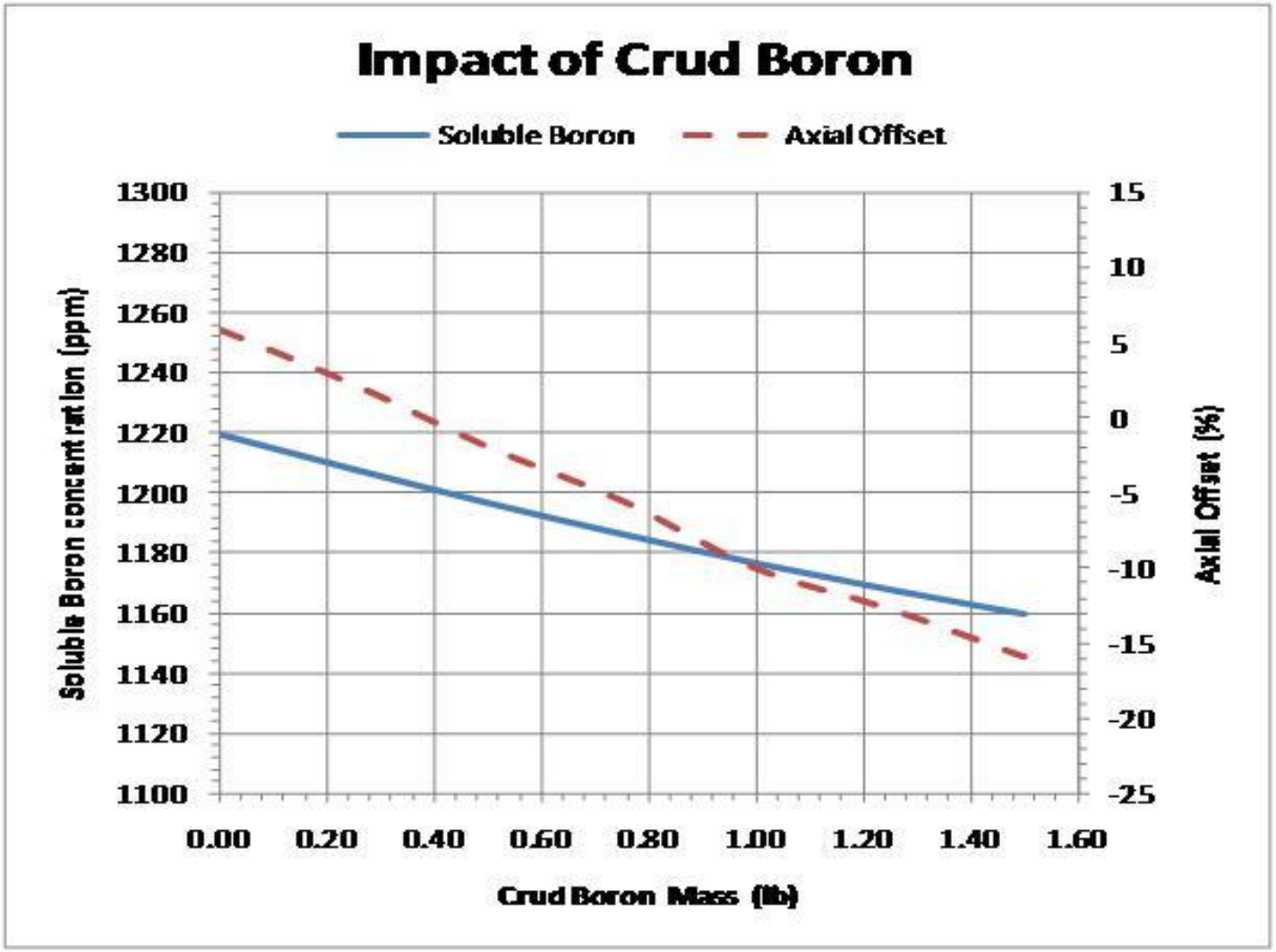
Boron/Crud Effect Evaluation



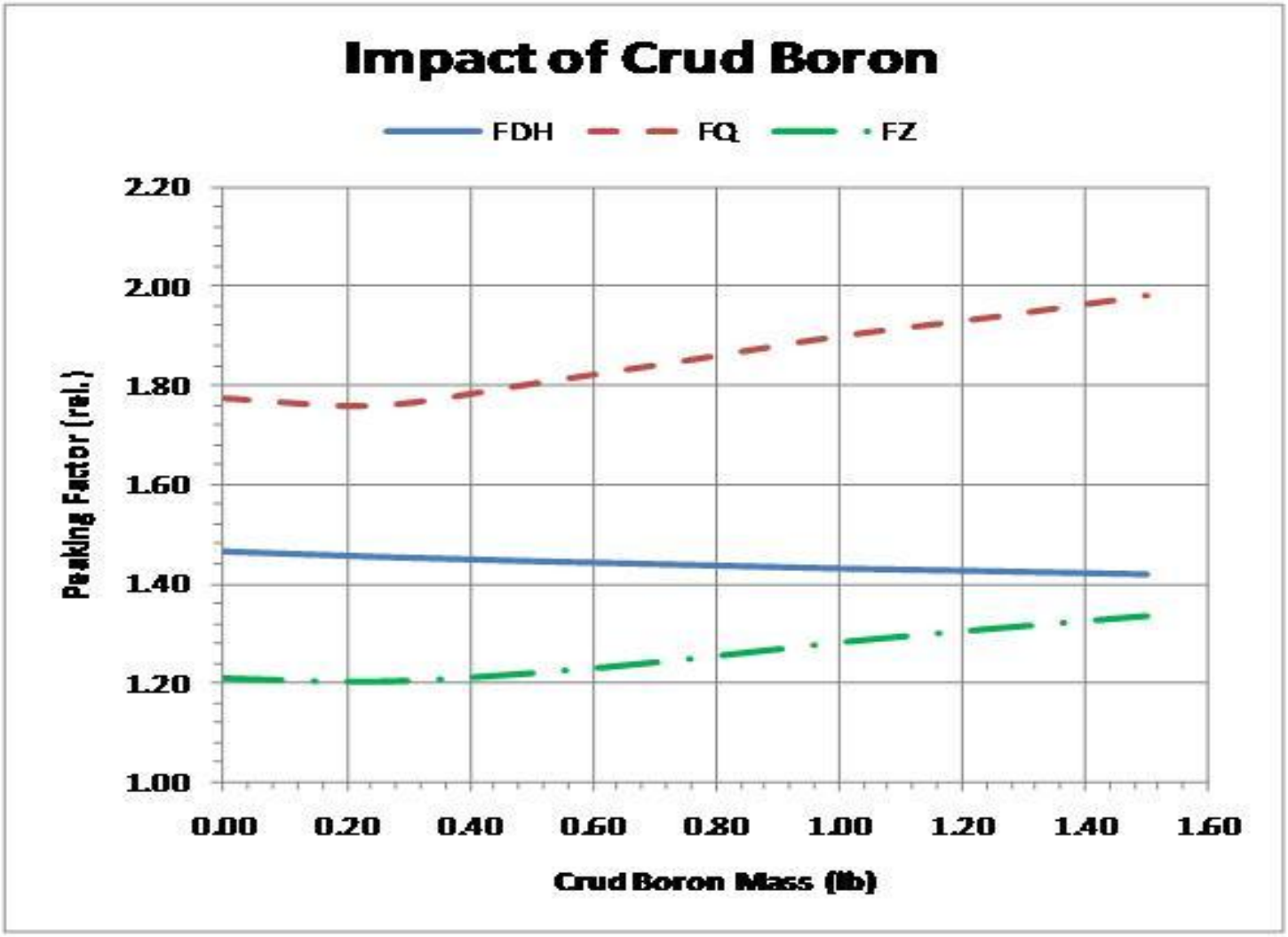
Boron/Crud Effect Evaluation



Boron/Crud Effect Evaluation



Boron/Crud Effect Evaluation

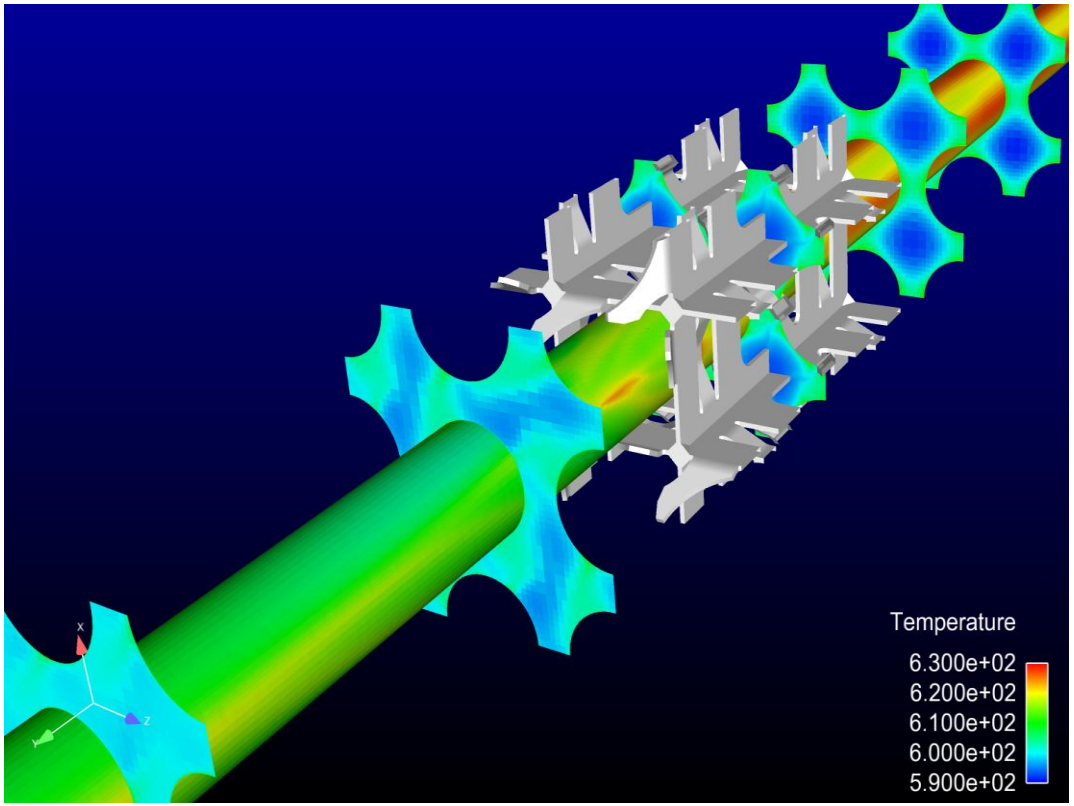


Summary of ANC9/VIPREW/BOA

- A prototype version of ANC9/VIPREW/BOA was developed for CIPS evaluation
- Sensitivity of core power distribution to boron distribution evaluated using the linked codes
- Code linkage is being improved using LIME approach
- Increasing model capability for more detailed crud analysis is under development
  - Local crud deposit thickness for Crud Induced Localized Corrosion (CILC)

ANC9/VIPREW/BOA

“Coupled Computational Fluid Dynamics and MOC Neutronic Simulations of Westinghouse PWR Fuel Assemblies with Grid Spacers”, NURETH 14-254



3x3 pin PWR fuel

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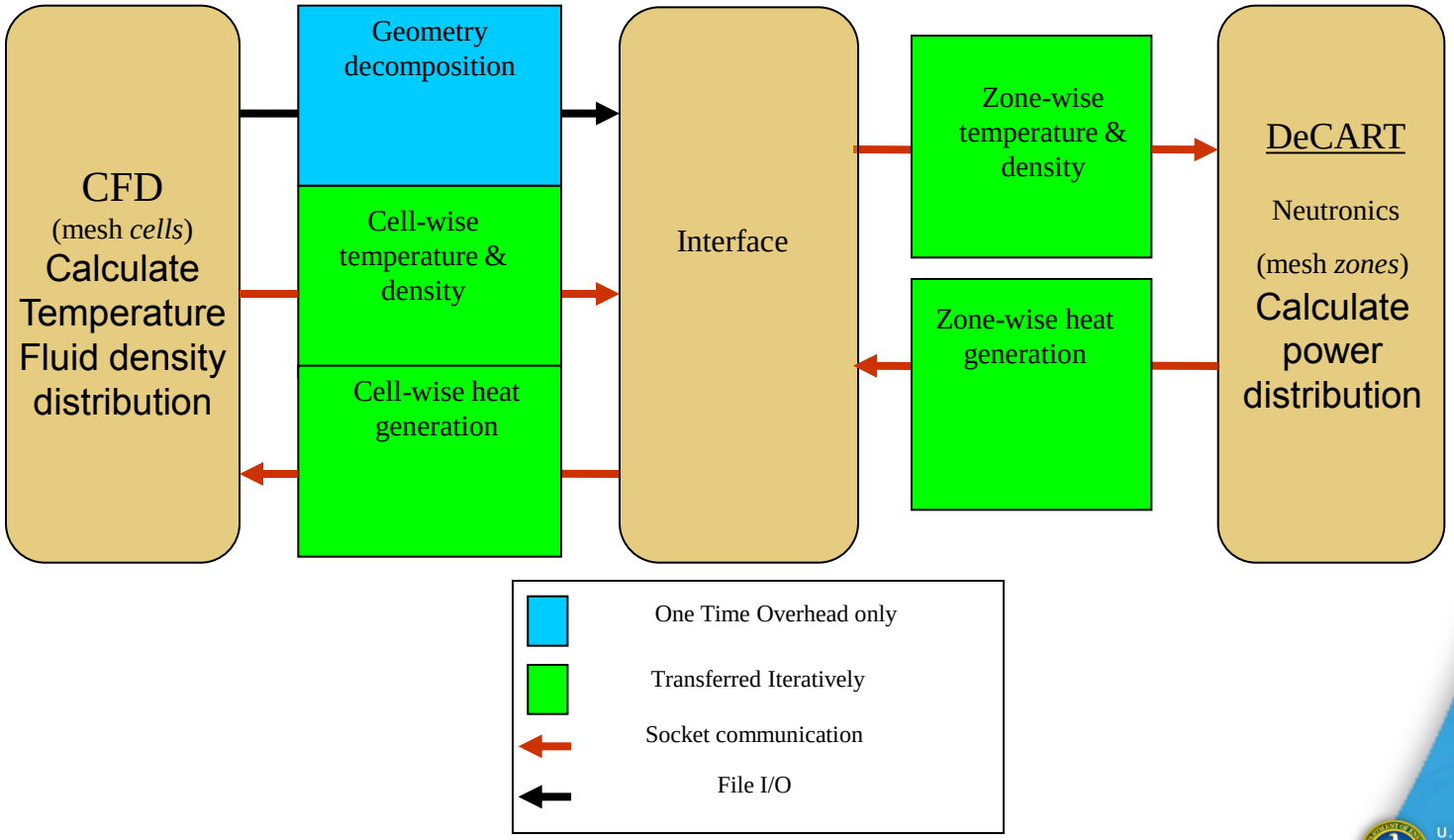
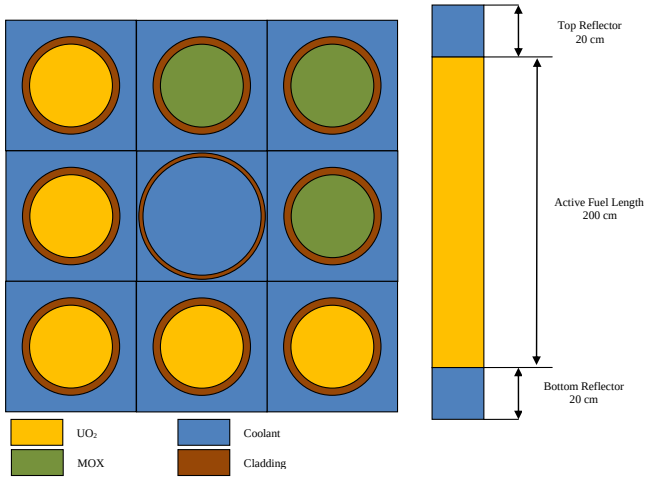
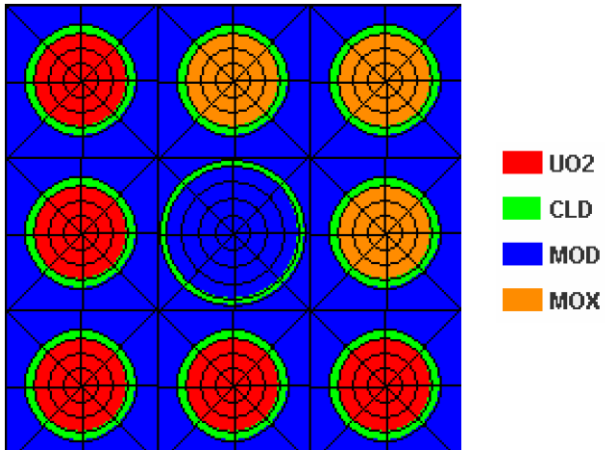
Neutronic Coupling with CFD



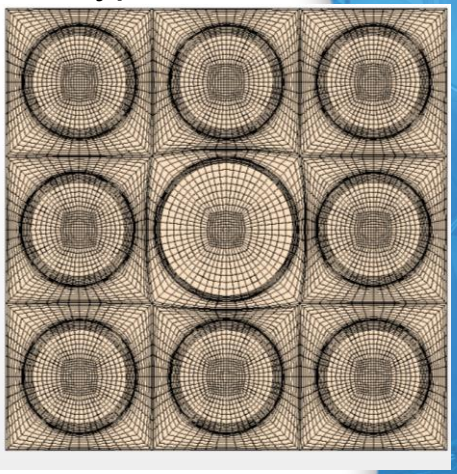
Neutronic Coupling with CFD

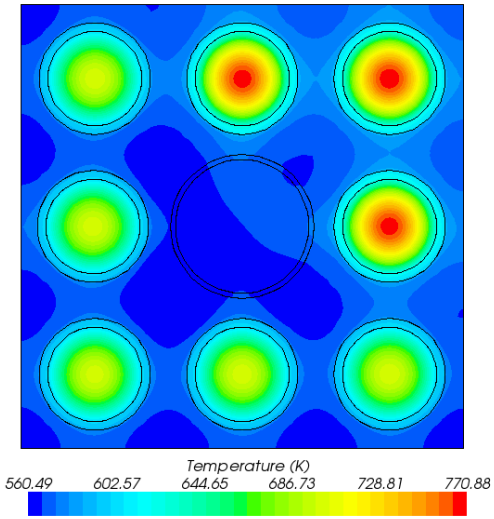


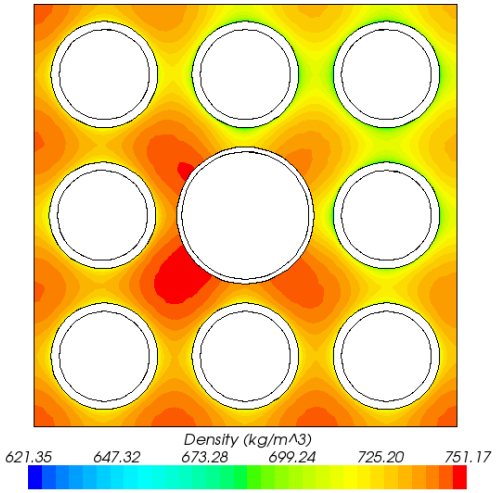
Typical DeCART Fuel Pin Mesh

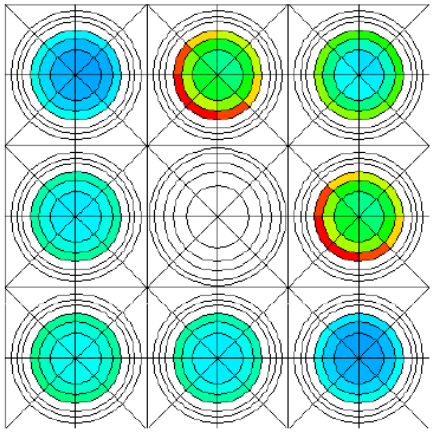


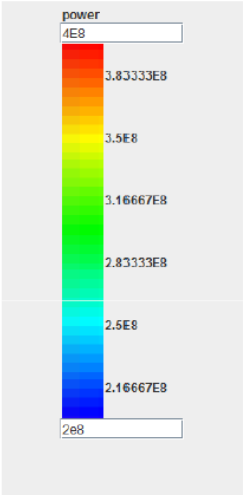
Typical CFD Mesh





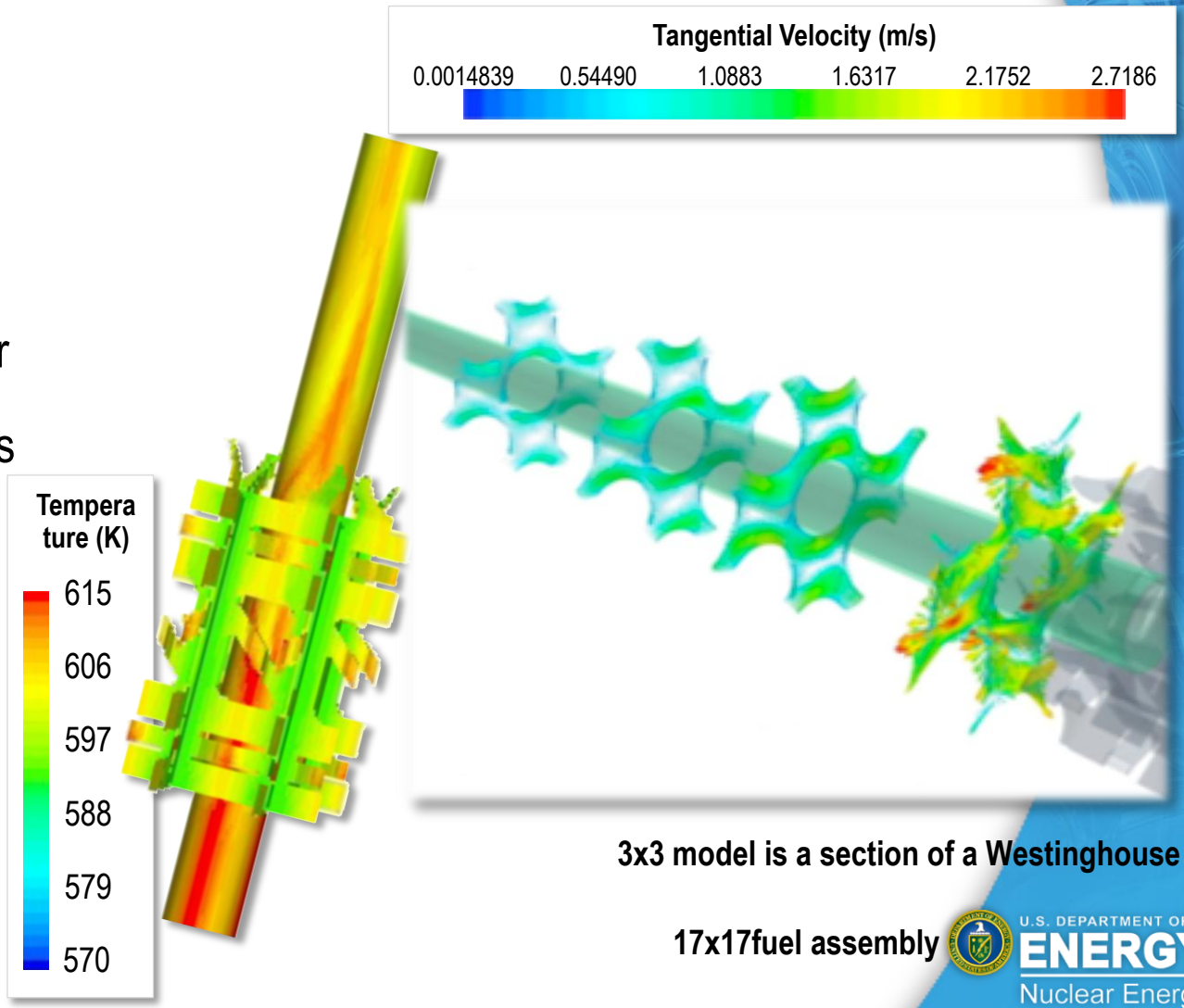






Neutronic Coupling with CFD

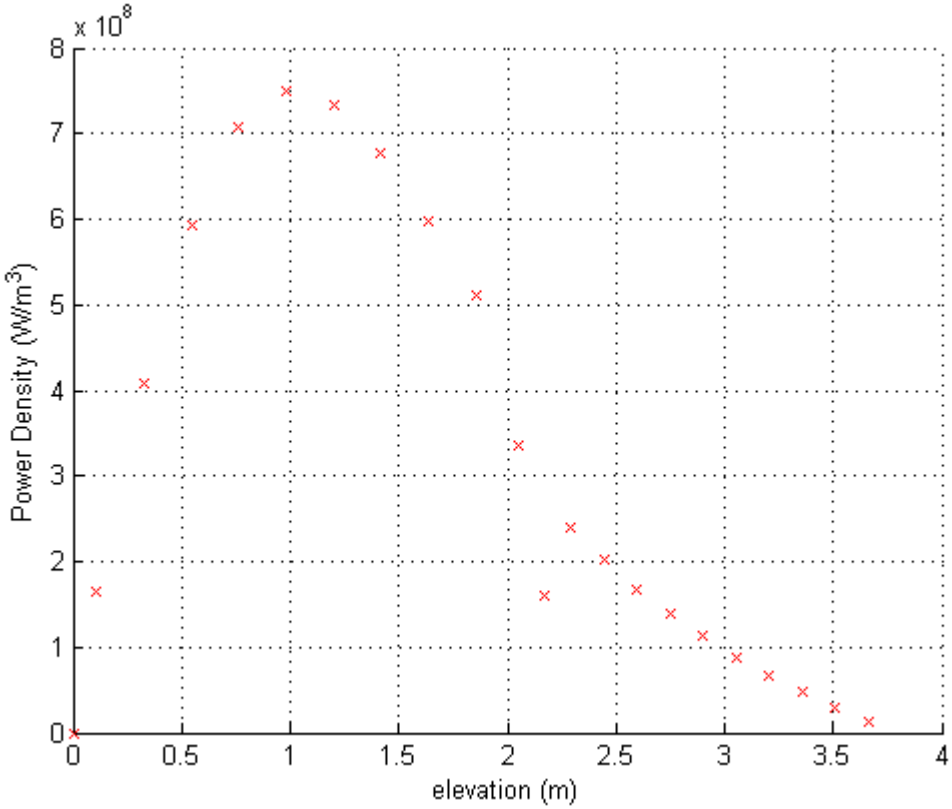
- Results: 3x3 coupled results
- Significance
  - Integrates state of the art practices in reactor physics and thermal hydraulics
  - Preliminary coupled simulation results show increased margin which could allow for power uprates



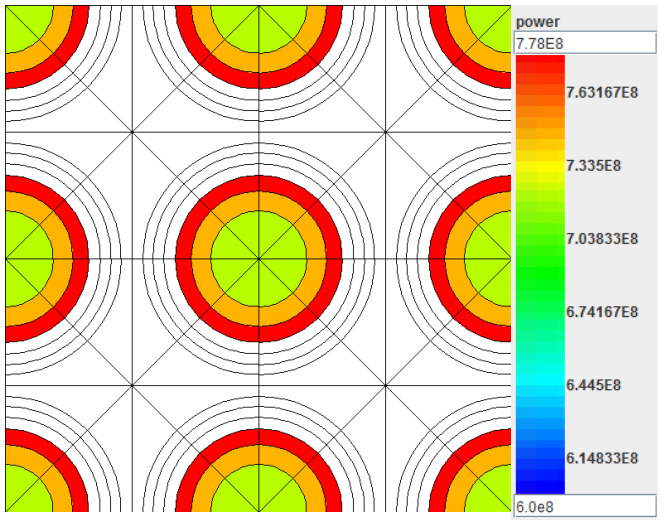
3x3 model is a section of a Westinghouse 17x17fuel assembly

Neutronic Coupling with CFD

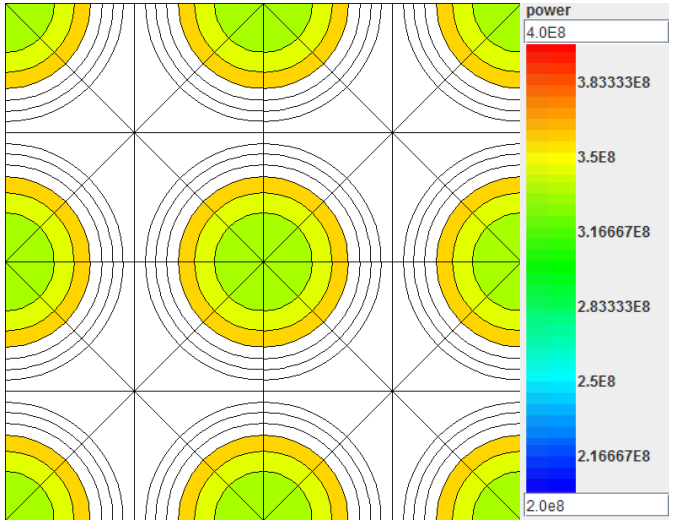
- Axial power distribution as the result of the coupling shows a drop of the power at the spacer grid position. It is due to the neutron deduction effect of the spacer grid.



Neutronic Coupling with CFD

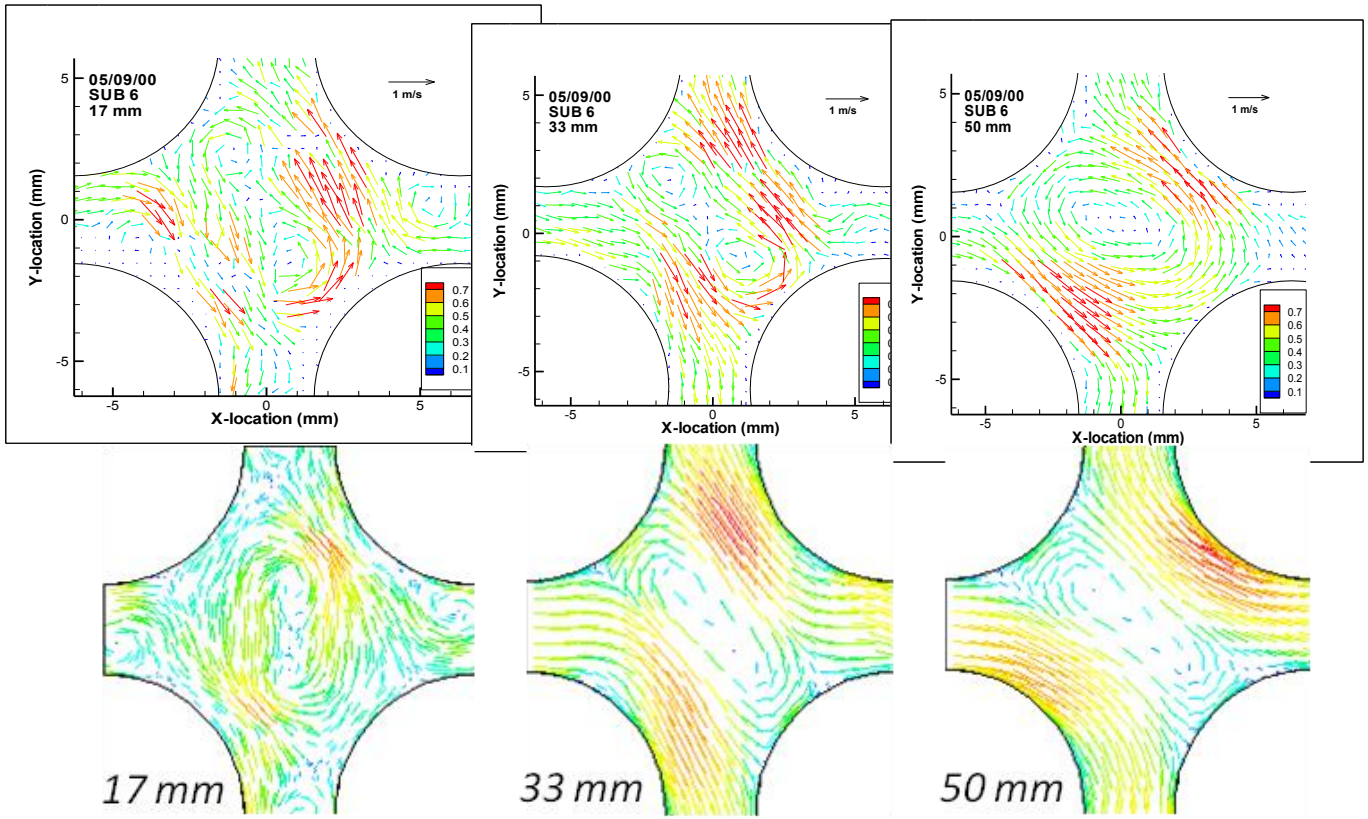


DeCART power distribution (W/m^3) at peak plane



DeCART power distribution (W/m^3) at grid spacer plane

Neutronic Coupling with CFD

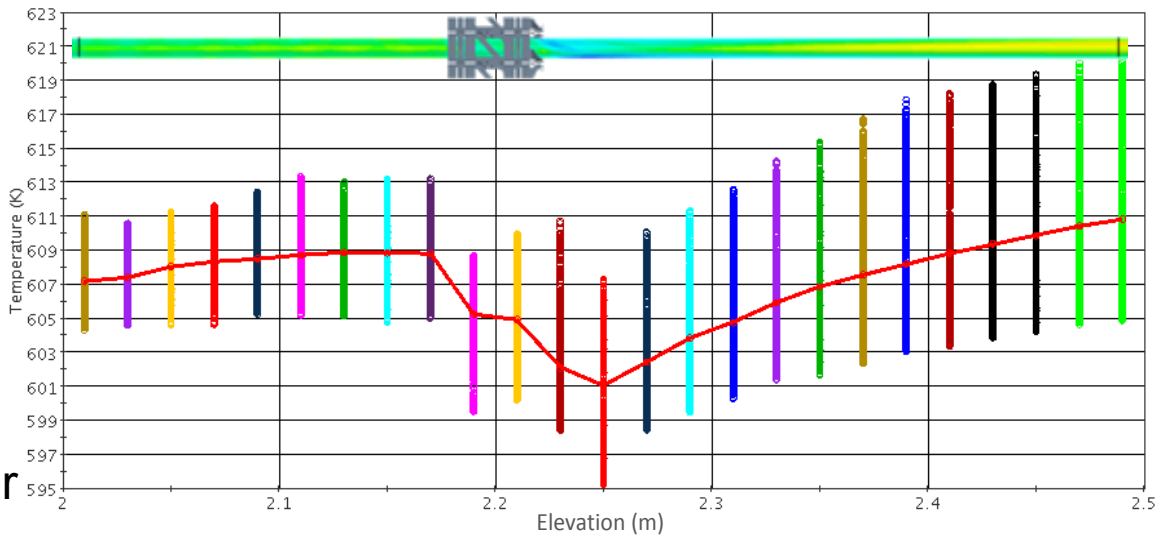


Test Data

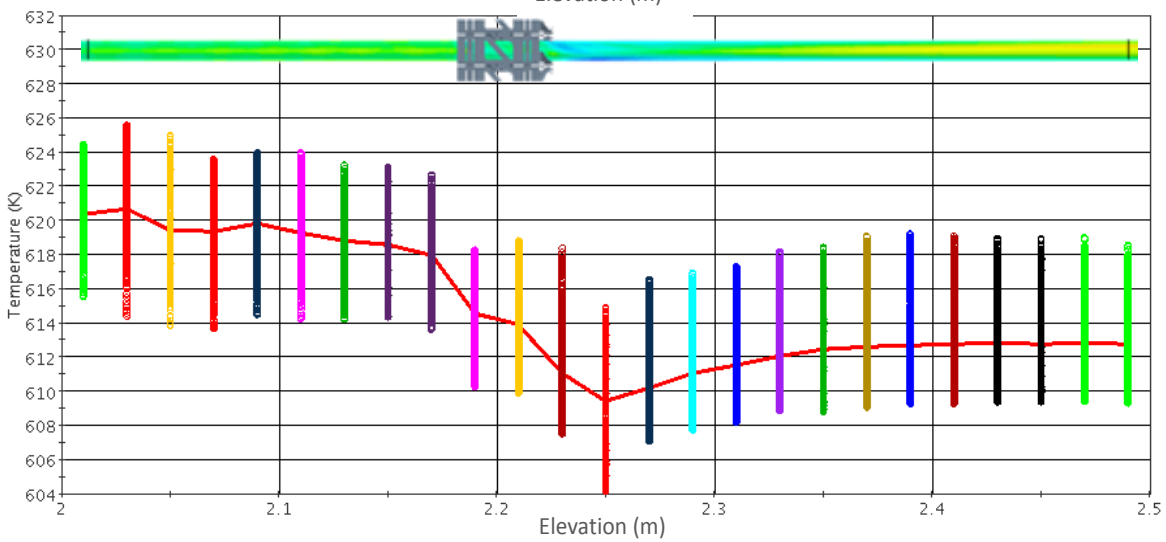
CFD data

Neutronic Coupling with CFD

Temperature distribution near the spacer grid on the central fuel rod

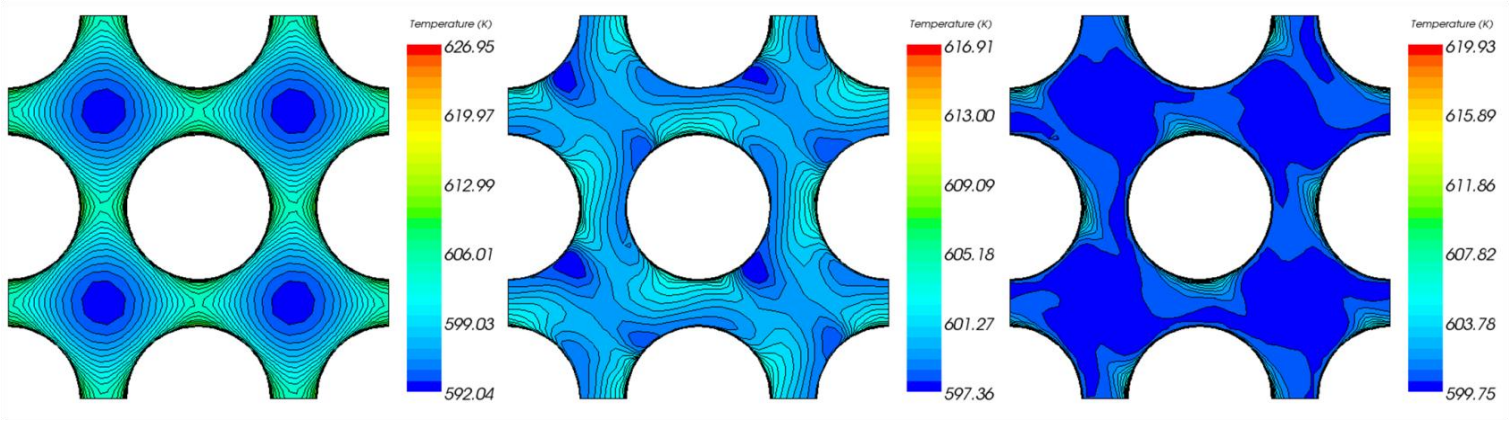


Decoupled results



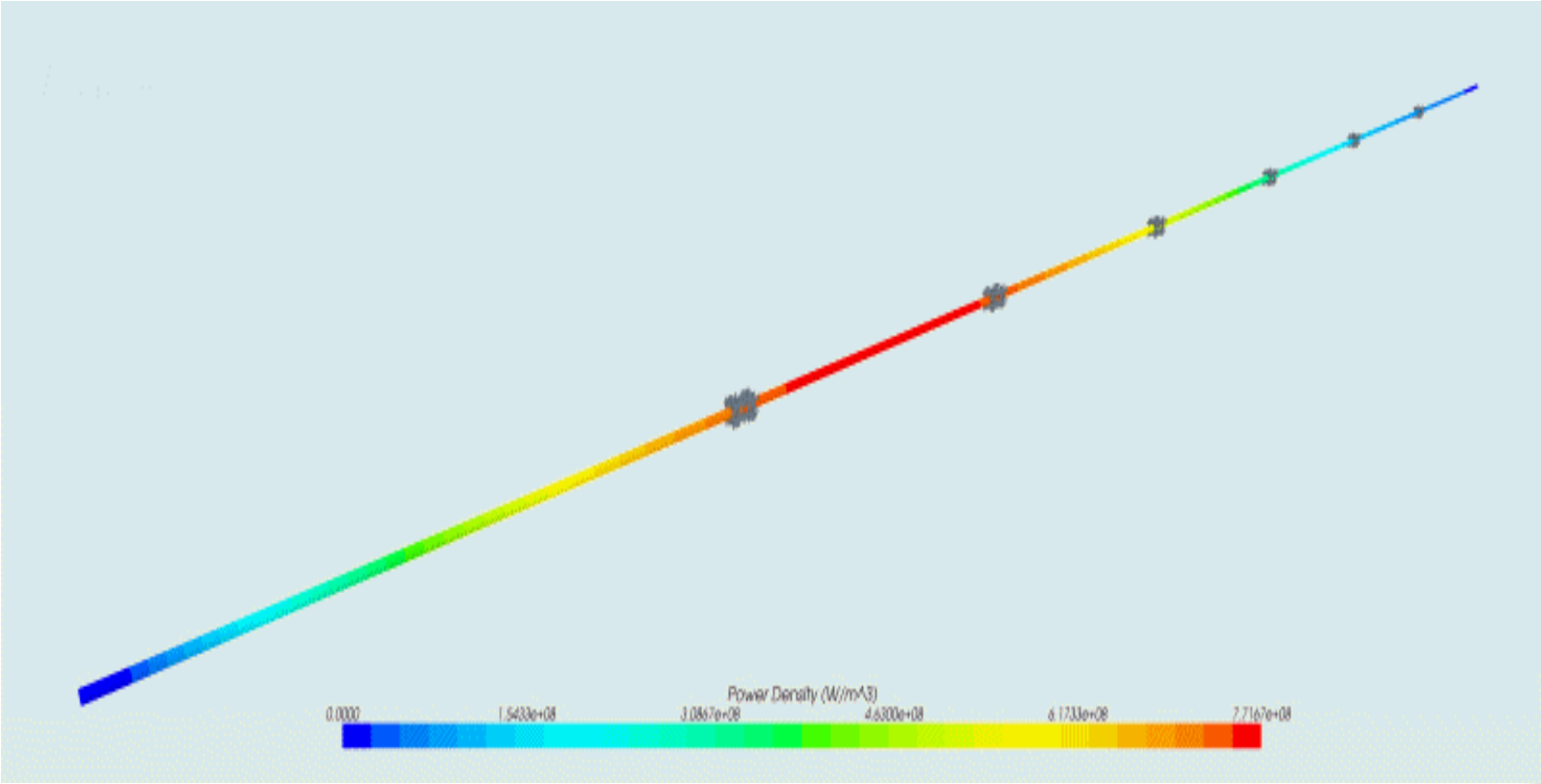
Coupled results

Neutronic Coupling with CFD



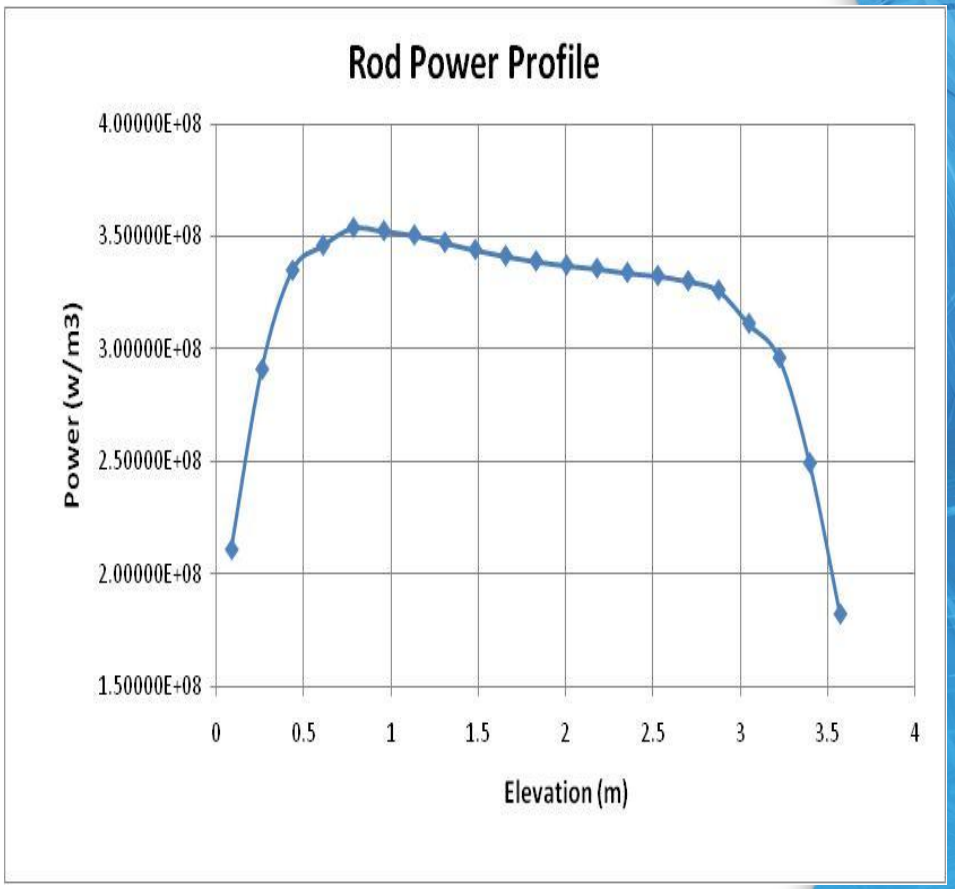
Fluid Temperature Distribution 50mm upstream of the spacer, 50mm and 100mm downstream, the mixing is clearly noticeable

Neutronic Coupling with CFD



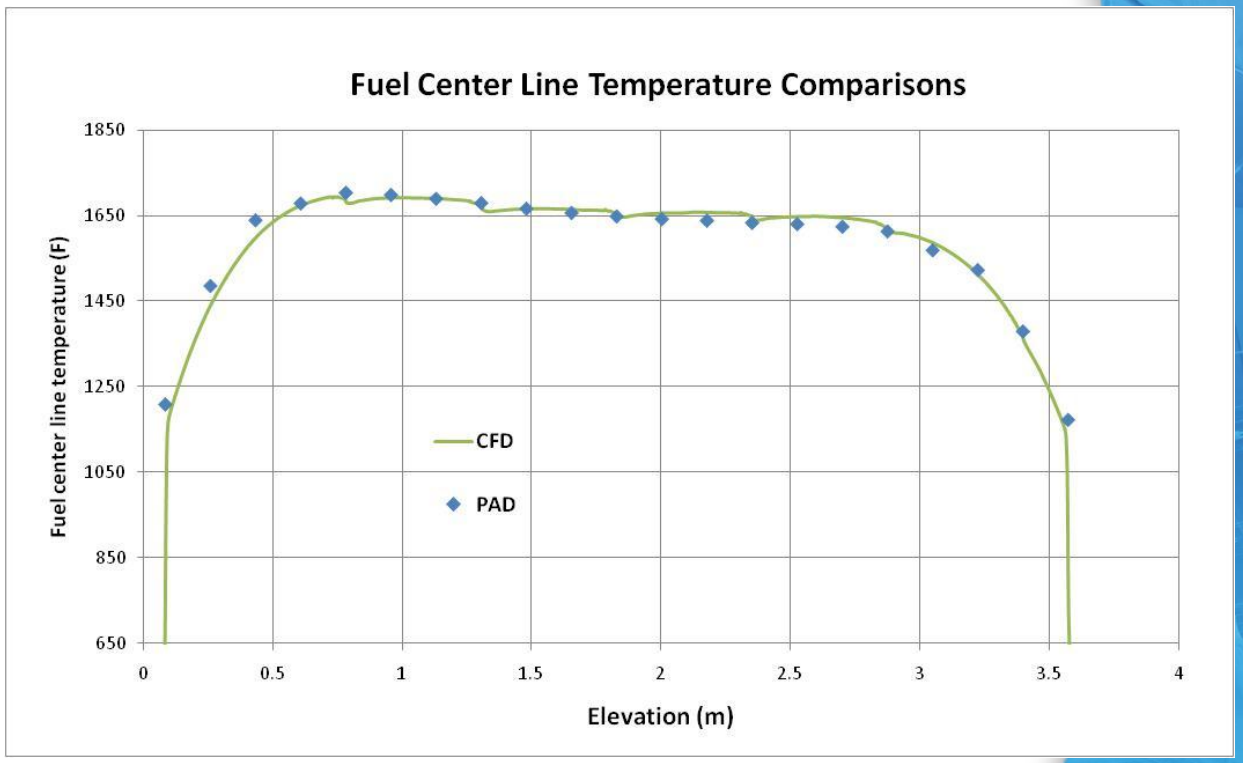
Fuel Center Line Temperature Prediction

- A initial run of the 3x3 pin CFD model was conducted to validate the fuel center line temperature predictions.
- The same calculation was done using Westinghouse internal fuel rod code: PAD.
- The same rod power profile was used in both models.



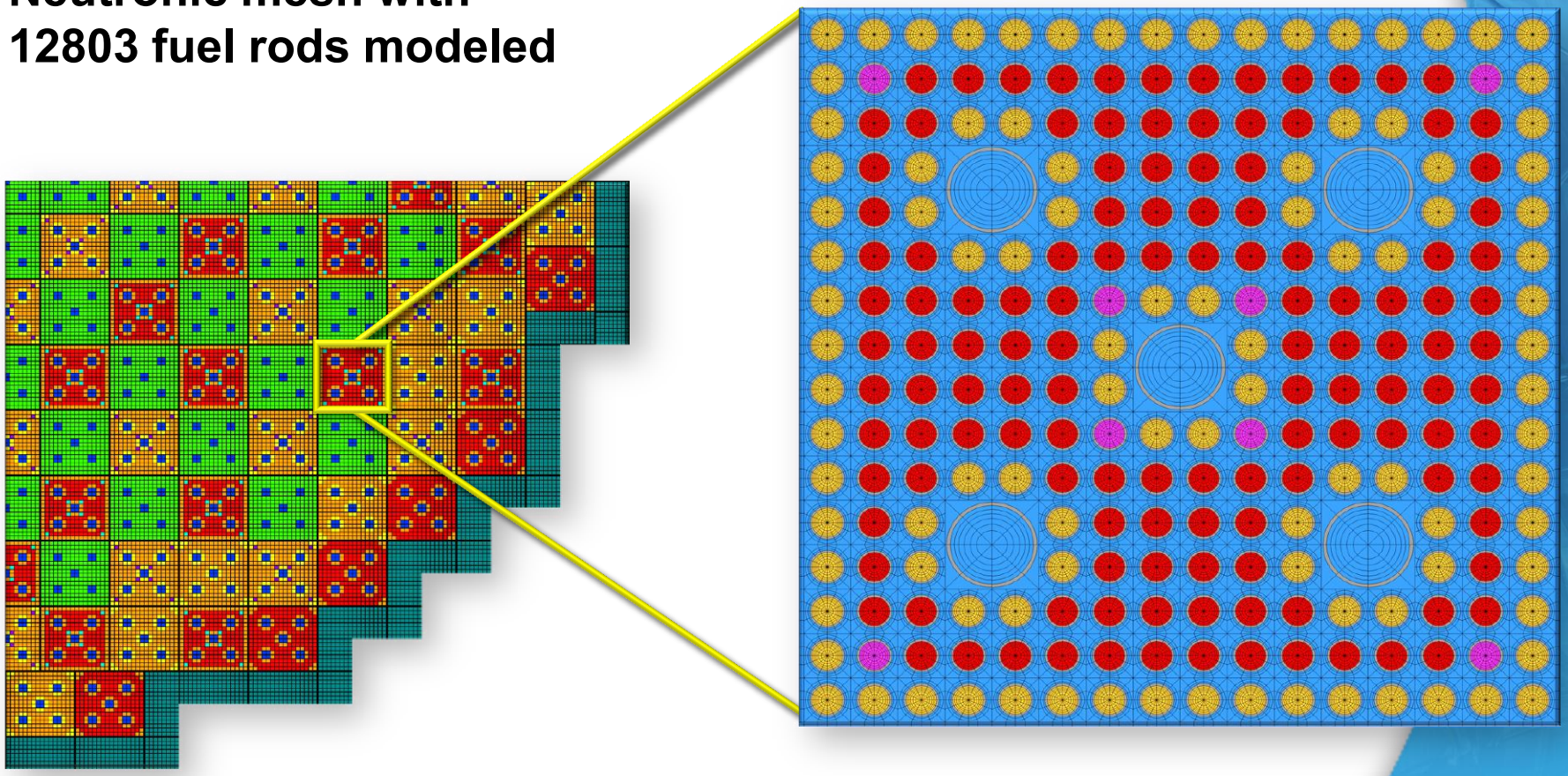
Fuel Center Line Temperature Prediction

- CFD result fits very well with the pad result.
- The drop of the temperature in the CFD plot demonstrates the impact of the mixing vanes on the fuel center line temperature.
- The 3x3 pin CFD model is being used to evaluate the fuel pellet temperature for transient events such as Rod Ejection and LOCA scenario where fuel is partially covered by coolant.



CE Reactor Quarter Core and 16x16 Fuel Assembly (Neutronic & CFD Coupling)

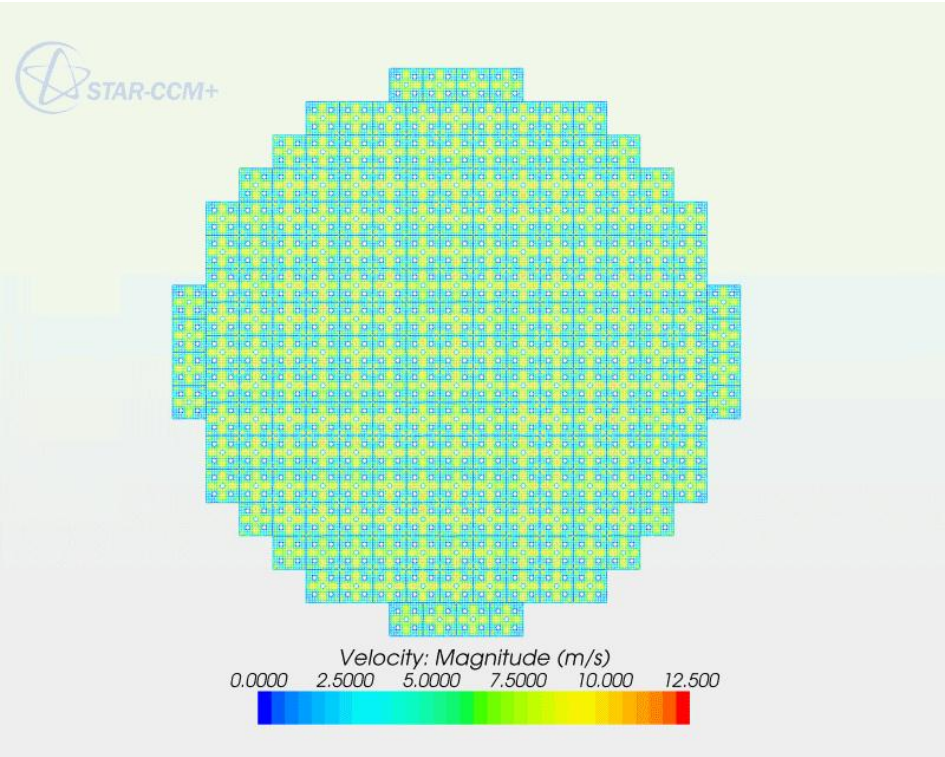
Neutronic mesh with 12803 fuel rods modeled



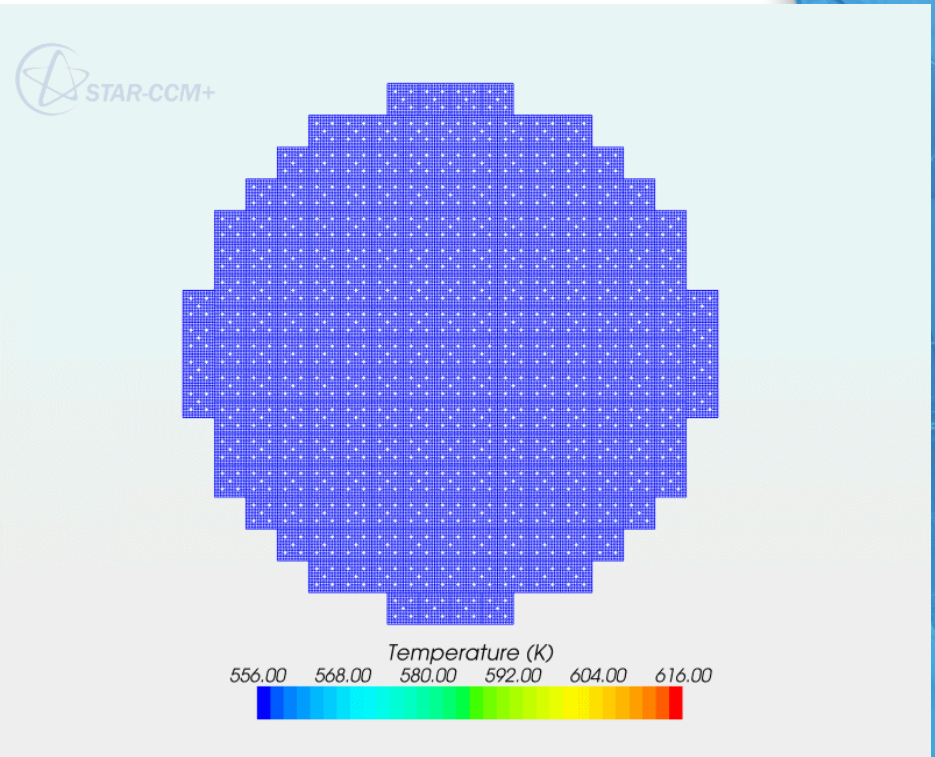
- Exact High Fidelity Representation

CASL-U-2011-0072-000-R

CE Reactor Quarter Core and 16x16 Fuel Assembly (Neutronic & CFD Coupling)

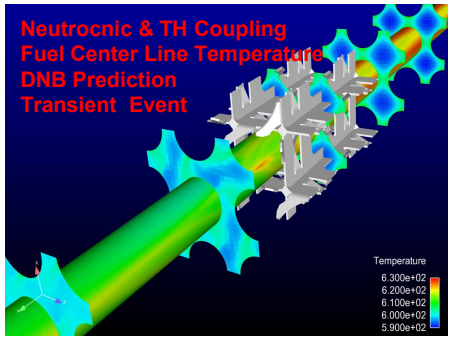


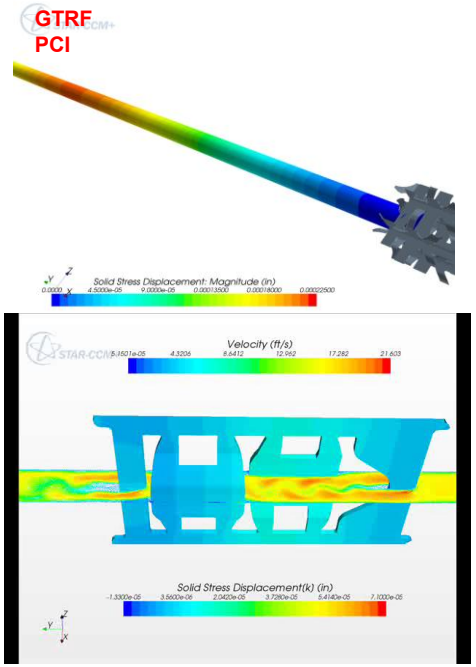
Core Coolant Velocity

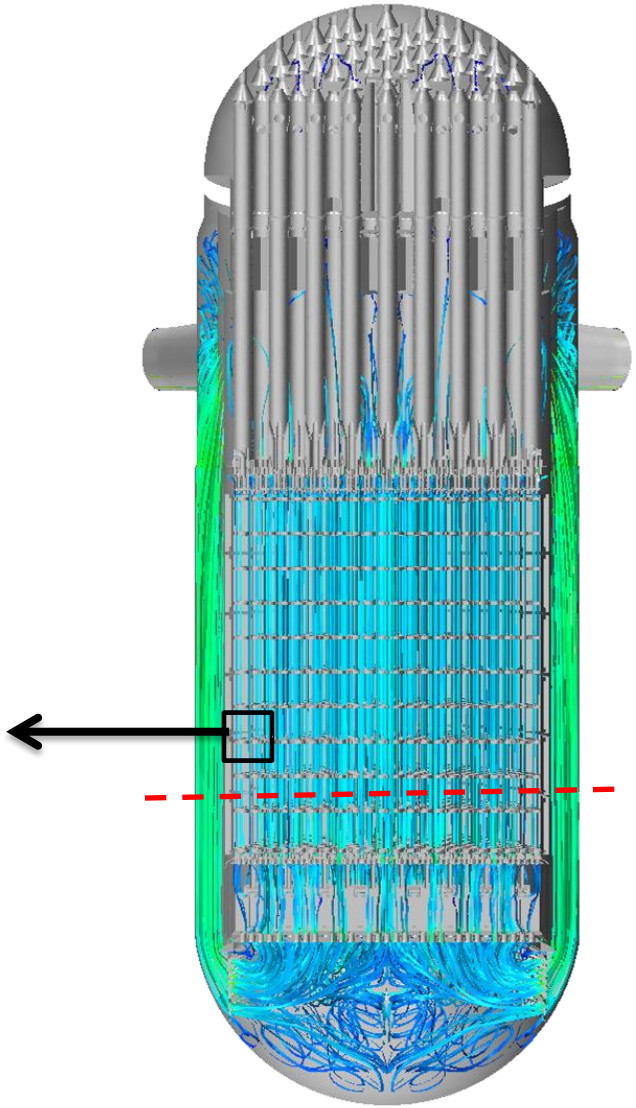


Core Coolant Temperature

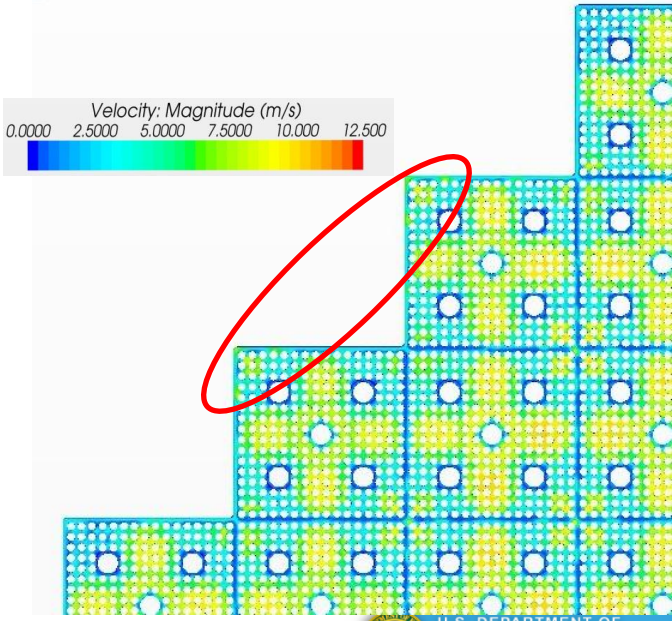
Coupling) From Vessel CFD Model to 3x3 Pin Multi-physics







Vessel CFD provides overall flow and temperature distributions. It also provide key indicators for GTRF, hot spot, crud & corrosion, under normal and transient condition.

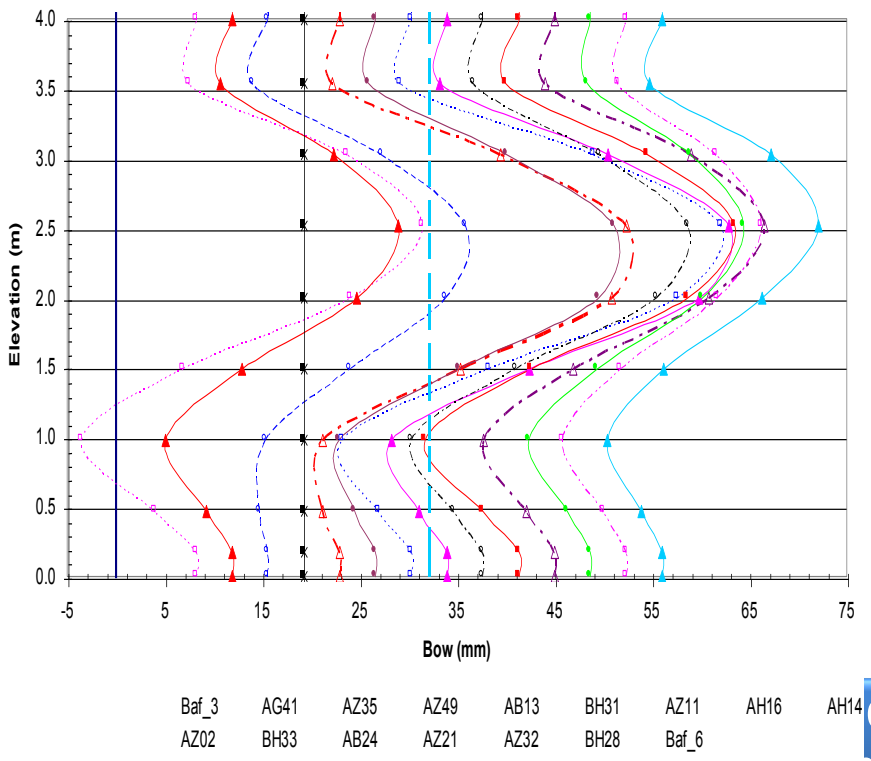


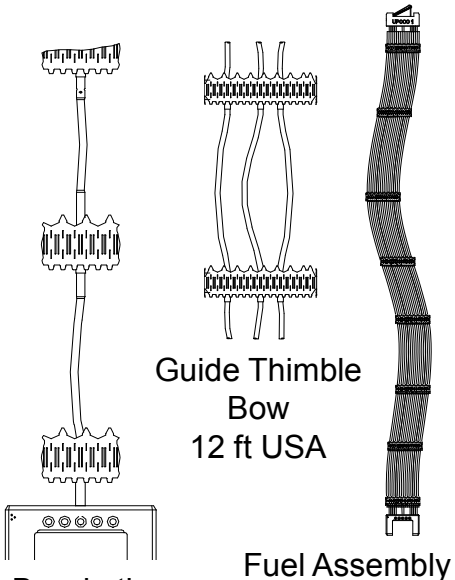
Vessel CFD Model

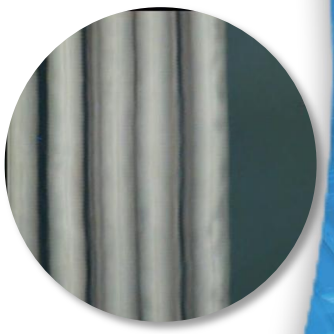
Fuel Assembly Distortion (FAD)

- Excessive axial forces caused by radiation-induced swelling lead to distortion or structural failure
- Power uprates and increased burnups:
  - May increase fuel distortions, alter core power distributions, fuel handling scenarios,

Figure 6-4: U1EOC6 out-of-core FA bowed shapes (Table 6-8)



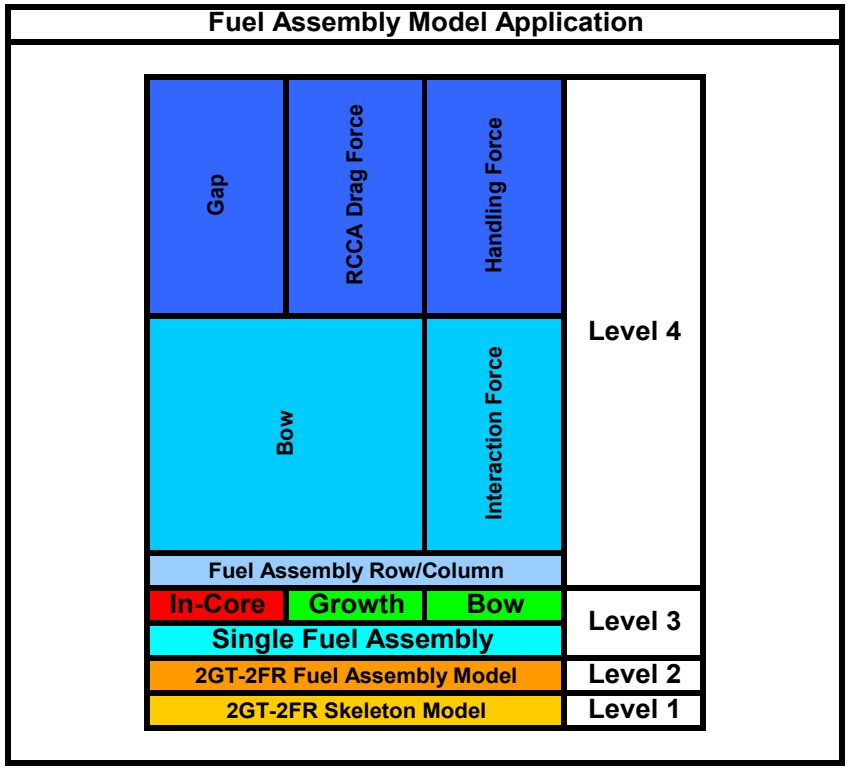


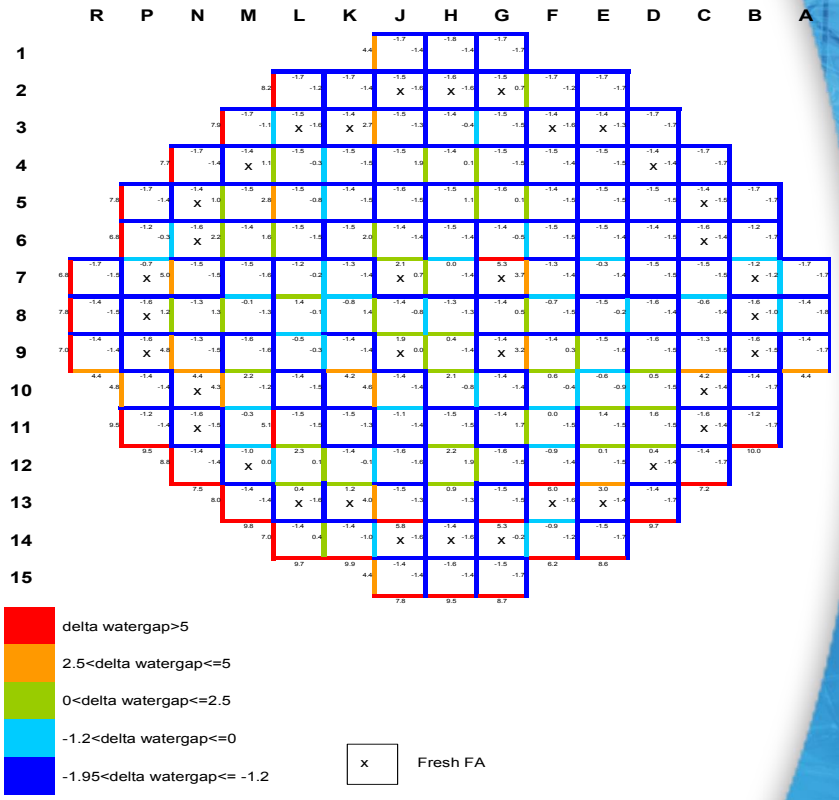


Rod
bow

distortion and impact on
ns and safety analyses

Link 3D FEA of Fuel in Core to Neutronics/TH





Predicts in-core assembly bow

Bow Data from Core

Westinghouse Uses SAVAN Code

Pellet Clad Interaction (PCI)

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Robert Montgomery
Pacific Northwest National Laboratory

CASL Roundtable
NC State University
August 9, 2011

CASL-U-2011-0072-000-R

Outline

- PCI background
  - *Coupled thermal-mechanical-chemical process that leads to clad breach*
  - *Discussion of prerequisites for PCI*
- Brief survey of occurrences
  - *Prevalent in both BWRs and PWRs*
- Motivation for CASL consideration of PCI
- Current computational approach
  - *Falcon*
- What is MPO attempting to do differently?

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Nuclear Energy

What is Pellet Clad Interaction (PCI)?

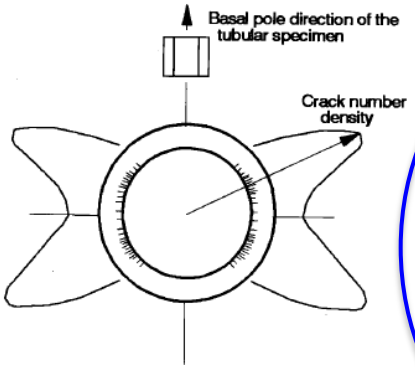
* A complex thermal-chemical-mechanical materials interaction process that occurs in LWR fuel rods

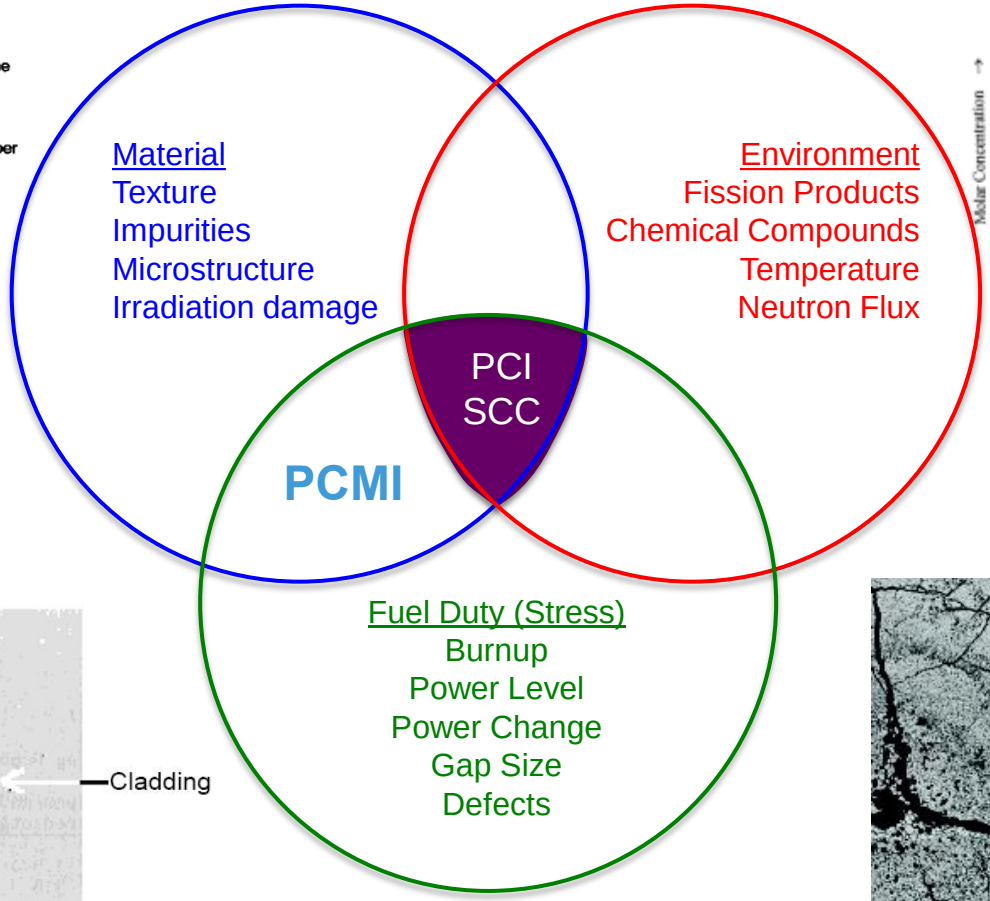
* Often involves Stress Corrosion Cracking (SCC) of zirconium alloy cladding at the cladding inner surface

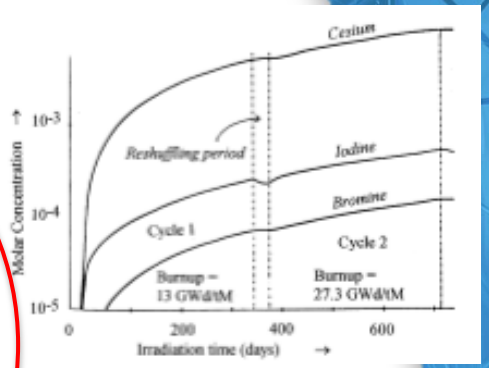
* Through-wall cladding cracks provide pathway for fission product release to the coolant

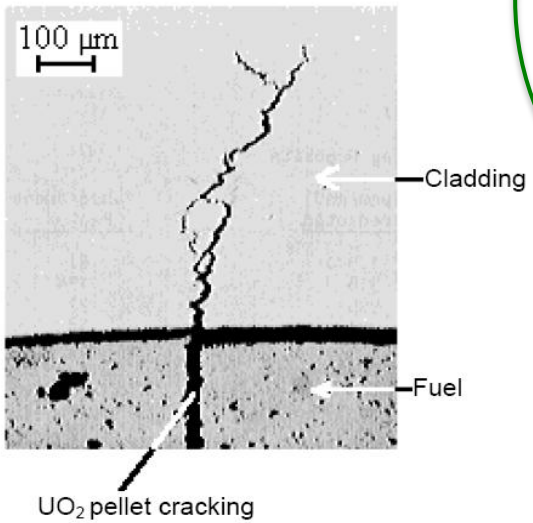
* An important fuel failure mode for normal operation and anticipated operational occurrences (AOOs)

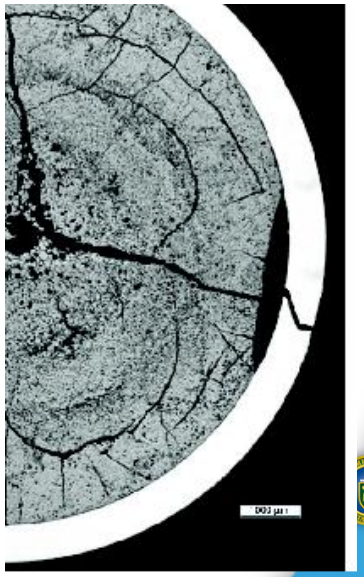
PCI is an Integral Mechanism











Overview of PCI (SCC and MPS) Failure Process

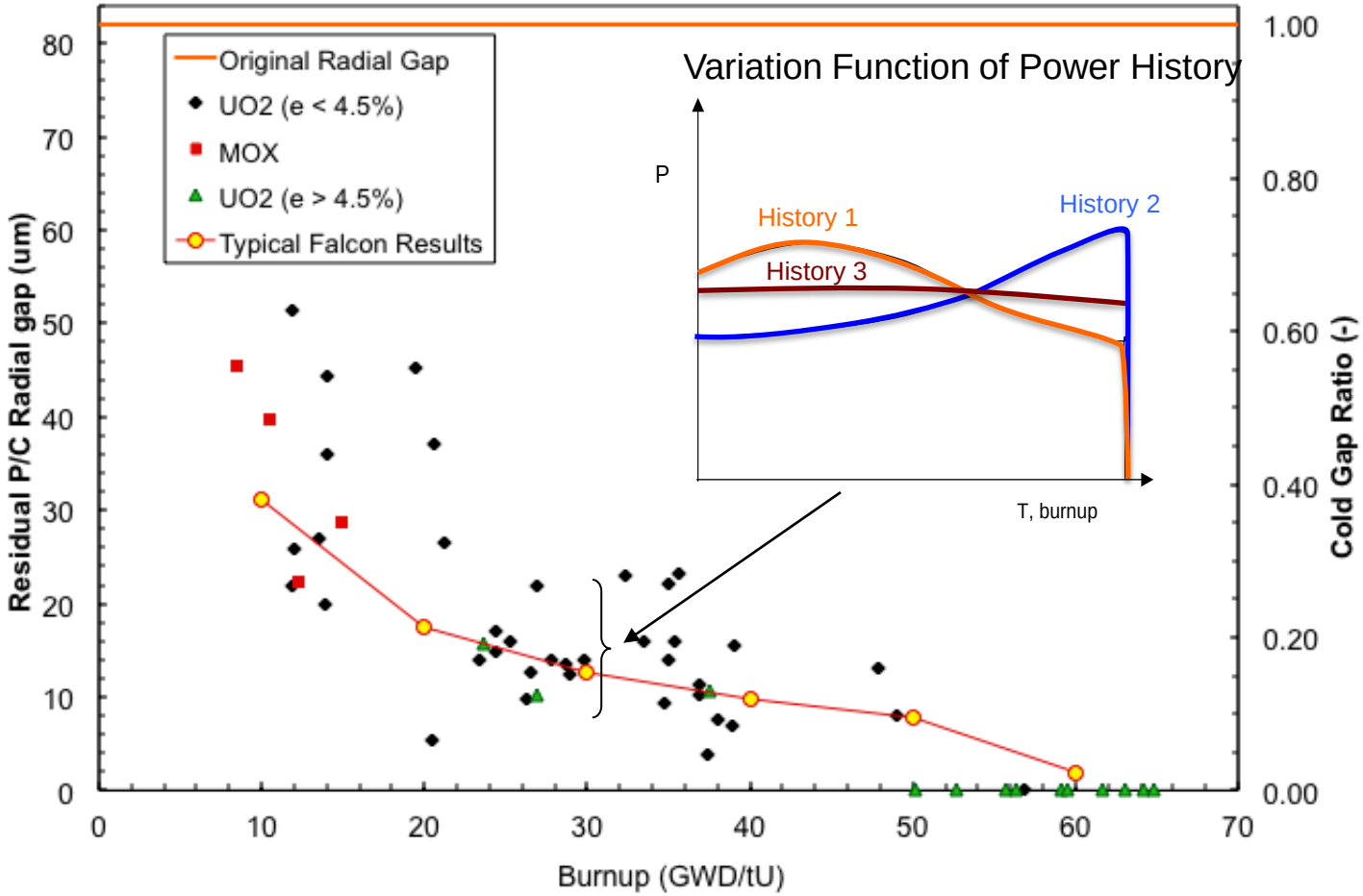
- PCI Failure Mechanism in LWRs
  - PCMI = Pellet Cladding Mechanical Interaction => Cladding Stress State
  - Stress + Corrosive fission products + Material susceptibility => Stress Corrosion Cracking (SCC)
  - Time to failure depends on local stress state, fission product conditions, and pellet/cladding material behavior

- Local stress state depends on:
  - Fuel conditioned state + power change (amount and rate)
  - Power Change $\Rightarrow$ Pellet Temperature Increase $\Rightarrow$ Pellet Thermal Expansion Strain $\Rightarrow$ Gap Closure $\Rightarrow$ Cladding Strain
  - Geometric considerations (pellet cracks, missing pellet surface defects, etc.)
  - Mechanical response of pellet and cladding (thermal creep, interfacial friction, etc.)

Overview of PCI Failure Process (cont'd)

- State of pellet and cladding interaction is a complex function of the prior irradiation history
  - Role of Pellet
    - Densification => opens gap; Relocation/pellet cracking, Thermal expansion, Swelling => closes gap
  - Role of Cladding
    - Thermal/irradiation creep => closes gap or induces plastic strain
  - Role of fission products
    - Production/release/decay => availability of reactive species for SCC
- Leads to processes of <u>conditioning</u> (able to withstand power change with minimal change in stress) or <u>deconditioning</u> (power change will induce large increase in stress)
  - Defined by residual (or cold) pellet-cladding gap (larger -> conditioned, smaller-> deconditioned)

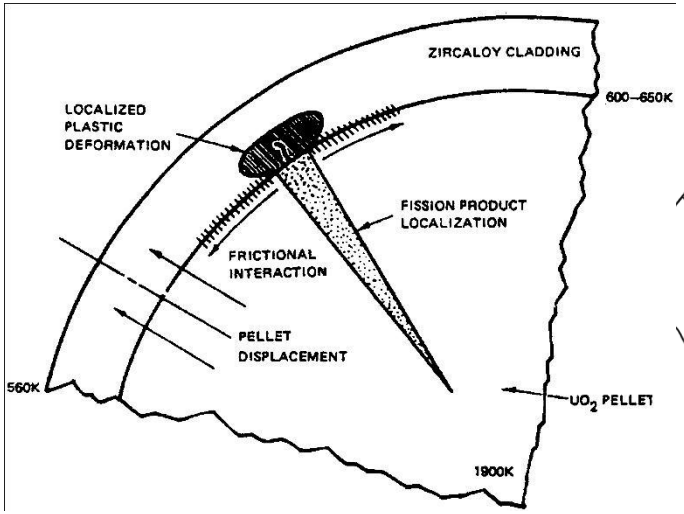
Data on Conditioned State in PWR Fuel

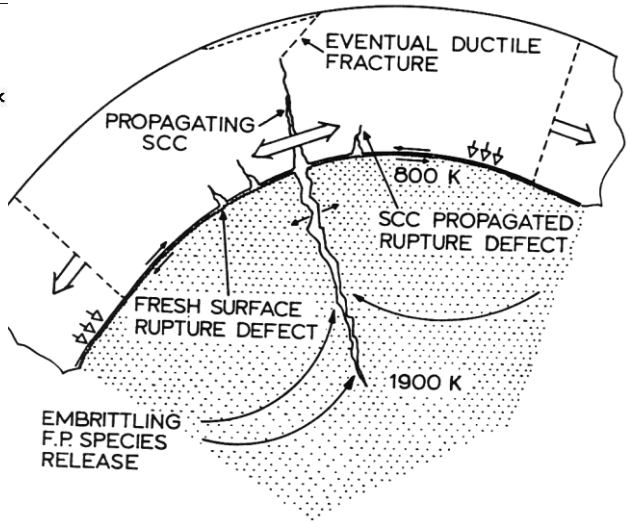


Overview of PCI-SCC Failure Process

- Fuel cracks provide direct pathway for fission product transport to cladding inner surface
- Causes a stress concentration field in cladding
  - Mechanical interaction with cladding through shear strain transfer

- SCC results in low strain failure with intergranular crack pattern (tree-branching)
- SCC process composed of slow incubation, followed by fast propagation
- PCI exhibits stochastic behavior
  - Not all tests at given nominal conditions result in failure





Brief PCI History

- First PCI failure identified in 1963 in GETR (BWR - Lyons)
  - About the same time, failures identified in Canadian NPD, CANDU and UK HBWR
- PCI linked to stress corrosion cracking (SCC) - some form of chemical attack by fission products on the cladding inner surface
  - Fission product species tested; I_2 (volatile) causes stress corrosion cracking (Rosenbaum - 1966)
- Early efforts to prevent PCI involved two major efforts
  - Impose power ramp restrictions (based on operating experience and ramp testing)
  - Develop fuel rod design improvements (based on separate effects and ramp testing)

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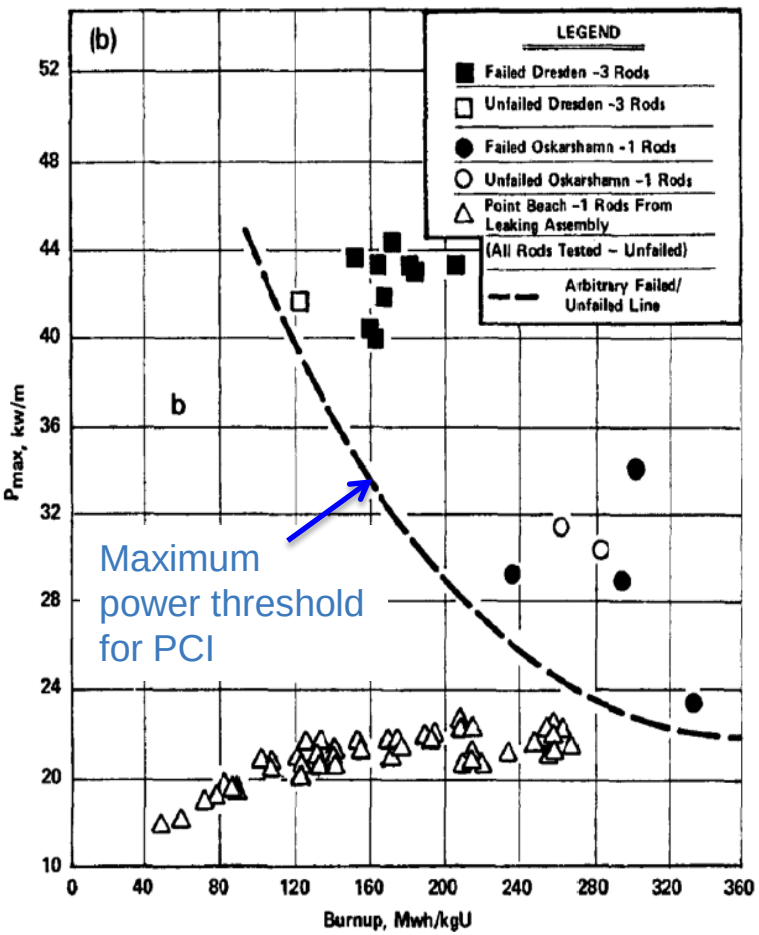
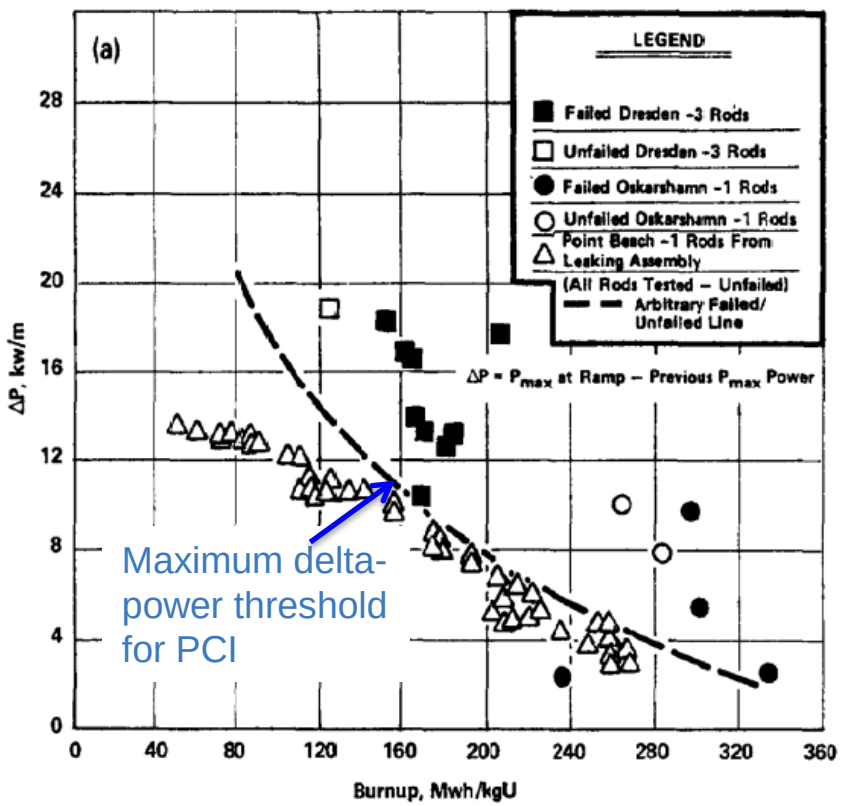
Operating Events with Multiple PCI Failures

- BWR Events
  - Historical – Oskarshamn-1 (Cycle 2, July 1975), Dresden (Cycle 3, Oct 1974), Oyster Creek (Cycle 10, 1986)
  - Recent – Hatch 1 (Cycle 21, October 2003), La Salle 2 (Cycle 9, 2002)
- PWR Events
  - Historical – Maine Yankee (Cycle 1, 1974), Point Beach 1 (Cycle 3, 1974), and Obrigheim (Cycle 6, 1974/75)
  - Recent – Braidwood 1 (Cycle 11, 2003)

PCI Failures at Dresden 3 and Oskarshamn-1





Examples of empirical relations for PCI Failure thresholds

Why Select PCI as a Challenge Problem?

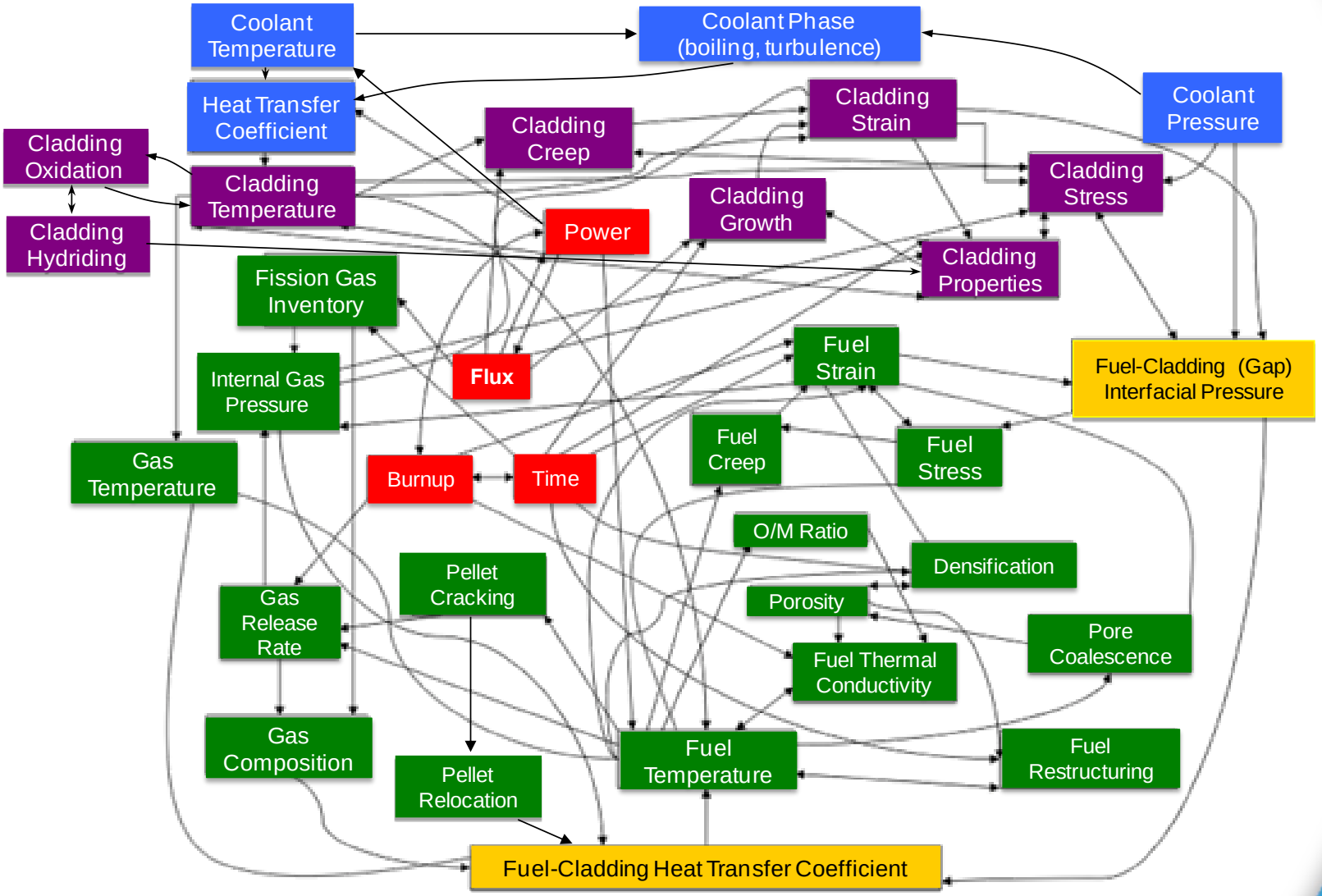
Quite simply, fuel rod failure by PCI is important; and CASL can do something about it:

- Widespread fuel failures are possible by PCI during normal or anticipated power maneuvers
  - Dresden and Oskarshamn events (>10 rods in multiple assembles from a single event)
- Current operating restrictions limit PCI failures to < 5% of all fuel rod failures, but… at a cost of lost EFPHs (16 to 50)
- Mitigation requires controls on the fuel design, fabrication process, and plant operations

Modeling PCI in LWR Fuel

- State of the art modeling approaches focus on
  - 2-D FEM methods with a mechanistic representation of the coupled thermal/mechanical behavior
  - Falcon represents the most widely used PCI analysis capability
  - Others include RODEX4, PAD/ANSYS, CYRANO3, etc.
- Falcon has unique capabilities for modeling local PCI effects Pellet-cladding interfacial forces in the R-θ plane
  - Discrete modeling of pellet cracks
  - Failure criterion based on Stress Corrosion Cracking (SCC) or empirically derived from ramp test data
- Applications have included evaluation of PCI failure potential for:
  - Steady state and transient operating conditions
  - Defective fuel pellets (missing pellet surface)
  - Tolerance stack up analysis

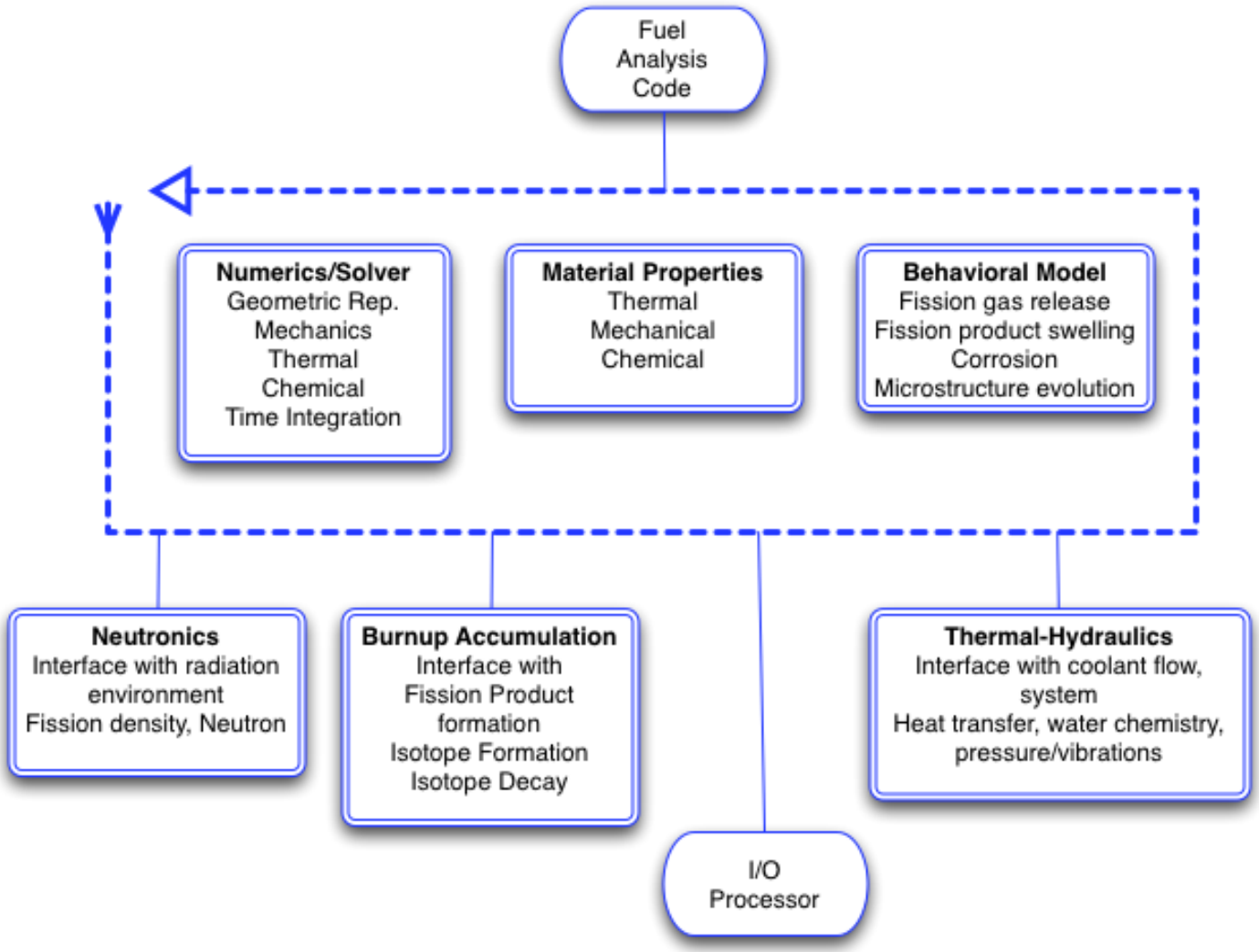
Complexity of Nuclear Fuel Simulation



Adapted from K. Lassmann, "The Structure of Fuel Element Codes," Nuclear Engineering and Design, 57 (1980), 17-39.

Simplified Fuel Performance Model Framework

Major Components of Nuclear Fuel Modeling Capability



Fuel Phenomena Important to PCI

- Pellet
  - Thermal Expansion (function of conductivity and expansion coefficients)
  - Cracking
  - Densification
  - Swelling (Solid and Gaseous)
  - Fuel Fragment Relocation
  - Interfacial friction/bonding between pellet and cladding
  - Fission Gas/Product Release/Decay
  - Fabrication Imperfections (e.g., MPS)
- Cladding
  - Stress Relaxation (thermal creep)
  - Creepdown (irradiation and thermal creep)
  - Chemical/metallurgical reactions leading to SCC of zirconium alloys

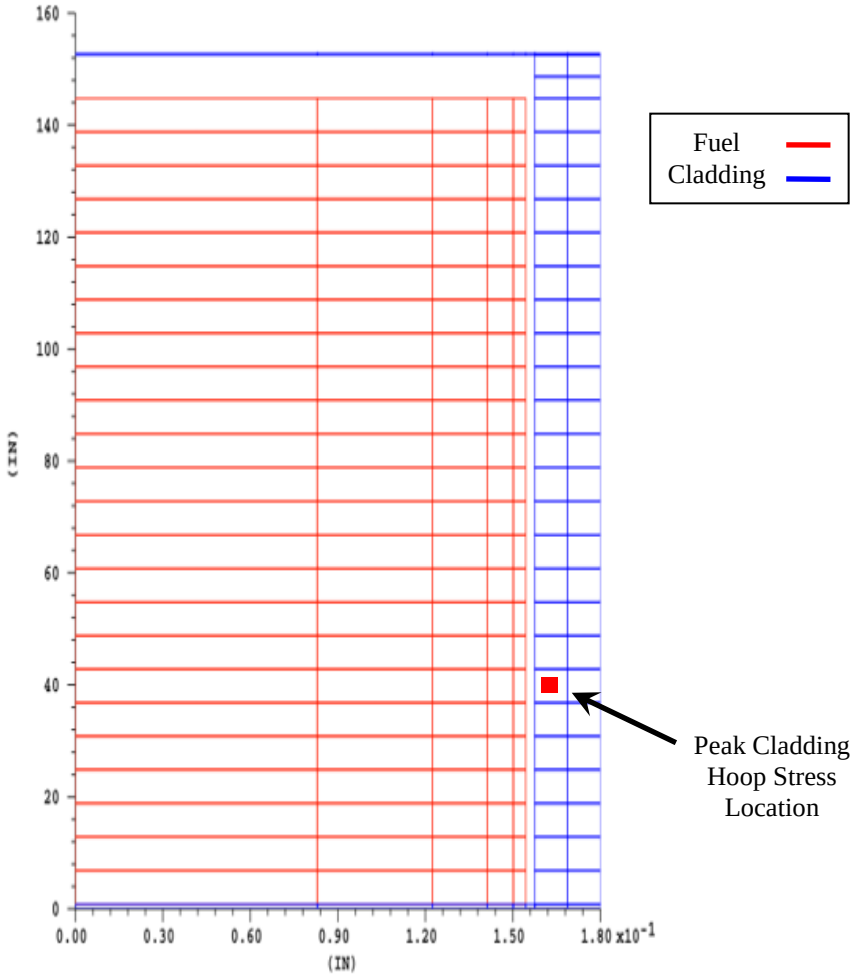
Many of these phenomena depend on the ever changing irradiation conditions (burnup, fluence, flux), power/temperature conditions, and material microstructure state (fission damage, neutron damage, chemical reactions, etc.)

Falcon PCI Analysis Approach

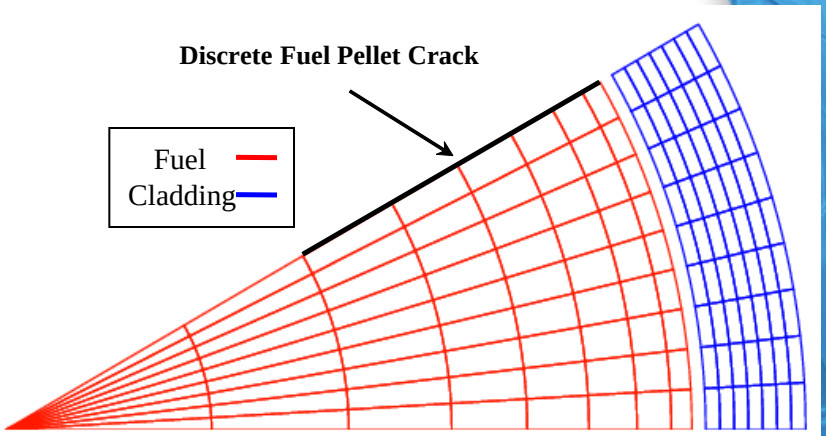
- Step 1. Base irradiation analysis (R-Z)
  - Use a full length R-Z model
  - Base depletion (including mid-cycle power changes) power history
  - Fresh cladding & initial fuel rod conditions
- Step 2. Startup/maneuver power ramp analysis (R-Z)
  - Use R-Z full length model
  - Startup/maneuver power history
  - Restart from the EOC conditions established by the base irradiation or period of lower (reduced) power operation
  - Peak cladding stress and its location are identified from R-Z restart analysis
- Step 3. Local effect PCI analysis (R-θ)
  - The axial node with the peak cladding hoop stress
  - Nodal startup power
  - Initial conditions established from the base irradiation (gap thickness, internal pressure, gas composition, burnup, T/H conditions, etc.)
  - Without or with MPS

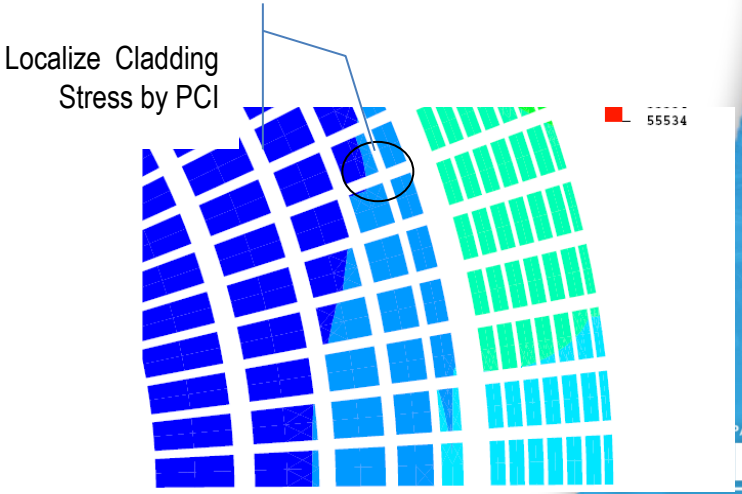
PCI analysis approach in FALCON

Step 1/Step 2: Full Length R-Z Analysis



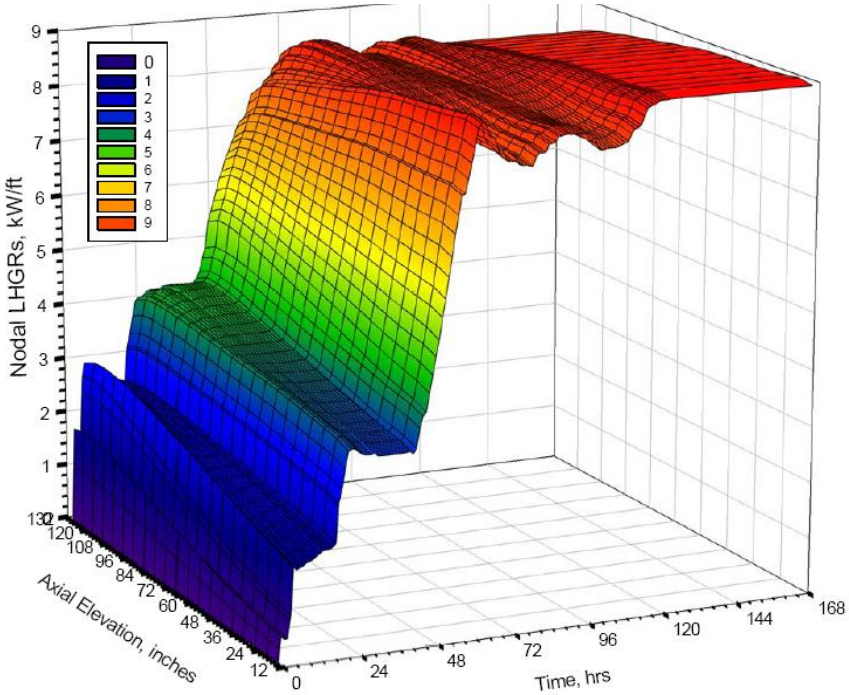
Step 3 PCI R-θ Analysis



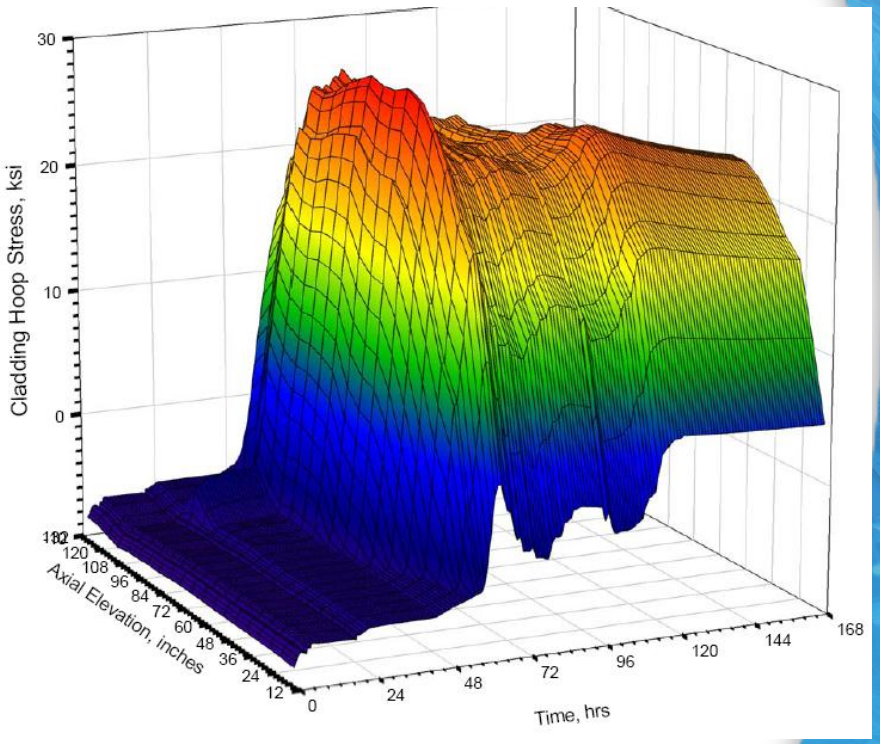


Results from Typical PWR Reactor Startup Analysis

Fuel Rod Nodal Power History

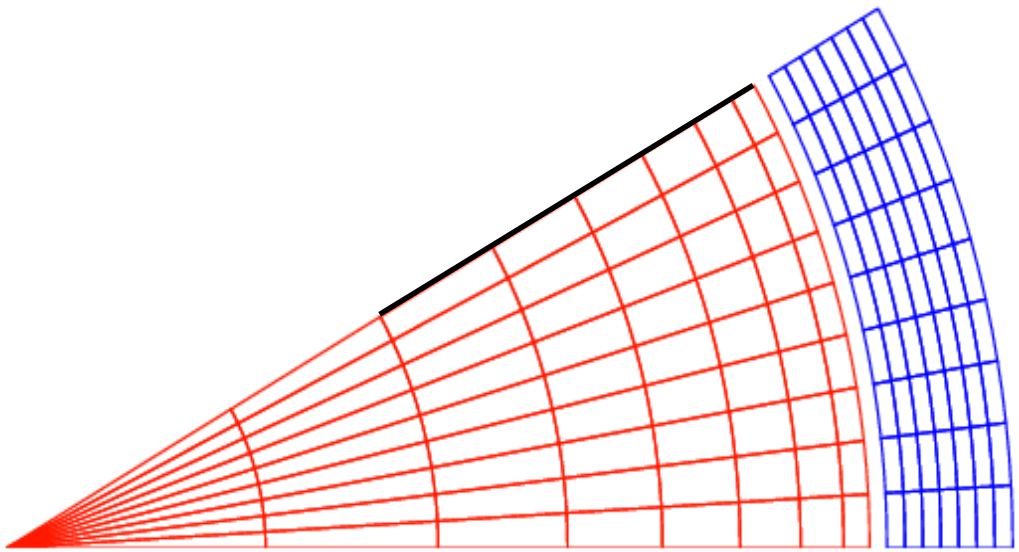


Cladding Hoop Stress History

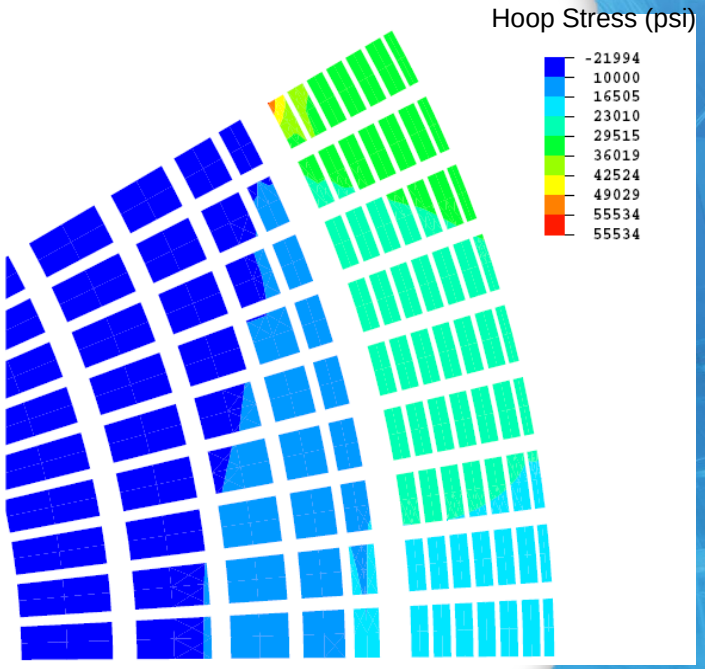


Typical Falcon Results for PCI

- Cladding hoop stress distribution during power ramp for "classical" PCI conditions



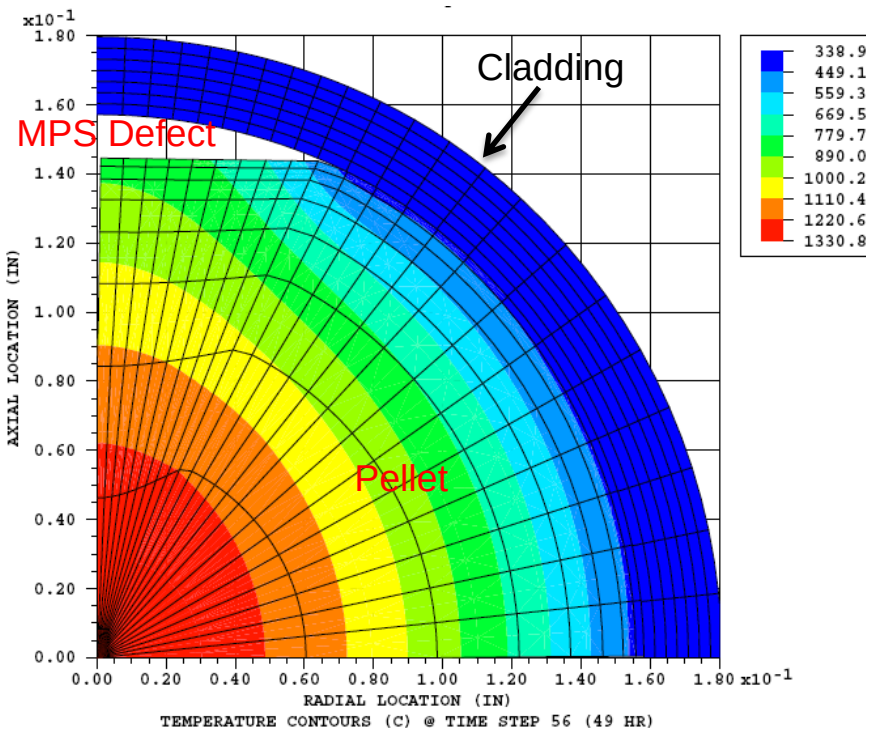
PCI R-θ Model



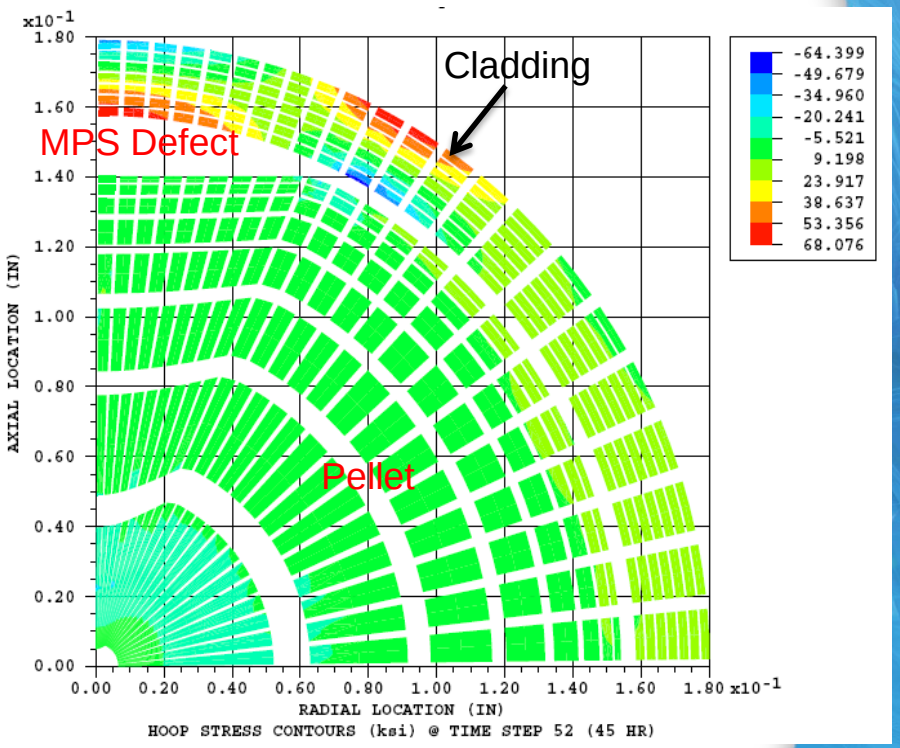
Hoop Stress Distribution

Typical Falcon Results for PCI-MPS

Pellet and Cladding Temperature Contour



Pellet and Cladding Hoop Stress Contour



How Can CASL/MPO Have an Impact?

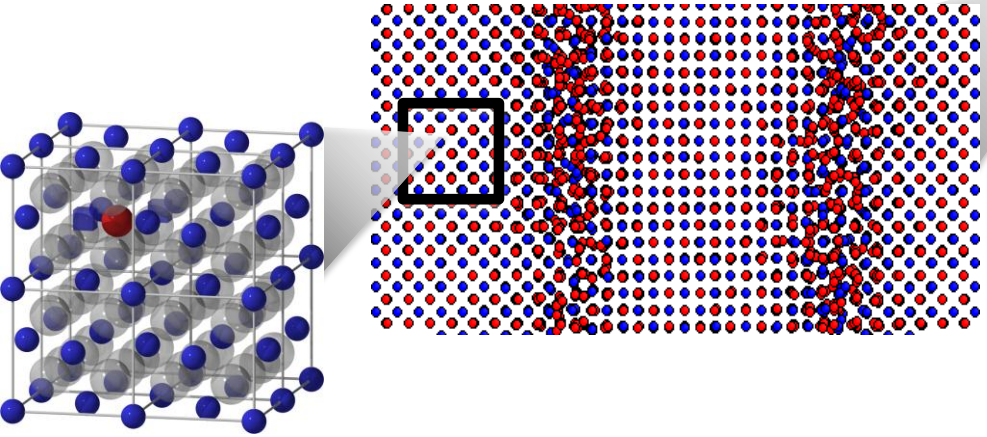
- Fundamental understanding of the key factors in the PCI process (e.g. role of MPS, SCC mechanism, improved clad/fuel creep models, etc.)

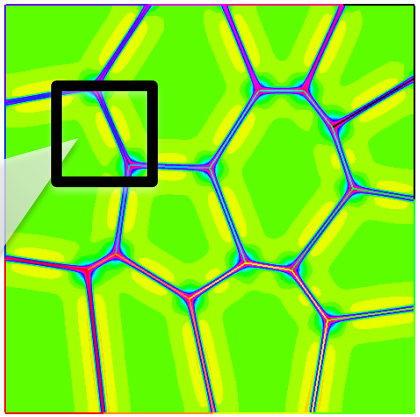
- Improved modeling and analysis can alleviate/facilitate solutions to PCI
  - Better fuel utilization (including guidance on MPS tolerances)
  - Optimized plant operations
  - Fuel design improvements – (including consideration of innovative designs - see Kurt Edsinger talk)

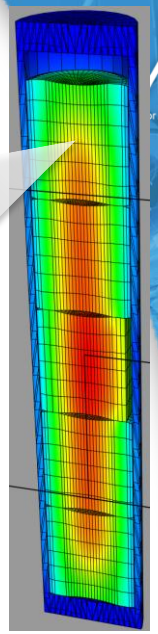
Materials Performance Optimization (MPO)

Enabling Improved Fuel Performance through Predictive Simulation

Challenging, multiscale processes impact nuclear fuel performance







Approach

- Provide physics-based materials models of fuel/clad/internals property evolution to enable predictive modeling of CRUD, GTRF and PCI within 3D, multi-physics, virtual reactor simulator
- Improved physics and chemistry insight delivered via constitutive relations
- MPO is comprised of a diverse group of computational materials scientists with a wide range of capabilities

Outcomes and Impact

- Predictive models of fuel failure, that quantitatively define operating margins & lifetime limits
- Validated predictions of fuel failure conditions
- Power uprates & increased fuel utilization

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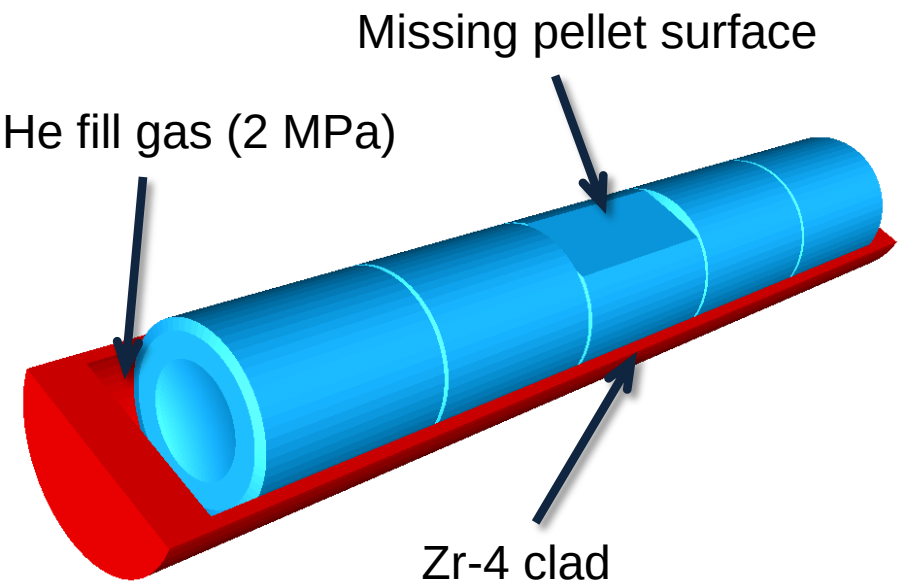
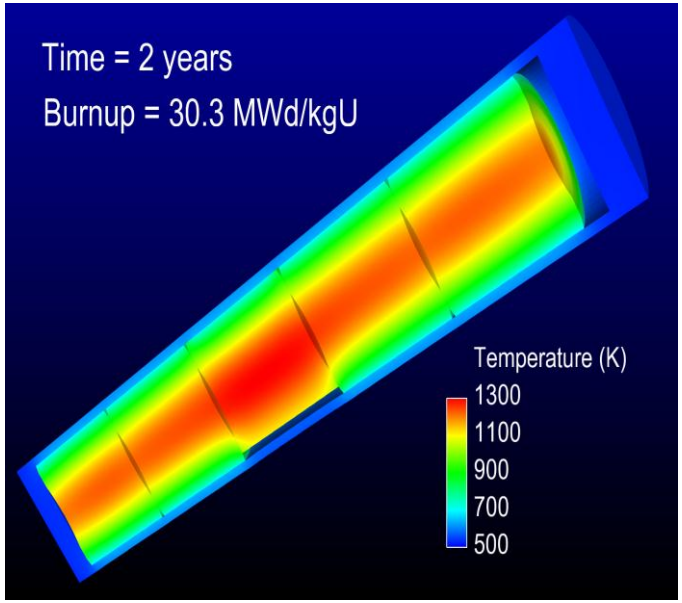
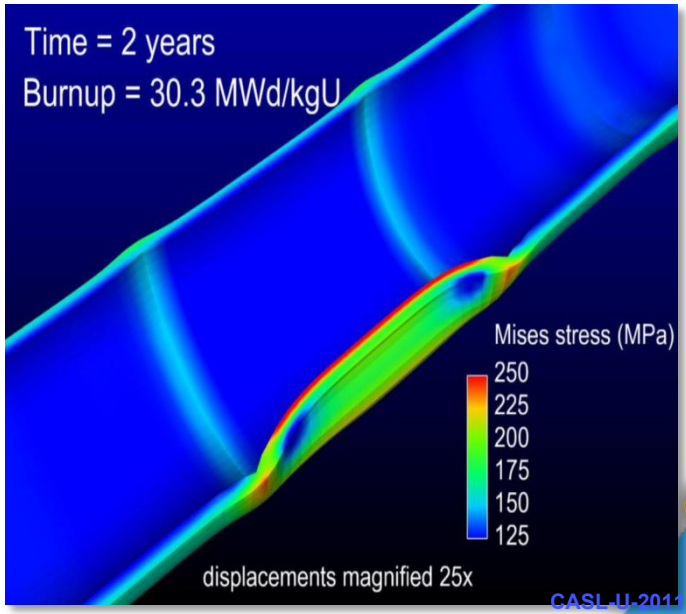
Peregrine Missing Pellet Surface simulations



- Defective (MPS) pellet placed midway between four intact pellets
- Simulation from fresh fuel state with a typical power history, followed by a late-life power ramp



Fuel Temperature



Von Mises Effective Stress

Summary

- The brief PCI background provides context for more detailed description tomorrow of how MPO is addressing the PCI challenge problem.

- The importance of input from thermal hydraulics and neutronics – as well as VUQ/data needs – were not discussed here, but ultimately required for complete and accurate assessment of PCI risk.
  - See VERA presentation tomorrow for discussion of coupling.

STRATEGIC PLAN

CASL Roundtable Meeting
August 9, 2011

Mario D. Carelli

CASL-U-2011-0072-000-R

Outline

- What It Is and It Is Not
- Strategic Plan Elements
  - Mission
  - Vision
  - Values
  - Goals
  - Planning
  - Organization
  - Execution of CASL Strategy
  - Roadmaps
  - Acceptance
  - Growth

What It Is and It Is Not

- It provides the “why”, “what”, and “who”

  It does not provide the “how”
- It is very high level and general, set goals and outcomes, it is brief!

  It does not provide details, they are in supporting documents
- It is a permanent, reference document

  It is not periodically updated – supporting documents are
- It is the driver of CASL activities and the reference for all CASL documents, directly or indirectly

If a major activity is not included in the Strategic Plan,

either

- The activity is not necessary and should be reconsidered

or

- The Strategic Plan is deficient and should be revised

Strategic Plan Elements

- MISSION
- VISION
- VALUES
- GOALS
- PLANNING
- ORGANIZATION
- EXECUTION OF CASL STRATEGY
- ROADMAPS
- ACCEPTANCE
- GROWTH

Mission

Provide leading edge Modeling and Simulation capabilities to improve performance of currently operating LWRs

- Develop integrated suite of codes running on some of the world's most powerful computers and capable of faithfully representing operational behavior of PWRs
- Verify such methodology against operational reactors
- Identify critical technical issues limiting operating reactors performance
- Apply CASL methodology to successfully resolve limitations

Vision

Be a game changer in the performance of operating nuclear plants and in the design of future plants

- CASL methodology will provide a deep insight in the modeling and phenomenological understanding of integrated behavior of nuclear reactors
- In the short term, it will allow operational improvements such as power uprates, higher burnup, lifetime extension
- In the long term, it will allow more efficient and safer reactor designs

Values

CASL will introduce new dimensions to the nuclear enterprise and open a new page in its collective advancement

- Technically: more realistic representation of reactor behavior allows to safely increase performance and make accidents more preventable with reduced consequences
- Institutionally: CASL is the archetype of complete cooperation by all elements of nuclear community: universities, laboratories, industry, reactor and fuel vendors, utilities, government and regulators

Goals

The wide ranging CASL Goals cover Organization, Collaboration, Technical, Relevance, Community and Growth

O – Lean team organization with swift two-way communications and feedback

O – One roof collocation

C – Relationship with DOE and NRC

C – Interfacing with technical community at large

T – Develop, verify, apply VERA

T – Identify and assess challenge problems

T – Advance state-of-the-art (modeling, numerical techniques, design solutions, products, e.g. advanced fuels)

R – Be a key contributor to improving reactor operation and design development

R – Address nuclear industry issues

C – Relationship with universities and secondary schools

C – Relationship with local and national public organizations

G – Expand from PWR starting basis (e.g. BWR, SMR, severe accidents, fuel cycle)

Planning

Assemble the best team capable of delivering CASL objectives in full satisfaction of key stakeholder objectives within the allotted time and resources.

– CASL Team is uniquely qualified in
  - Leading edge expertise in phenomenological modeling, computational simulation, experimental investigation
  - World class computational resources
  - Demonstrated proficiency in uncertainties evaluation and quantification
  - Experience in nuclear plants and fuel design, licensing, construction and operation
  - Experience with working together with DOE and NRC

– Key stakeholders are industrial (reactor, fuel and commercial codes vendors , utilities), institutional (DOE, NRC), educational (universities, secondary schools), public

Organization

CASL is built to satisfy the goal of a lean, efficient organization with swift two-way communication and feedback to fulfill stated goals

- Board of Directors
- One layer management
- Technical Focus Areas
- Operations
- Advisory Councils (science, industry, education, commercialization, communications)

CASL Organization

CASL-2011-048-O

Published: 7/11/11

Board of Directors
Ernest Moniz, Chairman

U.S. Department of Energy

COUNCILS

- **Science** — John Ahearne, Chairman
- **Industry** — John Gaertner, Chairman
- **Education** — John Gilligan, Chairman
- **Commercialization** — Jeff Cornett, Chairman
- **Communications** — Ken Nemeth, Chairman

Director
Doug Kothe

Deputy Director Ronaldo Szilard
Chief Scientist Paul Turinsky
Chief Strategy Officer Mario Carelli

Program Manager
Jeff Banta
Collaboration and Ideation Officer
April Lewis

Startup Manager
Gil Weigand
Partnership Manager
Jeff Cornett
Legal Project Manager
Jud Hightower

Operations
Operations Manager
Doug Kothe (interim)
Finance Officer
Victoria Shope
Administrative Support
Linda Weltman (executive)
Marsha Henley
Contracting Authority
Jo Ann Fitzpatrick
Quality Manager
Matt Sieger
VOCC Project Manager
John Shaw Jr.
VOCC IT & Cyber Security
Teresa Robison
Web & Database Design
Lara James
IT Project Manager
Brian Beal
Export Control
Rolf Migun / Sam Howard

Technical Focus Areas

MPO
Materials Performance & Optimization
Chris Stanek
Sid Yip
Brian Wirth

VUQ
Validation & Uncertainty Quantification
Jim Stewart
Dana Kelly

AMA
Advanced Modeling Applications
Jess Gehin
Zeses Karoutas
Stephen Hess

RTM
Radiation Transport Methods
Bill Martin
John Wagner

THM
Thermal Hydraulics Methods
Rob Lowrie
Rich Martineau

VRI
Virtual Reactor Integration
John Turner
Randy Summers

www.casl.gov

Consortium for Advanced Simulation of LWRs

Westinghouse

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Execution of Strategy

The CASL strategy execution evolves from the VERA development to its release to the technical community through a rigorous iter of verification and validation

- VERA development and verification
- Successful resolution of challenge problems
- Validation and uncertainties quantification
- Test stands at the three industrial core partners: EPRI, TVA, Westinghouse
- Release to technical community, observing proper intellectual property, commercialization and export control considerations

Challenge Problems

Table 1. Key Phenomena Limiting Improved Reactor Performance

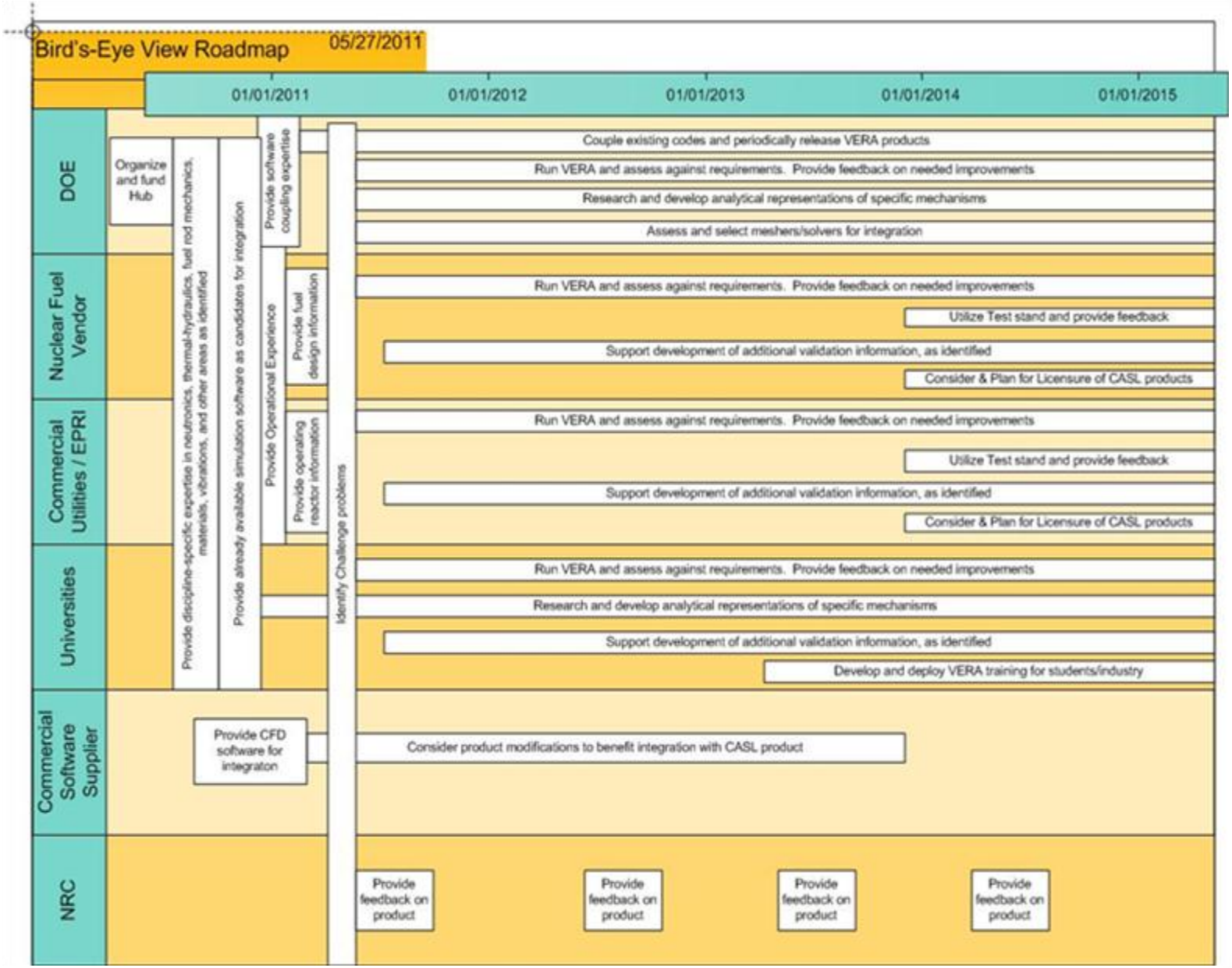
Phenomena	Power Uprate	Higher Burnup	Life Extension
Operational			
CRUD-Induced Power Shift (CIPS)	X	X	
CRUD-Induced Localized Corrosion (CILC)	X	X	
Grid-to-Rod Fretting Failure (GTRF)		X	
Pellet Clad Interaction (PCI)	X	X	
Fuel Assembly Distortion (FAD)	X	X	
Safety			
Departure from Nucleate Boiling (DNB)	X		
Cladding Integrity during Loss of Coolant Accidents (LOCA)	X	X	
Cladding Integrity during Reactivity Insertion Accidents (RIA)	X	X	
Reactor Vessel Integrity	X		X
Reactor Internals Integrity	X		X

-

Roadmaps

Bird's Eye and VERA Roadmaps provide focus and control of the overall program

- Bird's Eye roadmap defines route to successful completion of key stakeholders objectives
- VERA roadmap defines the key feeds



CASL
Consortium for Advanced Simulation of LWRs

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Acceptance

The ultimate strategic objective is that at the end of the 5-year period CASL generated products are accepted by the stakeholders

- *DOE:*
  - Satisfied objectives set forth in FOA ,as subsequently elaborated
  - Close coordination (weekly calls, periodic reviews)
- NRC
  - Periodic reviews to eventually lead to approval of VERA applications
- Industry
  - Operators adopt case technology to uprate plants performance
  - Designers adopt CASL technology to improve current designs and guide future designs
- Collaborations
  - Other organizations establish collaborations/partnerships with CASL

Growth

Following successful completion of its first 5-year mission, CASL will extend its technology and expertise to other areas than PWR operation

- Already contemplated in proposal
  - BWRs
- Solicited in first year or ORNL operation
  - Integral SMRs
  - Severe Accidents
  - SNF Evaluation
- Discussed collaborations
  - LMRs (with NEAMS)

DOE Light Water Reactor Sustainability (LWRS) Program

Dr. Ronaldo Szilard

Idaho National Laboratory
ronaldo.szilard@inl.gov

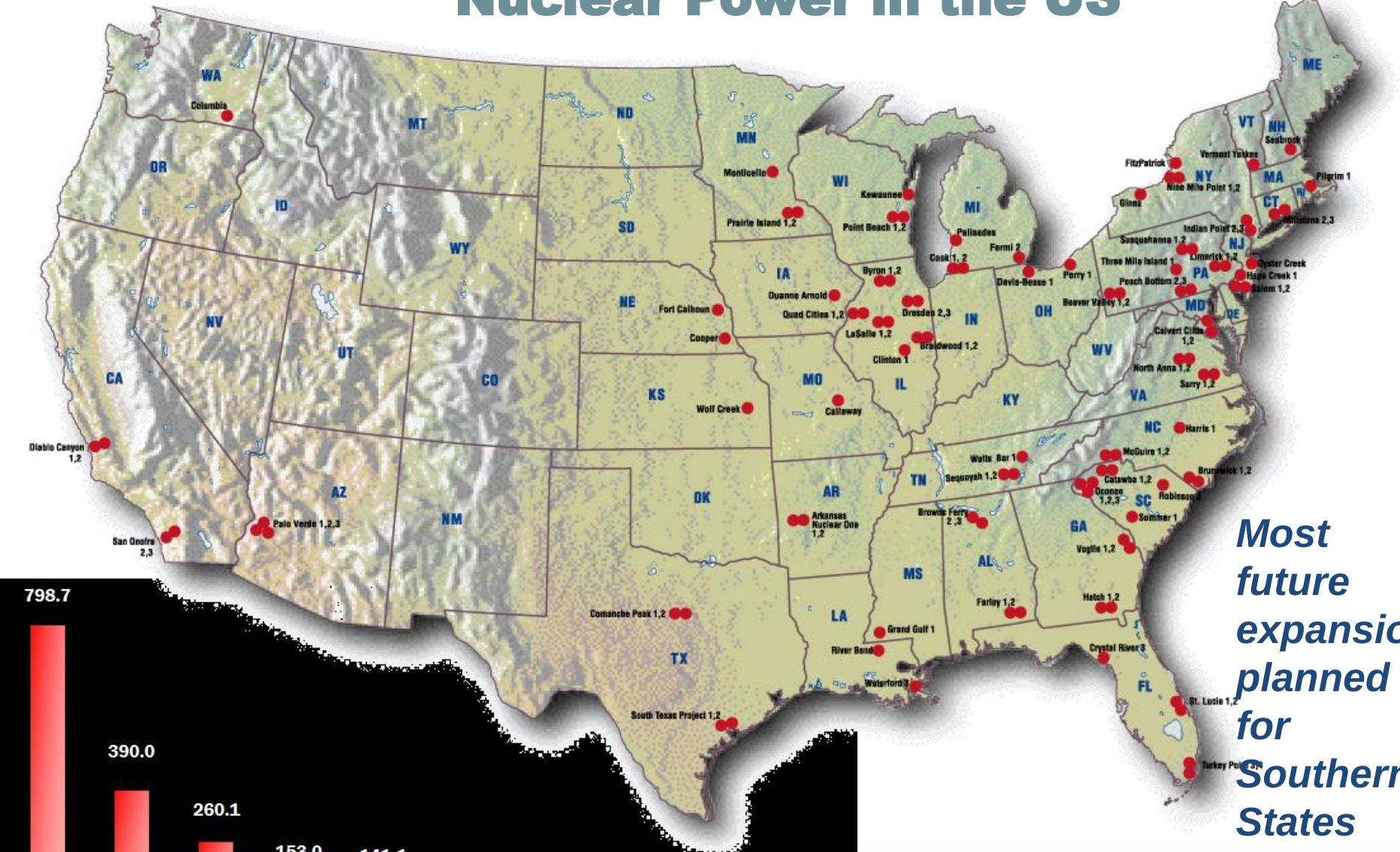
Light Water Reactor Sustainability

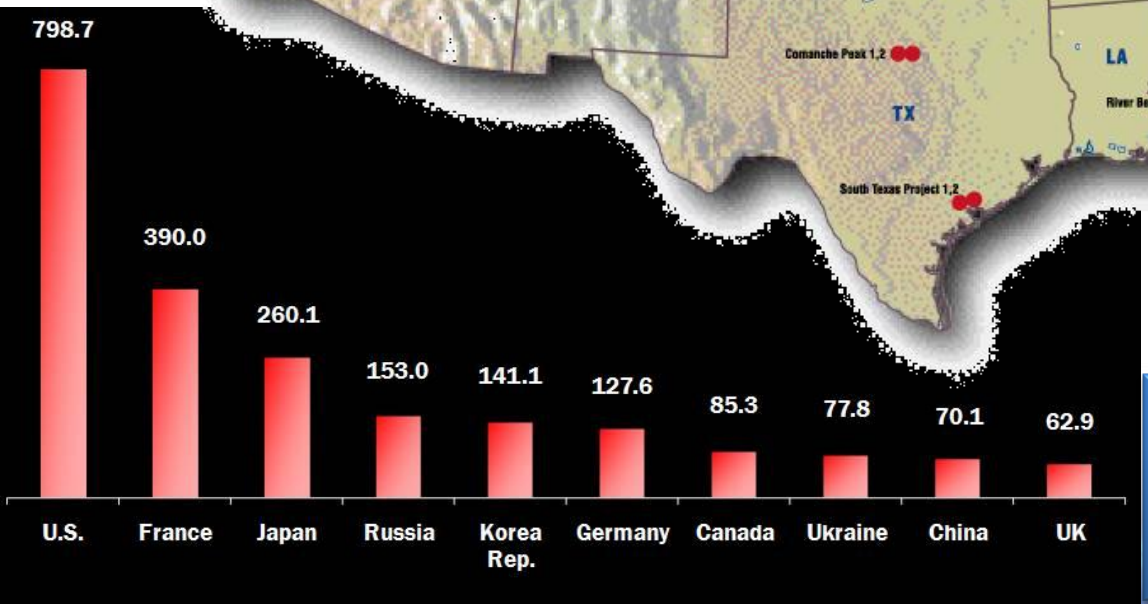
1st Annual CASL Round Table Meeting
NCSU, Raleigh, NC
August 9-11, 2011

Light Water Reactor Sustainability R&D Program

CASL-U-2011-0072-000-R

Nuclear Power in the US





Most future expansion planned for Southern States

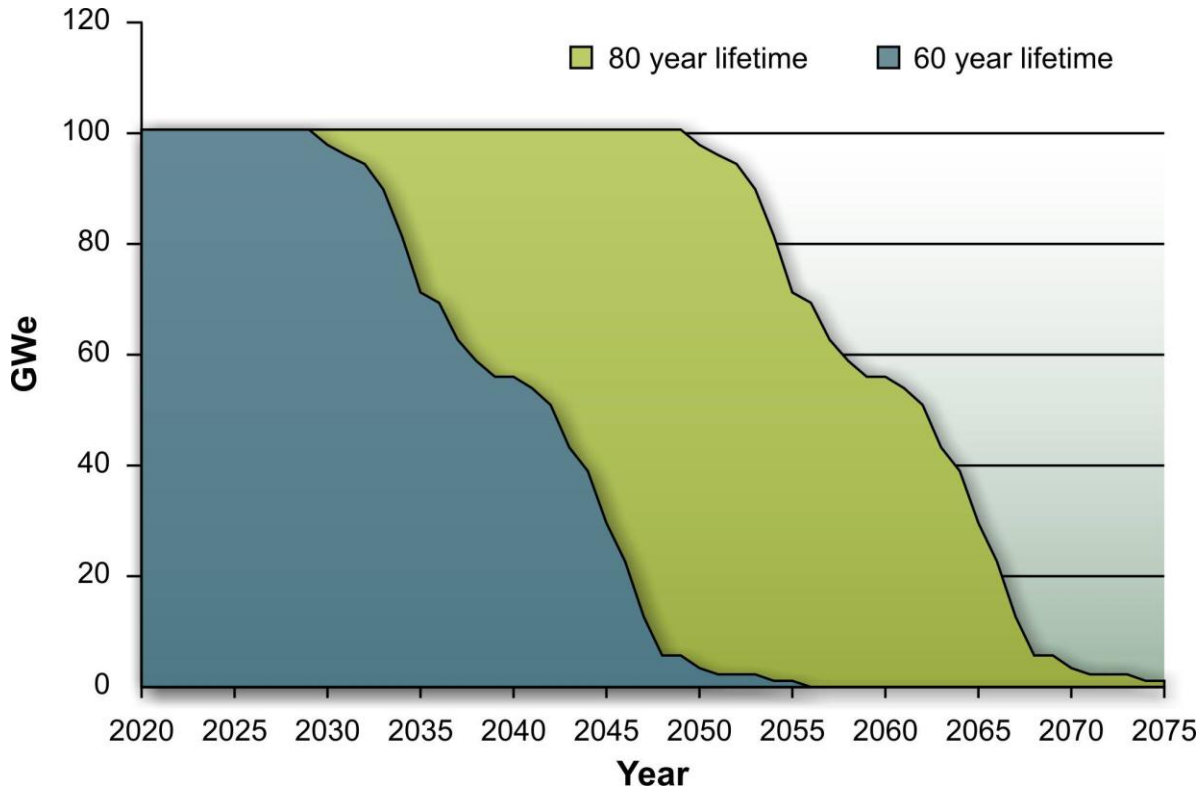
Top 10 Nuclear Generating Countries 2009, Billion kWh

Source: www.nei.org (International Atomic Energy Agency, 5/10)

SAND2012-8072-000-R

LWRS Program Key Driver

- **The key driver is the potential for production of 2000 GWe-years of low-cost electricity from extending the life of the current nuclear power plants.**



U.S. Nuclear Energy

Increasing cumulative capacity delivering at a high capacity factor

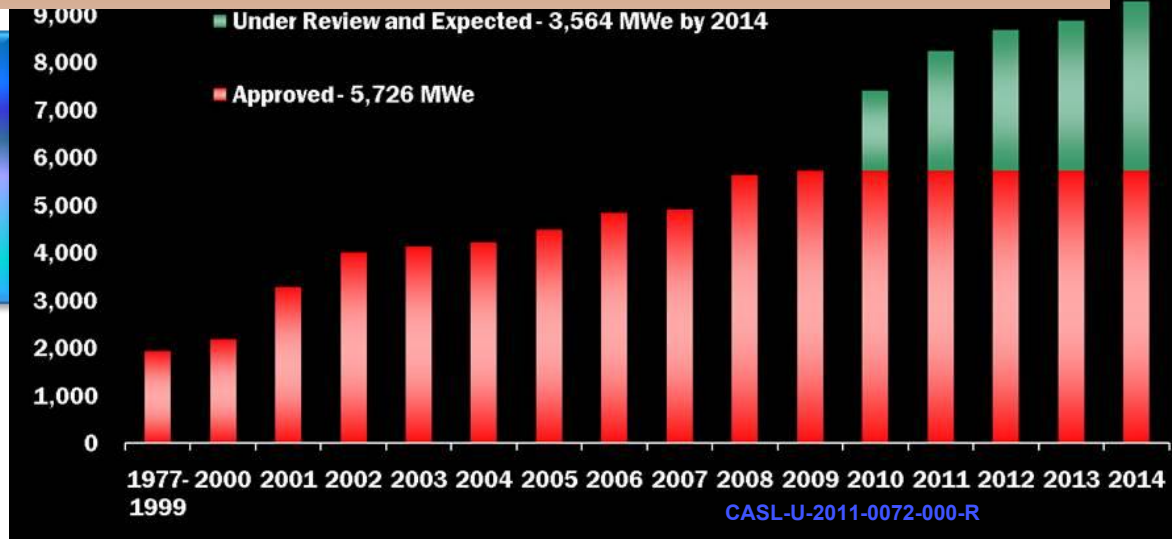
U.S. nuclear industry capacity factors 1971-2009 (percent)

Source: www.nei.org (Energy Information Administration, 5/10)

Safety + Economics

Cumulative Capacity Additions at U.S. Nuclear Facilities 1977-2014

Source: www.nei.org (Nuclear Regulatory Commission, 6/10)

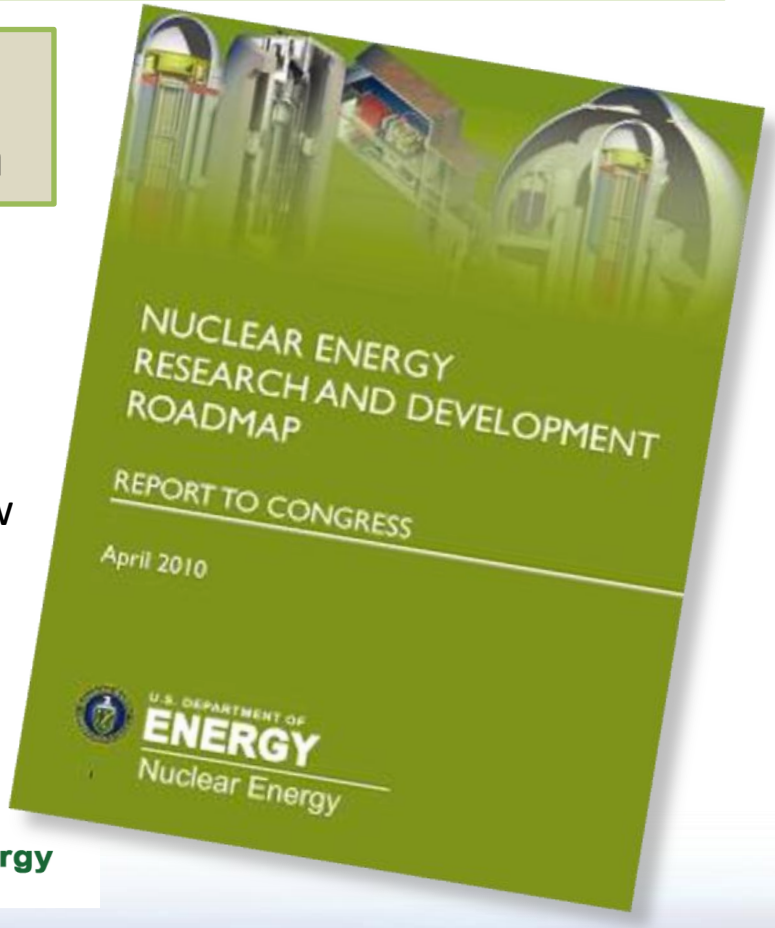


DOE Nuclear Energy Roadmap is the Foundation for LWRS Program Planning and Key Activities

R&D Objective #1 of DOE Nuclear Energy Roadmap is to Extend Life, Improve Performance, and Maintain Safety of the Current LWR Fleet

R&D Objective #1 — Light Water Reactor Sustainability (LWRS) Program

- Vision - Enable existing nuclear power plants to safely provide clean and affordable electricity beyond current 60-year license limit
- Program Goals
  - Develop fundamental scientific basis to allow continued safe long-term operation
  - Develop technical and operational improvements that contribute to long-term economic viability

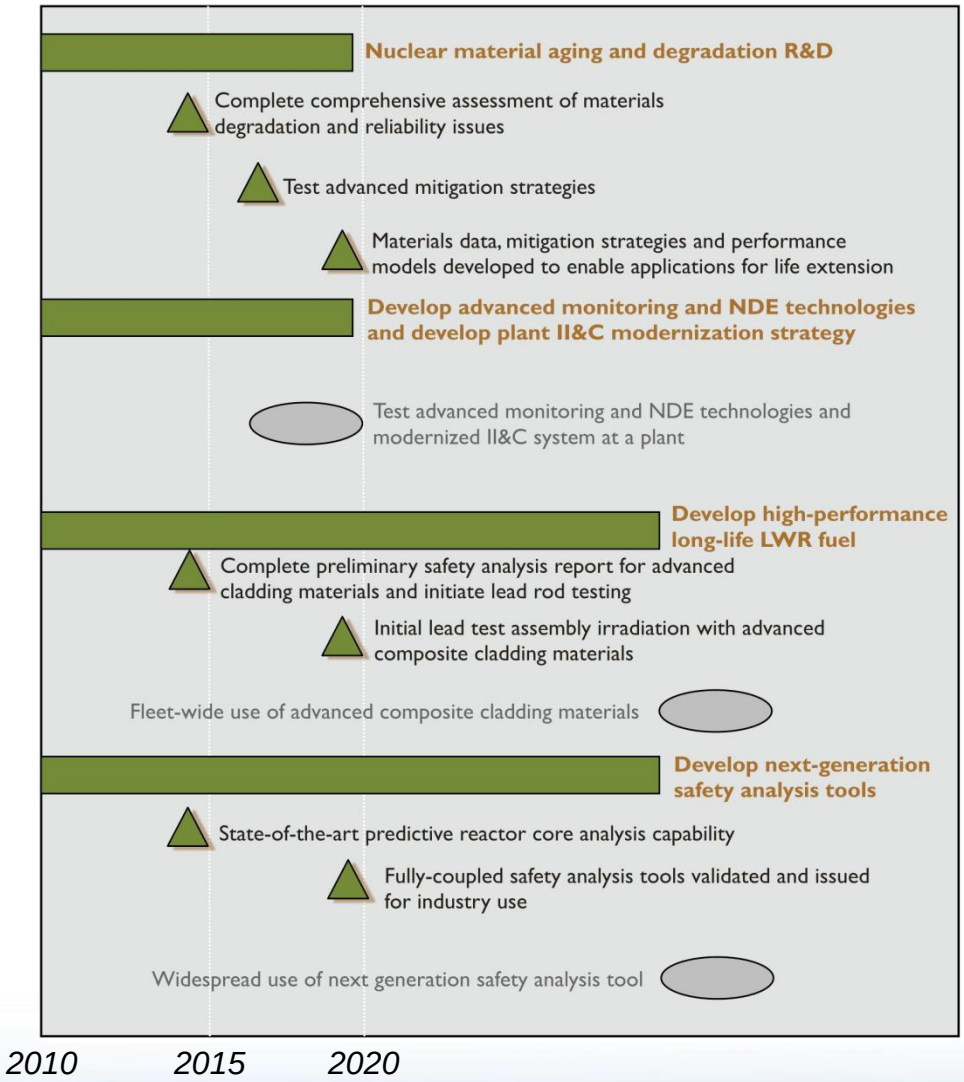


LWRS Light Water Reactor Sustainability

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

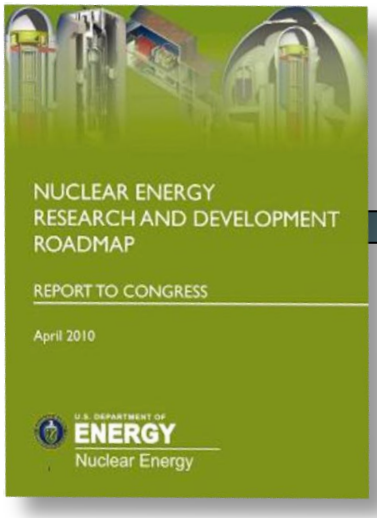
CASL-U-2011-0072-000-R

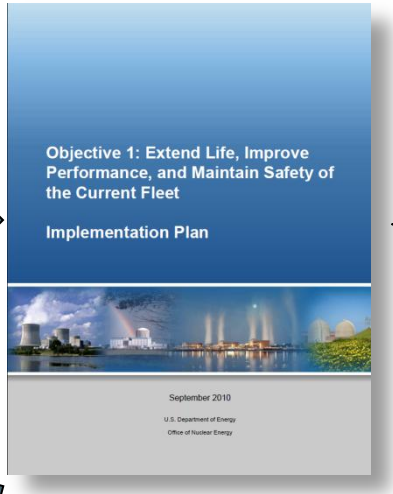
DOE NE R&D Roadmap: Deliverables for Objective 1

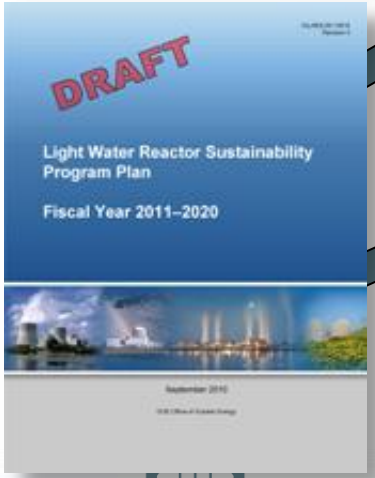


LWRS
Light Water Reactor Sustainability

DOE Nuclear Energy Roadmap is the Foundation for LWRS Program Planning and Key Activities







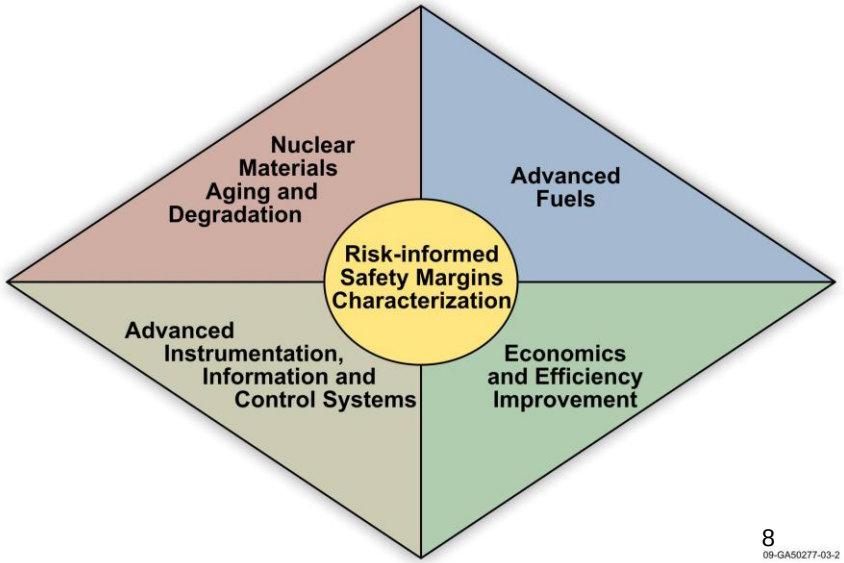
- *LTO / LWRS Joint Strategy Plan*
- *Nuclear Materials Aging and Degradation R&D Plan*
- *Advanced Instrumentation, Information, and Control Systems R&D Plan*
- *Risk-Informed Safety Margins Characterization R&D Plan*
- *Advanced LWR Fuel Development R&D Plan*
- *Economics and Efficiency Improvements R&D Plan*

LWRS
Light Water Reactor Sustainability

LWRS Program Scope

Scope

- Nuclear Materials Aging and Degradation
- Risk-Informed Safety Margin Characterization (RISMC)
- Advanced Instrumentation and Controls
- Advanced LWR Fuel Development
- Economics & Efficiency improvements
- *Synergy with Energy Innovation M&S Hub (CASL)*



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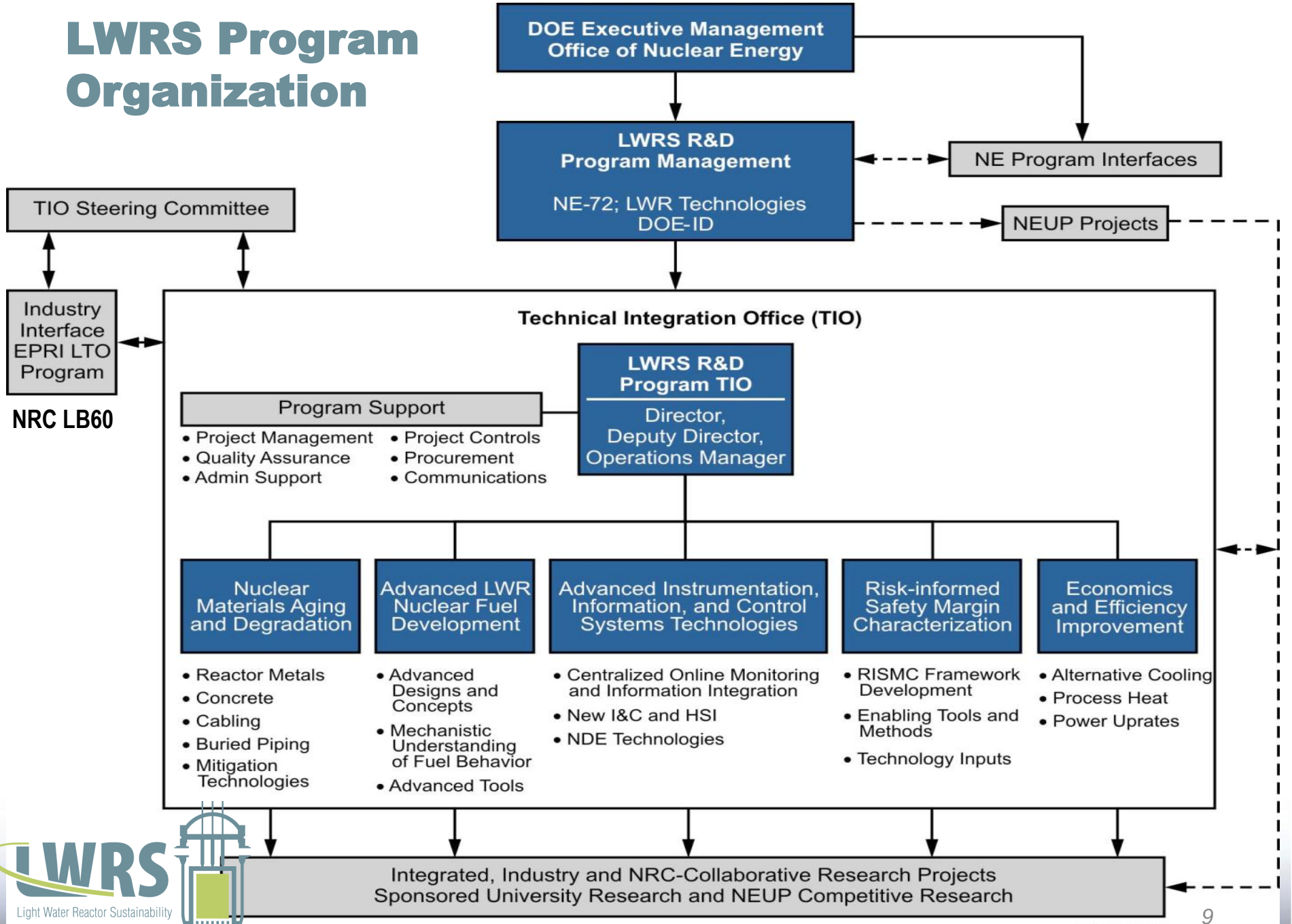
LWRS Program Organization



LWRS
Light Water Reactor Sustainability

LWRS Program: An Integrated Collaborative R&D Program

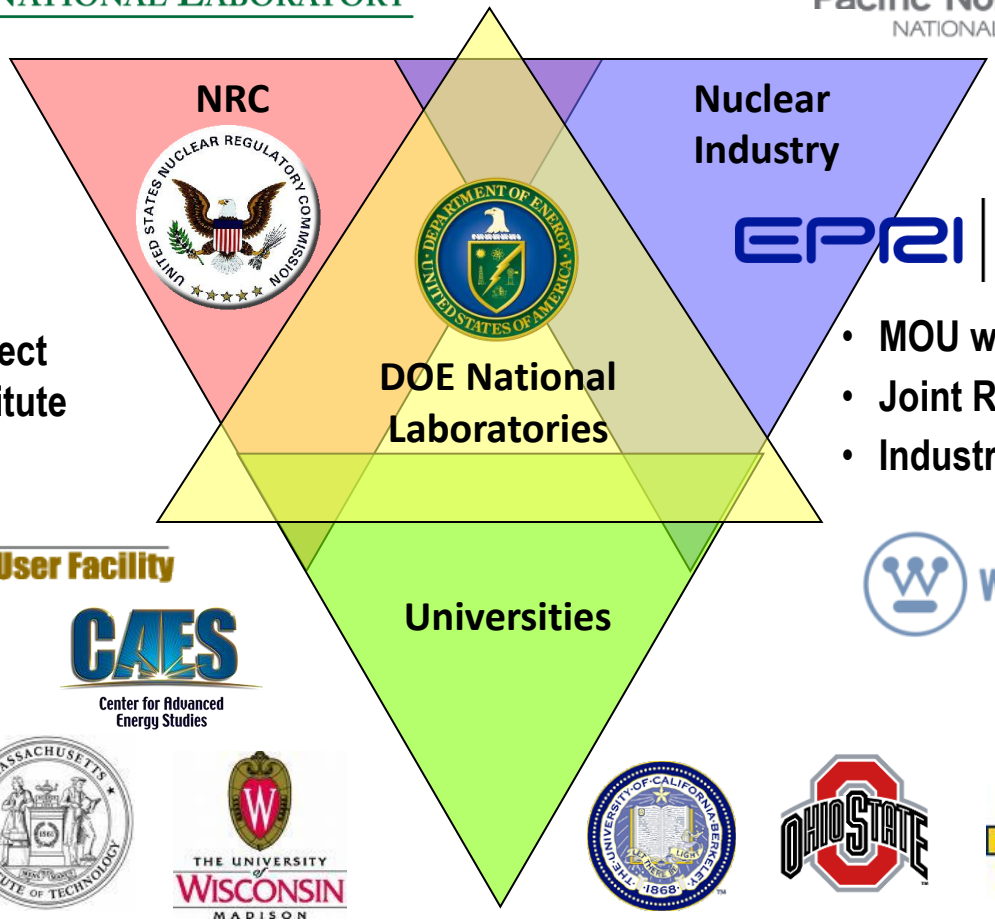
Idaho National Laboratory

Oak Ridge National Laboratory

Pacific Northwest National Laboratory

- MOU with NRC

- International Partners
  - Halden Reactor Project
  - Materials Aging Institute



EPRI ELECTRIC POWER RESEARCH INSTITUTE

- MOU with EPRI
- Joint R&D Plan
- Industry pilot projects

Westinghouse

ATR National Scientific User Facility

CASL

CAES Center for Advanced Energy Studies

UCSB

OSU Oregon State University

Massachusetts Institute of Technology

The University of Wisconsin Madison

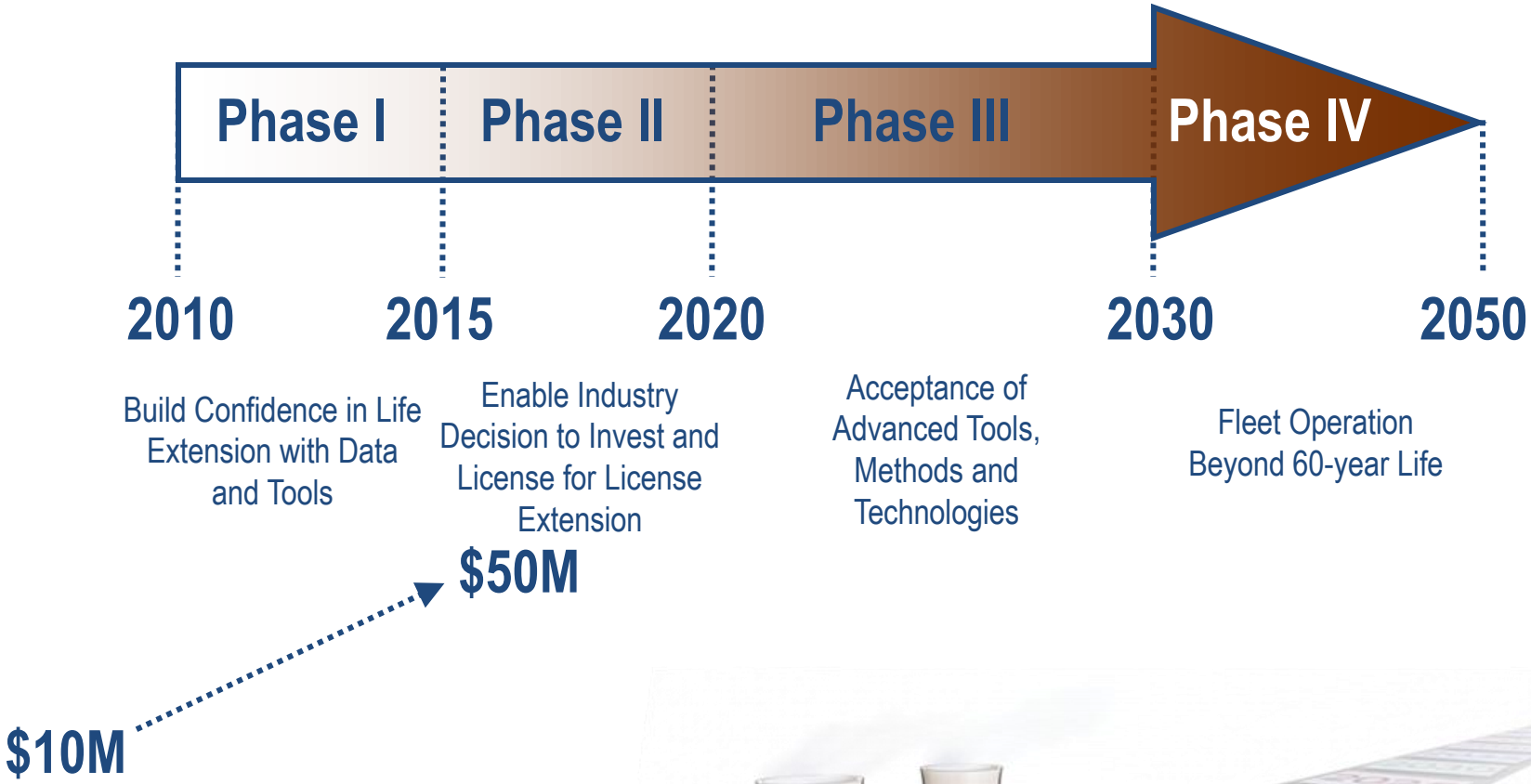
The University of California Berkeley

Ohio State

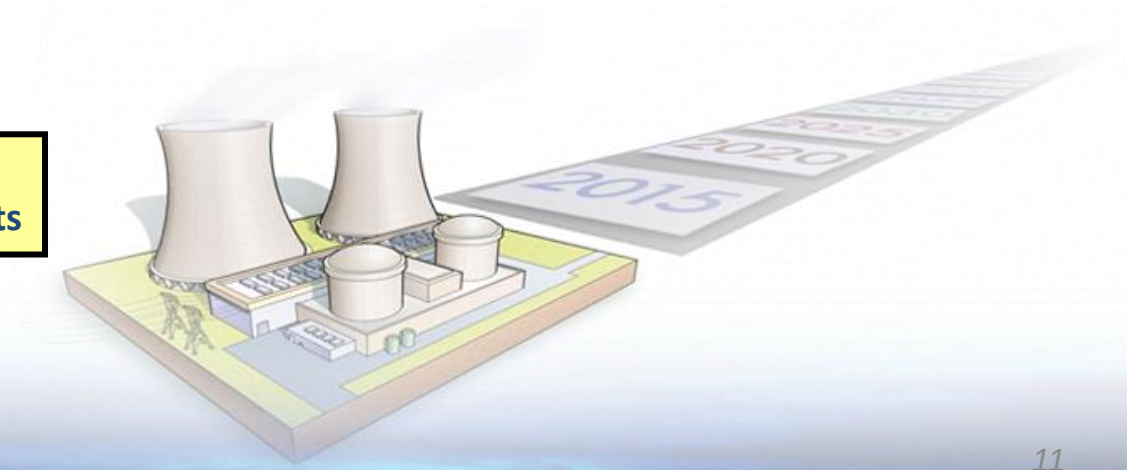
Michigan

LWRS Light Water Reactor Sustainability

LWRS Program Schedule Supports Investment & Licensing Decisions for Long-Term Operation



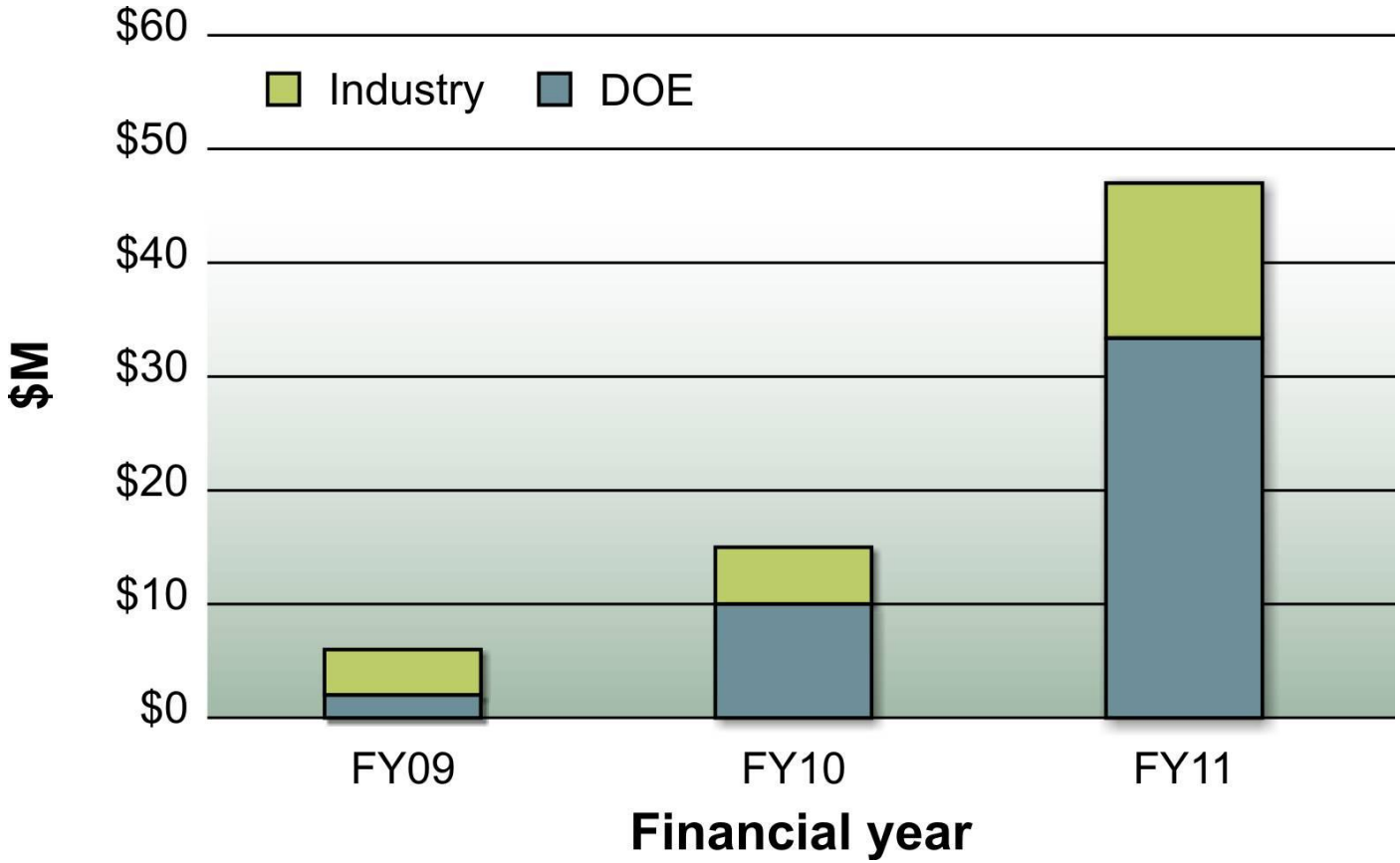
Large Payoff: Moderate R&D Cost Leveraging High Capital Investments



LWRS
Light Water Reactor Sustainability

CASL-U-2011-0072-000-R

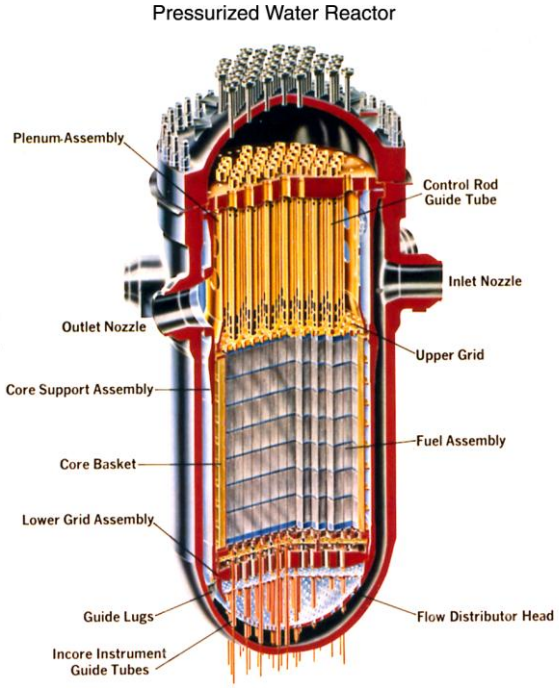
Industry Cost-Share – Stakeholder funded R&D and in-kind contributions

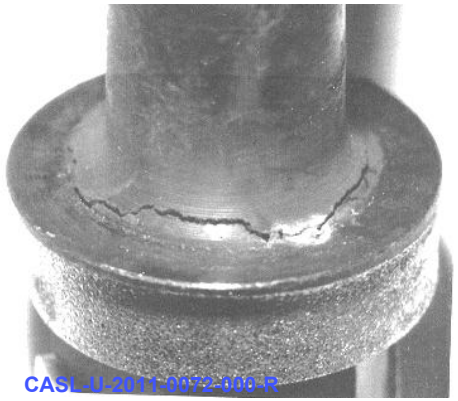


Large Payoff: Moderate R&D Cost Leveraging High Capital Investments

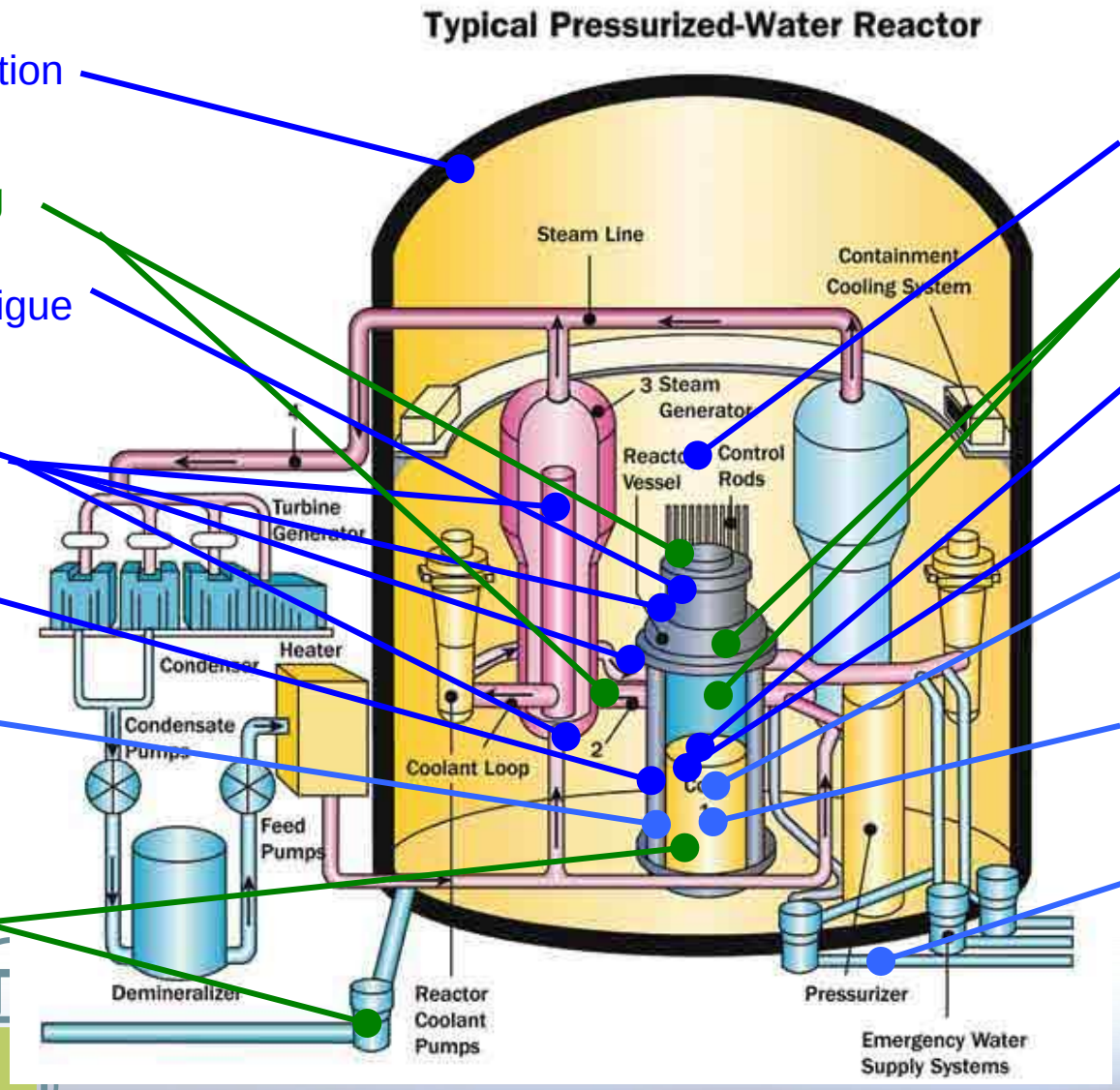
Extending the Service Life of Today's LWR Fleet May Create New Material Challenges

- Extending reactor life to beyond 60 years will likely increase susceptibility and severity of known forms of materials degradation and potentially introduce new forms of degradation
- The LWRS R&D effort seeks to provide the scientific basis for understanding and predicting materials aging and degradation within components, systems, and structures
  - Reactor metals (RPV's, internals, steam generators, balance of plant, and weldments)
  - Concrete
  - Buried piping
  - Cabling
  - Mitigation, repair and replacement technologies





The LWRS Materials Aging and Degradation R&D Pathway Encompasses the Entire Plant



Concrete Degradation

Repair welding

Environmental Fatigue

Crack initiation in Ni-base alloys

High fluence effects on RPV

Surrogate materials and attenuation

Advanced replacement alloys

Analysis of cable degradation

Thermal annealing

Mechanisms of IASCC

High fluence IASCC

Swelling of core internals

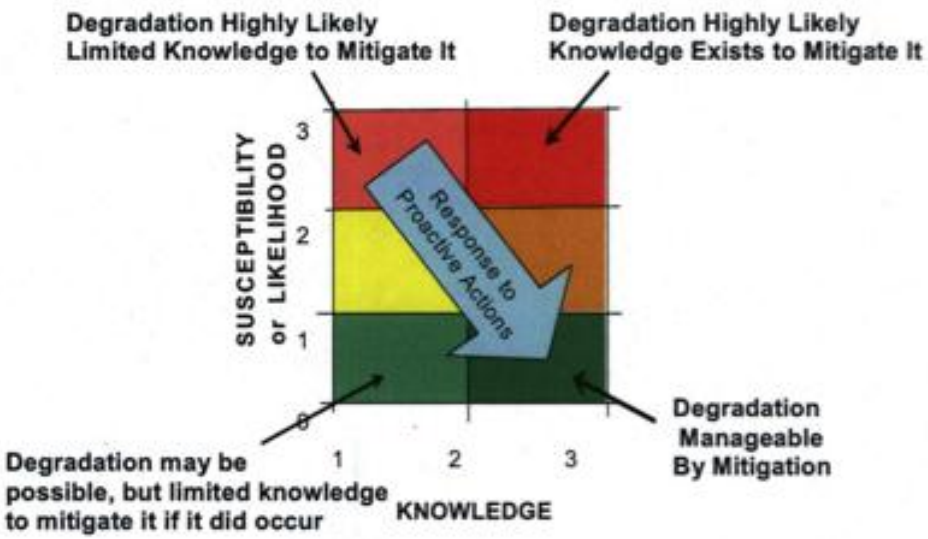
High fluence phase transformations

Buried piping analysis

LWRS
Light Water Reactor Sustainability

Materials research must also identify other or new topics before they become life-limiting

- **"Knowing the unknowns" is a difficult problem that must be addressed.**
- **This is a particularly difficult issue for such a complex and varied material/environment system.**
- **An organized PMDA approach is being employed.**
- **Together with the NRC, the LWRS is working to expand the initial activity (*NUREG/CR-6923)* to broader systems and longer lifetimes**
  - Core internals and primary piping
  - Pressure Vessel
  - Concrete
  - Cabling



***P**roactive **M**aterials **D**egradation **A**ssessment Matrix*

CASL-U-2011-0072-000-R

DOE/EPRI/CENG Nuclear Plant Life Extension Demonstration (NPLED) Project

- **In August 2009, Industry LTO Advisors asked EPRI to identify a generic pilot plant to investigate license renewal issues**
- **Constellation Energy (CENG) offered Ginna Station and Nine Mile Point Unit 1 Station as industry pilot plants**
- **Activity will be collaboration among U.S. DOE, EPRI, and CENG, to be conducted through DOE LWRS and EPRI LTO Projects**
- **Project has 3 year planned duration with option for extension**
- **Scope:**
  - Reactor Vessel Internals Enhanced Aging Inspection
  - Comprehensive Containment Assessment
  - Investigation of Surveillance Samples for Projecting Reactor Vessel Life
  - Medium and low voltage power cable aging in adverse environments
  - Buried piping degradation
  - Spent Fuel Pool aging issues
  - I&C challenges

CENG Pilot Plant Selection

- **2 CENG plants operating in their Periods of Extended Operation (beyond 40 years)**
  - Ginna (PWR) and NMP1 (BWR)
- **Ginna activities conducted in September/October 2010:**
  - Containment ISI external inspection
- **Ginna activities occurring in Spring 2011 outage:**
  - Lead plant for MRP-227 Reactor Vessel Internals Inspection
  - Containment Integrated Leak Rate Test
- **NMP1 has an extensive RFO planned for Spring 2011**

CENG
a joint venture of
Constellation Energy
EDF

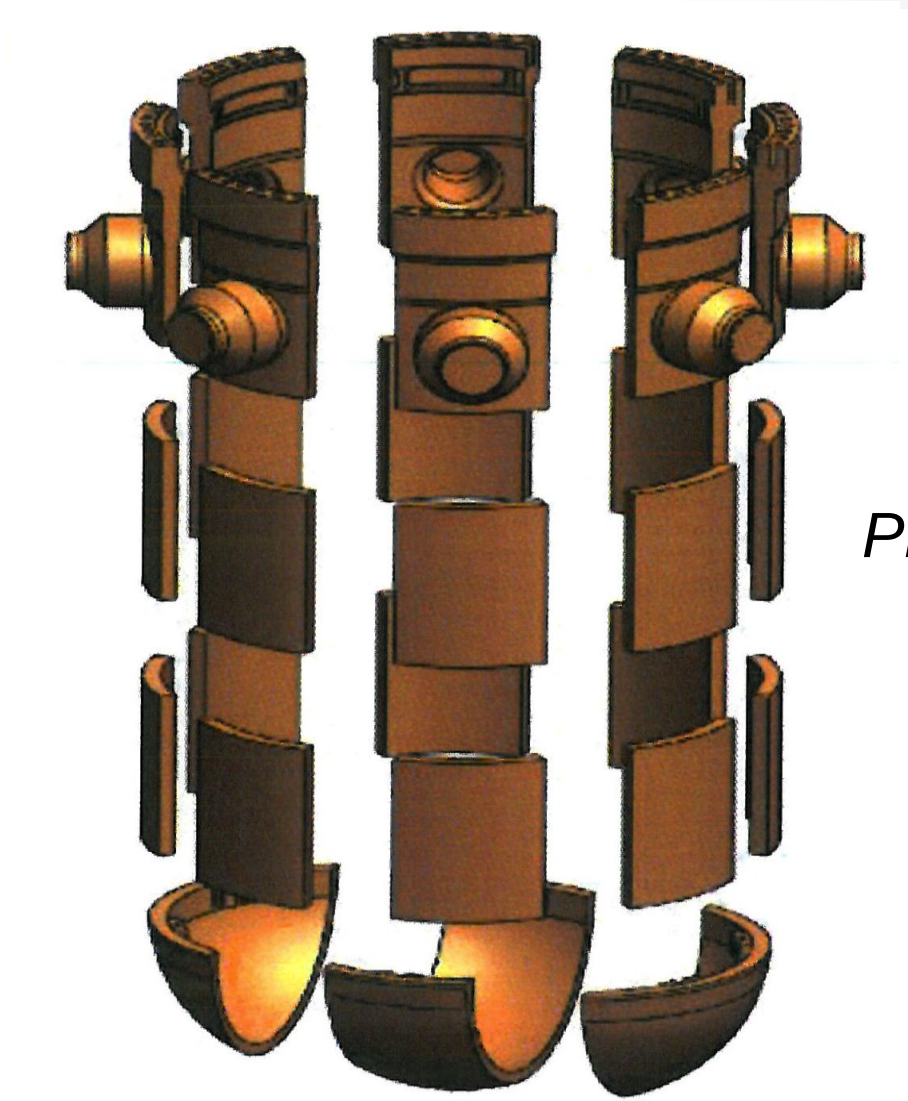
The decommissioning of the Zion 1&2 Nuclear Power Plants provides a timely opportunity to examine materials degradation

- **In support of extended service (and current operations), ORNL is coordinating and contracting activities with Zion Solutions.**
- **In collaboration with the US NRC, EPRI, and others a list of materials for "harvesting" is being compiled and feasibility examined.**
- ***Structures and components***
  - ***Thru-wall RPV sections***
  - ***Cabling***
  - ***Concrete bore samples***
  - ***Internals***
  - ***Access to observations on stored fuel***

Zion Nuclear Power Plant

LWRS
Light Water Reactor Sustainability

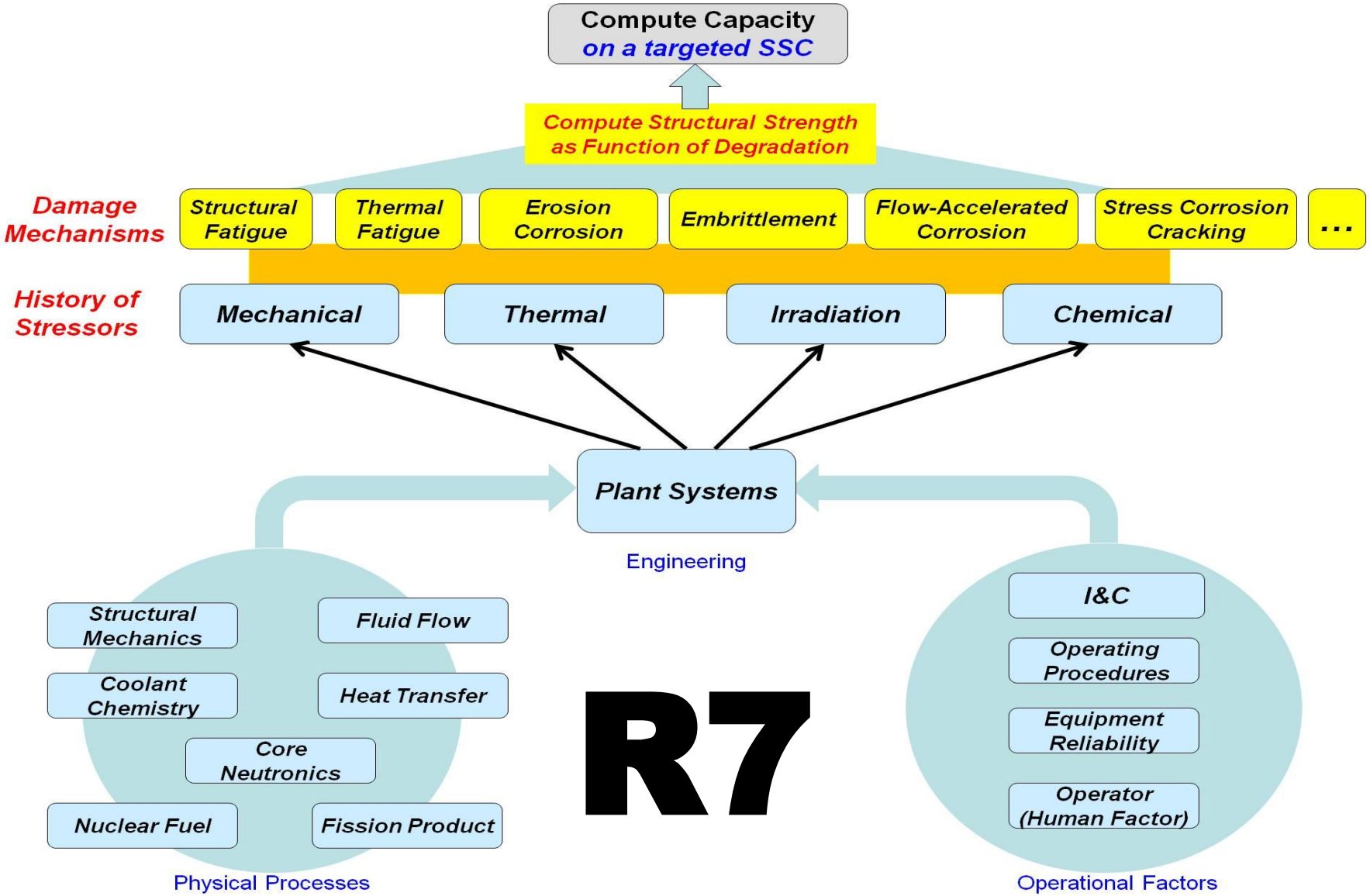
The Zion RPV's may provide invaluable material



Proposed Segmentation Plan

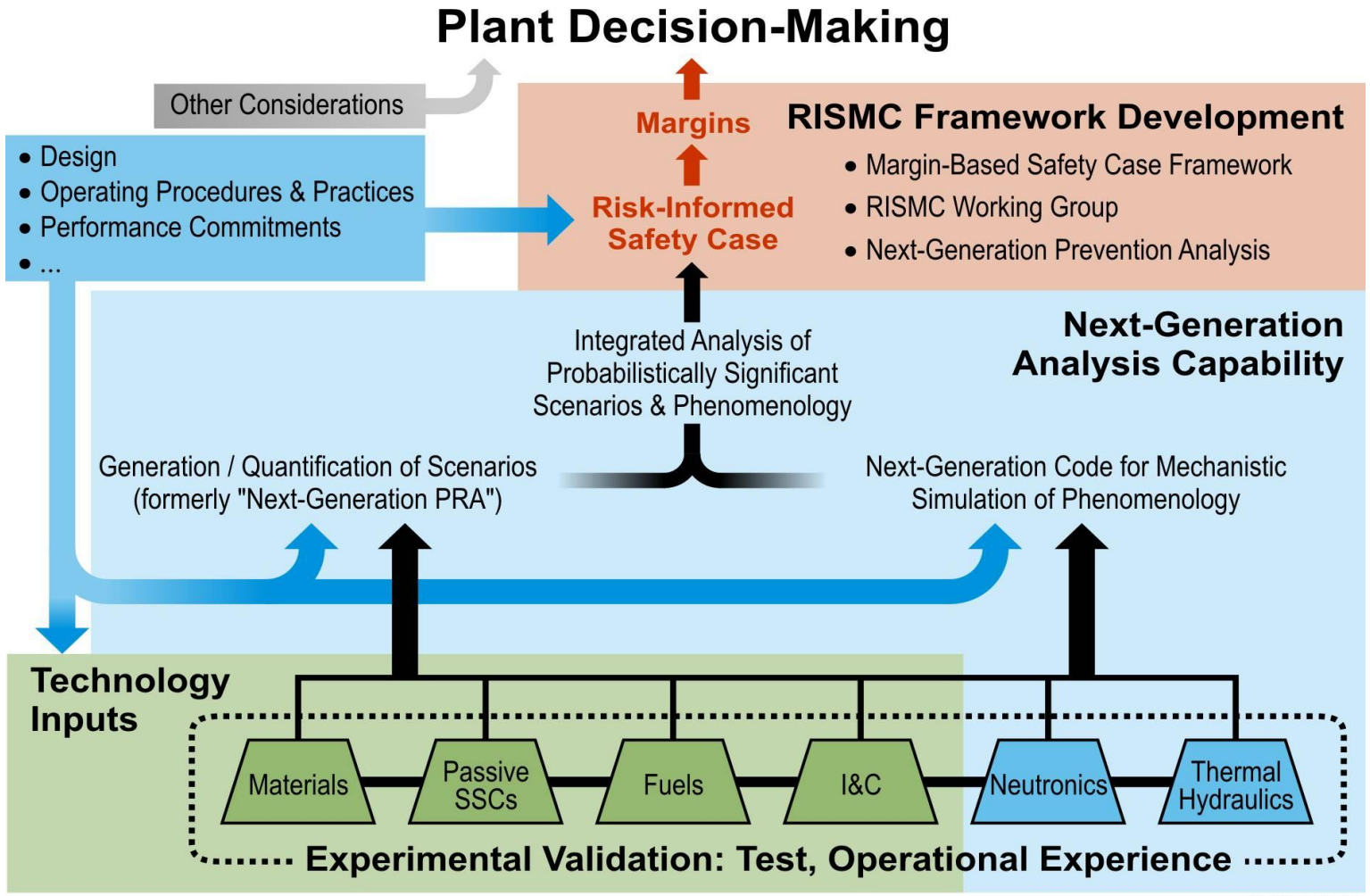
Characterization of safety margin is central to decision making in plant operational performance, power uprate, and life extension

09-GA50617-01-5


Compute Capacity
on a targeted SSC
Compute Structural Strength
as Function of Degradation
Damage Mechanisms
Structural Fatigue
Thermal Fatigue
Erosion Corrosion
Embrittlement
Flow-Accelerated Corrosion
Stress Corrosion Cracking
...
History of Stressors
Mechanical
Thermal
Irradiation
Chemical
Plant Systems
Engineering
Structural Mechanics
Fluid Flow
Coolant Chemistry
Heat Transfer
Core Neutronics
Nuclear Fuel
Fission Product
Physical Processes
R7
I&C
Operating Procedures
Equipment Reliability
Operator (Human Factor)
Operational Factors

Risk-Informed Safety Margin Characterization (RISMC)

Combining Probabilistic and Mechanistic Modeling to provide Integrated Quantification of Uncertainty



10-GA50039-03g

Advanced Information, Instrumentation & Controls (IIC) R&D

- Current technology for IIC is not sustainable – will become a limiting factor for continued operation
- Recent replacements and modernizations using digital technologies are perceived as unsuccessful.
- Regulatory uncertainty and a risk-averse industry reinforce the status quo of outdated and antiquated analog I&C.
- ALWR licensing will not change current IIC limitations.
- Asset owners and vendors recognize that the needed change is not occurring and is not likely to occur without substantial federal involvement.

From this…

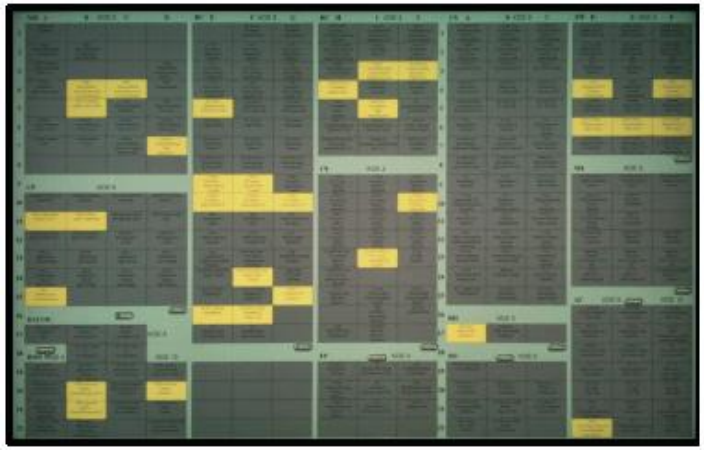
…to this!

- The commercial nuclear power industry will undertake modernization as a result of this program.
- Confidence will be created in the process of developing and deploying technology through this program to support utility and regulatory decisions.
- A federally funded and supported IIC Laboratory will form the basis for multi-party agreements used for research, development, demonstration, test & evaluation.

IIC Pilot Projects Provide Valuable Industry Input

Example: Alarm Systems

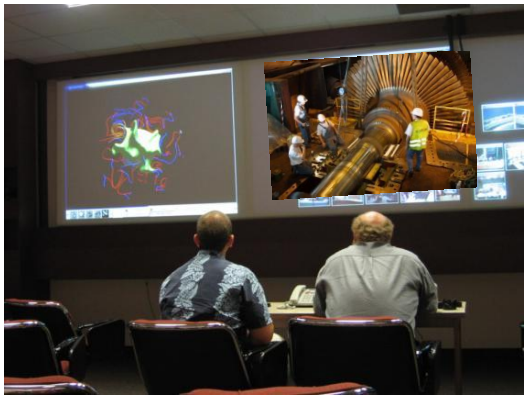
- Analog systems beyond service lifetimes
  - Fundamental alarm technology developed in the 1960s
  - Replacement parts difficult to obtain
  - Alarm systems very complex to maintain
- Overabundance of binary state alarm annunciator tiles
  - Typical plant features over 1000 individual alarm tiles
- Ineffective filtering of alarms leads to nuisance alarms that can overload operators
- Digital replacement systems have tended to be like-for-like replacements, not improved systems that intelligently filter alarms or help operator focus on most important alarms



IIC Pilot Projects Provide Valuable Industry Input

Example: Outage Control Center – Shared task visualization in coordination with the use of new technologies, allows for real time information flow, coordination of work groups and tasks, management of work progress, safety oversight, and increased efficiency/decreased down time.

Operations Control Center



Work Execution Center

Outage Field Activities

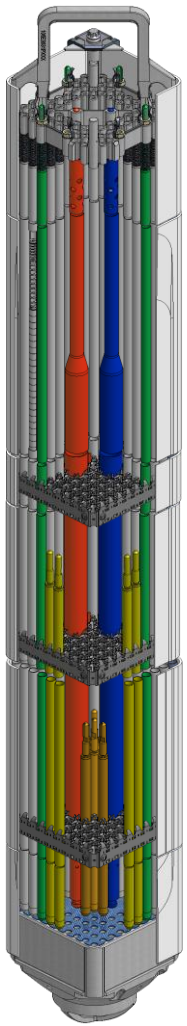
Advanced Nuclear Fuels

Goals:

- Improve the fundamental scientific understanding and prediction of the behavior of nuclear fuel pellets, cladding, and the fuel-coolant system under extended burn-ups for normal and transient conditions
- In public-private collaborations apply this information developing and demonstrating very advanced fuels with improved safety margins, and potential for higher fuel burn-ups and performance
- Develop predictive tools for advanced nuclear fuel performance
- Speed implementation of new fuel technologies to industrial application

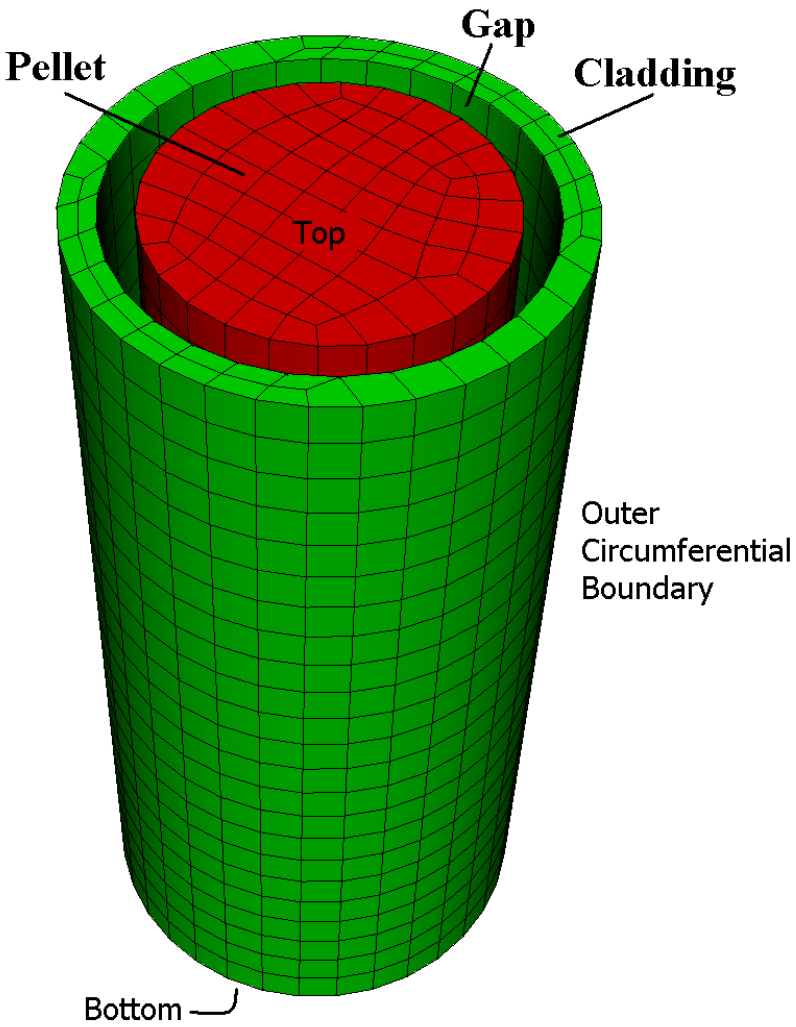
Specific planned activities:

- Begin the development of new long-life fuel designs with advanced fuel and cladding materials
- Develop predictive tools of advanced nuclear fuel performance
- Develop a model for fuel cracking at the mesoscale level with sufficient understanding to develop a predictive model for fission gas release

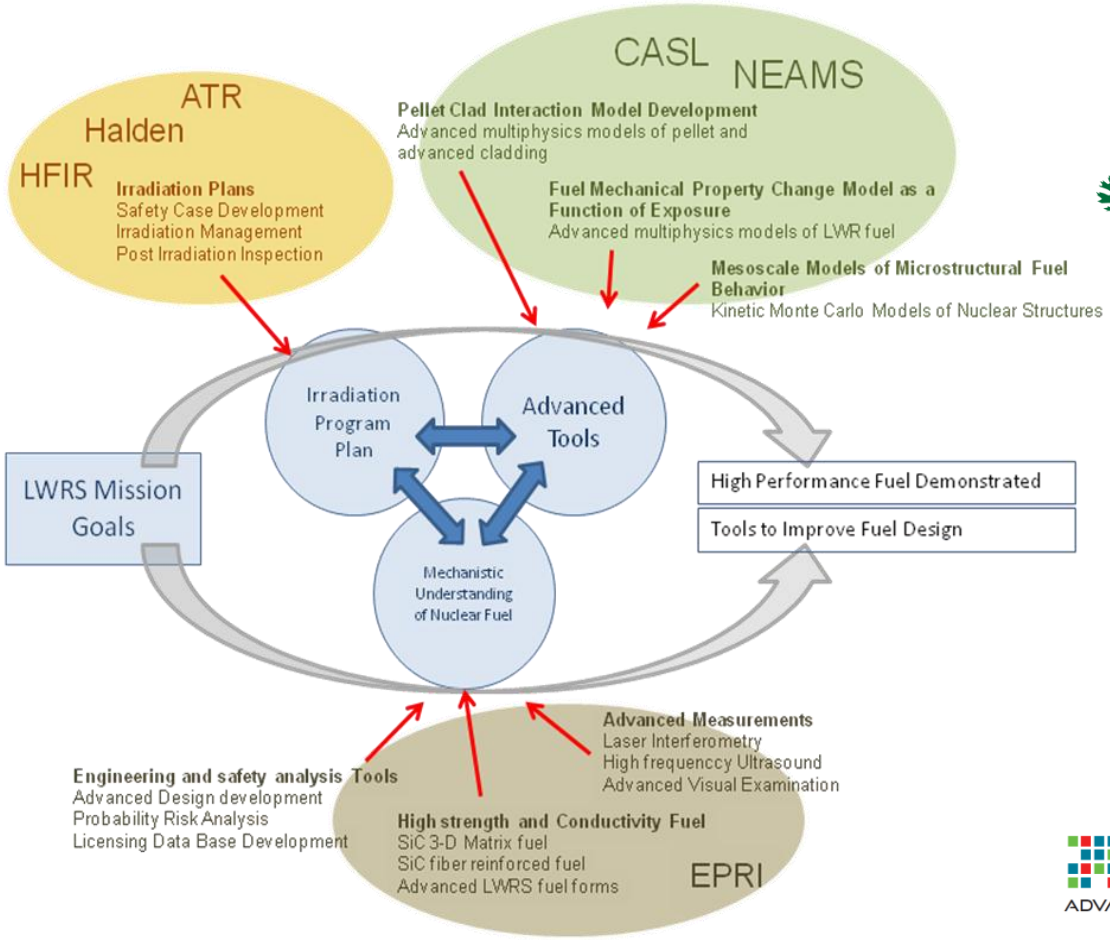


Advanced Fuel Designs & R&D Concepts

- Advanced fuels
  - UOX variants (additive fuels, >5% U-235, enriched gadolinium)
  - Alternate fuels (UN, UC, hydride)
  - Novel designs (annular fuel, innovative shapes, liquid metal bond)
  - Dopants for PCI, thermal conductivity
- Advanced Cladding
  - optimized next generation zirconium alloys
  - Silicon carbide (SiC)
- Modeling and Simulation
  - Address fuel performance issues through basic scientific understanding
  - Accelerate design to implementation



A multiple stakeholder strategy



Idaho National Laboratory

Oak Ridge National Laboratory

NEAMS

CASL

EPRI Electric Power Research Institute

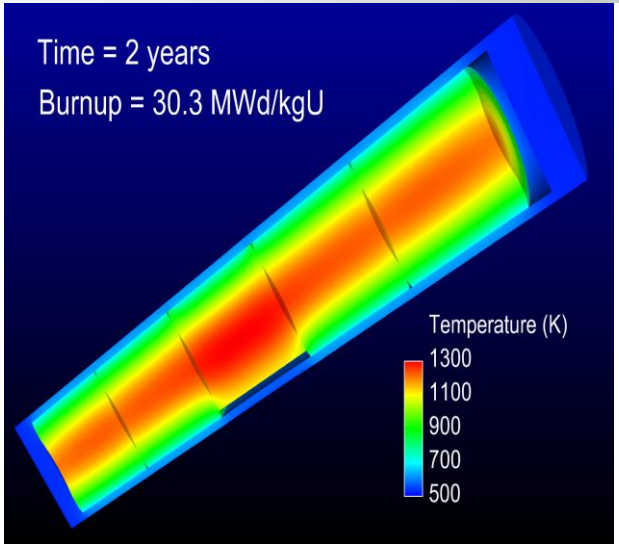
ATR National Scientific User Facility

AMSO Advanced Modeling & Simulation Office

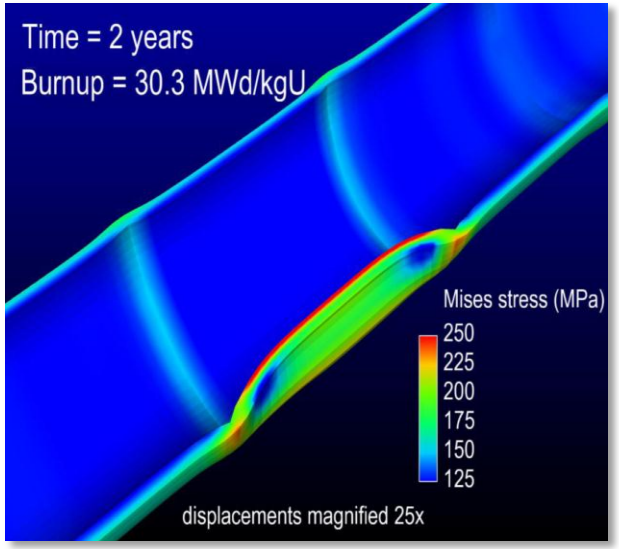
Fuel Performance Modeling:

High-resolution model for fuel/clad behavior and response to a missing pellet surface condition

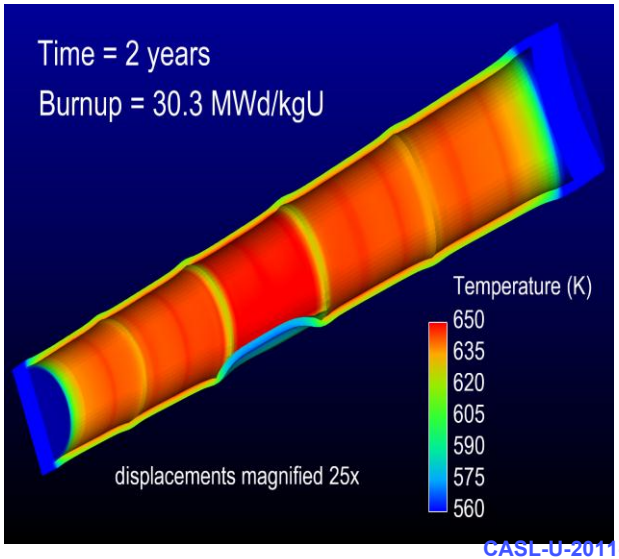
High resolution, 3D fuel performance calculation reveals the impact of a missing pellet surface on stress state, temperature profile, etc. (*i.e.* full nuclear fuel performance) as a function of fuel history.



Fuel Temperature



Stress

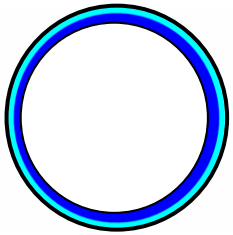


Clad Temperature

SiC Cladding Development

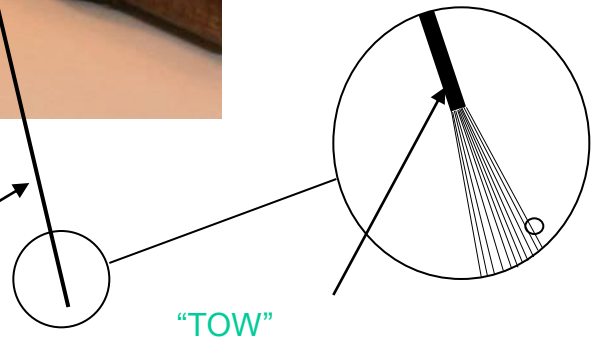
- Develop high performance, high burnup nuclear fuels with improved safety, clad integrity and fuel cycle economics
- Design, develop and test a multilayered SiC clad fuel that significantly increases fuel performance. Key characteristics include:
  - strength retention to at least 1500°C, appears to be DNB proof, and therefore can facilitate power uprates of 30% or more.
  - minimal exothermic water reaction or H_2 release during LOCA's,
  - fully retains fission gases – no creep and FG retention to at least 5000 psi
  - composite layer solves ceramic "brittleness" problem
  - Can operate in LWR coolant for over 10 years with no appreciable corrosion
    - Zirc alloys embrittle after 5 years operation and are therefore limited by regulation to 62 gwd/t
  - When coupled with increased U_{235} loading, can double the burnup to 100 gwd/t
  - Very hard, resists fretting and debris failure, further reduction in operational failures

SiC TRIPLEX CLADDING



FILAMENT WINDING

MONOLITHIC DENSE SiC TUBE



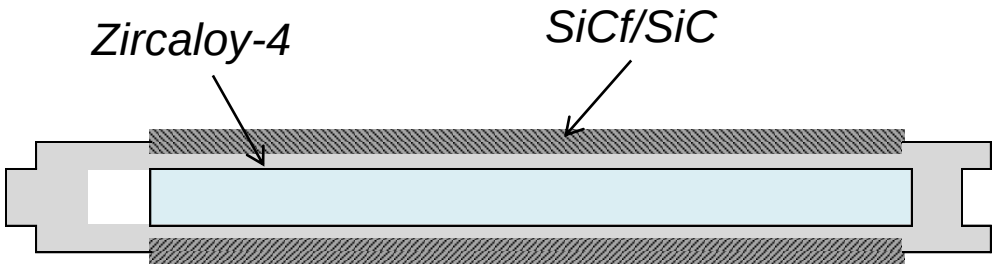
SiC FIBER TOW

"TOW" (500-1000 FIBERS)

Ceramic Composite Cladding (SiC) Development

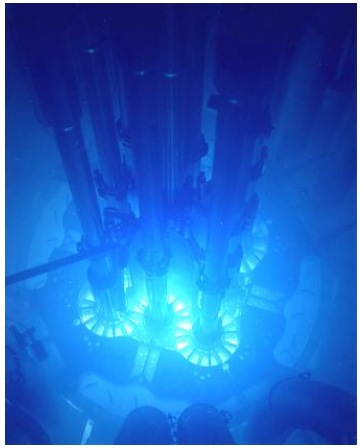
- ***Collaborative efforts with INL, EPRI, Westinghouse, MIT & ORNL***

- ***Fueled irradiations on-going at HFIR for ceramic matrix composite clad with UO_2 and UN based on MOX testing samples***
- ***ATR irradiations planned for unfueled and fueled experiments in FY-11***
- ***Start of Halden Reactor Project irradiation planning in FY-11***
- ***MIT PWR coolant experiment planning in FY-11***



SiC Cladding Schedule

- 2010 - selection of technology, second generation of nuclear fuel cladding design,
- irradiation design for Advanced Test Reactor, Oak Ridge HFIR irradiations of first generation fuel cladding
- 2011 - irradiation in Advanced Test Reactor, pre and post irradiation examination of second generation fuel cladding, testing advanced fuel forms to maximize benefits of advanced cladding, licensing basis development, planning for Halden reactor fuel failure experiments, planning for transient fuel testing at ATR and HFIR
- 2012 - fueled irradiation results of third generation cladding, transient testing of advance cladding, planning of fuel failure experiments at Halden reactor project - Norway
- 2013 - irradiation of advanced fuel form and advanced fuel cladding
- 2015 - demonstration of fuel assembly performance, fuel failure testing at Halden reactor, licensing basis defined, support for LWRS license extension decisions
- 2020 - demonstration of commercial lead test assembly, demonstration of high power density capability, licensing application for commercial use
- 2025 - demonstration of full core reload and power up-rated reload



Economics and Efficiency Improvement

	Phase I	Phase II	Phase III
	Building Confidence in Life Extension with Data and Tools	Enable Industry Decision to Invest and License for Life Extension	Applications of Scientific Solutions to Address Issues in Life Extension Decision Making and Continuing Technology Development
Alternative Cooling Technology	Preserve once-through technology and develop water conservation technology for wet cooling tower	Cost reduction and efficiency improvement for alternative and new cooling technology	Demonstration of alternative and new cooling technologies
Non-electric Applications	Technology and economics viability	Interface design	Pilot demonstration of process heat applications
Power Uprate	Collaborate with other pathways to enable 10 GWe extra capacity addition through power uprates, with a stretch goal of 20 GWe		

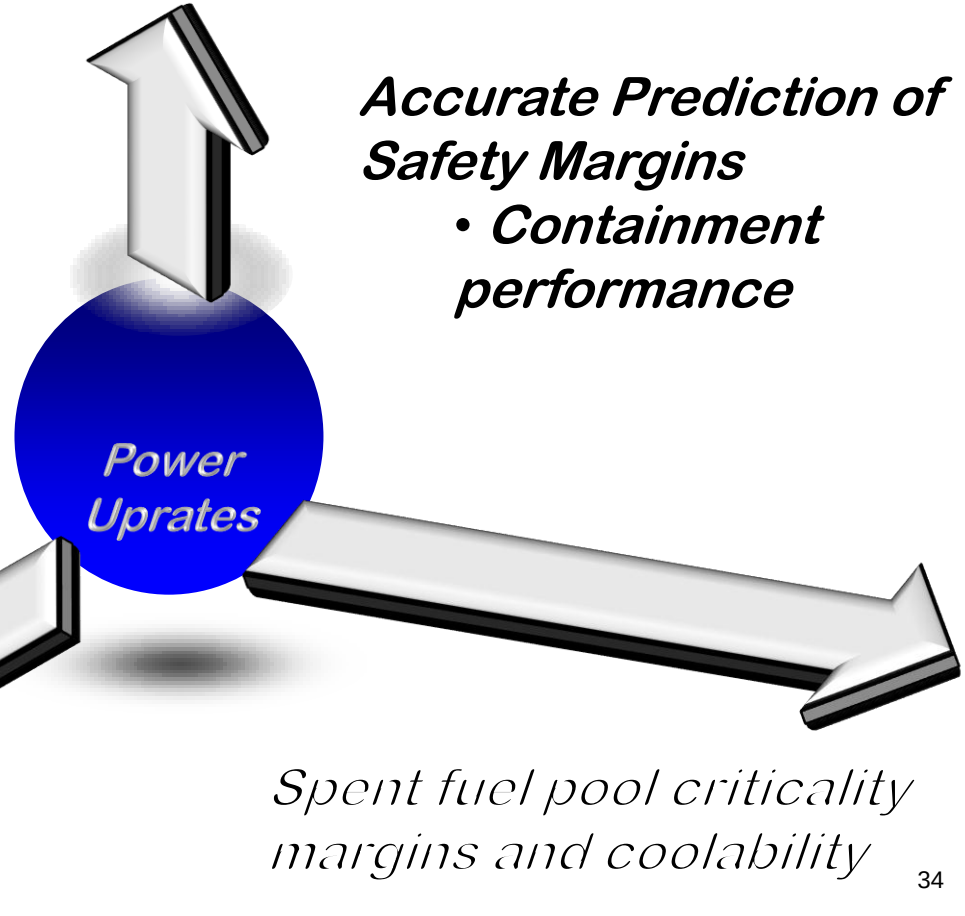
2010 2015 2020 2025 2030

Power Uprates

High-Power Density Cores
- ***DNB characterization***

- **Improved analysis methodology**
- ***Mitigation Strategy: advanced component designs (dryers and separator)***

Accurate Prediction of Safety Margins
- ***Containment performance***



Address Adverse Flow Effects

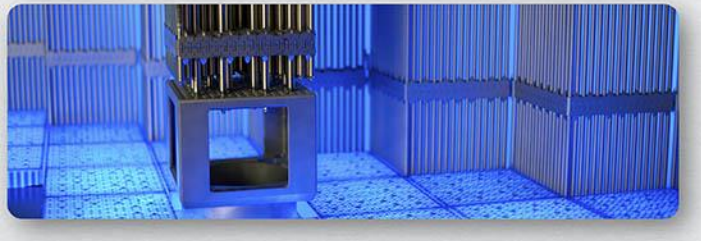
Spent fuel pool criticality margins and coolability

CASL-U-2011-0072-000-R

LWRS

Light Water Reactor Sustainability

CASL-U-2011-0072-000-R



ELECTRIC POWER RESEARCH INSTITUTE

Advanced LWR Fuels

Kurt Edsinger

Director, Fuel & Chemistry

CASL Round Table

Raleigh, NC

CASL-U-2011-0072-000-R

Agenda

- Background
- Some Early Research
- Whitepaper / Roadmap on Breakthrough Fuel Designs
- CASL Connection

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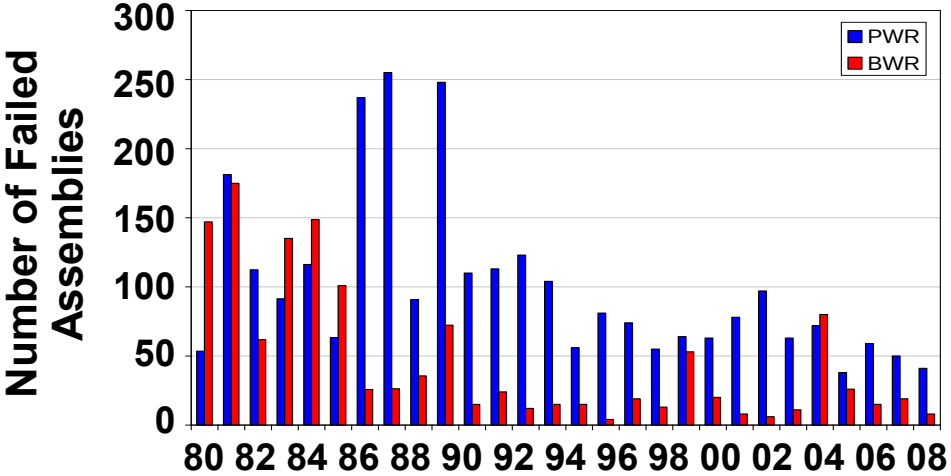
Industry Still Focused on Zero Failures

INPO Board Sets Goal

"Zero by 2010"

"Take high impact actions to significantly improve fuel cladding performance in support of Industry 2010 goals"



2006 2007 2008 2009 2010 2011

CNOs pledge support

INPO review visits begin

EPRI Technical Guidelines

Zero Failures

"Driving to Zero"

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What Changed?

- Funding from EPRI's LTO program on small SiC cladding effort
- Funding from EPRI's Technology Innovation (TI) program on SiC channels
- General sense of broadening mission (?)
- Roadmaps…

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EPRI Effort in SiC Development

EPRI became engaged in 2008

- Sponsored research in
  - End-plug seal
  - Fuel rod design / performance assessment
  - Cost-benefit evaluations
  - Structural applications

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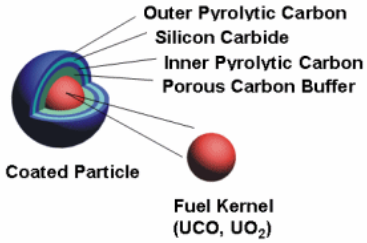
Silicon Carbide

- Attractive for many applicatons
  - High temperature
    - Turbines and combustors
  - Armor
  - Nuclear
    - Tristructural Isotropic (TRISO) Fuel
    - Nuclear fusion



- Development for use as a conventional fuel clad material
  - Initiated between Ceramic Tubular Product (CTP) and Westinghouse
  - Triplex cladding demonstrated good in-core performance

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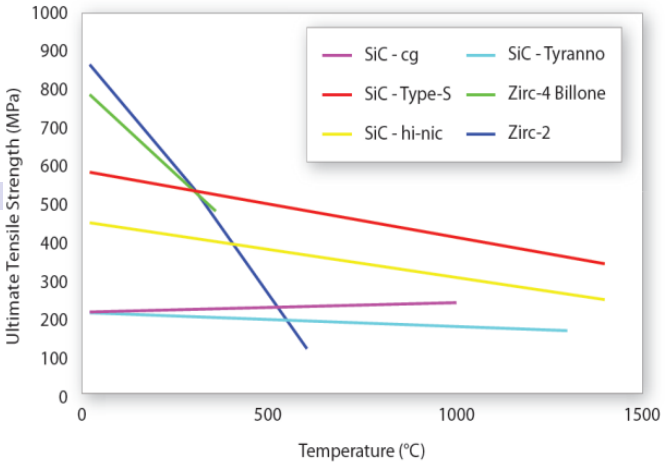
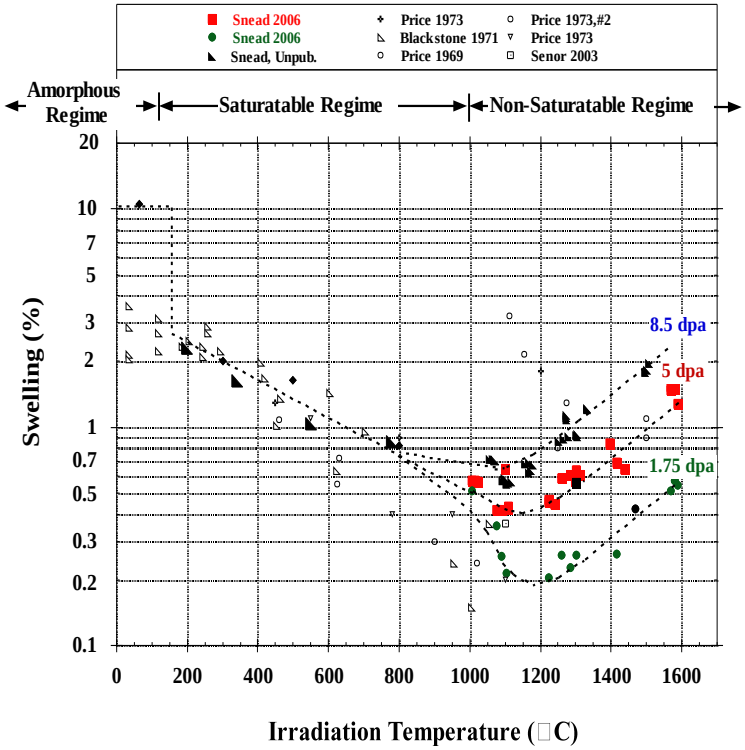
Silicon Carbide (cont'd)

- Used in the re-crystallized form
  - Extrusion, CVD, CVI, PIP
- No significant degradation upon exposure to neutron irradiation at temperatures of technological interest (150-1200°C)
  - Amorphization below 150°C
  - Irradiation induced volumetric swelling
- Test shows excellent wear resistance





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End Seal Development

"Silicon Carbide doesn't melt"

- Multilateral program with DOE, Westinghouse, CTP, MIT and EPRI
  - Initial (borosilicate) sealing formula failed in MIT test reactor
  - New seal concepts screened in autoclave; surviving samples tested in MIT test reactor
- One (PNNL) diffusion bond sample (Ti-SiC) survived, all others debonded
  - Differential volumetric expansion one possible cause for failure; DOE program to evaluate irradiation properties of bonding phase
- In need of a better approach…
  - Edison Welding Institute (EWI)?

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Fuel Rod Design / Performance

- Incorporated SiC properties modules into Falcon
- Analyzed peak power rod over typical 3 cycles in a PWR
  - 4 mil and 3 mil radial pellet-clad gaps with 10% central hole in UO_2
- Compared Falcon results with MIT's FRAPCON results for both Zr-4 and SiC clads
- Provided critical perspectives on the SiC analysis results:
  - Pellet-clad gap closure and clad hoop stress
  - Clad stress-strain behavior representing the clad as monolithic vs. multi-layer composite

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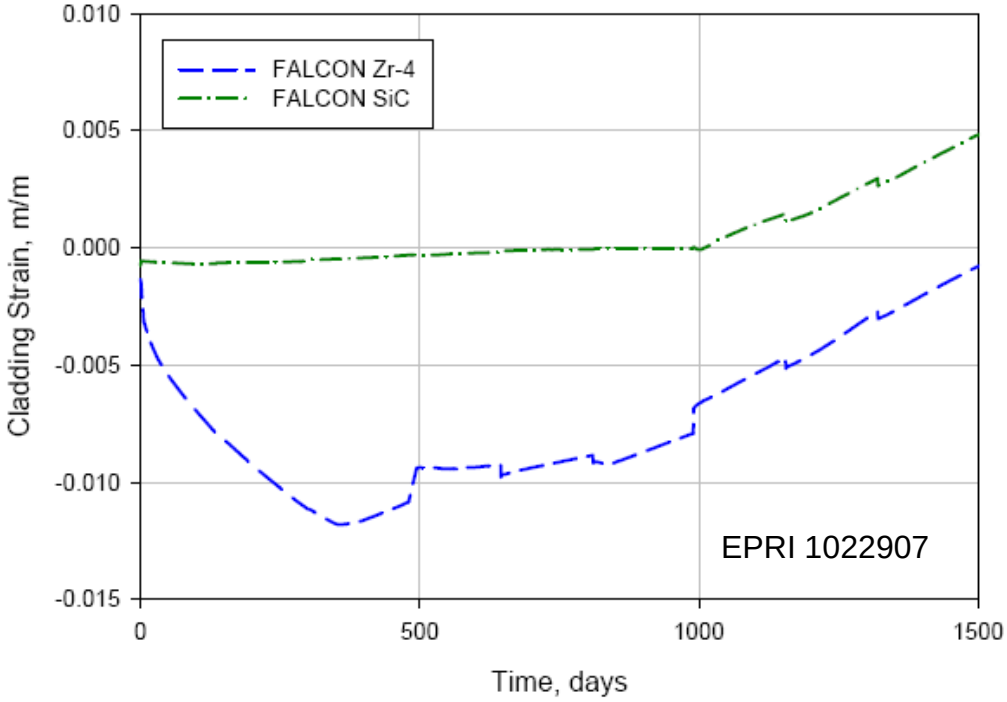
Fuel Rod Design / Performance

Annular pellet needed to control fuel center line temperature

- 4-mil pellet-clad gap closes in ~1000 days (~2 PWR cycles)
- Monolith SiC survives additional 150 days of exposure before failing:
  - Maximum burn-up achievable ~ 69 GWd/t (lower than current Zirlo license burn-up limit)
- Multi-layer SiC clad may be able to sustain much higher hoop stress
  - Burn-up ~ 80 GWd/t (and even beyond) possible, but needs to be demonstrated



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Cost-Benefit Evaluation

- Evaluation being conducted in 3 phases
  - Define a feasible fuel rod design
  - Evaluate core designs for longer cycle or higher energy output
  - Cost-benefit
- Core design for 62 and 100 GWd/MTU peak rod burn-up
  - ~50 and ~80 GWd/MTU batch average
- Two strategies
  - Longer cycle length at current power density
  - Same cycle length at higher power

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Cost-Benefit Evaluation

18 Month Cycles (non-uprated)

Clad	Batch Size	Ave Enrichment (w/o)	Relative U235 Mass per reload batch	Discharge Burnup (MWD/KgU)	Batch Fab Cost (M$)	Batch Enriched U Cost (M$)	Batch Total Fuel Cost (M$)	Level Fuel Cost ($/MWh)
Zirc	84	4.52	1.0	44.8	7.89	91.2	117.3	8.79
SiC	84	4.77	0.95	49.6	7.89	87.4	113.5	8.50
SiC	64	5.71	0.87	65.2	6.01	82.3	105.6	7.91
SiC	52	6.96	0.86	80.1	4.88	84.1	105.7	7.91

EPRI 1022908

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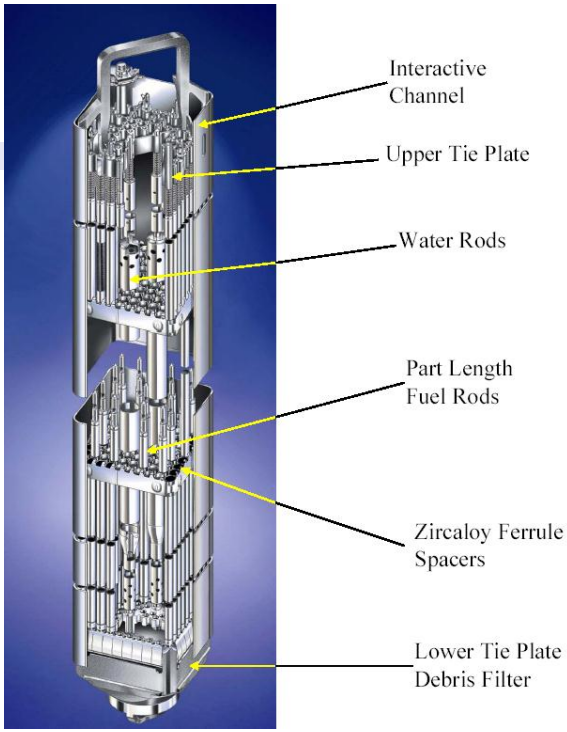
SiC for Structural Applications

- Existing zirconium based BWR channels are susceptible to channel bow
  - Flux gradient
  - Shadow corrosion
- SiC is dimensionally stable to very high fluences after initial volumetric swelling
- Much simplified requirements compared to clad
  - Could provide information for cladding development
- Joint project with the US DOE Idaho National Laboratories (INL)



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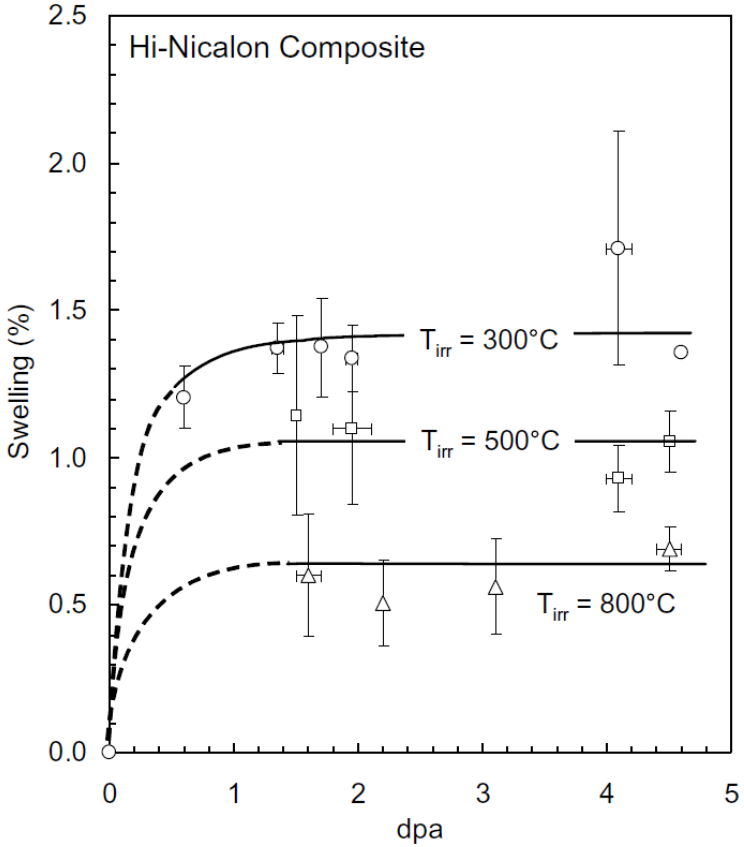
SiC for Structural Applications (cont'd)

Major issues

- Initial irradiation induced volumetric swelling
  - ~1.5% by volume
  - Saturates after ~6 months of irradiation
- Ability of components to resist fragmentation



G. Newsome et al., J. of Nuc. Mat., 371 (2007) 76-90

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Breakthrough Fuel Designs

- Identify key technical barriers in properties of current fuel/cladding materials (62 GWd/MT rod average burnup limit)
- Consider fuel with revolutionary potential for
  - Power uprate
  - Higher discharge burnup
  - Improved safety margins
- Candidate fuel designs and material should have the potential of being implemented at LWRs in ~10 years
  - Large existing technical database / strong existing R&D activity
  - High fuel reliability
  - Significant economic benefits

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Key Barriers

- Cladding corrosion, hydriding and irradiation-induced embrittlement
  - Surpass evolutionary changes
- Low fuel thermal conductivity
  - Limits power maneuvering flexibility and power uprate
- Total fuel rod surface area
  - Limits power uprate (concerns of DNB margin and boiling related AOA/CIPS, crud/corrosion)
- 5% enrichment limit
  - Limits average batch discharge burnup (particularly long cycle length cores) and fuel burnup extension
- LOCA criteria on cladding oxidation/hydriding and hydrogen generation

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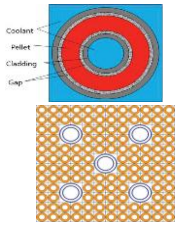
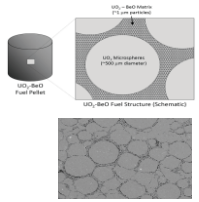
Technologies for Increasing Margins

New Fuel Technology	Main Function	Potential Benefits	Status	Main Concerns
>5% Enriched Fuel	Loading more fissible U-235 in fuel rods (5-7%)	Increase dicharge burnup, reduce waste volume and improve fuel economics	-Past studies suggest potential "cost saving" with 70 GWd/MTU -Utilities industry interested generally, but afraid… -Japanese industry proposing collaboration	Most regulatory
Dual Cooled Fuel 	Increase total fuel surface area >30%	May achieve 20% power uprate while: - Reducing fuel centerline temperature by 40% - Reducing surface heat flux and increasing DNB margin	- Conceptual design (for 50% uprate) by MIT/Westinghouse - KAERI performed detailed designs for 20% uprate - Fabrication and 1st irradiation of rods completed - Additional testing and irradiation planned	Fabricability, reliaibility
SiC Clad	Cladding resistant to steam interaction and melting	Largely improves LOCA safety margins in core melting down and hydrogen bubble buildup; allows for long term core residence	-LTO funding for feasibility study -DOE funded research last 4 years -Supporting data from other high temperature reactor programs	Fabricability, reliability
BeO Additive Fuel 	Use networked BeO to conduct heat in fuel to rod surface	May allow power rate and improve fuel rod T/M properties	-Conceptual design by IBC Advanced Alloys -Some lab fabrication studies at universities	Replacing too much uranium, reliability
Metal Fuel	Higher uranium loading for the same volume	Will improve fuel thermal conductivity and reduce waste volume	IBC Proposal	Volatile reaction with coolant if exposed
Hydride Resistant Zr-Clad	Optimize alloy chemistry and process for corrosion and hydriding resistance	Increase corrosion and hydriding margins for High Burnup Fuel (>62 GWd/MTU rod avg.)	-PWR alloys (M5, Zilo) need demonstration -BWR Zr-2 alloy needs improvement for >62 GWd/MTU applications	None

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Utility Perspective

- "Safer Fuel" should be the priority
  - SiC is only one example

- >5% enrichment challenges relate to infrastructure and licensing
  - Japanese industry funded extensive IAE study on barriers to increasing enrichment above 5%
  - Potential to improve fuel economics and waste volume reduction
  - Essentially required for many advanced fuel designs

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Utility Perspective (cont'd)

- Dual Cooled Fuel:
  - Active area of development with KAERI conducting design, fabrication, and testing (co-sponsored by KHNP)
- BeO Additive and Metal Fuel:
  - Some small-scale efforts underway
- Hydride Resistant Zr-clad:
  - Gap in research on "revolutionary" concepts

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Leveraging CASL

- New fuel design / geometry
- Power uprate (DNB margin, AOA/CIPS, crud/corrosion)
- Cladding corrosion, hydriding and irradiation-induced embrittlement
- LOCA criteria on cladding oxidation/hydriding and hydrogen generation
- Fuel thermal conductivity
- 5% enrichment limit

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Together…Shaping the Future of Electricity

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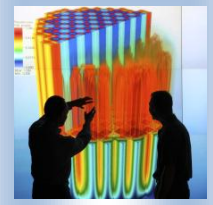
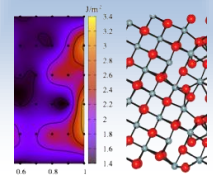




Virtual Reactor Integration Focus Area

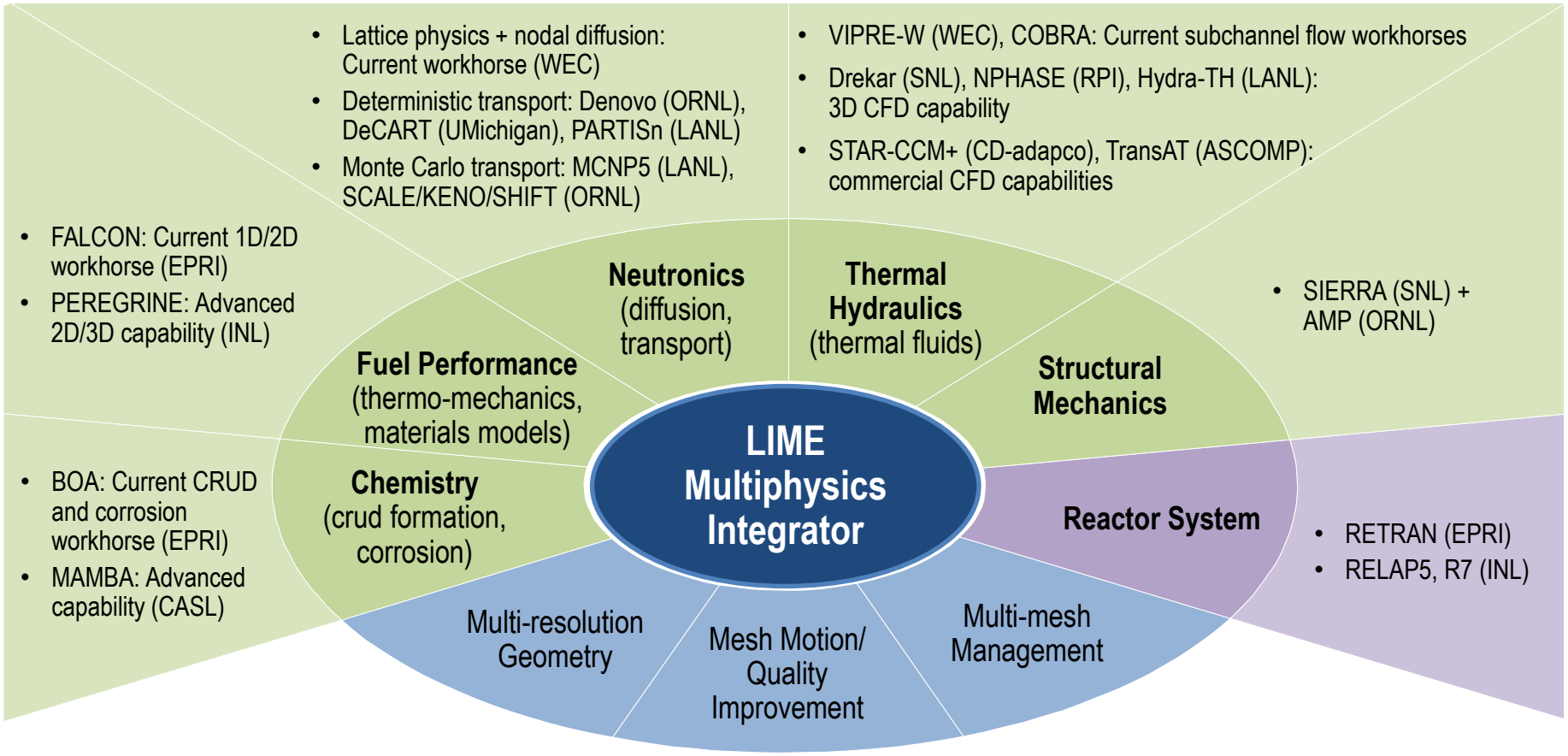
John Turner (ORNL), Lead
Randy Summers (SNL), Deputy Lead

CASL
Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL-U-2011-0072-000-R

The VERA Physics Simulation Suite combines advanced capabilities with mature, validated, and widely-used codes.



What's the "roadmap" for VERA development?

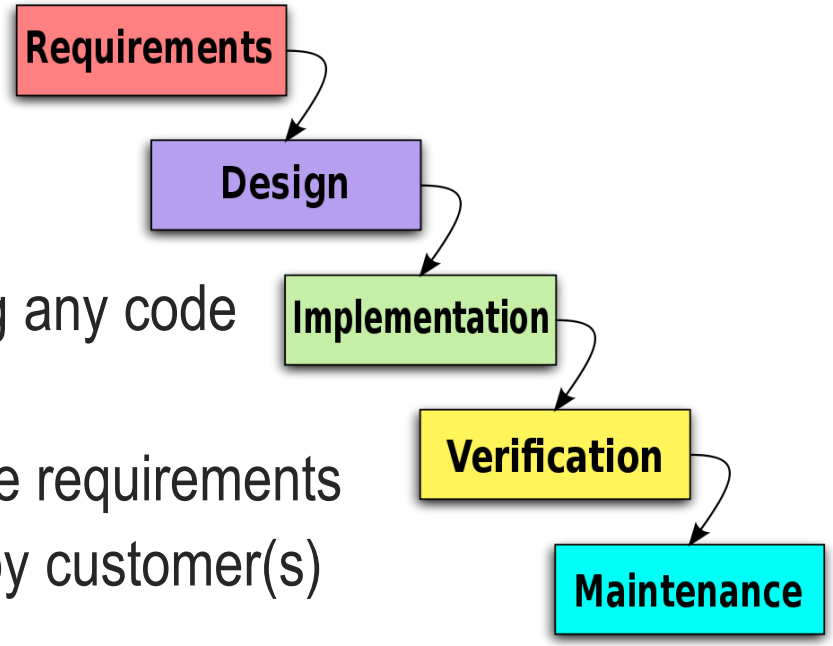
Writing software is easy

- "Writing songs is easy. Writing great songs is hard."
  - Bono (? couldn't verify)
  - also "Look, I'm sick of Bono and I AM Bono."
- Writing software is easy. Writing great software is hard.
  - single author, team, geographically-dispersed team
  - single user (self), targeted users, broad user community
  - research/exploration, prototype, production, real-time operation, regulatory environment
  - serial, shared-memory parallel, distributed-memory parallel, large-scale parallel, heterogeneous

Goal for CASL product(s) is extremely ambitious

Challenge-problem driven development (1 of 3)

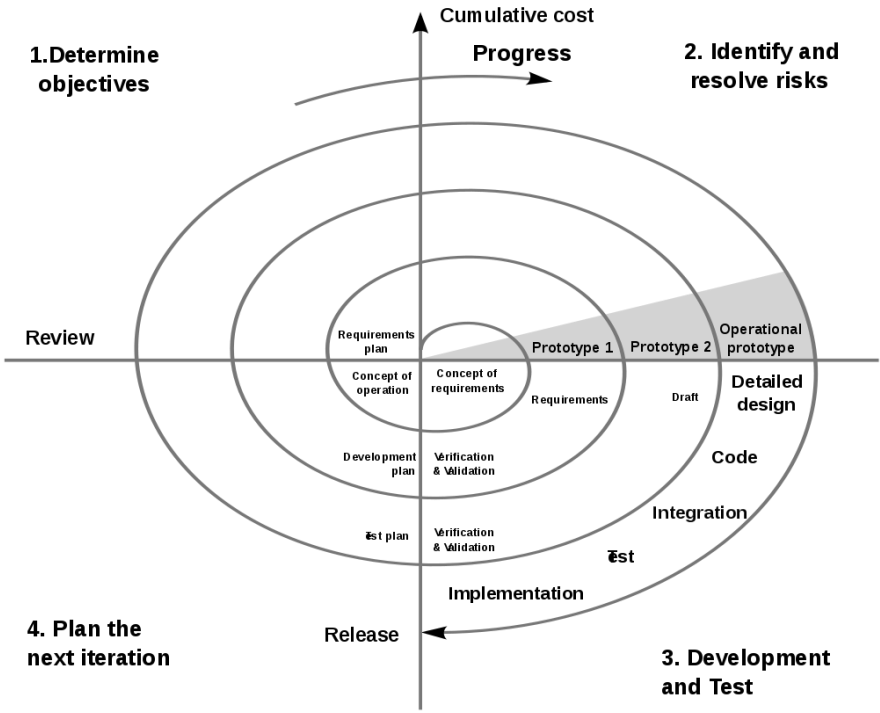
- one end of the software development spectrum…
  - imagine all ways the end product will be used
    - often becomes “all ways the product might ever be used”
  - fully design entire system before writing any code
  - implement the design
  - verify that the implementation meets the requirements
  - deliver the product to the grateful, happy customer(s)



Often called the “waterfall” model.

Challenge-problem driven development (2 of 3)

- at the other end of the spectrum is agile / lean / iterative development…
  - meet with customer
    - determine needs and priorities
  - implement only what is absolutely necessary, in order of priority, delivering working product frequently
  - product evolves



Agile methods fix Time (fixed iterations, fixed releases) and Effort (fixed team size) and vary Scope (functionality) based on iterative feedback.

Challenge-problem driven development (3 of 3)

- CASL is following a challenge-problem driven plan
  - use specific relevant problems to drive development of broadly-applicable capability
- could be viewed as large-scale iterative development
- more appropriate for program with significant R&D component(s)
- feedback from customers / users on priorities is critical

What is the VERA Roadmap?

- VRI should not define the VERA roadmap – it requires CASL-wide participation
  - VRI has put in place a solid software process, and is implementing a solid build / test infrastructure
  - VRI is defining the VERA architecture
    - including coupling, programming model, and platform strategies
  - AMA sets priorities
  - MPO, RTM and THM set the pace for delivery of new capability
  - VUQ informs the entire process, assesses progress

However, we had to start somewhere…

VERA 0.5 (12/2010)

Baseline	Initial Advanced
ANC9	Star-CCM+
VIPRE-W	DeCART

LIME, Trilinos (NOX, ML, etc.), DAKOTA

VERA 1.0 (03/2011)

Baseline	Initial Advanced	Advanced
BOA		
ANC9	Star-CCM+	
VIPRE-W	DeCART	Denovo

LIME, Trilinos (NOX, ML, etc.), DAKOTA

RELAP5	Geometry / Mesh / Data Transfer

VERA 1.5 (09/2011)

Baseline	Initial Advanced	Advanced
BOA		Drekar
ANC9	Star-CCM+	SCALE
VIPRE-W	DeCART	Denovo

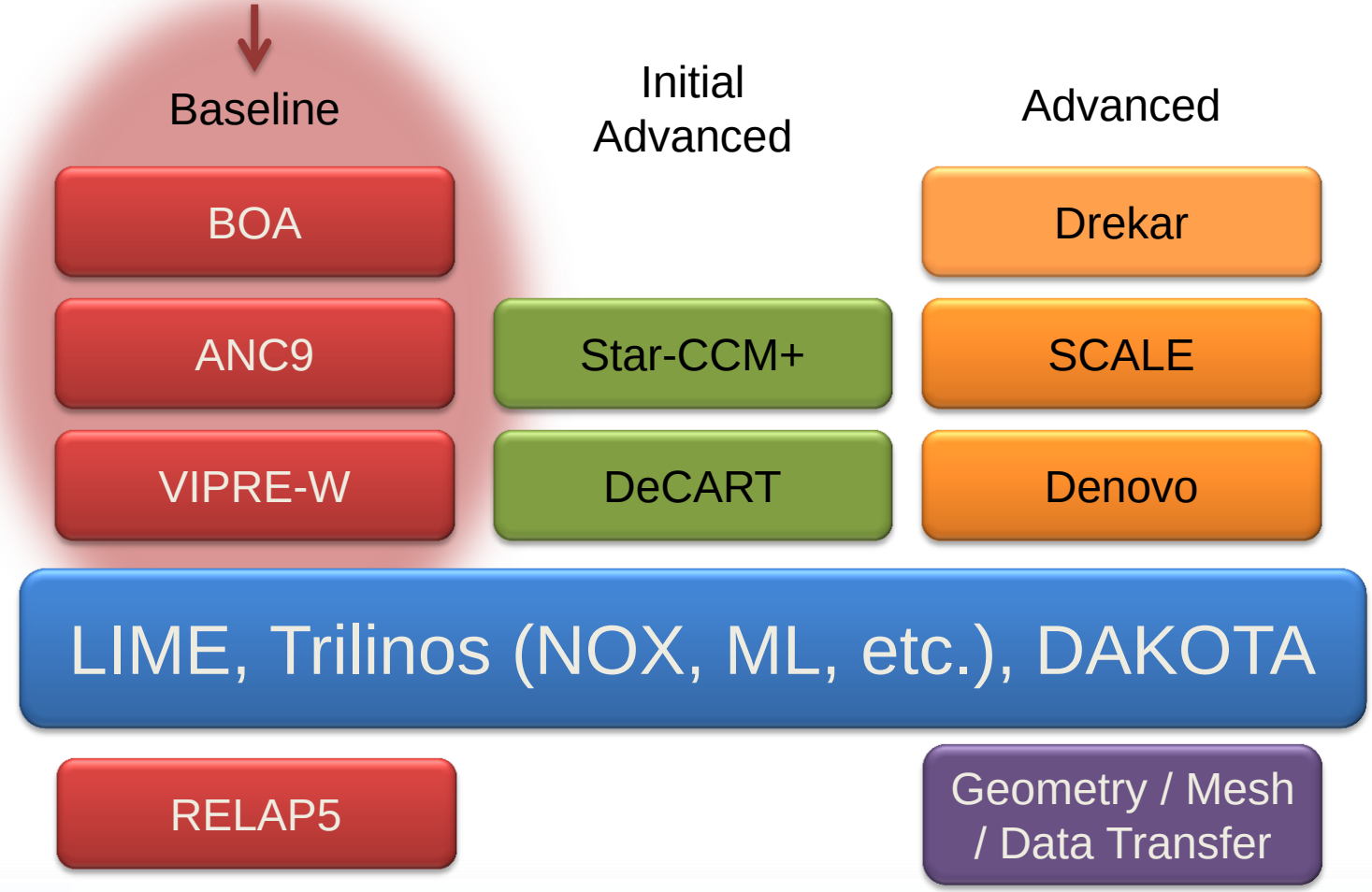
LIME, Trilinos (NOX, ML, etc.), DAKOTA

RELAP5

Geometry / Mesh / Data Transfer

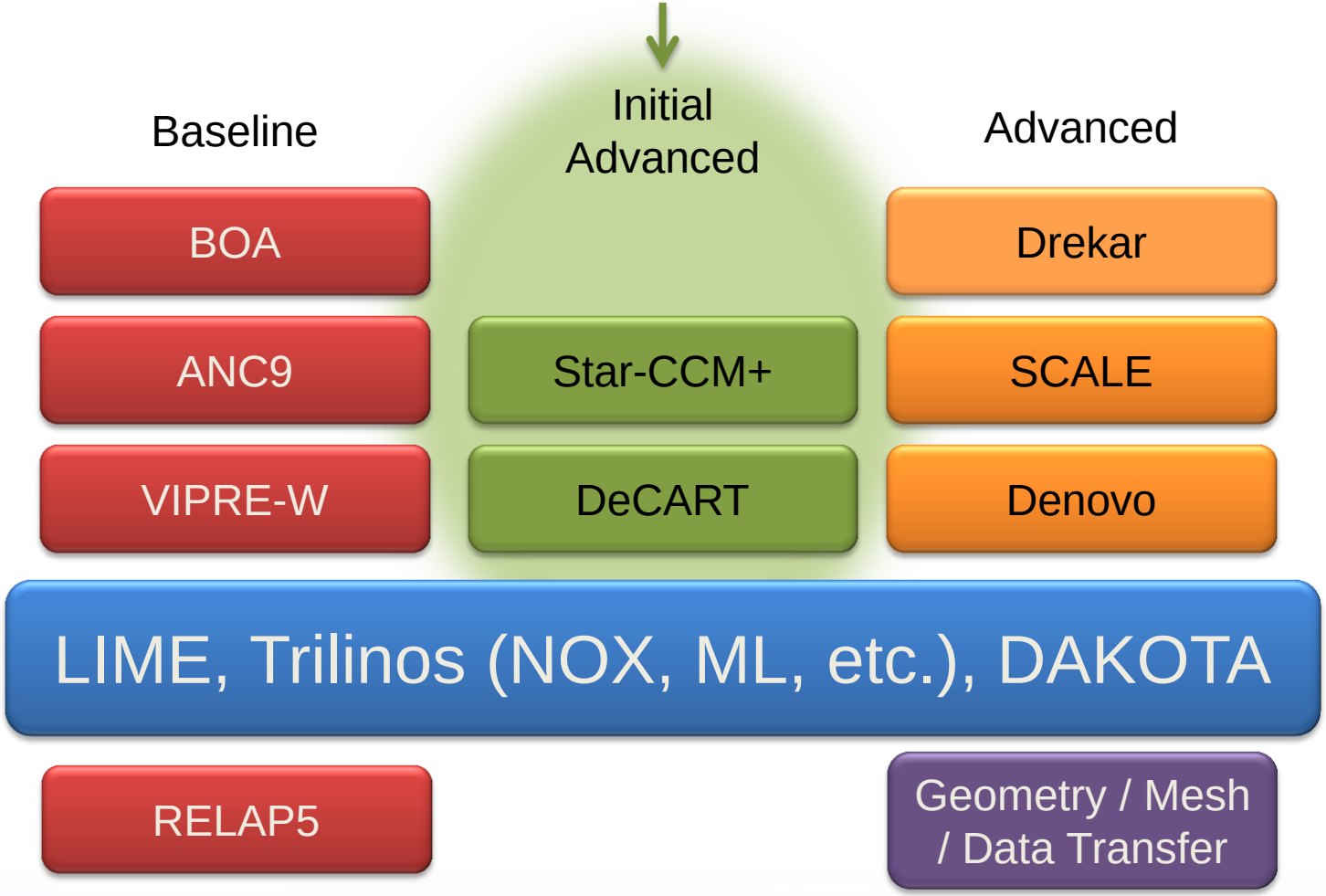
VERA 1.5 (09/2011)

Presentation 1:
Rod Schmidt & Jeff Secker



VERA 1.5 (09/2011)

Presentation 2:
Ben Collins



VERA 1.5 (09/2011)

Presentation 3:
Jay Billings & Greg Davidson

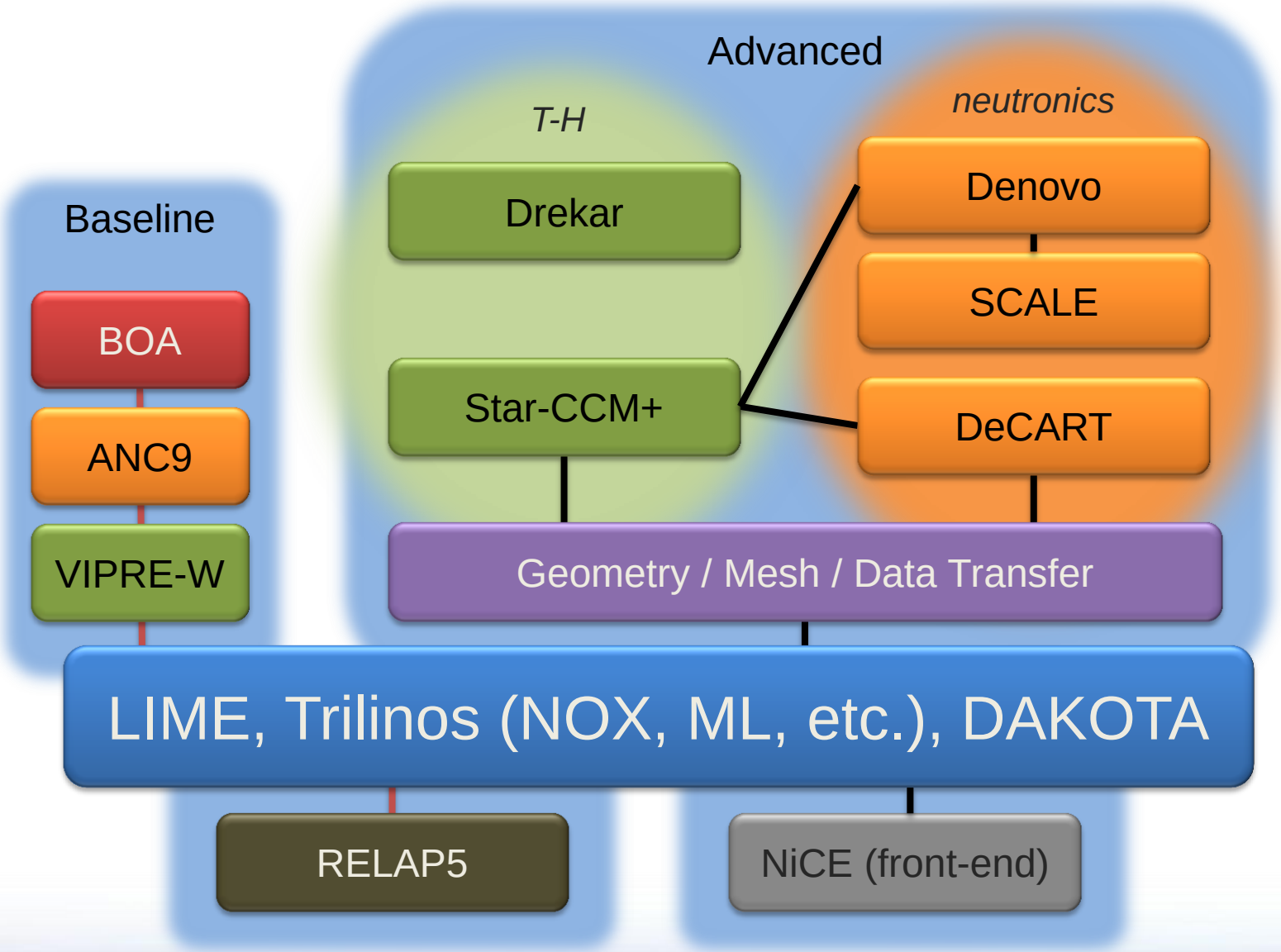
Baseline	Initial Advanced	Advanced
BOA		Drekar
ANC9	Star-CCM+	SCALE
VIPRE-W	DeCART	Denovo

LIME, Trilinos (NOX, ML, etc.), DAKOTA

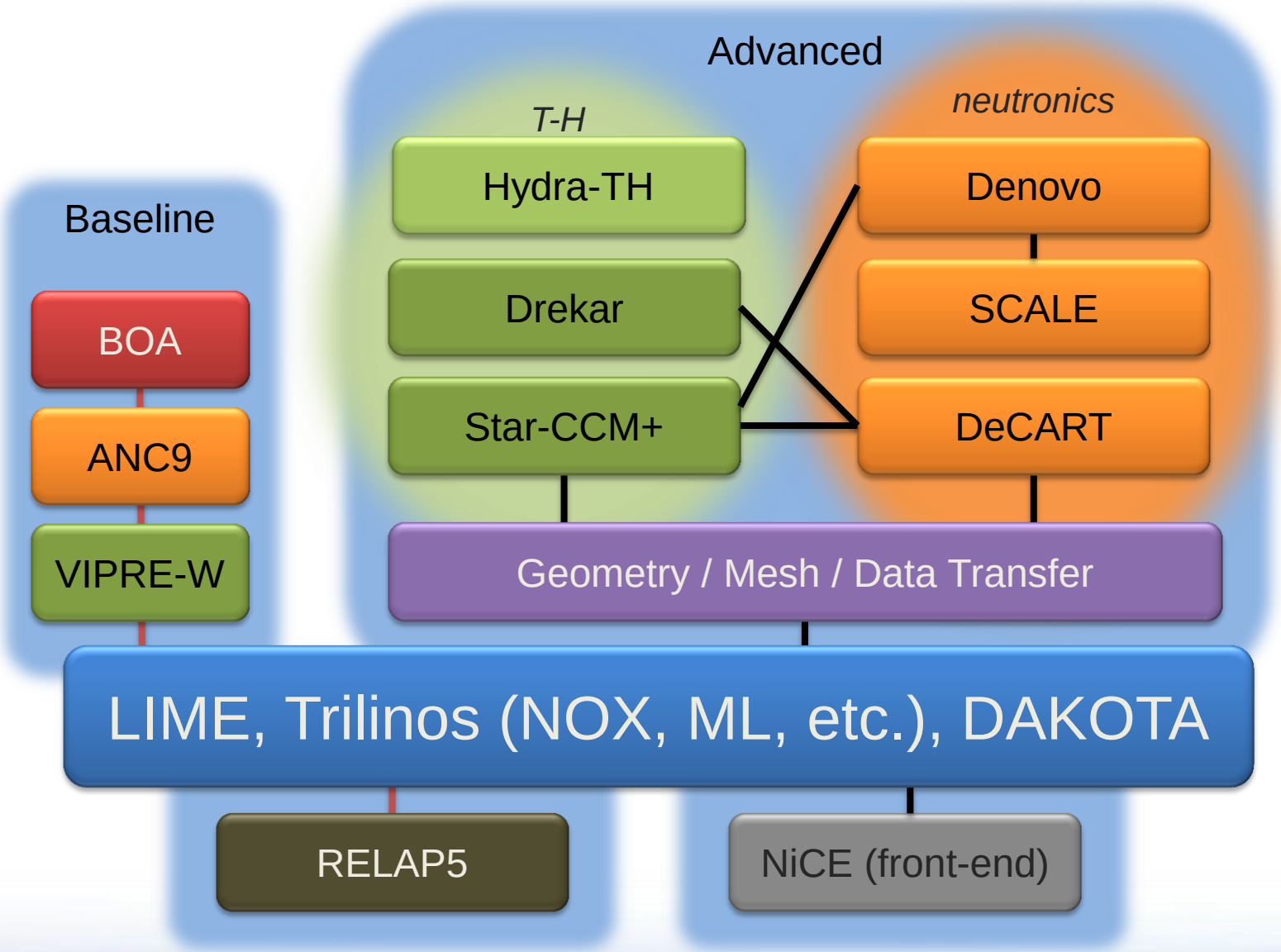
RELAP5

Geometry / Mesh / Data Transfer

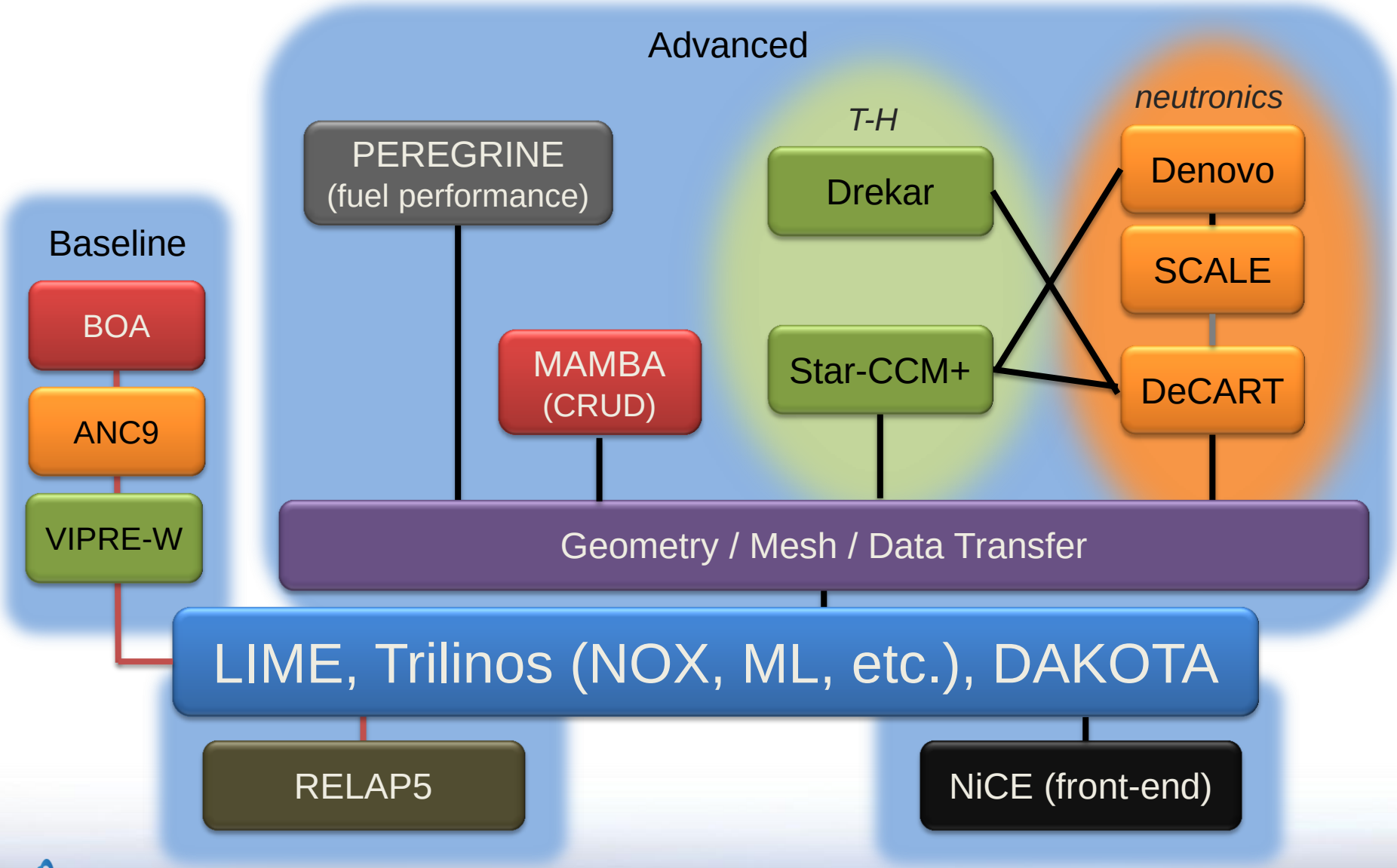
VERA 1.5 (09/2011)



VERA 1.x (12/2011)



VERA 2.0 (03/2012)



Based on Y1 experience, VRI will evolve LIME in Y2 while adding new components and improving coupling

Supplemental

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Sid Yip
Brian Wirth

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Validation & Uncertainty Quantification
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AMA
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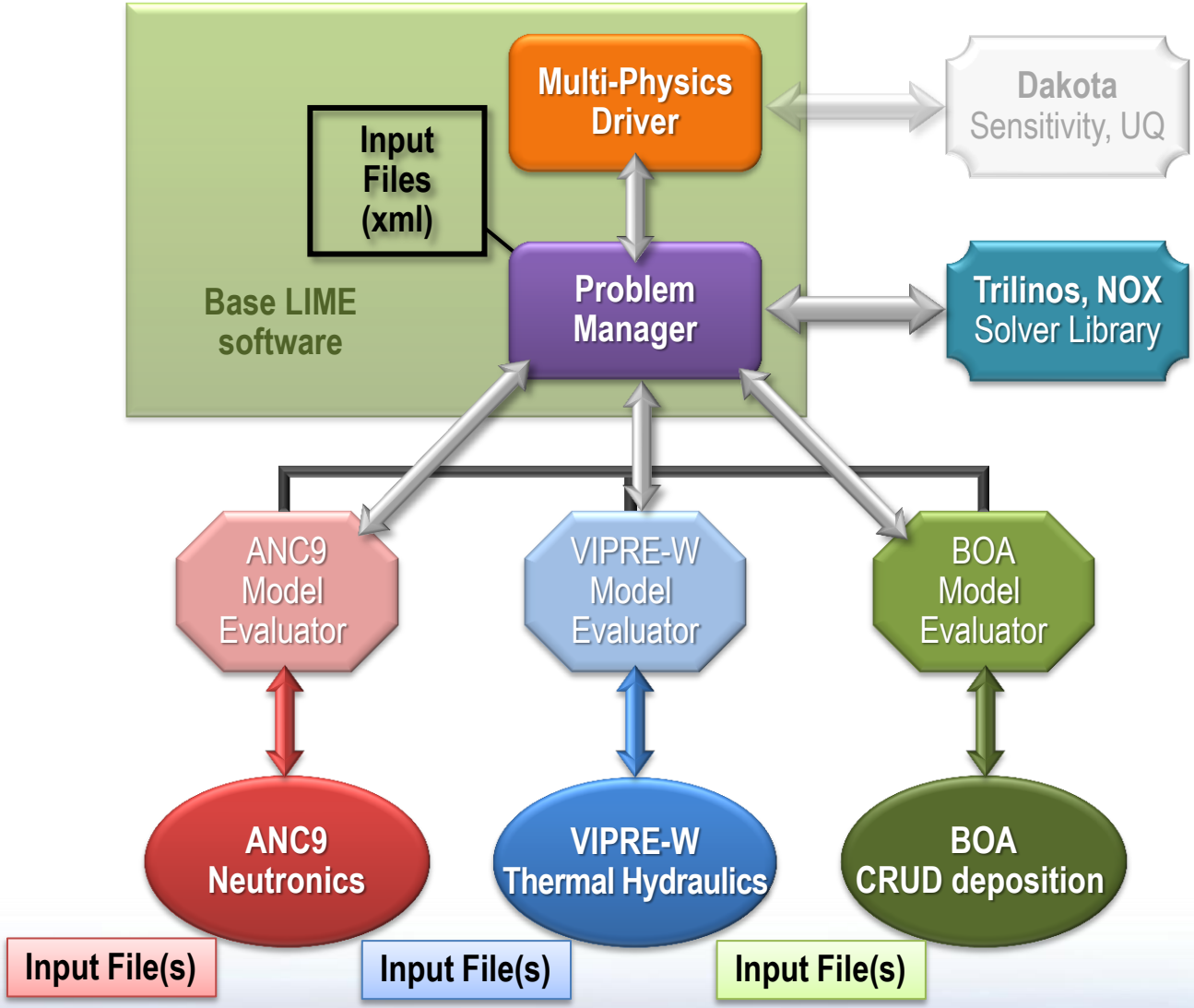
Jess Gehin
Zeses Karoutas
Stephen Hess

RTM
Radiation Transport Methods
Bill Martin
John Wagner

THM
Thermal Hydraulics Methods
Rob Lowrie
Rich Martineau

VRI
Virtual Reactor Integration
John Turner
Randy Summers

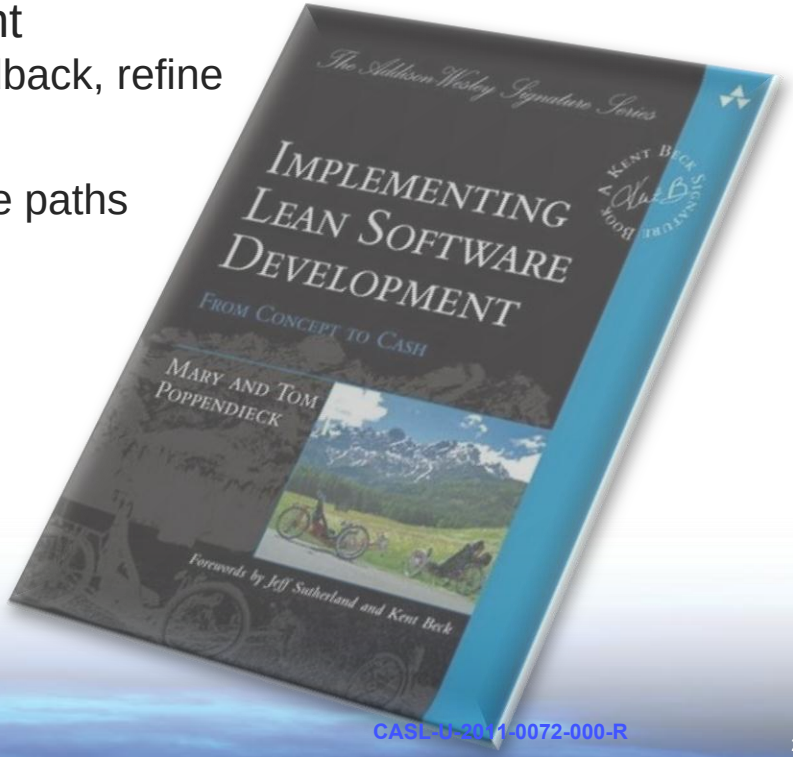
LIME-based coupling diagram for ANC-VIPRE-BOA



Lean Software Development

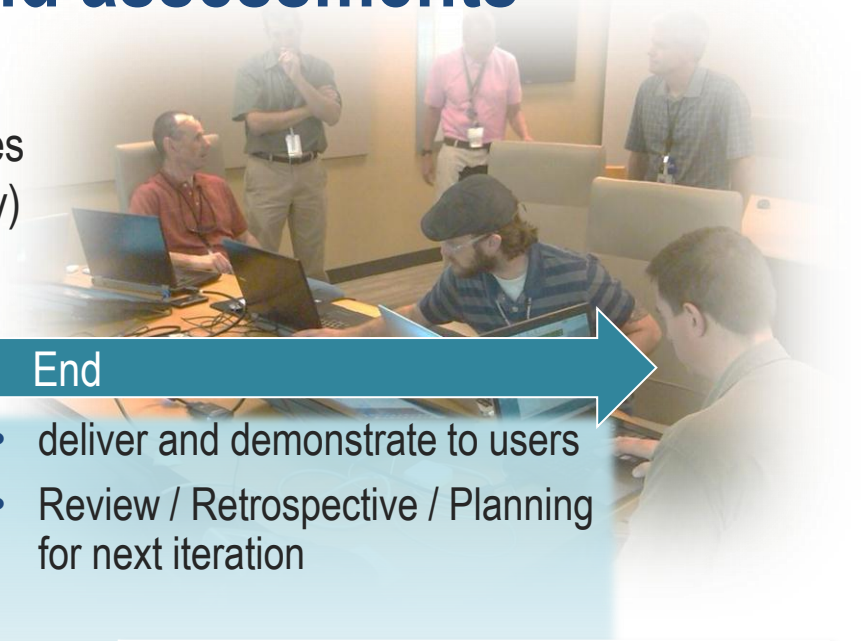
- Motivation for Lean Software Methods:
  - Lean Manufacturing (e.g. Toyota Production System)
- Seven Principles of Lean:

1. eliminate waste
   - for software, waste is partially completed work, churn due to changing requirements, extra features, etc.
2. build quality in
   - test-driven development, continuous integration and automated testing
3. amplify learning through iterative development
   - sketch design, prototype, assess, customer feedback, refine
4. defer commitment
   - delay irreversible decisions and/or follow multiple paths
5. deliver fast
   - short release cycles, limit work in progress
6. respect people
   - team should design and refine processes
   - no single “Best Way”
7. optimize the whole



CASL is using a modified Scrum-ban process, with semi-annual major releases and assessments

- based on methodologies being used by partners
- combine attributes of Scrum and Kanban methodologies
- customized for CASL and refined as needed (iteratively)



Start

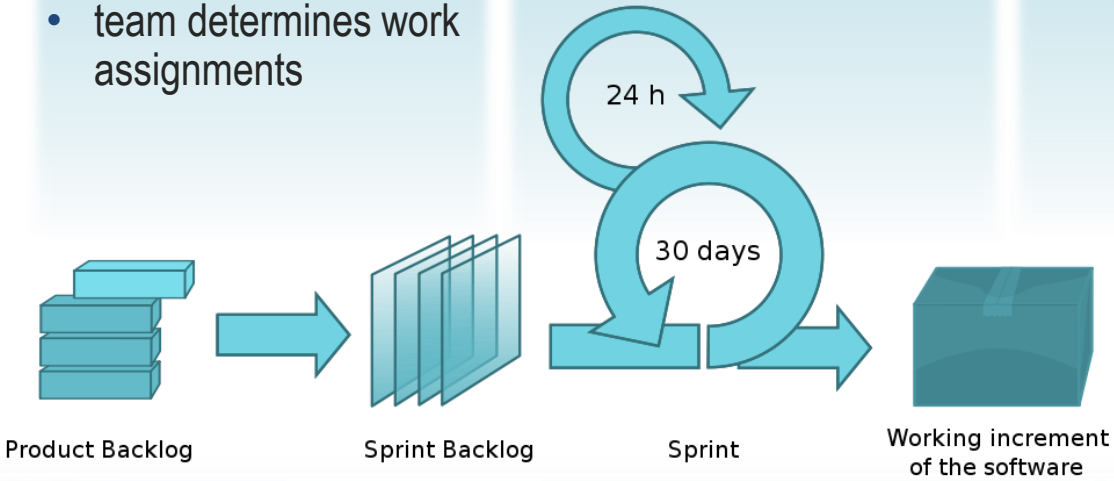
- users prioritize goals for next 4-week iteration
- team determines work assignments

Execute

- two 30-minute standup meetings each week

End

- deliver and demonstrate to users
- Review / Retrospective / Planning for next iteration



Scrum: http://en.wikipedia.org/wiki/Scrum_%28development%29

Desirable attributes

- emphasis on collaboration and adaptability
- constant communication / interaction
  - both within team and with user community
- accommodates changing requirements & unpredictability

Agility + Formality

Development of a LIME-based ANC-VIPRE-BOA multi-physics simulation capability in VERA

J. Secker, P. Hilton, B. Coulter, D. Paterline, R. Milanova, C. Beard, K. Beatty, Y. Sung (Westinghouse)

K. Belcourt, R. Schmidt (SNL)

C. Baker (ORNL)

J. Westacott (CSA)

Presented by: Rod Schmidt (SNL)

Jeff Secker (Westinghouse)

CASL-U-2011-0072-000-R

This is a New Coupled Code Application

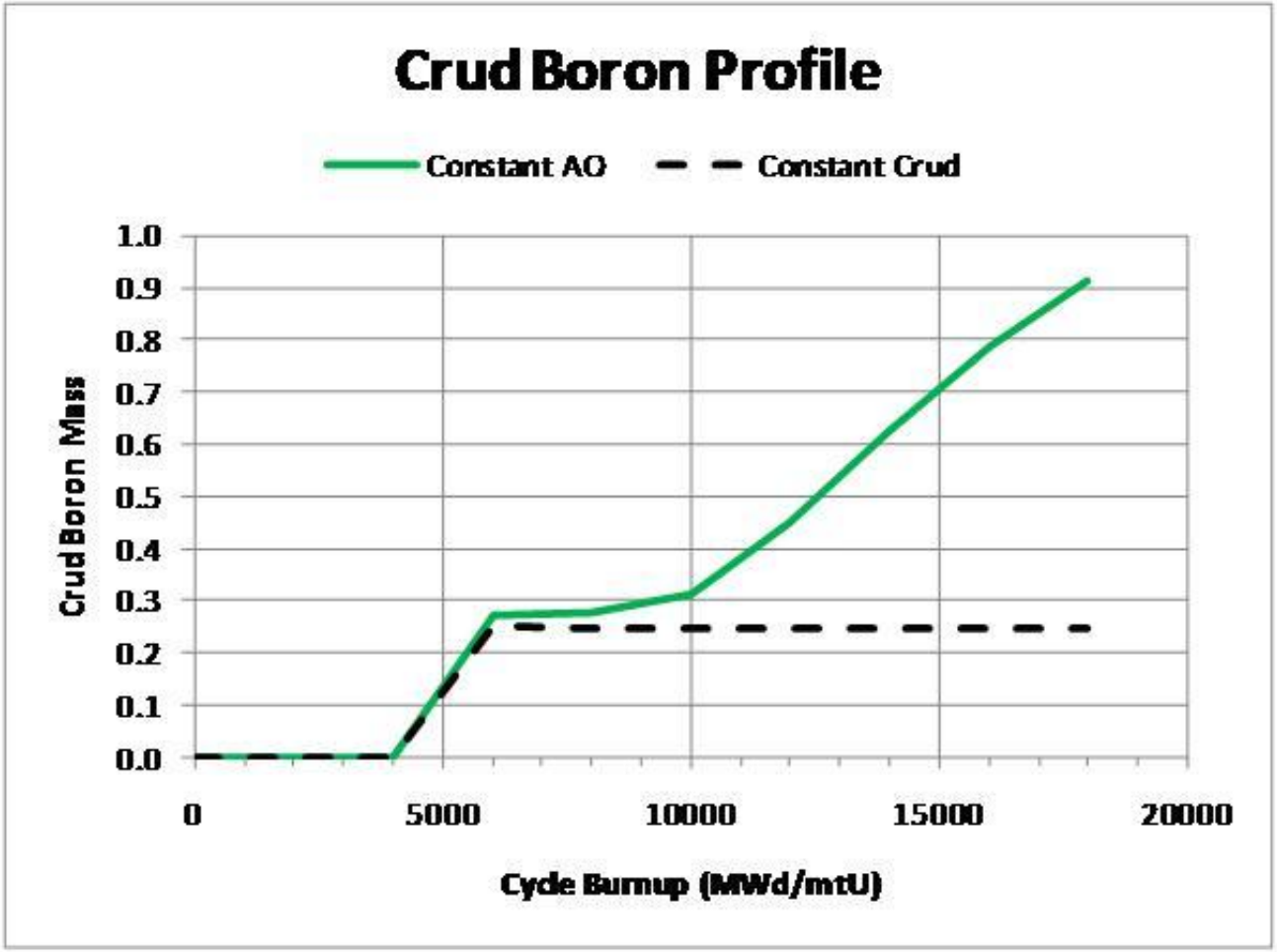
- Westinghouse previously coupled ANC and VIPRE-W with RETRAN (system model) for accident analysis - RAVE
  - Transients are short duration - do not require fuel depletion
- This CASL application utilizes the coupling for all ANC applications including core depletion
  - Requires some additional software updates
- Coupling with BOA is also a new, first time application

ANC9/VIPRE-W/BOA

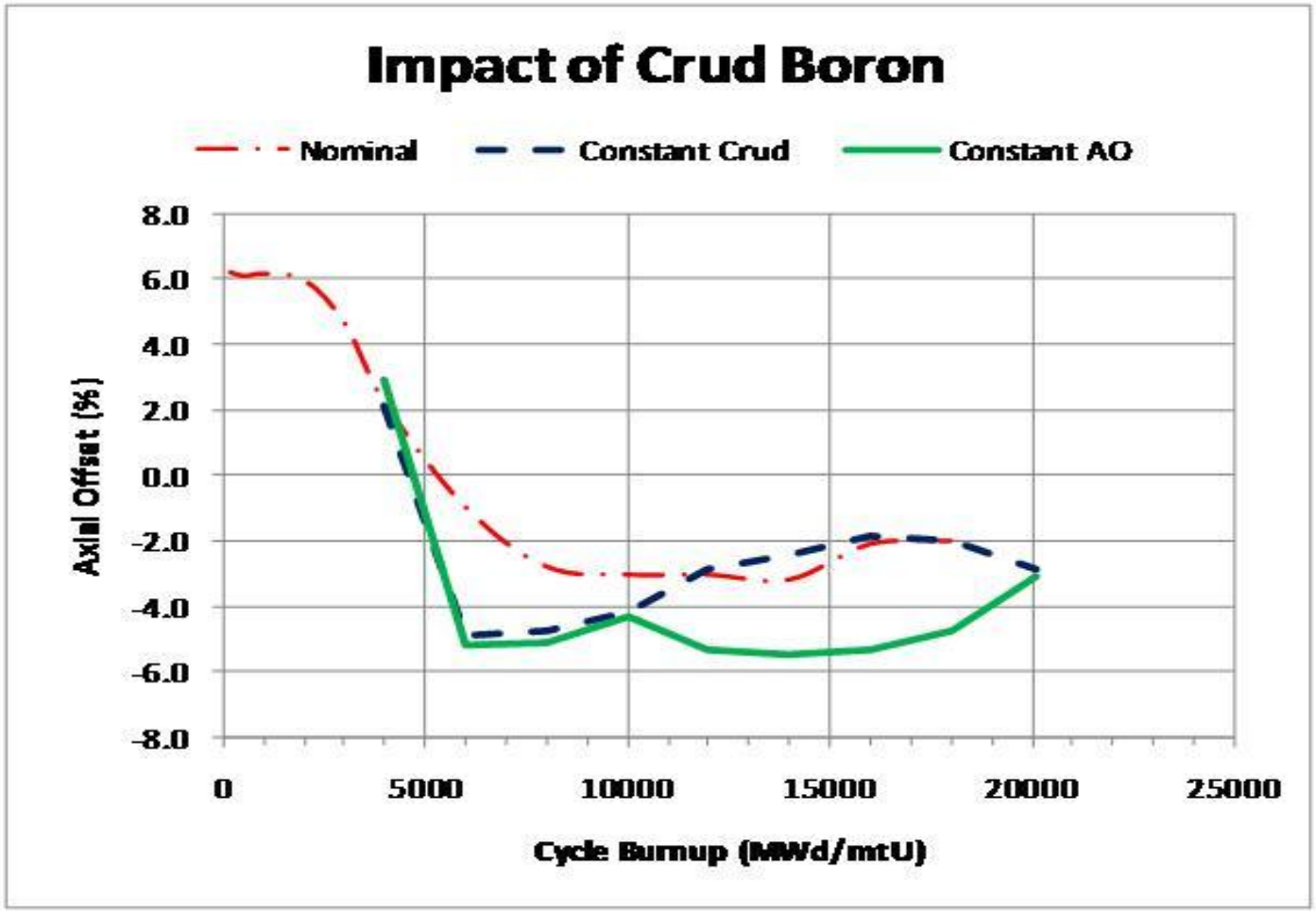
Background: Boron/Crud Effect Evaluation (i.e. Is it important?)

- Case description
  - Case 1: Depletion at full power without crud deposition (standard calculation)
  - Case 2: Assumed a boron distribution to slightly reduce the core axial offset at 6000 MWd/MTU and the boron distribution held uniform for the remainder of the cycle
  - Case 3: Started as the second case, but varied the amount of boron to keep the core-wise axial offset at a constant value
- Effect of boron mass is evaluated

Boron/Crud Effect Evaluation



Boron/Crud Effect Evaluation



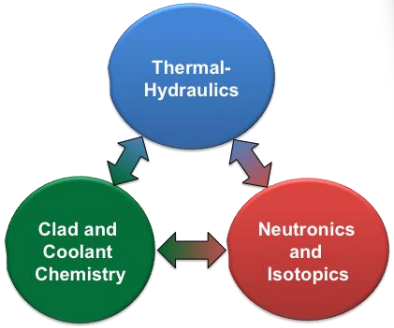
A coupled ANC-VIPRE-BOA multi-physics code will provide immediate value-added capability

- Leveraging current codes to provide better capability in the near term is a crucial first step toward achieving longer term goals.
  - Deepens understanding of physical problem and industry needs
  - Promotes acceptance and buy-in by industry partners
  - Utilizes proven technology that is already successfully applied for PWR design and operation as first step
  - Fosters industry experience with and confidence in high-performance computational technologies
- Targets the CRUD Induced Power Shift (CIPS) challenge problem.

Near-term impact important to long term goals

Objectives

- The goal of this work is to produce and demonstrate a LIME-based coupled ANC9-VIPRE-BOA multi-physics simulation capability useful to industry.
  - ANC9, *Westinghouse* Neutronics code
  - VIPRE-W, *Westinghouse* Thermal-Hydraulics code
  - BOA, *EPRI code for predicting* Crud deposition



- Previously, WEC developed a PVM-based approach to couple ANC and VIPRE called "ANCKVIPRE". This software provided a starting point for this more expanded work
- Provides the computational basis for L1 Milestone: L1:CASL.P2.03 (Crud: Quarter-Core Modeling of Watts Bar 1 Cycles 1-3 with Coupled VIPRE/ANC/BOA in VERA)

Preliminary tasks for each stand-alone code

- Transfer of each code (VIPRE, ANC, ANCKVIPRE, BOA) to CASL
  - both legal and technical issues
- Perform initial build and test
  - must demonstrate correct behavior and results on CASL computers
- Commit to CASL "git" repository
- Create "stand-alone" wrap of each code under LIME
  - Initial refactoring of source code
- Adapt build for Cmake test harness and incorporate into nightly build and test
  - Not initially done for all codes. Now is the standard
  - Required significant adaptations to build system in some cases

On the Relative Size and Complexity of ANC9, VIPRE-W, and BOA

- "Legacy" codes with extensive development and application history. Designed to be built as stand-alone applications (i.e. binary), and the WEC customized build-system reflects this bias.
  - leverages makefiles, ANT, imake, and home-made scripts
- ANC-9
  - Depeneant on 9 external libraries (sylib, nfdlib, CoreStore, nexus, codeif, . . .)
    - C, C++, JAVA, and Fortran
  - 742 Fortran files (physics and driver libraries)
    - ~245,000 lines of actual code (i.e. not comments)
- VIPRE-W
  - Dependent on 2 external libraries (sylib, nfdlib)
    - C, C++, and Fortran
  - 185 Fortran files (physics and driver libraries), 1 C file
    - ~38,000 lines of actual code (i.e. not comments)
- BOA
  - 106 Fortran files
    - ~40,000 lines of actual code (i.e. not comments)

Multi-physics code coupling was organized into two stages

1. LIME-based coupling of ANC-VIPRE
   - Coupling just 2-codes was important to develop confidence and identify challenge areas
   - Initial goal to reproduce previous ANCKVIPRE results
2. LIME-based coupling of ANC-VIPRE-BOA
   - Requires newest versions of ANC (9.4) and BOA, plus
   - New capabilities added to ANC9.4
     - read ppp files from BOA, depletion while coupled to Vipre . . .)

- In each case, the customized LIME-related software had to be written and appropriate changes made to each code to interface correctly.
  - Multi-physics driver
  - Model Evaluators and Transfer Operators
  - Physics code refactoring

What is LIME?

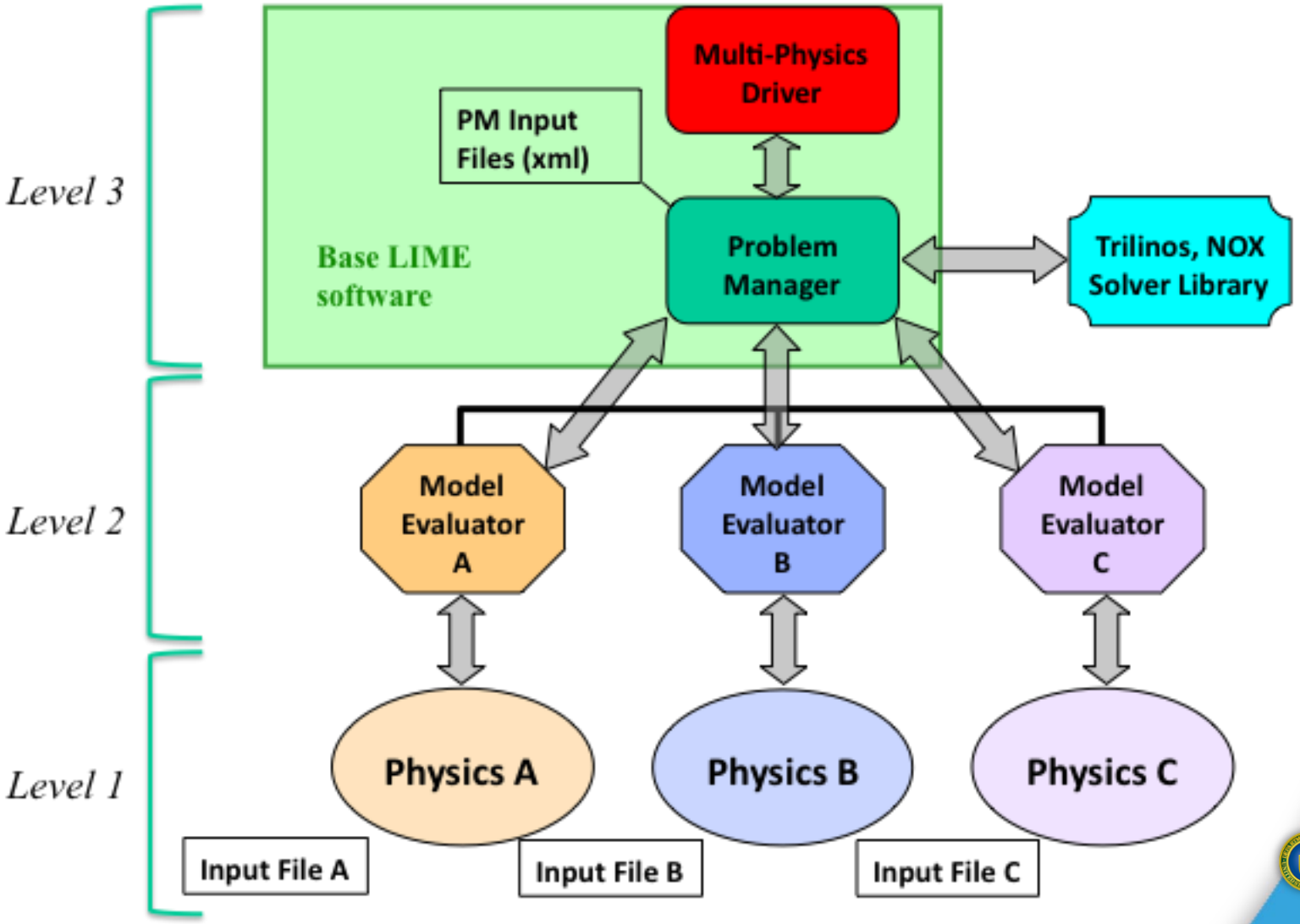
LIME is:

- an acronym for Lightweight Integrating Multi-physics Environment for coupling codes.
- a tool for creating multi-physics simulation code(s) that is particularly useful when computer codes are currently available to solve different parts of a multi-physics problem.
- intended to provide
  - key high-level software,
  - a well defined approach (including example templates),
  - and interface requirements for participating physics codes

  to enable the assembly of these codes into a robust and efficient multi-physics simulation capability.

LIME is one part of VERA

Key Components of a Simple Generic Application Created using LIME



Perspective: How Big is LIME?

- The LIME src directory currently contains 16 C++ files

LIME_Broadcast_File.cpp	LIME_Model_Evaluator.hpp
LIME_Broadcast_File.hpp	LIME_PrePostOperator.cpp
LIME_Data_Transfer_Operator.hpp	LIME_PrePostOperator.hpp
LIME_Elimination_Module.hpp	LIME_Problem_As_Operator.hpp
LIME_Fortran_Name_Macros.hpp	LIME_Problem_Manager.cpp
LIME_Hierarchy_Problem_Manager.cpp	LIME_Problem_Manager.hpp
LIME_Hierarchy_Problem_Manager.hpp	LIME_Strings.cpp
LIME_Model_Evaluator.cpp	LIME_Strings.hpp

that reflect ~ 2000 lines of C++ code

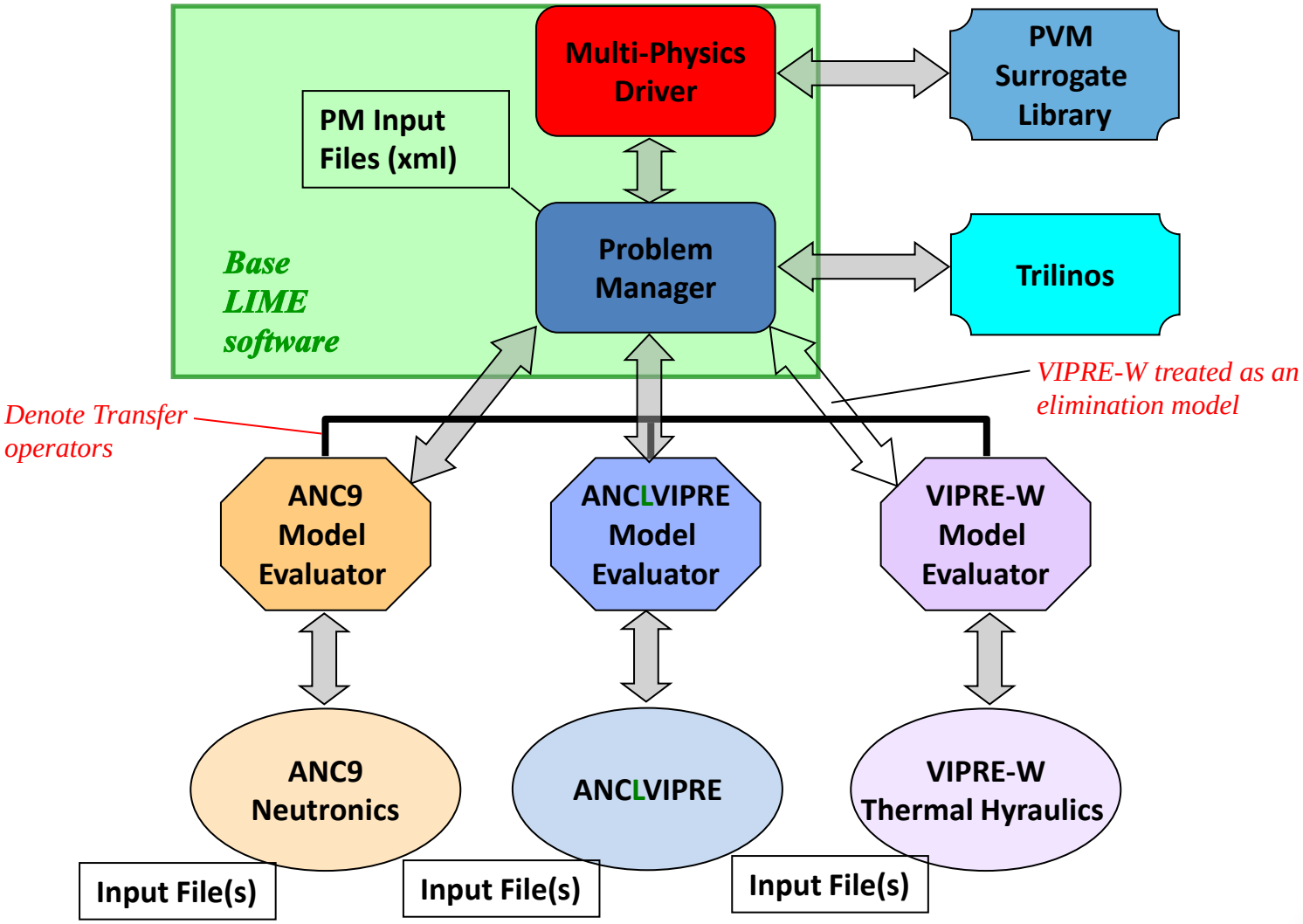
- LIME currently depends on several Trilinos packages

LIME is small compared to ANC, VIPRE, or BOA

Stage 1: LIME-based coupling of ANC-VIPRE

- **Key Challenges**
  - How to replace the PVM based process management and data transfer approach used in ANCKVIPRE without significant code mods to ANC or VIPRE
  - Deal with name clashes, shared resource (file descriptors and streams) conflicts, and shared global data problems, including those stemming from use of common blocks in the Sylib library.
- **Some key elements of current approach**
  - Create a thread-safe shared memory PVM surrogate library for message passing and process management interfaces used by WEC codes.
  - Move the common block data into C structures and allocate one C structure for each of the WEC codes that access the Sylib data.
  - Insert C interface between the call to Sylib and the implementation of the Sylib subroutine (required creating thread-safe sylib mods).
  - Write the MPDriver to run each WEC application in it's own thread
  - Passing thread specific C structure down into the Fortran CASL routines.

LIME-based coupling diagram for ANC-VIPRE



Summary of LIME-based coupled ANC-VIPRE Application

- Reimplemented PVM in thread safe shared memory form
- Thread-safe version of sylib library created and available to WEC
- Library versions of WEC applications required some modifications to source in addition to high-level restructuringLIME driver runs each WEC application in it's own thread and links against the PVM surrogate
- Successfully reproduces previous ANCKVIPRE results identically.

Phase 1 ANC-Vipre coupled App. Completed

LIME-based coupling of ANC-VIPRE-BOA

- **Challenges**
  - Requires most recent version of ANC (version 9.4, reads ppp files)
    - 9.4 uses new CoreStore lib (not backward compatible with 9.2.3)
    - 9.4 not capable of doing depletion when coupled to VIPRE
  - Transfer of BOA code (EPRI) to CASL
    - Mostly just legal details
  - A new (to LIME) time integration strategy needed for ANC-VIPRE-BOA
  - Disruptions in work schedules and staff availability
- **Some key elements of current approach**
  - Expand Phase-1 ANC-VIPRE coupling to include BOA
  - Adapt time integration scheme in LIME Problem Manager to accomodate unique aspects of ANC-VIPRE-BOA coupling
    - basically a new hierarchical fixed point iteration scheme
  - Modifications of ANC 9.4 to handle depletion when coupled

LIME-based coupling diagram for ANC-VIPRE-BOA

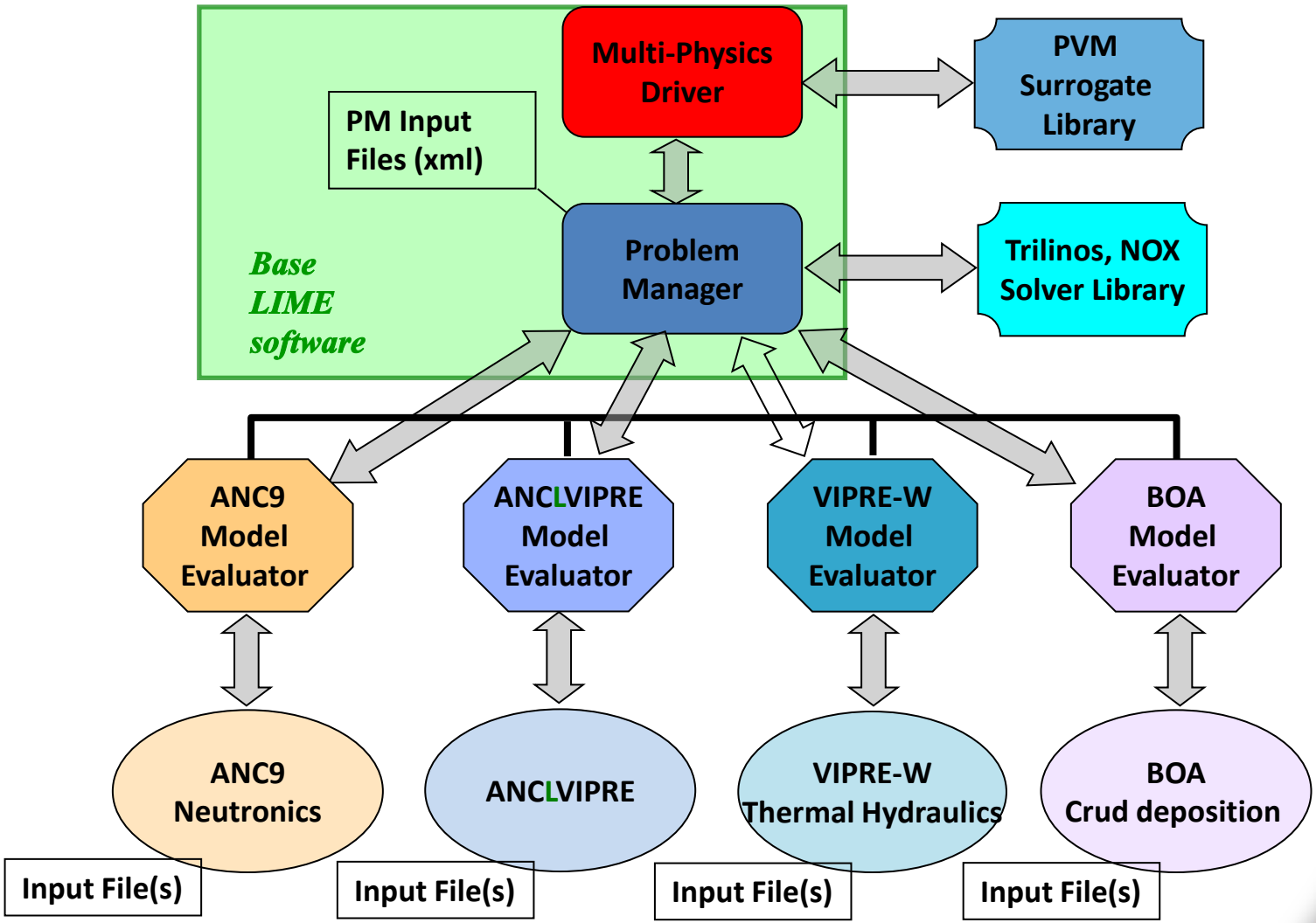
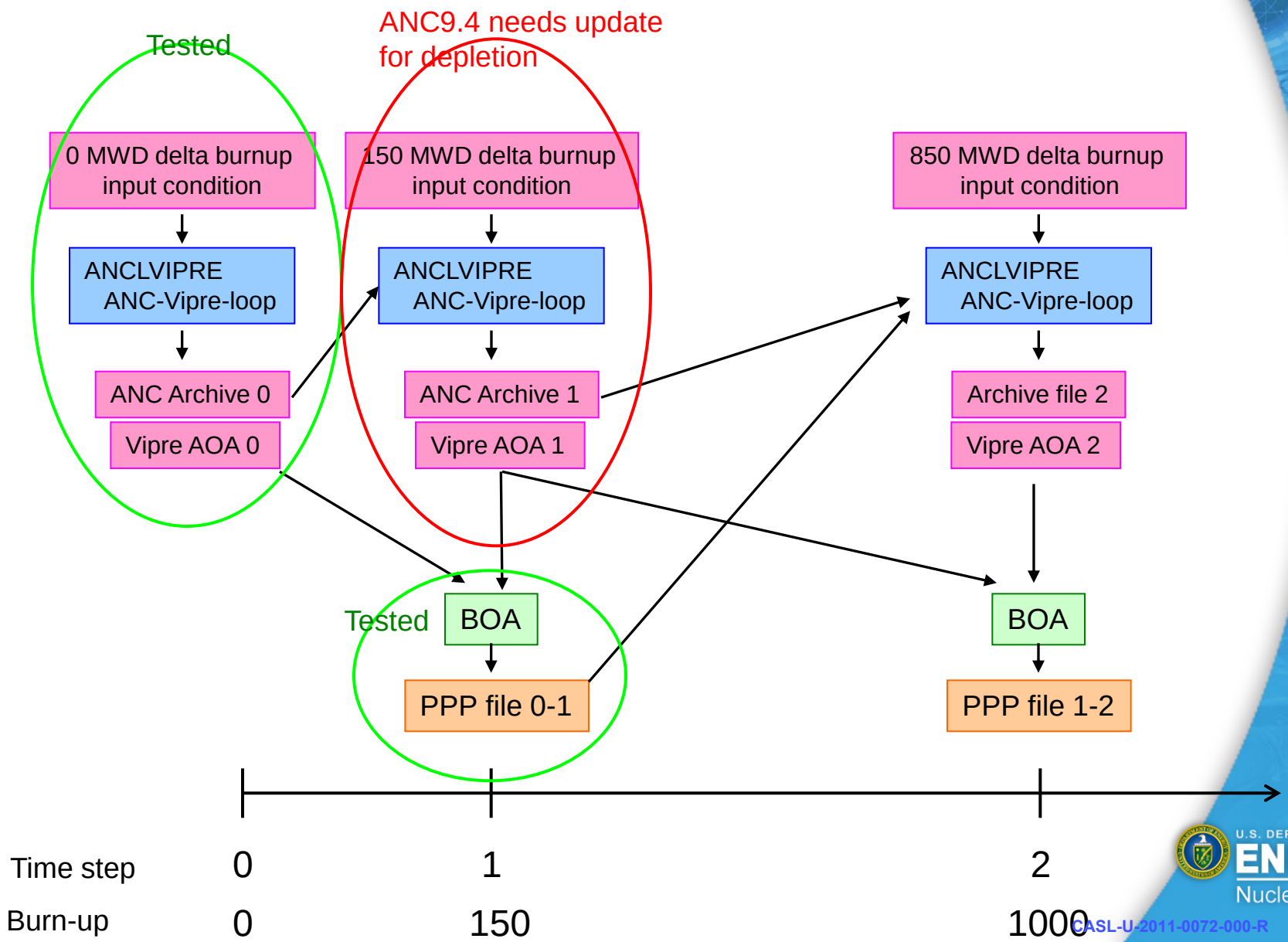


Illustration of Coupling Operations for Time-Stepping ANC-VIPRE-BOA



Status Summary

- VIPRE-W, ANC9.2.3, ANCKVIPRE, delivered to CASL
- Codes successfully compiled and executed in CASL computing environment. LIME-based ANC-VIPRE coupling complete and tested.
- BOA delivered to CASL, successfully built and tested standalone
- Created and tested all customized LIME software (MEs, multiphysics drivers, transfer functions) for ANC-VIPRE-BOA coupling
- ANC-VIPRE linkage updated by VRI using LIME
- Watts Bar Unit 1 identified as reference plant
- ANC9.4 delivered to CASL
  - Caused some additional re-work to compile and re-link to VIPRE/BOA
    - 9.4 uses CoreStore 1.2 lib instead of version 1.1
  - Additional ANC9.4 revisions just completed by Westinghouse and sent to CASL
- Base input files for Watts Bar ANC9, VIPRE, BOA completed and delivered to CASL
- Initial code linkage (ANC-VIPRE-BOA) underway

Success is not far away

Coupling of DeCART with STAR-CCM+
Current Status and Work Going Forward

Prof. Thomas Downar, University of Michigan
Brendan Kochunas, University of Michigan
Mathieu Hursin, University of Michigan
Benjamin Collins, University of Michigan
Robert Brewster, CD-adapco
Emilio Baglietto, CD-adapco

CASL-U-2011-0072-000-R

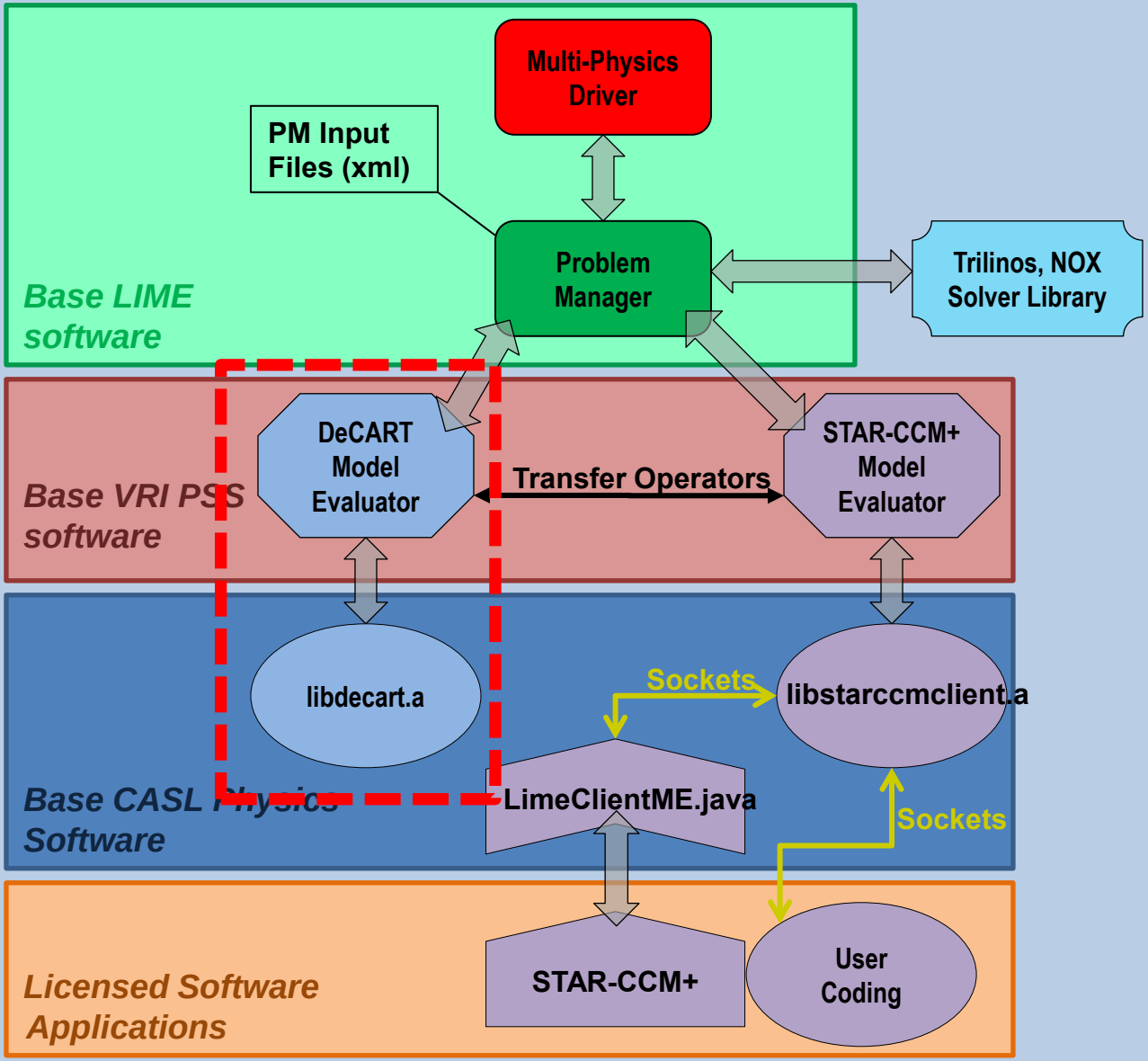
Personnel & Responsibilities

- Prof. Tom Downar (UMich) is point of contact and managed overall execution.
- Brendan Kochunas (UMich) was primarily responsible for developing the parallel data transfer and integrating the codes into VERA.
- Dr. Mathieu Hursin (UMich) was responsible for developing initial coupling strategy that is currently in VERA.
- Dr. Ben Collins (UMich) will be responsible for the continuing development of the coupling.
- Dr. Robert Brewster (CD-adapco) was responsible for supplying CFD models and technical support to UMich as needed.
- Dr. Emilio Baglietto (CD-adapco) was responsible for managing activities within CD-adapco to insure the necessary support was provided and also gave expert feedback on results

Overview

- Integrating DeCART and Star-CCM+ into VERA
- Existing: Serial Coupling in VERA
- Developing: Parallel Coupling Outside of VERA
- Planned: Parallel Coupling without File I/O
- Data Mapping
- Path Forward
- Conclusions

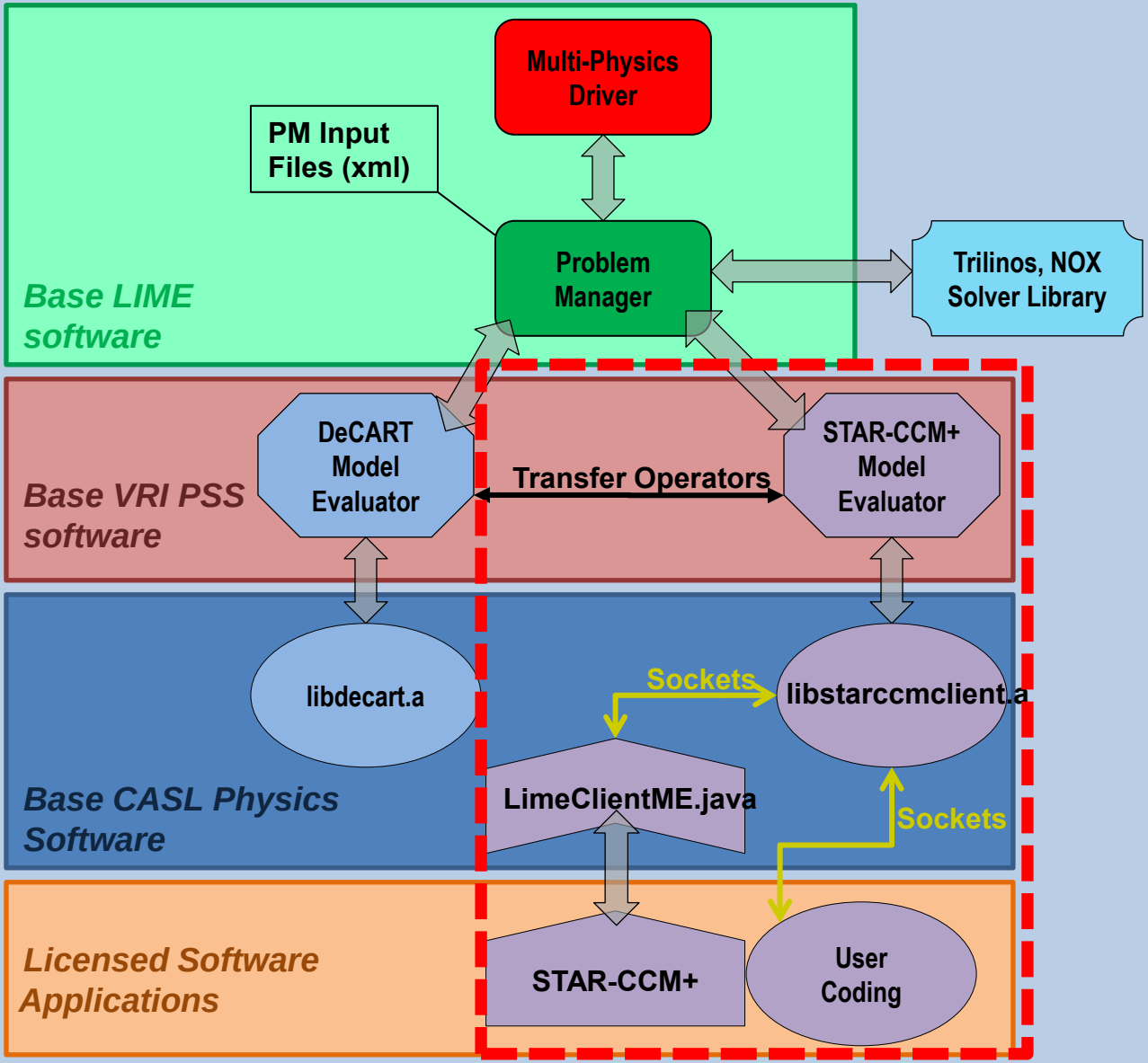
VERA (DeCART / Star-CCM+ Coupling)



Integrating DeCART into VERA

- Minor refactoring of top level routines
- Included ability to pass in MPI communicators and command line arguments
- Modified initialization procedure

VERA (DeCART / Star-CCM+ Coupling)

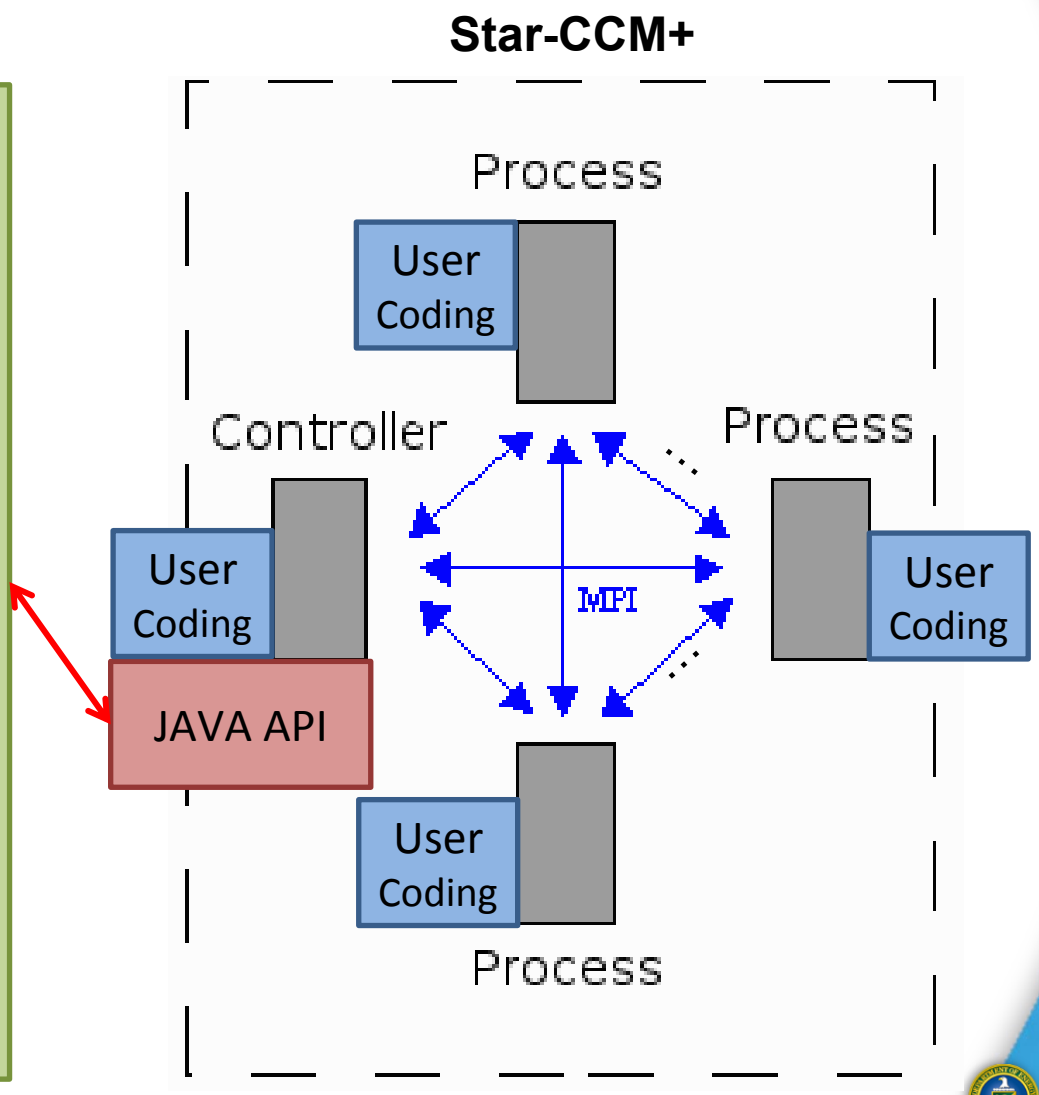


Integrating Star-CCM+ into VERA

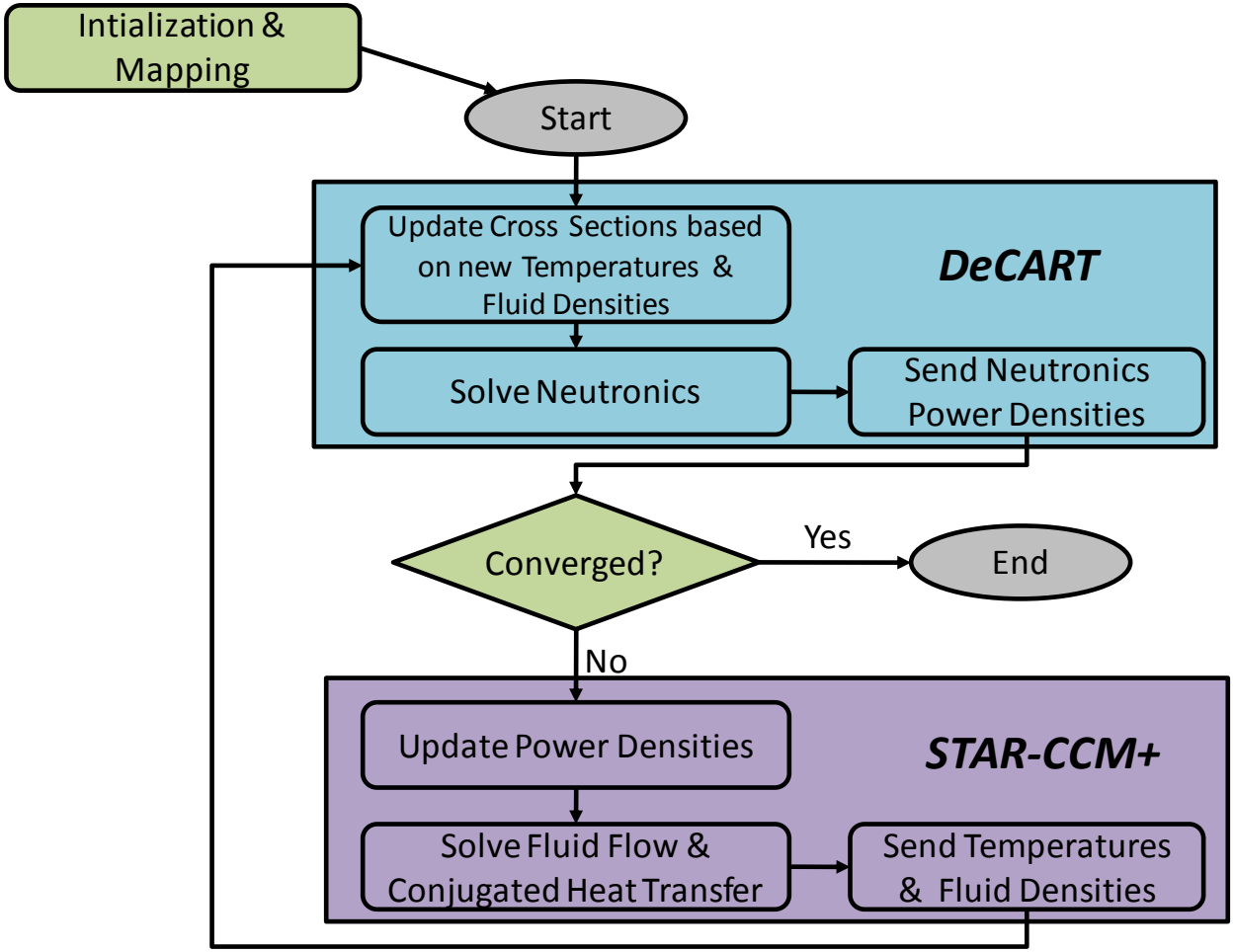
Model Evaluator

- Develop library to communicate with JAVA API
- JAVA API controls iteration sequence in STAR-CCM+

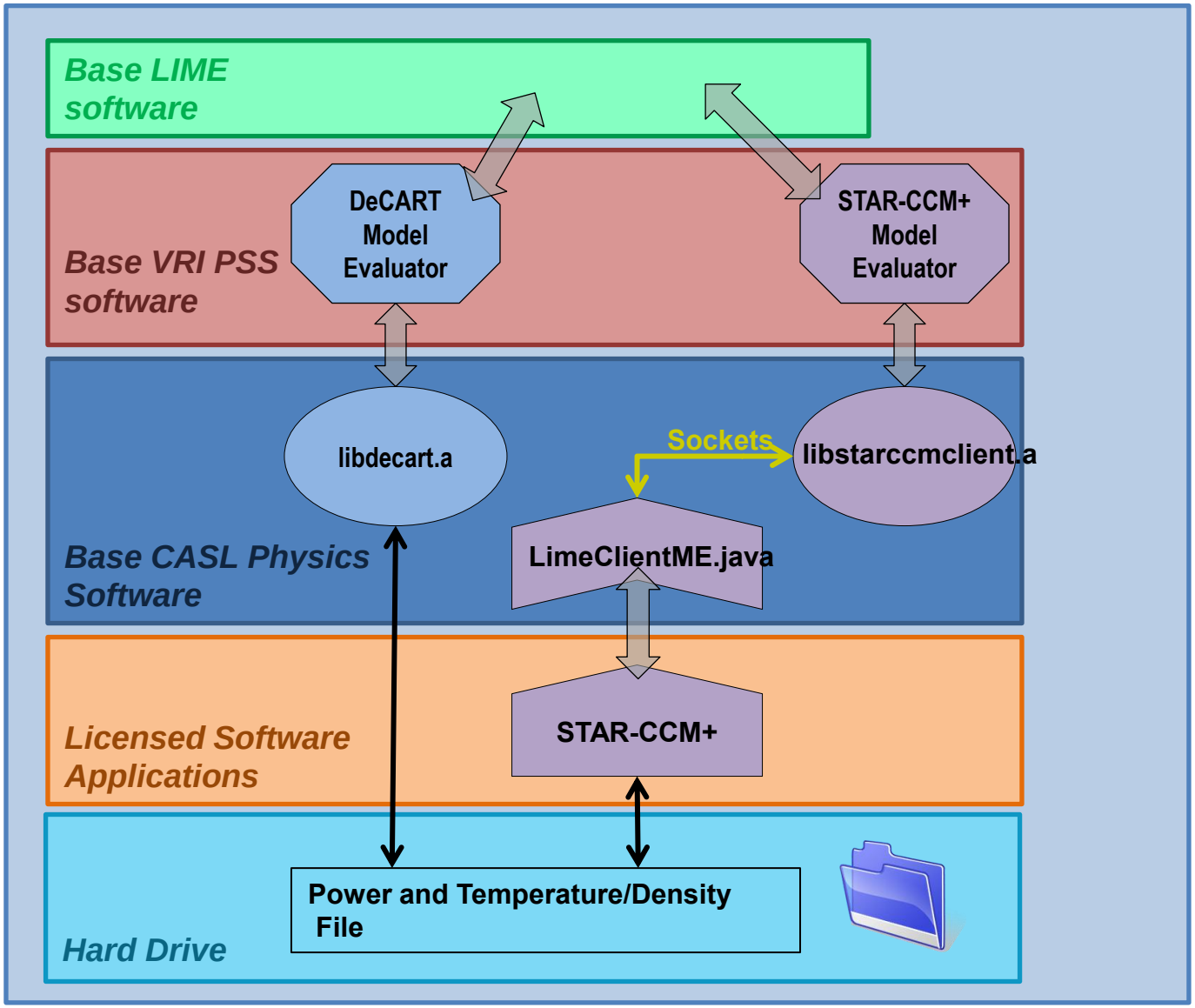
- Current:
  - Data transfer using File I/O
- Goal:
  - Data Transfer using Socket and MPI communication



Existing: Serial Coupling in VERA



Existing: Serial Coupling in VERA

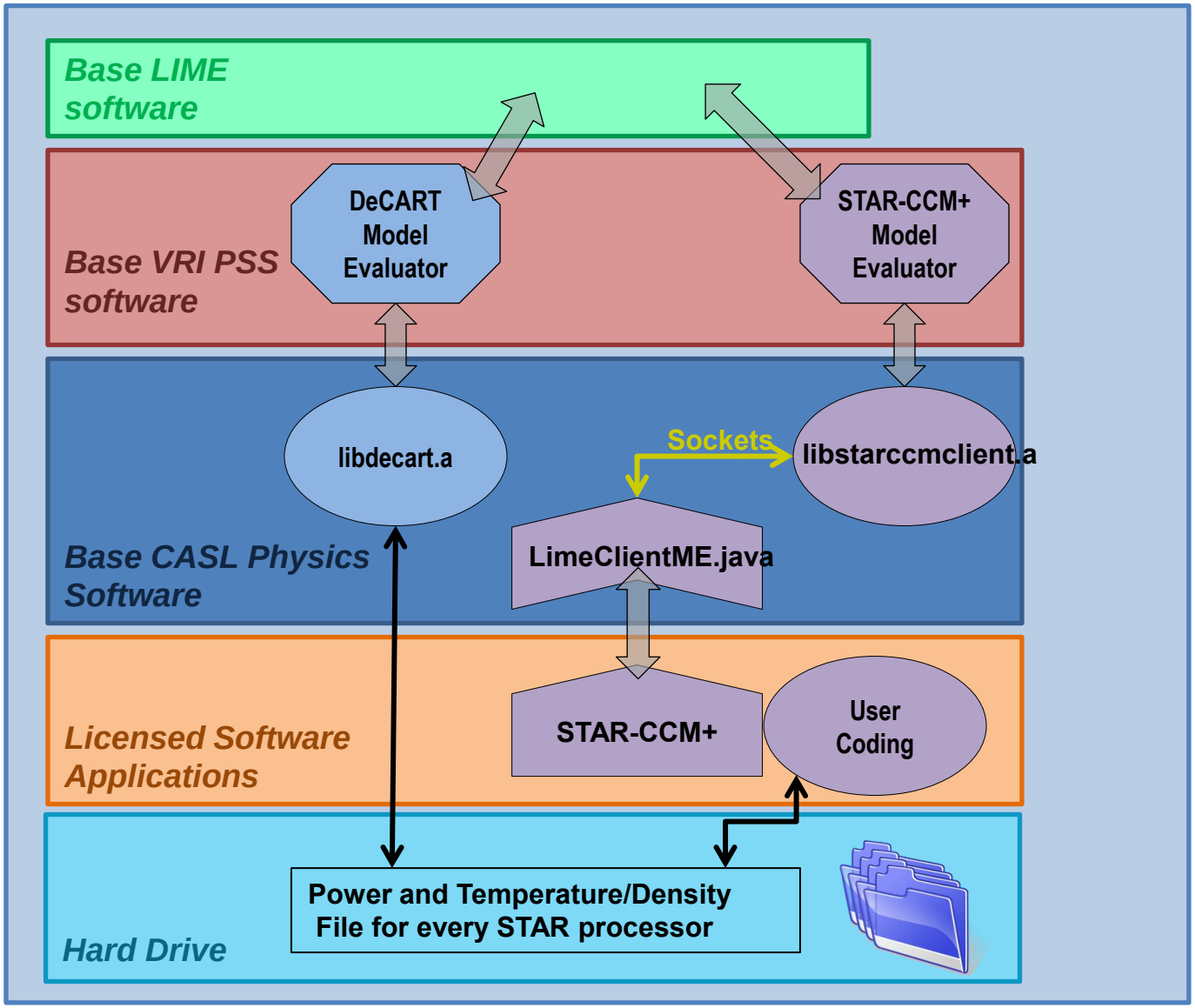


Developing: Parallel Coupling Outside of VERA

- Instead of writing a single file with all data, multiple files are written for each STAR-CCM+ process
  - User coding

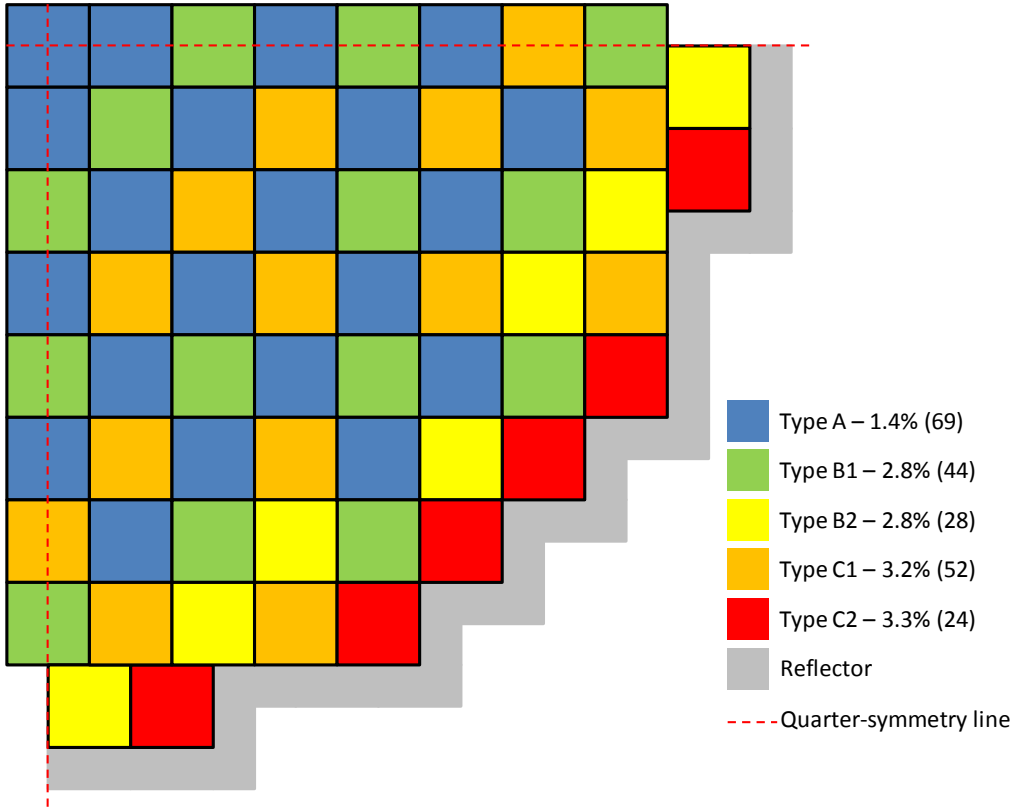
- Iteration strategy is the same
- Iterations are not automated
  - Residuals must be monitored by user
  - User must decide when to perform a data transfer
  - Codes are run as separate jobs on cluster

Developing: Parallel Coupling Outside of VERA

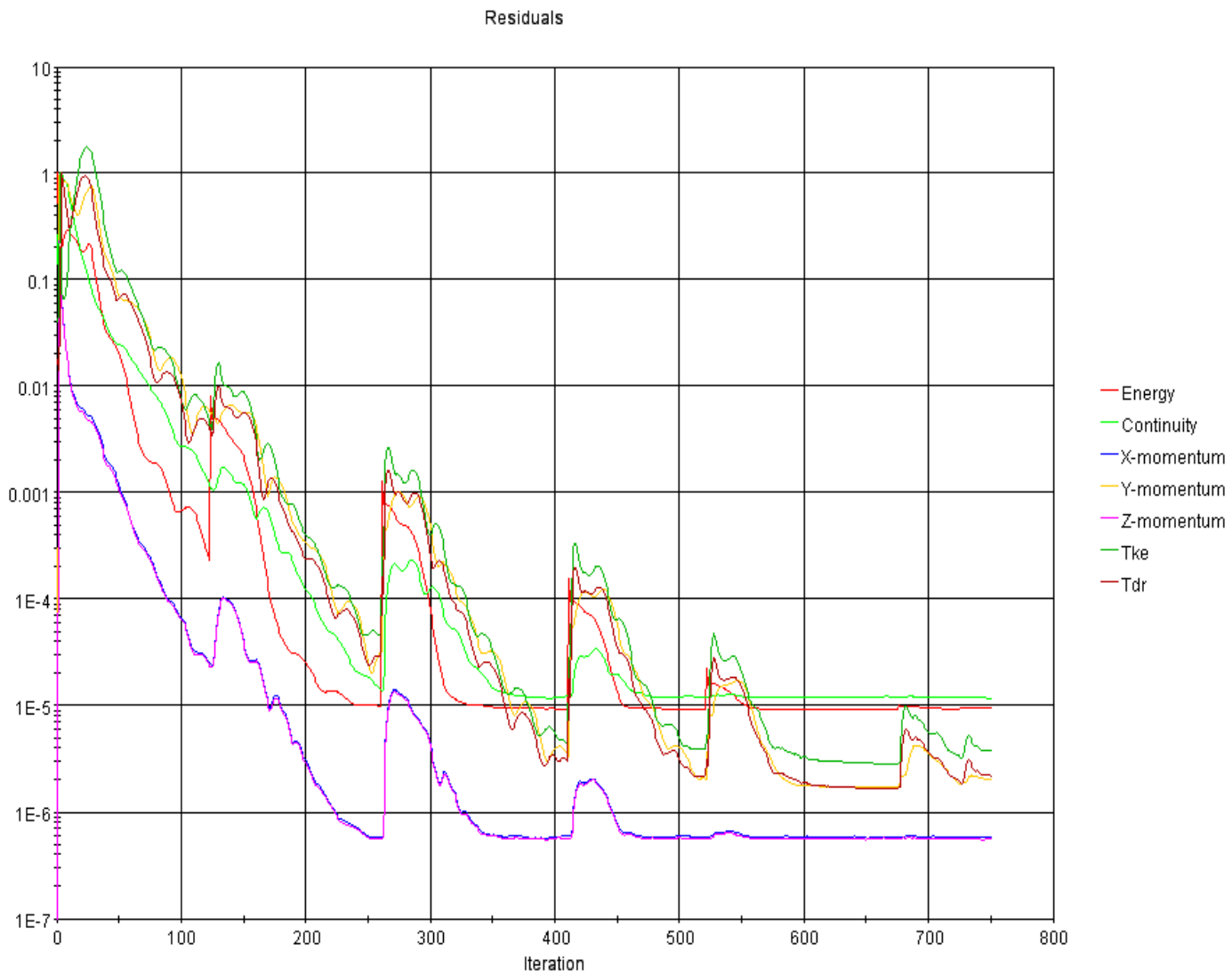


Calculation Details

- Quarter core PWR model
  - DeCART coupled to STAR-CCM+
    - STAR-CCM+ was run with 256 processors
    - DeCART was run with 80 processors
  - Solved with a Fixed Point Gauss-Seidel iteration.

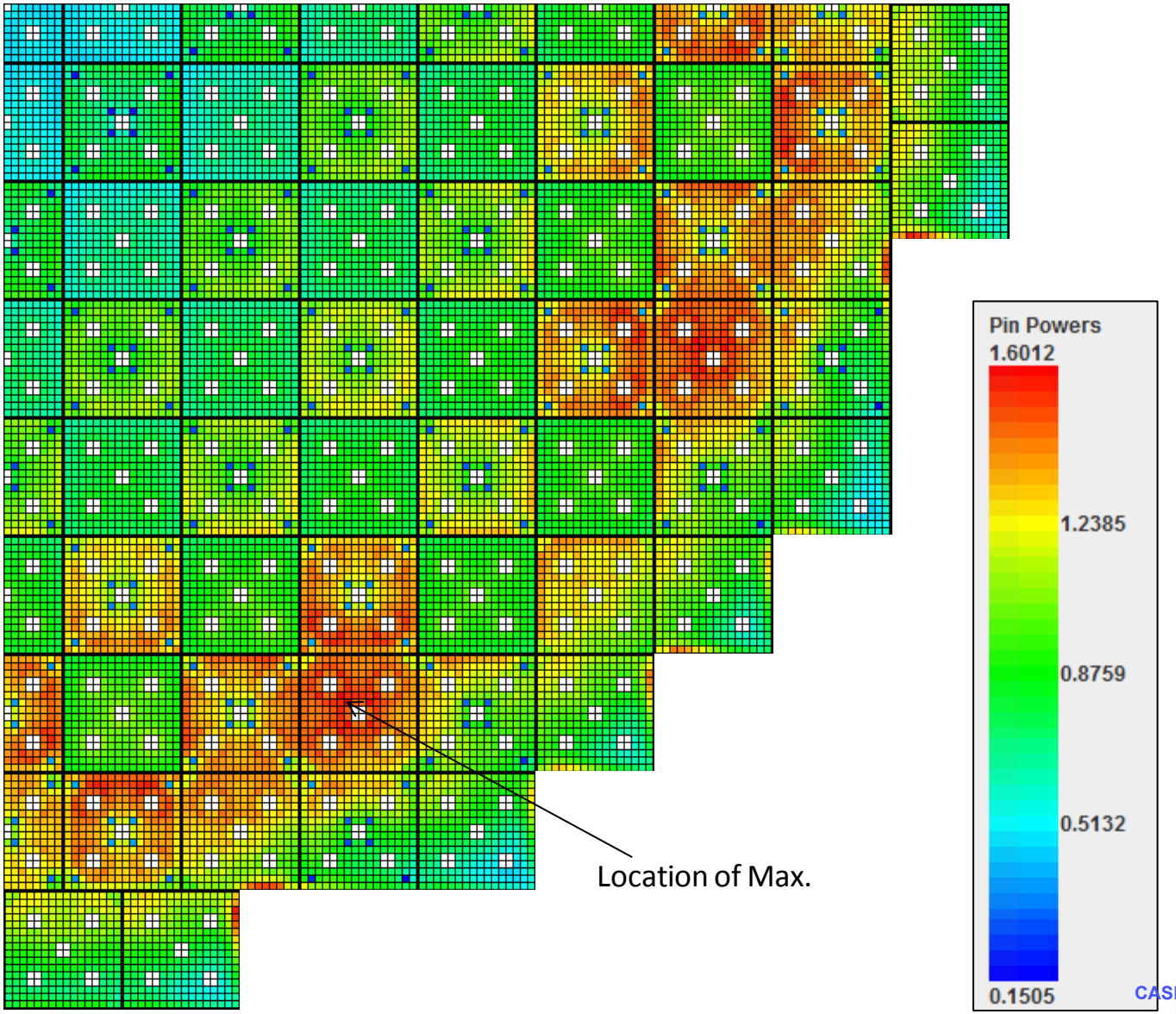


Coupled Calculation with Parallel File I/O



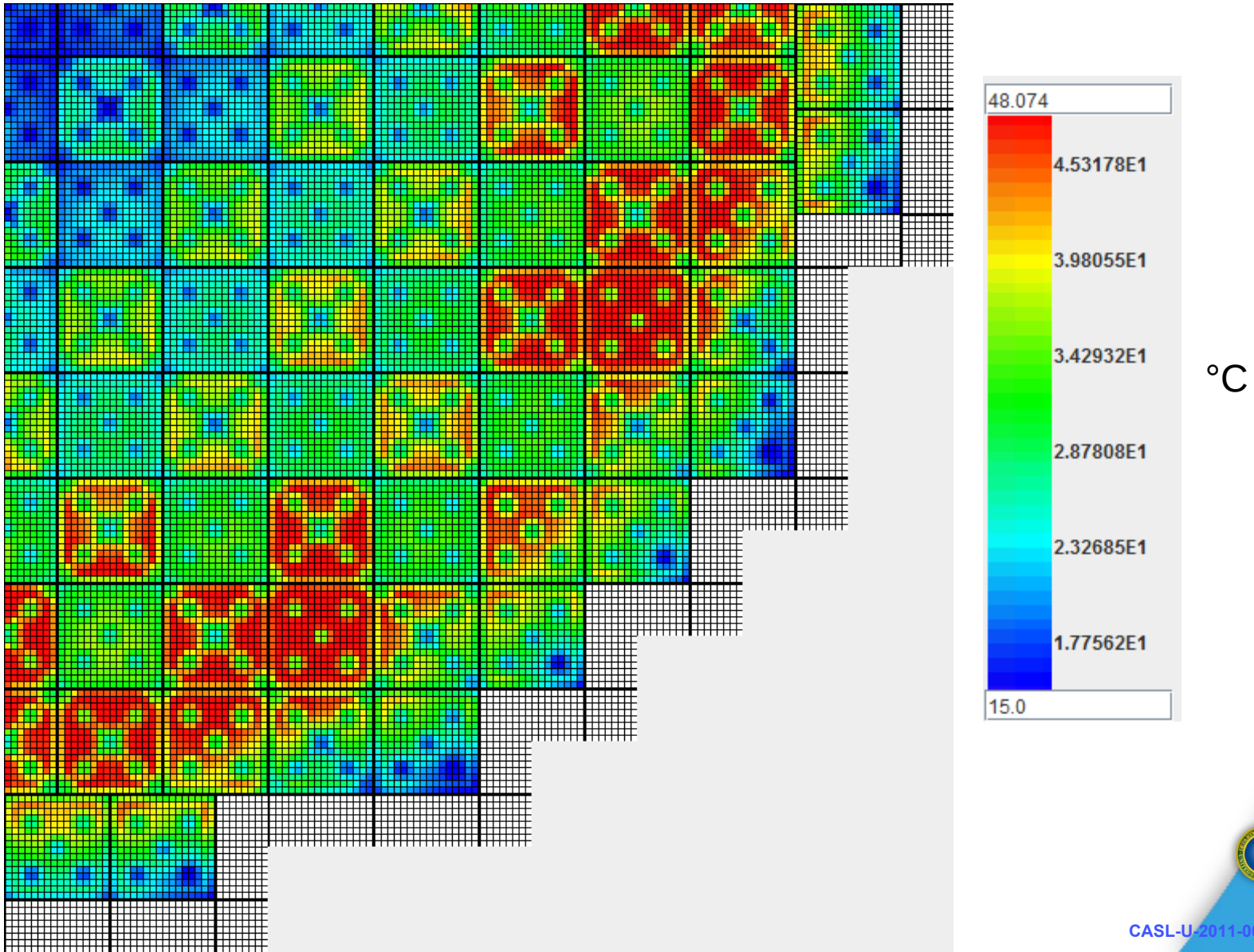
Coupled Results

Axially Integrated Pin Powers

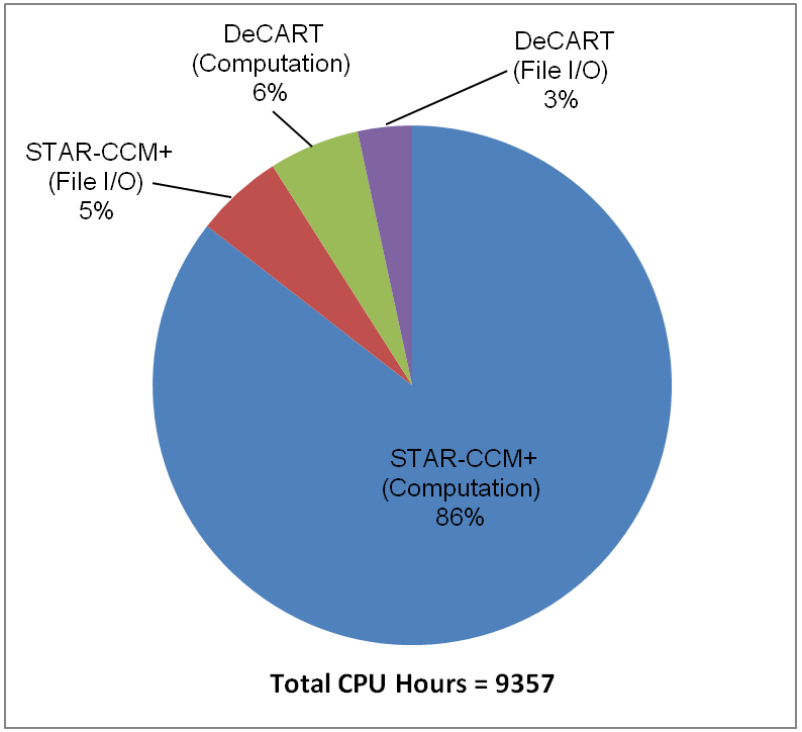


Coupled Results (cont.)

Temperature Rise (°C)



Computational Performance



CPU Hour Requirements of Coupled Simulation by Component Task

Times for Different Calculations

Calculation Component	Est. Real Time (min)	CPU Hours
DeCART Fixed Point Iter.	105.57	140.76
STAR-CCM+ Fixed Point Iter.	399.00	1702.40
DeCART Total (Coupled)	633.43	844.58
STAR-CCM+ Total (Coupled)	1995.00	8512.00
Total (Coupled)	**2628.43**	**9356.58**
DeCART Total (Stand-alone)	**86.59**	**115.46**

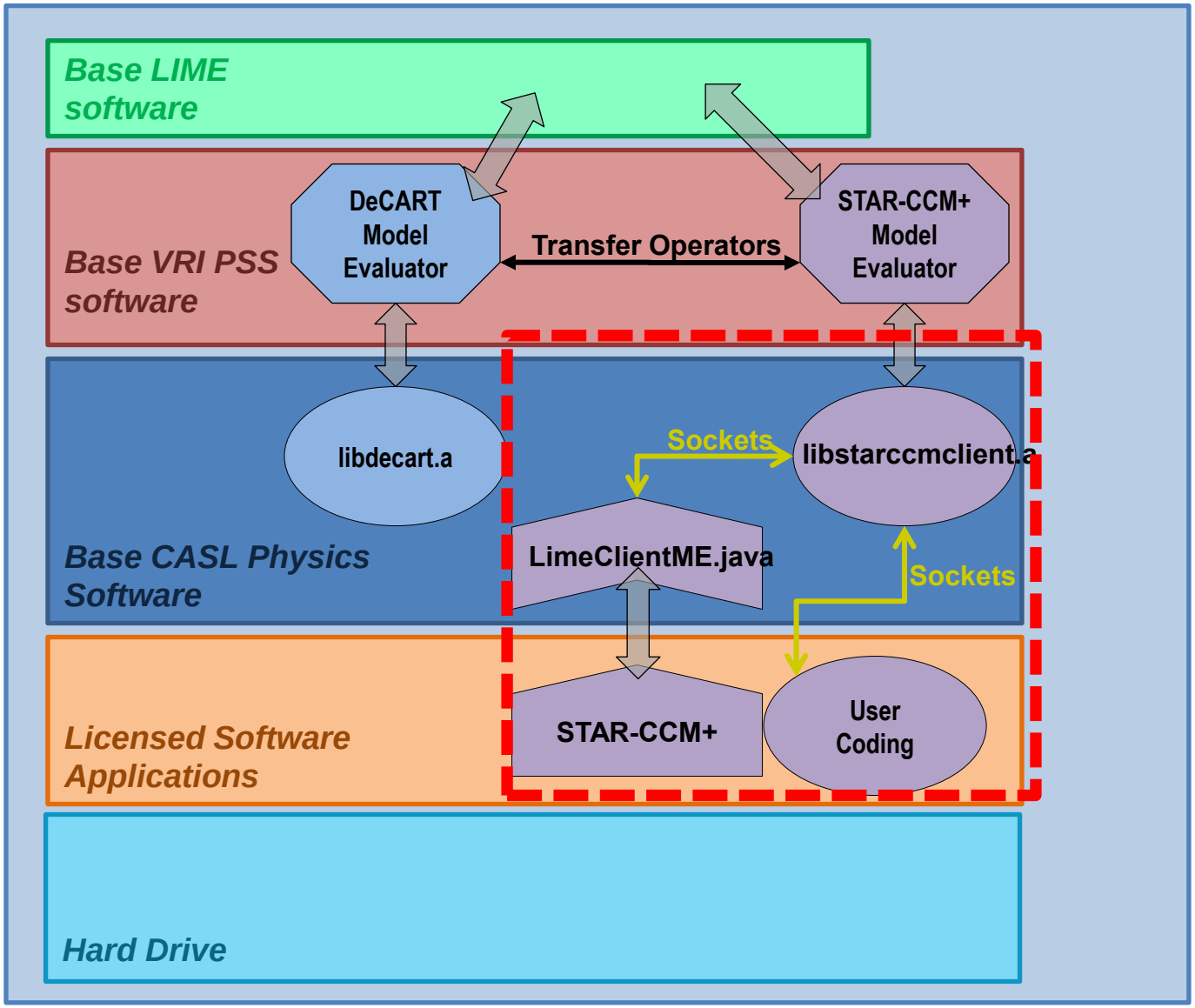
100x computation time needed for CFD!

Planned: Parallel Coupling without File I/O

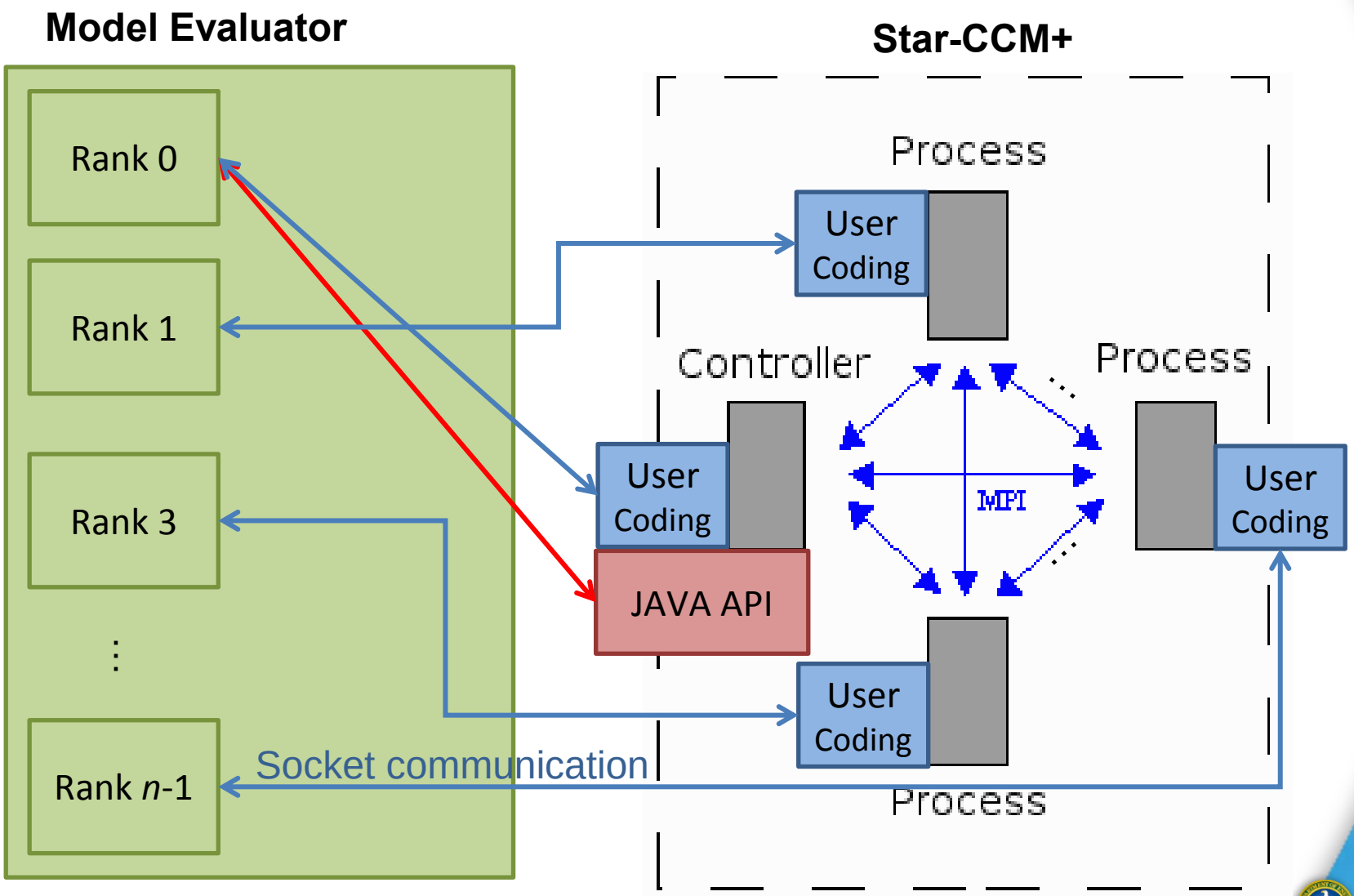
- Time spent doing file transfer is 8% of total runtime
- Disk requirements are roughly 50 GB

- Model Evaluators pass data using MPI
- User coding will be needed in STAR to pass data to the model evaluator using socket communication

Planned: Parallel Coupling without File I/O



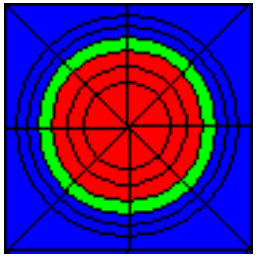
Planned: Parallel Coupling without File I/O



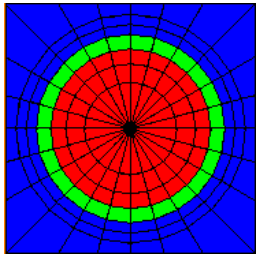
Data Mapping

- Data is mapped using centroid values
- CFD mesh requires a much finer mesh than neutronics
- Conformal mesh between DeCART and STAR-CCM+ has been tested

DeCART mesh

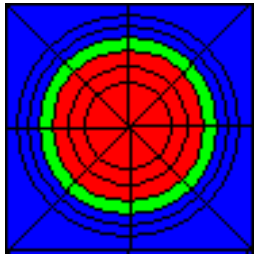


STAR-CCM+ mesh

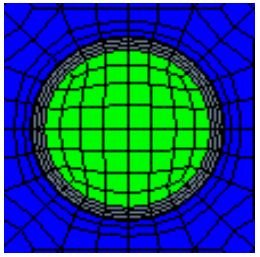


- Non-conformal mesh works but does not enforce conservation laws (~0.5% Error)

DeCART mesh



STAR-CCM+ mesh



Conclusions

- DeCART and STAR-CCM+ have been implemented into VERA
  - The integration of STAR-CCM+ demonstrates that commercial codes can be integrated into VERA
- Serial File I/O Coupling is implemented into VERA
  - Serial File I/O is very time consuming and limits size of problems that can be run
- Parallel File I/O Coupling has been developed
  - Quarter core coupled problems are possible
- Path Forward
  - Implement parallel file I/O into VERA
  - Improve data mapping algorithms
  - Eliminate need for file I/O to increase efficiency
  - Optimize convergence algorithms

Questions?

CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

HPC Updates to Scale for Cross Section Processing

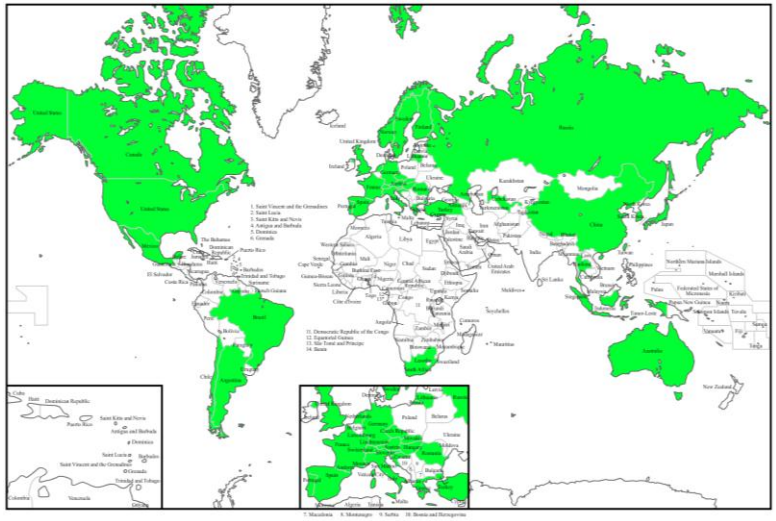
Jay Jay Billings, ORNL
Scale Modernization Team

August 10th 2011

CASL-U-2011-0072-000-R

Talk in Brief

- A bit about Scale (and its role in the VRI)
- HPC Showstoppers in Scale 6.0
- "Hmm… Upgrades"
  - *Changes to Scale for "Scale4CASL" release*
  - *Cross sections only, not depletion*
- On-going and Future Work
  - *Projects funded by the NRC, the Division, and the Directorate*



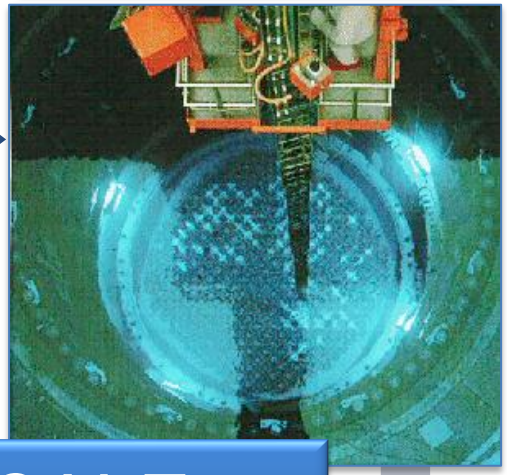
Scale Map of the World

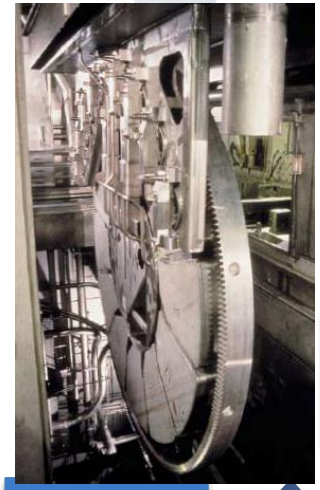
A Bit About Scale

Applications of SCALE

Material Processing & Fuel Fabrication

Commercial and Research Reactors





Recycling

Storage

Transportation

Disposal

Slide courtesy of Brad Rearden

Scale Modernization Team

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ORNL-RNSD

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Jordan Lefebvre
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Donald Newell
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Funded by NRC, DOE, ORNL and CASL across multiple projects

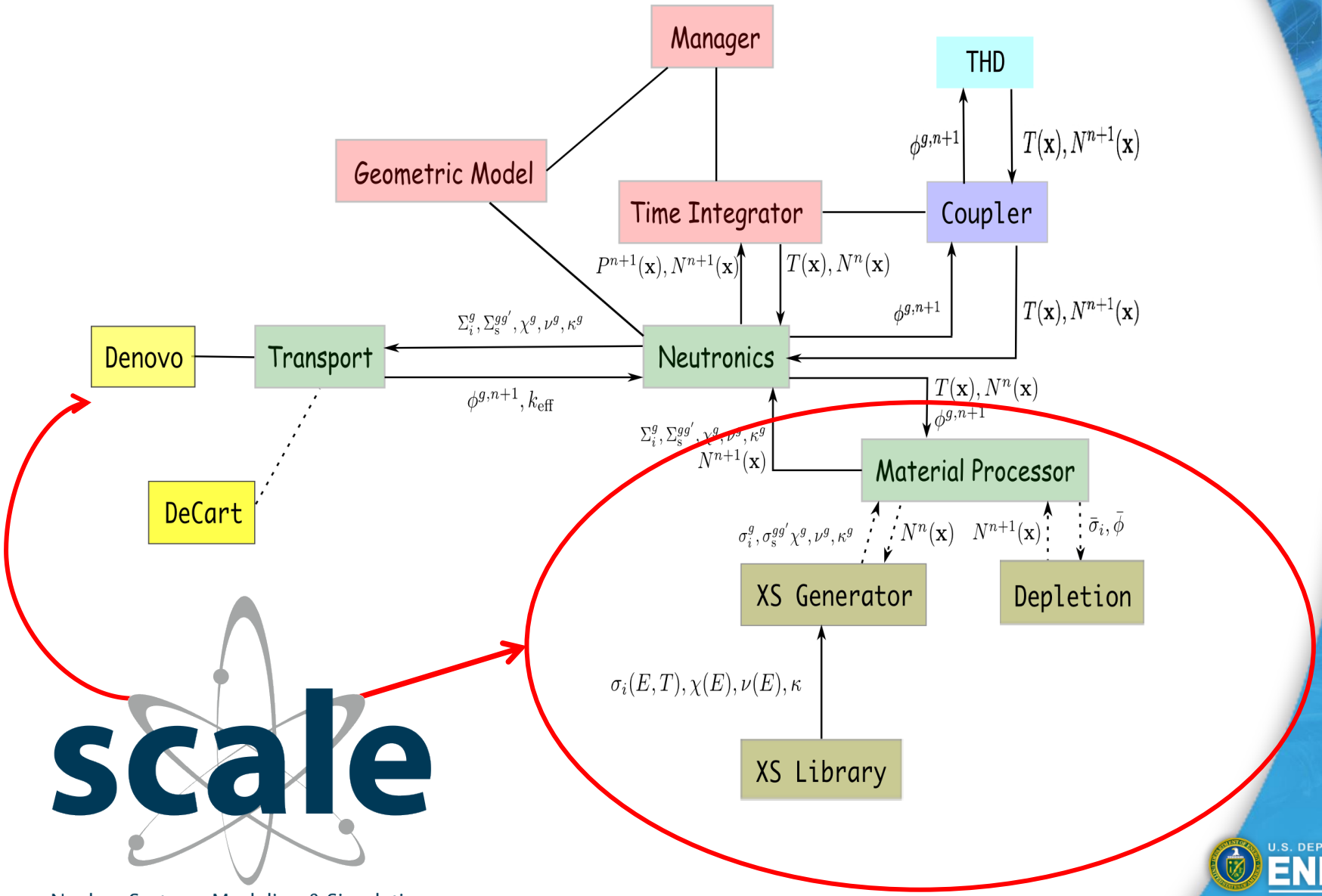
Lester Petrie
ORNL-RNSD

Brad Rearden
ORNL-RNSD

Mark Williams
ORNL-RNSD

CASL-U-2011-0072-000-R

"The CASL Problem"



scale

Nuclear Systems Modeling & Simulation

CASL

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY

Nuclear Energy

HPC Showstoppers in Scale 6.0

Consider a Full Core Problem….

A full Westinghouse PWR core in Scale modeled with 1" resolution would have…

- Roughly 7.6 million cross section cells:
  - $50{,}952\ rods\ \times 150\,\frac{cells}{rod} \approx 7.6M$
- Roughly 500 million depletion zones
  - $50{,}952\ rods\ \times 264\,\frac{pellets}{rod}\ \times 5\,\frac{rings}{pellet}\ \times 8\,\frac{sectors}{ring}\ \approx 500M$

Running the Numbers

How long would it take?

- Scale 6.0 is not an HPC code! It only executes *sequentially.*
- Roughly 30s per cross section cell, depending on method = 230M seconds
- Roughly 5s per depletion zone = 2.5B seconds

That's 87 years.

Running the Numbers 2

What would it look like computationally?

- Tons of I/O
  - Nearly 64M reads and writes of the AMPX library
- A loose confederation of Fortran executables passing files
  - Execution flow determined at run time
  - Could not couple to another code (very easily)
- Only capable of compiling with the Intel Compilers
- **NO** unit tests on 500k lines of code (but plenty of system tests)

Showstoppers

- 87 years to do cross sections and depletion because of sequential execution
  - 7 years for cross sections
  - 80 years for depletion
- Not easily coupled to the rest of the PSS
  - Would only work with Intel compilers, (not on HPC systems)
  - Wouldn't be testable as an embedded code!

Simply put: CASL could kiss high-resolution HPC goodbye

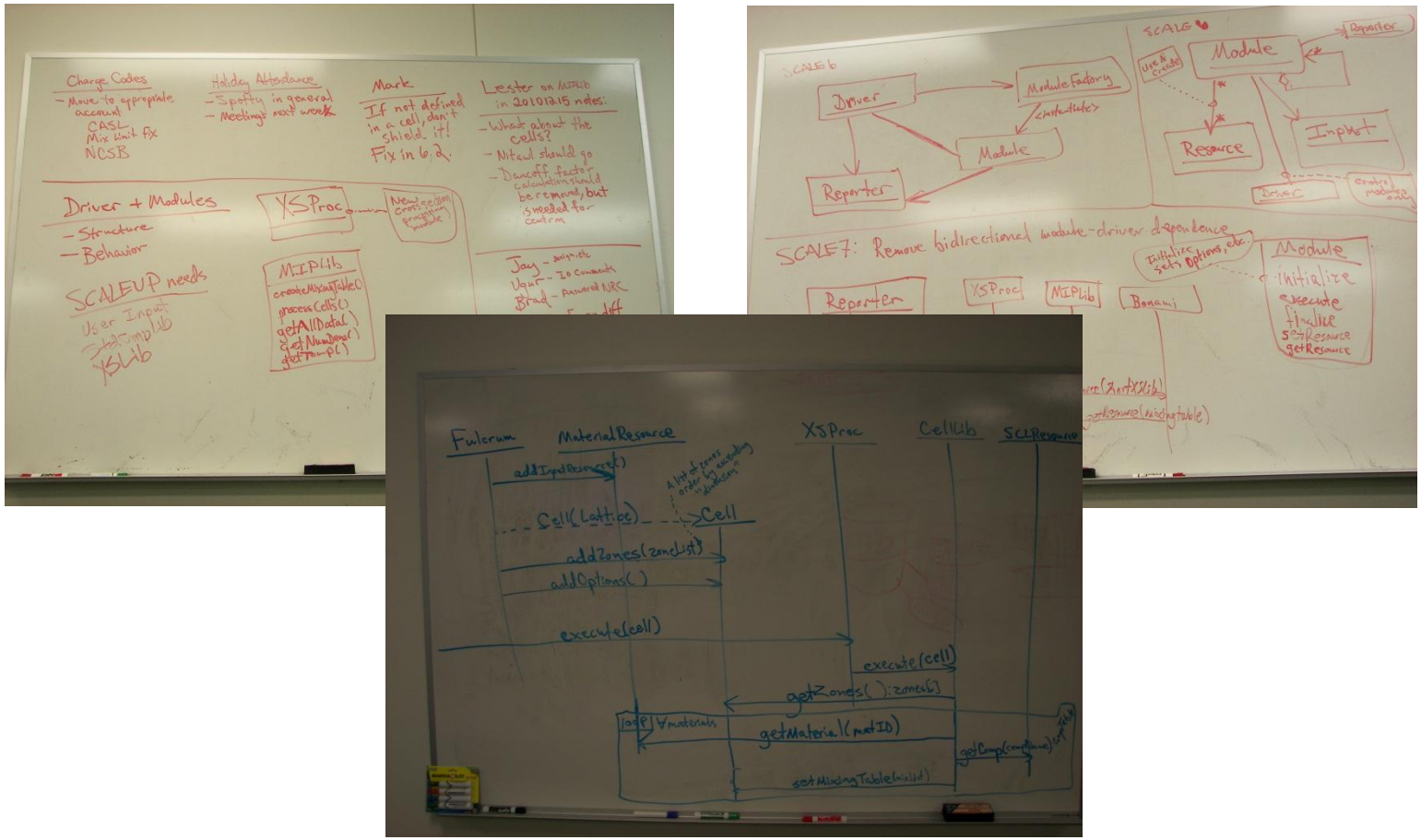
“Hmm… Upgrades.”

Development Process

We developed a simple process based on best practices:

- Plan, plan, plan
  - Identify deliverables, milestones, babies and staff absences
- Iterative and flexible
- Leverage Object Oriented Programming, Model-Driven and Test-Driven Development
  - UML and CTest + QtTest
- Meet three times weekly, two hours per meeting
- Document everything digitally
  - IBM Rational modeling tools and transformation engine
  - GForge/RTC/Fogbugz
  - Mediawiki
  - Doxygen
  - Photos

Development Process 2



Getting together actually works!

Development Guidlines

We stuck to some guidelines:

- Can't just throw out tried-and-true Scale components
- Accept changing requirements
- Create a parallel code by design, not optimization
- All new code will be C++ with Fortran bindings as needed
  - And work with GCC!
- All new code must be covered with unit tests
- Everything must be documented at least a little bit
- Above all, work together and have fun

High-Level Tasks

- Create a well-defined Module base class
  - What do all Modules do?
- Create a "Cell" data class to hold cross section, depletion data
  - LatticeCells only for CASL, other types to follow
- Eliminate extra I/O
  - Separate Module-to-Module data transfer from user I/O
  - Remove all I/O from Modules
    - Send important information to a "Reporter"
  - Create unique, standard implementations of "Resources"
- Cover everything with unit tests
  - C++, C and Fortran code
- Modify BONAMI-IR to work with new infrastructure

Results: Minus a six second startup in standalone mode, we can process Cells in 0.5 seconds!

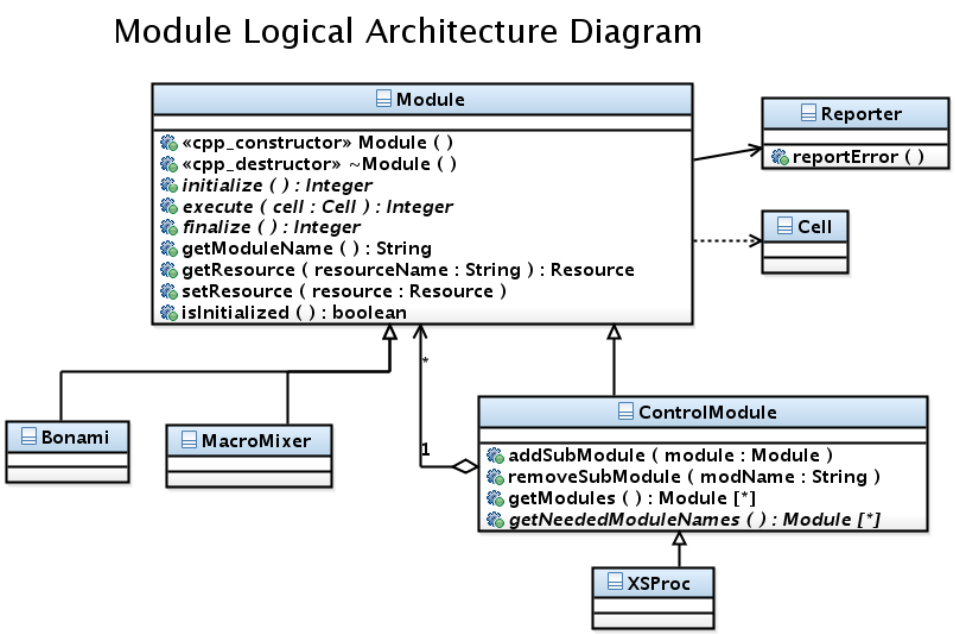
Defining a Module

Modules…

- Manipulate Cells (like a flyweight)
- Manage Resources and Reporters

ControlModules…

- Manage collections of Modules
- Execute in a pre-determined order

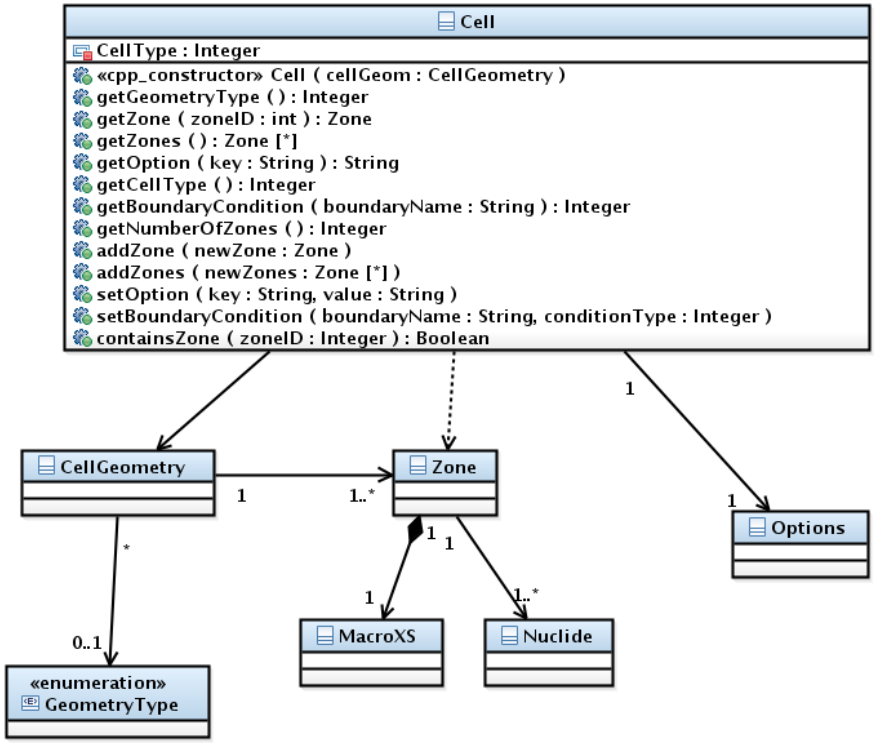


The Cell

Cells…

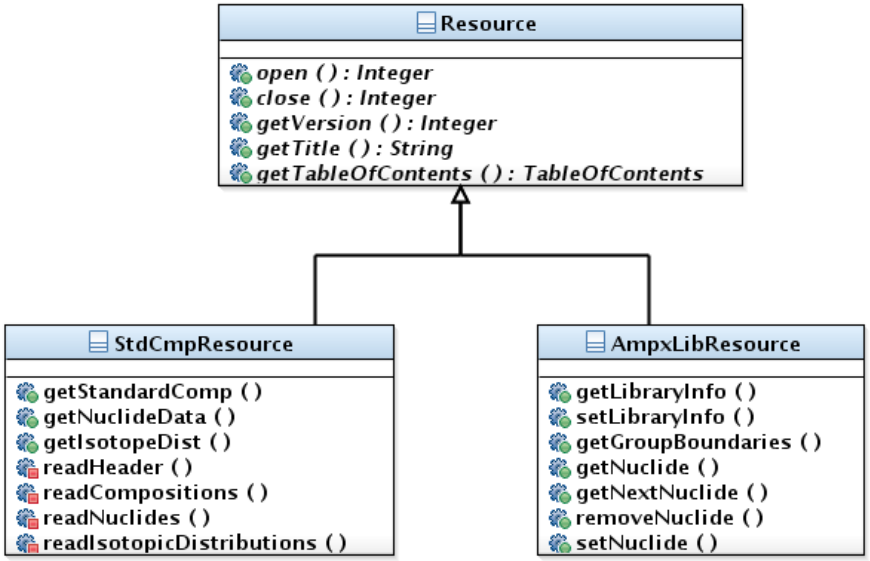
- Contain everything!
  - Geometry and Zones
  - Material Info (XS, fluxes)
  - Options and Tags
- Are completely independent and distributable

Cell Logical Architecture Diagram

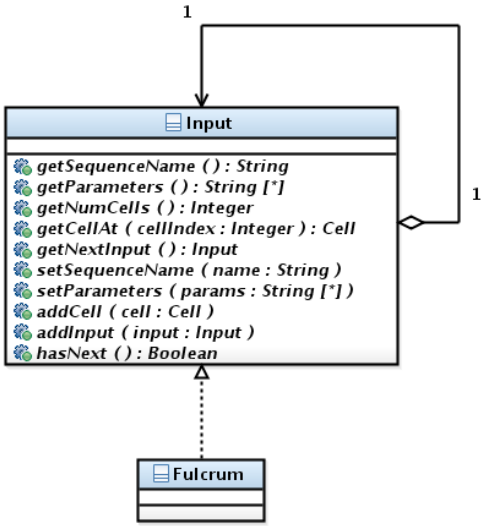


Data Resources and User IO

Resource Logical Architecture



Input Logical Architecture Diagram



Resources…

- Standardize reference data I/O, classes and access
- Provide unique, optimized implementations vs. 80 existing implementations

User Input

- Standardized Input reader (straight to Cells)
- Standardized error Reporting

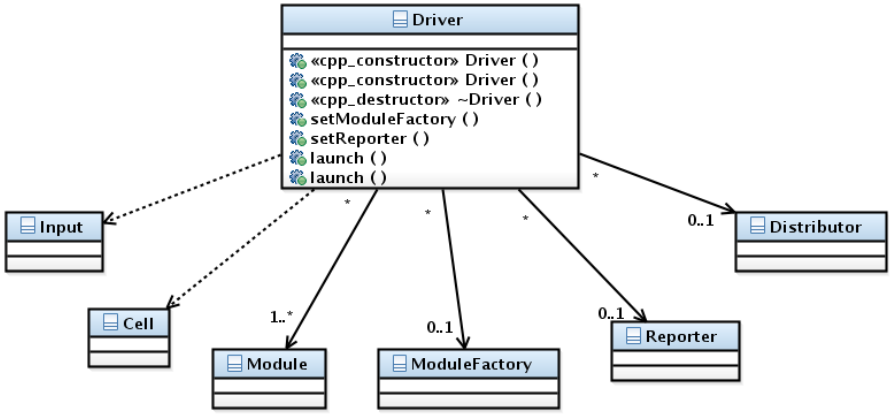
On-going and Future Work

NRC-Funded "Parallel Scale" & Embedded Self-Shielding Method (ESSM)

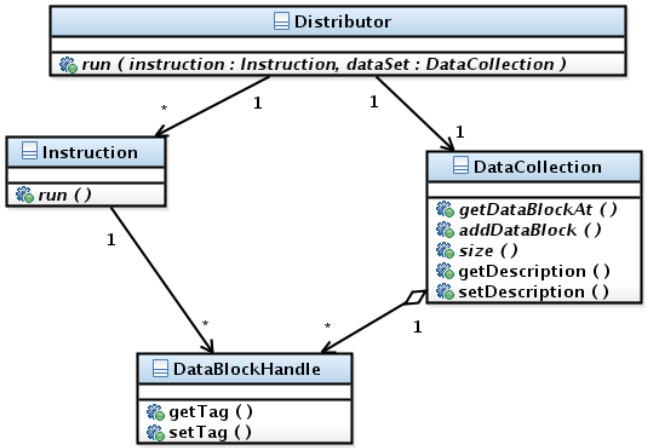
The NRC has graciously funded…

- Development of OpenMP and MPI based distribution mechanisms in Scale
  - OpenMP works great
  - Developing MPI version
  - Fixing parallel I/O bugs
- Embedded Self-Shielding Method
  - POC: Mark Williams

Driver Logical Architecture Diagram



Distributor Logical Architecture Diagram



Division and Directorate-Funded Efforts

- Template-based Input Processing
- Constructive Solid Geometry Package
- Development of new Resources and integration of all Resources into remaining Scale Modules

Future CASL Work

- Integration into Neutronics package, POC: Greg Davidson
- Integration of ORIGEN for depletion, POC: Kevin Clarno

Questions?

CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

The Neutronics/Denovo Package and TH Coupler
Wednesday, August 10, 2011
CASL Roundtable Meeting
Raleigh, North Carolina

Greg Davidson, Tom Evans, Stuart Slattery

CASL-U-2011-0072-000-R

Collaborators

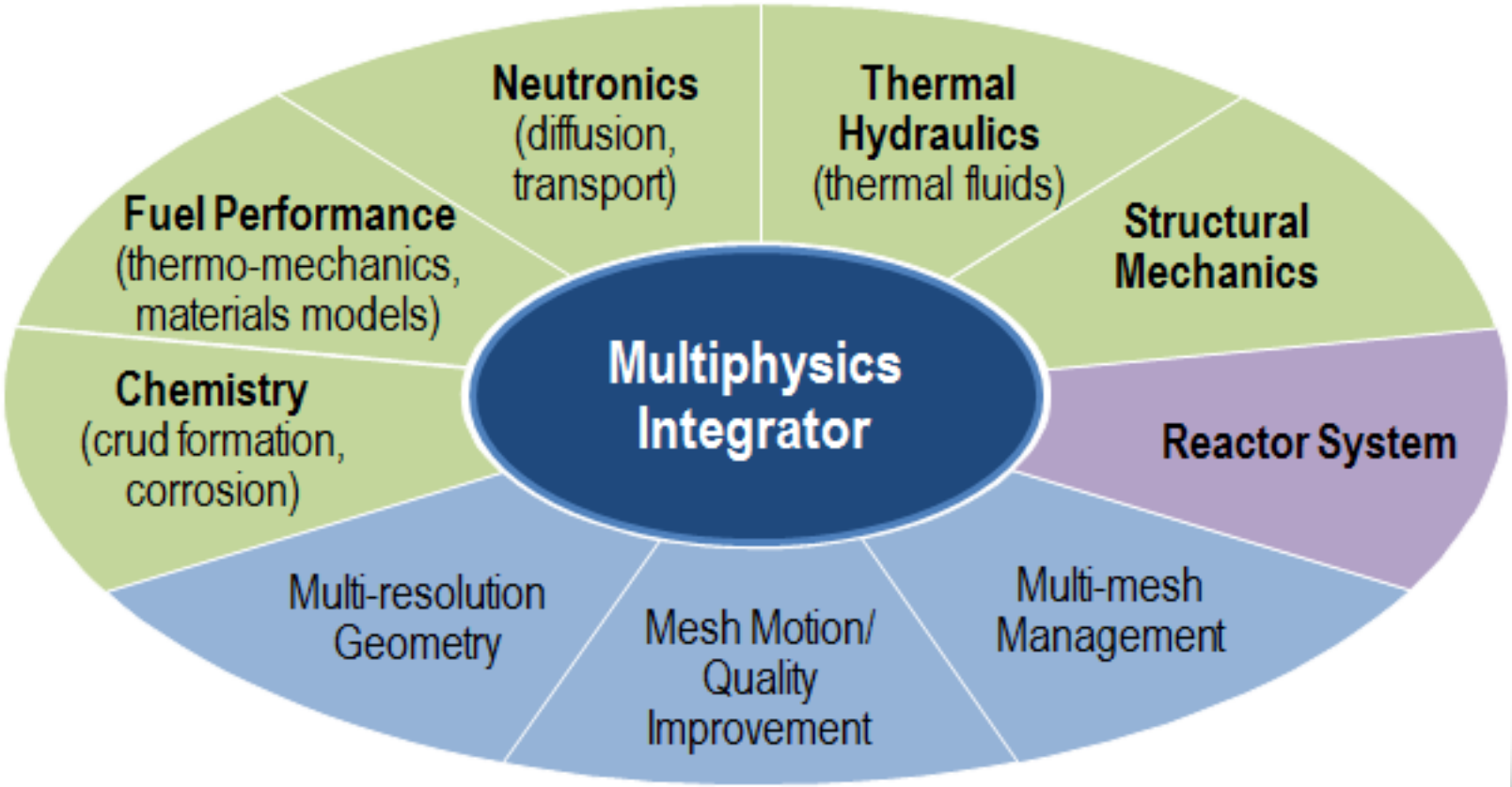
- *ORNL Staff*
  - Tom Evans
  - Greg Davidson
  - Josh Jarrell
  - Bob Grove
  - Chris Baker
  - Andrew Godfrey
  - Kevin Clarno
  - Douglas Peplow
  - Scott Mosher
- *CASL*
  - Roger Pawlowski
  - Brian Adams

Brendan Kochunis

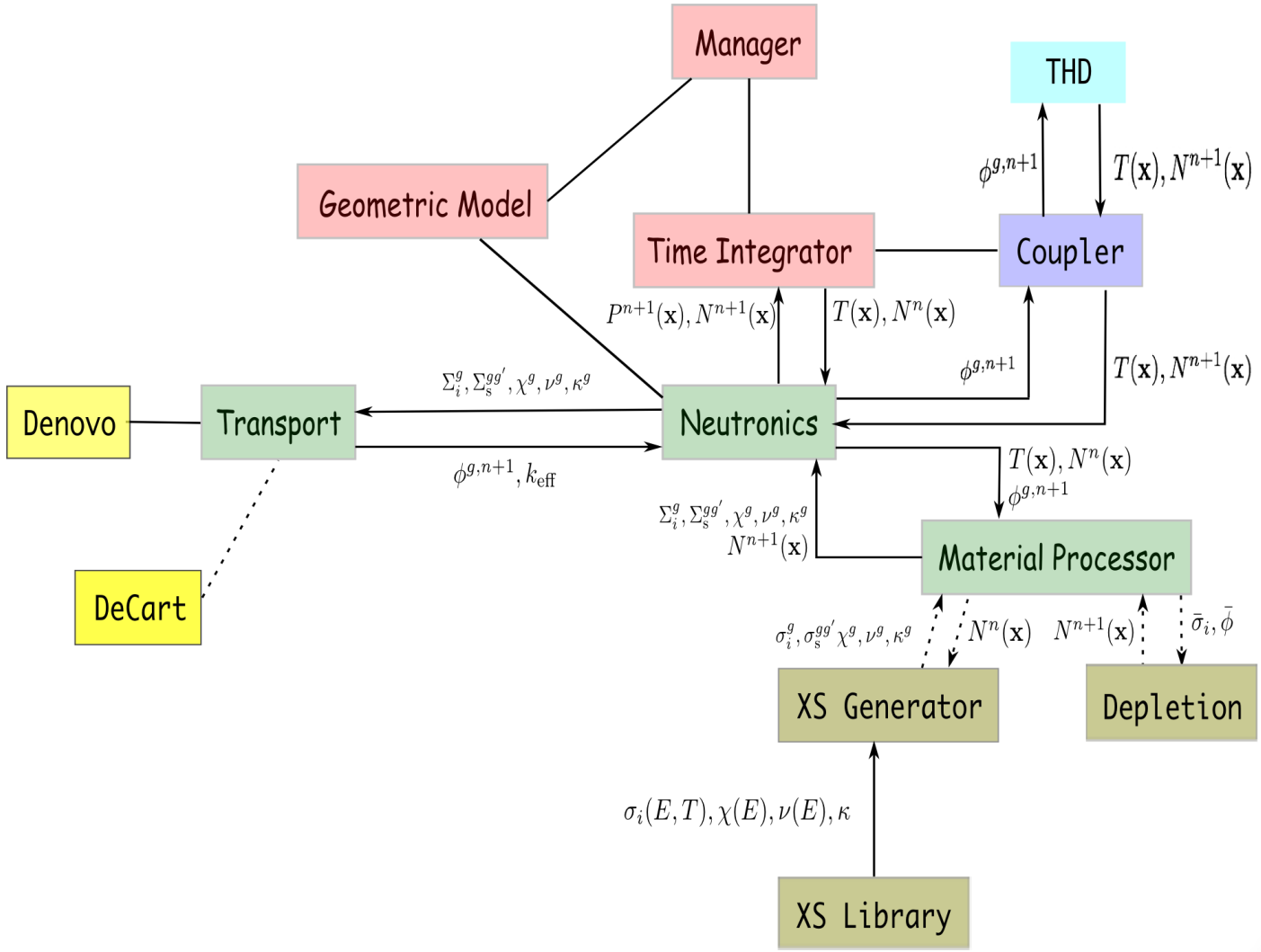
- *Students and Postdocs*
  - Stuart Slattery (Wisconsin)
  - Rachel Slaybaugh (Wisconsin)
  - Josh Hykes (North Carolina State)
  - Todd Evans (North Carolina State)
  - Cyrus Proctor (North Carolina State)
- *OLCF (NCCS) Support*
  - Dave Pugmire
  - Sean Ahern
  - Wayne Joubert

Virtual Reactor Simulation

Neutronics is one part of a complete reactor simulation



VERA (Virtual Environment for Reactor Applications) – Neutronics Package



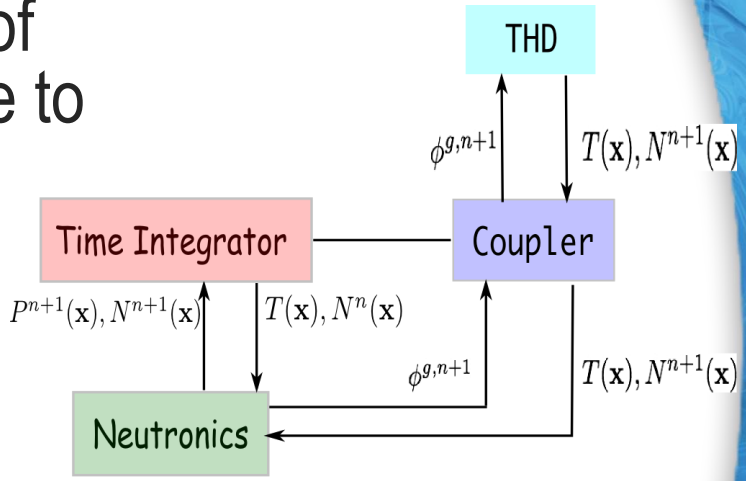
Denovo Capabilities

- State of the art transport methods
  - 3D/2D, non-uniform, regular grid S_N
  - Multigroup energy, anisotropic P_N scattering
  - Forward/Adjoint
  - Fixed-source/*k*-eigenvalue
  - 6 spatial discretization algorithms
    - Linear and Trilinear discontinuous FE, step-characteristics, theta-weighted diamond, weighted diamond + flux-fixup
  - Parallel first-collision
    - Analytic ray-tracing (DR)
    - Monte Carlo (DR and DD)
  - Multiple quadratures
    - Level-symmetric
    - Generalized Legendre Product
    - QR
- Modern, Innovative, High-Performance Solvers
  - Within-group solvers
    - Krylov (GMRES, BiCGStab) and source iteration
    - DSA preconditioning (SuperLU/ML-preconditioned CG/PCG)
  - Multigroup solvers
    - Transport Two-Grid upscatter acceleration of Gauss-Seidel
    - Krylov (GMRES, BiCGtab)
      - Multigrid preconditioning
  - Eigenvalue solvers
    - Power iteration (with rebalance)
      - CMFD in development
    - Krylov (Arnoldi)
    - RQI

Features of the Coupler

The coupler is designed to:

- Is designed to map a collection of points from one physics package to another.
- Is currently implemented for:
  - Denovo/Star-CCM+ coupling
  - Denovo/Drekar coupling
- Is general enough to support (with some additional development) any point-wise based couplings.
- Is general enough to support (with a fair bit of additional development) any coupling



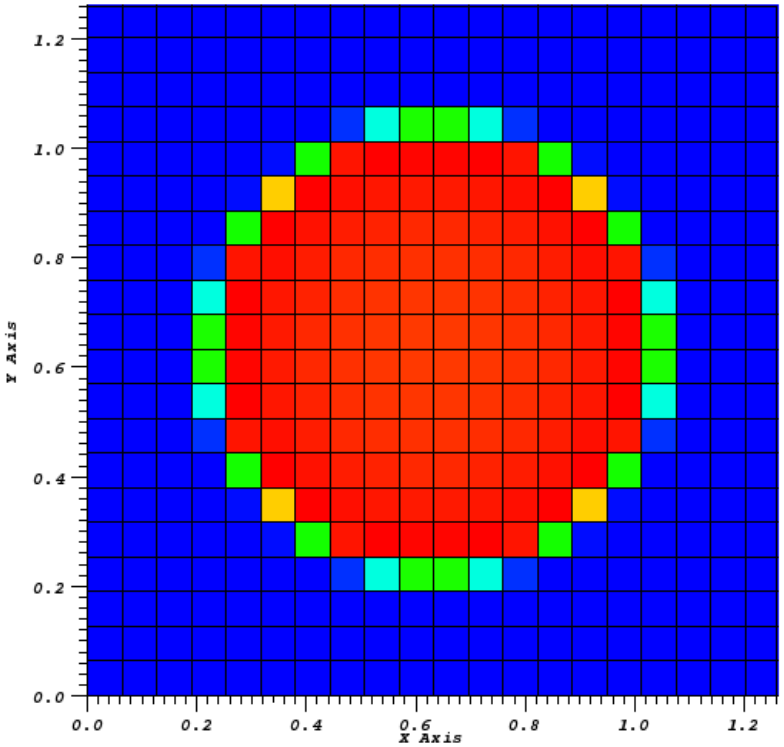
Coupler Setup

Coupling between Neutronics and THD is as follows:

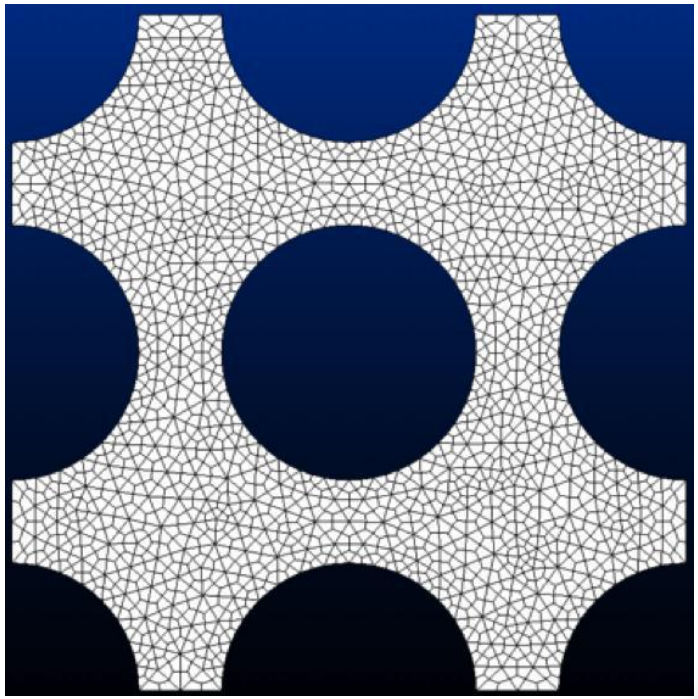
Neutronics Procs	THD Procs
Partition Neutronics	Partition THD
Instantiate Coupler	
Register Neutronics Object	Register Coupling Points

Building the Transfer Maps

Denovo Pincell Mesh



Drekar Pincell Mesh



Building the Transfer Maps

1. Every THD process sends a list of points to every Neutronics process (each point has a unique handle)
2. Every Neutronics process checks which points are in its domain and creates a local map

	THD Partition	Handle	X	Y	Z
Neutronics Partition 0	0	0	0.100	0.100	0.100
	1	1	0.110	0.100	0.100
Neutronics Partition 1	1	2	0.120	0.100	0.100
	4	3	0.130	0.100	0.100

Building the Transfer Maps

3. Every Neutronics process sends the points it owns back to the THD process
4. The THD processes assemble local maps

	Neutronics Partition	Handle	X	Y	Z
THD Partition 0	14	12	0.100	0.500	0.700
	26	102	0.110	0.500	0.700
THD Partition 1	12	33	0.110	0.600	0.700
	4	25	0.110	0.700	0.700

Building the Transfer Maps

Once finished:

- Every support point on the THD domain has been mapped to a Neutronics partition
- Every THD process knows which neutronics partitions own its points
- Every Neutronics process knows which points belong to which THD partition.
- Therefore, two-way mapping between partitions can be performed.
- This mapping stays constant as long as neither mesh or spatial partitioning changes.
- Any “point-wise” data can be transferred between physics packages

Transferring data

- Example: Transferring power to THD partitions
  - For every point in its local map, each Neutronics process computes the power at the point
  - The powers are sorted, packed into buffers, then sent to the appropriate THD process
  - Each THD process receives buffers of powers from each Neutronics process in its local map
  - The THD process writes those powers into the appropriate points

Neutronics/Star-CCM+ Coupling

- Star-CCM+ Coupling is file based
- The THD points are read in from a Star geometry file

Prostar Cell Id	Cell Index	Region Index	Volume (m^3)	X (m)	Y (m)	Z (m)
4.600e+002	0.000e+000	4.000e+000	1.397e-008	-1.522e-003	1.239e-002	1.000e-002
4.610e+002	1.000e+000	4.000e+000	1.397e-008	-1.419e-003	1.201e-002	1.000e-002
4.180e+002	2.000e+000	4.000e+000	1.397e-008	-1.522e-003	1.280e-002	1.000e-002
4.630e+002	3.000e+000	4.000e+000	1.397e-008	2.784e-003	1.223e-002	1.000e-002
1.948e+003	4.000e+000	4.000e+000	1.397e-008	-1.522e-003	1.239e-002	3.000e-002

Neutronics/Star-CCM+ Coupling

- The points are distributed to the neutronics processes and powers calculated as usual.
- Instead of distributing the powers back to the THD processes, it writes them to a Star-CCM+ power file

Enthalpy	X	Y	Z
0.745E+08	-0.141E-01	0.124E-01	0.100E-01
0.745E+08	-0.140E-01	0.120E-01	0.100E-01
0.745E+08	-0.141E-01	0.128E-01	0.100E-01
0.763E+08	-0.153E-01	0.122E-01	0.100E-01
0.745E+08	-0.141E-01	0.123E-01	0.300E-01

- Once the SCALE coupling is finished, the Coupler is ready to pass temperature data to the SCALE cross section processor

Using the Coupler

- Setup the neutronics object

```
Neutronics* neutronics;
if(on_neutronics)
{
      neutronics = new Neutronics("neut_input_file.inp");
      neutronics->setup();
}
```

- Setup the THD object

```
THD* thd;
if(on_thd)
{
      thd = new THD("thd_input_file.inp");
      thd->setup();
}
```

Using the Coupler

- Create the coupler and do setup

```
Coupler coupler(MPI_COMM_WORLD, comm_neutronics,
                comm_thd, neutronics, thd);
if(on_neutronics)
{
      coupler.register_neutronics(neutronics);
}
```

- Register the points from the THD package

```
if(on_thd)
{
      coupler.register_points(thd->get_points(),
                              thd->get_handles());
}
```

- Build the map

```
coupler->build_map();
```

Using the Coupler

- Perform the transport

```
if(on_neutronics)
{
      neutronics->transport();
}
```

- Transfer powers from the neutronics domain to the THD domain

```
coupler.transfer_power();
```

Future Work/Next Steps

- Add global balance data
  - Neutronics passes integrated global power (scalar) to THD that can be used to normalize the source yielding global conservation for codes with heterogeneous mesh representations
  - For non-strong coupling (T), there are no conservation requirements for THD ➔ Neutronics
- Couple SCALE XSProc package to Neutronics
  - This will allow temperature feedback from THD into cross sections
- Couple Drekar to Neutronics (both Denovo and DeCART)
  - This will allow massively-parallel CFD calculations without file-based coupling

Questions?

Materials Performance Optimization (MPO) Focus Area

Chris Stanek
Los Alamos National Laboratory

Brian Wirth
University of Tennessee

Sidney Yip
Massachusetts Institute of Technology

CASL Roundtable
NC State University
August 10, 2011

CASL-U-2011-0072-000-R

Attention span

Attention span is the amount of time that a person can concentrate on a task without becoming distracted. Most educators and psychologists agree that the ability to focus one's attention on a task is crucial for the achievement of one's goals.[1]

Length of the span

Estimates for the length of human attention span are highly variable and depend on the precise definition of attention being used.

- *Focused attention* is a short-term response to a stimulus that attracts attention. The attention span for this level is very brief, with a maximum span, without any lapse at all, that may be as short as 8 seconds.[2] This level of attention is attracted by a ringing telephone, or other unexpected occurrence. After a few seconds, it is likely that the person will look away, return to a previous task, or think about something else.
- *Sustained attention* is the level of attention that produces the consistent results on a task over time. If the task is handling fragile objects, such as hand-washing delicate crystal glasses, then a person showing sustained attention will stay on task and will not break any dishes, but a person who loses focus may break a glass or may stop washing the dishes to do something else. Most healthy teenagers and adults are unable to sustain attention on one thing for more than about 20 minutes at a time, although they can choose repeatedly to re-focus on the same thing.[2] This ability to renew attention permits people to "pay attention" to things that last for more than a few minutes, such as long movies.

Attention span, as measured by sustained attention, or the time spent continuously on task, varies with age. Older children are capable of longer periods of attention than younger children.[3]

For time-on-task measurements, the type of activity used in the test affects the results, as people are generally capable of a longer attention span when they are doing something that they find enjoyable or intrinsically motivating.[2] Attention is also increased if the person is able to perform the task fluently, compared to a person who has difficulty performing the task, or to the same person when he or she is just learning the task. Fatigue, hunger, noise, and emotional stress reduce time on task. Common estimates for sustained attention to a freely chosen task range from about five minutes for a two-year-old child, to a maximum of around 20 minutes in older children and adults.[2]

A different flavor of motivation:

- The first person to sit, after 11 minutes of applause for a Stalin speech, was sent to the gulag

Outline

- CASL/MPO background
  - Challenge problem focused
  - Balanced length scale approach

- Technical Results
  - Cross cutting areas: Zr-O-H thermodynamics, phase field hydrogen behavior, Zr-O-H pair potential derivation, atomistics of defect interaction in Zr, Zr creep
  - PCI: Peregrine, SCC and external interactions
  - CRUD: MAMBA, boron deposition model, Ni-O atomistics, CRUD phase thermodynamics
  - GTRF: SIERRA structural mechanics,

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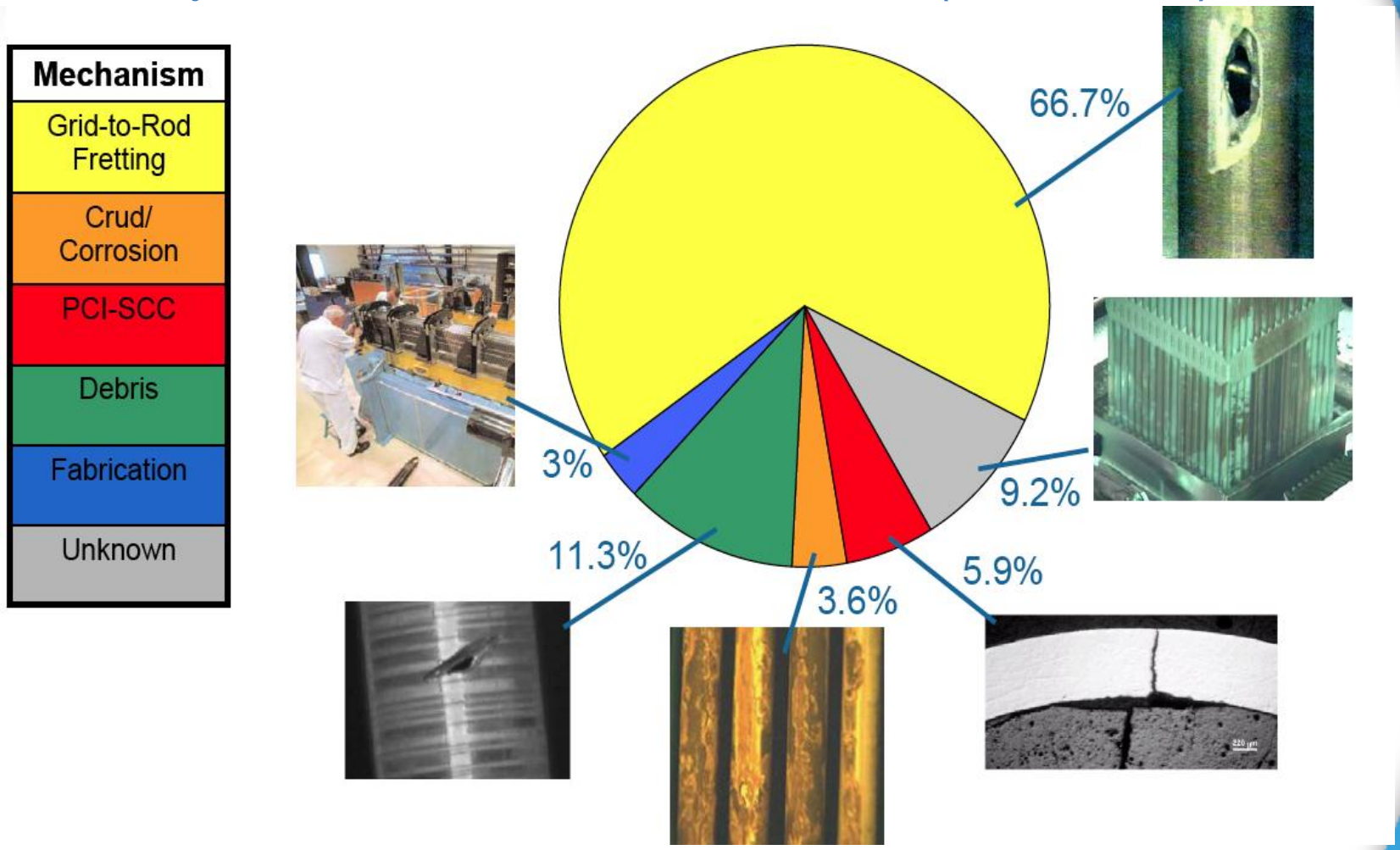
CASL Challenge Problems

Key phenomena limiting PWR reactor performance

	Power uprate	High burnup	Life extension
Operational			
CRUD-induced power shift (CIPS)	✕	✕	
CRUD-induced localized corrosion (CILC)	✕	✕	
Grid-to-rod fretting failure (GTRF)		✕	
Pellet-clad interaction (PCI)	✕	✕	
Fuel assembly distortion (FAD)	✕	✕	
Safety			
Departure from nucleate boiling (DNB)	✕		
Cladding integrity during loss of coolant accidents (LOCA)	✕	✕	
Cladding integrity during reactivity insertion accidents (RIA)	✕	✕	
Reactor vessel integrity	✕		✕
Reactor internals integrity	✕		✕

CASL Challenge Problems

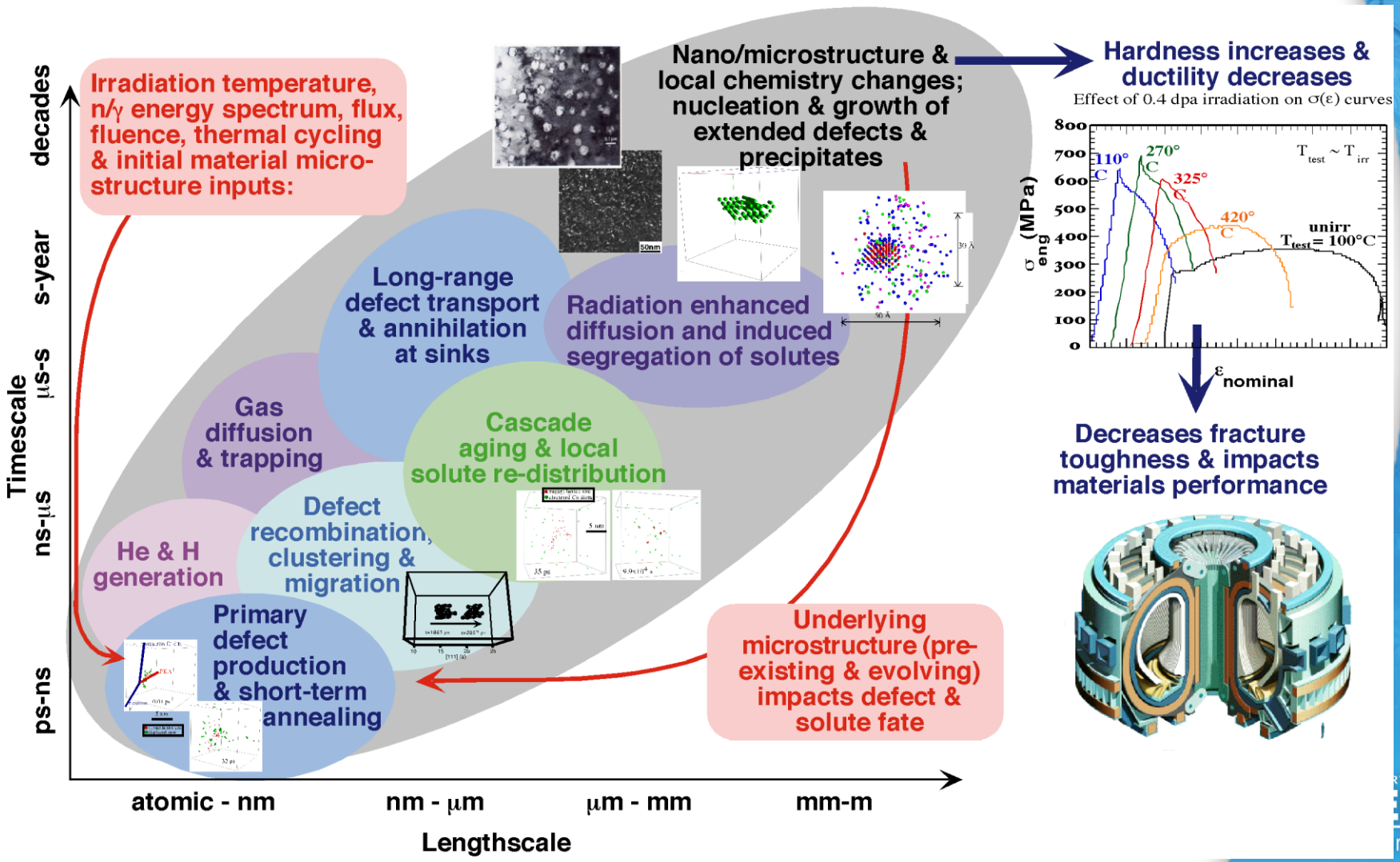
Summary of US fuel failure mechanisms (2000-2008)



* Edsinger, Stanek, Wirth, JOM **63, no. 8** (2011)

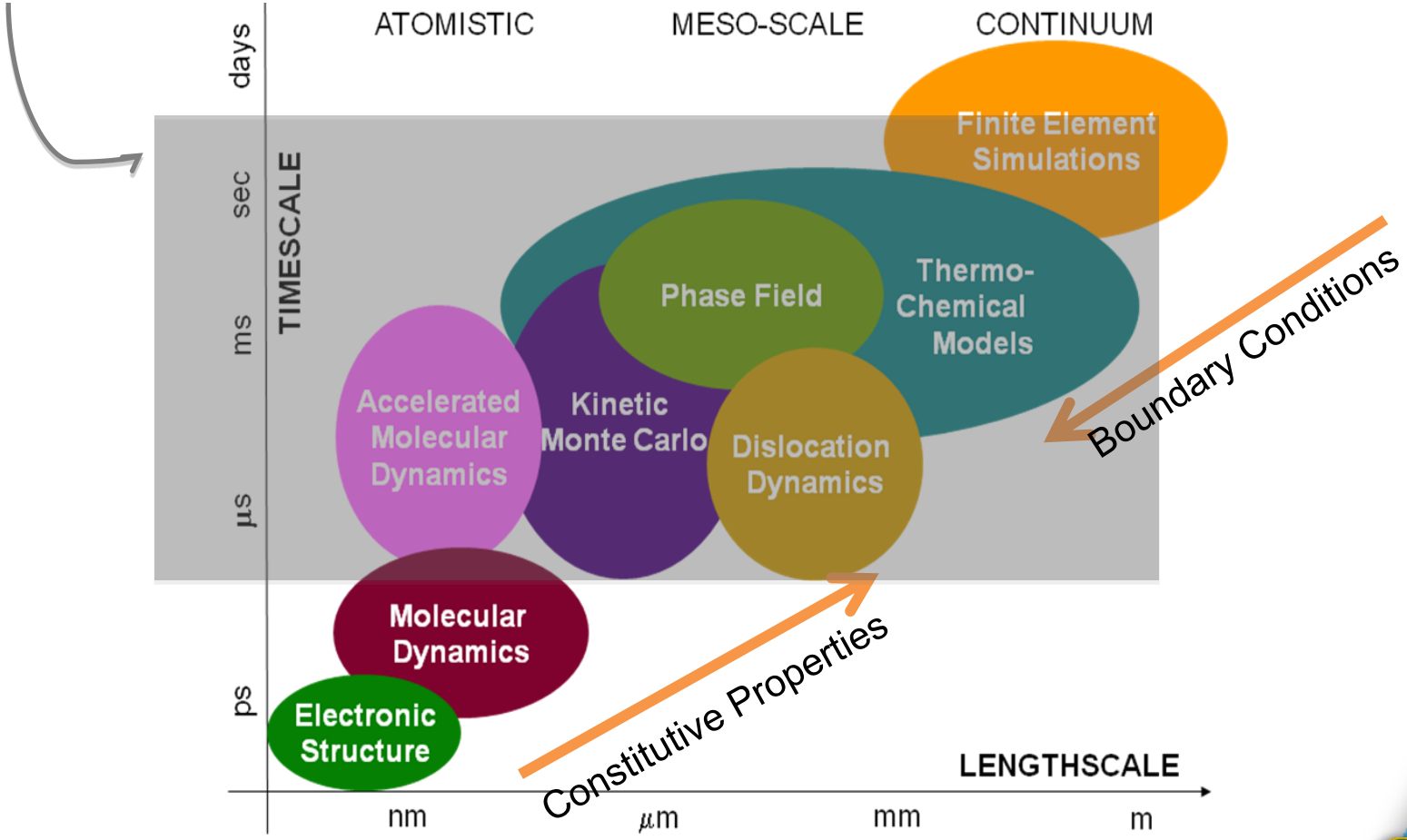
Fuel failure modes provide motivation for MPO activities

Materials performance in extreme radiation environments is controlled by multiscale processes



Multiscale Materials Modeling Approach

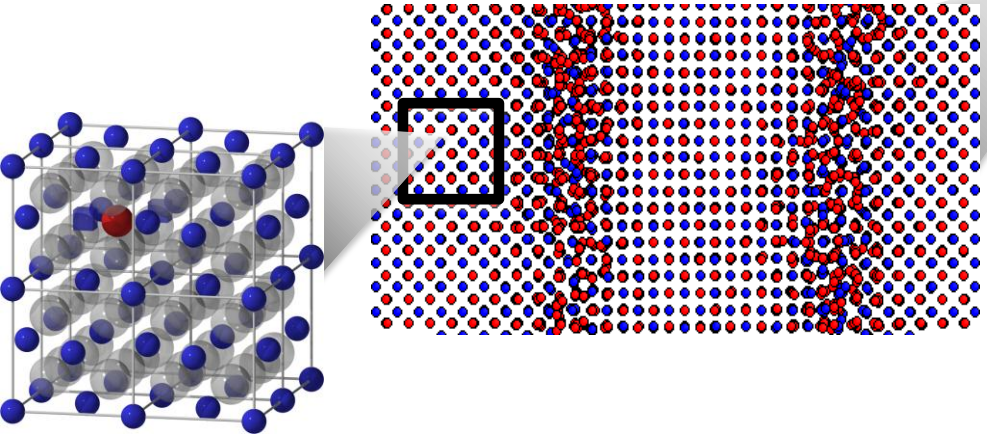
Our biggest scientific challenge is understanding the kinetics of coupled defect – solute/impurity evolution (not entirely unique to irradiation materials) with a wide range of kinetic rates

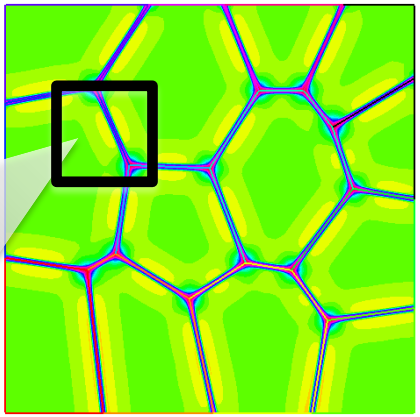


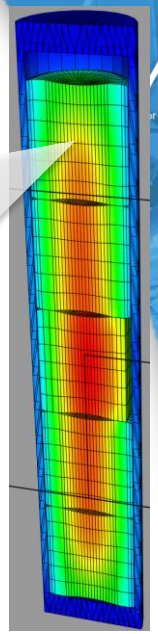
Materials Performance Optimization (MPO)

Enabling Improved Fuel Performance through Predictive Simulation

Challenging, multiscale processes impact nuclear fuel performance







Approach

- Provide physics-based materials models of fuel/clad/internals property evolution to enable predictive modeling of CRUD, GTRF and PCI within 3D, multi-physics, virtual reactor simulator
- Improved physics and chemistry insight delivered via constitutive relations
- MPO is comprised of a diverse group of computational materials scientists with a wide range of capabilities

Outcomes and Impact

- Predictive models of fuel failure, that quantitatively define operating margins & lifetime limits
- Validated predictions of fuel failure conditions
- Power uprates & increased fuel utilization

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MPO objective: *Deliver materials physics-based constitutive models to the virtual reactor for CASL challenge problems*

Near term effort

Incorporate available, engineering-scale fuel/clad/corrosion constitutive models into 3-D, high resolution coupled physics simulation capability (interfaced with virtual reactor);

Initiate a series of microscale activities to provide mechanistic/physical insight into complex degradation phenomena corresponding to challenge problems: PCI, GTRF and CRUD

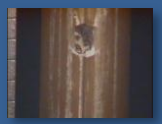
Intermediate and out-year effort

Microscale models will be used to refine physics-based constitutive relations that can address coupled environments of T, stress, reactivity, radiation, etc.

Improved constitutive models are then utilized by the virtual reactor for fully coupled neutronics, CFD/thermal hydraulics simulations of fuel behavior.

MPO Challenge Problems

GTRF



CRUD

PCI

Vera Integration (VI) Project: Initially define structural mechanics & coupled physics FEM modeling framework for GTRF, PCI and CRUD. Assess predictions versus experiment, interact with other FAs & guide advanced constitutive model development

GTRF:
* VI/FEM implementation

* Surface tribology

CRUD:
* Chemical kinetics
* Boron incorporation
* Thermodynamics of mixed oxides
* Thermal conductivity

CORROSION:
* General oxidation
* Hydriding
* Stress corrosion cracking

CLAD (& grid):
* atomistics /microstructure / hydrides / dislocations / strength-creep

Cross-cutting sub-groups:
* Potentials
* Clad microstructure
* Clad strength/properties

FUELS:
* Fuel pellet restructuring / fission gas release / fuel creep / pellet – clad interaction

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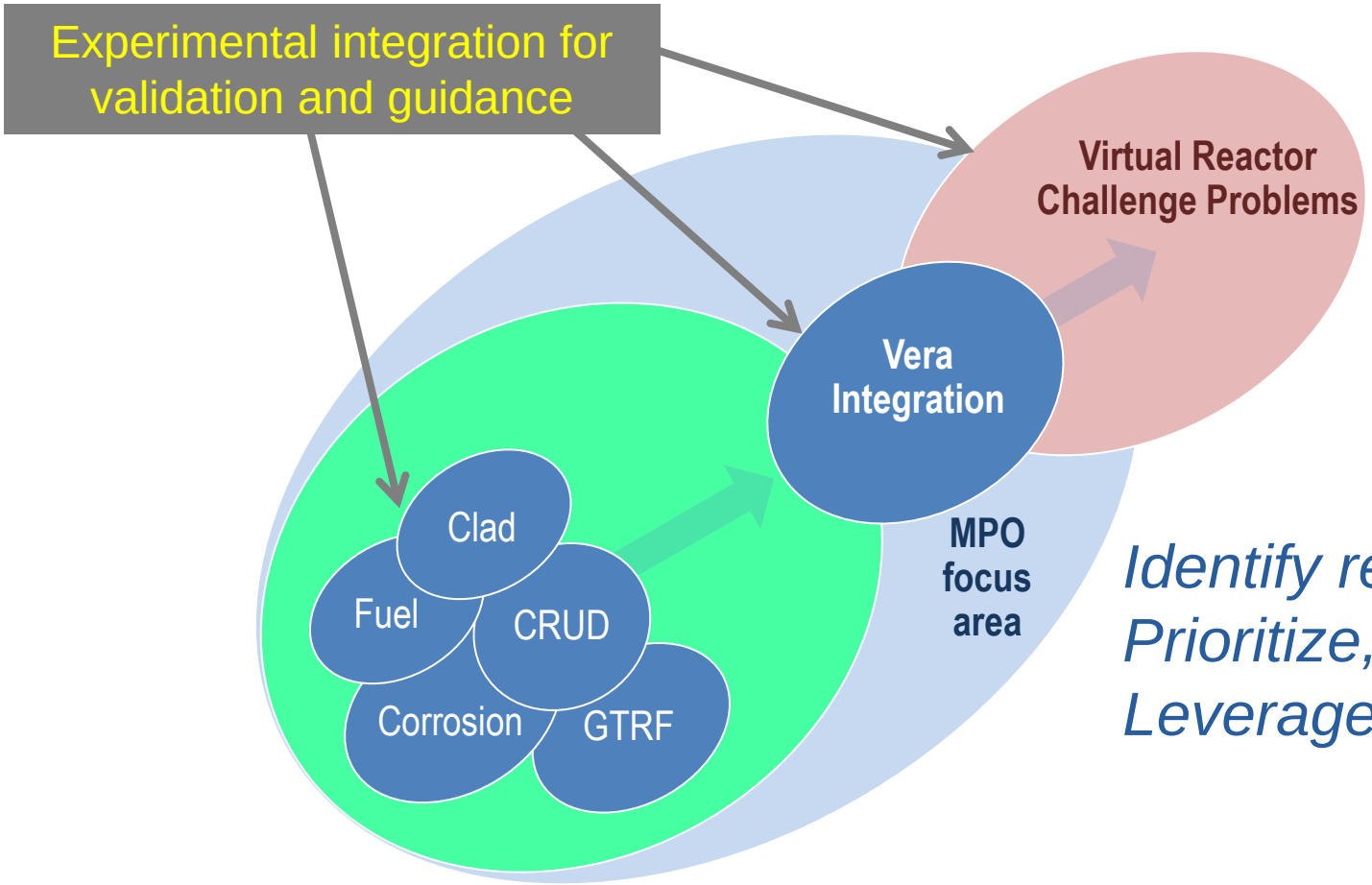
MPO aims to integrate microscale materials science into constitutive models for multiphysics virtual reactor challenge problems



Identify relevance, Prioritize, Leverage

Important to achieve balance between continuum and atomistic

Cross cutting technical results

- Zr-O and Zr-H thermodynamics
- Phase field/smooth boundary method for hydride formation/growth
- Zr-O-H “COMB” atomistic pair potentials
- Defect interactions in Zr
- Zr thermal and radiation creep

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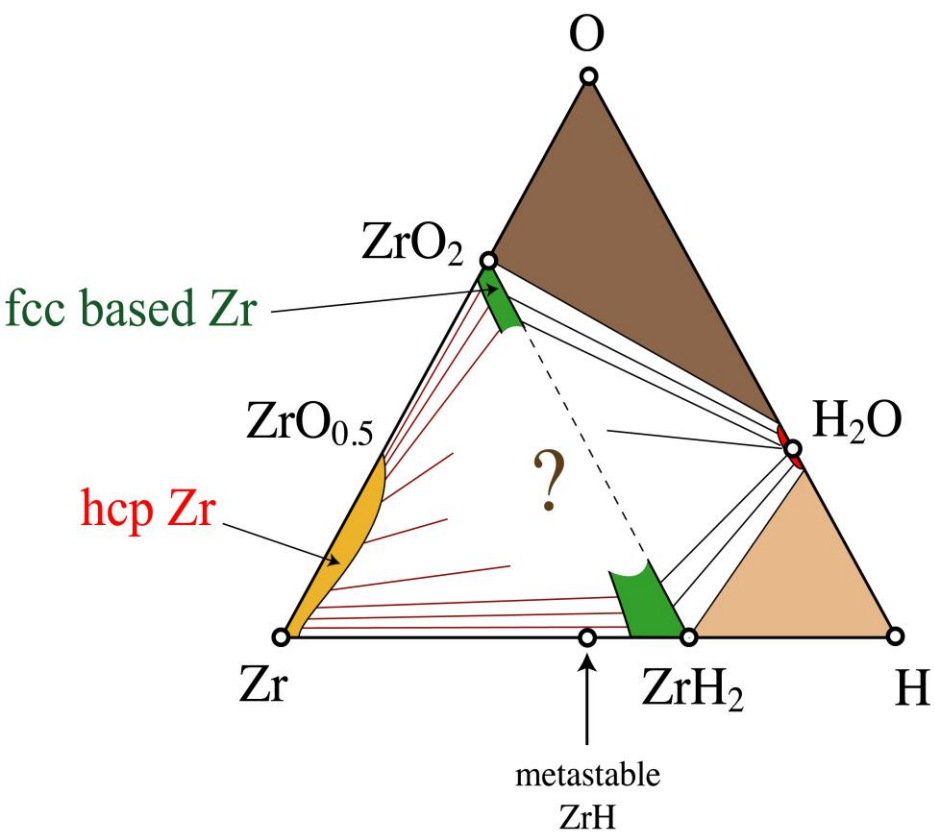
First-principles prediction of thermodynamic properties in the Zr-O-H system

Anton Van der Ven and Qingchuan Xu (Univ. of Michigan)

Continuum simulations of oxide formation on the clad surface as well as internal hydride nucleation and growth requires as input crucial thermodynamic and kinetic data, such as:



- Free energies of the relevant solid solutions, oxides and hydrides,
- Metastability of non-equilibrium hydrides
- The electronic structure of the various phases to establish whether corrosion product oxides and hydrides are metallic, semiconducting or insulating (important for setting up a physically relevant continuum level simulation of corrosion that accounts for electron transport)
- Oxygen and hydrogen diffusion coefficients in the various phases (hcp Zr and hydrogen diffusion in substoichiometric hydrides).

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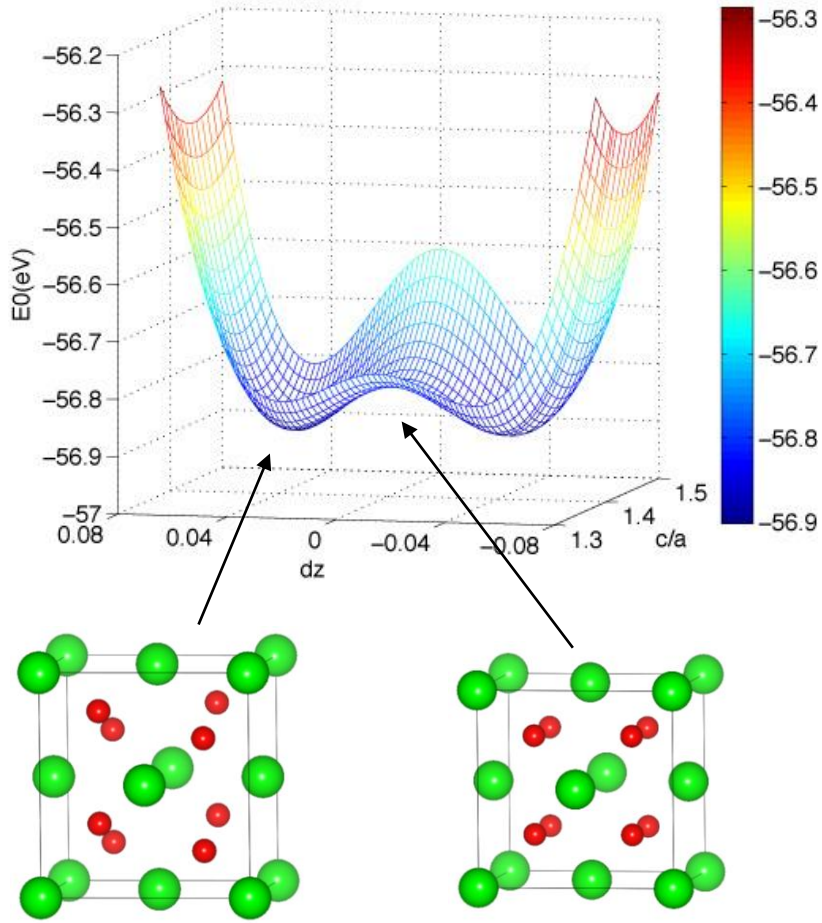
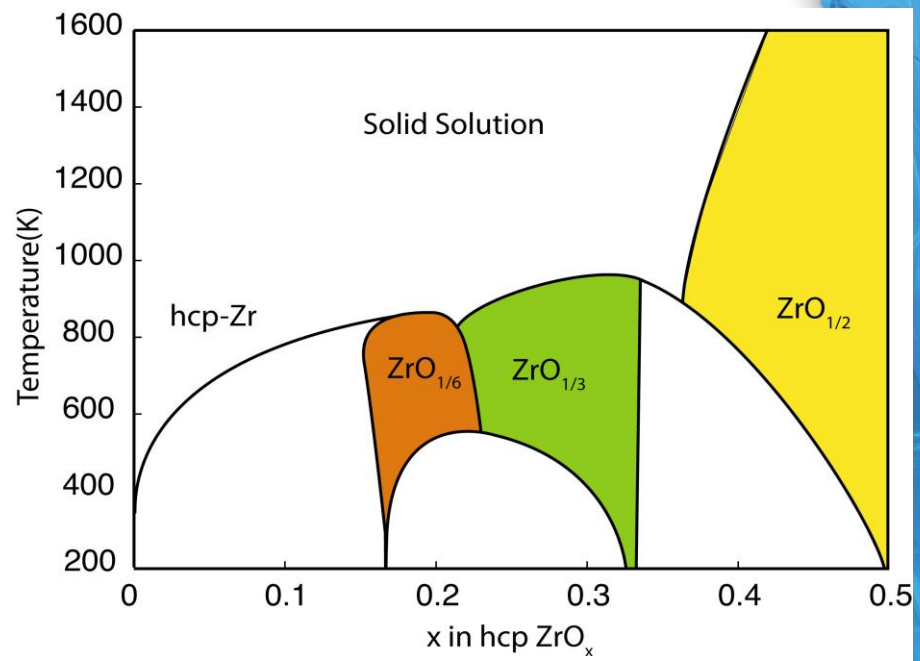
Thermodynamic properties of the binary Zr-O system

Anton Van der Ven and Qingchuan Xu (Univ. of Michigan)



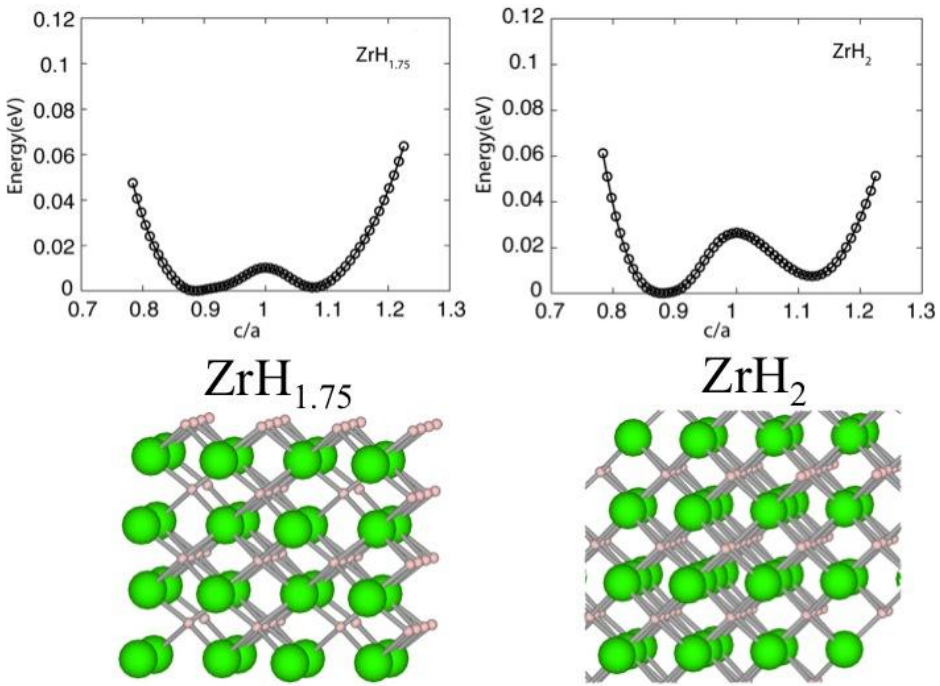
The energy of ZrO_2 as a function of c/a ratio and an internal shuffle variable that measures the extent with which alternating (110) planes of oxygen move up and down.



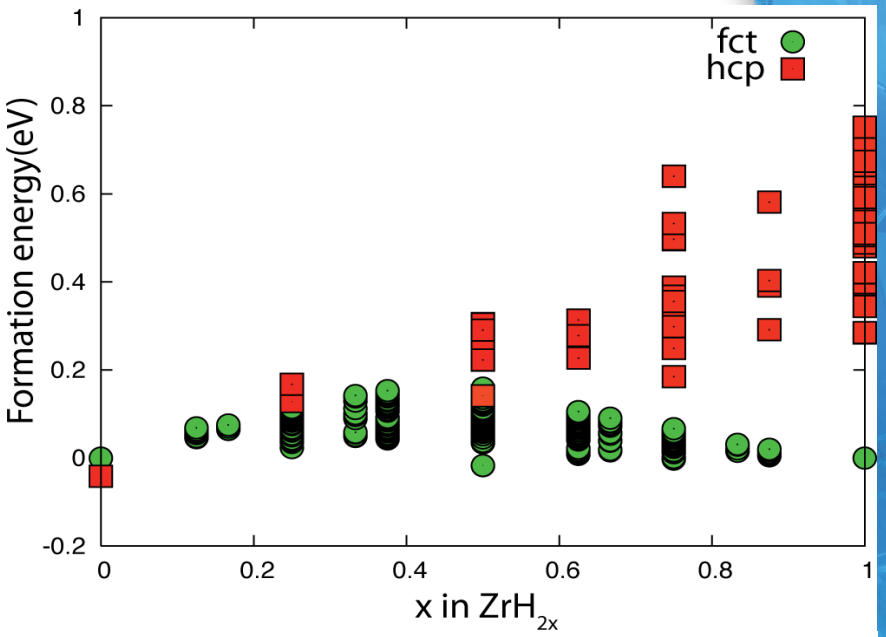
Calculated temperature composition phase diagram of ZrO_x within the hcp Zr crystal. Beyond x=0.5, the hcp form of ZrO_x transforms to ZrO_2 through a two-phase reaction (not shown).

Thermodynamic properties of the binary Zr-H system

Anton Van der Ven and Qingchuan Xu (Univ. of Michigan)



Variation of the energy of ZrH_{2-x} as a function of c/a ratio. The cubic phase is predicted to be mechanically unstable at zero Kelvin (i.e. does not reside at a local energy minimum). Extraction of hydrogen from ZrH_2, as in $ZrH_{1.75}$ above, results in a reduction in the energy difference between tetragonal and cubic symmetry



Formation energies of hcp Zr containing H in both tetrahedral and octahedral interstitial sites (red squares) and of tetragonally distorted fcc Zr with hydrogen over interstitial tetrahedral sites (green circles).

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Phase Field (Smooth Boundary Method) Simulation of Hydride Formation and Growth

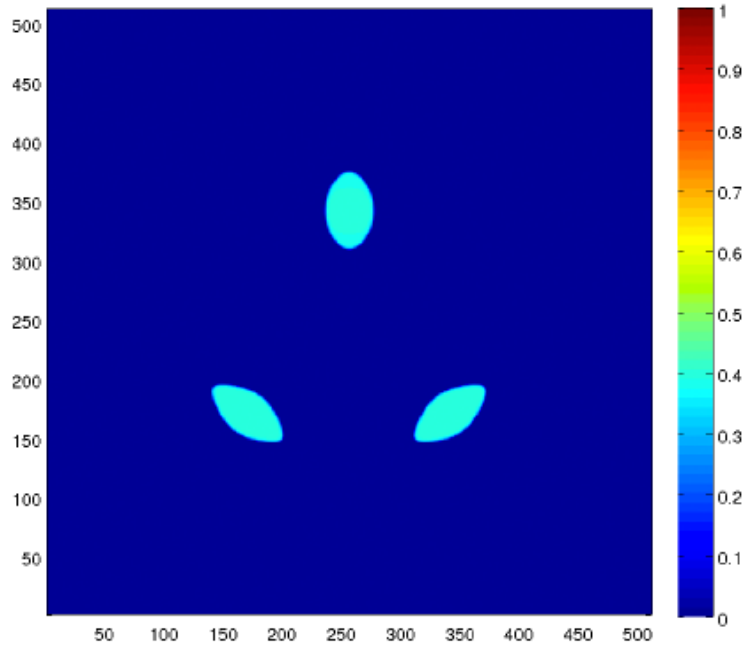
Andrea Jokisaari and Katsuyo Thornton (Univ. of Michigan)

Cladding embrittlement is related to increased hydrogen content during operation in the form of brittle zirconium hydride precipitates.

Array of hydrides in Zr – showing 3 orientations, from Bradbrook et al 1972

Initial phase field calcs (Guo) show 3 orientations.

A more realistic free energy functional is being developed.



$$E_{dis} = \frac{1}{2}\int_V \lambda_{ijkl} e^0_{ij}(\mathbf{x})\, e^0_{kl}(\mathbf{x})\, dV - \bar{\epsilon}_{ij}\int_V \lambda_{ijkl} e^0_{ij}(\mathbf{x})\, dV + \frac{V}{2}\lambda_{ijkl}\bar{\epsilon}_{ij}\bar{\epsilon}_{kl}$$

$$- \int_V \lambda_{ijkl} e^0_{ij}(\mathbf{x})\, \bar{\epsilon}_{ij}(\mathbf{x})\, dV + \frac{1}{2}\int_V \lambda_{ijkl}\bar{\epsilon}_{ij}(\mathbf{x})\, \bar{\epsilon}_{kl}(\mathbf{x})\, dV,$$

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COMB Pair Potential Derivation for Zr-O-H

Simon Phillpot (UF) and Stephen Foiles(Sandia)

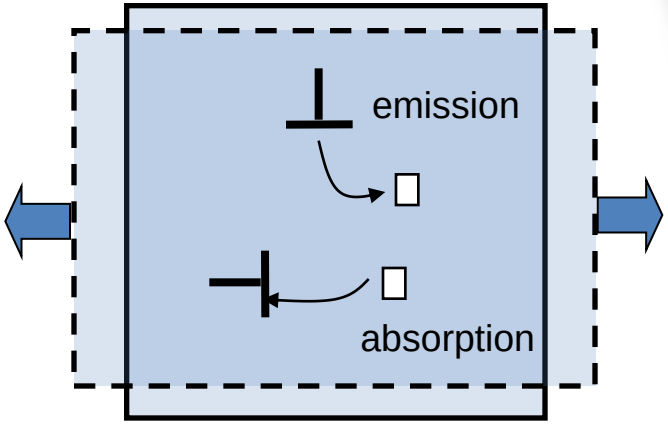
DFT unable to consider sufficiently many atoms for multidimensional defect interaction – thus pair potentials required (COMB).

Properties	Experiment	DFT	EAM [3]	AMEAM [7]	COMB
a (Å)	3.232 [1]	3.23 [4]	3.234	3.231	3.22
c (Å)	5.182 [1]	5.17 [4]	5.168	5.148	5.203
c/a	1.6033 [1]	1.6006 [4]	1.598	1.5932	1.6143
I_2 stacking fault {0001} [mJ/m^2]		200.3 [5]	198	26	213
I_1 stacking fault {1-100} [mJ/m^2]		145.8 [5]	174	13	115
$E_{vacancy}$ (unrelaxed, T=0) [eV]		2.077 [3]	1.762	1.75	2.00
E, Octa. Int. [eV]		2.84 [6]	2.88	3.57	3.87
E, Basal Crowdion [eV]		2.95 [6]	2.91	3.52	4.05
C_{11} (GPa)	155 [2]	156 [4]	147	144	157
C_{12} (GPa)	67 [2]	61 [4]	69	74	69
C_{13} (GPa)	65 [2]	62 [4]	74	67	60
C_{33} (GPa)	172 [2]	166 [4]	168	166	168
C_{44} (GPa)	36 [2]	26 [4]	44	33.4	40
Basal S.E. {0001} [J/m^2]		1.60 [4]	1.77	0.988	1.45
Prism S.E. {10-10} [J/m^2]		1.66 [4]	1.93	0.978	1.49

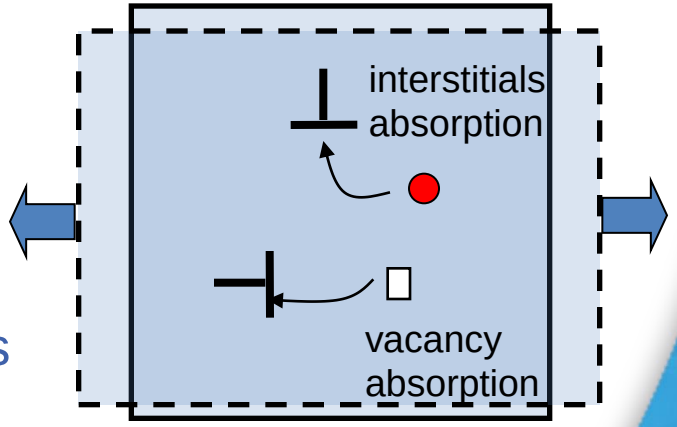
Mechanisms of Thermal and Irradiation Creep

Carlos Tome, LANL

Thermal creep: thermally activated vacancy diffusion
→ climb-controlled glide of dislocations
→ need to balance sources and sinks
→ relevant at high temperature or for close-to-yield stresses

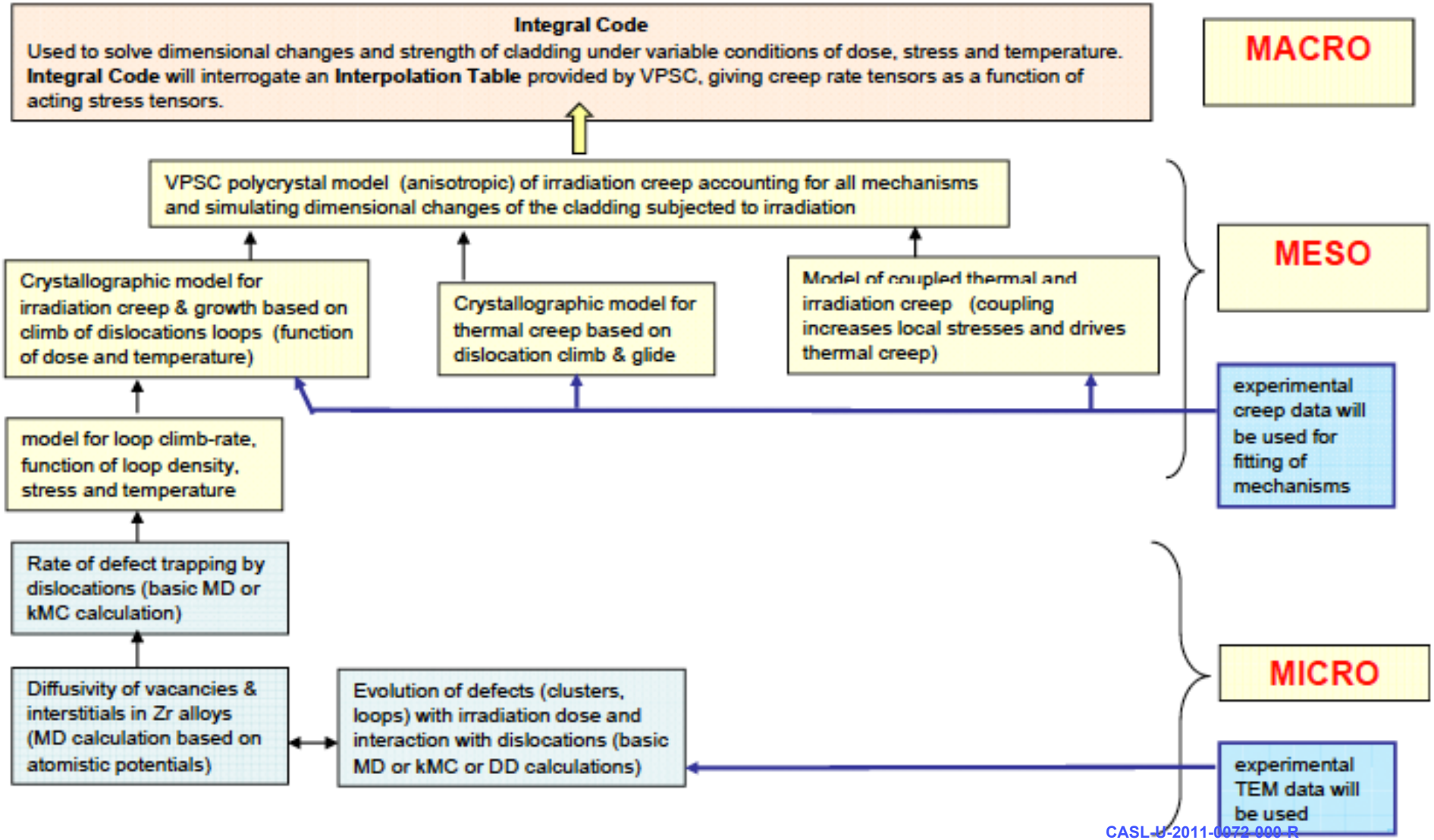


Irradiation creep: driven by super-saturation of vacancies and interstitials
→ climb of dislocation loops
→ climb and glide of edge dislocations
→ relevant at all irradiation temperatures



Multiscale Modeling of Thermal and Irradiation Creep in Zr

Carlos Tome, LANL

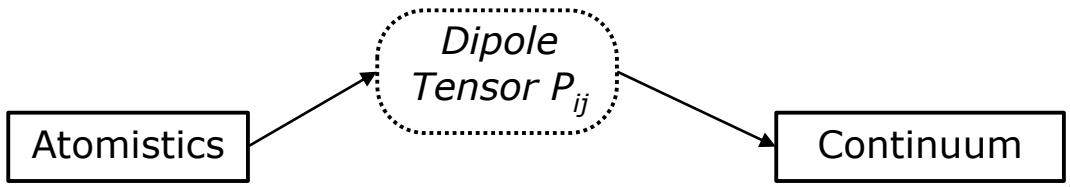


Atomistic characterization of point defects in Zr

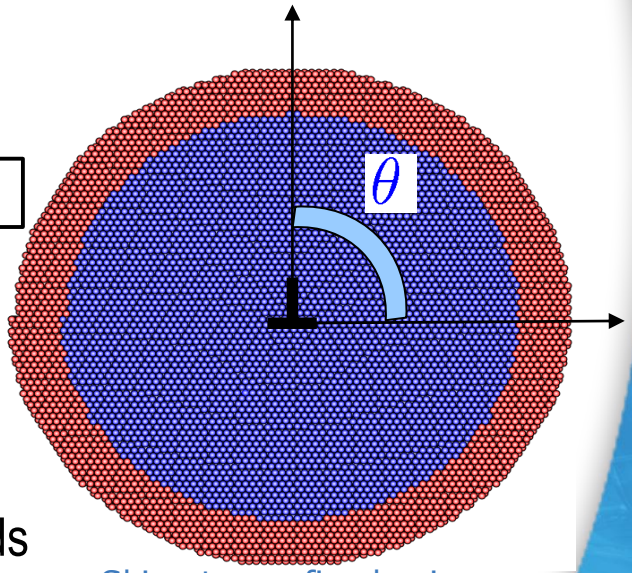
Subramanian et al. (LANL) Osetskiy, et al. (ORNL), Yildiz et al. (MIT)

GOAL: provide atomistic basis for modeling creep in cladding material

- Unit processes of creep – flow of defects into dislocation
- Flow of defects depends on energy landscape in field of dislocation
- Energy landscape obtained from atomistics is recast into continuum form in order to bridge scales



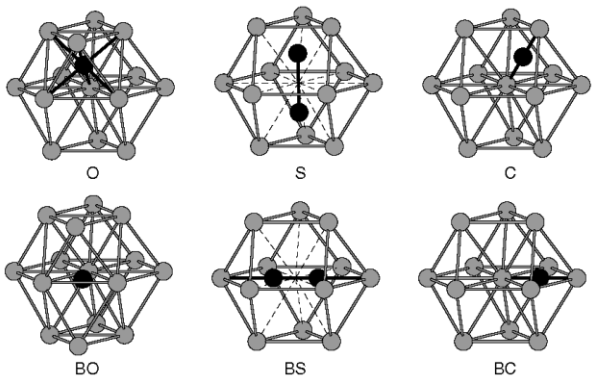
- Dipole Tensor P_{ij} :
  - ➔ Continuum property, computed from atomistics
  - ➔ Characteristic of a defect
- We use the Energy Derivative method, which yields accurate results for defects with long-range strain fields
- Introduce defects, compute energy from atomistics, and compare with theory



Skin atoms, fixed using anisotropic elasticity

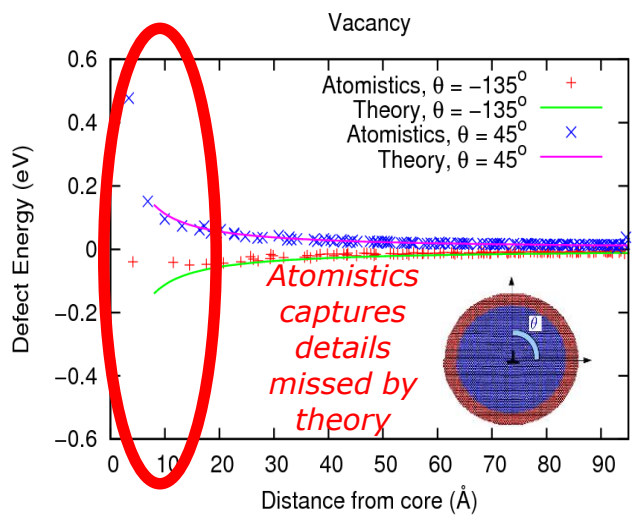
Atomistic characterization of point defects in Zr

Subramanian et al. (LANL) Osetskiy, et al. (ORNL), Yildiz et al. (MIT)

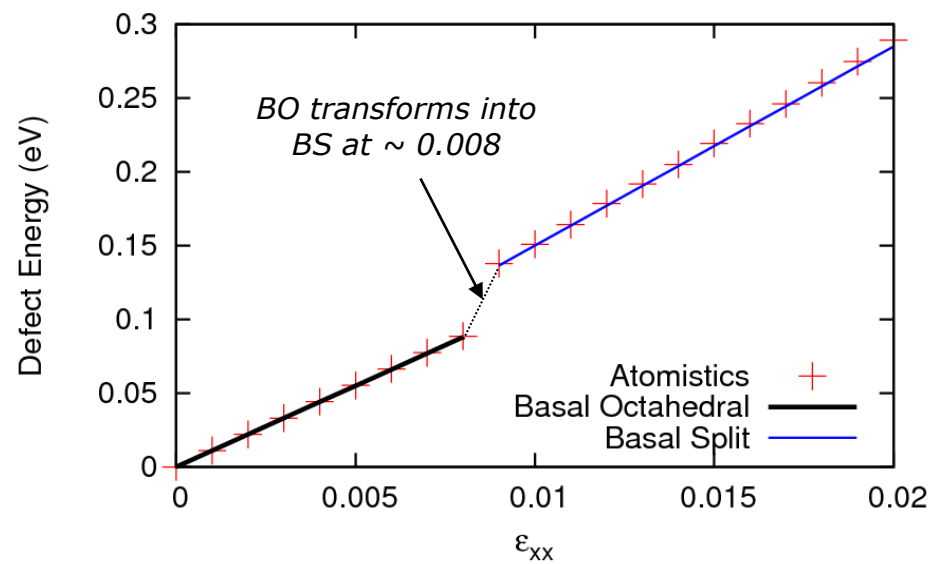


Types of self-interstitials

We can now predict defect-dislocation interaction with high accuracy, including effects that go beyond anisotropic linear elasticity



Defect energy in the field of a dislocation. Away from the core, atomistics matches continuum solution



Comparison of atomistics and continuum defect energies for interstitials. Excellent agreement is obtained for strains up to ~ 5% (full range not shown)

Viscoplastic Self Consistent (VPSC) Model

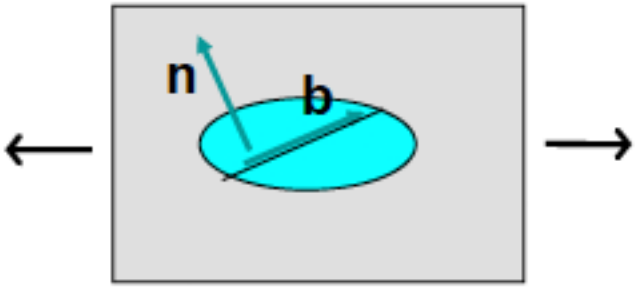
Carlos Tome, LANL

Each grain is treated as a visco-plastic anisotropic ellipsoidal inclusion embedded in a visco-plastic anisotropic Homogeneous Effective Medium.

Solve stress equilibrium equation for inclusion in the homogeneous medium.

→ Eshelby problem !

$$\sigma_{ij,j} = 0$$



Constitutive creep law for the grain

$$\dot{\varepsilon}_{ij}^{grain} = \dot{\varepsilon}_{ij}^{glide} + \dot{\varepsilon}_{ij}^{climb} = \dot{\gamma}_0^{gl} \sum_s m_{ij}^s \left(\frac{m_{kl}^s \, \sigma'_{kl}}{\tau_o^{glide}} \right)^{n_{gl}} +$$

$$\sum_k \rho^{(k)} b_i^{(k)} b_j^{(k)} \left(\Phi_0^{(int)} + \Delta\Phi_{(\sigma)}^{(int)} - \Phi_0^{(vac)} + \Delta\Phi_{(\sigma)}^{(vac)} \right)$$

Model gives the constitutive creep law for the polycrystal : $\bar{\dot{\varepsilon}} = \bar{M} : \bar{\sigma} + \bar{\dot{\varepsilon}}_0$

and the stress and creep rate in each grain: $\dot{\varepsilon}_{ij}^{grain}$ and σ_{ij}^{grain}

Applications of VPSC

- ACCELERATED GROWTH: Simulations showing that Irradiation Growth Rate increases in Zr alloys due to climb and growth of c-type interstitial loops

C.N. Tome, N. Christodoulou, *Philos. Mag.* **80** (2000) 1407

- Simultaneous action of Thermal and Irradiation Creep at the grain level lead to a coupling that gives a larger creep rate than the direct sum of both contributions taken separately

Turner, Tome, Christodoulou, Woo, *Philos. Mag.* **79** (1999) 28.

Upscaling to Peregrine:
Lookup Table Approach

A procedure to find the creep-rate tensor associated with an applied stress tensor

→Using the polycrystal model calculate response associated with regularly spaced stress states

→Create interpolation table

* given a stress state → $\bar{\sigma}_{ij}$
* find the 4 angles defining its direction → $\theta_1, \theta_2, \theta_3, \theta_4$
* find the closest angles in the Table → $\theta_i^{lower}, \theta_i^{upper} \quad (i = 1,4)$
* perform a Taylor expansion calculating incremental derivatives:

$$\dot{\varepsilon} = f_{(\theta_i)} \cong f_{(\theta_i^{lower})} + \sum_{k=1}^{4} \frac{f_{(\theta_i^{upper})} - f_{(\theta_i^{lower})}}{\theta_k^{upper} - \theta_k^{lower}} (\theta_k - \theta_k^{lower})$$

Deliver a subroutine for interpolatation of stress and strainrate

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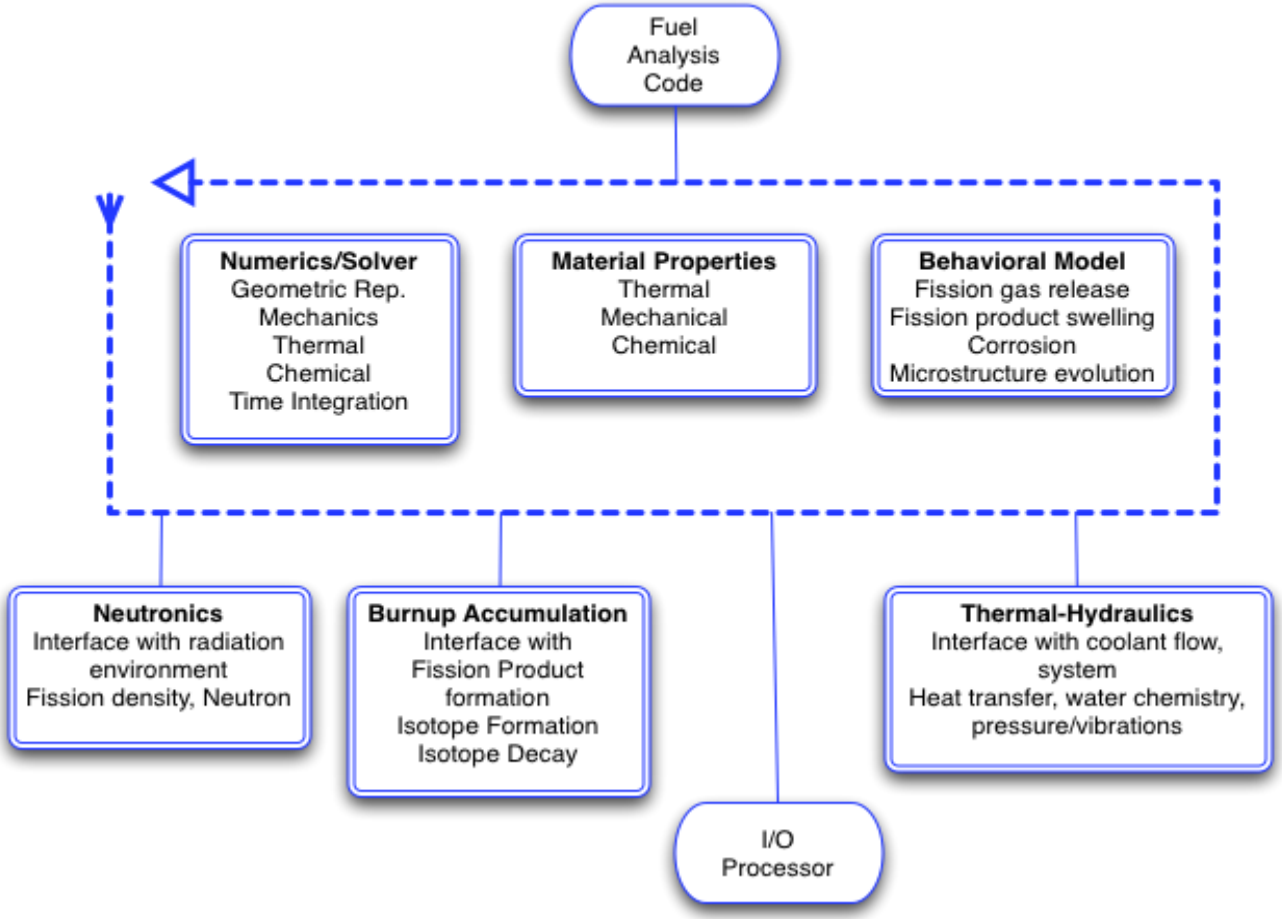
Fuel Performance Modeling:
PCI Challenge Problem

Major Components of Nuclear Fuel Modeling Capability



L2.MPO.P2.03

Deliver a Structural Mechanics Framework for PCI Challenge Problem -

"Peregrine"

Chris Stanek
LANL

Brian Wirth
UTK

Derek Gaston, Cody Permann, David Andrs Jason Hales, Steve Novascone, Rich Williamson and Rich Martineau
INL

Robert Montgomery*, Joe Rashid, Bob Dunham, Dion Sutherland
Anatech

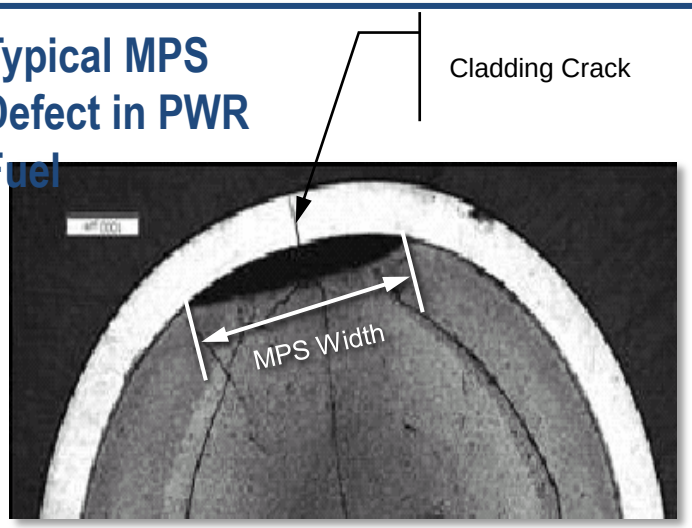
Currently at Pacific Northwest National Laboratory

CASL-U-2011-0072-000-R

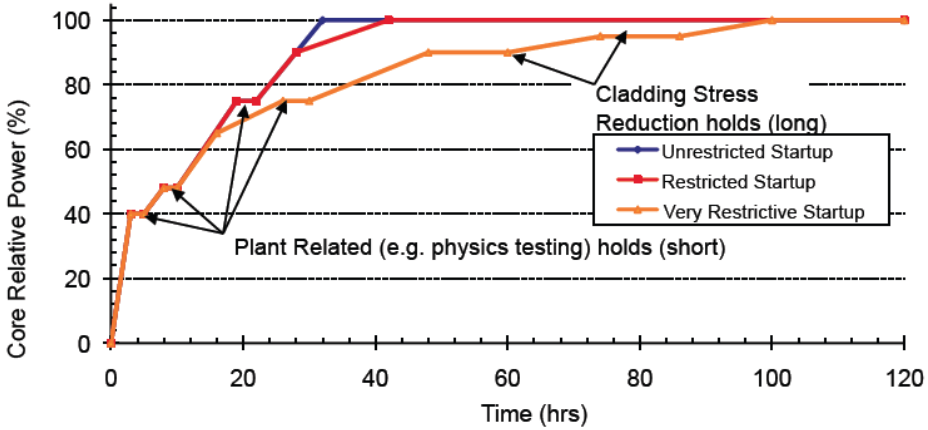
New 3D multiphysics fuel performance simulation capability to assess Pellet Clad Interaction (PCI)

- PCI limits reactor performance associated with power uprates, higher burnup and manufacturing quality assurance around missing pellet surface (MPS) chips and operating flexibility during power changes
- Current capability: MOOSE-based BISON
- CASL-developed capability = Peregrine (based on MOOSE)
- 3D fuel performance model is critical to assess complex, coupled physics and irregular geometries responsible for PCI fuel failures and reactor performance

Typical MPS Defect in PWR Fuel



Impact of MPS Defect on Power Operation



Figures from Robert Montgomery (Anatech)

Peregrine 3D fuel performance model being developed for CASL

Current MOOSE-BISON Capability

General Capabilities

* 3D and 2D axisymmetric fully-coupled thermomechanics
* Large deformation mechanics
* Steady and transient operation
* Parallel computation
* Meso-scale informed material models
* Species diffusion

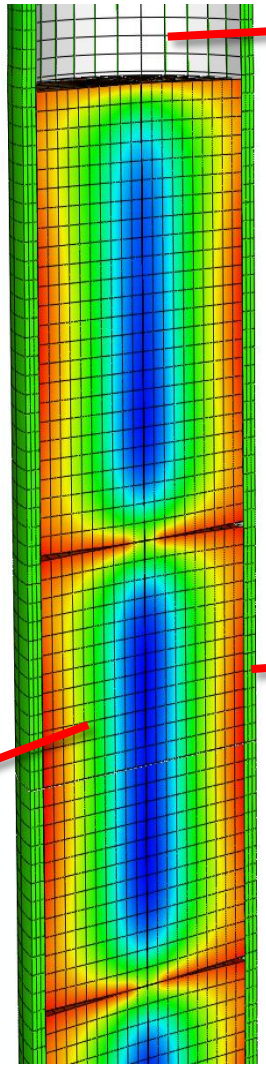
Gap/Plenum Behavior

* Gap heat transfer with kg= f (T, n)
* Mechanical contact
* Plenum pressure as a function of:

- evolving gas volume (from mechanics)

- gas mixture (from FGR model)

- gas temperature approximation



Oxide Fuel Behavior

* Temperature/burnup dependent conductivity
* Thermal expansion
* Volumetric heat generation (fission)
* Two-stage fission gas release
* Solid and gaseous fission product swelling
* Densification

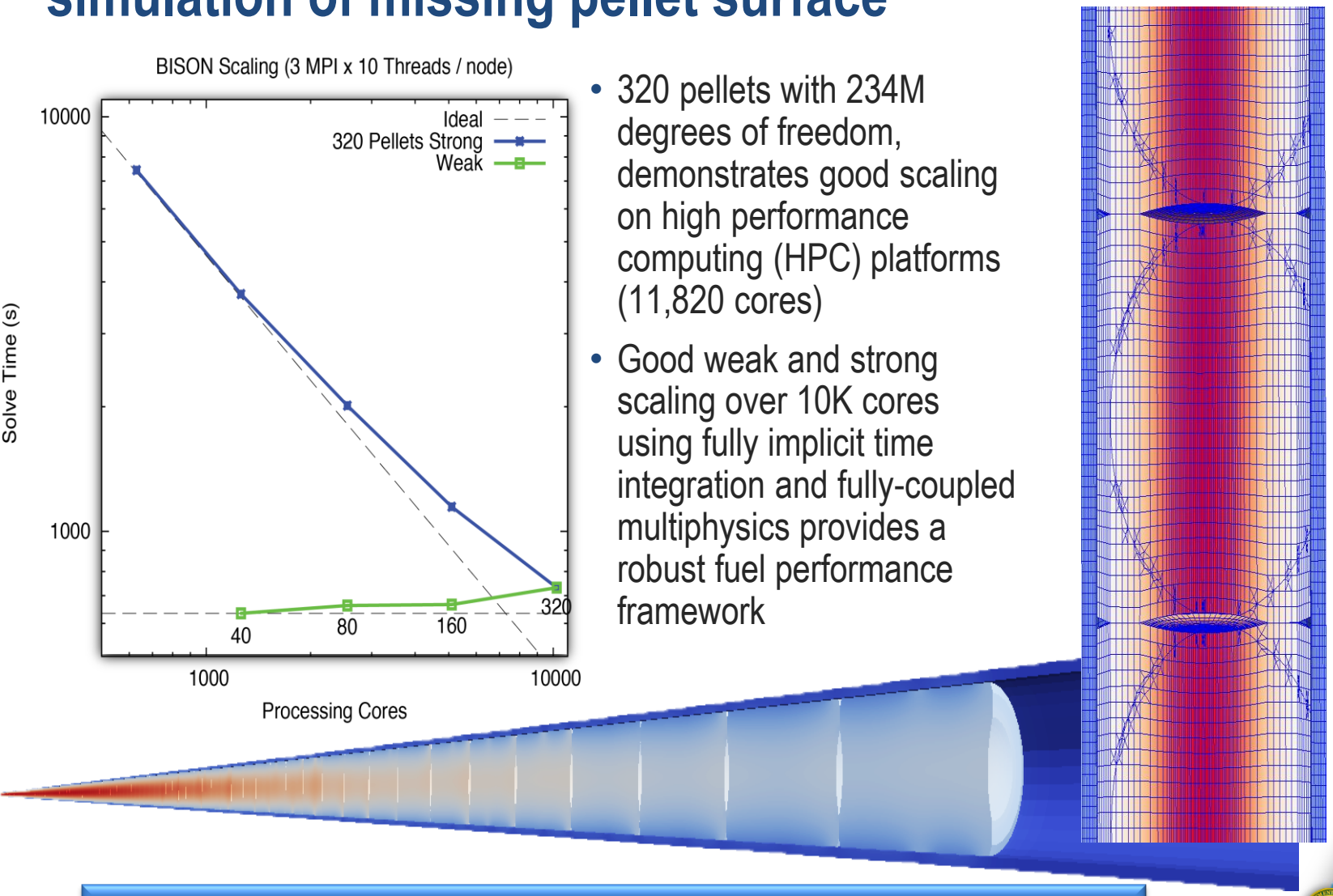
Cladding Behavior

* Thermal and irradiation creep
* Thermal expansion
* Plasticity

Solid foundation for the development of Peregrine

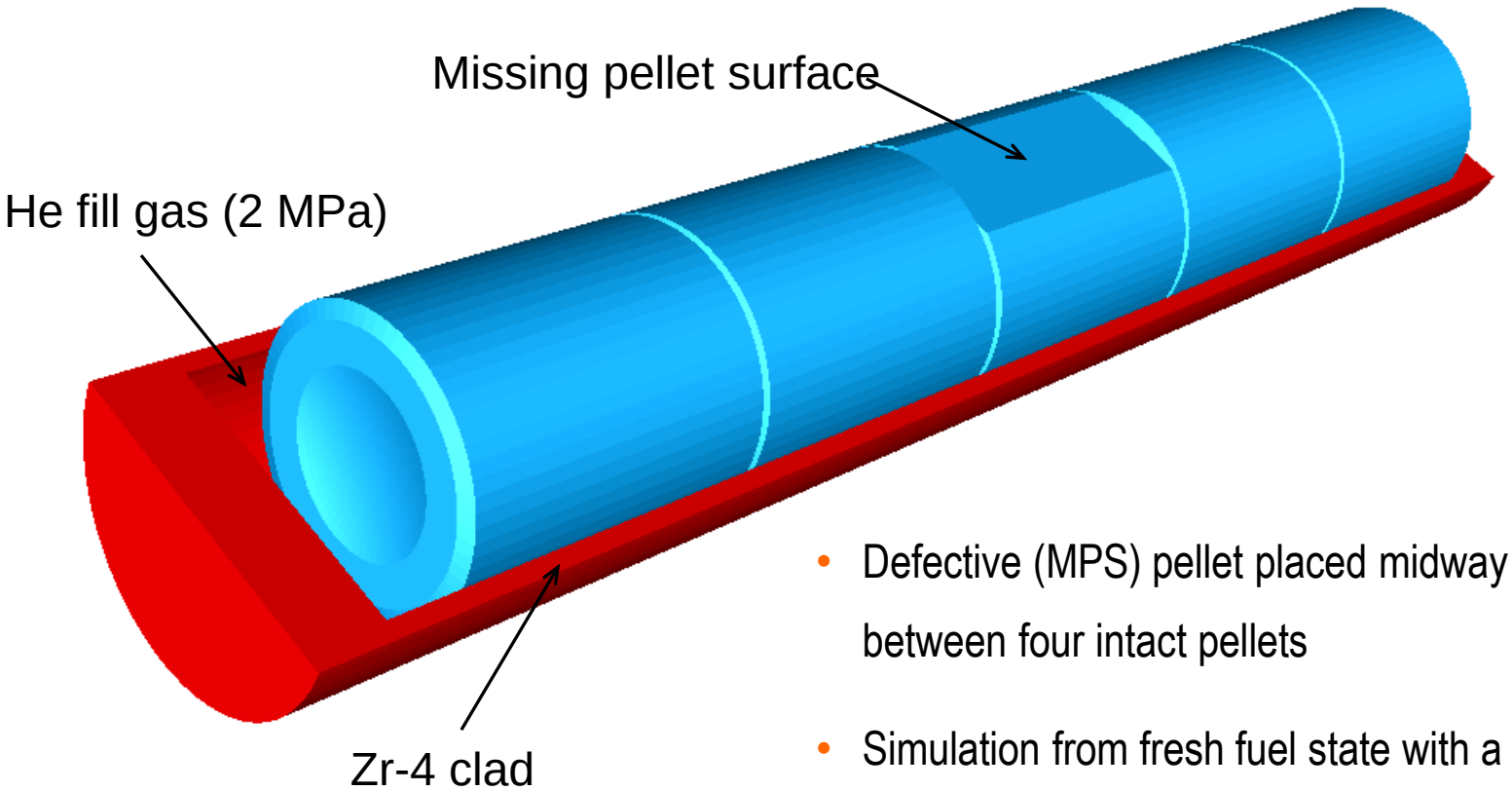
Full length, 320 fuel pellet fuel pin & high resolution simulation of missing pellet surface

- 320 pellets with 234M degrees of freedom, demonstrates good scaling on high performance computing (HPC) platforms (11,820 cores)
- Good weak and strong scaling over 10K cores using fully implicit time integration and fully-coupled multiphysics provides a robust fuel performance framework



MOOSE-based fuel performance models scale to HPC environments

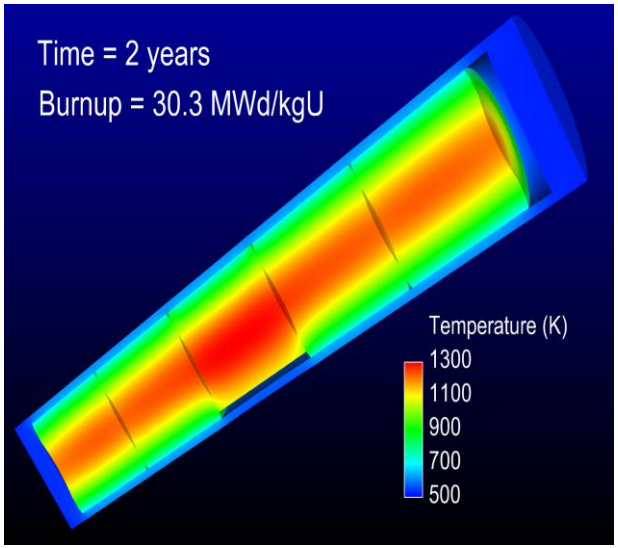
High Resolution 5-pellet MPS Simulation



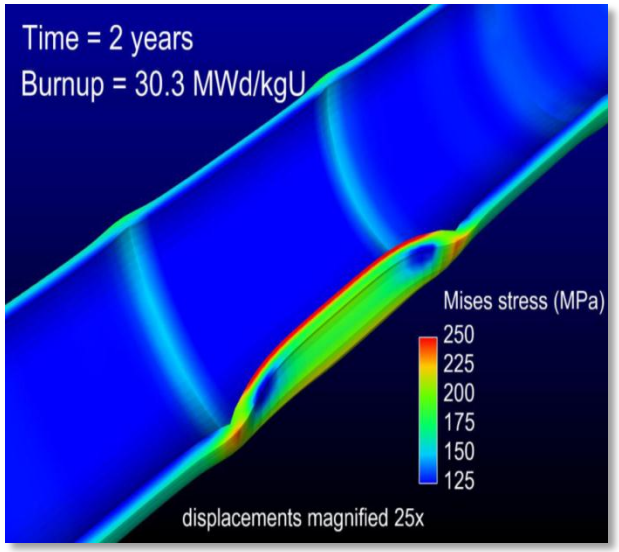
- Defective (MPS) pellet placed midway between four intact pellets
- Simulation from fresh fuel state with a typical power history, followed by a late-life power ramp

High-resolution model for fuel/clad behavior and response to a missing pellet surface

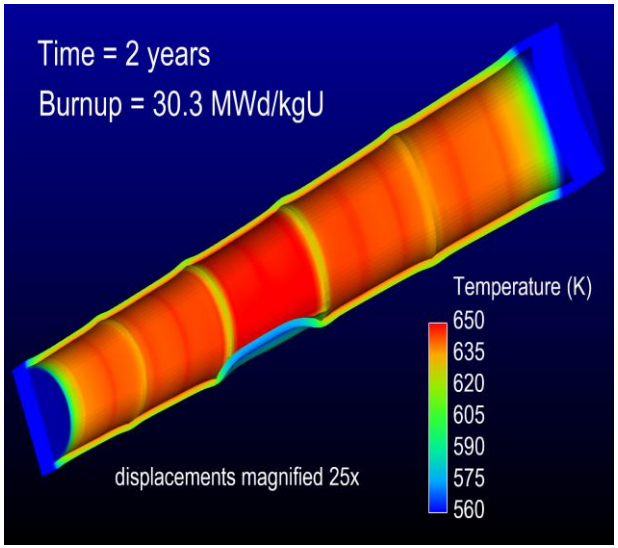
High resolution, 3D fuel performance calculation reveals the impact of a missing pellet surface on stress state, temperature profile, etc. (*i.e.* full nuclear fuel performance) as a function of fuel history.



Fuel Temperature



Von Mises Effective Stress



Clad Temperature

Development of Peregrine 3D fuel performance model will enable evaluation of PCI fuel failures

Outcomes and benefit to nuclear power industry

- HPC-scaling of the Peregrine fuel performance model will enable efficient consideration of complex phenomena
- Flexible framework will be used to systematically assess fuel performance during normal and transient operations and off-normal conditions:
  - *Evaluate effect of pellet irregularities on fuel performance*
  - *Optimize power maneuvers improving operational margins*

Peregrine fuel performance simulations will help eliminate PCI fuel failures

Next steps

- Building on BISON, develop Peregrine using industry standard, validated models
- Define and implement directed lower-length-scale modeling approaches to develop improved, physics based models of fuel and clad property evolution
- Contribute to efficient evaluation of innovative fuel designs and best estimate vs conservative reactor operation
- Couple to MNM, VRI, and AMA focus areas for full implementation and analysis

Peregrine – BISON Distinction

- BISON is an INL general purpose fuel performance code developed in the MOOSE environment, that can be readily applied to a variety of fuel and reactor types, including oxide fuel in LWRs, metallic and oxide fuel in SFRs, TRISO fuel in AGRs, etc.

- Peregrine fuel performance code will be comparatively rigid and will be an open source, validated PWR fuel performance model.

- Under CASL NDAs, Peregrine will be compared directly to Falcon for a comparable set of validation tests.

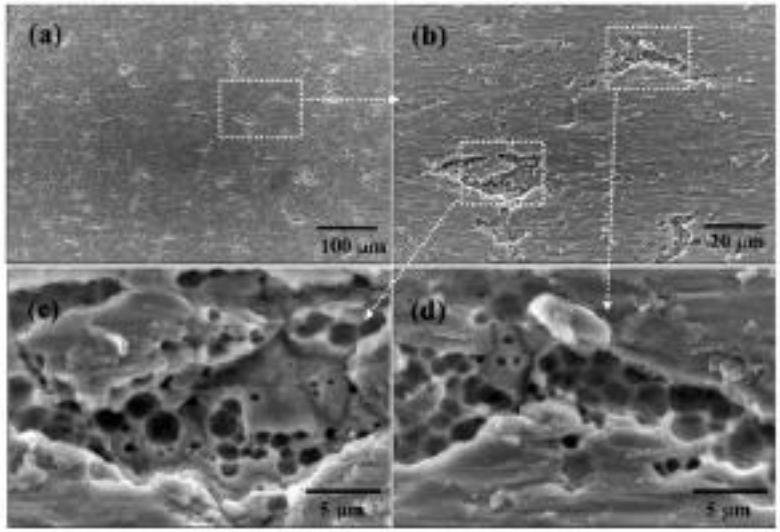
- Peregrine will be designed and architected to accept and utilize proprietary material data and/or models, where appropriate

- Finally, Peregrine will not incorporate any embedded mesocale models e.g. MARMOT (MOOSE-based phase field modeling code). Rather, individual physics models or parameters in existing models will be produced by CASL for use in Peregrine.

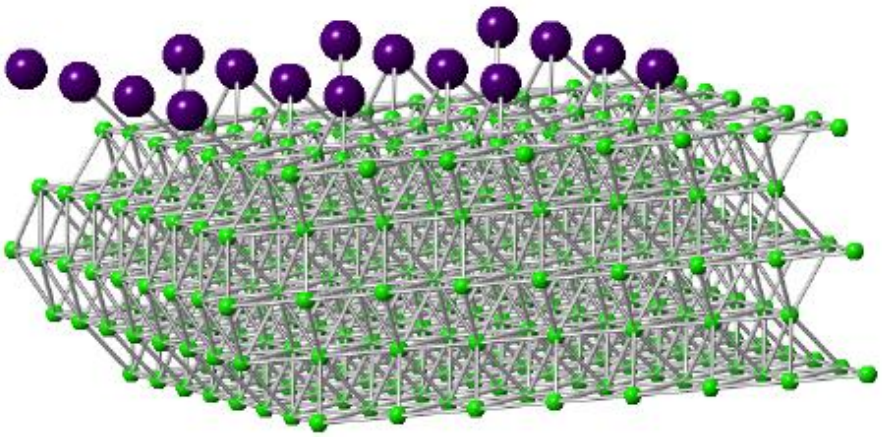
Investigation of I-influenced SCC in Zr Clad

Matt Rossi and Chris Taylor, LANL

- Use of atomistics for crack initiation/propagation as well as I permeation through surface oxide layer



ZrI_x pits caused by I corrosion of Zr, pits weaken triple point and GBs, pit coalescence leadto cracking



I interaction with Zr surfaces

	Reactants	Products	ΔE (eV)
$Zr + I_2 \Leftrightarrow ZrI_2$	$Zr + I_2$	ZrI_2	-4.59
$ZrI_2 + I_2 \Leftrightarrow ZrI_4$	$ZrI_2 + I_2$	ZrI_4	-6.78
$2ZrI_2 + I_2 \Leftrightarrow 2ZrI_3$	$2ZrI_2 + I_2$	$2ZrI_3$	-9.50
$2ZrI_3 + I_2 \Leftrightarrow 2ZrI_4$	$2ZrI_3 + I_2$	$2ZrI_4$	-5.24

All Zr-I reactions are exothermic. Results suggest that ZrI_2-I bonding is stronger than ZrI_3-I, ZrI_2 is least stable of the three ZrI_x species, prefers higher I-coordination.

Exploration of new SCC model at PCI wkshp

MPO Strategic Vision for Modeling Nuclear Fuel Performance

Phased approach, closely comparing modeling predictions to power & test reactor data to verify models and identify shortcomings

Phase 1:

Develop 3D nodal representation of fuel & cladding in structural mechanics/chemistry code suite that implements industry/EPRI material databases & empirical models, and identifies mechanism for physics coupling (e.g., fluids, neutronics)

- Verification/validation path against industry codes

Phase 2: Compare 3D predictions to reactor data

* Identify short-comings in the materials databases/models (e.g., constitutive & creep models of clad and fuel) & begin model refinement
* Develop improved coupling framework
* Implement a Uncertainty Quantification framework

MPO Strategic Vision for Modeling Nuclear Fuel Performance (cont'd)

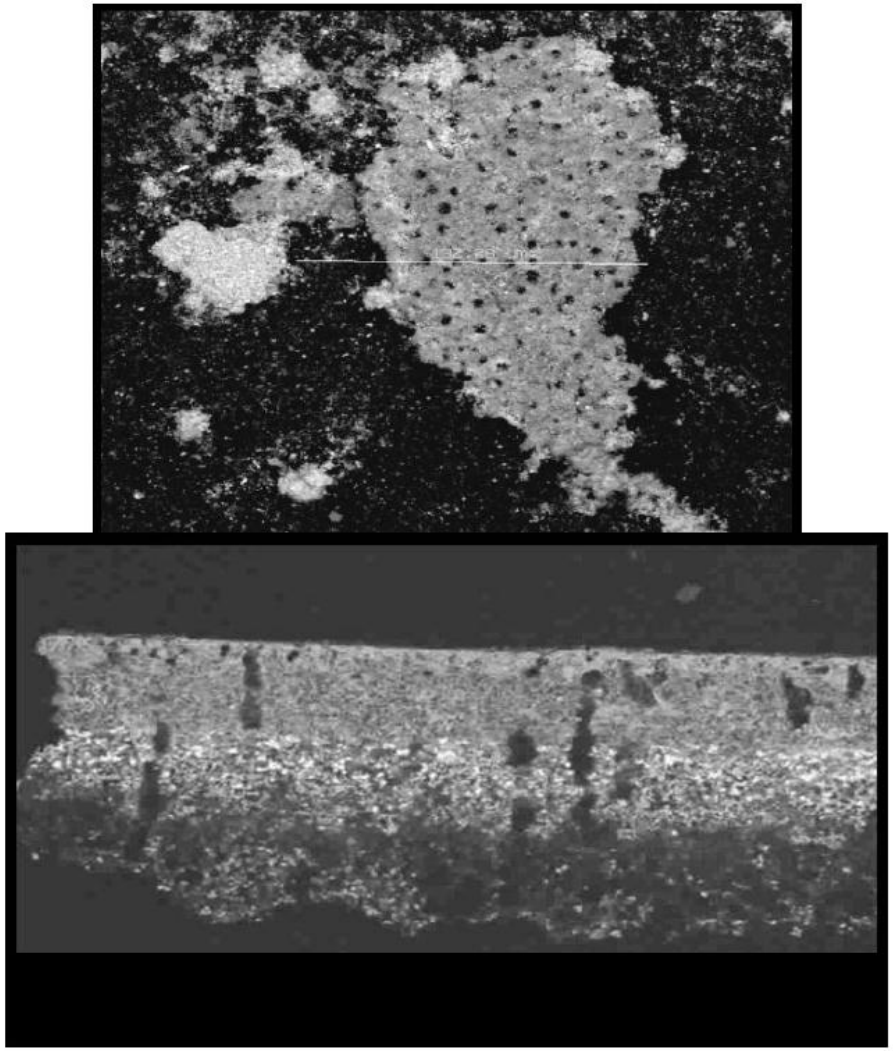
Phase 3: Utilize improved, coupled 3D code with emerging improvements in material property models to:

* compare with test & power reactor data
* assess the effects of operating conditions, over-power transients, etc. on fuel performance

Phase 4: Predict reactor operating window (e.g., power level & gradients, ramp changes, fuel burnup history, etc.) and margins to avoid fuel failures using CASL developed 3D, high-fidelity simulation tool with integral UQ framework

CRUD

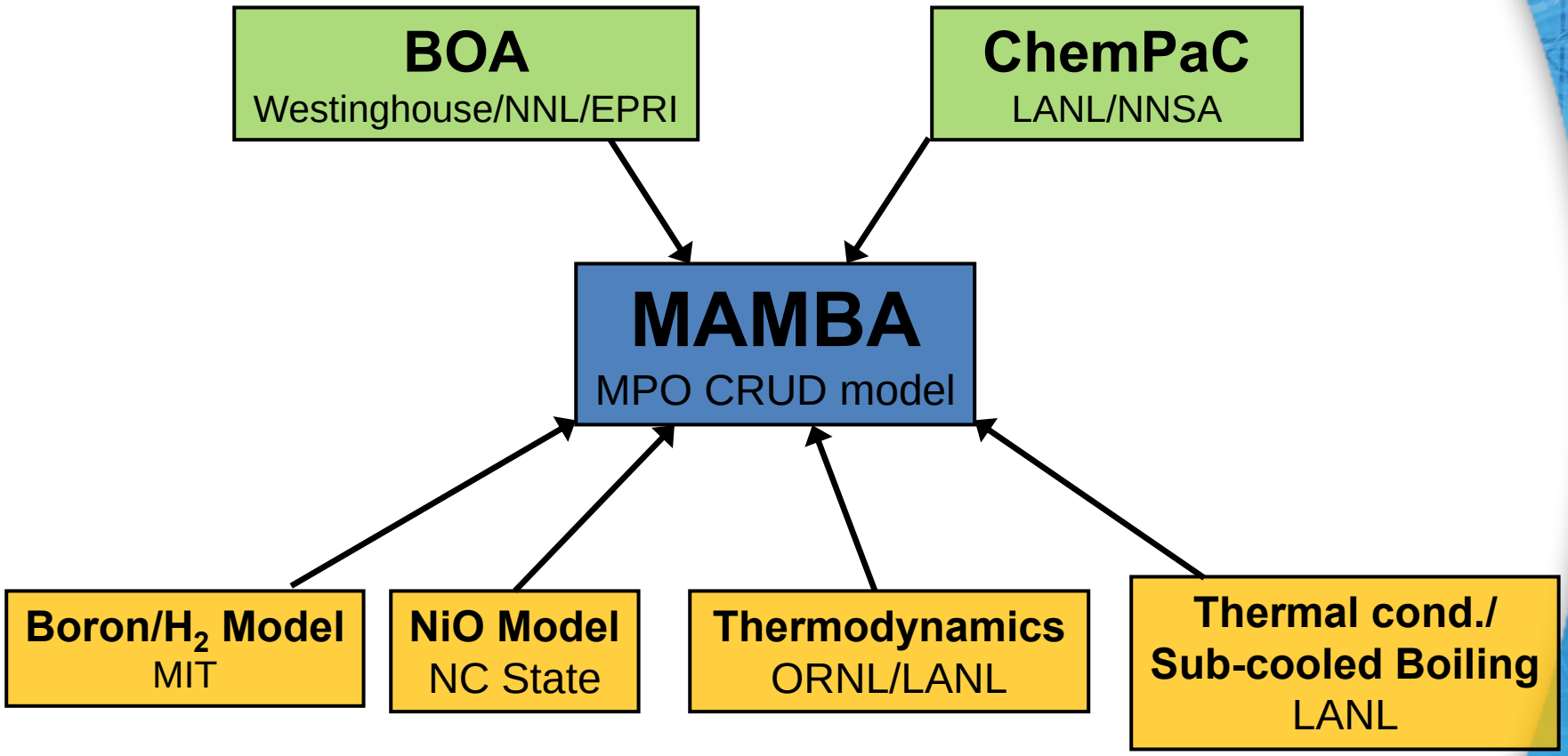
- Corrosion deposits from balance of plant surfaces
- Not all crud is bad
  - Thin crud should improve heat transfer
- However, significant deposits can cause problems
  - Accelerated cladding corrosion - failure
  - Axial Offset (PWRs)
  - Large releases at shutdown – elevated radiation fields (PWRs)



Micrographs provided by K. Edsinger, EPRI

Material Framework for CRUD Test Problem

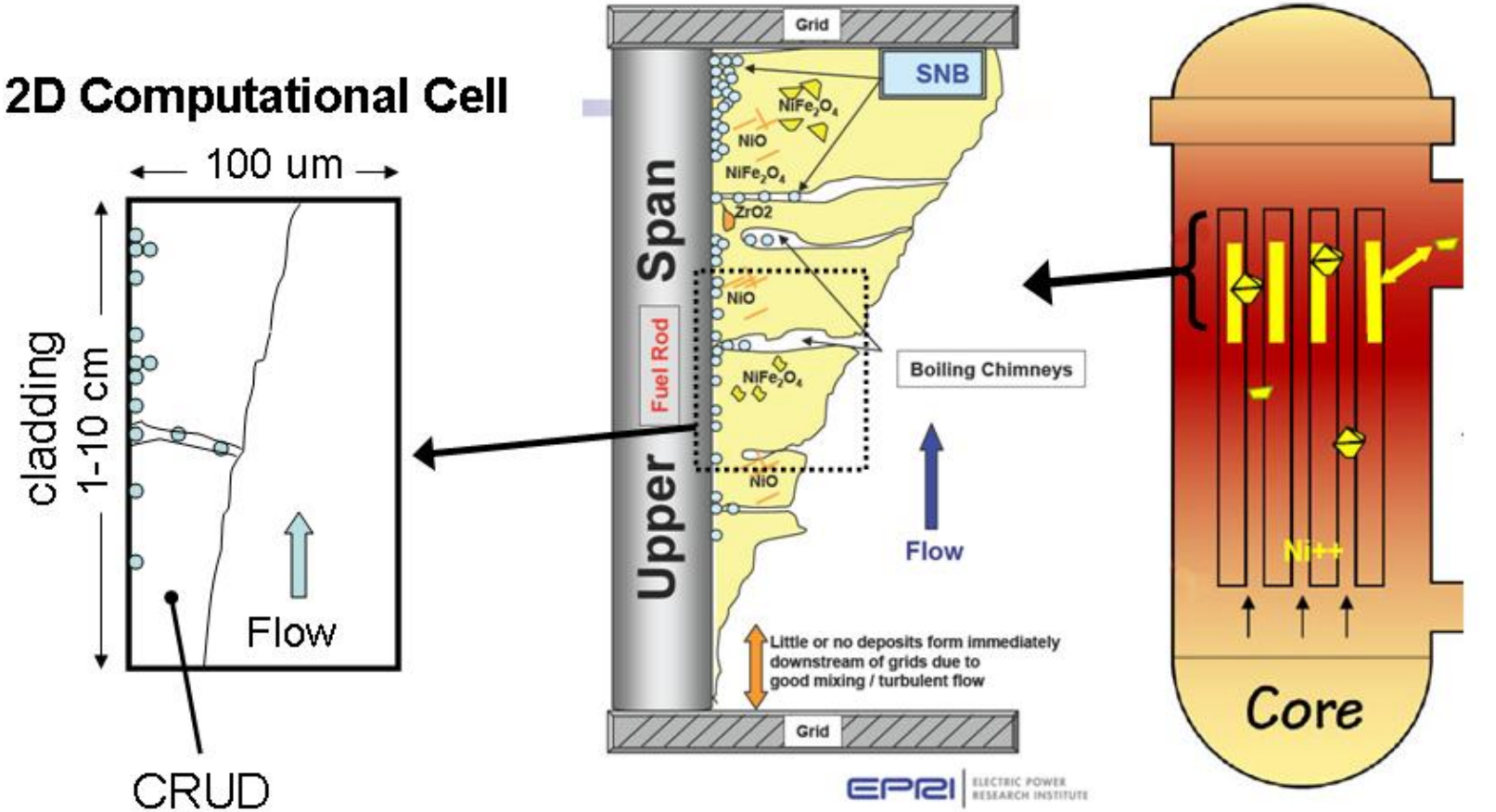
Brian Kendrick (LANL), Mike Short (MIT), Dennis Hussey (EPRI)



MAMBA = MPO Advanced Model for Boron Analysis

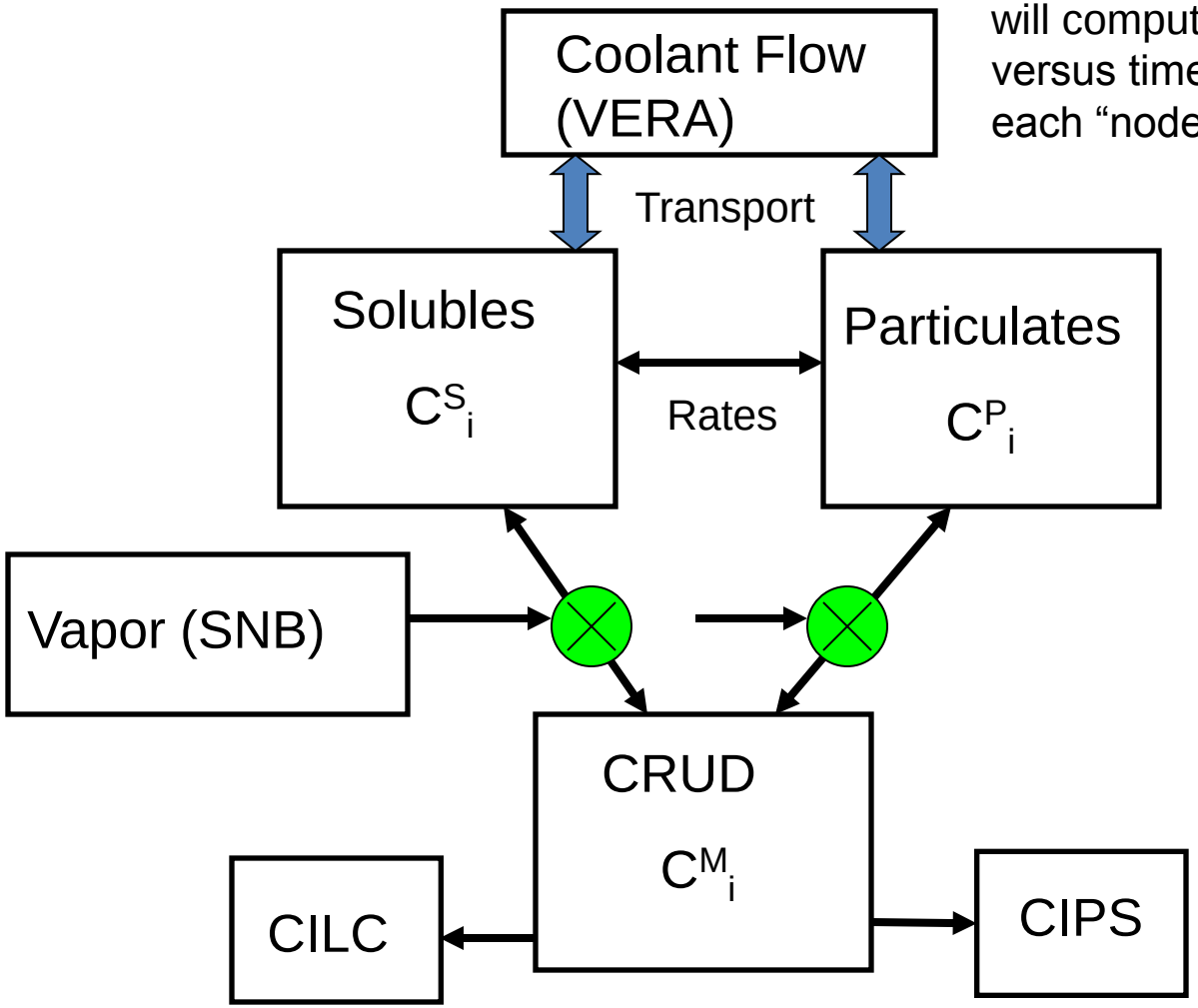
MAMBA's 2D Computational Cell

Brian Kendrick (LANL)



MAMBA flow chart: phases, interfaces, and submodels

Chemical kinetics mechanisms will compute species concentrations versus time for "local conditions" at each "node" within computational cell



Primary Species:

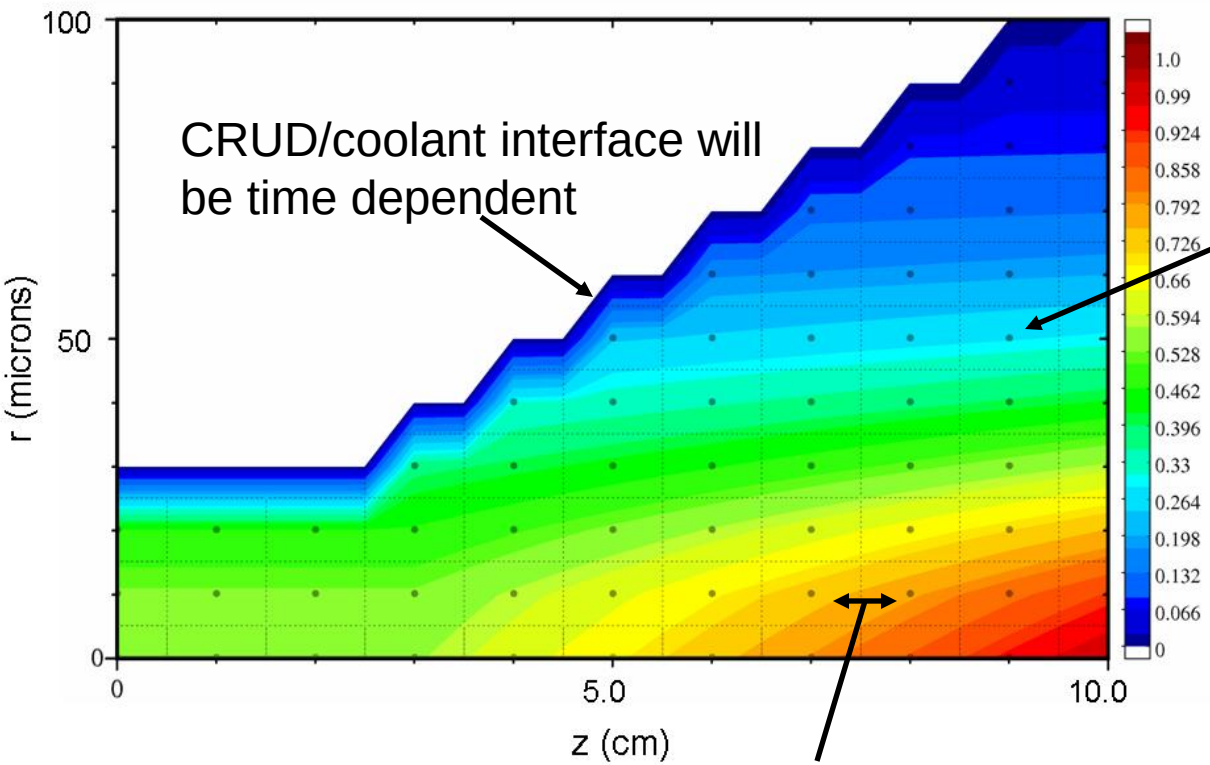
C_1 = Ni
C_2 = Fe
C_3 = Zr
C_4 = Zn
C_5 = B
C_6 = Li
C_7 = Cr
C_8 = Co
O and H implied

MAMBA example/preliminary calculation

Brian Kendrick (LANL)

CRUD deposition: static 2D model

Colored contours: normalized boron concentration



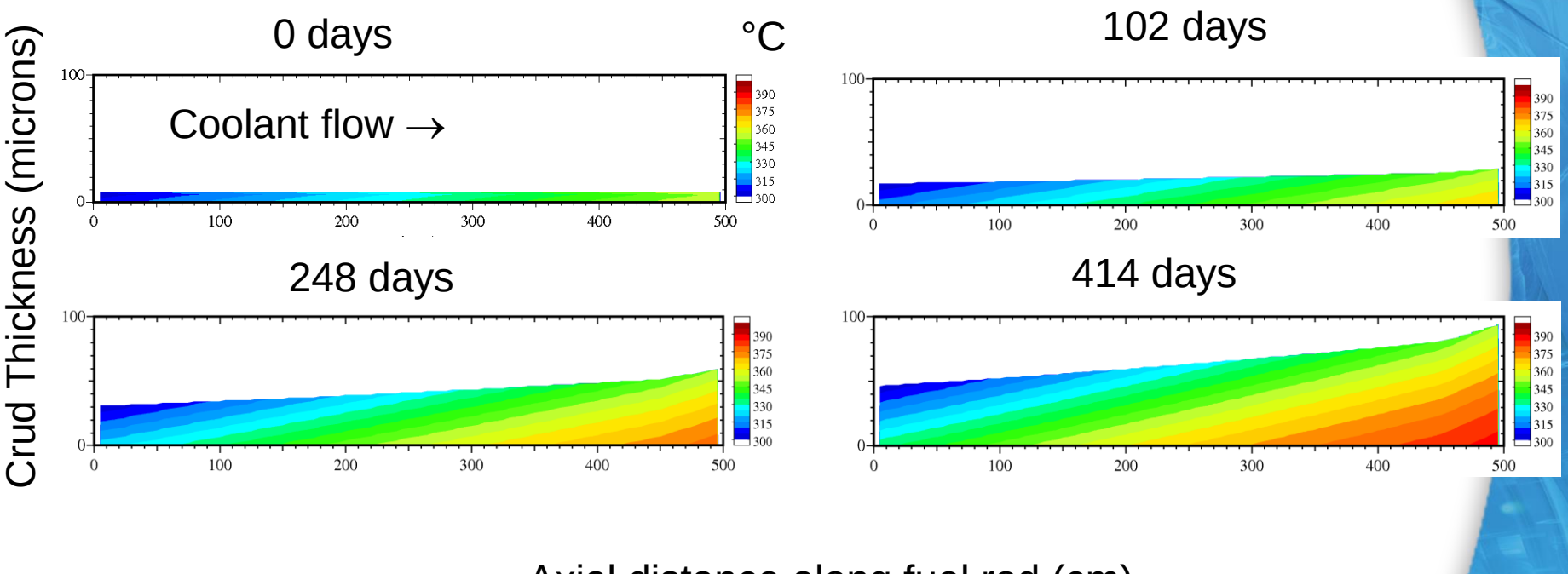
CRUD/coolant interface will be time dependent

Compute node and volume element

Particle/Heat Transport between nodes: 2D numerical solution

MAMBA example/preliminary CRUD simulation

Temperature distribution (colored contours)



Primary inputs:
* heat flux from cladding surface, heat transfer rate due to SNB
* coolant temperature along crud surface (300-350°C)
* thermal conductivity and heat capacity of crud
* surface deposition rate of particulate Ni/Fe oxides
* deposition rate of boron within crud
* coolant concentrations of particulate Ni/Fe oxides, boron, and other species

MAMBA Future Work

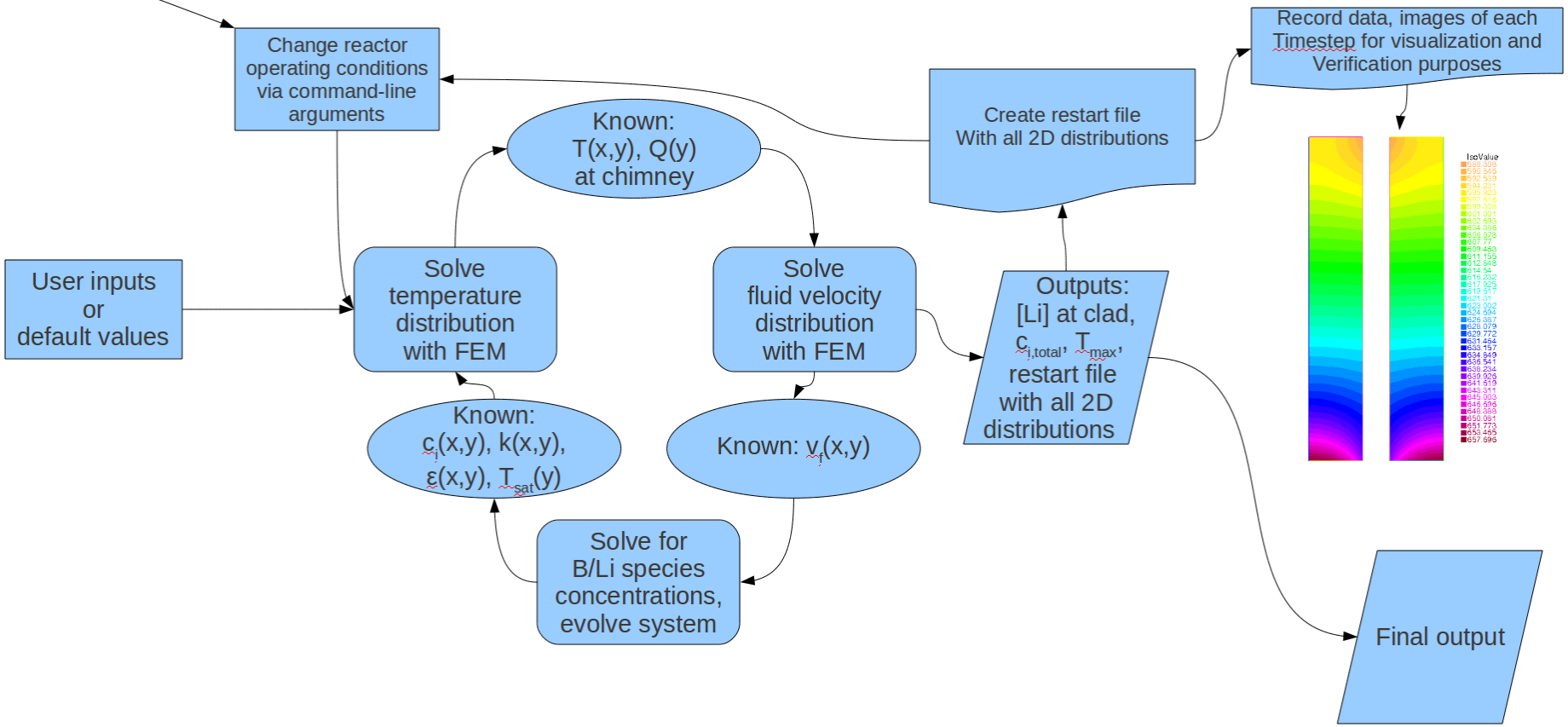
- Develop improved SNB model / couple to 2D wick boiling sub-model (M. Short)
- Incorporate time dependent micro-structure: porosity, chimney density/radius
- Incorporate crud microstructure dependent thermal conductivity and heat capacity
- Develop multi-phase chemical kinetics/transport models for species of interest (Ni, Fe, B, Li, Zn, Zr, Cr, ….).
- Validate MAMBA code against crud test problem (iterate)
- Explore coordination between MAMBA and THM
- Develop and refine interface between MAMBA ↔ VERA
- Develop and refine interface between MAMBA ↔ BOA

Primary Risk = *lack of experimental data will impede validation of MAMBA*

MAMBA Boron Deposition Model

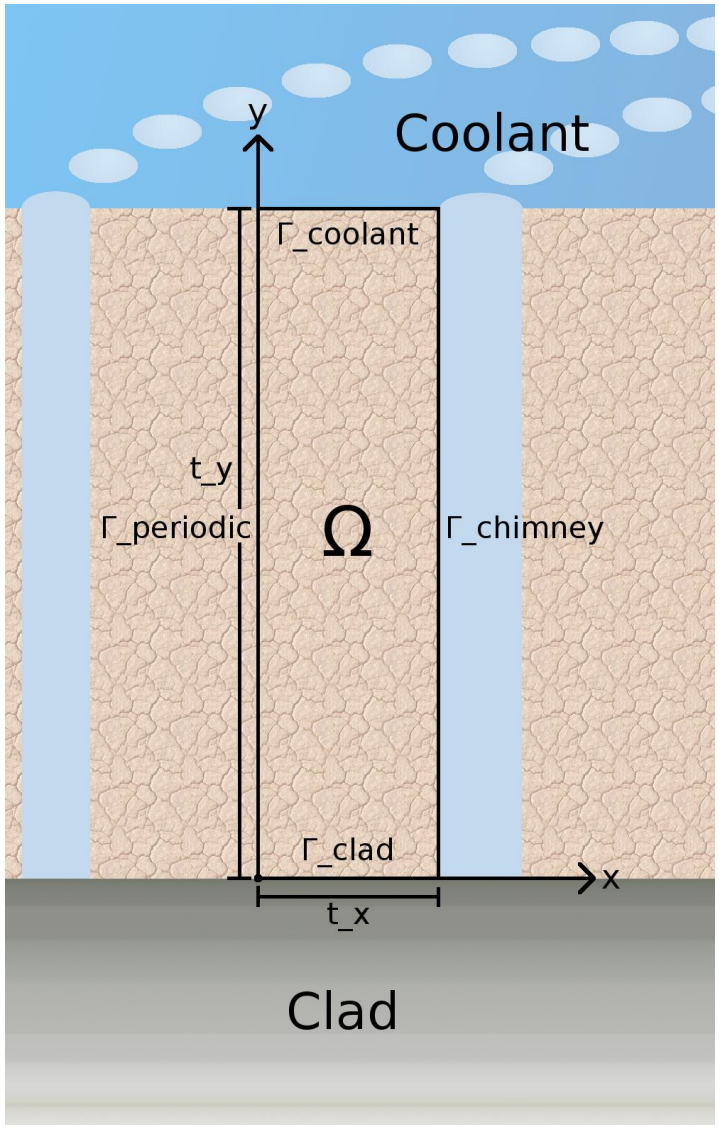
Mike Short (MIT)

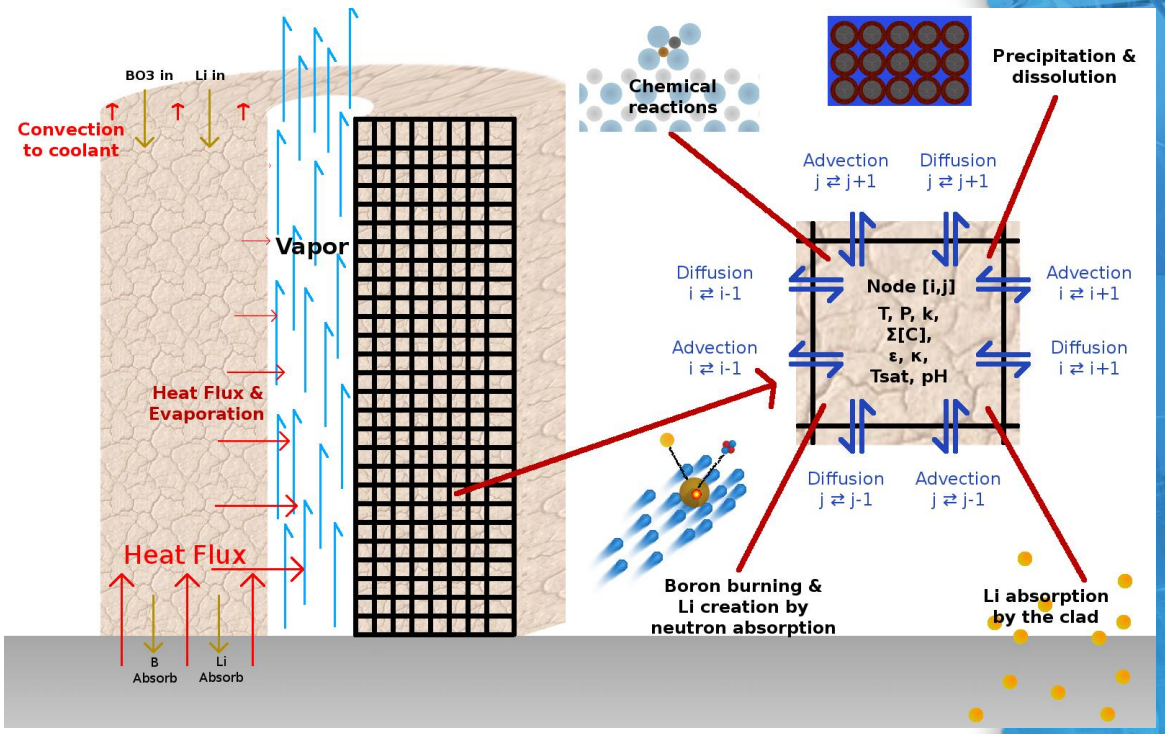
- Assumes steady state T, v & C profiles
- Calculates 2D distributions in 1-2 minutes using coupled, iterative FEM



Boron Model Functionality

Mike Short (MIT)



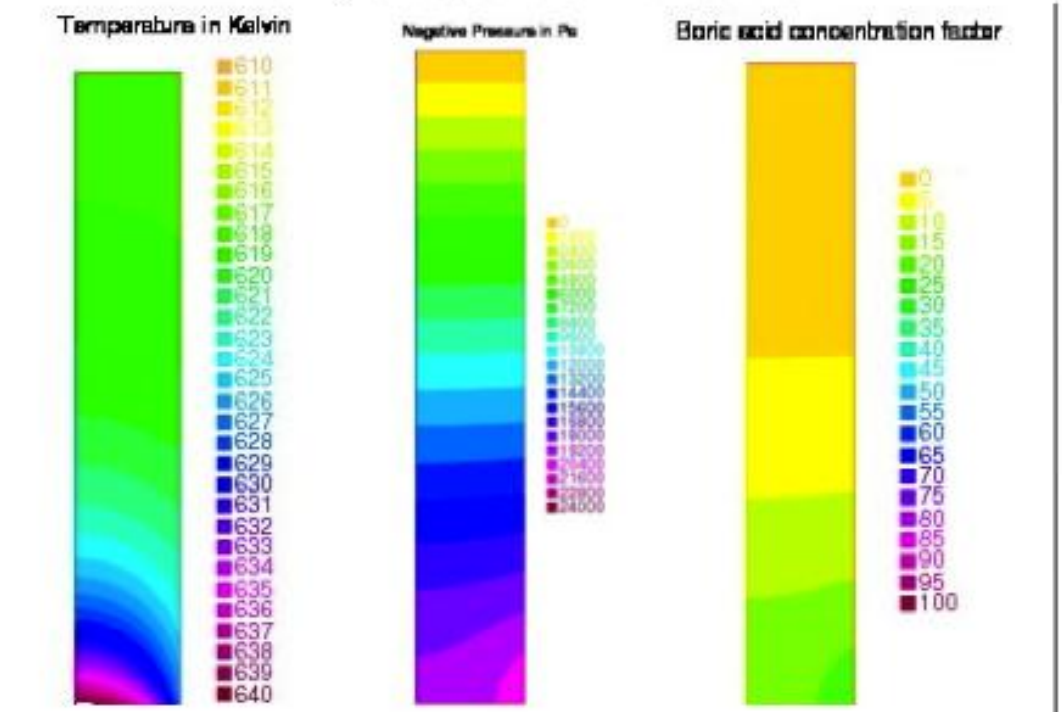


$$-\nabla\cdot(k(\Omega)\nabla T(\Omega))=0 \quad -\nabla\cdot(\kappa(\Omega)\nabla P(\Omega))=0 \quad u=-\kappa(\Omega)\nabla P(\Omega)$$

$$\frac{dm_{total}}{dt}=\sum_{i=1}^{4}\left[\sum_{s=1}^{4}\frac{dm_{i,flow}}{dt}+\sum_{i\neq j}^{4}\frac{dm_{i\to j}}{dt}-\sum_{i\neq j}^{4}\frac{dm_{j\to i}}{dt}-\frac{dm_{i,burn}}{dt}\right]$$

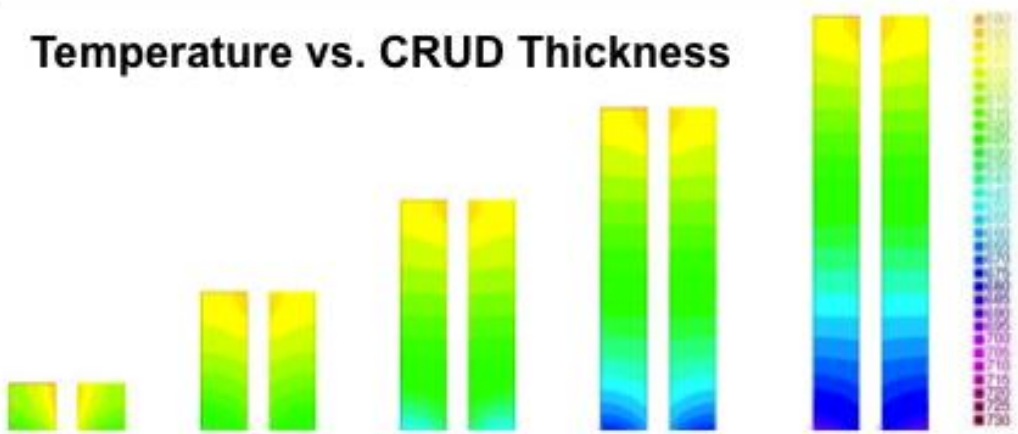
Preliminary Boron Model Results

Fully Coupled Simulations

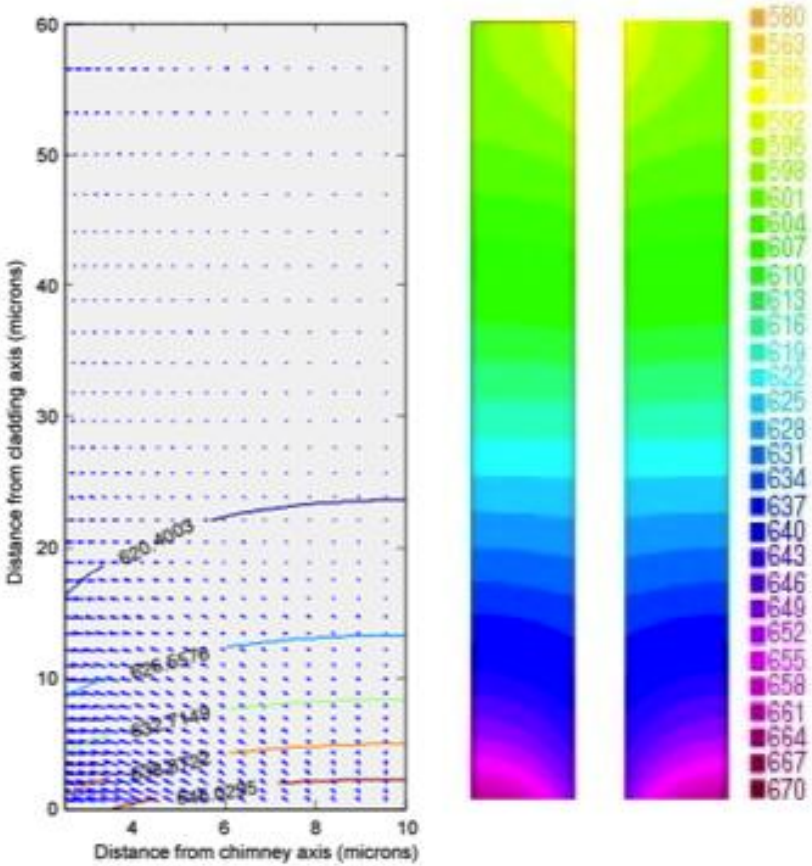


Temperature Velocity BO_3 Concentration

Temperature vs. CRUD Thickness



Model Verification

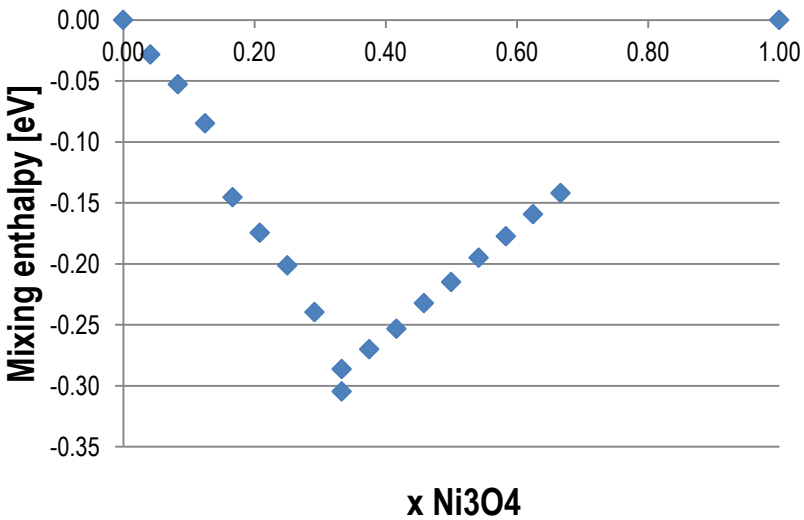


ul Haq [JNM 2011] MAMBA BDM

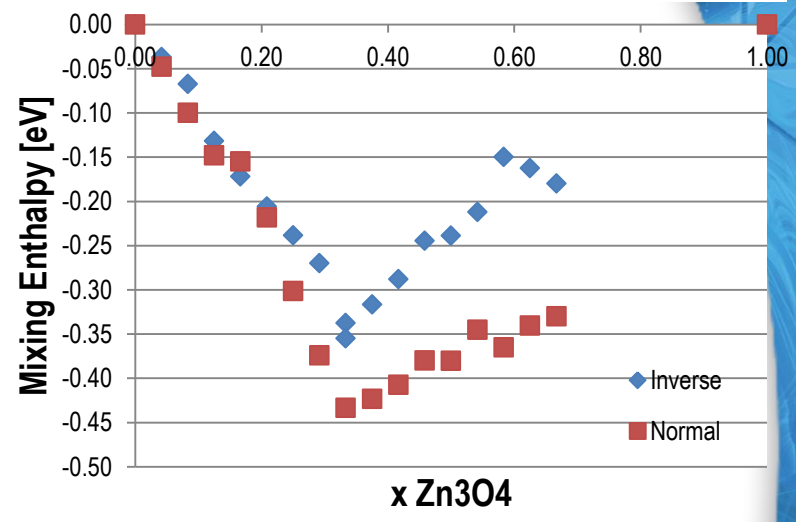
Density functional theory calculations applied to Fe_3O_4, Ni_3O_4 $NiFe_2O_4$, $ZnFe_2O_4$ and $Ni_{0.5}Zn_{0.5}Fe_2O_4$ Spinel phases

David Andersson (LANL)

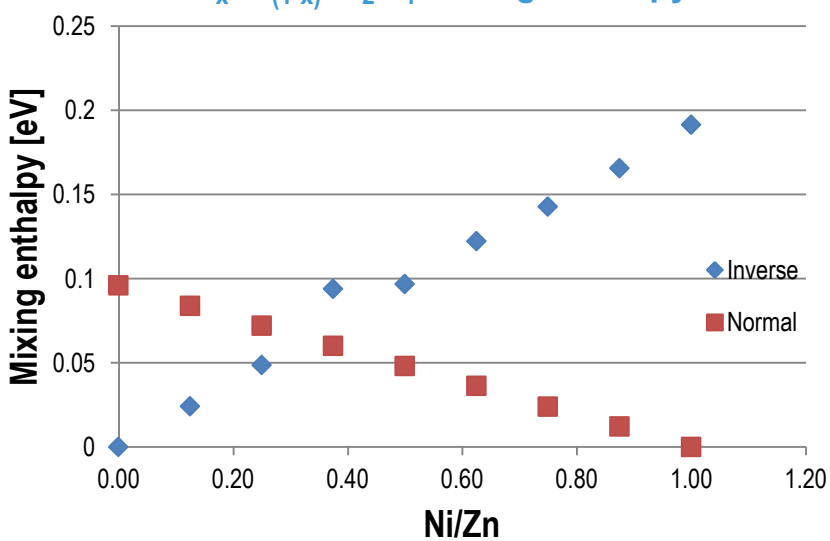
$Ni_{3x}Fe_{3(1-x)}O_4$ mixing enthalpy



$Zn_{3x}Fe_{3(1-x)}O_4$ mixing enthalpy



$Ni_xZn_{(1-x)}Fe_2O_4$ mixing enthalpy



Relative stability of Ni_2FeBO_5, $\Delta\mu(Ni_2FeBO_5)$ [eV/atom]

	NiO, $NiFe_2O_4$, O_2, B and Li	NiO, Fe_2O_3, O_2, B and Li	$NiFe_2O_4$, FeO, O_2, B, Li	$NiFe_2O_4$, Fe_2O_3, O_2, B, Li
$\Delta\mu(Ni_2FeBO_5)$	-0.71	-0.73	-0.18	-0.66
	$NiFe_2O_4$, Fe_2O_3, O_2, LiB_2O_7, Li	$NiFe_2O_4$, Fe_2O_3, O_2, LiB_2O_7, Li_2O	$NiFe_2O_4$, Fe_3O_4, O_2, LiB_2O_7, Li_2O	NiO, Fe_3O_4, O_2, LiB_2O_7, Li_2O
$\Delta\mu(Ni_2FeBO_5)$	0.24	0.08	0.15	-0.02
	NiO, Fe_2O_3, LiB_2O_7, Li_2O	NiO, $NiFe_2O_4$, LiB_2O_7, Li_2O		
$\Delta\mu(Ni_2FeBO_5)$	0.01	0.02		

Only "realistic" case for Ni_2FeBO_5

Calculated non-stoichiometry reactions for spinel phases

$A_1B_2O_4$	O_I (eV)	V_O (eV)	A_I (eV)	V_A (eV)	B_I (eV)	V_B (eV)
Fe_3O_4	3.46	-0.49/2.31	-0.003/3.73	1.71	N/A	N/A
$NiFe_2O_4$	4.15	-0.38/2.42	4.85/7.65	3.57	0.62/4.36	4.95
$ZnFe_2O_4$	4.45	-0.16/2.64	--	3.16	--	4.45

Preliminary observations from the DFT calculations and directions for future work

David Andersson (LANL)

- Positive mixing enthalpy for $Ni_{1-x}Zn_xFe_2O_4$ implies limited solubility for $NiFe_2O_4$-$ZnFe_2O_4$.
- Possible non-stoichiometry reactions for oxygen vacancies in Fe_3O_4, $NiFe_2O_4$ and $ZnFe_2O_4$ and Fe interstitials in Fe_3O_4, to be further explored.
- At low T both $Ni_{3x}Fe_{3(1-x)}O_4$ and $Zn_{3x}Fe_{3(1-x)}O_4$ are stoichiometric compounds. At high T $Ni_{3x}Fe_{3(1-x)}O_4$ may exhibit some solubility for $x<1/3$.
- Undertake quantitative comparison with existing CALPHAD models and experiments.
- B incorporated as Ni_2FeBO_5 or LiB_2O_7 into the CRUD. Preliminary results indicate that LiB_2O_7 is preferred under most conditions. Ni_2FeBO_5 only emerges as the stable phase is in equilibrium with NiO, Fe_3O_4, O_2 and Li_2O.
- Add Ni_2FeBO_5 and LiB_2O_7 to existing CALPHAD models and perform accurate calculations of phase equilibria.
- Future work: Model refinement, comparison to experiments, model validation and expand spinel calculations to include $NiCr_2O_4$ and $FeCr_2O_4$.
- Challenges: Complicated compounds for DFT, issues with accuracy could emerge during the validation and/or incorporation to CALPHAD models.

Toward a first principles understanding of CRUD deposition

A. M. Dongare, C. J. O'Brien, J. Eapen, and D. W. Brenner (NC State)

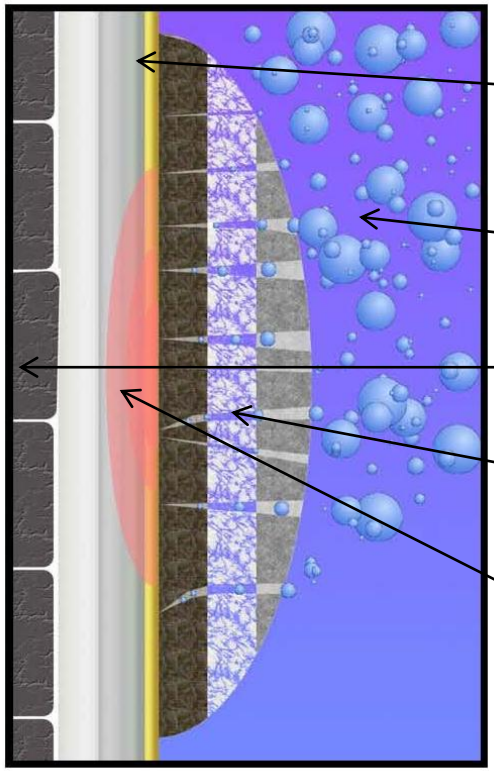


Figure courtesy of Michael Short, MIT

- A new first principles approach is being developed for predicting conditions leading to CRUD deposition due to sub-cooled boiling.
- In our modeling the growth of metal clusters from a variety of candidate species is used as a surrogate for surface deposition.

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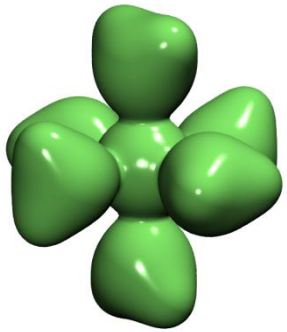
First Principles Study of CRUD solvation

- Thermodynamic stabilities can be used to determine which species are driven to deposit as CRUD.
- First principles quantum chemical methods are used to compute free energies of formation of clusters/species (ΔG_{FP})



Electron density iso-surface for $Ni^{+2}(H_2O)_6$

(NWCHEM)

B3LYP/ LANL2DZ

$$\Delta G_{tot} = \Delta G_{FP} + \Delta G_{MD}$$

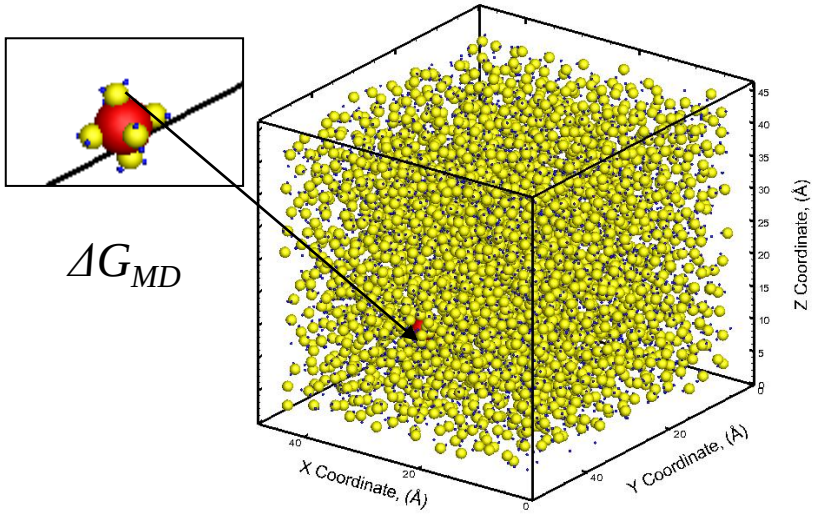
Prior model reactions for dissolution of NiO in water

$$NiO_{(cr)} + 2H^+ \rightarrow Ni^{2+} + H_2O \quad \text{- (A)}$$

$$NiO_{(cr)} + H^+ \rightarrow Ni(OH)^+ \quad \text{- (B)}$$

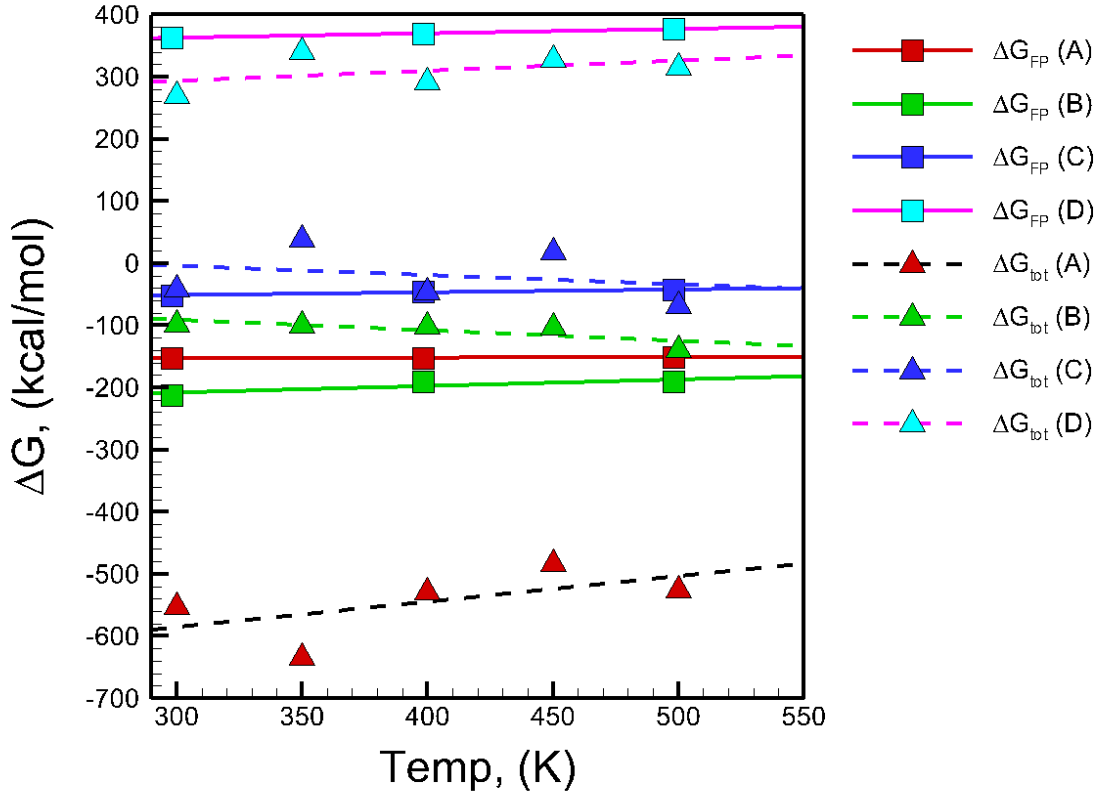
$$NiO_{(cr)} + H_2O \rightarrow Ni(OH)_2^0 \quad \text{- (C)}$$

$$NiO_{(cr)} + 2H_2O \rightarrow Ni(OH)_3^- + H^+ \quad \text{- (D)}$$



MD simulations for solvation free energies of $Ni^{+2}(H_2O)_6$ clusters

CRUD Reaction Thermodynamics



$$NiO_{(cr)} + 2H^+ \rightarrow Ni^{2+} + H_2O \quad \text{- (A)}$$

$$NiO_{(cr)} + H^+ \rightarrow Ni(OH)^+ \quad \text{- (B)}$$

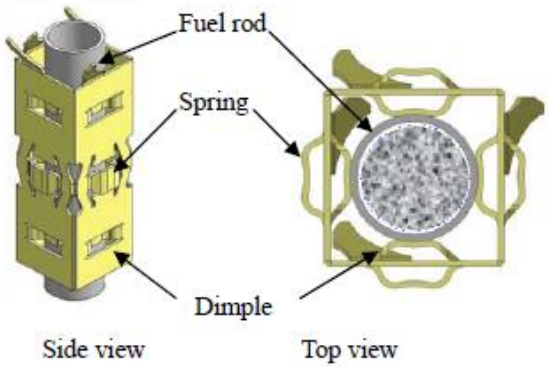
$$NiO_{(cr)} + H_2O \rightarrow Ni(OH)_2^0 \quad \text{- (C)}$$

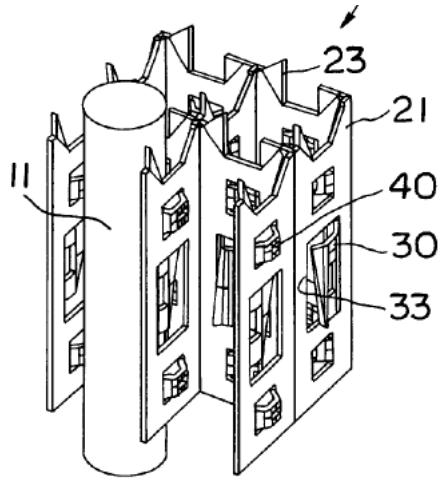
$$NiO_{(cr)} + 2H_2O \rightarrow Ni(OH)_3^- + H^+ \quad \text{- (D)}$$

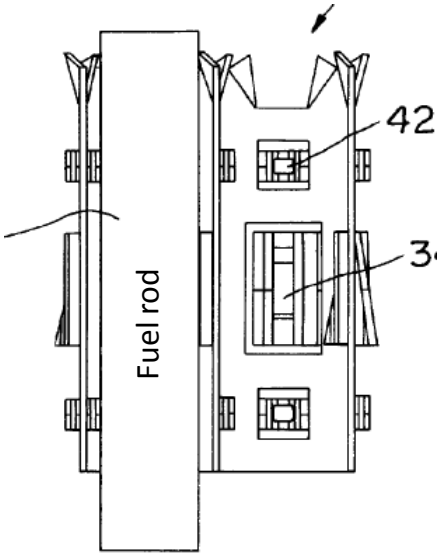
- Reaction (A) is stable in the presence of a solvent, but is less thermodynamically favorable by roughly an order of magnitude if the solvent is removed.

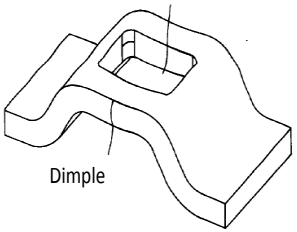
These results suggests that reactions in the presence of bubbles (due to sub-cooled boiling) correspond to a missing solvent and may therefore help to drive the CRUD deposition

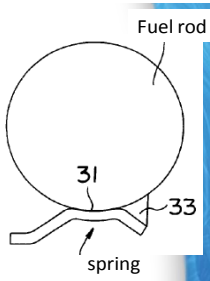
GTRF: Spacer Grid with Springs/Dimples

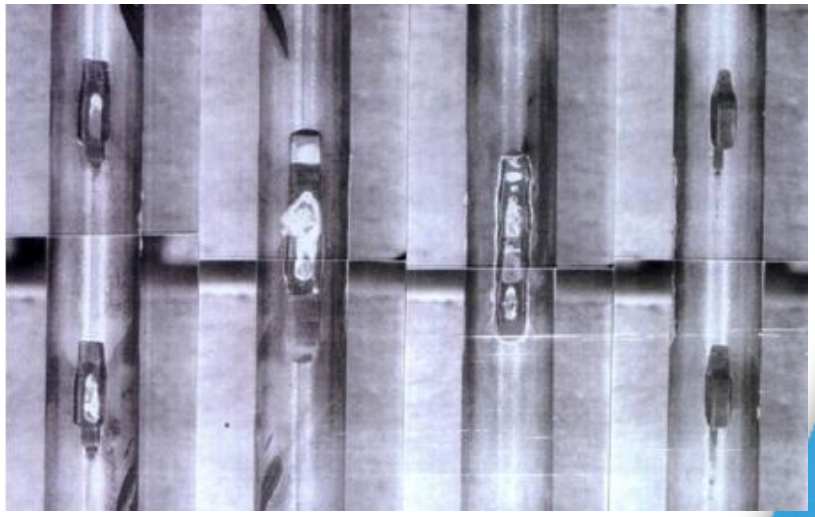












16x16 KOFA fuel rods (Kim, 2010)

GTRF Prediction – Current State-of-the-Art

- T/H analysis to determine velocity
- Correlate to turbulence PSD
- Approximate turbulence force as Gaussian Band-Limited White Noise Signal acting on fuel rods

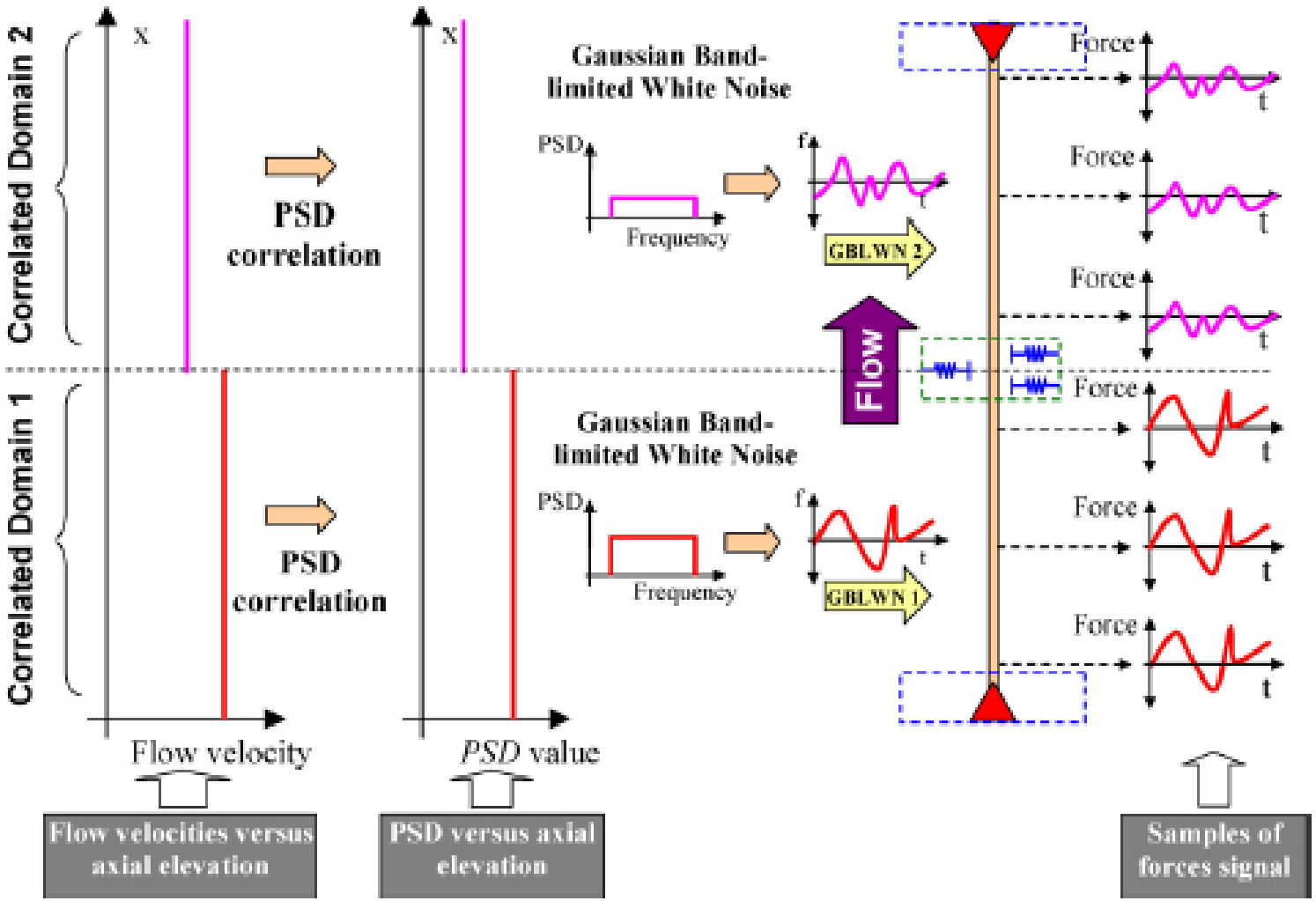
- CFD analysis to determine velocity and stresses in coolant
- Determine tractions acting on fuel rods

- Elastic beam vibration analysis, accounting for gaps
- Determine normal contact and friction forces, and sliding distances at supports (springs and dimples)

- Determine wear depth in fuel clad using wear correlation

$$\frac{dV(t)}{dt} = \kappa_V \frac{dW(t)}{dt} = \kappa_V \frac{d[F(t)l(t)]}{dt}$$

Workflow in the WEC VITRAN code
- Rubiolo and Young (2009)



Structural mechanics approach: High-fidelity, fluid structural interaction tool to predict gap, turbulent flow excitation, rod vibration and wear

- High Fidelity, 3-D Structural Mechanics/Fluid Structure Interaction
  - Turbulent flow excitation
    - Want CFD
  - Gap
    - Determine deformation of fuel rod and spacer grid through out fuel cycles
    - 3D finite element (implicit)
  - Structural dynamics (rod vibration)
    - Rod stiffness change due to creep-down
    - Inelastic deformation due to irradiation creep, etc. affecting vibration response
    - 3D finite element (explicit or implicit?)
    - Contacts, friction models
  - Fluid-structure interaction modeling
    - Not done to-date
    - Is it important to capture?
    - Is it feasible to capture?

- Predict Wear
  - Fretting wear
    - Analogous to high cycle fatigue
    - Loads on wear area due to vibration contacts at springs and dimples are important
  - Other considerations
    - Other sources of load, PCI, fission gas, etc., affecting stresses at the wear sites
    - Material state, e.g., due to irradiation damage, affects wear behavior
    - Friction models

L2:MPO.P2.02

Phenomena Relevant for GTRF that Evolve in Time

Spacer grid deformation
Fuel clad deformation
→ Gap between rod and spacer grid

Material state at contact region (e.g. irradiation hardening)
→ Wear Model

Turbulence force (pressure and shear) on rod
Fission gas pressure, PCI, nominal fluid pressure
→ Stress and deformation state in contact/fretting wear regions
→ Wear Model

Time

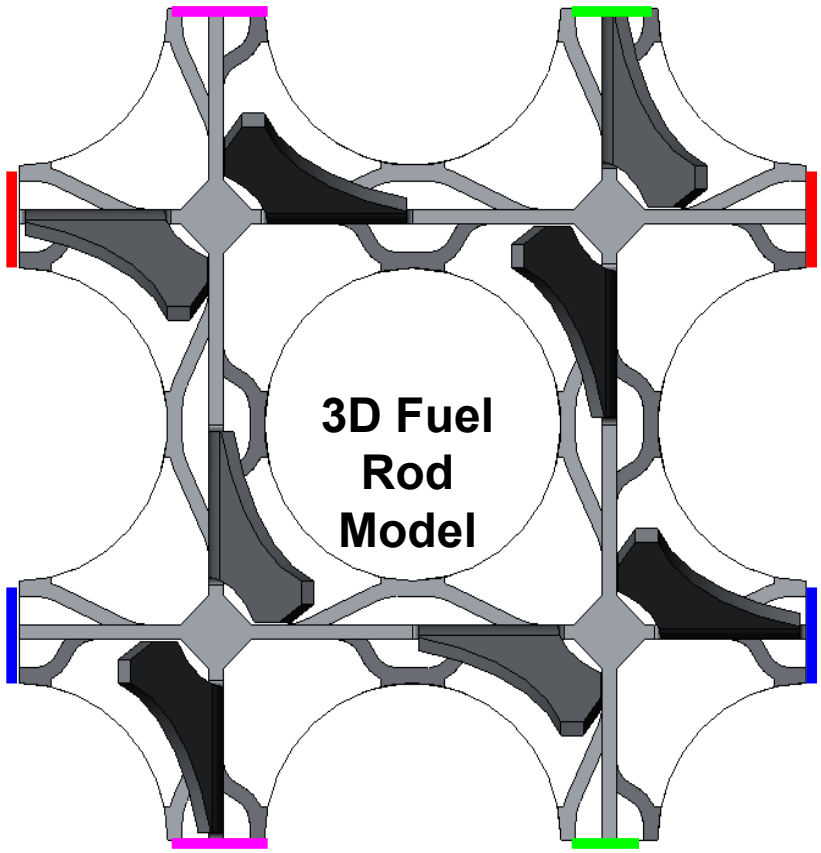
Modeling Challenges

- Time Scale
  - Inelastic deformation (irradiation creep, corrosion/hydriding, growth) – long time scale
  - Structural vibration – short time scale
- Material constitutive models
- CFD – fluid forces (pressure and shear stress) on rod are stochastic
  - Building deterministic box – need help with statistics on contact stress and deformation for wear model (e.g., may be stochastic FEM, spectral SFEM, etc.)
- Rod vibration
  - Structurally - vibration is elastic on current configuration that has undergone large deformation
  - Locally – inelastic deformation in contact region

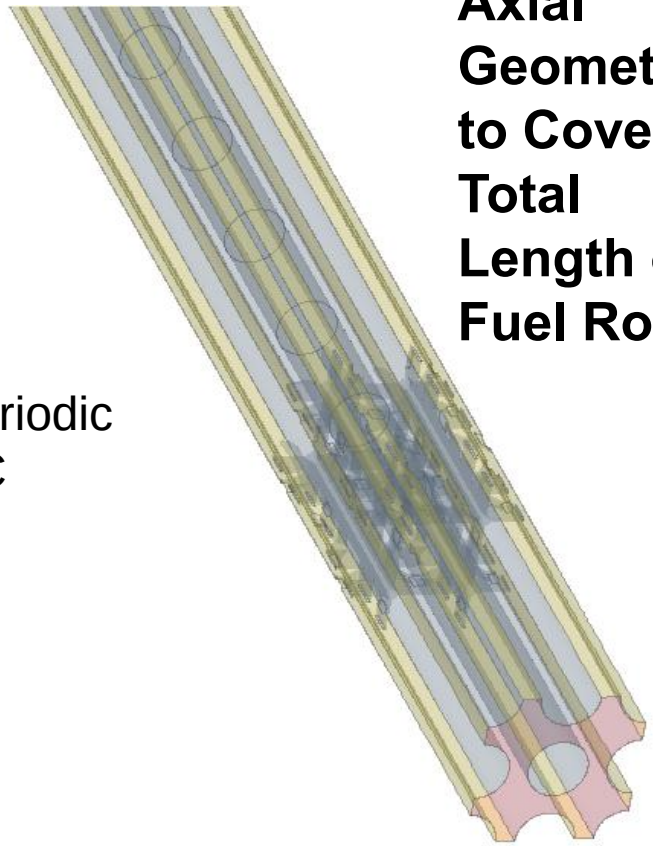
L2:MPO.P2.02

3x3 Bench Problem for GTRF Challenge Problem

Radial Geometry



Periodic
BC



Axial Geometry to Cover Total Length of Fuel Rod

L2:MPO.P2.02

Simple Structural Dynamics Problems to Establish Modeling Capability/Experience for 3x3 Bench Problem

- Salinas/ABAQUS Explicit
  - Hollow closed-end cylinder loaded by excitation forces (elastic)
    - 3D finite element
    - Supported at ends by stiff linear and torsional spring at one node
    - Construct forces using an assumed constant turbulence PSD
    - Use isotropic temperature-dependent elastic constants
    - Assume through-wall and axial temperature distributions
    - Solve problem by time history (modal analysis?)
  - Add internal pressure (elastic)
    - Solve dynamic problem by time history (modal analysis?)
  - Add solid cylindrical blocks inside cylinder (elastic)
    - Define contact surfaces to avoid material interpenetration
    - Solve dynamic problem by time history (modal analysis?)
  - Add square box at mid span (elastic)
    - Define contact surfaces
    - Use Coulomb friction model
    - Solve dynamic problem by time history (modal analysis?)

- Adagio/ABAQUS Standard
  - Hollow closed-end cylinder loaded by excitation forces (elastic with residual plastic strain)
    - 3D finite element
    - Supported at ends by stiff linear and torsional spring at one node
    - Construct forces using an assumed constant turbulence PSD
    - Use isotropic temperature-dependent elastic-plastic model
    - Preload cylinder by internal pressure to yield plastically through wall, then unload to create residual plastic strain
    - Assume through-wall and axial temperature distributions
    - Solve dynamic problem by time history
  - Add internal pressure
    - Solve dynamic problem by time history
  - Add solid cylindrical blocks inside cylinder
    - Define contact surfaces to avoid material interpenetration
    - Solve dynamic problem by time history
  - Add square box at mid span
    - Define contact surfaces
    - Use Coulomb friction model
    - Solve dynamic problem by time history

L2:MPO.P2.04 – Milestone

Conduct 3-D, high resolution, coupled fluids/materials demonstration and assessment of GTRF challenge problem (co-owned by VRI)

- Contributing FAs and Projects: MPO-GTRF, MPO-Clad, MPO-VI, VRI-CPI, THM-CFD
- Technical POC: Sam Sham
- MPO
  - GTRF, Sham (ORNL) - lead
    - Hayrapetian, Demkowicz (MIT) – micromechanical wear modeling
    - El-Azab (FSU) – microstructure
    - Blau (ORNL) - tribology
    - Lu (WEC) – VITRAN cognizant engineer, GTRF test loop data

Wear Model Development

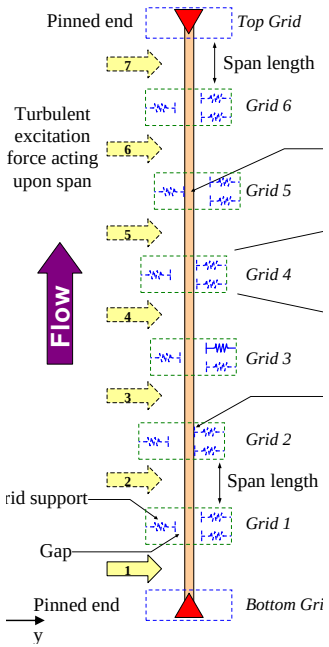
  - VI, Wirth (UT) – lead
    - Sham, Li, Nath (ORNL) – constitutive models, finite element implementation
    - Lu, Hu, Wang, Thouless (UM) – material models, finite element analysis
    - Hu (UM) – CASL summer intern – sensitivity analysis
  - CLAD
    - Tome (LANL), Sham (ORNL) – advanced MPO material models

Finite Element Material Models, Gap Prediction, GTRF Analysis Framework

- VRI
  - CPI, Sham (ORNL) – lead
    - Crane (SNL) – structural analysis (Sierra/adagio)
    - Turner (SNL) – CFD/structural analyses data interface
    - Sham, Nath (ORNL) – test problem formulation/definition, structural analysis

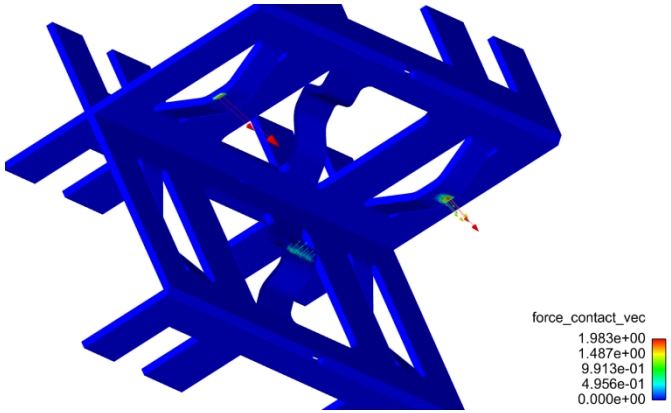
Structural Dynamics Analyses

3D Analyses - High Fidelity Prediction of Rod Failure Caused by GTRF Wear



WEC/VITRAN

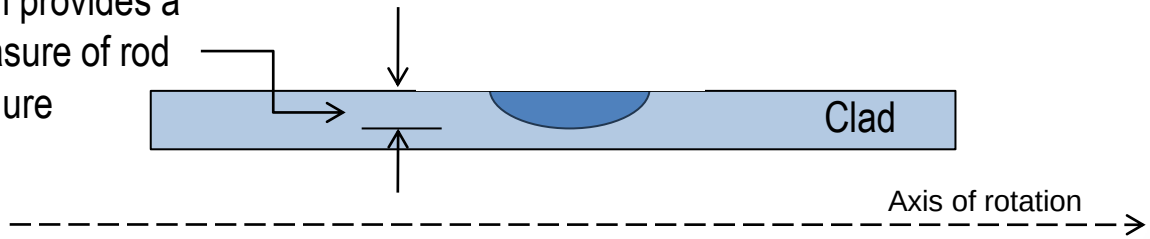
- Point contact at wear site
- 1D model
- Can predict wear volume



3D model

- Obtain contact tractions over wear area
- Can predict wear depth profile using new MPO initial wear model

Wear depth provides a direct measure of rod failure



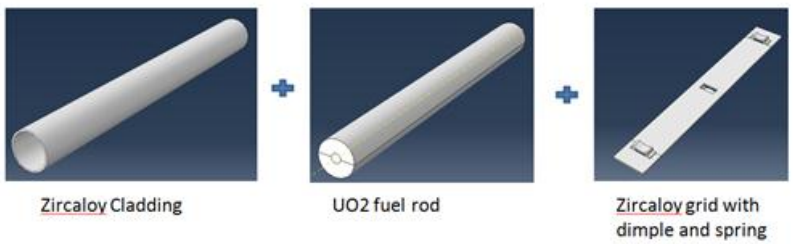
Inherent ambiguity in using wear volume to predict rod failure

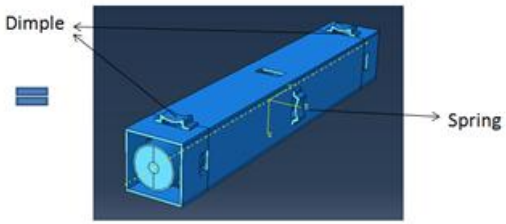
Incorporation of Creep Model

Wei Lu and Michael Thouless (Univ. of Michigan)

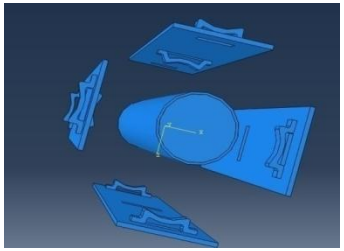
Mechanical Engineering
University of Michigan

This study demonstrated that it was possible to incorporate a creep model into a GTRF analysis to compute the evolution of the normal stresses at the contact. This will provide the basis for a subsequent project to incorporate this normal stress into a wear model.

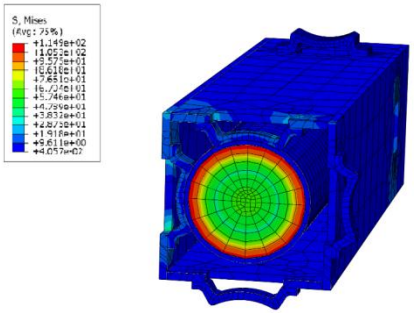




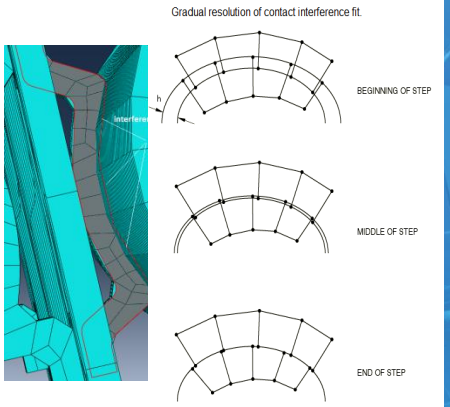
The model is composed of three parts: UO_2 fuel rod, zircaloy cladding, and four zircaloy plates with punched dimples and springs



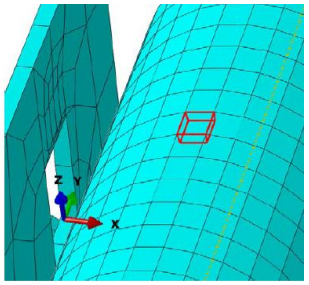
A unit spacer grid comprises four plates. Each plate has two punched dimples on one side and one punched spring on the other side.

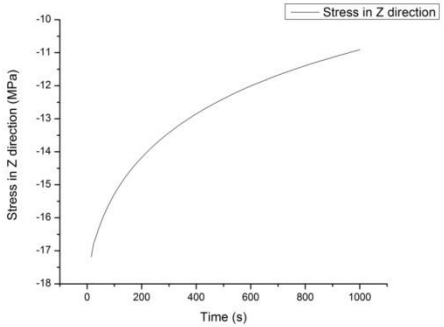


The temperature distribution



A shrink-fit method to gradually resolve the interference distance





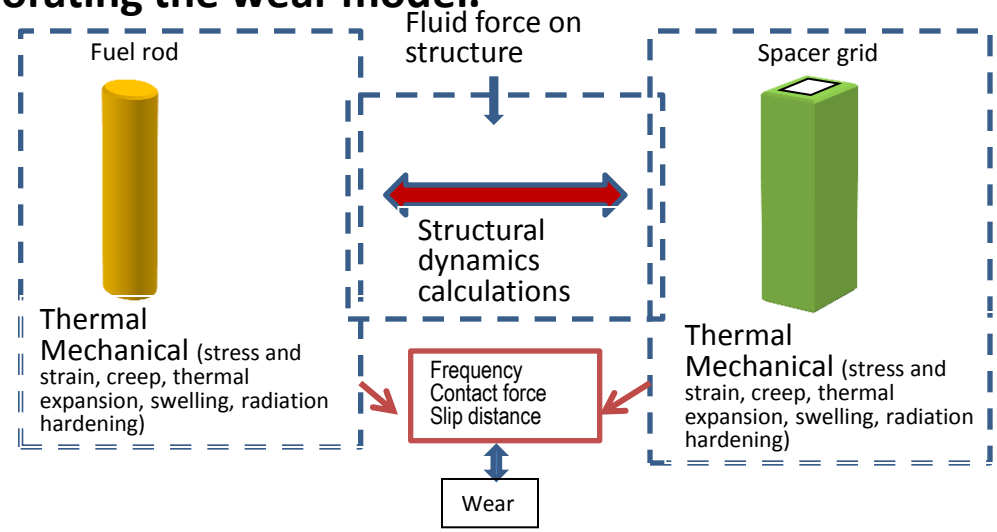
The stress relaxation of an element in the cladding in contact with the spring. The negative stress means compression

Nuclear Energy

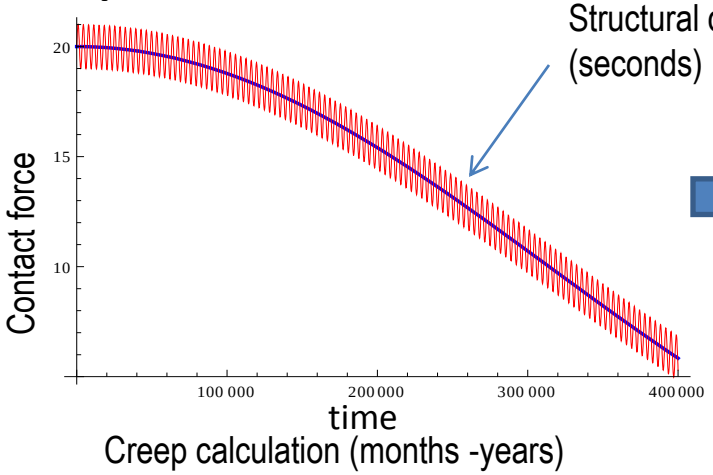
CASL-U-2011-0072-000-R

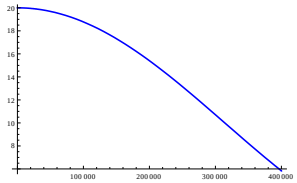
Future Work

Develop and demonstrate structural-mechanics framework for evolution of pin-grid contact incorporating the wear model.



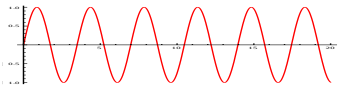
Develop the framework for multi-time-scale calculations and integration





Creep calculation gives time average contact situations

Interface with dynamics



Interface with wear model

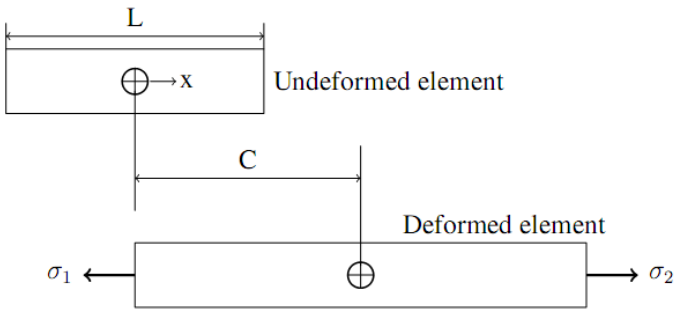
Structural dynamics calculation at given sampling time to get frequency, amplitude of contact force, slip distance.

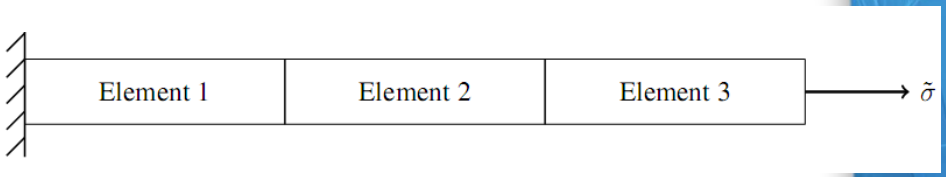
Wear model gives prediction of local interference change

Initial Work on Discrete Element Model

Mike Demkowicz (MIT)

- Discrete elements with continuous displacement field defined within the element
- Quasi-static simulation





- Future work:
  - Complete 1D model (adding dynamics and simulating fracture)
  - Develop 2D DEM wear model (fracture and contact interaction)
  - Transition to 3D (further application of model to common wear problems, such as the Mindlin analysis)
  - Incorporate additional effects into wear model (e.g. coupling with models from CRUD and CORROSION teams)

Mindlin analysis:

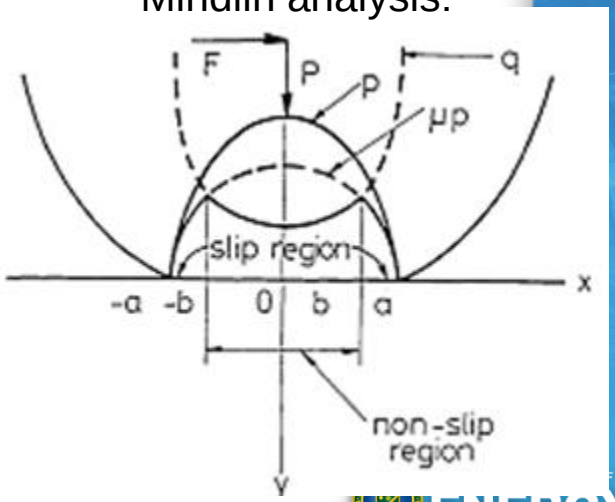
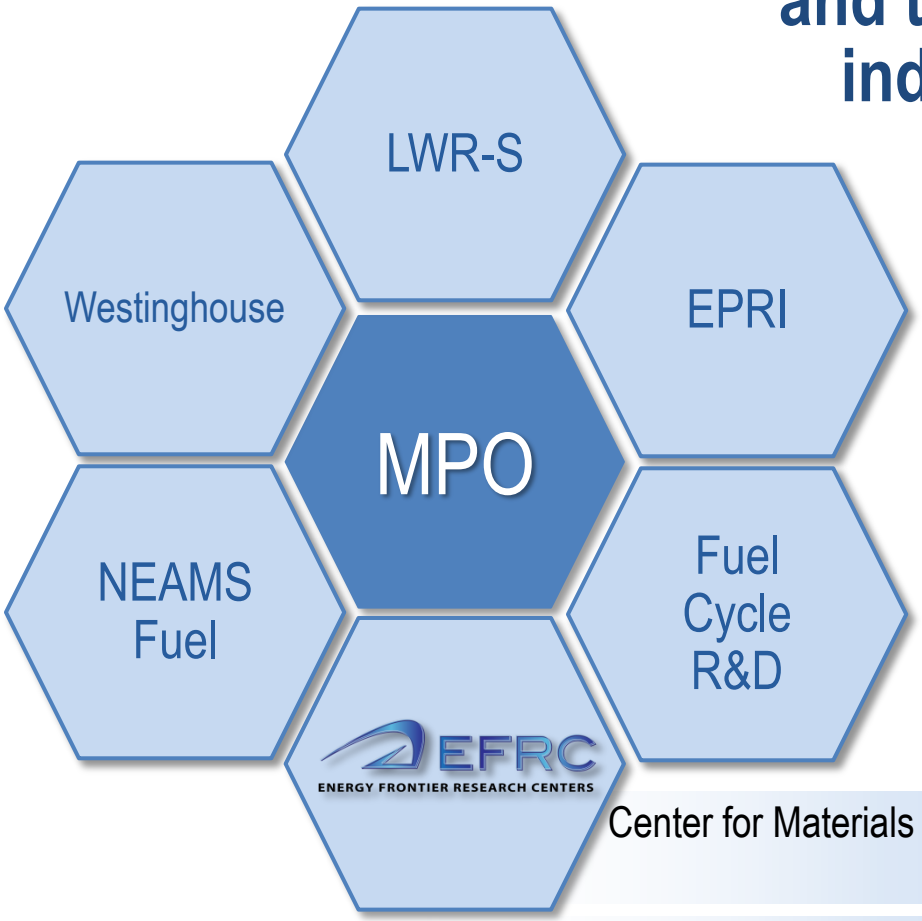


Image from Waterhouse, Intl. Matl. Rev. 37 (1992)

MPO can not do everything required, and thus will leverage existing DOE, industry, and university programs



Aggressive strategy requires cooperation with Office of Science, Office of Nuclear Energy, etc., programs for the development improved fundamental physics, mechanics and chemistry models

Center for Materials Science of Nuclear Fuel
INL/NCState/UF/FSU

Extreme Environmental Tolerant Materials via Atomic Scale Control of Interfaces
LANL/MIT

Center for Defect Physics of Structural Materials
ORNL

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Virtual Office Community, and Computing (VOCC) Project Update

Roundtable Presentation

August 10, 2011

April Lewis
CASL Collaboration and Ideation Officer
VOCC Laboratory Manager

CASL-U-2011-0072-000-R

Talking Points

- Facility Readiness Update
  - VOCC One Roof, Huddles, Collaboration Portal, etc.
- Governance
  - Facility Access
  - Reservation Application
  - Training
- Issues and Impacts

Collaborative Discussion

Virtual Office, Community, and Computing (VOCC)

Lab	Status	Training Required	Limited Access	Comment
VOCC Labs		✓	✓	Access Training
Battlefield of Ideas(BOI)				
I-WAIT			✓	Pipe work for cooling unit in HPC server room
CASPER Lab		✓	✓	
IVAC Lab		✓	✓	
I-CREATE Lab		✓		MIPS in repair, adding digital signage, etc. for WALDO
Telepresence (Oak and Aspen)		✓		

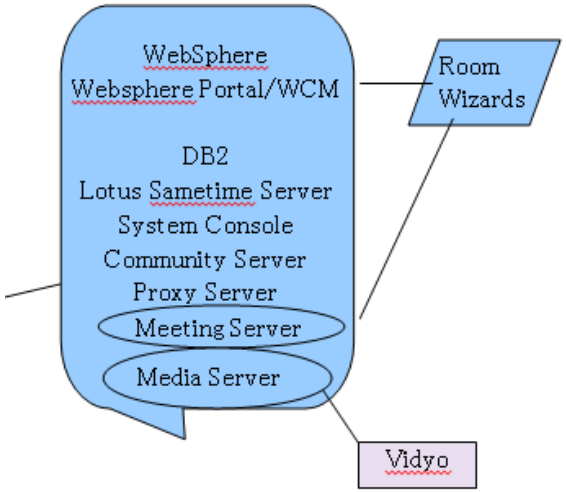
Huddle Status

- 68% deployed ORNL(2), INL, NCSU, WEC, UMICH
- MIT scheduled for next week(8/15-17, 2011), SNL and LANL in planning, Site Visit to SNL in July, Site visit to LANL 8/ 21-23, 2011
- All Huddles deployed and invoiced by September 30, 2011
- Huddles in 2012 proposed EPRI and DOE HQ
- Aspen Huddle down for 3 days, replaced codec and tested system back online.
- New issue: experiencing network “packet filtering” on ORNL network this week

Unified Communications

Collaboration Portal

- Three servers 2 VM's per server, portal exceptions approved
- Second round of setup'/config. This week start integrating portal with AD. Final setup on server ports.



Social Information Connection

Governance

CONSORTIUM FOR ADVANCED SIMULATION OF LIGHT WATER REACTORS DIVISION
Virtual Office, Community, and Computing Facility
Operational Requirements and Guidelines

Proc. No. CASL-001
Page No. 7 of 14
Rev. No. 0

4.12.2. If sensitive data is printed to either of these printers, it is the responsibility of the printer user to remove all printed matter from the bins and then cycle the printer to delete the information in the volatile memory.

4.12.3. Any printed matter left in the printer bins unclaimed will be handled as if sensitive and disposed of accordingly.

4.13. **Storage Areas**

4.13.1. Mobis (pronounced "mo-bees") are available for use by any VOCC user. The Mobis provide convenient storage that is mobile and lockable. Since there is a limited number, use of the Mobis should be coordinated with the VOCC IT Coordinator, which includes making a reservation for use or use over an extended timeframe. The Mobis are restricted to use inside of the VOCC facility. When a user is finished with the Mobi, the key is placed back in the lock for the next user.

4.13.2. Storage lockers are available in Room F322. These lockers vary in size and can be used for storing laptops, cell phones, other electronic devices, etc. These lockers are intended for use to store items that will not be allowed in the VOCC facility during sensitive discussions. However, they are currently also being made available for general storage use by VOCC users on a short-term basis (daily use maximum). Since there is a limited number, use of the Mobis should be coordinated with the VOCC IT Coordinator, which includes making a reservation f over an extended timeframe. When a user is finished with the locker, the key is plac lock for the next user.

4.14. **Electronic Writable Media and Devices**

4.14.1. All thumb drives, portable hard drives, and storage media (CD-ROMs, DVDs, memo to be connected to or read by VOCC computers must be scanned prior to use. VOC a scanning station for this purpose. A sticker will be placed on each item to signif use with VOCC equipment.

4.15. **VOCC Facility Access Control Requirements**

4.15.1. All VOCC facility users are responsible for complying with the access control requir in this section and the VOCC facility usage requirements.

4.15.2. Access to the VOCC facility will be limited to persons with work activities in colla directly relevant to, or specified by CASL-funded scope and execution plans. The CA office shall determine and indicate the VOCC access status for all CASL personne Directory.

4.15.3. The VOCC Operations Manager will be the control point for synchronizing the VO access list with the CASL Directory. The CASL CIO shall server as backup for Personnel will be included on the VOCC proximity card access list according to tl access status in the CASL Directory.

4.15.4. All personnel not on the VOCC proximity card access list are considered to be a (reference 4.15.10)

4.15.5. ORNL Visitor Control will maintain the VOCC proximity card access list at the directi VOCC Operations Manager, with the CASL CIO providing backup. The CASL Direct access list will be periodically examined (at least quarterly) to ensure all staff on the a are consistent and in compliance with CASL's constantly-changing requirements and scope.

4.15.6. Each person must individually pass their badge over the proximity card reader, hear a "beep", and be provided with a green light in order to gain access. "Tailgating" into the VOCC facility is not allowed. "Tailgating" is the practice of one individual using their badge to gain access to the facility

Completed VOCC Operational Requirements and Guidelines Document, foundation for facility Access training.

4.12.2. Access to the VOCC facility will be limited to persons with work activities in collaboration with, directly relevant to, or specified by CASL-funded scope and execution plans. The CASL Director's office shall determine and indicate the VOCC access status for all CASL personnel in the CASL Directory.

4.12.3. The VOCC Operations Manager will be the control point for synchronizing the VOCC proximity access list with the CASL Directory. The CASL CIO shall server as backup for this function. Personnel will be included on the VOCC proximity card access list according to their indicated access status in the CASL Directory.

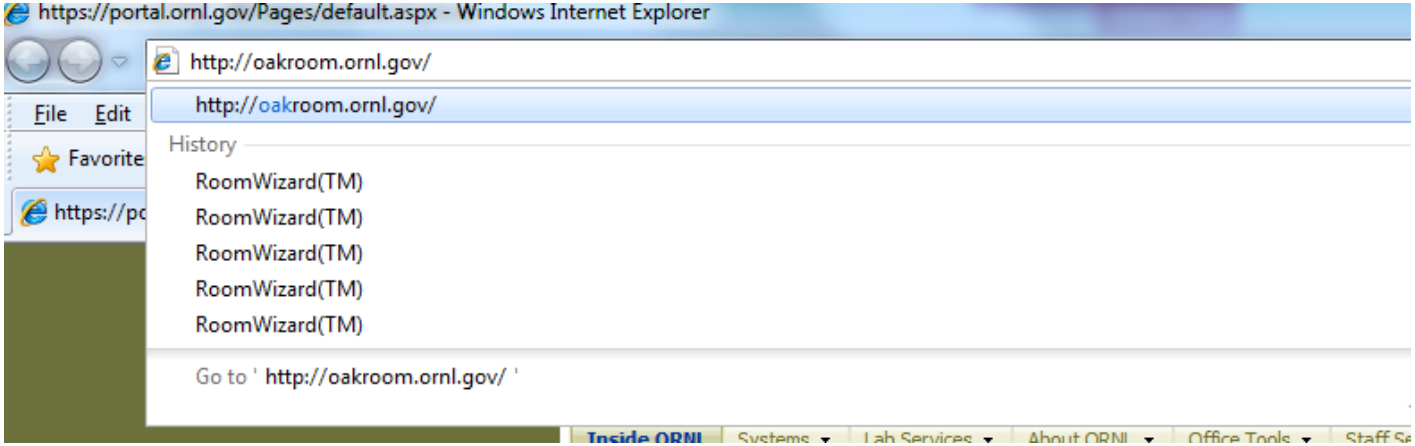
4.12.4. All personnel not on the VOCC proximity card access list are considered to be a VOCC visitor. (reference 4.12.10)

4.12.5. ORNL Visitor Control will maintain the VOCC proximity card access list at the direction of the VOCC Operations Manager, with the CASL CIO providing backup. The CASL Directory and the access list will be periodically examined (at least quarterly) to ensure all staff on the access list are consistent and in compliance with CASL's constantly-changing requirements and scope……

Access, Training, Metrics

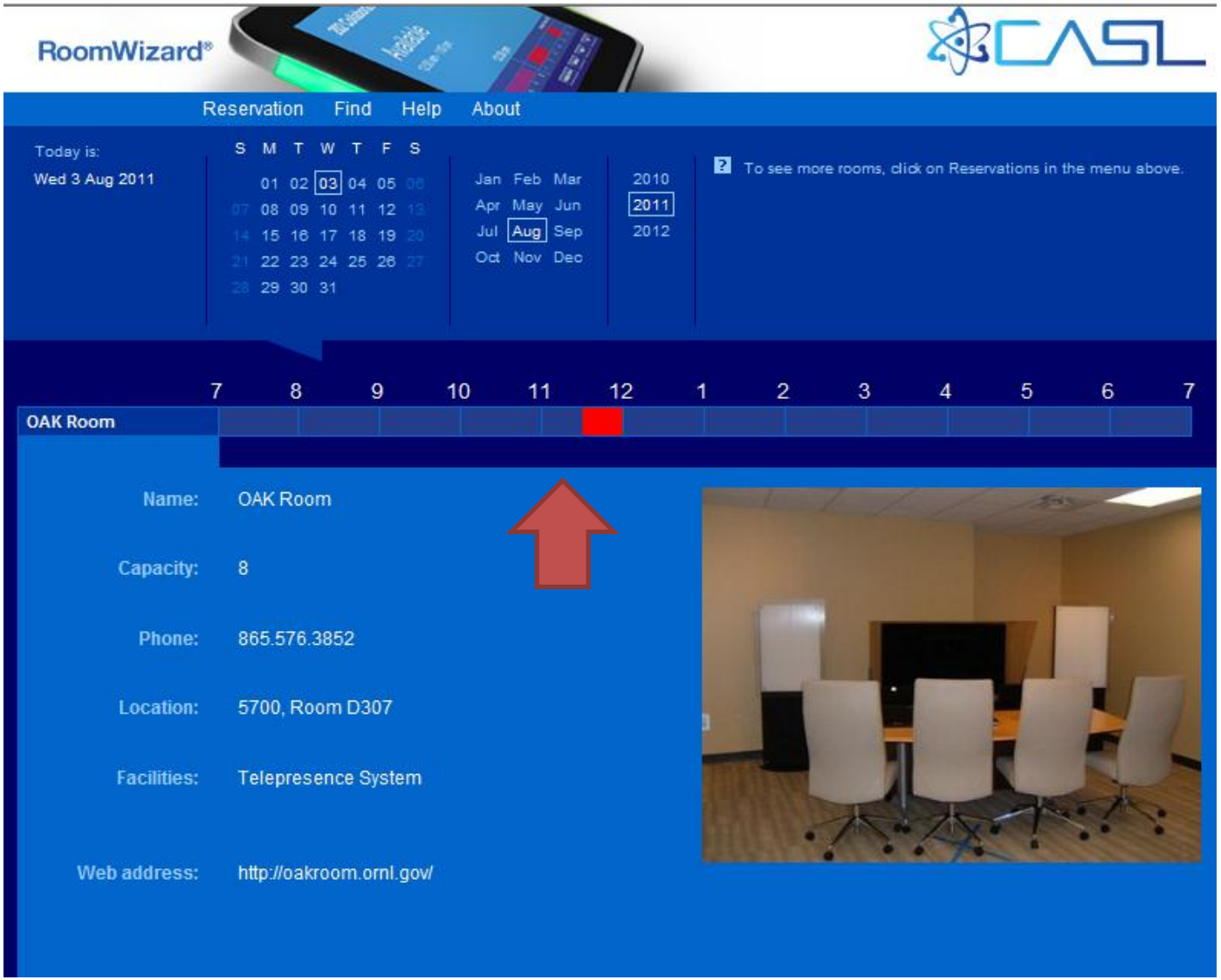
Virtual Office, Community, and Computing

- RoomWizards are online and can be reserved via an Internet Browser
- Venue name is in the URL address
  - For example: http://oakroom.ornl.gov
- Venue Names: IDEATE1, IDEATE2, IDEATE3, IDEATE4, IDEATE5, IDEATE6, IVACLAB, ICREATELAB, CASPERLAB, OAKROOM, ASPENROOM



Virtual Office, Community, and Computing

Click the appropriate time for your meeting on the timescale



Virtual Office, Community, and Computing

- To complete the reservation, fill out the form. Include your email address and check the box for E-mail receipt to receive an email with the details of the reservation. Click Save to make the Reservation

RoomWizard®

Reservation Find Help About

Today is: Thu 4 Aug 2011

To complete the reservation, fill out the form below.
To enter more info, use the advanced reservation form.

OAK Room

Purpose: CASL Roundtable Presentations Pl
The purpose of the reservation

Click here to use the advanced reservation form

Host: First Name Teresa Last Name Robison
The person responsible for the reservation

Host E-mail: robisontk@ornl.gov
Host's or reserver's e-mail address

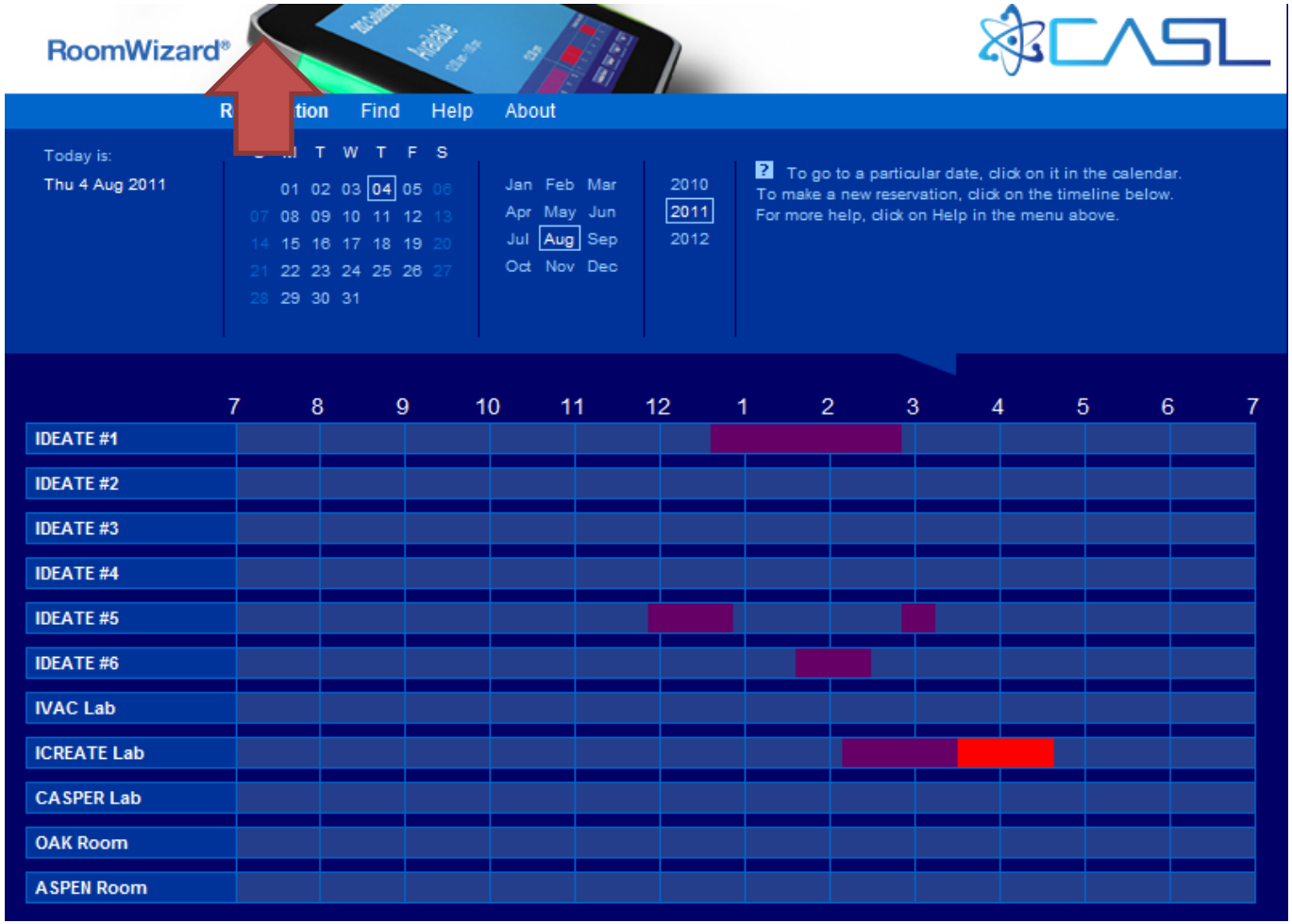
E-mail receipt
Send me an e-mail with the details of this reservation

Time: 3:00 pm - 4:00 pm
Start time End time

Save — Make the reservation
Quit — Don't make the reservation

Virtual Office, Community, and Computing

- To reserve other Venues, Click the Reservation button to retrieve a list of all VOCC venues
- Reservation view shows what Venues are available by date
- Detailed instructions are available



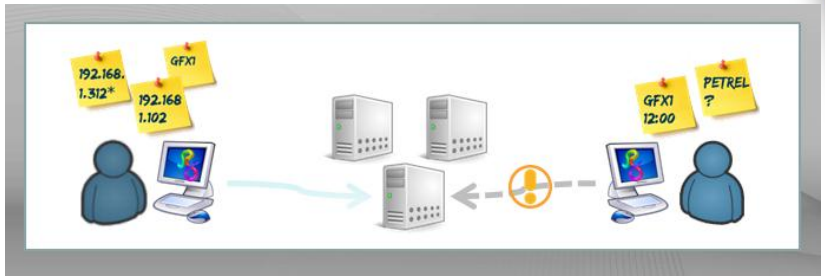
Individual Components

- Data Architecture
  - Remote Connect Configuration, RGS and Connection Broker software
- Collaboration Portal
  - Web Manager, Media Service,
- Room Wizards
- Network plans for joining ORNL domain
  - Firewall issues
  - Network connectivity, authentication,

What are we working on now?

RGS and Connection Broker

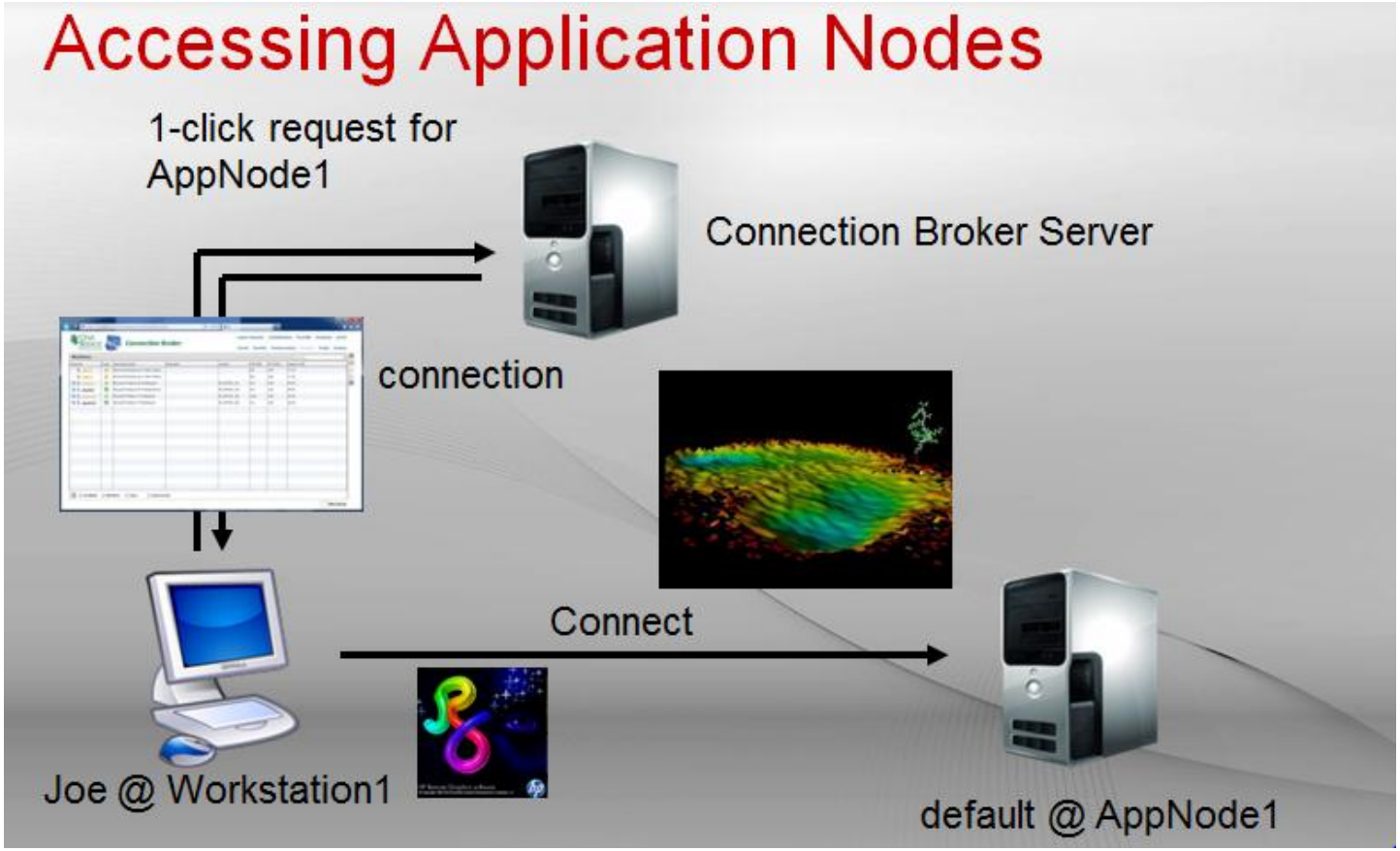
- **HP's RGS is used for the remote desktop access**
  - Workstation → workstation for collaboration
  - Workstation → application node for display capabilities
- **RGS features**
  - High-performance, low bandwidth
  - Remote video, mouse, keyboard, audio (optional USB, text copy/paste)
  - Collaboration (1<->many)
  - Secure



- **Connection Broker offers Web based access for remote visualization**
  - Easy for users to find each other and collaborate
  - Easy for users to find their resources
  - Easy to connect and work with RGS

Managed or Mediated Graphics Collaboration

Managed Access for limited Viz. licenses



Sample Execution

Content Management

Off Use Screen Content Management

ISSUES and Impacts

CYBER.CYBER…CYBER

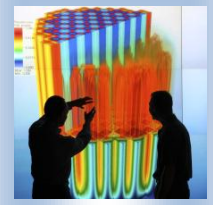
Reconfiguration of ORNL Networks

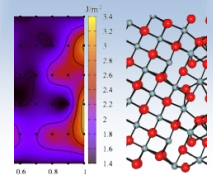
Virtual Office, Community, and Computing (VOCC)

"Have questions or want additional information?"

- VOCC Contacts:
  - April Lewis, Collaboration Ideation Officer, VOCC Project Manager, VOCC Laboratory Manager
  - John Shaw, VOCC Operations Manager (acting)
    - Handles the day to day operations(equipment, people, etc)
  - Teresa Robison, VOCC IT Coordinator and Division Cyber Security Officer
    - Assist VOCC Project manager with IT issues, supports VOCC Operations Manager with Vidyo Instruments and scheduling.

VOCC Project Contacts





Radiation Transport Methods (RTM) Summary of Projects

CASL Roundtable, Raleigh
August 9-11, 2011

Bill Martin
University of Michigan
RTM Lead, CASL

John Wagner
Oak Ridge National Laboratory
RTM Deputy Lead, CASL

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL-U-2011-0072-000-R

RTM consists of 5 projects

- **Sn** (discrete ordinates) – the primary development path for deterministic transport
- **MOC** (Method of Characteristics) – the alternative development path for deterministic transport
- **Monte Carlo and hybrid methods** – the development path for stochastic transport and advanced hybrid transport methods
- **General transport** – methods development that supports all transport effort
- **Coupled transport** – multiphysics coupling with neutronics

RTM projects build upon the initial transport capability deployed in VERA

Overall Strategy for RTM

- **Pursue three independent transport approaches to deliver 3D pin-resolved transport for production calculations:**
  - Sn and MOC are complementary deterministic transport capabilities and both are being developed for VERA-TR.
  - Monte Carlo is (now) the benchmark transport capability
  - Hybrid Monte Carlo is the advanced transport capability
- **Explore improvement of existing transport capabilities applicable to deterministic or stochastic transport:**
  - Advanced energy condensation methods (vs multigroup)
  - Transient discretization methods
- **Explore advanced coupling methodologies:**
  - High-order/low-order coupling with CMFD
  - High-order/low-order coupling with Variable Eddington Factors
  - Advanced solvers to support high-order/low-order multiphysics coupling

Brief descriptions of RTM sub-projects

- **3D Sn transport**
  - 3D Sn transport development
  - Unstructured mesh development for Sn transport
- **MOC transport**
  - Improved 2D/1D scheme for MOC
  - 3D MOC feasibility
- **Monte Carlo and hybrid transport**
  - Hybrid Monte Carlo transport methods
  - Monte Carlo Parallelization
  - Hybrid transport with functional Monte Carlo
  - Improved temperature feedback for Monte Carlo
- **General transport**
  - Discrete Generalized Multigroup Method
  - Transient methods for MOC transport
- **Coupled transport**
  - Multiphysics Coupling Based on Effective Low-Order Transport
  - Nonlinear Acceleration of Neutron Transport Criticality Problems
  - Advanced iterative methods for nonlinear multiphysics coupling

Sn Transport Sub-Projects

- 3D Sn transport development (Tom Evans, ORNL)
- Unstructured mesh development for Sn transport (Max Rosa, LANL)

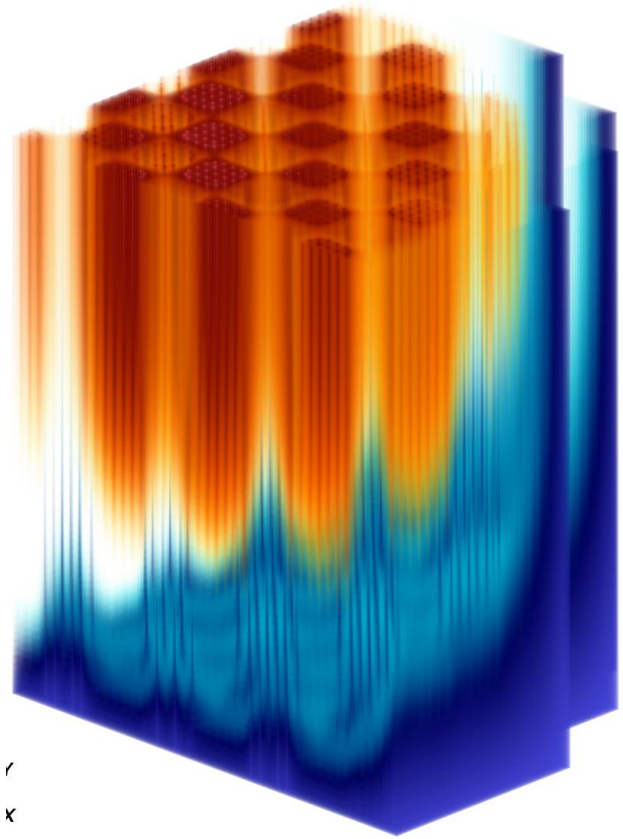
S_N Transport Project – Denovo

Staff

- Tom Evans, ORNL (PI)
- Greg Davidson, ORNL
- Josh Jarrell, ORNL
- Steve Hamilton, ORNL
- Wayne Joubert, ORNL
- Jae Chang, LANL
- Max Rosa, LANL

Students/PostDocs

- Stuart Slattery, Wisc. (PhD)
- Rachel Slaybaugh, Wisc. (PhD)
- Todd Evans, NCS (Postdoc) Collaboration through VUQ
- Cyrus Proctor, NCS (Phd) Collaboration through VUQ



Objectives and Strategies

- Develop deterministic neutron transport capabilities:
  - Full core simulation including pin-resolved transport
  - Multigroup cross section generation
  - Lattice physics
  - Depletion
- Accommodate capability development in RTM
  - Hybrid transport methods
  - Unstructured mesh development
  - Transient methods development
  - Ultrafine energy groups

Approach

- Use the Denovo code framework for the following tasks:
  - Provide 3D, S_N, regular-grid transport with sub-cell interface treatments
  - Provide unstructured grid S_N transport using the Capsaicin Poblano library
  - Provide a Neutronics package coupled to SCALE for cross section processing and depletion
- Build LIME ModelEvaluators and TransferOperators that can be used to integrate the neutronics components into VERA for coupled-physics simulations

Significant Results/Highlights

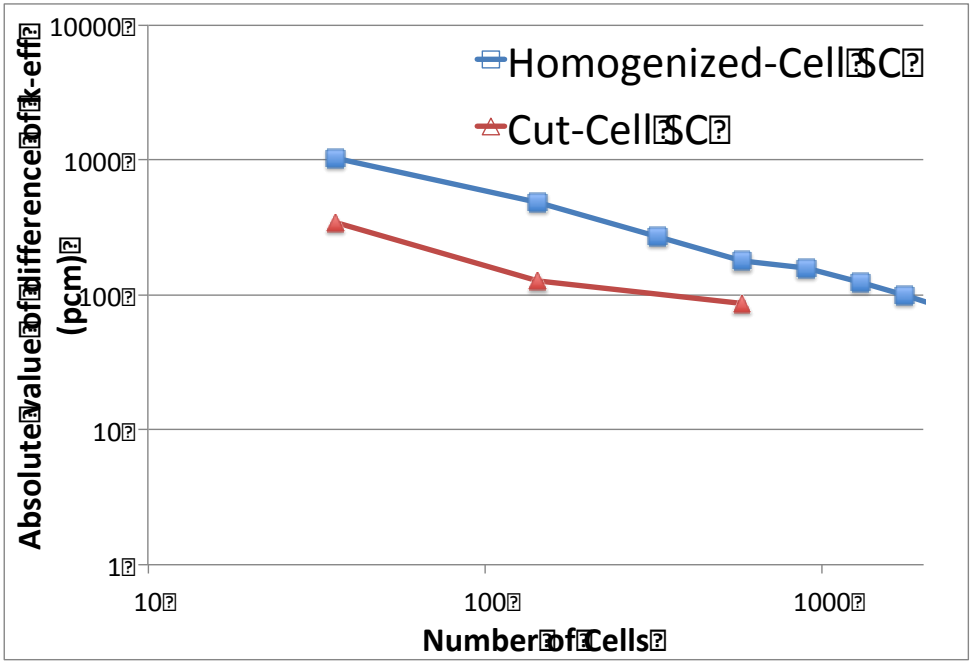
- L3:MNM.Rad.Y1-2.01: Demonstrate full-core, pin-homogenized, 3-D transport capability
  - Completed 3/31/2011 (described next)
- Talk presented at HPC Users Forum: “CASL: Neutronics and 3D S_N Transport,”, April 6, 2011.
- Best Paper Award, ANS Winter Meeting 2010: “Massively Parallel Solutions to the k-Eigenvalue Problem, “ Davidson, Evans, and Slaybaugh.
- Also contributed to several VRI milestones (described in other presentations).

L3:MNM.Rad.Y1-2.01: Demonstrate full-core, pin-homogenized, 3D deterministic transport

- Successfully ran the C5G7 (unrodded) 3D and 2D benchmarks
- Performed 3D Quarter Core Simulations (A. Godfrey, AMA):
  - Radial zoning varied from 12x12 per fuel pin to 4x4.
  - Axial zoning varied from 15.24 cm to 0.2 cm.
- Conclusions:
  - LD and TLD perform much better than SC when using coarse axial zoning
  - Good results are achieved (< 40 pcm) with LD using 4x4 radial zoning, 15.24 cm axial zoning, and QR 2/4 quadrature → 42 min runtime using 960 cores
  - 6x6 with QR 6/6 achieved best results at 15.24 cm axial (9 PCM)
  - At 2.54 cm LD is still sufficiently more accurate than SC
  - SC requires ~1 cm axial zoning to approach LD results
  - Running a 1.6G-cell problem is feasible (190KCPU-hours)

Future Work – PoR-3

- RTM.SN.P3.01: Denovo development, full-core, pin-homogenized, deterministic transport (L3)
  - execution of the 2D C5G7 test problem (or equivalent problem) using cut-cells,
  - comparison of 2D cut-cell and macro-mixed cell approaches,
  - execution of 3D test problems (from a selection of C5G7, PWR900 core, and 1/4 core cases) using macro-mixed cell meshing,
  - comparison of 3D results to published benchmarks or Monte Carlo-based solutions where appropriate.
- Completed work
  - 2D Cut Cell paper accepted, "A Cut-Cell Approach for 2D Cartesian Meshes that Preserves Orthogonal Grid Sweep Ordering," Jarrell, Grove, and Evans, ANS Winter Meeting, 2011
  - 2D cut cells implemented and tested



Reduction in number of cells using cut-cell treatment in a lattice.

Future Work – FY12

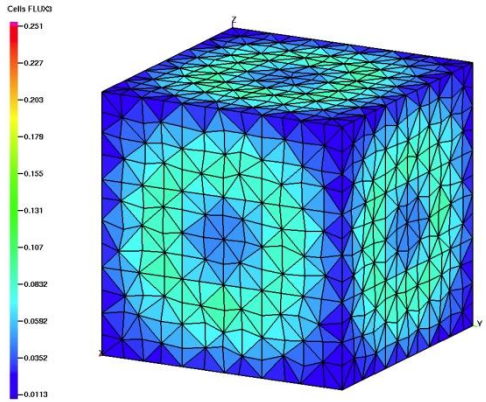
- Develop consistent, hybrid SN/MoC method for 3D deterministic transport
  - Solve IFBA/Gad problems
  - Provide necessary fidelity for full core depletion
- Submit following journal papers (all currently in preparation):
  - Multilevel energy decomposition
  - QR quadratures for reactor calculations
  - 2D cut cells
  - Multigrid energy preconditioning + RQI
- Full neutronics coupling (including cross section processing and depletion)

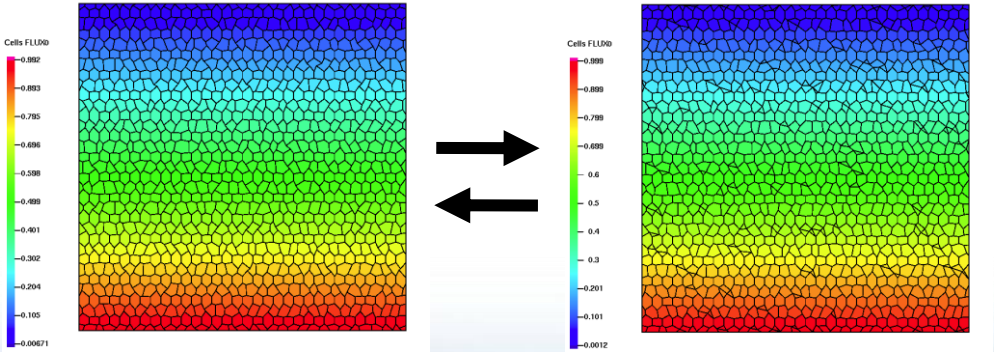
Hurdles

- Budget and funding levels may not be commensurate with all required tasks
  - In addition to RTM work, we have significant deliverables in VRI
  - Unfunded mandate (but a critically important obligation) for student support

Unstructured mesh for 2D Sn

- PI: Massimiliano (Max) Rosa Co - PI: Randal S. Baker
- Collaborators: Jae H. Chang, James S. Warsa
- Use Capsaicin methodology to provide parallel multigroup Sn transport capability on unstructured meshes to VERA - TR
  - Capsaicin is a parallel, unstructured mesh, multigroup Sn code for fixed source problems
  - Eigenvalue problems solved as non - linear fixed - point iteration (JFNK, Accelerated fixed - point)
  - Can detect non - convex mesh, compute on convex mesh, then project back to non - convex mesh
  - Provide interface specification and libraries for VERA-TR (Denovo) to access this capability





L4 milestones

- SN.01.05 - Capsaicin source code deposited into CASL repository (9/30/10)
  - Capsaicin source code available under nfi006 project folder as of March 2011
  - Delay partly due to intellectual property (IP) issues and especially to bureaucratic hurdles in obtaining access to computational resources at ORNL (Max Rosa was granted access to some computational resources in February of 2011)
  - We plan to make Capsaicin available under the CASL git repository recently made available on casl-dev.ornl.gov (Max Rosa is waiting for access to the server)
- SN.01.06 - Capsaicin successfully running its neutronics acceptance tests on leadership architecture at ORNL (12/31/10)
  - Milestone completed in March of 2011 (on frost)
  - While waiting for access to computational resources at ORNL further tests were added to Caspsaicin's suite of neutronics acceptance tests and committed into Capsaicin source code by the end of 2010

L4 milestones (cont)

- SN.01.07 - VERA - TR successfully running Capsaicin's neutronics acceptance tests on unstructured meshes (3/31/11)
  - Currently postponed as milestone for POR - 3 (9/30/2011)
  - A first specification for the interface to Caspsaicin's neutronics module Poblano was agreed upon in early March and implemented and tested in Capsaicin at the end of March 2011
  - Recently started work to support the Denovo team in writing a new solver option which calls the interface to Poblano
  - Communication between the Capsaicin and Denovo teams is critical for the development and implementation of the interface

- SN.01.08 - VERA-TR running a 2D lattice physics benchmark problem with the same data on both structured and unstructured meshes (6/30/11)
  - Will have to be pushed into FY 2012 (see next slide)
  - Definition of 2D lattice physics benchmark problem will require closer collaboration and interaction between the Capsaicin and Denovo teams

Plans for FY 2012

- Complete unstructured mesh development for 2D Sn transport in VERA-TR
  - Expand SN.01.08 milestone to contemplate also comparison with a structured mesh calculation using cut cells
  - In case overhead associated with interface approach turns out to be limiting from an application's performance stand point consider alternative approach of implementing unstructured mesh solver option directly in VERA - TR
- Write report which summarizes implementation of 2D unstructured mesh capability within VERA-TR
- Investigate implementation of a 3D unstructured mesh capability within VERA-TR
  - Can leverage on the existing 3D Sn transport capability on linear tetrahedral finite elements available in Capsaicin
  - Research on 3D DFEM for polyhedral finite elements

MOC Transport Sub-Projects

- Improved 2D/1D scheme for MOC (Ed Larsen, Michigan)
- 3D MOC feasibility (Tom Downar, Michigan)

Improved 2D-1D Method for DeCART

Staff

- Ed Larsen, UM (PI)
- Tom Downar, UM
- Han-gyu Joo, SNU

Students/PostDocs

- Blake Kelley, UM (PhD student)

The Project

- The 3D lattice physics code DeCART uses a “2D-1D” discretization method in which 2D MOC in the radial (x,y) plane is combined with 1-D nodal diffusion in the axial (z) direction.
- The 1-D nodal diffusion model is inaccurate for strong axial variations, due e.g. to control rods or part-length burnable absorbers.
- This project will develop, implement, and test a new 2D-1D method that overcomes this and other deficiencies in the current method.

Approach

- In addition to the inaccuracies mentioned above, DeCART fails to iteratively converge when the mesh (particularly, the axial mesh) becomes too fine. We have discovered two reasons for this:
  - Most importantly, the equations solved in DeCART do not limit to the Boltzmann transport equation in the fine mesh limit.
  - The CMFD acceleration method used in DeCART does not accelerate the transverse leakage terms between the 2-D slices. For problems in which these slices become thin and the transverse leakage terms become large, an inconsistency can occur in the accelerated scattering sources and unaccelerated transverse leakages.
- We have undertaken a study of these (intertwined) issues and devised ways to overcome them.
- The new method preserves the basic 2D-1D methodology.

Results

- To deal with the issues of accuracy and consistency, it is necessary to modify the transverse leakage terms so that the 2D-1D method properly limits to the Boltzmann transport equation for fine meshes. We have devised several ways to do this.
- It is necessary to devise an improved CMFD acceleration method in which the (unknown) transverse leakages are accelerated, together with the coarse cell-averaged scalar fluxes. We have done this also. The new “boundary CMFD” acceleration method has been tested successfully in 1-D. We are confident that it will work in multi-D.
- When implemented in DeCART, the new method should yield numerically consistent solutions of the 3-D Boltzmann transport equation. Also, the new method should be much more parallelizable than the current method.

Challenges

- The new 2D-1D and CMFD methods will not be minor variants of the current methods in DeCART. The implementation of these methods will not be easy.
- The new 2D-1D method will require more computer storage, to store angle-dependent transverse leakages. We see no way to avoid this.

Milestones

- The goal during the first year was to derive the underlying equations that describe the new 2D-1D model and implement the improved methodology into a prototype version of DeCART.
- We have gained a proper understanding of the problems associated with the current 2D-1D method and devised alternative approaches to fix the problems.
- It has been decided that the new method should be directly implemented in the full DeCART code – not in a “prototype” (test) code. This strategy should result in a faster long-term implementation in DeCART.
- Blake Kelley is now “learning the code.”

Milestone: PoR-3

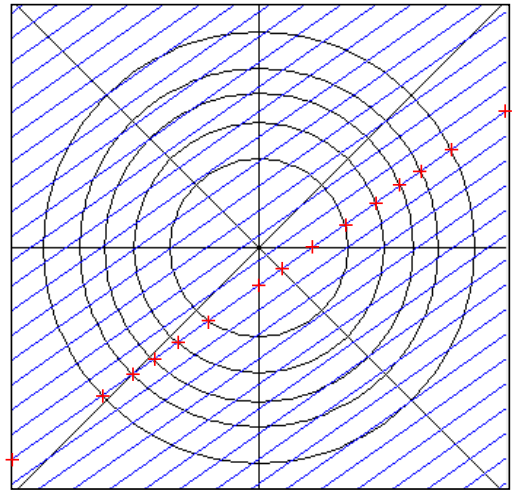
- Because of the decision to implement the method in the full DeCART, a working version of the new method will not likely be running at the end of PoR-3. However, we hope to have one running soon after this.

Future Work

- The new 2D-1D method will be fully implemented in DeCART as soon as possible. It will be tested on several different problems of interest, and based on the results will be modified as necessary to deal with (i) unnecessary excessive run times, (ii) unnecessary excessive storage requirements.
- The new 2D-1D method will not be a minor modification of the existing method, and the new CMFD method will not be a minor modification of the existing CMFD method.
- The resulting work will form the basis for Blake Kelley's PhD project and will become available for general use in DeCART.

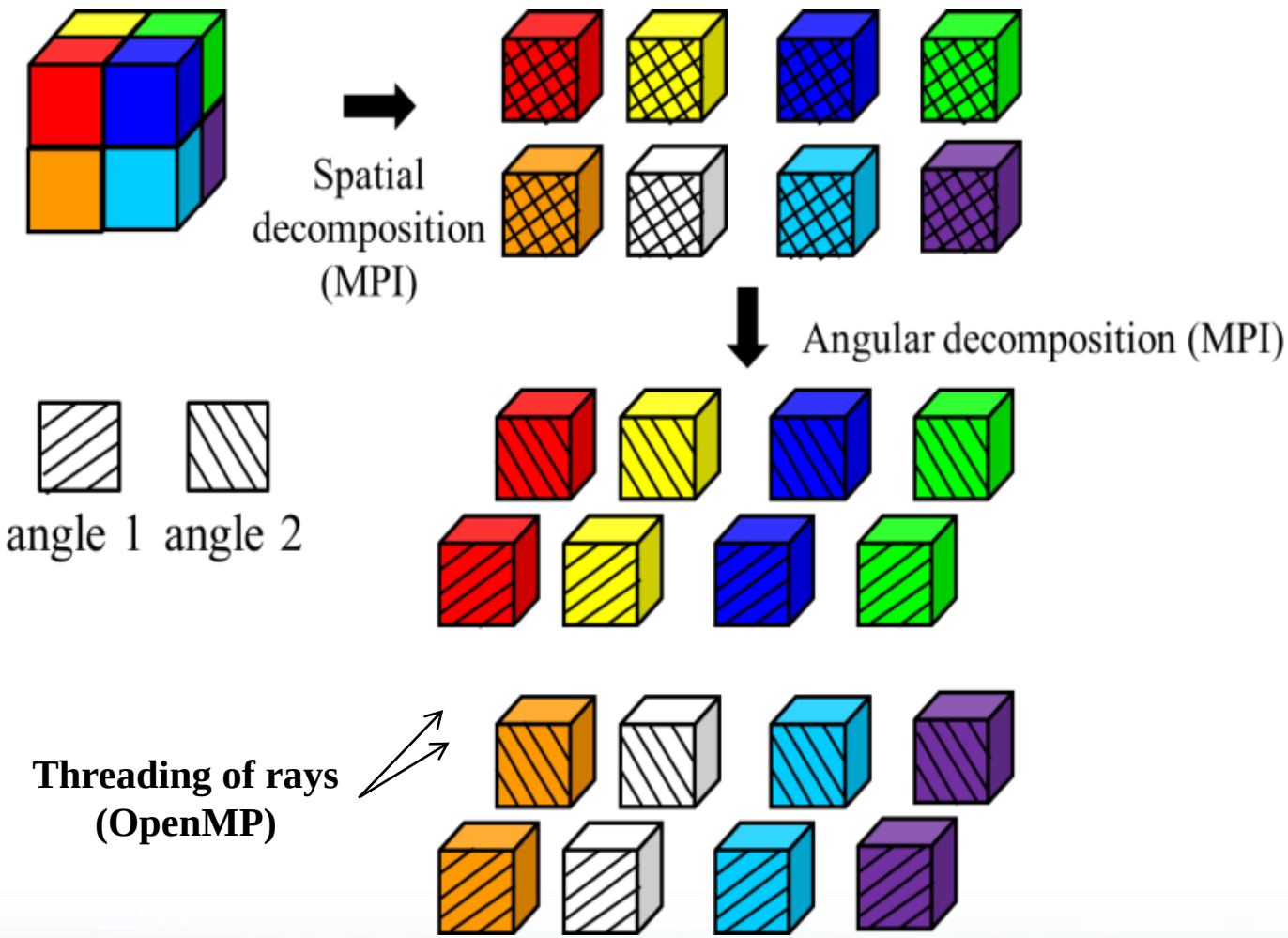
3D MOC feasibility

- PI: Tom Downar (Michigan)
- Co-PI: Bill Martin
- PhD student: Brendan Kochunas

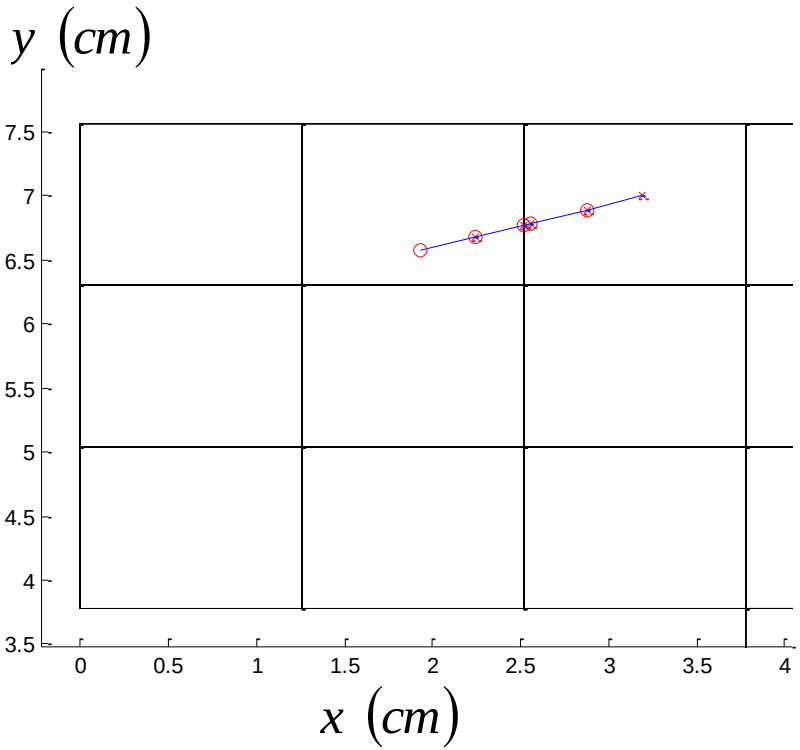


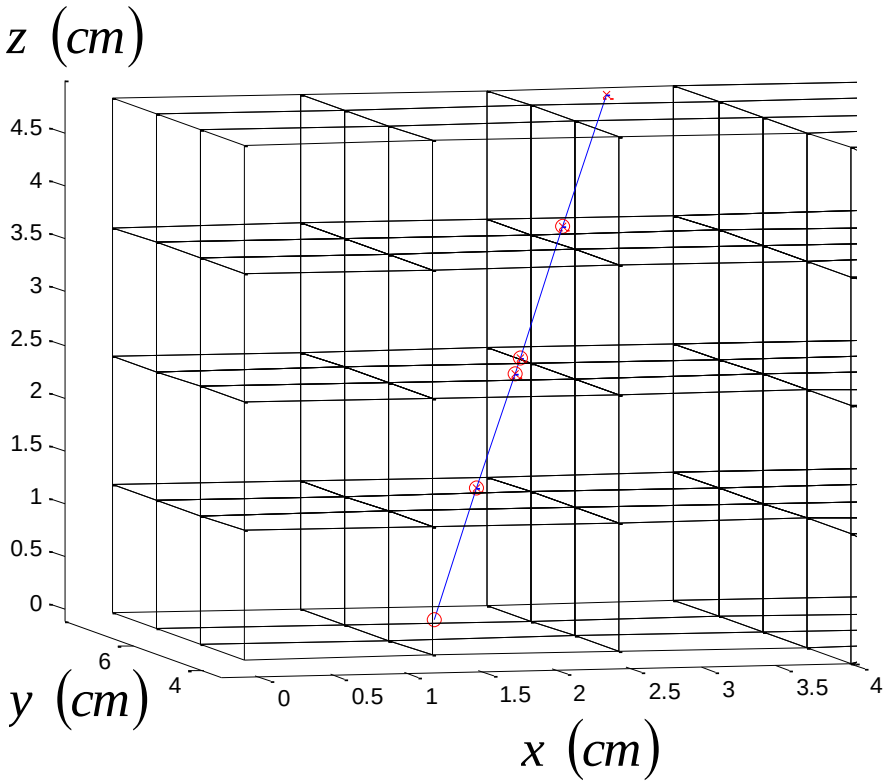
Objective: *Develop and evaluate scalable parallel algorithms for solving the neutron transport equation in 3D using MOC.*

Parallel Algorithm for 3D MOC

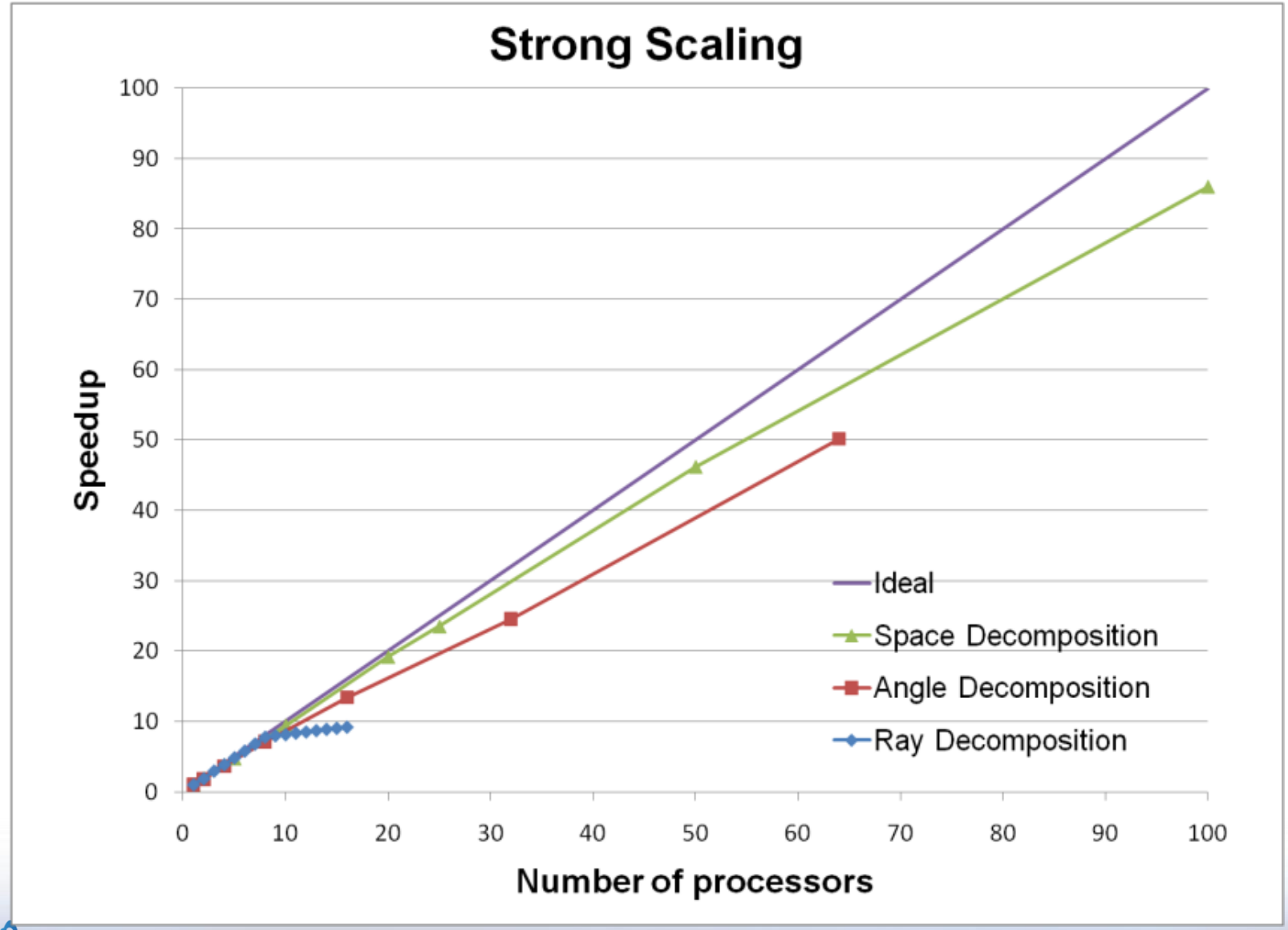


3D MOC – Modular Ray Tracing

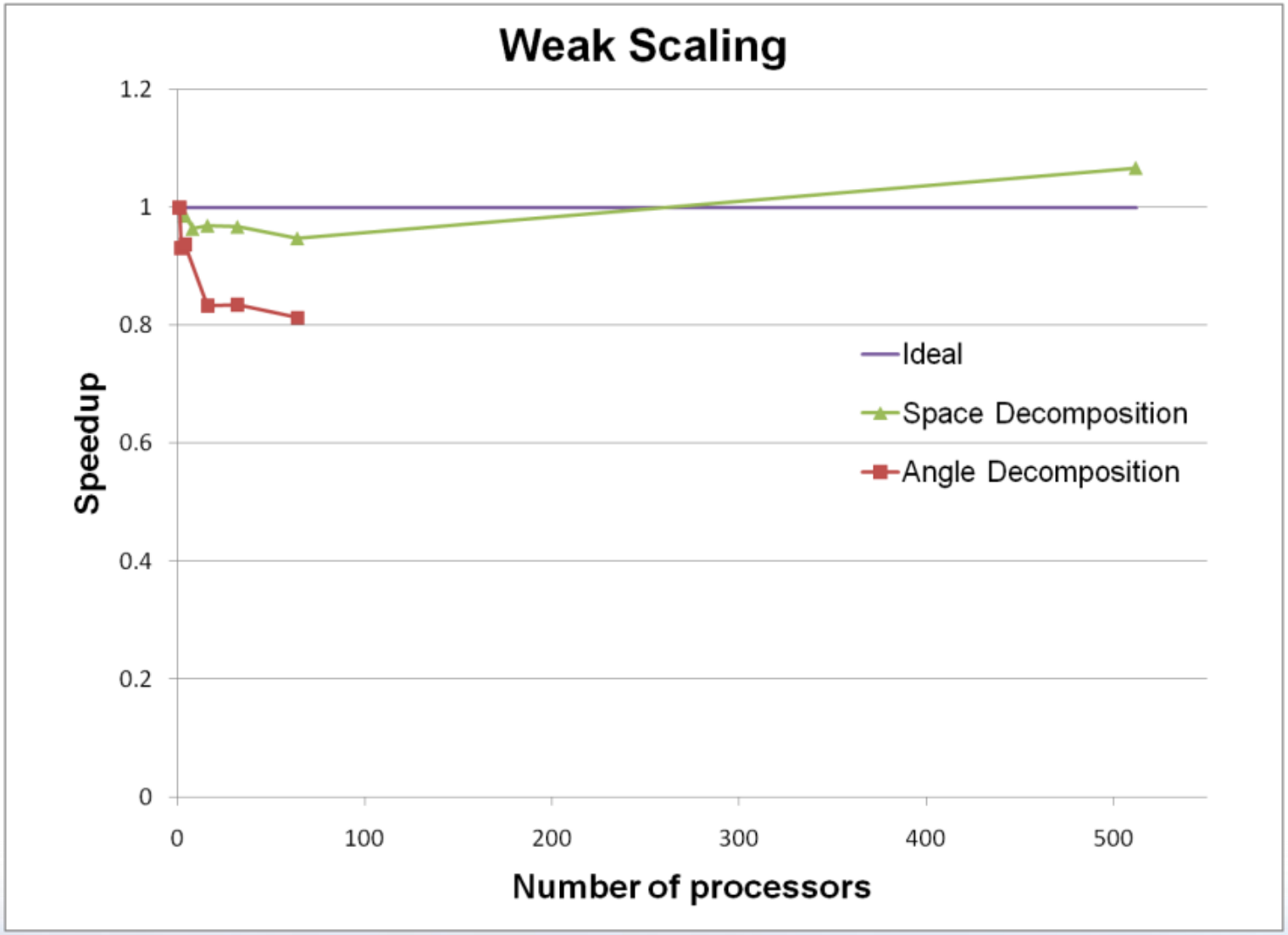




3D MOC – Preliminary Results (strong scaling)



3D MOC – Preliminary Results (weak scaling)



What's Next for 3D MOC?

- Extended geometries
- Investigate parallel decomposition in energy
- Multi-level CMFD acceleration
- Begin V&V to baseline results of 3D MOC
- Scaling studies up to *O*(100K) processors.

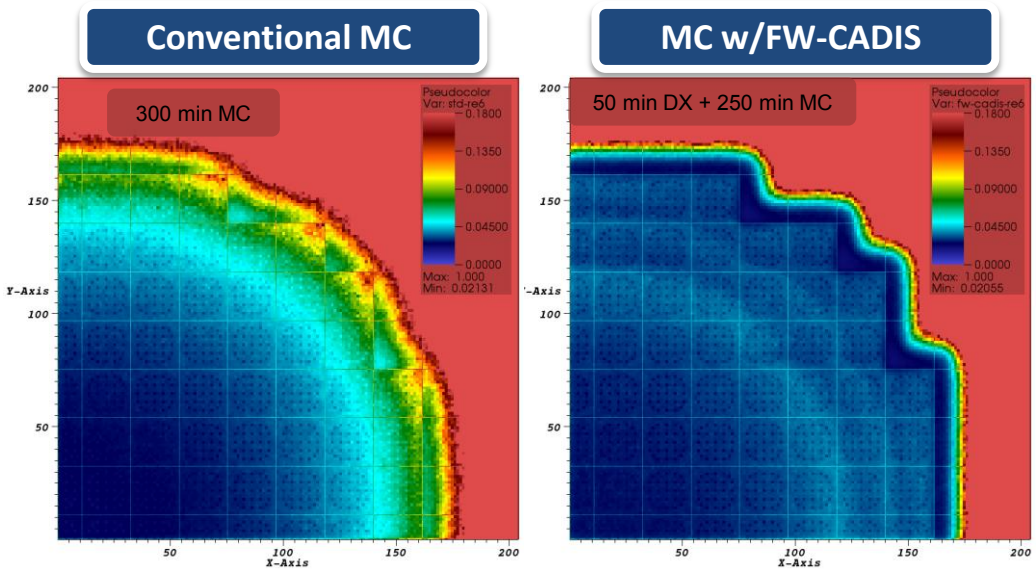
Monte Carlo/Hybrid Transport Sub-Projects

- Hybrid Monte Carlo transport methods (John Wagner, ORNL)
- Monte Carlo Parallelization (Ben Forget, MIT)
- Hybrid transport with functional Monte Carlo (Ed Larsen, Michigan)
- Improved temperature feedback for Monte Carlo (Bill Martin, Michigan)

Hybrid Monte Carlo transport methods

Staff

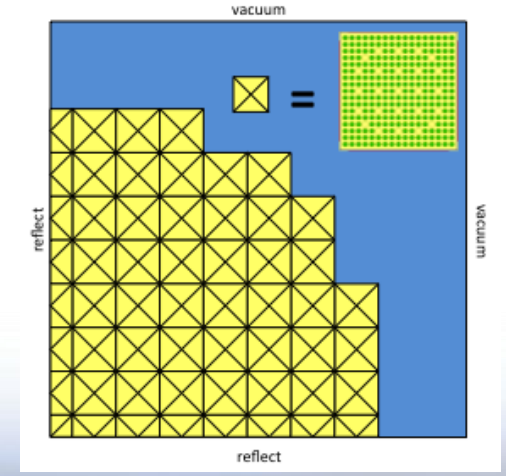
- John Wagner, ORNL (PI)
- Scott Mosher, ORNL (Co-PI)
- Tom Evans, ORNL
- Douglas Peplow, ORNL



Statistical uncertainties in group 6 fluxes (0.15 to 0.275eV)

Students/PostDocs

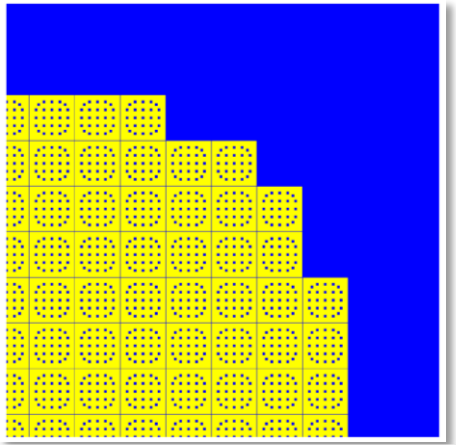
- Brenden Mervin, UT (PhD)
- Nicholas Sly, UT (PhD)
- Ahmad Ibrahim, UW (PhD) (summer 2011)
- Qiong Zhang, NCSU (PhD) (summer 2011, collaboration w/VUQ)



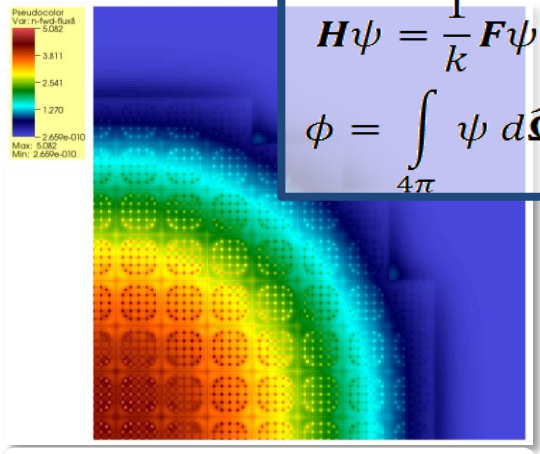
Goal, Objective, Approach

- Goal – overcome one of the principal barriers (i.e., slow, non-uniform convergence of system-wide MC estimates throughout a reactor) to being able to utilize high-fidelity MC for reactor analyses.
- Objective – achieve substantial improvements in computational efficiency and reliability in determining high-precision fluxes throughout the problem space in MC k-eigenvalue problems.
- Approach
  - Identify test problems and develop and verify models
  - Extend FW-CADIS method for flux convergence in k-eigenvalue problems and demonstrate initial implementation
  - Evaluate methods for improving source convergence
  - Initiate development and investigation of alternative hybrid methods
  - Define source and tally convergence performance metrics and initiate performance evaluation

FW-CADIS method has been extended to accelerate reactor eigenvalue problems



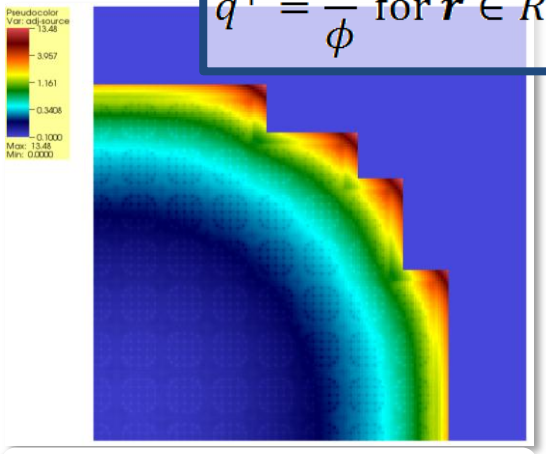
1: construct DX model



$$\boldsymbol{H}\psi = \frac{1}{k}\boldsymbol{F}\psi$$

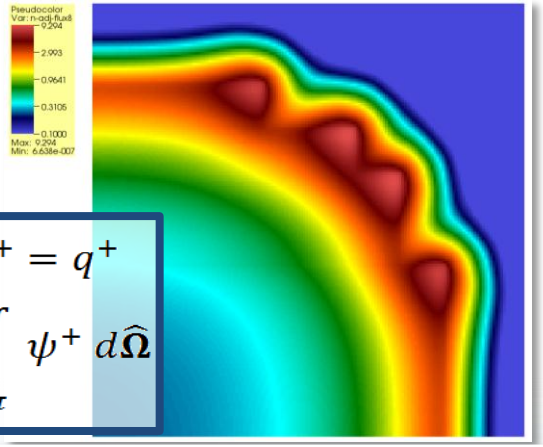
$$\phi = \int_{4\pi} \psi \, d\hat{\boldsymbol{\Omega}}$$

2: solve DX eigenvalue equation



$$q^{+} = \frac{1}{\phi} \text{ for } \vec{\boldsymbol{r}} \in R$$

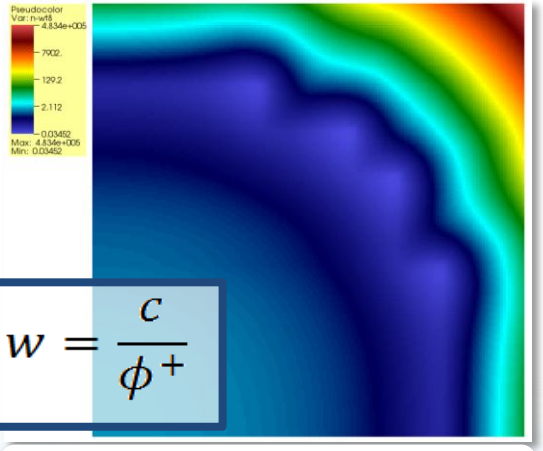
3: construct adjoint source



$$\boldsymbol{H}^{+}\psi^{+} = q^{+}$$

$$\phi^{+} = \int_{4\pi} \psi^{+} \, d\hat{\boldsymbol{\Omega}}$$

4: solve DX fixed-source adjoint eqn

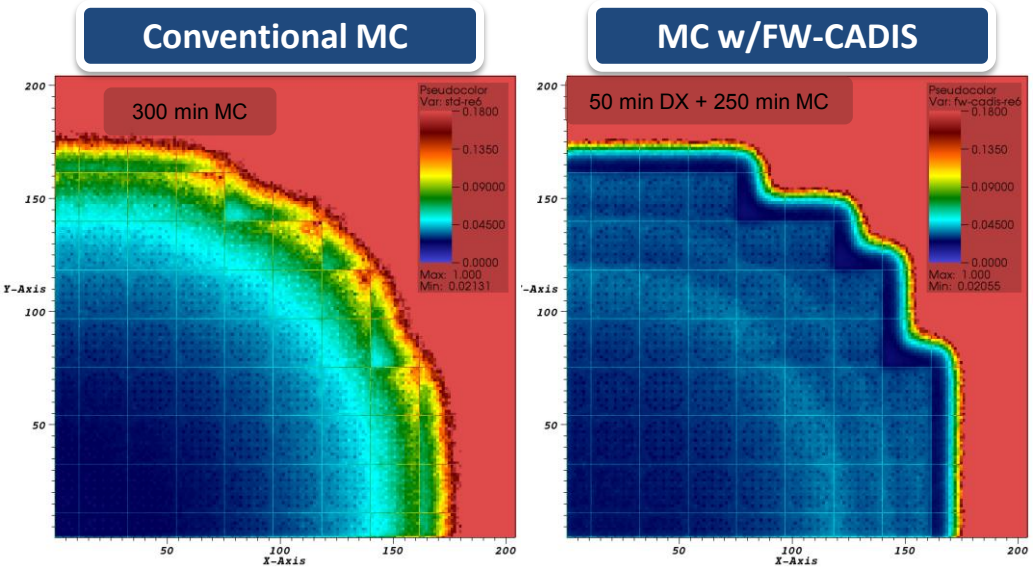


$$w = \frac{c}{\phi^{+}}$$

5: construct weight windows

J.C. WAGNER and S.W. MOSHER, "Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Reactor Analyses," *Trans. Am. Nucl. Soc.* **103**, 342-344 (2010).

Hybrid methods – FW-CADIS helps overcome prohibitive computational time requirements



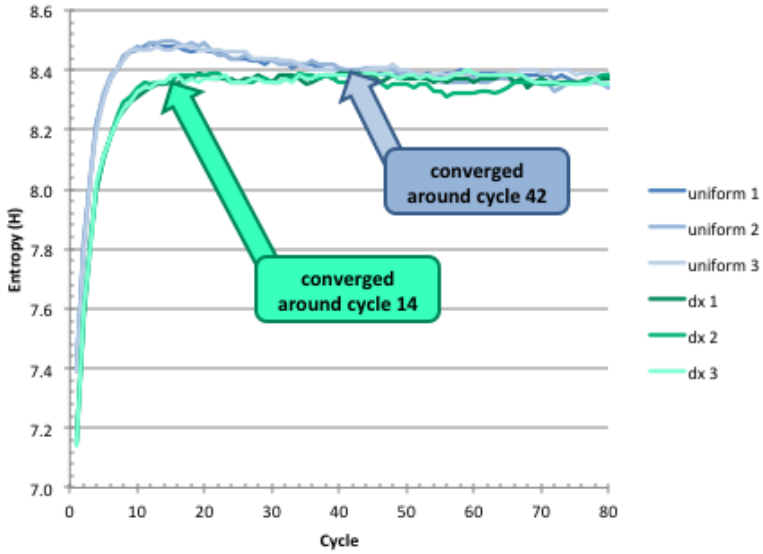
Statistical uncertainties in group 6 fluxes (0.15 to 0.275eV)

	MCNP	FW-CADIS
Uncertainty range	0.6 – 16.2%	1.0 – 6.6%
Time to < 2% uncertainty	323 hrs	45 hrs
Speed up (includes Denovo run time)	-	7.1*

*depending on computational parameters, the speed-up varied between 6 and 10

FW-CADIS deterministic solution can be exploited in other ways:

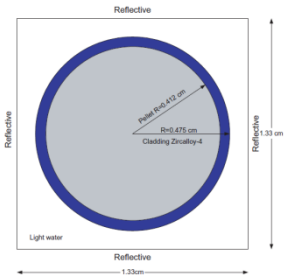
- Generate initial fission source and *k* for MC
  - accelerate source convergence
  - improve convergence reliability

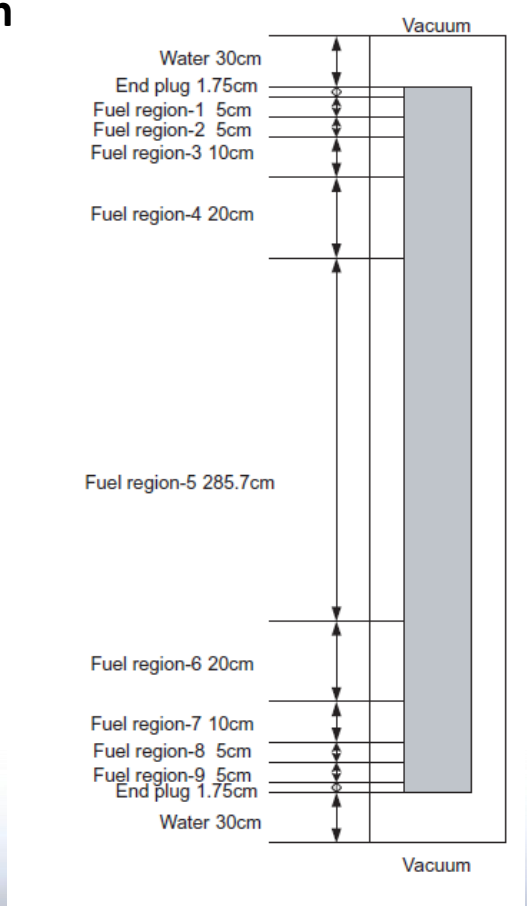


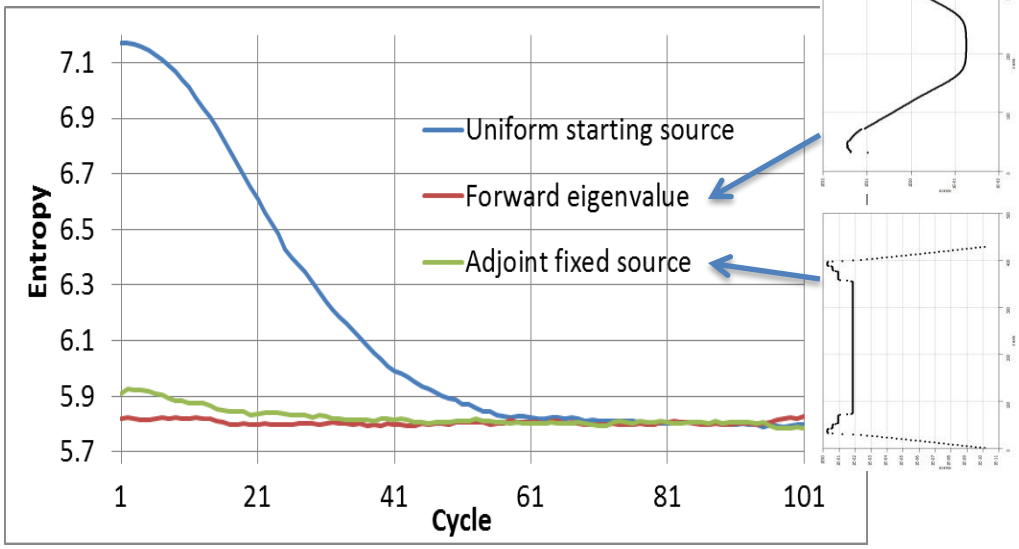
- Select domain boundaries
  - improve parallel load balancing
  - reduce Monte Carlo run time

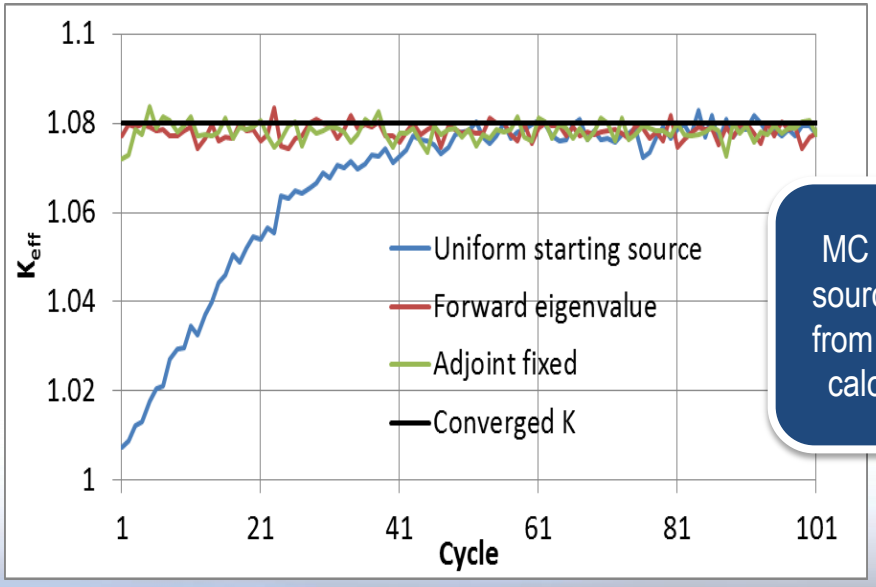
Hybrid methods – source convergence acceleration with deterministic-based starting sources

- **OECD/NEA Source Convergence Test Problem #2 – pin-cell array with irradiated fuel symmetric axial composition**





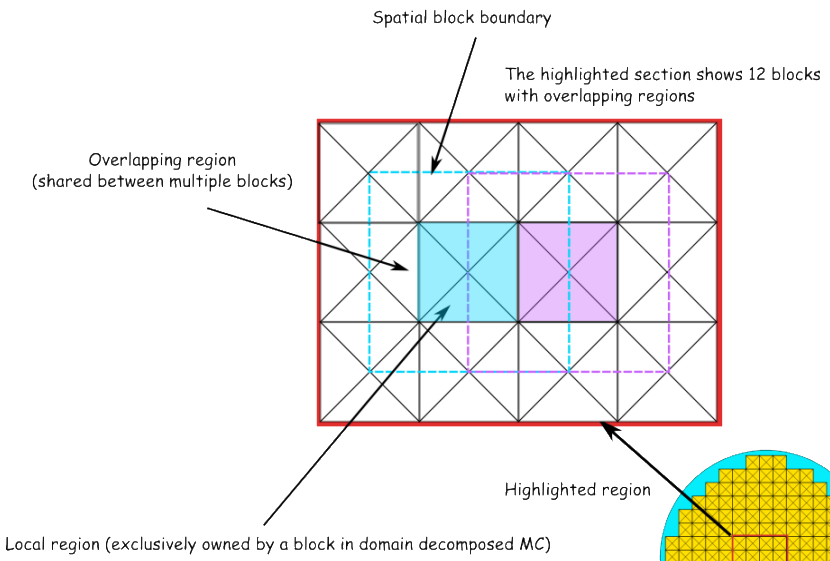


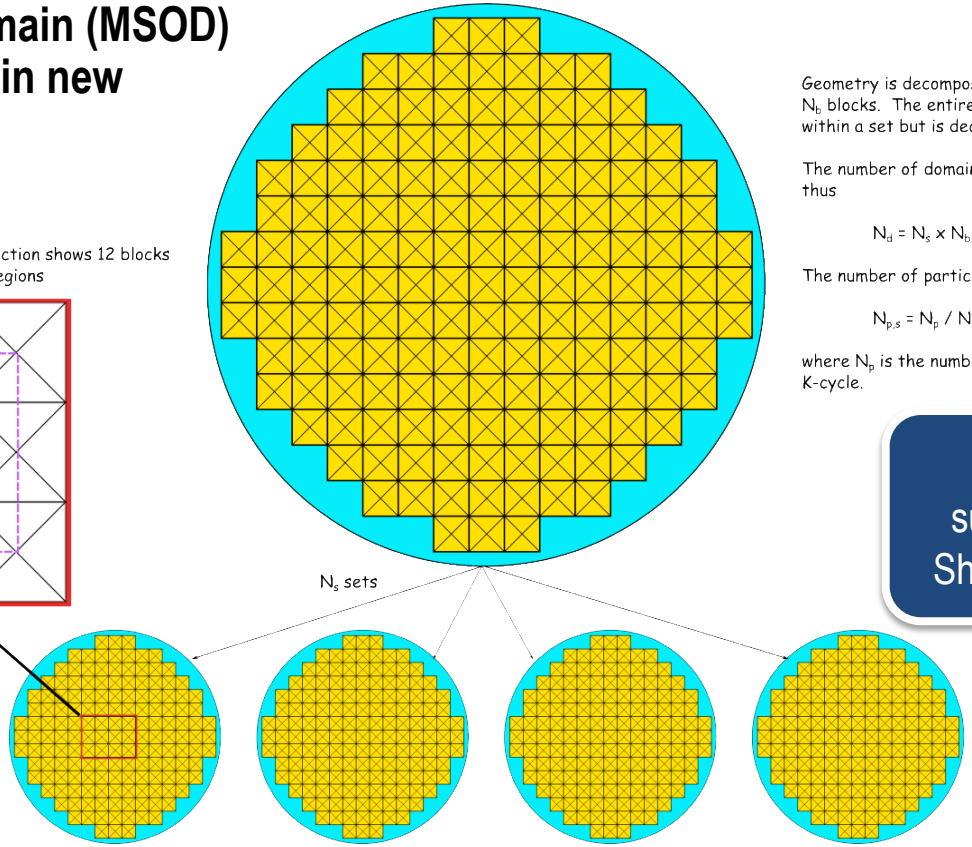


MC starting source taken from Denovo calculation

Domain decomposition parallelism development to overcome prohibitive memory requirements

Novel multi-set overlapping domain (MSOD) parallel algorithm implemented in new Monte Carlo code - *Shift*





Geometry is decomposed into N_s sets, each with N_b blocks. The entire geometry is represented within a set but is decomposed across blocks.

The number of domains (processes) in a problem is thus

$$N_d = N_s \times N_b$$

The number of particles per set is

$$N_{p,s} = N_p / N_s$$

where N_p is the number of requested particles per K-cycle.

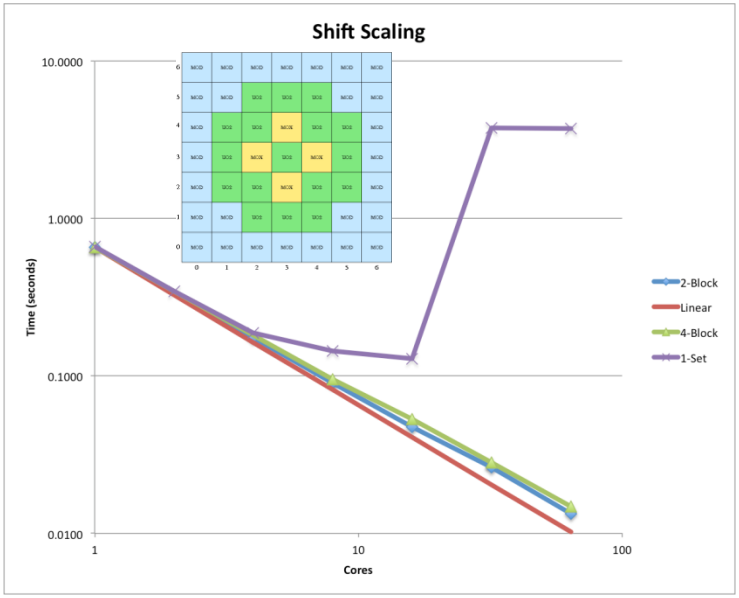
ORNL LDRD supported initial Shift development

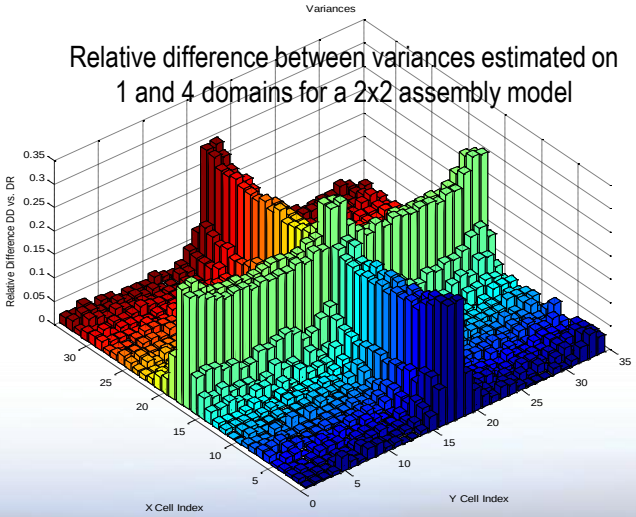
Pictorial representation of MSOD parallel decomposition. Here the core geometry is decomposed into $N_s = 4$ sets. Each set has N_b blocks with overlapping regions such that the total number of parallel domains is $N_b \times N_s$. Particles are decomposed across sets where the number of particles per set is $N_{p,s} = N_p / N_s$. Each block can define an overlapping domain (shown in inset) to reduce block-to-block communication for particles that scatter at the interfaces between blocks.

J. C. WAGNER, D.E. PEPLOW, S.W. MOSHER, T.M. EVANS, J.A. TURNER, "Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses," Joint Int. Conf. on Supercomputing in Nuclear Applications + Monte Carlo (SNA+MC2010), Tokyo, Japan, October 17-21, 2010.

New DD MC code, Shift, under development to implement hybrid and parallel methods

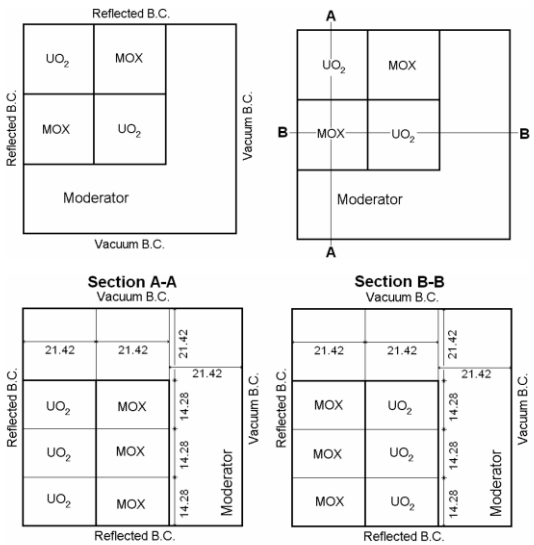
- Designed from outset for use on massively parallel platforms
  - Domain replication and domain decomposition (MSOD); in *Denovo* code base
  - Performing parallel scaling studies
- *Scale* geometry
- Implementing hybrid methods
  (Shift + Denovo in common code base)
- Approaches for efficient variance estimation
  - Evaluating batches vs. neglecting variance contributions from particles that leave domains
- Implementing continuous energy physics
- Implemented Shannon Entropy
- Testing, verification and validation

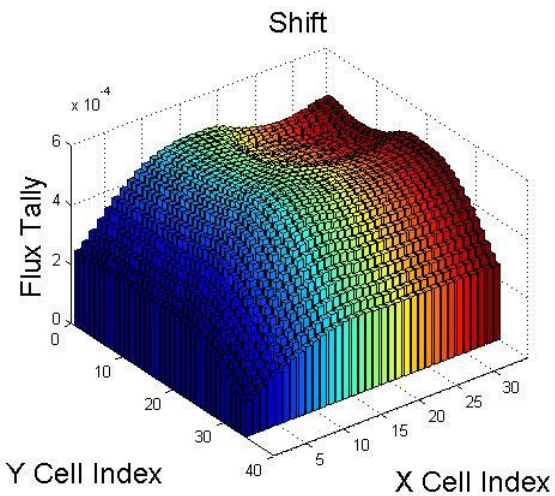


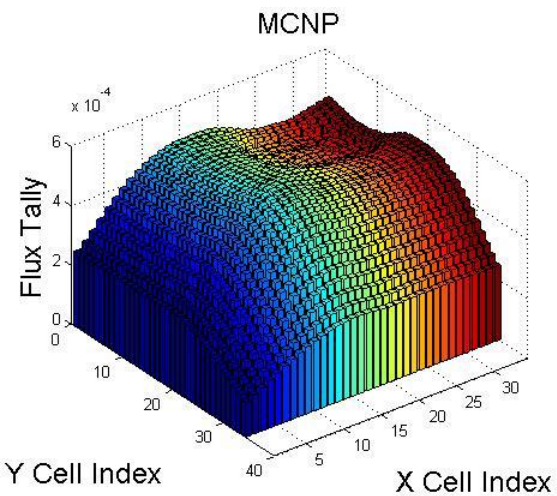


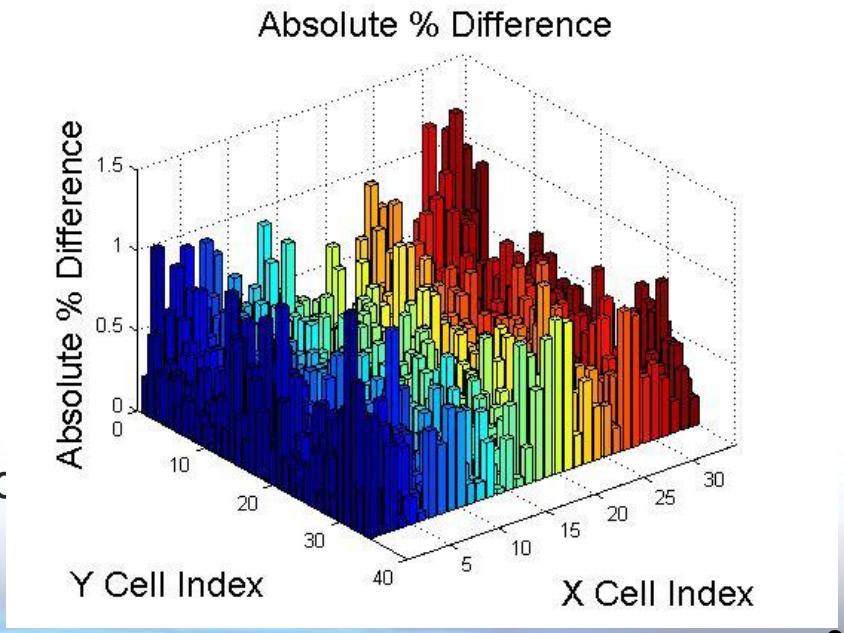
Example of Shift testing – 3-D C5G7 Benchmark

Figure 1. Modified three-dimensional configuration









- Compared k_{eff} values and flux tallies between Shift and MCNP using domain replication
  - Results agree within statistical uncertainties
  - 30,000 particles, 1200 cycles, 500 skipped
  - Center control rods fully inserted
  - Tally over the 4 fuel assemblies; 1 tally per pin cell
- Upcoming: Variance calculation and continued benchmarking.

Significant Results/Highlights

- FW-CADIS method extend and demonstrated to accelerate convergence by 6-10X [2-D ¼ PWR core]
- New MC DD algorithm (MSOD) developed, initial scaling studies performed (frost)
- Use of deterministic-based MC starting sources demonstrated to improve efficiency and reliability
- New hybrid Scale sequence developed for testing
- Publications:
  - ***Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Reactor Analyses*, *Trans. Am. Nucl. Soc.* 103, 342-344 (2010)**
  - ***Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses*, SNA+MC2010, October 17-21, 2010**
  - ***Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses*, *Progress in Nucl. Sci. Tech*, accepted for publication (2011).**
  - ***Acceleration of Monte Carlo Criticality Calculations Using Deterministic-Based Starting Sources*, *Trans. Am. Nucl. Soc., accepted for publication, Nov. 2011***
  - ***Several papers planned for PHYSOR 2012***

Current and Future Work

POR-3

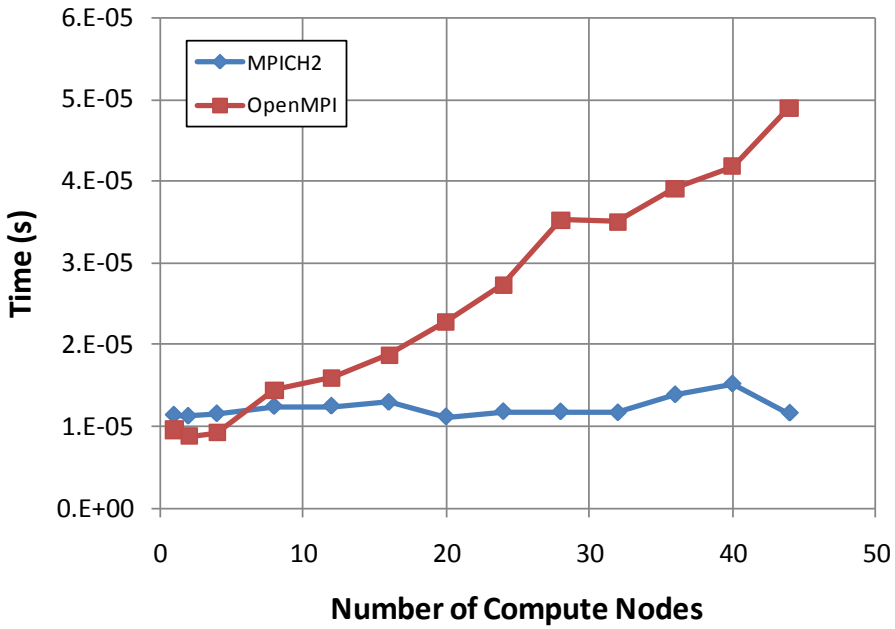
- **L3:MNM.Rad.Y1-2.03**: Issue report on status and development path for Monte Carlo and hybrid methods, including plans for V&V and UQ (originally June 30, 2011; revised to Sept. 30, 2011)
- **L3:RTM.MCH.P3.02**: Preliminary results with FW-CADIS using Shift for benchmark/test problems (Sept. 30, 2011)

POR-4

- Complete integration & testing of hybrid methods and MC DD algorithm in Shift
- Complete integration & testing of MC DD algorithm in Shift
- Collaborate with UM on hybrid methods implementation/testing in Shift
- Submit PHYSOR and/or journal articles on the following
  - MC DD algorithm and scaling studies in Shift
  - FW-CADIS for reactor analysis
  - Hybrid methods for acceleration of MC source convergence
  - Variance estimation strategies for MC DD

Monte Carlo Parallelization

- PI: Benoit Forget (MIT)
- PhD student: Paul Romano
- Data decomposition for parallel MC
  - **Decompose data across nodes**
  - **Assign particles to processors (may be multiple processors/node)**
  - **When particle crosses a boundary, fetch its data when needed**
  - **Examining MPI-2 (one-sided communication) vs MPI-1**
  - **Will consider continuous energy physics and second order geometries**
  - **Building theoretical model**



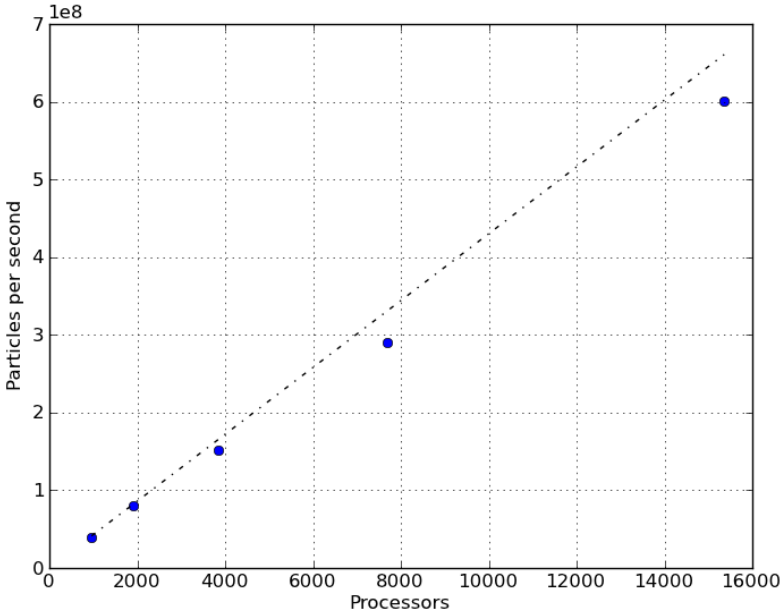
- **MPI-2 timing study**
- **3D mesh, 100x100x100, 1 group**
- **No data decomposition**

Monte Carlo Data Decomposition

- PI: Benoit Forget (MIT)
  - PhD Student: Paul Romano
- Year 1 milestones
  - Explore efficiency of data decomposition
  - Develop scalable fission bank algorithm
    - Load balancing possibilities
  - Proof-of-concept MC code
- Year 2 milestones
  - Develop semi-empirical model to study efficiency of data/domain decomposition

Fission Bank Algorithm

- Each node only gets a small fraction of the fission bank
- Nodes communicate with each other at the end of each cycle to evenly distribute particles
  - Sorted locally
  - Conserves reproducibility
  - Load balancing can be done easily by sending more/less particles to processors



Weak-scaling on Jaguar on a 20x20 pin array with vacuum boundary conditions

OpenMC

- Modern architecture (Fortran 2003)
- Unified grid energy structure
- Second order constructive geometry
- Distributed fission bank
- Most reactions are represented

- Ongoing work
  - General tally implementation with timing capabilities
  - Semi-empirical model development for data decomposition

Hybrid Transport – Functional Monte Carlo

Project Members

Staff

- Ed Larsen, UM (PI)
- Bill Martin, UM
- Han-gyu Joo, SNU

Students/PostDocs

- Jinan Yang, UM (postdoc)
- Min-jae Lee, SNU (PhD)
- Emily Wolters (UM PhD Jan 2011, now at ANL)
- Kendra Keady, UM (PhD)
- Changyuan Liu, UM (PhD)

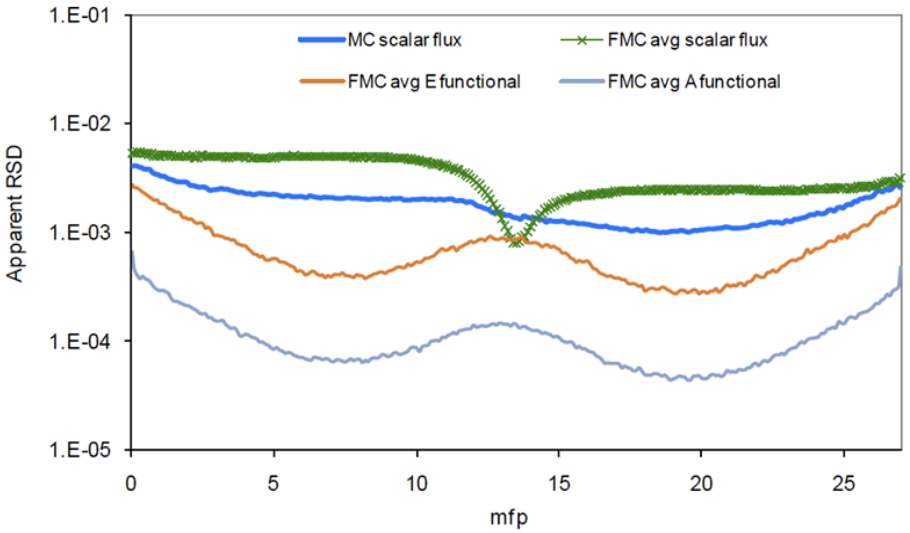
What is FMC, and why are we doing it?

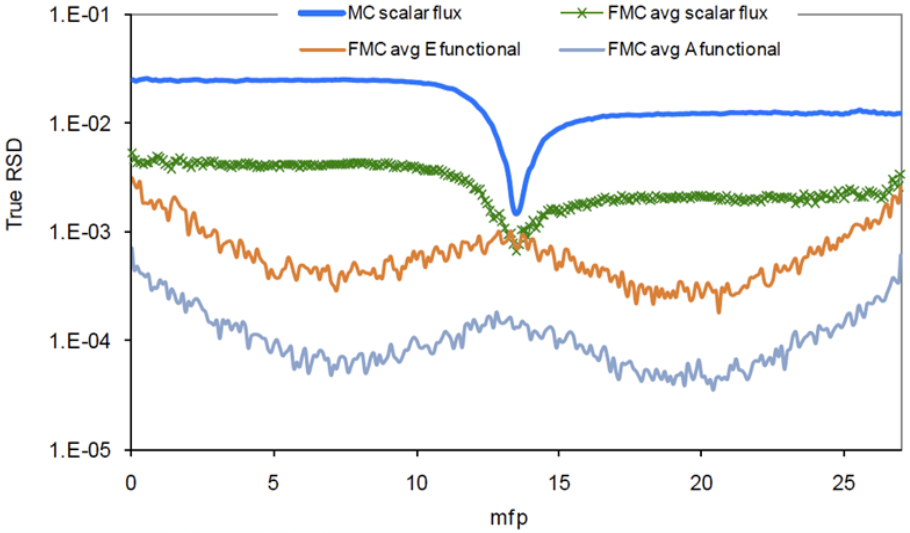
- Functional Monte Carlo (FMC) is a hybrid transport methodology in which Monte Carlo does not directly estimate neutron fluxes but estimates certain nonlinear functionals – which have:
  - (i) the character of multigroup cross sections,
  - (ii) smaller statistical errors than estimates of the neutron flux.

  After the functionals are estimated by Monte Carlo, "exact" deterministic low-order equations containing the functionals are solved to obtain volume-averaged estimates of neutron fluxes. These estimates contain only statistical errors.
- This is an entirely new approach to transport simulations, which offers to overcome many disadvantages of Monte Carlo for optically thick systems (such as commercial reactor cores). The objective of this project is to develop, implement, and test FMC for realistic problems and assess how it can be used advantageously.

Results

- Statistical errors in the FMC eigenfunction and eigenvalue estimates are greatly reduced from standard Monte Carlo.
- The disparity between the apparent and real relative standard deviations is essentially eliminated.
- For optically thick systems in which standard Monte Carlo estimates of the eigenfunction "wobble," the FMC eigenfunctions exhibit no discernable wobbling.
- The "CMFD-based" FMC methods are easier to implement but usually have larger statistical errors.





Challenges

- Because this hybrid computational approach is entirely new and different; no theoretical basis exists for assessing the worth of a new method before implementing and testing it.
- Learning from experience what works and does not work, and are trying to be guided by intuition. The lack of an underlying theory is a hindrance.
- Preliminary results suggest that 2-D FMC estimates may have more statistical noise than 1-D estimates. (But this is not certain.)

Milestones – past year

- Establish a proof of principle for relatively simple configurations (1D and 2D) and provide a basis for deciding which path to follow for 3D heterogeneous configurations.
- These tasks were addressed by implementing, testing, and comparing about 10 different FMC methods. Most numerical comparisons were done in 1-D test codes, although Min-jae Lee implemented two simpler CMFD-based methods in a 2-D ORNL multigroup code. From the 1-D comparisons, we have singled out two methods that seem most promising for 2-D and 3-D.

Milestone: PoR-3

- Jinan Yang has begun implementing the candidate 2-D FMC methods in SHIFT, an ORNL multigroup Monte Carlo code in the SCALE package. The goal is to implement and test several methods on at least on a one-group model of a typical LWR assembly with homogenized “coarse” cells.

Future Work

- Several 2-D FMC methods will be implemented and tested in Shift. This effort will include:
  - general multigroup anisotropic scattering problems and applications where the coarse spatial cells are not homogenized.
  - the testing and comparison of solutions from these methods on realistic 2-D problems.
- The results of this work will illuminate the pros and cons of the FMC method for practical problems. This will indicate ways in which the method can be used most effectively.

On-the-Fly temperature feedback for Monte Carlo

- PI: Bill Martin (Michigan)
- Co-PI: Tom Downar
- PhD student: Eva Sunny
- Collaborators: Forrest Brown (LANL) and Gokhan Yesilyurt (ANL)

Motivation

- Monte Carlo codes depend on temperature-dependent cross sections for accurate simulation of temperature effects (i.e., Doppler broadening).
- NJOY is used to generate cross section datasets at temperatures of interest, say 300K, 1200K, etc. for every isotope in an MCNP simulation.
- High fidelity multiphysics simulation may require cross section datasets at every 5-10K, at least for key isotopes such as U238, FPs, and transuranics.
- Assuming ~ 130 MB/dataset/degK for all isotopes in a typical PWR depletion, this yields ~ 26 GB for 200 datasets covering the temperature range 300K to 2300K. This may require decomposition of the cross section data as well as spatial decomposition for geometry and tallies.
- The OTF dataset is ~ 2 GB for all isotopes and all temperatures in 1K increments from 77K to 3200K.

Brief description of OTF Methodology

- The Adler-Adler resonance cross section representation was chosen as the functional model for the OTF expansion because it is equivalent to:

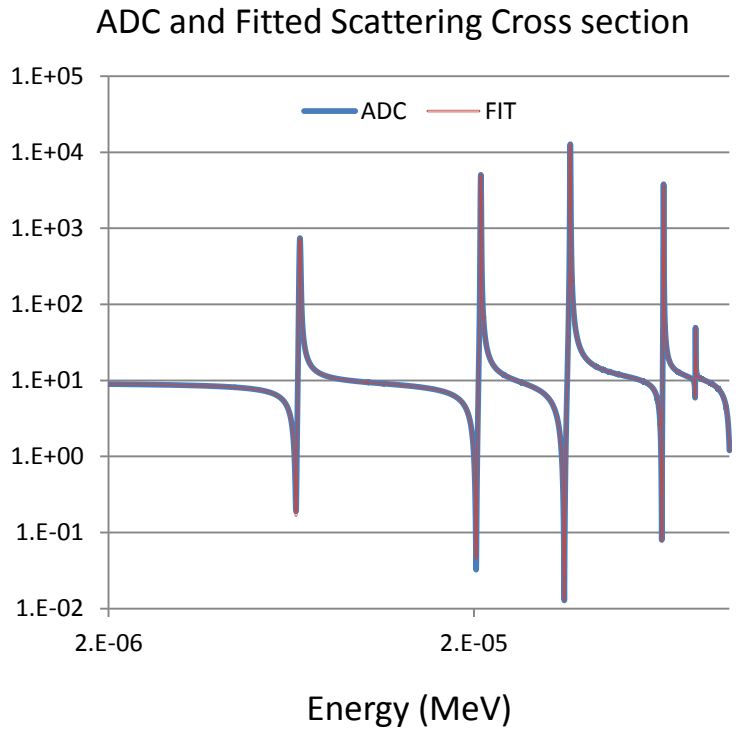
$$\sigma^x(T) = A + \sum_i f_i(T) E_i + \sum_i h_i(T) F_i$$

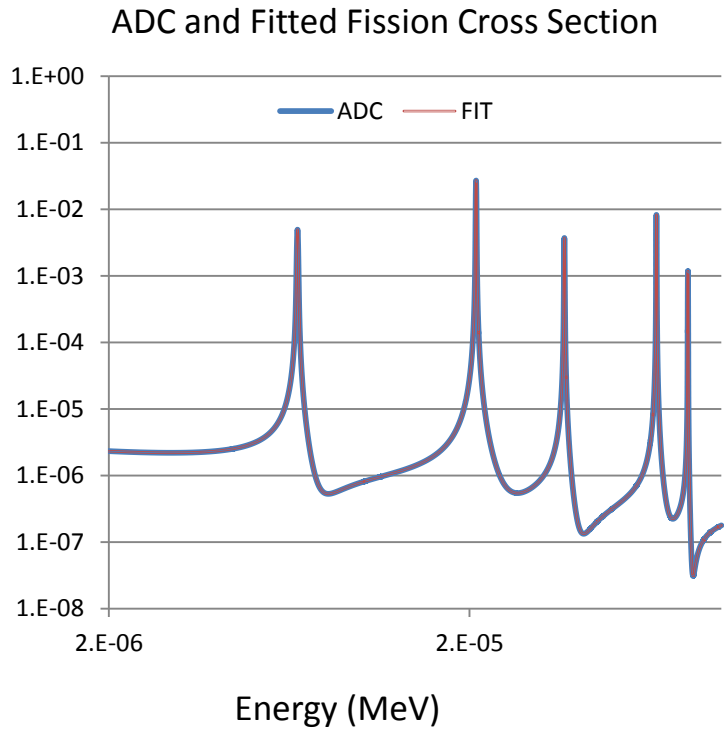
- The $f_i(T)$ and $h_i(T)$ functions contain all temperature dependence and are obtained by examining the temperature dependence of the resonance cross sections. The resultant expansion can be expressed as follows:

$$\sigma^x(T) = \sum_{n=1}^{6} \frac{f_n}{T^{n/2}} + \sum_{n=1}^{6} g_n T^{n/2} + c$$

- The 13 constants (c, f_n, *and* g_n) are regressed to match exact Doppler broadened data for every neutron energy E and temperature T.
- The entire OTF dataset consists of 13 coefficients for every isotope, every cross section type, and every neutron energy (20k) and is ~ 5 GB total for 50 isotopes . It is equivalent to generating NJOY cross section libraries for every 1K temperature increment.
- The resultant OTF expansion applies to all isotopes, even C and H.

Results for OTF Doppler broadening

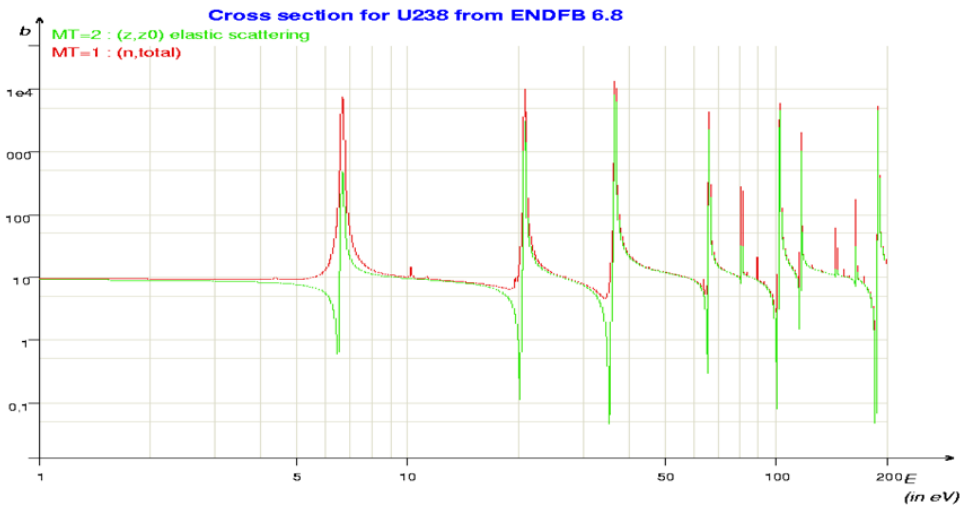




OTF fit to U238 resonance scattering and fission cross sections in the energy range 1 eV to 80 eV

Resonance upscattering

- Doppler broadening performed by NJOY only broadens the reaction cross sections, e.g., $\sigma_a(E)$ or $\sigma_s(E)$
- The scattering kernel $\sigma_s\left(\mu, E' \to E\right)$ is not broadened and the asymptotic slowing down kernel is used for heavy nuclei. MCNP allows the free gas scattering kernel to be used up to 400 kT, which is ~ 10 eV at room temperature. However the free gas scattering kernel assumes the scattering cross section is a constant. Well, ….



- Resonance upscattering can have a ~200-300 pcm effect on keff for LWRs and ~700 pcm effect for VHTRs. Our goal is an OTF method to treat resonance upscattering.

Milestones

L4 Due	Description	Status
09/30/2010	Understand S(a,b) and rejection methods for handling resonance upscattering	Completed
12/31/2010	Develop test Monte Carlo code	Completed
06/30/2011	Decide how to incorporate resonance upscattering into MCNP5	Rejection technique implemented in MCNP5 at LANL in July 2011
09/30/2011	Decide how to incorporate OTF Doppler broadening for all isotopes in MCNP5 based on NEUP grant	Meeting in Ann Arbor with G. Yesilyurt (ANL) and F. Brown (LANL) on Sept 7 to discuss this topic

FY12 tasks

- **OTF Doppler broadening**
  - Develop prototype OTF dataset for U238 cross sections including capture, fission, scattering, and total. Name this isotope U238*.
  - Develop prototype MCNP5 capability to read OTF cross sections and compare MCNP5 runs on benchmark suite with U238 at library temperature T versus U238* at temperature T.
  - Construct OTF library for ~20 other isotopes and test.
- **Resonance upscattering**
  - Compare S(a,b) approach versus rejection approach for accuracy and efficiency.
  - Investigate alternative methods not unlike Yesilyurt's 13-term expansion to parameterize the Doppler-broadened double-differential scattering kernel to incorporate upscattering

General Transport Sub-Projects

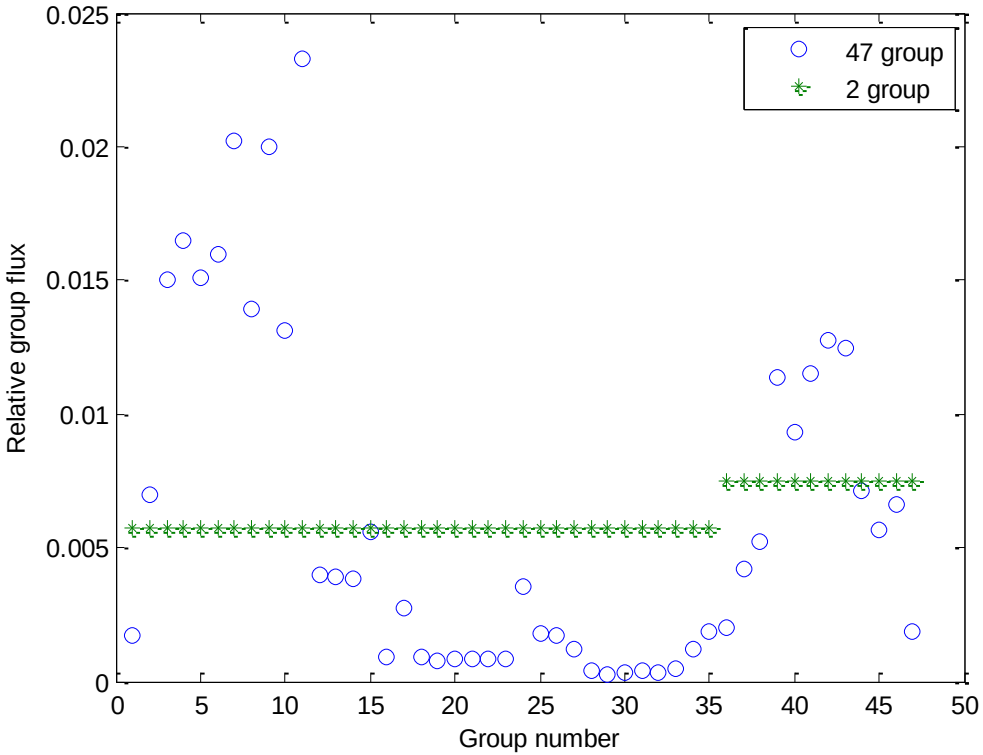
- Discrete Generalized Multigroup Method (Ben Forget, MIT)
- Transient methods for MOC transport (John Lee, Michigan)

Discrete Generalized Multigroup (DGM) – an Alternative Energy Condensation Method

- PI: Benoit Forget (MIT)
  - PhD Students: Lei Zhu and Matt Everson
  - Master's Student: Nate Gibson
- Year 1 Milestones
  - 1D/2D SN testing on fine group structures (<100 groups)
  - Algorithm improvement for ultra-fine group (11,288 groups)
  - Energy-based acceleration
- Year 2 Milestones
  - Study use of recondensation technique for self-shielding
  - Explore improvements for high order spatial schemes

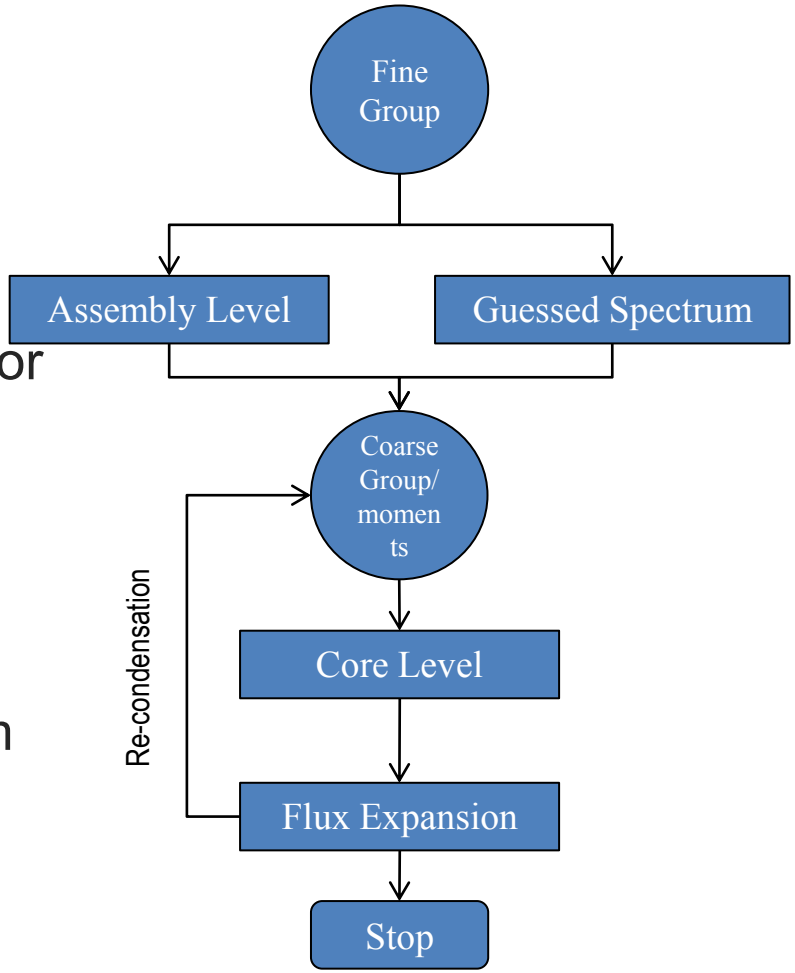
Basic approach

- Expand discretized energy variable using orthogonal polynomials
  - Zeroth order is equivalent to a coarse multigroup method
  - Higher order expansions provide spectral shape for a fine group structure
- Higher order equations are only coupled to coarse group equations sytem
  - For the cost of a coarse group calculations, we can get an idea of the fine group spectral shape



Recondensation

- The new flux can be used to recondense the parameters
  - Iterative process will converge to exact fine group solution for certain spatial schemes (flat angular flux)
  - Iterative process will improve solution for higher order spatial schemes
  - Faster convergence than standard multigroup since you can isolate up-scattering with the coarse groups
- Tested on modified C5G7 with 70 groups
  - 2 group pin power errors (rms) from lattice condensation were reduced from 4.9% to 1.0% with one iteration
- Current work
  - Explore improvements for higher order spatial schemes
  - Implementation in Denovo



Ultra-fine group

- Generated the 11,288 group library defined by CEA
- Infinite medium code with DGM was developed
- Bondarenko flux used for initial spectral guess
- Convergence was obtained for ~300 coarse groups for pins with uranium and plutonium (overlapping resonances)
  - 9-10 recondensation iterations needed for full convergence
- Current work
  - Implement in 1D cylindrical for pin cell
  - Compare with current self-shielding models

Transient methods for MOC transport

- PI: John Lee (Michigan)
- Co-PI: Tom Downar
- PhD student: Adam Hoffman

L4 Milestones and Status

1. Determine development test codes to implement and test time-stepping schemes.

- DeCART was selected as a test code.
- Denovo will be incorporated in the future studies.

2. Identify candidate time-stepping schemes.

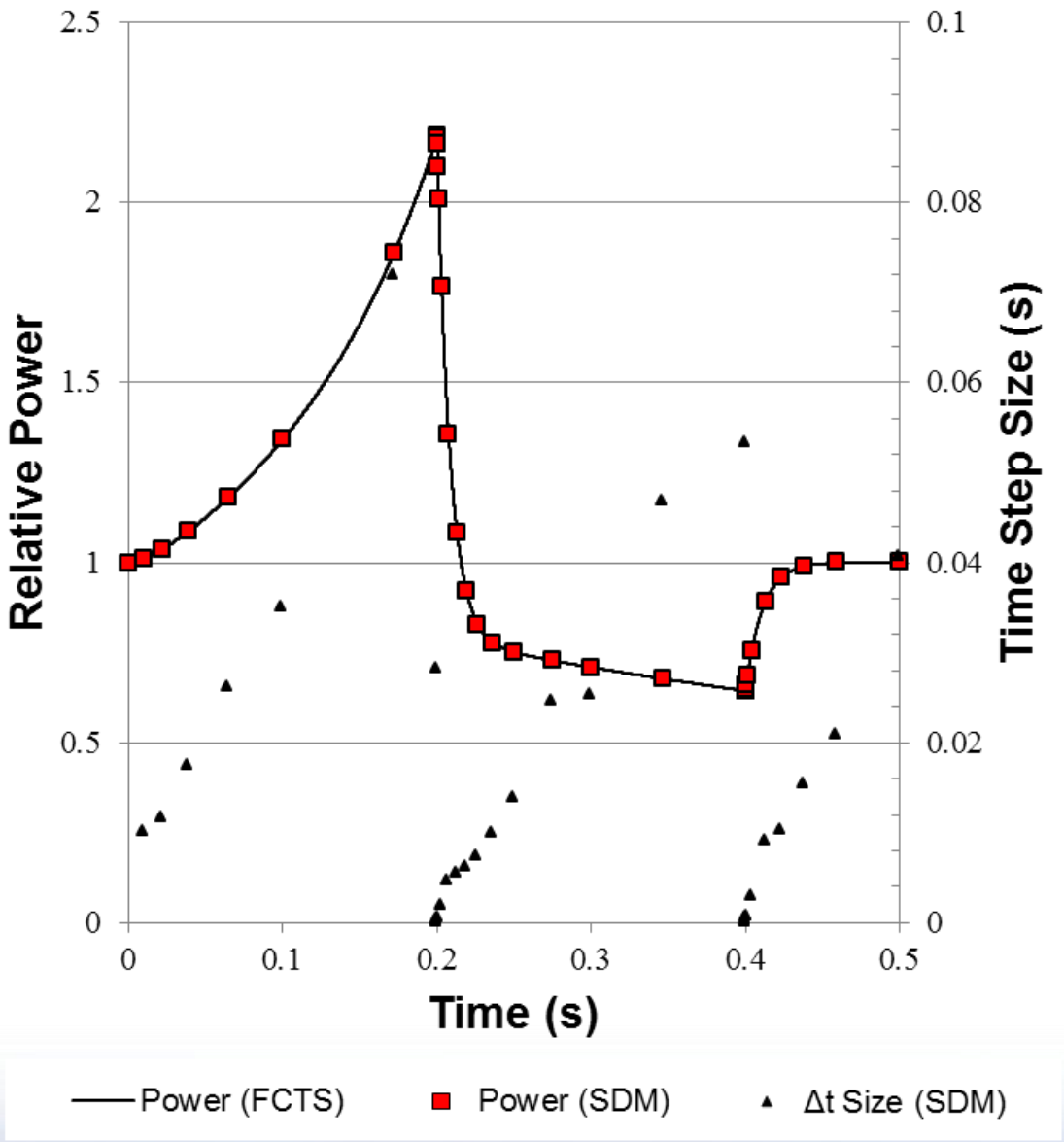
- The step doubling method (SDM) with the theta method and backward differentiation formula (BDF) were selected.
- Both approaches are amenable to parallelized adaptive time-stepping.
- Future work will investigate characteristic methods that span time and space.

L4 Milestones and Status (continued)

3. Implement time-stepping schemes into test codes.

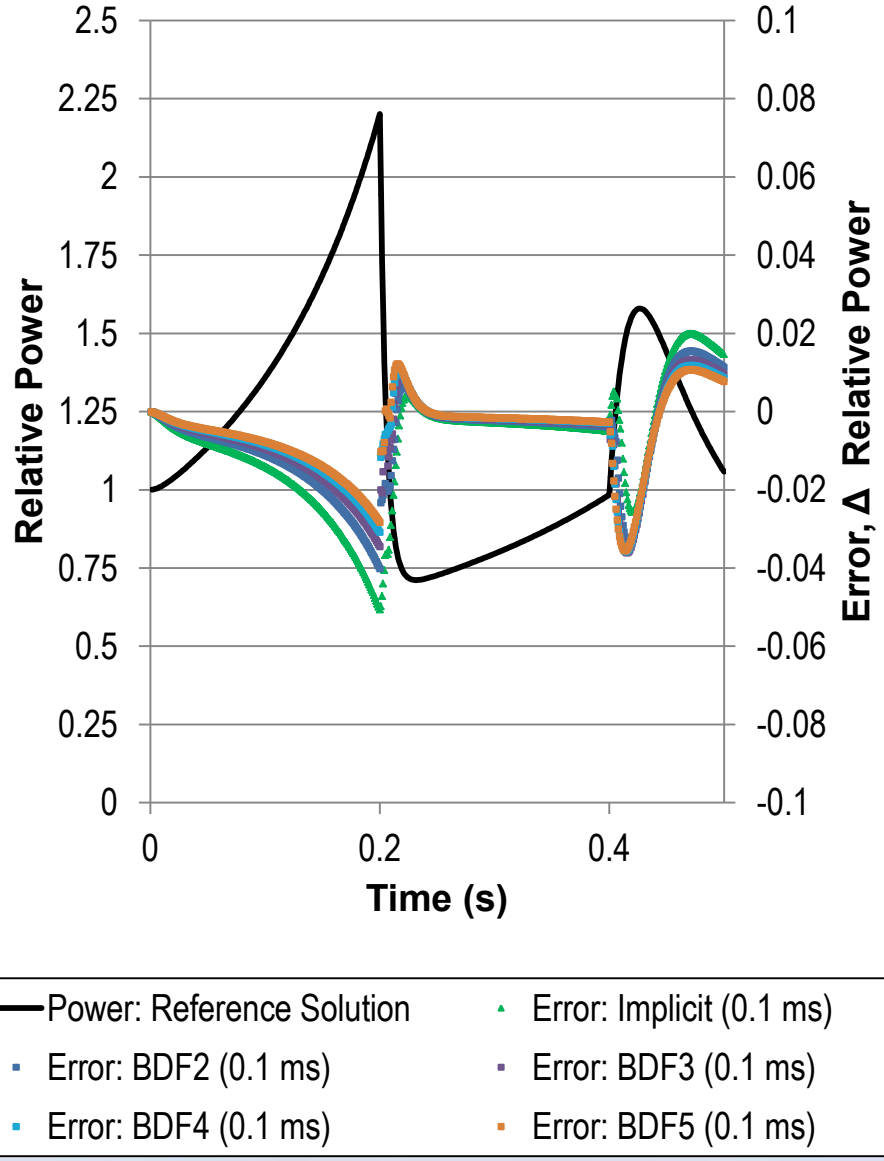
- Adaptive time-stepping via SDM has been implemented in DeCART
  - Method has been parallelized to use an arbitrary number of processor groups, although two groups is ideal.
  - SDM builds on the widely-used theta method to efficiently model transients with varying time scales while monitoring temporal truncation error and avoiding the need for pilot runs.
- Time integration by BDF has been implemented in DeCART
  - BDF has proven to be more accurate than the theta method for a common time step size.
  - Current implementation only supports constant time steps
  - Near-term future work will incorporate adaptive time-stepping, both in serial and parallel modes.

Computational results - SDM



Demonstration of adaptive time stepping by SDM for the modified TWIGL benchmark.
A. J. Hoffman, B. Kochunas, J. C. Lee, "Parallelized Adaptive Time Stepping Using the Step Doubling Method in DeCART," *Trans. Am. Nucl. Soc.* **104**, 877 (2011).

Computational results – implicit Euler vs BDF



Comparison of implicit Euler solution and BDF solutions of varying order for a constant time step for a modified TWIGL problem.

L4 Milestones and Status (continued)

4. Improvements in the DeCART transient method.

- Alternatives to the assumption in DeCART that the angular flux time derivative is isotropic:

$$\frac{\varphi_g^n(\mathbf{r},\mathbf{\Omega}) - \varphi_g^{n-1}(\mathbf{r},\mathbf{\Omega})}{\Delta t} \cong \frac{\bar{\phi}_g^n - \bar{\phi}_g^{n-1}}{4\pi\Delta t}$$

  - An alternate treatment has been implemented in DeCART which assumes that the spatial dependence of the angular flux along a segment is unchanged over the previous time step but normalized to preserve the average scalar flux.

$$\frac{\varphi_g^{n-1}(s)}{\bar{\phi}_g^{n-1}} \cong \frac{\varphi_g^n(s)}{\bar{\phi}_g^n}$$

  - Although these formulations are in agreement in diffusive problems, some discrepancies are apparent in regions where diffusion theory is known to be inadequate, e.g. near control rods.
- There is a need to develop more accurate transient models for benchmarking and assessing the adequacy and limitations of various approximations.

L4 Milestones and Status (continued)

5. Recommend future development path for transient capability in Denovo and DeCART.

- DeCART is acceptable for production transient modeling but not high fidelity benchmarking. To achieve better accuracy, two approaches will be investigated:
  - Avoid making assumptions about the angular dependence of the time derivative. This will necessitate storing angular data and approximating the spatial dependence of the angular flux from the previous time step.
  - Incorporate time dependence along a characteristic for an exact treatment of neutron time-of-flight.
- Need to have robust adaptive time stepping algorithms in Denovo and DeCART for computational efficiency.
  - Efficient use of HPC resources while permitting the user to monitor temporal truncation error and avoid the need to perform pilot simulations to estimate appropriate time step sizes.
  - These methods also provide an additional avenue for parallelization, potentially improving scalability beyond steady-state capability.

Coupled Transport Sub-Projects

- Multiphysics Coupling Based on Effective Low-Order Transport (Dimitriy Anistratov, NCSU)
- Nonlinear Acceleration of Neutron Transport Criticality Problems (Ryosuke Park, INL – now at LANL)
- Advanced iterative methods for nonlinear multiphysics coupling (Tim Kelley, NCSU)

Multiphysics Coupling Based on Effective Low-Order Transport Problems

- PI: Dmitriy Anistratov (NC State University)
- Students
  - Octavian Geagla (MS student)
  - Apil Tamang (PhD student, joined the project in June, 2011)
- Goals
  - The goal is to reduce computational costs and improve multiphysics coupling
  - Development of flexible and efficient multi-level methodology for adequate coupling and solving multiphysics equations based on effective low-order transport problems
  - The computational costs will be decreased, because of low dimensionality of this special effective low-order transport problem and fewer recalculations of the high-order multigroup transport problem

Approach and Progress

- **Approach**
  - Formulation of few-group and one-group low-order transport problems that are able to capture exactly necessary transport effects
  - Formulation of a hierarchy of multigroup low-order equations that can generate averaged data for an effective low-order transport problem.
  - Multiphysics equations are coupled with an effective one-group transport problem
- **Main Results and Progress**
  - Development of multi-level nonlinear diffusion acceleration method for solving k-eigenvalue, multigroup transport problems in 1D (M&C 2011, Rio)
  - Formulation of the methodology for multiphysics coupling in 1D geometry based on the QD method including
    - spatial and temporal discretization of equations
    - methodology for solving system of nonlinearly coupled equations
  - Currently work on implementation and analysis on the formulated methodology

Key L4 milestones

- 12/31/10
  - Formulation of a multi-level methodology for coupling neutron transport and multiphysics equations in 1D geometry
  - Accomplished
- 3/31/11
  - Implementation of the multi-level methodology for solving transport equation coupled with multiphysics equations in 1D geometry.
  - Partially accomplished
- 6/30/11
  - Analysis and testing of multi-level methodology for solving transport equation coupled with multiphysics equations in 1D geometry
  - Partially accomplished

PoR-3 and beyond

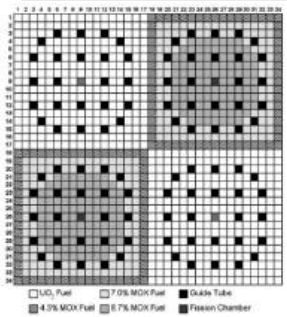
- Milestones for PoR-3
  - The multi-level methodology in 1D geometry will be tested and analyzed to determine the way for developing a methodology for 2D.
- Next Year Plan
  - Prototype multi-level methodology for multiphysics coupling in 2D.

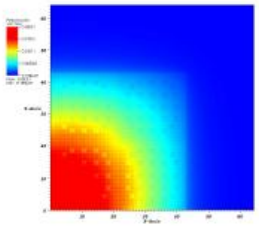
Nonlinear Acceleration of Neutron Transport

- PI: Ryosuke Park (INL)
- Nonlinear diffusion acceleration to accelerate criticality problems
  - **High-order/low-order coupling with CMFD at low-order to preserve reaction and leakage rates**
  - **Low order operator is a diffusion equation, amenable to efficient multilevel solvers**
  - **Low-order operator is coupled to the multiphysics and iteration feeds the physics back into the high order equation, avoiding complexity of coupling to angular fluxes**

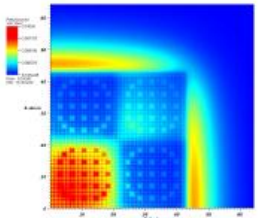
Performance of JFNK-eigenvalue acceleration scheme

	Tran. Sweep	CPU total in sec	k_{eff}
NDA-PI(0)	39	1158.7	1.18619353
NDA-PI	4	400.8	1.18649578
NDA-JFNK	6	214.0	1.18650041

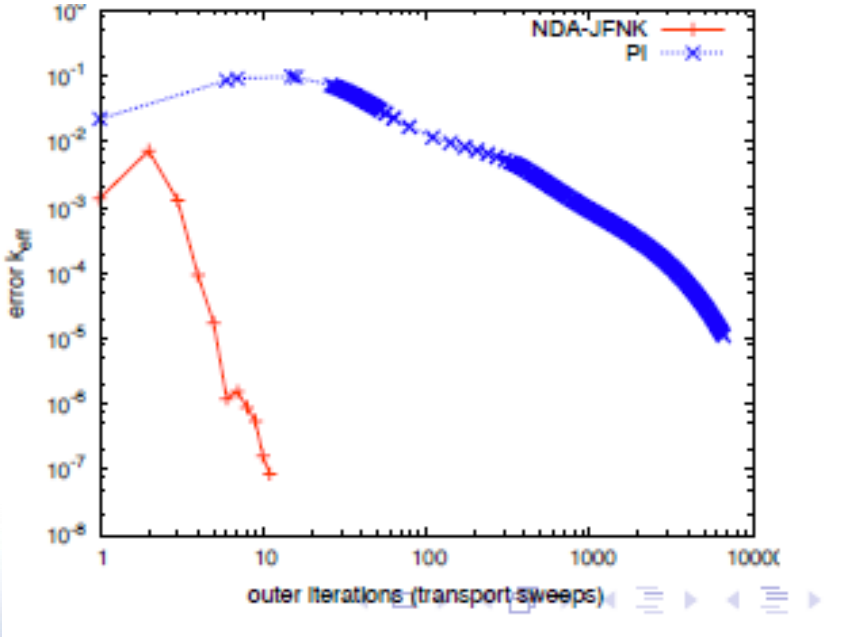




fast flux



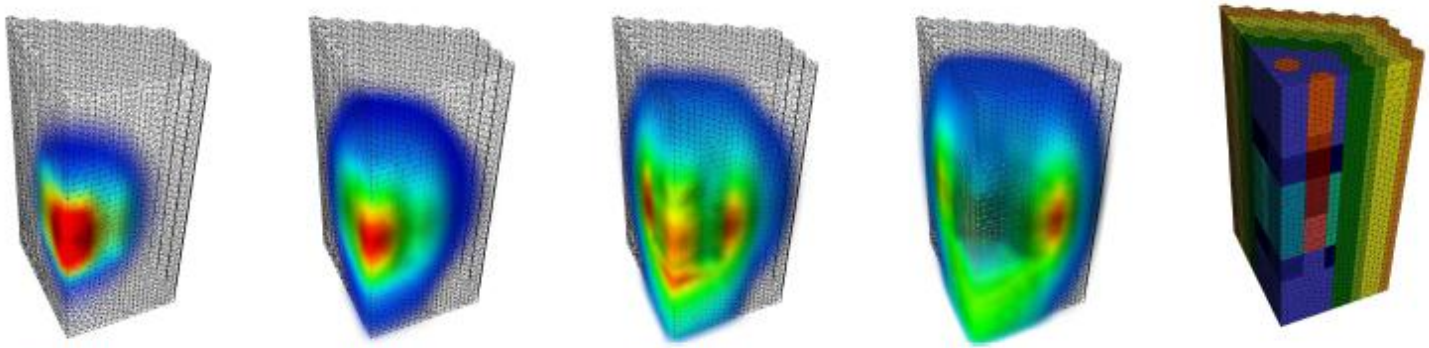
thermal flux



Computational results

Result Takeda Benchmark

3D, 4-group small core with $\pi/4$ symmetry



group1 group2 group3 group4 material

	T. S.	CPU time	# Element	k_{eff}	% error
NDA-JFNK(Flat)	7	190	20157	0.833943	4.4
NDA-JFNK(Flat)	7	1859	128552	0.858211	1.6
NDA-JFNK(linear)	27	709	20157	0.869975	0.25
NDA-JFNK(linear)	13	2724	128552	0.872174	1.1e-4
PI	385	78540	128552	0.872237	7.3e-3

S8 (80-direction) reference keff = 0.872173

- Linear source is much more accurate than flat source.
- Linear source increases # of transport sweep by a factor of 2-4.
- Larger the element size is, more transport sweeps are required for the linear source case.

PoR-3 and beyond

- Discussions are underway with INL, Michigan, and Sandia to initiate an effort to couple DeCART and Drekar via the MOOSE framework.
- This will allow tight coupling with existing JFNK machinery in MOOSE and will facilitate algorithm development for coupled multiphysics with DeCART and Monte Carlo.
- This would be a first step towards:
  - a high-order/low-order transport methodology with Monte Carlo as the high-order and DeCART as the low-order transport (with CMFD) for example.
  - coupling of DeCART to BISON for materials feedback
- This could take advantage of the nonlinear keff acceleration work reported earlier.
- This would leverage/complement a separate project at INL to couple Monte Carlo and Bighorn via MOOSE to perform fully coupled analyses of ATR.

Advanced iterative methods for nonlinear multiphysics coupling

PI: C. T. Kelley (NCSU)
PhD Student: Jeff Willert
Collaborators: Dana Knoll (LANL), Tom Evans (ORNL), Roger Pawlowski (Sandia)

Objectives:

- Apply Jacobian-Free Newton-Krylov (JFNK) methods to nonlinear accelerators
  - Nonlinear Diffusion Acceleration (NDA)
  - Quasi-Diffusion Acceleration (QD)
- Compare JFNK-NDA/QD to preconditioned GMRES
- Apply to hybrid methods, eg MC for high-order equation

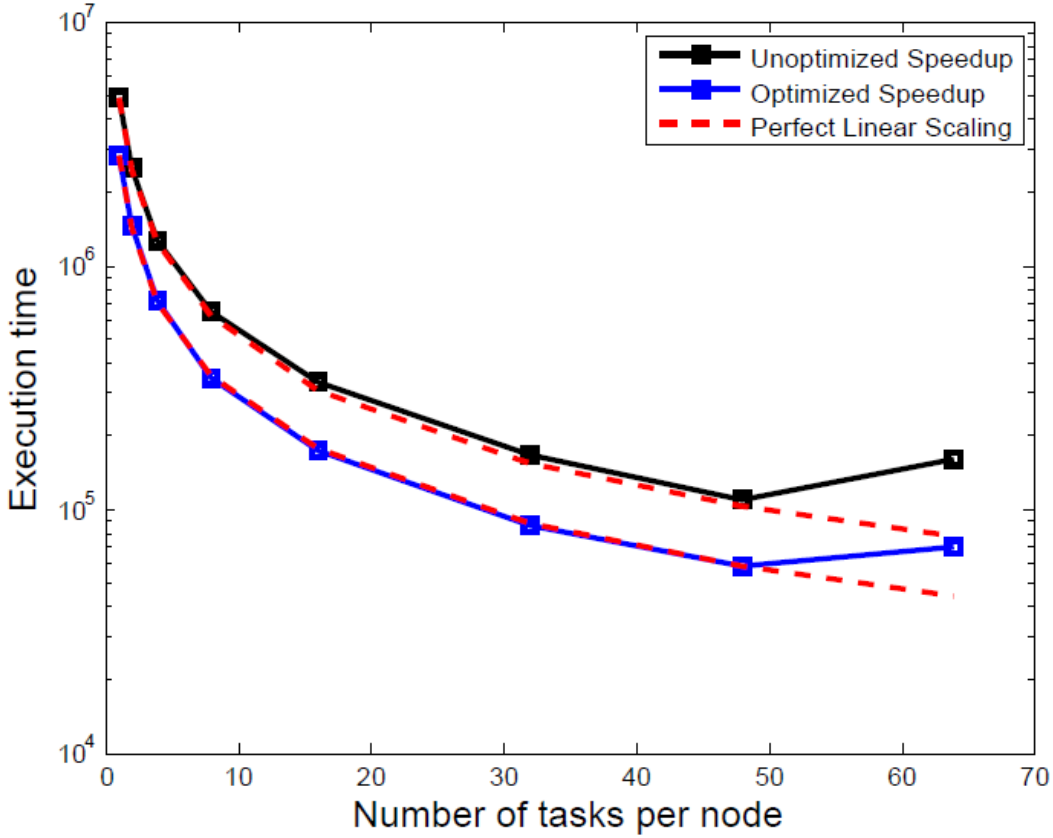
Challenges:

- Finite-difference Jacobians won't work with MC
- High-order MC flux must be differentiated in low-order equation

Results

- Analytic Jacobian-Vector product (1, 2, 3D)
  - Will (in principle) accept MC high-order flux
  - No finite-difference error
- First round of comparisons with JFNK-NDA vs GMRES (1D)
  - MATLAB 1-D code complete; used to test ideas
  - JFNK seems better, need to try more preconditioners
- Preliminary results with MC on GPU
  - MC high-order sweep on GPU
  - NDA/QD works well with source iteration
  - JFNK in progress
  - Challenge: need to smooth/filter MC high-order flux

Multi-core Scaling for QD-accelerated Monte Carlo



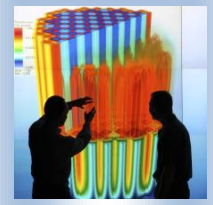
- Simple 1D problem
- Matlab code transliterated to C
- MPI scales well on 12 core Opteron
- OpenMP scales better on SMT dual core (4x vs 3x)

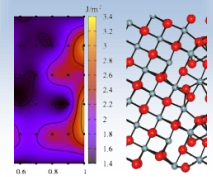
Milestones

- MATLAB codes for 1D
  - Multi-group, anisotropic, NDA (done)
  - Hybrid solver prototype (now in C/OpenCL with GPU)
  - One group hybrid solver (in progress)

Work for Next Year

- Complete MATLAB prototype code (1D)
- JFNK+NDA/QD in C/OpenCL/Fortran (1D, 2D)
- Smoothing of MC high-order flux with integration into JFNK-NDA/QD (2D)
- Begin development of convergence analysis/theory for hybrid method.





Radiation Transport Methods (RTM) FY12 and Long-Term Planning/Strategy

CASL Roundtable, Raleigh
August 9-11, 2011

Bill Martin
University of Michigan
RTM Lead, CASL

John Wagner
Oak Ridge National Laboratory
RTM Deputy Lead, CASL

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL-U-2011-0072-000-R

Overall Strategy for MNM-RTM thus far… just reviewed

- **Pursue three independent transport approaches to deliver 3D pin-resolved transport for production calculations:**
  - Sn and MOC are complementary deterministic transport capabilities and both are being developed for VERA-TR.
  - Monte Carlo is (now) the benchmark transport capability
  - Hybrid Monte Carlo is the advanced transport capability
- **Explore improvement of existing transport capabilities applicable to deterministic or stochastic transport:**
  - Advanced energy condensation methods (vs multigroup)
  - Transient discretization methods
- **Explore advanced coupling methodologies:**
  - High-order/low-order coupling with CMFD
  - High-order/low-order coupling with Variable Eddington Factors
  - Advanced solvers to support high-order/low-order multiphysics coupling

MNM-RTM consists of 5 projects

- **Sn** (discrete ordinates) – the primary development path for deterministic transport
- **MOC** (Method of Characteristics) – the alternative development path for deterministic transport
- **Monte Carlo and hybrid methods** – the development path for stochastic transport and advanced hybrid transport methods
- **General transport** – methods development that supports all transport effort
- **Coupled transport** – multiphysics coupling with neutronics

RTM projects build upon the initial transport capability deployed in VERA

Overall Strategy for RTM … looking forward

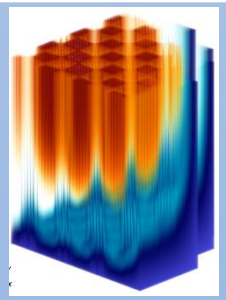
- **As we complete first year, it is appropriate to reassess**

- **Are the current strategy and milestones appropriate?**
  - **Yes, no changes?**
  - **Mostly, minor tweaks needed?**
  - **No, major changes required?**

- **Is the current scope right?**
  - **Radiation transport, but where do other Neutronics needs fit?**
    - **Problem-dependent multi-group cross-section library development**
    - **Depletion/decay**
    - **Multi-physics code coupling**
    - **Etc...**

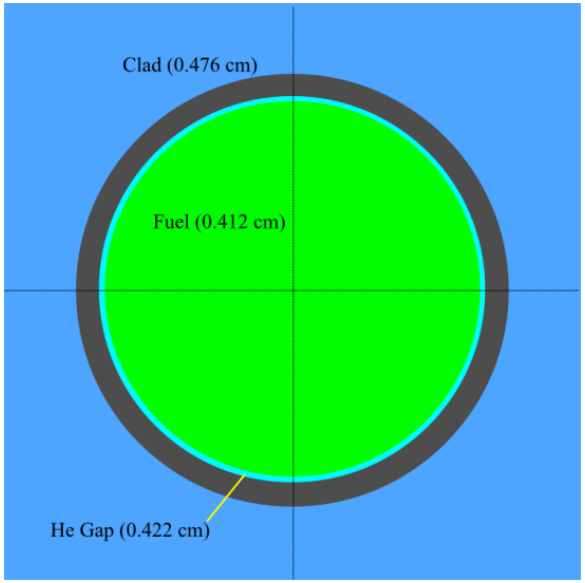
- **What can we realistically accomplish / support?**

RTM capability roadmap

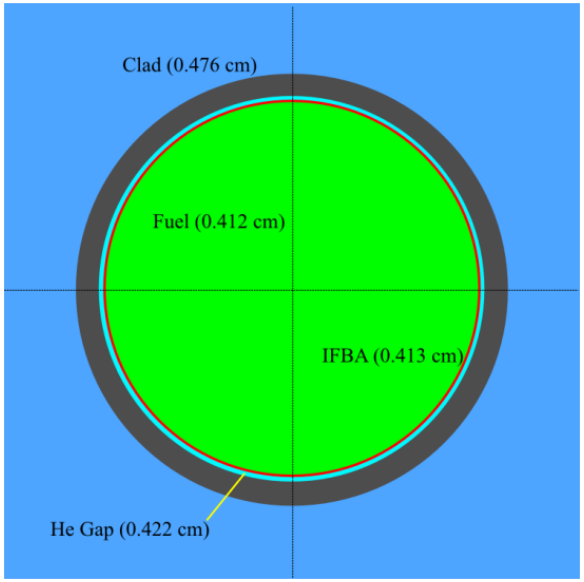
Year 1	Year 2	Year 3	Year 4	Year 5
 Full-core 3D homogeneous pin-cell Sn transport Full-core 2D/1D resolved pin-cell MOC transport with T-H coupling	← We are here Full-core 3D homogeneous pin-cell Sn transport with T-H coupling	Full-core 3D pin-resolved transport – both Sn and MOC Prototype transient 3D transport capability – Sn and/or MOC	Full-core 3D pin-resolved transport – both Sn and MOC – with T-H coupling Prototype 3D hybrid Monte Carlo transport	Transient full-core 3D pin-resolved transport – Sn and/or MOC – with T-H coupling Full-core 3D hybrid Monte Carlo transport with T-H coupling

Y3 Capability Challenge – Full-Core 3D Pin-Resolved Transport

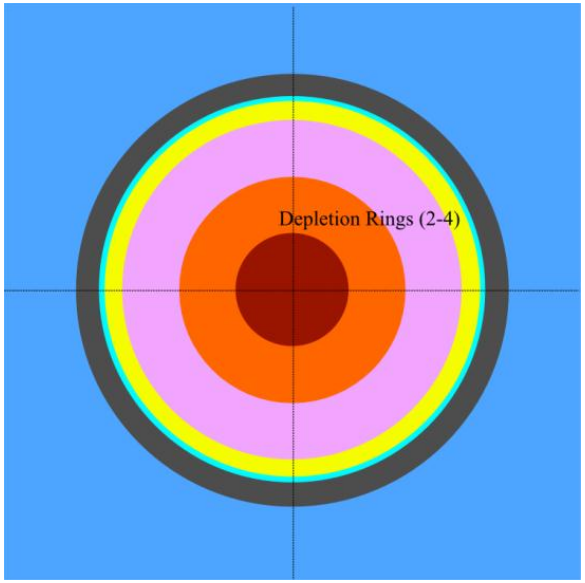
PWR Fuel Pin Types



regular fuel pin



IFBA fuel pin



regular fuel pin with depletion rings

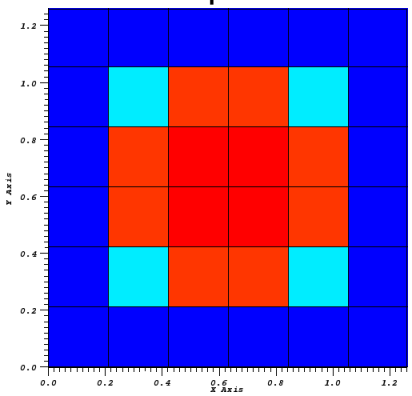
3D transport must resolve fine-scale complexity, especially for depletion

Deterministic Radiation Transport

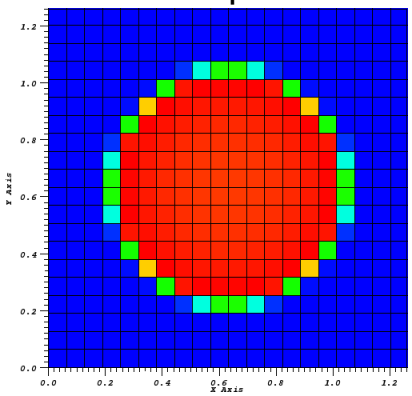
Are We at Risk for Achieving Full-Core 3D Pin-Resolved Transport in Y3?

- 2D: good methods in place for foreseeable future
  - MOC
- 3D: currently no single candidate that can solve full-core problems with fully resolved pins using a consistent approach
  - IFBA / Gd
  - Depletion (rim effects)
- We do have approximations that work to varying degrees
  - 2D/1D MOC
  - 3D regular grid with macro-mixing

6×6 pin cell



20×20 pin cell



Medium and long term consistent approaches must be investigated

Potential Deterministic Approaches

- **3D MOC**
  - No theoretical barrier
  - Implementation and parallel scaling issues
  - Very high cost; may preclude use in medium term
- **2D/1D MOC**
  - Consistency issues; research required
  - Axial resolution/behavior unclear
  - Best prospect for solving 3D IFBA/depletion in short term
  - Parallelization remains an issue
- **Regular Grid S_N**
  - Demonstrated for regular fuel pins
  - Will **not** work for IFBA (500×500 cells per pin required)
  - Limited utility for highly resolved depletion
- **S_N w/embedded MOC**
  - Potential for consistent 3D approach for all problems
  - No existing implementation yet; research required
  - May be too expensive to be practical
- **Unstructured S_N**
  - Meshing 3D IFBA/depletion layers problematic
  - High user setup costs
  - Memory/time intensive
  - Parallelization issues need to be researched
  - Not viable to meet Y3 Milestone

No single answer yet, but a roadmap can be formulated

3D Deterministic Transport Roadmap Requirements

- Must address all classes of problems
  - IFBA
  - Rim effects – PCI
  - Depletion – radial burnup, Gd
- AMA constraints on user setup
  - May preclude approaches that require extensive meshing
- Target must include non-HPC platforms
  - Clusters on order of 1000 cores must be capable of doing significant simulation
  - Does not preclude HPC as platforms for the future (today's HPC is tomorrow's cluster!)
- Fit within CASL budget and priorities
- Full-core 3D pin-resolved transport by Y3

Constraints moving forward

Full-Core 3D Pin-Resolved Det. Transport Roadmap

- 2D/1D MOC
  - Continue research for more consistent coupling between 2D MOC and 1D axial treatment
  - V&V of existing technique must continue to fully vet capability
  - Short term approach
- Structured S_N
  - Continue use of existing regular grid S_N for initial class of AMA problems where applicable
  - Needed to support hybrid MC capabilities
  - Short term approach
- S_N w/embedded MOC
  - Development and testing in FY12.
  - Decision point at end of FY12 on continuing with full implementation
  - Medium/long term approach
- 3D MOC
  - Continue on-going research into feasibility
  - Decision point at end of FY12 or early FY13 on continuing with full implementation
  - Long term approach
- Unstructured S_N
  - Feasibility study on meshing/solver costs for fully resolved 3D unstructured with decision point on continuation in first half of FY12
  - Decision-pending approach

Full-Core 3D Pin-Resolved Det. Transport Summary

- Continue using existing 2D/1D MOC and regular grid S_N in short term
  - Vet limitations with continuing V&V activities
- Research and development investment in FY12
  - Consistent 2D/1D MOC
  - S_N w/embedded MOC
  - 3D MOC
- Decision points in FY12
  - Determine meshing, memory, and runtime costs/requirements for unstructured S_N in first quarter
  - Feasibility of 3D MOC and S_N w/embedded MOC approaches based on research, development, and testing results

Hybrid Monte Carlo Radiation Transport

Hybrid MC Challenges – Are We at Risk for Achieving Full-Core MC Transport in Y4?

- Prohibitive computational time requirements
  - Tally convergence
    - Non-uniform: uncertainty increases with distance from core center
    - Must run batch of simulations to estimate true uncertainties (cycle-to-cycle correlation)
  - Source convergence
    - Slow in large systems and w/ high dominance ratio
    - Can be difficult to identify/confirm
- Prohibitive memory requirements
  - High fidelity → high information density
    - $O(10^9)$ tally bins in fuel is not unreasonable
    - Too much tally information to store on every processor
- Others…
  - Statistical uncertainty propagation
  - Efficient tallying strategies to support multi-physics coupling

Significant challenges, but there is hope – see presentations from recent ANS Panel Session on MC Reactor Analyses

193	(assy/core)
× 264	(rods/assy)
× 4	(radial bins/rod)
× 4	(azimuthal bins/rod)
× 24	(axial bins/rod)
× 200	(groups or reaction rates)

= 3.91×10^9 tally bins	

Approaches to Overcome Barriers

Hybrid Methods

- **FW-CADIS**
  - Initial results promising; good prospect for 3D CE MC Rx analyses
  - Further testing, optimization, research required
  - Implementation in Shift
- **FMC/CMFD**
  - Initial results promising
  - Implementation and testing in multi-D (plans to implement in Shift)
  - Research required

Parallelism

- **Data Decomposition**
  - No existing implementation yet; research required
  - May be too expensive to be practical
- **Domain Decomposition**
  - Builds on experience from ASCI
  - MSOD developed and algorithm implemented in Shift
  - Research, scaling studies and testing required

Platform

- **Shift**
  - New hybrid MC code developed from outset for use on massively parallel systems
  - CASL Hybrid MC platform
  - Needs many user features / capabilities, e.g., depletion

Numerous challenges, but a roadmap has been formulated

Hybrid MC Transport Roadmap Requirements

- Must address all classes of problems
  - IFBA
  - Rim effects – PCI
  - Depletion – radial burnup, Gd
- AMA constraints on user setup, reliability, and run time
- Target is HPC platforms
  - Hybrid MC not currently expected to be mainline capability
- Fit within CASL budget and priorities
- Prototype full-core 3D pin-resolved capability by Y4

Constraints moving forward

Full-Core 3D Hybrid MC Roadmap

- FW-CADIS Hybrid Methods
  - Continue research, implementation in Shift, and testing
  - Complete studies related to source convergence; evaluate use of lower-order deterministic solutions
  - Short term approach
- FMC / CMFD Hybrid Methods
  - Continue research, implementation in Shift, and testing
  - Medium term approach
- Domain Decomposition Parallel
  - Complete research and testing in FY12
  - Decision point at end of FY12/early FY13 on viability
  - Medium term approach
- Data Decomposition Parallel
  - Continue on-going research into feasibility
  - Decision point at end of FY12/early FY13 on continuing on with full implementation
  - Long term approach
- Shift
  - Continue developing needed capabilities, V&V, and testing
  - Deploy initial capability to VRI and AMA in FY12

Full-Core 3D Hybrid MC Summary

- Continue current hybrid MC efforts and Shift development
  - Vet limitations with continuing performance testing activities
- Research and development investment in FY12
  - Hybrid methods
  - Parallel schemes
- Decision points in FY12 / FY13
  - Needs to continue hybrid methods work beyond FY13
  - Feasibility of data parallelism and domain decomposition approaches based on research, development, and testing
  - Identification and prioritization of remaining R&D needs

Summary

- This talk focused only on preliminary thoughts related to a Roadmap for achieving full-core 3D pin-resolved transport with deterministic and hybrid MC methods
- The goal of this talk was to socialize the issues and stimulate discussion

Panel Discussion

- **Are the current strategy and milestones appropriate?**

- **Is the current scope right?**
  - **Radiation transport, but where do other Neutronics needs fit?**
    - **Problem-dependent multi-group cross-section library development**
    - **Depletion/decay**
    - **Multi-physics code coupling**
    - **Etc...**

- **What can we realistically accomplish / support?**

Thermal Hydraulic Methods

Robert Lowrie (LANL), Lead
Richard Martineau (INL), Deputy

DOE Annual Review
Oak Ridge National Laboratory
August 18, 2011

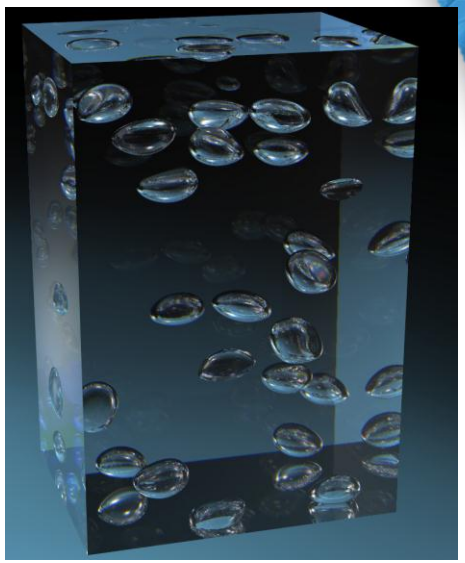
CASL-U-2011-0072-000-R

Thermal Hydraulic Methods

Delivers thermal-hydraulic simulation tools to VERA

Objectives and Strategies

- Deliver next-generation T-H simulation tools to VERA, interfaced with the latest VUQ technologies, and accommodate tight coupling with other physics
- Computational Fluid Dynamics (CFD) Project: Deliver to VERA non-proprietary, scalable, verified and validated component-scale CFD tools
- Interface Tracking Methods (ITM) Project: Generate microscale simulation results and experimental data for CFD closure models and validation



Requirements Drivers

- Advances in THM needed to attain the mesh and physics fidelity required for detailed investigation of CASL Challenge Problems
- Key requirements:
  - Scalable implicit algorithms for turbulent multiphase flow, from microscale through component length scales
  - Ability to mesh and analyze quickly complex geometries
  - Subgrid models that are focused on specifics of Challenge Problems
- Leverage capabilities from NE, Office of Science, NNSA, and others

Outcomes and Impact

- VERA will have the following CFD capability:
  - single- and multiphase
  - subgrid models, tuned to PWRs
  - coupled with and targeted towards specific reactor physics
- Primary success metric: Using the capabilities developed to gain new insight into the CASL Challenge Problems
- The new code, results, and experimental knowledge base will
  - lead to a greater understanding of T-H issues in reactor problems
  - form a repository for future open research and development

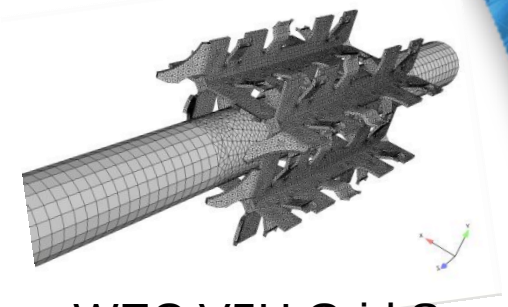
THM Highlights

- Identified 2 non-proprietary HPC codes for further development, each with unique capabilities
  - SNL's Drekar code computed turbulent CFD excitation forces for 3x3 GTRF problem. Contributed to GTRF L1 milestone.
- Defined ITM test cases and performed initial simulations of turbulent flows with wall-attached bubbles
- Published sensitivity study of CFD to multiphase / boiling parameters
- CASL special session at NURETH-14, the premier T-H conference, with 9 papers on advanced thermal hydraulics
- Recently hired former Director for CFD Technology of SIMULIA (leading commercial code)
  - Author of Hydra-TH code, a basis that will accelerate CFD development

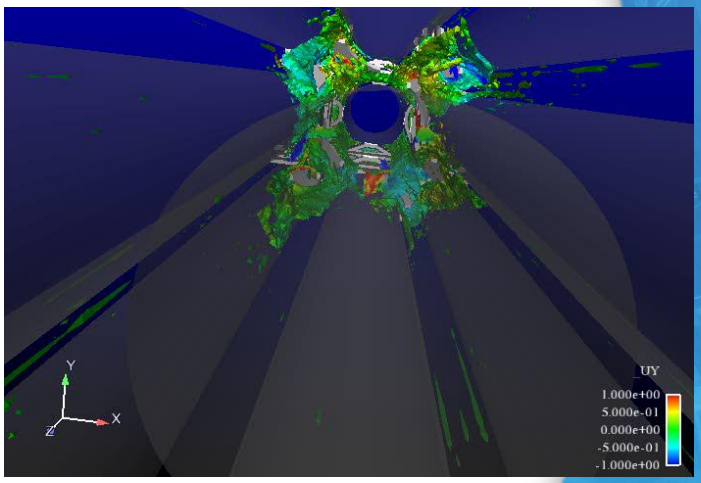
SNL's Drekar Computed Turbulent CFD Excitation Forces for 3x3 GTRF Problem

L3 THM.CFD.P2.04

- SNL Staff: J. Shadid, T. Smith, R. Pawlowski, E. Cyr, P. Weber, and D. Turner
- Targeted the Grid-to-Rod Fretting (GTRF) Challenge Problem: Fluid/Structure Vibration Wearing of Pin Cladding.
- WEC Benchmark with experimental data for validation.
- Demonstration of a scalable higher-order accurate CFD 3x3 pin capability will:
  - Increase accuracy over current CFD simulations
  - Enable VUQ assessment of CFD and vibration analysis
  - Reduce the margins of uncertainty, allowing for power up-rates, life extensions and future reactor design.
  - Build connections THM – VRI - VUQ and transfer technology within CASL partnership
- Published at NURETH-14



WEC V5H Grid Spacer



Drekar parallel LES Simulation

CFD plays a critical role in majority of Challenge problems

THM Challenges

- Meshing complex geometries for large-scale computations is very labor intensive
  - *Path forward: Evaluating Boxer and Spider "shrink-wrap" approach*
- Lack of confidence and robustness in 3-D turbulent multiphase methods for boiling flows, with sparse data under PWR conditions and little HPC experience with such methods.
  - *Path forward: Formulate experimental plan, evaluation of multiphase formulations and codes.*
- Ensuring that commercial and non-proprietary tools complement one another.

Year 1 THM Challenges and Roll-ups

- Non-proprietary HPC platform for team software development of CFD not initially identified
  - *Now have 2 massively parallel codes (Drekar and Hydra-TM), each with unique capabilities*
- Coordination of 12+ organizations, with few individuals that have collaborated with one another, compounded by contract delays
  - *Some sub-teams now beginning to form*
  - *11/12 contracts recently completed, with one foreign contract remaining*
- IP issues with geometry and data
  - *Lack of experience with very large datasets that contain protected data*
  - *Universities generally will not have access to proprietary geometries (ongoing issue)*

THM Next Steps

- CFD Project (focuses on component-scale):
  - Further application, development, and release of SNL's Drekar CFD code version 1.0 to CASL. Integration with intrusive VUQ technologies for grid-spacer inverse design.
  - Deployment and testing of LANL's Hydra-TH CFD code; application to "fast meshing" technologies.
  - Measure sensitivity of CFD flow results to phase-to-phase heat/momentum transfer parameters and to boiling models
  - Assessment of multiphase codes; develop migration path of models to our HPC codes
  - Identify fast-running capability for depletion calculations: sub-channel? coarse-grid CFD?
- ITM Project (focuses on microscale)
  - Large-scale, detailed simulations of subcooled flow nucleate boiling
  - Application of VUQ methodologies to results from ITM test cases simulations
- Specific Challenge Problem focus:
  - Determine degree of required FSI coupling for GTRF and requirements on geometry resolution (gaps)
  - Assess coupling mechanisms with MPO on CRUD formation
- Solidify/establish collaboration plans with NEAMS, Relap-7, Naval Reactors, CEA/EDF, and others.
- Coordinate experiments at MIT, CCNY, and TAMU

EXTRAS

CASL
Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

THM Team and Budget

Organization	Annual Budget ($K)	Primary Focus in THM
Los Alamos	570	CFD methods and development, multiphysics (Hydra-TH code)
MIT	389	Experiments, ITM, modeling
RPI	200	ITM, CFD, modeling (NPHASE-CMFD code)
Sandia	200	CFD development, scalable algorithms (Drekar code)
Oak Ridge	200	CFD methods and development
Idaho	188	Multiphase flow methods development
Texas A&M	150	Experiments, modeling
U. Michigan	100	Uncertainty quantification
NC State	88	ITM Simulations (PHASTA code); Upscaling CFD to sub-channel
Notre Dame	75	ITM simulation (FTC3D code)
City College NY	75	Experiments, ITM simulation (FELBM code)
ASCOMP	60	ITM/CFD Simulations (TransAT code), modeling
TOTAL	**2295**	

THM has experts in simulation, modeling, and experiments

Thermal Hydraulics

Jul-Jan 2010 Plan of Record

Activities

- Workshop 2010 Aug. 23-24
- Deliver initial version of Implementation Plan for VERA-CFD
  - Requirements document and overview of plan
  - Documentation of Drekar CFD code
  - Description of ITM methodology and codes
  - VUQ methodology for THM
- Begin definition of ITM test cases

Budget

CFD Development	$403K
ITM & Experiments	$367K
TOTAL	**$770K**

Challenges and Risks

- Coordination of 12+ organizations, most with small funding levels
- Formulate meaningful requirements while waiting for high-level input from AMA and VRI
- Ensure that commercial and non-proprietary tools complement one another

Milestones

- Document implementation plan for next-generation flow simulation capability (L3)
- Define at least 2 ITM test problems (L4)
- ITM simulations of turbulent flows with wall-attached bubbles (L4)
- Documentation of uncertainty sources and system response quantities in T-H simulations (L4)

Thermal Hydraulics

Jan-Jul 2011 Plan of Record

Activities

- Code development and application of SNL's Drekar code to GTRF
- Development of CFD and ITM test cases and generation of initial results
- Measure sensitivity analysis of multiphase / boiling parameters

Budget

CFD Development	$537K
ITM & Experiments	$489K
TOTAL	**$1,026K**

Challenges and Risks

- Delays in subcontracts not in place
- Mesh generation a challenge, particularly for GTRF
- Lack of use of many codes on leadership computer systems

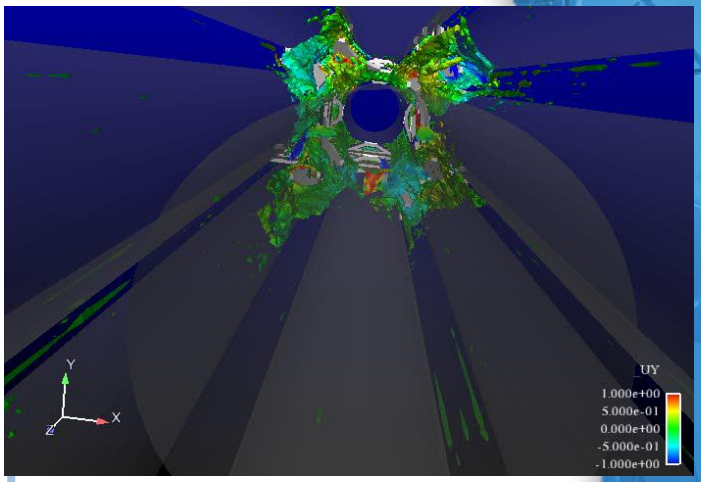
Milestones

- Compute Turbulent CFD Excitation Forces for 3x3 GTRF Problem using SNL Drekar code (L3). Fed GTRF L1 milestone.
- Measure sensitivity of CFD to multiphase / boiling parameters (L3)
- Define ITM test cases (L3)
- Evaluate NPHASE (L3) -- delayed

Computational Fluid Dynamics (CFD) Project

Activities

- Development of SNL's Drekar CFD code
  - Stabilized FEM, fully implicit, intrusive UQ
- Development of LANL's Hydra-TH code
  - Hybrid projection method, mixed meshes
- Application of above codes to GTRF and CRUD
- Evaluation of multiphase algorithms from NPHASE
- Development of Discrete Equation and Diffuse Interface Methods
- Benchmark definitions and baseline calculations
- Upscaling CFD results to subchannel



Challenges and Risks

- Meshing complex geometries remains very labor intensive
- Lack of confidence and robustness in 3-D turbulent multiphase methods for boiling flows, with sparse data under PWR conditions
- IP issues with geometry and data. Lack of experience with very large datasets that contain protected data. Many partners will likely never have access to these geometries.
- Determination of multiphase closure parameters relevant to PWRs

L3 Milestones

- Establish collaboration plan with NEAMS, Relap-7, NR, CEA/EDF for thermal hydraulics
- Upscale CFD models of rod bundle geometries to subchannel
- Deployment and testing of Hydra-TH CFD code
- Release Drekar CFD code version 1.0 (PoR-4)
- Define thermal fluid benchmark problems and provide baseline CFD simulations (PoR-4)

Interface Tracking Methods (ITM) Project

Activities

- Definition of test cases and “challenge simulations”
- Test case simulations using TransAT, PHASTA, FTC3D
- Define coordinated experimental plan; setup of experiments
- Sensitivity studies to target important closure parameters

Challenges and Risks

- Benefits of upscaling results to CFD parameters remains to be demonstrated
- Other reactor physics not accounted for in current ITM codes
- Experiments have limited ability to match PWR flow conditions, and not all partners have access to proprietary geometries

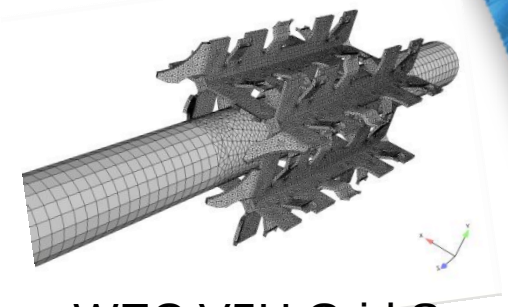
L3 Milestones

- Measure sensitivity of CFD flow results to phase-to-phase heat/momentum transfer parameters and to boiling models
- Application of verification methodology to preliminary results from ITM test cases simulation
- Evaluate capabilities and improve ITM models in PHASTA code on a leadership computer system
- Define a Complete Simulation of Subcooled Flow Nucleate Boiling (PoR-4)

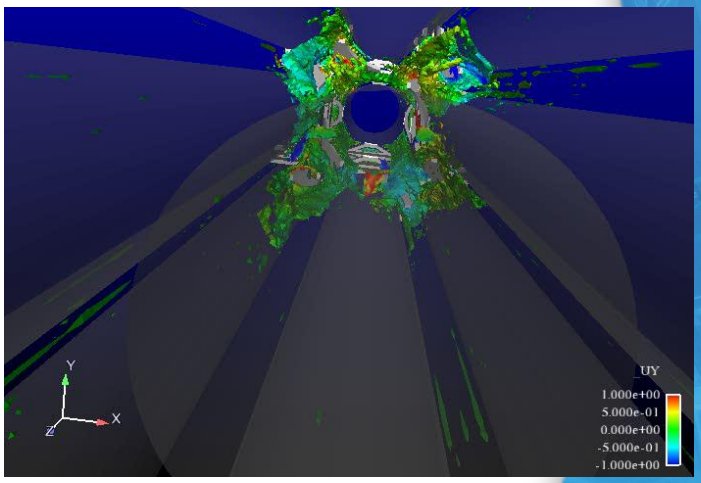
SNL's Drekar Computed Turbulent CFD Excitation Forces for 3x3 GTRF Problem

L3 THM.CFD.P2.04

- SNL Staff: J. Shadid, T. Smith, R. Pawlowski, E. Cyr, P. Weber, and D. Turner
- Targeted the Grid-to-Rod Fretting (GTRF) Challenge Problem: Fluid/Structure Vibration Wearing of Pin Cladding.
- WEC Benchmark with experimental data for validation.
- Demonstration of a scalable higher-order accurate CFD 3x3 pin capability will:
  - Increase accuracy over current CFD simulations
  - Enable VUQ assessment of CFD and vibration analysis
  - Reduce the margins of uncertainty, allowing for power up-rates, life extensions and future reactor design.
  - Build connections THM – VRI - VUQ and transfer technology within CASL partnership
- Published at NURETH-14



WEC V5H Grid Spacer



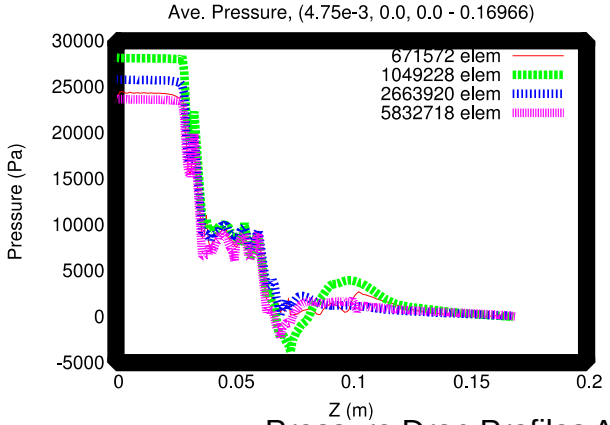
Drekar parallel LES Simulation

CFD plays a critical role in majority of Challenge problems

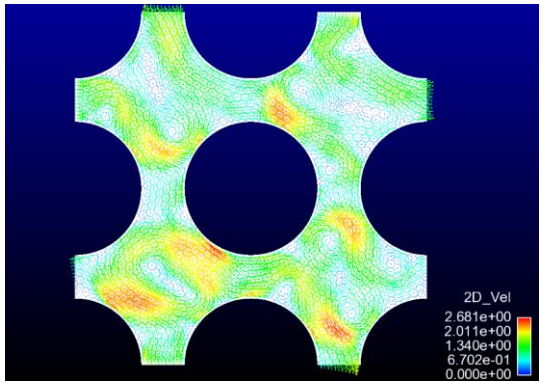
Initial Results: SNL Drekar Code

FEM LES CFD

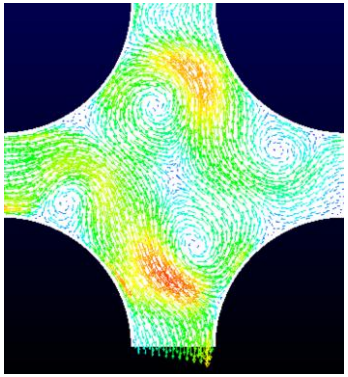
- Time-averaged LES solution



Pressure Drop Profiles Across Mixing Vane

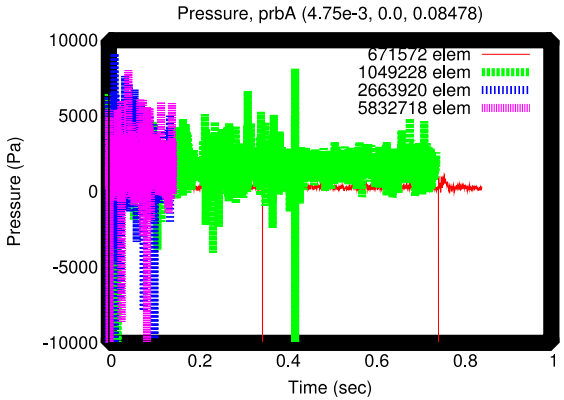


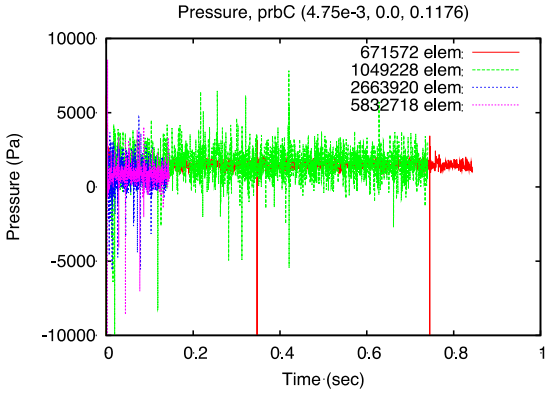
Cut-plane Velocity Vectors Downstream Of Mixing Vane

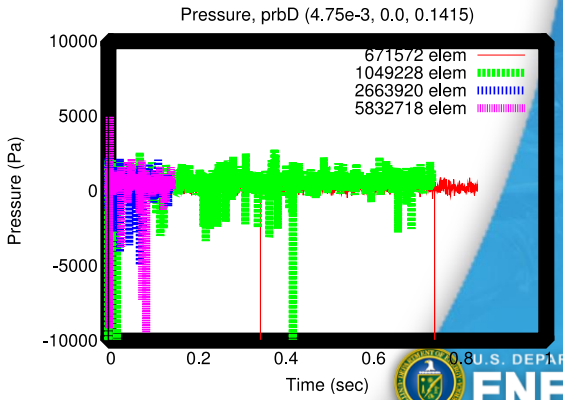


Detail Lower-left Quadrant Velocity Vectors

- Unsteady Pressure Field



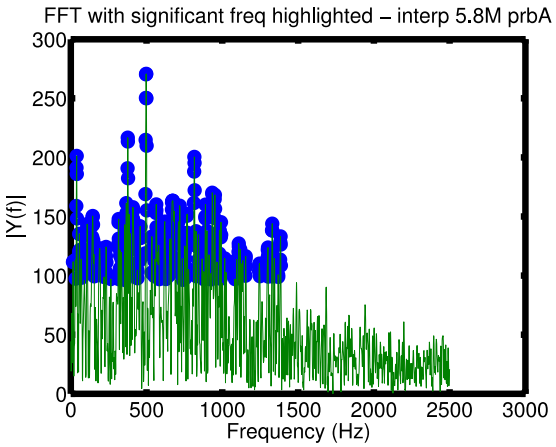


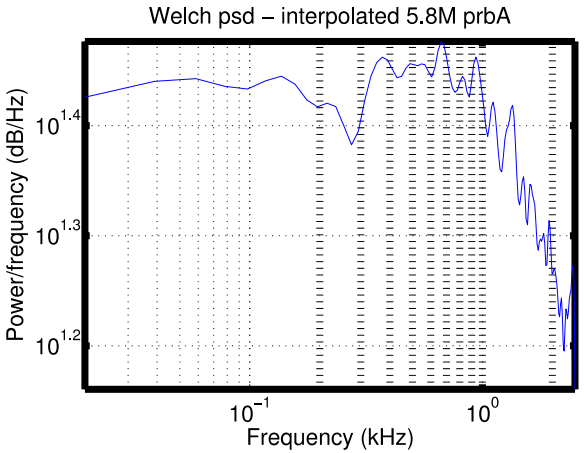


Initial Results: SNL Drekar Code

FEM LES CFD

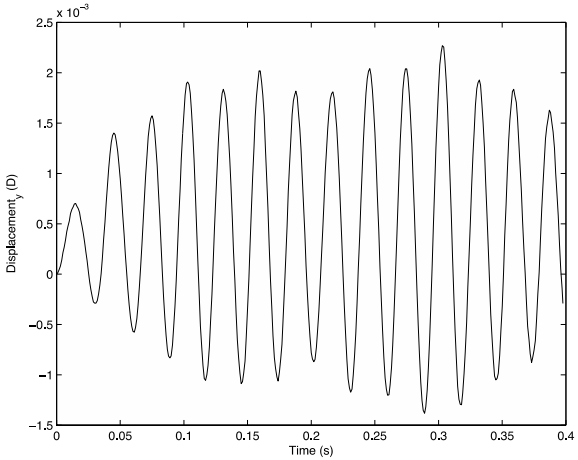
- Analysis of LES Pressure Field (FFT & PSD)

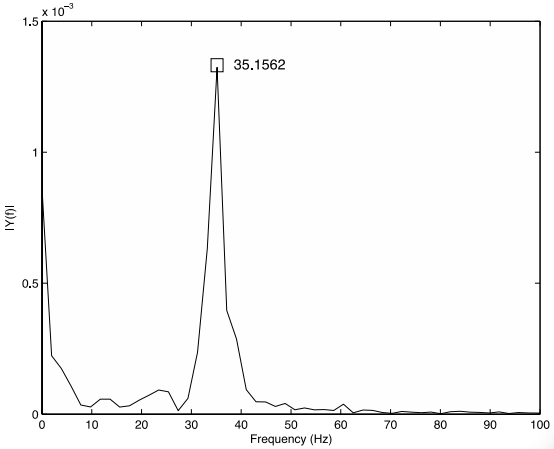




- Demo of Drekar LES Forcing of Structural Vibration (Sierra/Presto). Solid Zircaloy Rod

Displacement of rod in y-direction from LES forcing





FFT of vibrational response of rod

Next Steps for Drekar

- Detailed Investigation of temporal and spatial order of accuracy/verification with turbulence on 3x3 model (coordinated with VRI-GTRF & VUQ)
- Demonstrate CFD – Neutronics coupling using Drekar, Denovo and VERA/LIME (coordinated with VRI)
- Demonstrate large-scale parallel conjugate CFD and heat transfer studies
- Additional physics model development (LES/RANS, multiphase-flow models, etc…)
- Carry out optimization and scaling studies on Jaguar (currently run on up to 9600 cores for short time 3x3 simulation)
- Optimize solvers (physics-based preconditioners, one-step Newton, modified Newton, semi-implicit, etc.)
- Demo 5x5, 17x17 sub-assemblies, and ¼ core reactor simulations
- Release Code to CASL Partnership

Closure relations for VERA-CFD to come from experiments and ITM/DNS Simulations

Mass $$\nabla \cdot \vec{u} = \dot{m}\left(\frac{1}{\rho_\ell} - \frac{1}{\rho_v}\right)\delta_S$$

Phase change and surface tension forces are represented as delta functions at the interface

Momentum (Navier-Stokes)

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla\cdot(\rho\vec{u}\vec{u}) = -\nabla P + \nabla\cdot\mu(\nabla\vec{u} + \nabla^{\perp}\vec{u}) + \rho\vec{g} + \sigma\kappa\vec{n}\delta_S$$

Energy $$\frac{\partial(\rho c_p T)}{\partial t} + \nabla\cdot(\rho c_p \vec{u} T) = \nabla\cdot\lambda\nabla T + \dot{m}h_{\ell v}\delta_S$$

- Examples of ITMs: volume of fluid, level-set, front-tracking, …
- CASL codes implementing ITMs include STAR-CCM+, TransAT, PHASTA, FTC3D, …
- Wish to test ITM capabilities in these codes. Therefore developed six ITM Test Cases

ITM Test Cases – Tests ability of ITM codes

Physical phenomena	Test Case #	Objective	Relevance	Capabilities tested	Database	Developed by
Single-phase turbulence and heat transfer	1	Predict friction factor of turbulent flow over a flat wall with a pattern of small hemispherical solid obstacles	Subcooled boiling in PWR hot channel at axial locations between the onset of nucleate boiling and the point of net vapor generation	Single-phase CFD without interface tracking, heat and phase change	Numerical database generated by CASL	MIT/Ascomp
	2	Predict axial location of onset of subcooled nucleate boiling (point where $T_w \approx T_{sat}$)	Onset of nucleate boiling in PWR hot channel	Single-phase CFD with heat transfer, but without interface tracking and phase change	Traditional correlations for heat transfer coefficient and pressure	Ascomp/MIT

ITM Test Cases – Summary (2)

Physical phenomena	Test Case #	Objective	Relevance	Capabilities tested	Database	Developed by
Single bubble	3a	Predict growth and detachment of single air bubble under flow conditions	Subcooled boiling in PWR hot channel before and after point of net vapor generation	Interface-tracking and CFD, no heat transfer and phase change	n/a	RPI
	3b	Predict growth and detachment of single bubble under subcooled pool boiling conditions	Subcooled boiling in PWR hot channel before and after point of net vapor generation	Interface-tracking and CFD with heat transfer and phase change (both evaporation and condensation) including a microlayer evaporation model	Experimental database generated by CASL	MIT/Ascomp
	3c	Predict growth and detachment of single bubble under subcooled flow boiling conditions	Subcooled boiling in PWR hot channel before and after point of net vapor generation	Interface-tracking and CFD with heat transfer and phase change (both evaporation and	Experimental database generated by CASL	CCNY

ITM Test Cases – Summary (3)

Physical phenomena	Test Case #	Objective	Relevance	Capabilities tested	Database	Developed by
Multiple bubbles	4	Predict the void fraction distribution dependency on bubble deformability in a turbulent up-flow	Subcooled boiling in PWR hot channel after net vapor generation	Interface tracking and CFD, no heat transfer and no phase change	n/a	Notre Dame Univ. / TAMU

- *Focus is on phenomena relevant to the CASL challenge problems; in particular, we have emphasized boiling, which is key to CRUD and DNB*
- *Test key interface-tracking and turbulence simulation capabilities*
- *Reasonably 'easy', to fit within the first 1.5 years of CASL project. Test cases do not aim at prototypical PWR fuel assembly conditions.*

ITM Test Cases – Why they matter

- *Distinguish between the various ITM codes available to CASL, and algorithms/assumptions (e.g. compressibility, soft interface) implemented in those codes.*
- *Test the particular package 'software-hardware-user' of different groups within CASL.*
- *Serve as a test-bed for new VUQ approaches, which may be developed by the VUQ focus area.*
- *Be a first step towards 'numerical experiments' that will support the development of closure relations for VERA-CFD.*

Future Work

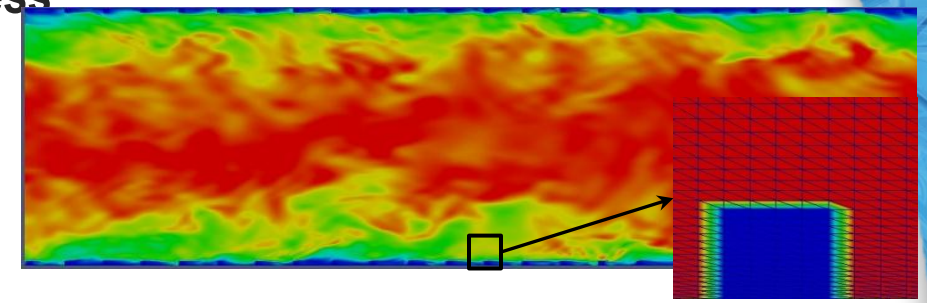
- *Complete definition of ITM Test Cases 3a and 3c*
- *Complete databases in support of ITM Tests Cases*
- *Complete simulations of ITM Test Cases using the CASL ITM codes*
- *Develop ITM Challenge Simulation:*
  - *Focus on subcooled flow boiling at PWR prototypical flow conditions and geometry (properly scaled)*
  - *Include combined turbulence, interface tracking, heat transfer and phase change (both evaporation at the wall and condensation in the flow core)*
  - *Could resolve transport of chemical species (relevant to CRUD)*
  - *Between 1 and 10 billion grid points*
  - *Will be used as an "engine" for development of closure relations for VERA-CFD*

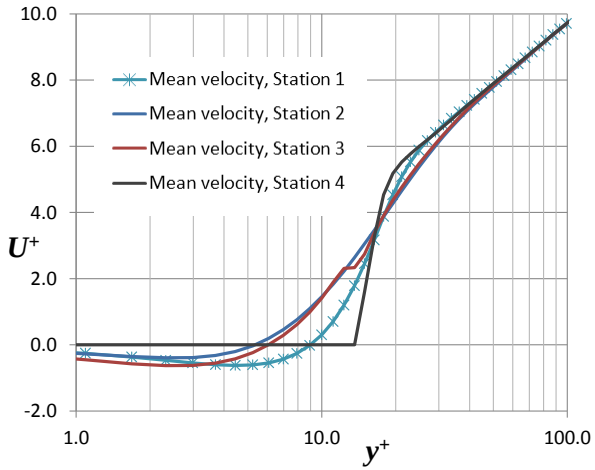
ITM Benchmark #1: PHASTA simulations

Igor Bolotnov (NCSU)

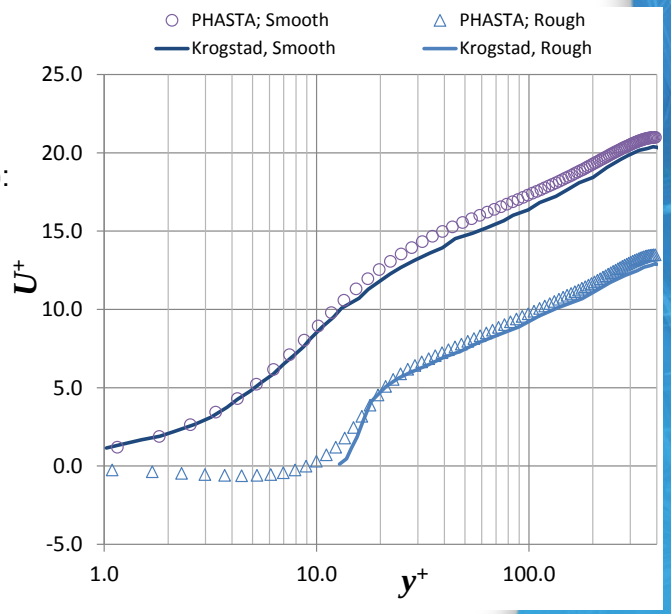
Channel flow with rectangular roughness, Re_T = 400

- Computational mesh: 22M elements
- 6000 processors on Jaguar used

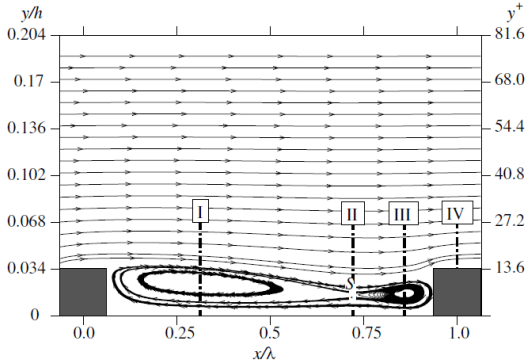




Law of the wall comparison with smooth and rough simulations of Krogstad et al. (2005):



Measuring stations are consistent with Ashrafian et al. (2004):



4-year timeline for VERA-CFD capabilities

✓ Initial single-phase turbulent excitation forces for GTRF analysis on 3x3 AMA problem

Single-phase capability in VERA; improved GTRF and CRUD analysis

Use upscaled ITM for improved subcooled boiling analysis

Are coupled surface reactions needed for CRUD analysis?

7/1/11 — 7/1/12 — 7/1/13 — 7/1/14 — 7/1/15

Initial single-phase heat transfer multipliers for CRUD analysis on 3x3 AMA problem

What degree of FSI coupling is needed for GTRF? Gap resolution?

Initial 3-D multiphase capability, coupled into VERA

Improved DNB analysis, coupled under VERA

ITM Simulations and Supporting Experimental Activities in CASL

Jacopo Buongiorno
Associate Professor of Nuclear Engineering
Massachusetts Institute of Technology
(617-253-7316, jacopo@mit.edu)

9-10 August 2011, NCSU

CANES Center for Advanced Nuclear Energy Systems

CASL-U-2011-0072-000-R

Motivation

In VERA-CFD, two-phase flow will be described by the "two-fluid" phase-averaged approach

Mass (*k* = liquid or vapor)

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \vec{v}_k) = \Gamma_k$$

Momentum

$$\frac{\partial(\alpha_k \rho_k \vec{v}_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \vec{v}_k \vec{v}_k) = -\alpha_k \nabla P - \frac{\vec{\tau}_{w,k} p_{w,k}}{A} - \alpha_k \rho_k \vec{g} + \Gamma_k \vec{v}_k + \vec{F}'''_{i,k}$$

Energy

$$\frac{\partial[\alpha_k \rho_k (h_k + \frac{v_k^2}{2})]}{\partial t} + \nabla \cdot [\alpha_k \rho_k \vec{v}_k (h_k + \frac{v_k^2}{2})] = \frac{q''_w p_{w,k}}{A} + \alpha_k \rho_k \vec{v}_k \cdot \vec{g} + \Gamma_k (h_k + \frac{v_k^2}{2}) + \vec{F}'''_{i,k} \cdot \vec{v}_k + Q'''_{i,k}$$

...which requires many closure relations for the wall-to-flow and phase-to-phase exchange terms

CASL-U-2011-0072-000-R

Motivation (2)

Sensitivity analyses (U-Michigan) on STAR-CD EMP model have shown that key parameters in subcooled flow boiling (e.g. void fraction, heat transfer coefficient and pressure drop) depend strongly on wall-to-flow heat transfer closure relation, in particular:

- *bubble departure diameter*
- *bubble departure frequency*
- *bubble growth and wait times*
- *nucleation site density*
- *areal void fraction*

CASL-U-2011-0072-000-R

Motivation (3)

Large uncertainties are hidden in these closure relations

Example of closure relation used by CFD codes for wall-to-flow heat transfer is the partitioned heat flux model

$$q''_{tot} = q''_e + q''_q + q''_c$$

$$q''_e = \frac{\pi D_b^3}{6} \rho_g h_{fg} f_b N_{SD}$$

$$q''_q = \left(t_w f_b\right) A_q \frac{2k_l (T_w - T_{sat})}{\sqrt{\pi \alpha_l t_w}}$$

$$q''_c = A_{1\phi} h_{turb} \left(T_w - T_{sat}\right)$$

Requires input for:

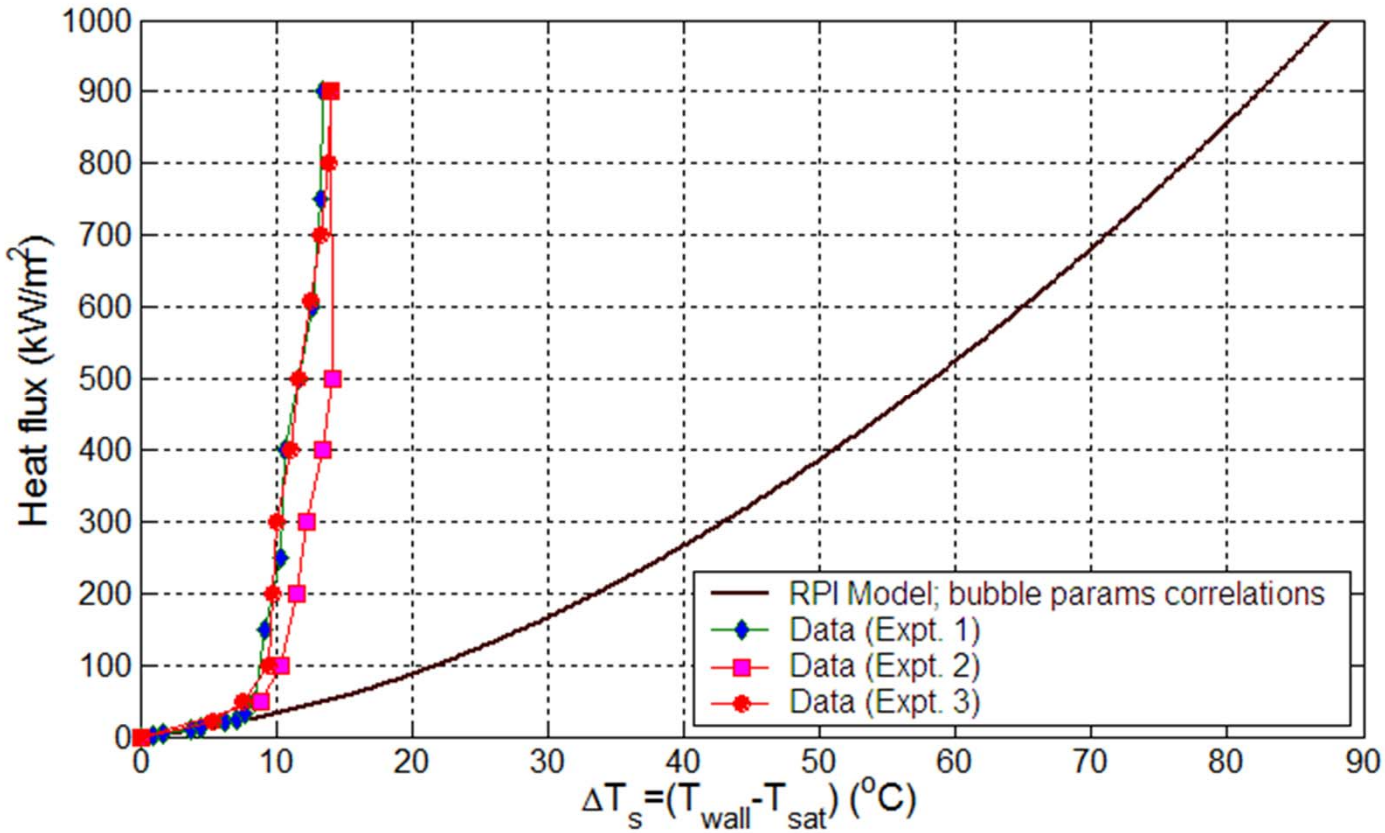
- bubble departure diameter
- bubble departure frequency
- bubble growth and wait times
- nucleation site density
- areal void fraction

Model comes with default correlations for bubble parameters

CASL-U-2011-0072-000-R

Motivation (4)

Predictions of this model with default correlations for bubble parameters… are off by as much as 1000%!!



HOW TO IMPROVE FIDELITY OF CLOSURE RELATIONS?

High-fidelity closure relations may come from numerical simulations with interface tracking

ITM - Background

Closure relations for VERA-CFD could come from simulations with interface tracking methods (ITM)

Mass $$\nabla \cdot \vec{u} = \dot{m}\left(\frac{1}{\rho_\ell} - \frac{1}{\rho_v}\right)\delta_S$$

Phase change and surface tension forces are represented as delta functions at the interface

Momentum (Navier-Stokes)

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla \cdot (\rho\vec{u}\vec{u}) = -\nabla P + \nabla \cdot \mu(\nabla\vec{u} + \nabla^{\perp}\vec{u}) + \rho\vec{g} + \sigma\kappa\vec{n}\delta_S$$

Energy $$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho c_p \vec{u} T) = \nabla \cdot \lambda \nabla T + \dot{m} h_{\ell v}\delta_S$$

- Examples of ITM: volume of fluid, level-set, front-tracking, …
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CASL-U-2011-0072-000-R

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Physical phenomena	Test Case #	Objective	Relevance	Capabilities tested	Database	Developed by
Single-phase turbulence and heat transfer	1	Predict friction factor of turbulent flow over a flat wall with a pattern of small hemispherical solid obstacles	Subcooled boiling in PWR hot channel at axial locations between the onset of nucleate boiling and the point of net vapor generation	Single-phase CFD without interface tracking, heat and phase change	Numerical database generated by CASL	MIT/Ascomp
	2	Predict axial location of onset of subcooled nucleate boiling (point where $T_w \approx T_{sat}$)	Onset of nucleate boiling in PWR hot channel	Single-phase CFD with heat transfer, but without interface tracking and phase change	Traditional correlations for heat transfer coefficient and pressure	Ascomp/MIT

CASL-U-2011-0072-000-R

ITM Test Cases – Summary (2)

Physical phenomena	Test Case #	Objective	Relevance	Capabilities tested	Database	Developed by
Single bubble	3a	Predict growth and detachment of single air bubble under flow conditions	Subcooled boiling in PWR hot channel before and after point of net vapor generation	Interface-tracking and CFD, no heat transfer and phase change	n/a	RPI
	3b	Predict growth and detachment of single bubble under subcooled pool boiling conditions	Subcooled boiling in PWR hot channel before and after point of net vapor generation	Interface-tracking and CFD with heat transfer and phase change (both evaporation and condensation) including a microlayer evaporation model	Experimental database generated by CASL	MIT/Ascomp
	3c	Predict growth and detachment of single bubble under subcooled flow boiling conditions	Subcooled boiling in PWR hot channel before and after point of net vapor generation	Interface-tracking and CFD with heat transfer and phase change (both evaporation and	Experimental database generated by CASL	CCNY

ITM Test Cases – Summary (3)

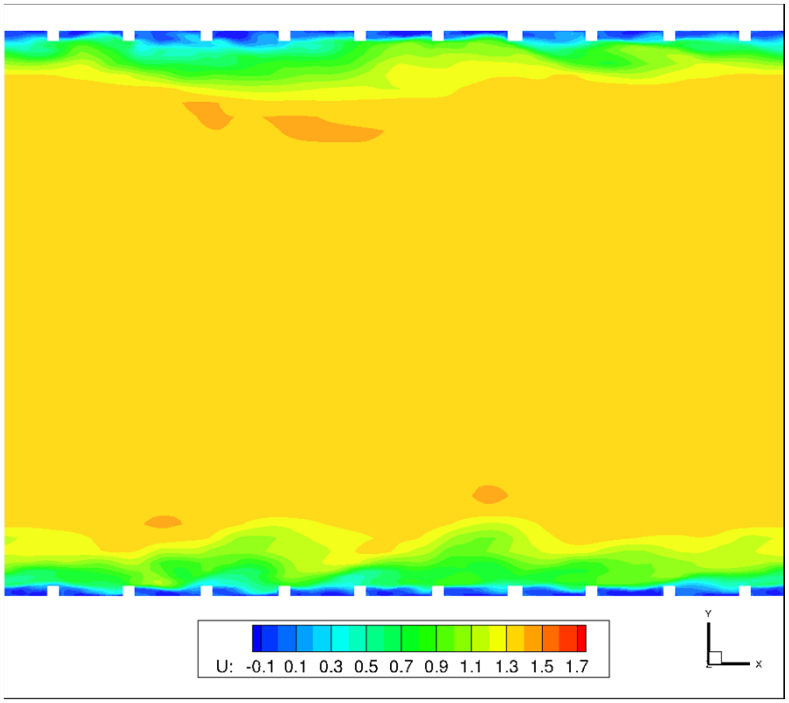
Physical phenomena	Test Case #	Objective	Relevance	Capabilities tested	Database	Developed by
Multiple bubbles	4	Predict the void fraction distribution dependency on bubble deformability in a turbulent up-flow	Subcooled boiling in PWR hot channel after net vapor generation	Interface tracking and CFD, no heat transfer and no phase change	n/a	Notre Dame Univ. / TAMU

- *Focus is on phenomena relevant to the CASL challenge problems; in particular, we have emphasized boiling, which is key to CRUD and DNB*
- *Test key interface-tracking and turbulence simulation capabilities*
- *Reasonably 'easy', to fit within the first 1.5 years of CASL project. Test cases do not aim at prototypical PWR fuel assembly conditions.*

CASL-U-2011-0072-000-R

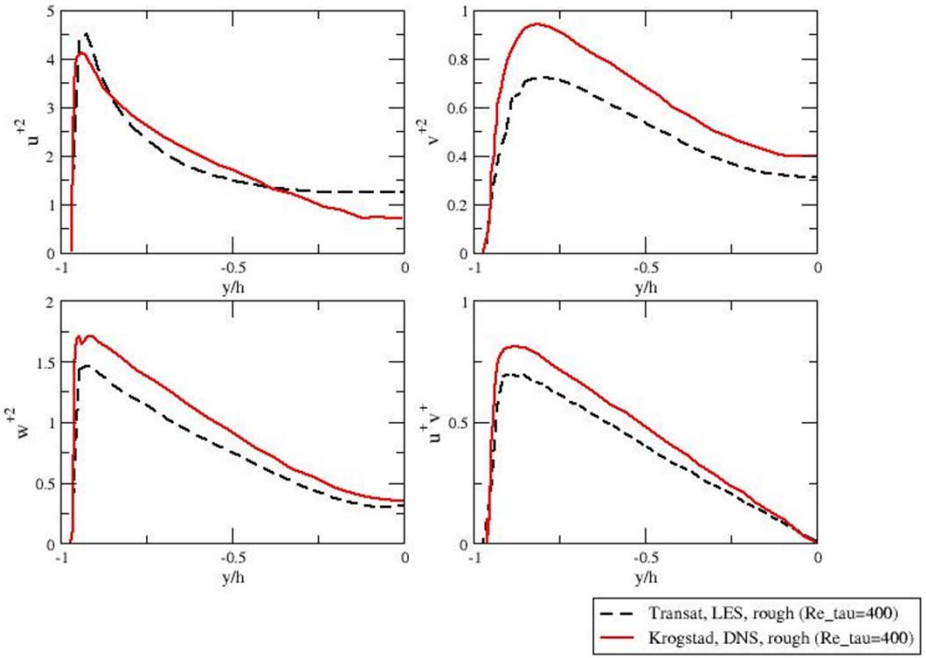
ITM Test Cases – Some initial results (1)

ITM Test Case 1: Krogstad's reference flow between parallel channels with rectangular roughness elements; LES simulation run with TransAT on Jaguar



↑

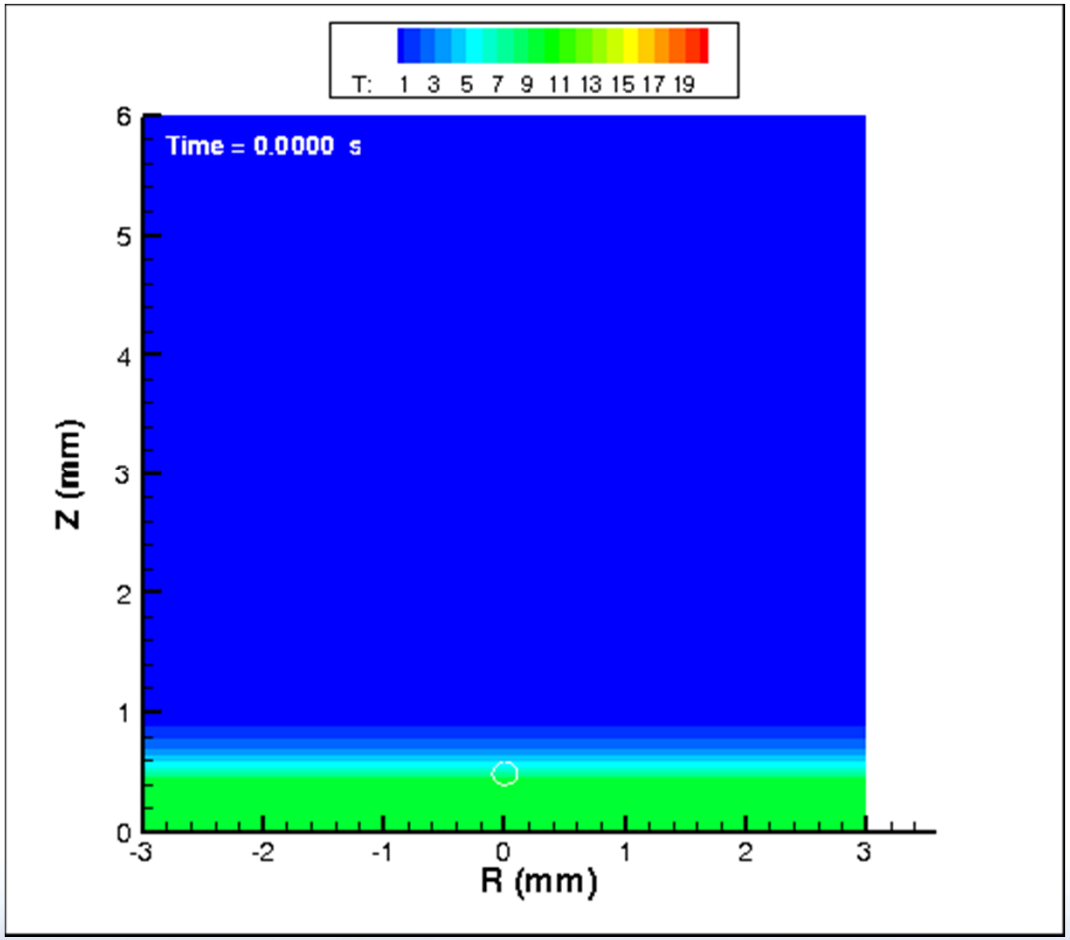
VIDEO



ITM Test Cases – Some initial results (2)

ITM Test Case 3a: growth and detachment of reference steam bubble off heated wall; level-set simulation run with TransAT on Jaguar

VIDEO →



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ITM Test Cases – Why they matter

- *Distinguish between the various ITM codes available to CASL, and algorithms/assumptions (e.g. compressibility, soft interface) implemented in those codes.*
- *Test the particular package 'software-hardware-user' of different groups within CASL.*
- *Serve as a test-bed for new VUQ approaches, which may be developed by the VUQ focus area.*
- *Be a first step towards 'numerical experiments' that will support the development of closure relations for VERA-CFD.*

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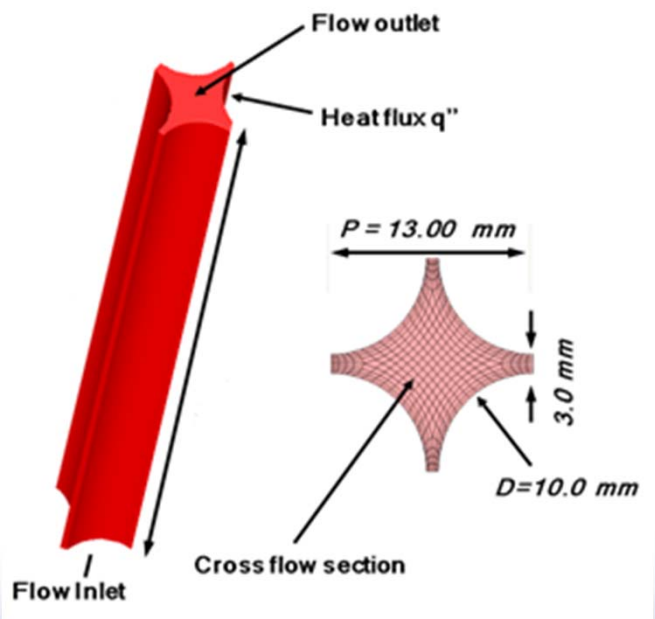
Next Step – Develop ITM Challenge Simulation

- Subcooled flow boiling in PWR 2x2 (or 3x3) subchannel with prototypical flow conditions and geometry (properly scaled)
- Include combined turbulence, interface tracking, heat transfer and phase change (both evaporation at the wall and condensation in the flow core)
- Simulate rate at which vapor bubbles form and grow, depart and move along and away from the wall, and recondense as they move into the colder core of the subchannel
- Could resolve transport of chemical species (relevant to CRUD)
- Between 1 and 10 billion grid points, run on Jaguar
- Will be used as an "engine" for development of closure relations for VERA-CFD



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How to validate ITM results?

Want to know:

- bubble departure diameter
- bubble departure frequency
- bubble growth and wait times
- nucleation site density
- areal void fraction
- velocity, temperature and phase distributions

in both POOL and FLOW boiling

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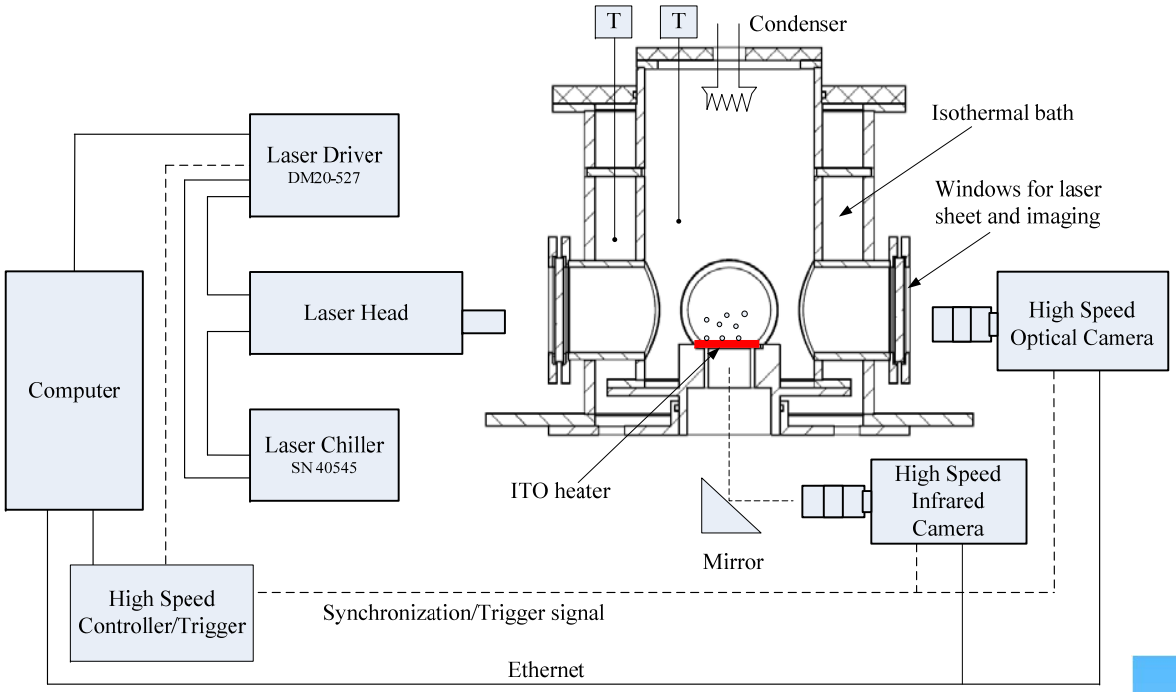
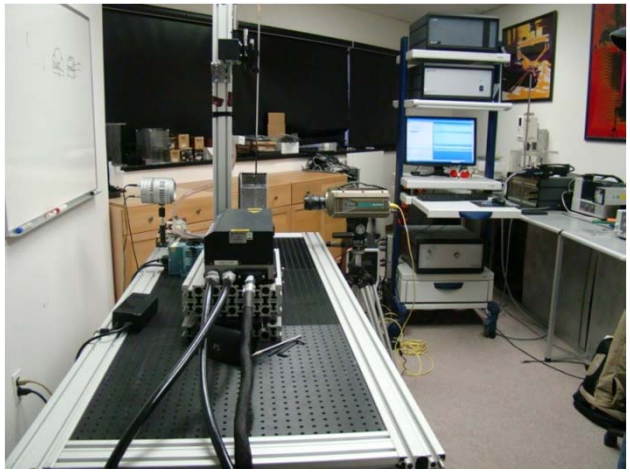
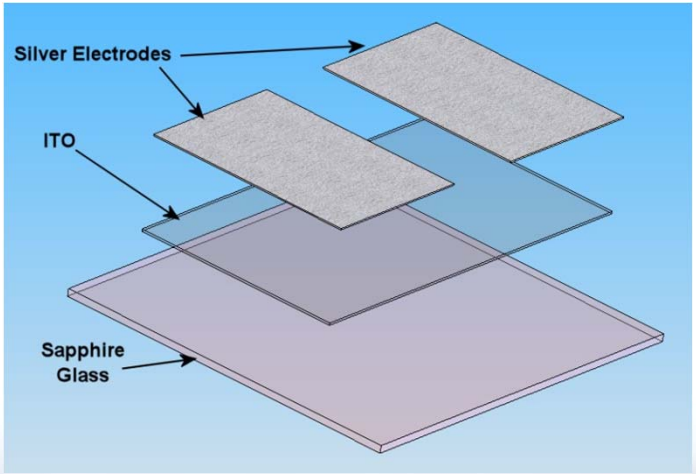
Pool boiling facility with synchronized IR, PIV and HSV





Special transparent heater design (ITO on sapphire substrate) enables access/imaging of bubbles from the side as well below the boiling surface



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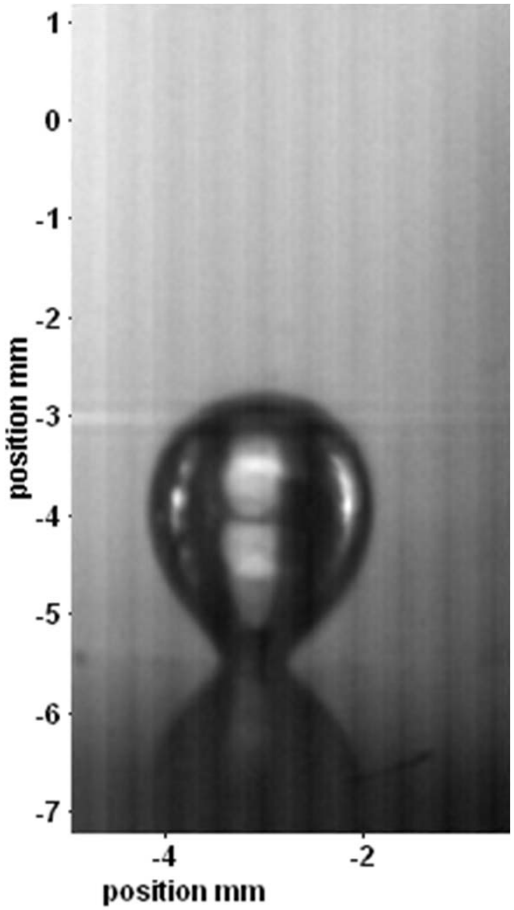
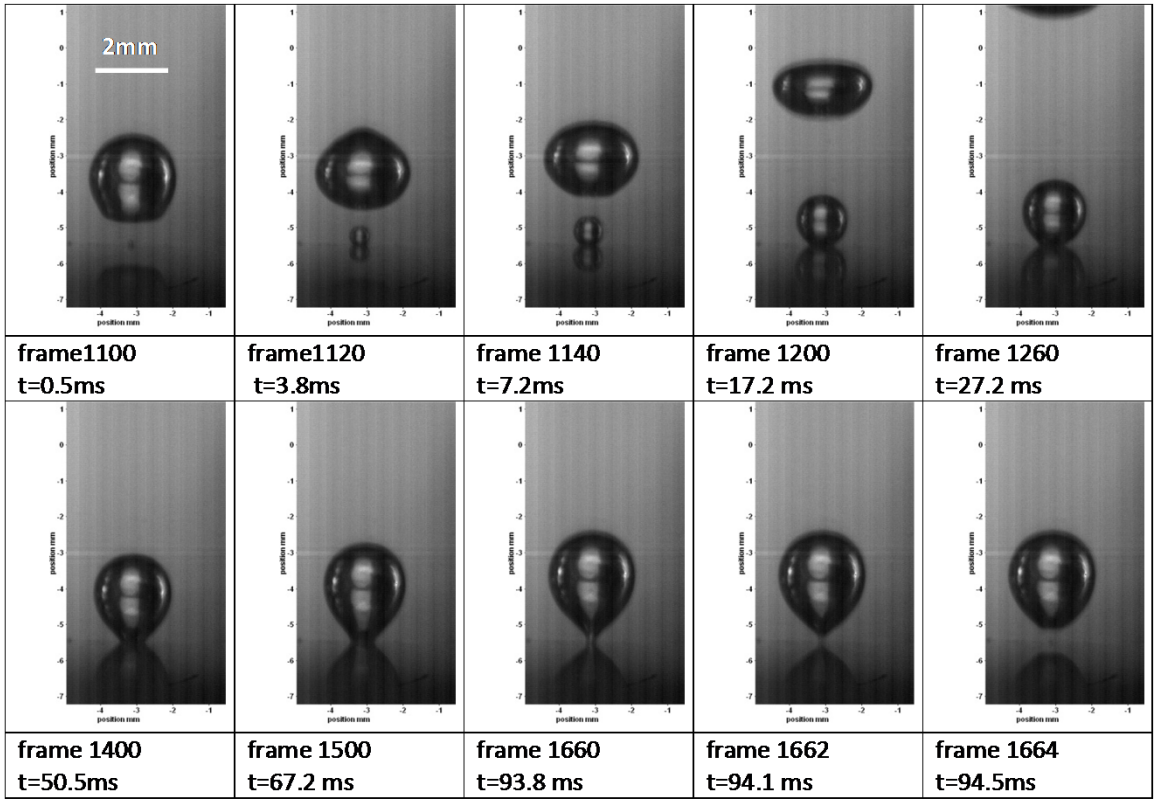
Examples: High-Speed video

Gives *bubble shape (phase distribution)* near boiling surface

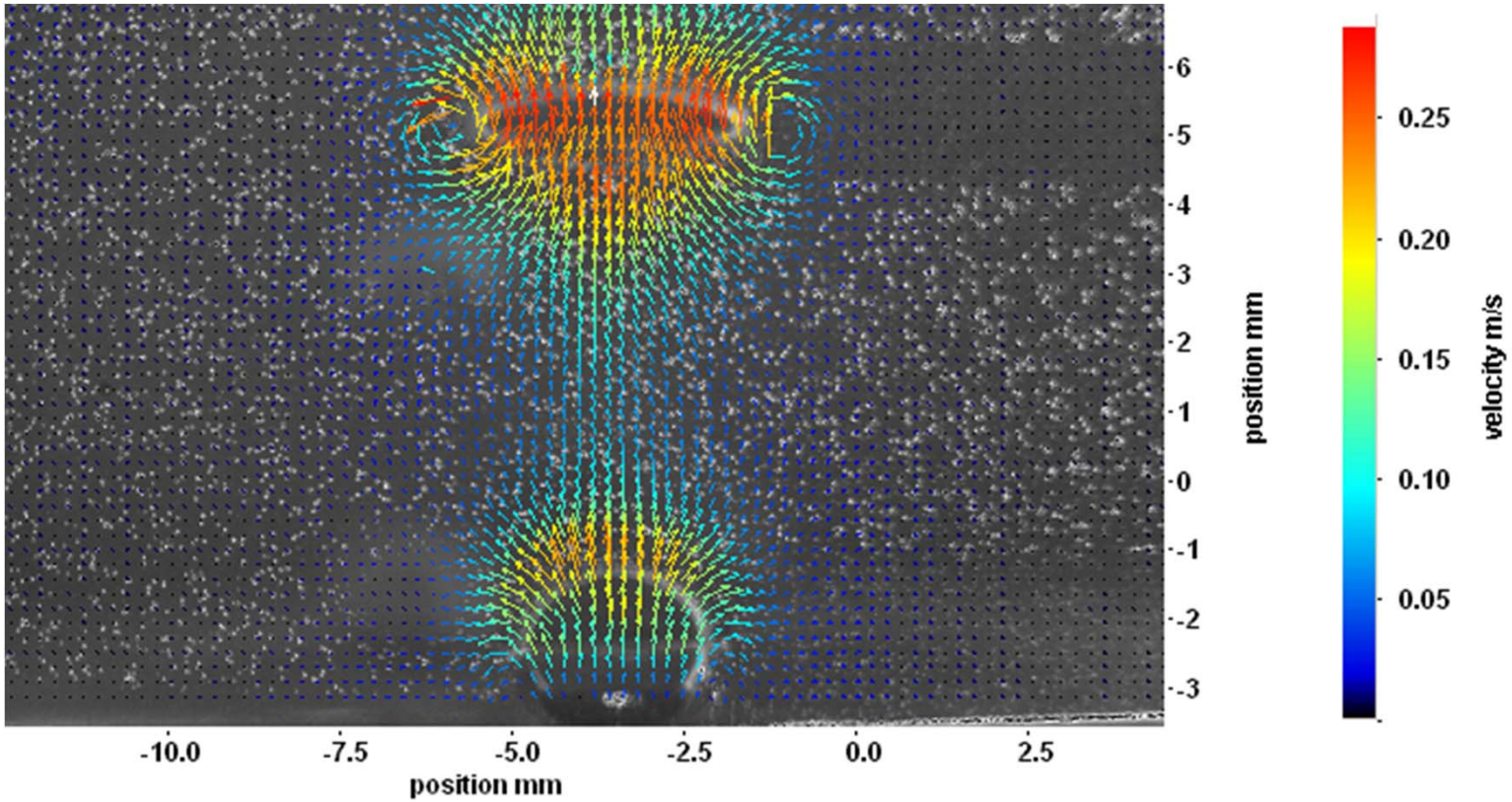


T≈100ºC, q"≈12 kW/m^2, 6000 fps



Examples (2): Two-Phase PIV

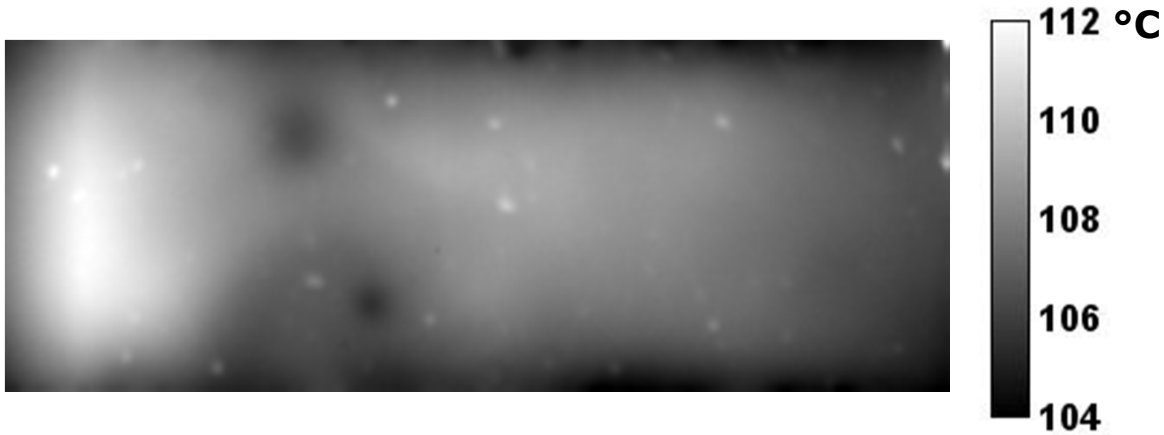
Gives *velocity distribution* near growing bubble



Examples (3): High-Speed IR Thermometry

IR images give the *nucleation site density*

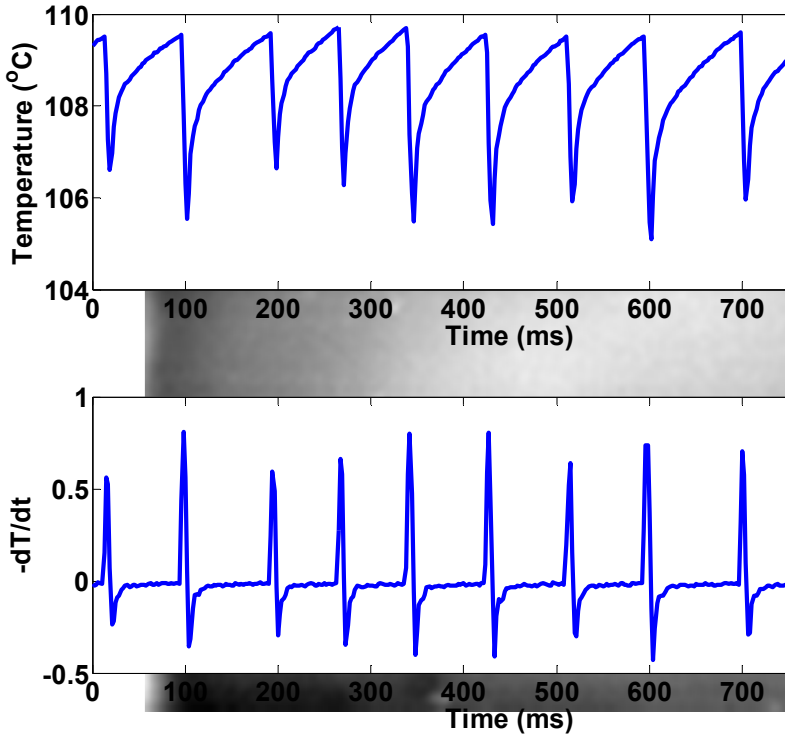
DI water
at q"=50 kW/m²
(ΔT_s~8.5°C)
1000 fps

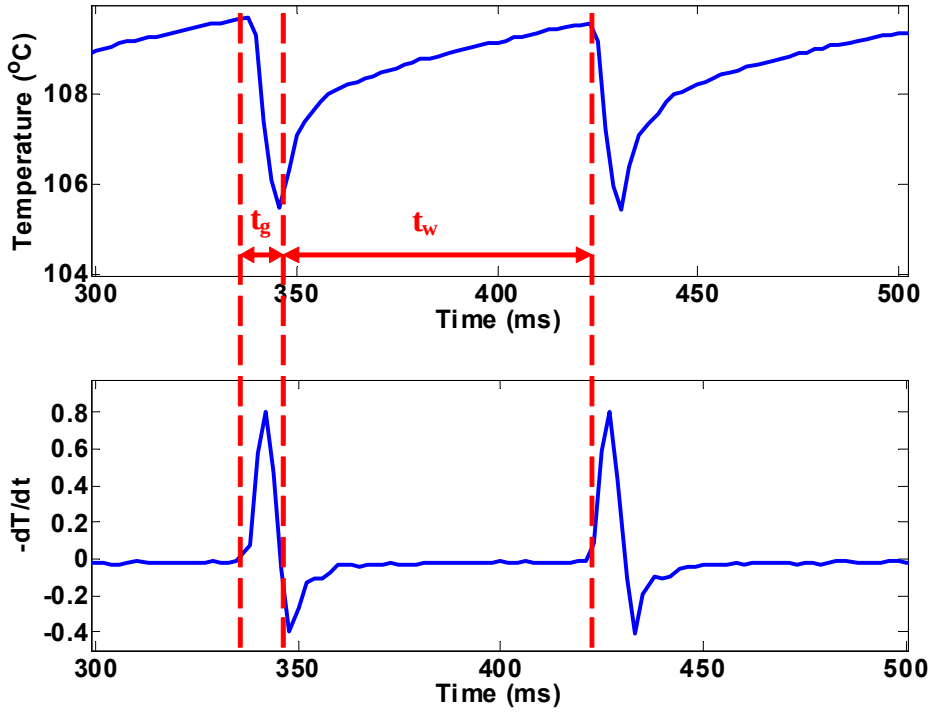


DI water
at q"=250 kW/m²
(ΔT_s~10.3°C)
1000 fps

Examples (4): High-Speed IR Thermometry

IR images give the *bubble frequency, growth time and wait time*

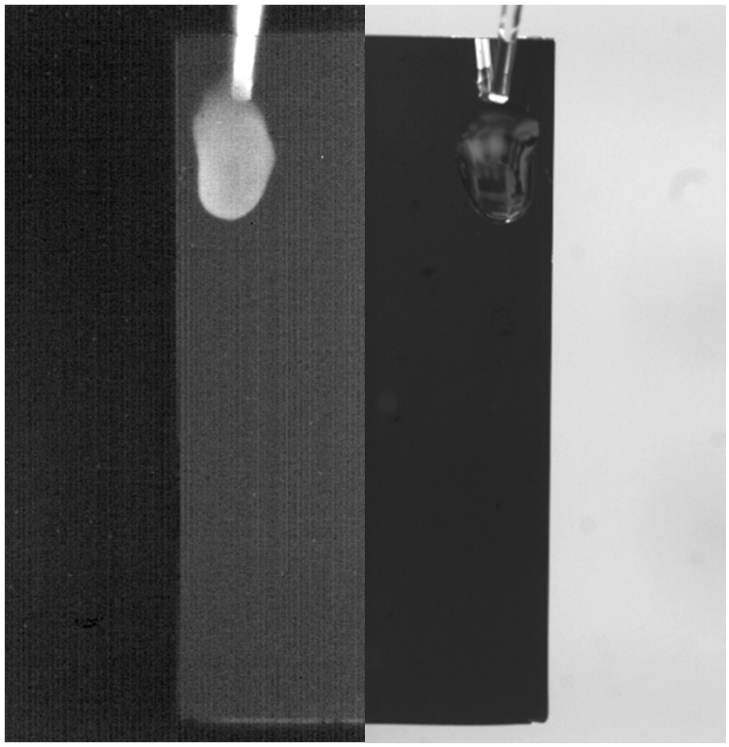




Examples (5): High-Speed IR Thermometry

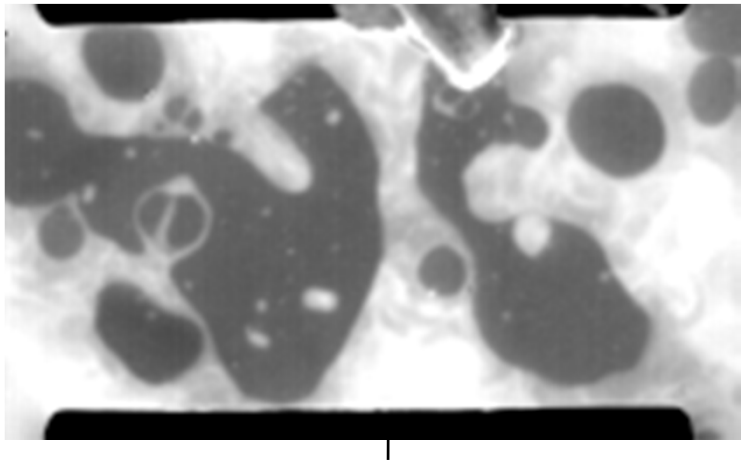
IR images give also the *areal void fraction*

Droplet sliding on surface of Si wafer

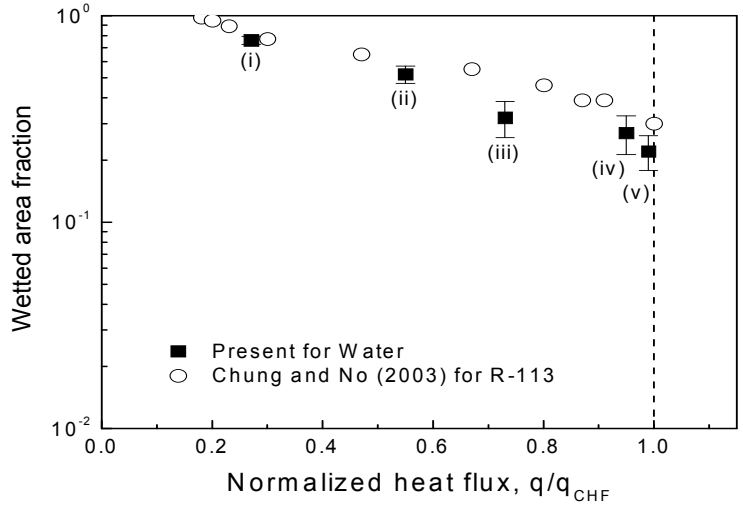


IR (from behind the wafer)

HSV (from above the wafer)

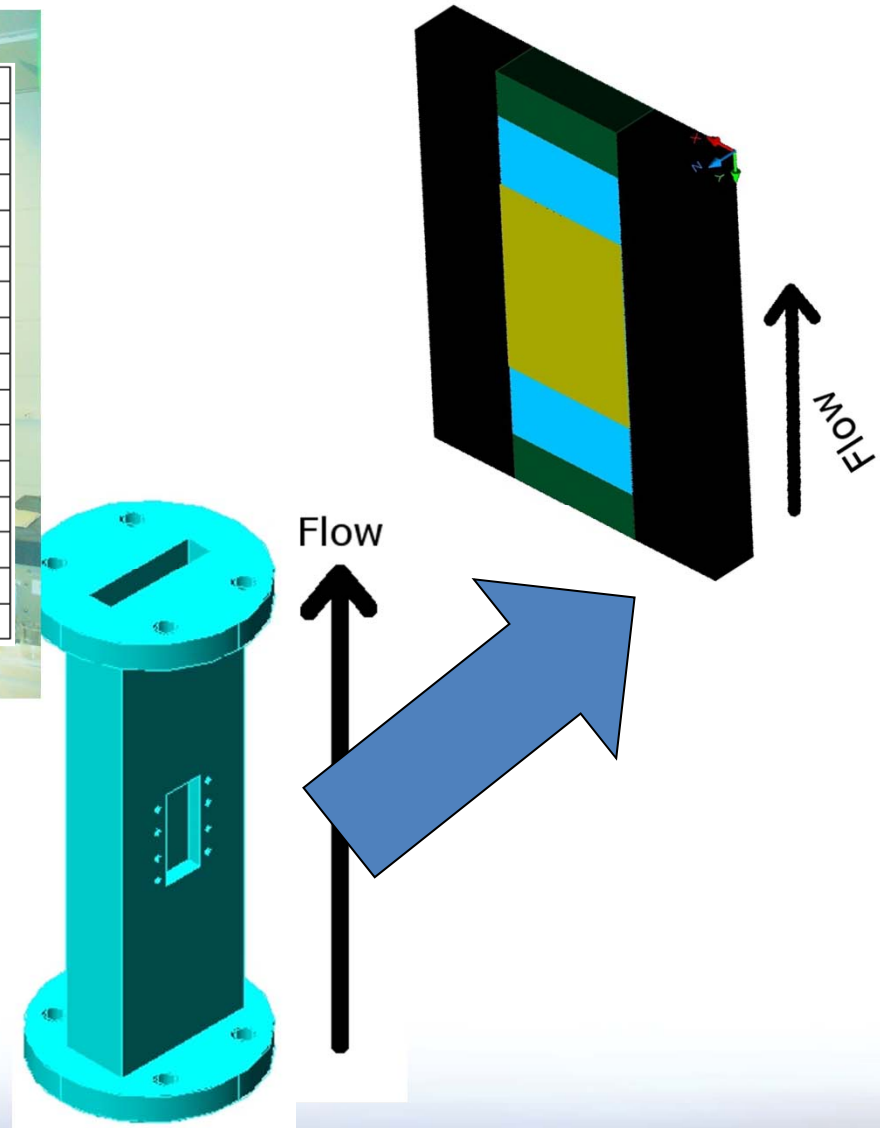


Dynamics of areal void fraction in high-heat-flux nucleate boiling



Flow boiling facility with synchronized IR, PIV and HSV

Parameter	Experiment Range	PWR Range
Reynolds Number	$0\text{-}1\times10^5$	$2\times10^5\text{-}5\times10^5$
Prandtl Number	1.1-6.2	0.9-1.2
Froude Number	0-25	0-217
Boiling Number	0-10	0-0.25
Equilibrium Exit Quality	-0.24 to 0	-0.38 to -0.15
Water velocity	0-2m/s	2-5m/s
Mass Flux	0-1500kg/m^2-s	1500-3500kg/m^2-s
Temperature	25-150°C	286-324°C
Pressure	0.1-0.4MPa	15.5MPa
Subcooling	0-75°C	21-58°C
Hydraulic Diameter	16mm	12mm
Wetted Perimeter	110mm	30mm
Heated Perimeter	15mm	30mm
Heat Flux	0-2MW/m^2	0-0.45MW/m^2
Channel Area	450mm^2	88mm^2



Quartz test section with ITO on sapphire substrate heater insert

CASL-U-2011-0072-000-R

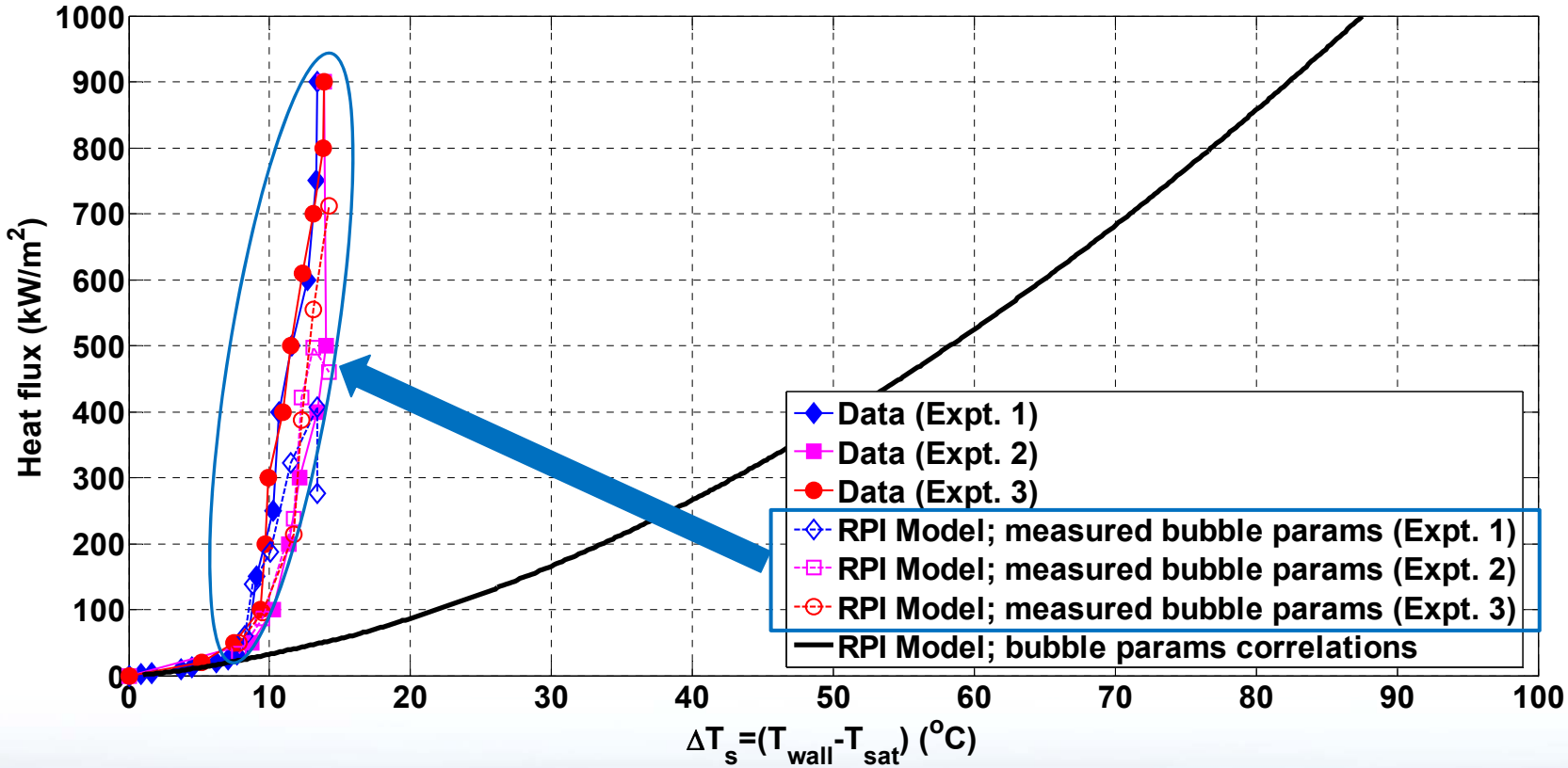
Flow boiling facility with synchronized IR, PIV and HSV

The most comprehensive set of subcooled flow boiling measurements to date

Publications:	Euh (2010)	Situ (2004, 2008)	Basu (2002)	Thorncroft (1998)	Del Valle (1985)	Estrada-Perez (2010)	Díez (2005)	This Work
Departure Diameter	No	Yes, HSV	No	Yes, HSV	Yes, HSV	No	No	Yes, HSV, IR
Departure Frequency	Yes, HSV	Yes, HSV	No	Yes, HSV	No	No	No	Yes, HSV
Growth Time	Yes, HSV	Yes, HSV	No	Yes, HSV	Yes, HSV	No	No	Yes, HSV
Growth Rate	Yes, HSV	Yes, HSV	No	Yes, HSV	No	No	No	Yes, HSV
Wait Time	Yes, HSV	Yes, HSV	No	Yes, HSV	No	No	No	Yes, HSV
Sliding Velocity	No	No	No	Yes, HSV	No	Yes	No	Yes, PIV, HSV
Phase Slip	No	No	No	No	No	Yes, HSV, PIV	No	Yes, HSV, PIV
Nucleation Site Density	No	No	Yes	No	Yes, HSV	No	No	Yes, IR, HSV
Onset of Nucleate Boiling	No	No	Yes, HSV, PI	No	Yes, HSV, PI	Yes	Yes	Yes, PI, EB
Heat Transfer Coefficient	No	No	No	No	No	No	Yes, IR, PI	Yes, IR, PI
Liquid 2D Velocity Field	No	No	No	No	No	Yes, PIV	No	Yes, PIV
Liquid 2D Temperature Profile	No	No	No	No	No	No	No	Yes, PLIF
Heater 2D Temperature Profile	No	No	No	No	No	No	Yes	Yes, IR
Heat Flux	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
System Pressure	Yes, PG	Yes, PG	Yes, PT	Yes, PT	Yes	No	Yes	Yes, PT
Inlet temperature	Yes, TC	Yes, TM	Yes, TC	Yes, TC	Yes, TC	Yes	Yes	Yes, TM
Outlet temperature	Yes, TC	Yes, TC	Yes, TC	Yes,TC	Yes, TC	Yes	Yes	Yes, TM
Flow Rate, Mass Flux	Yes, FM	Yes, FM	Yes, FM	Yes, FM	Yes, FM	Yes	Yes	Yes, FM

There is a chance this may actually work!

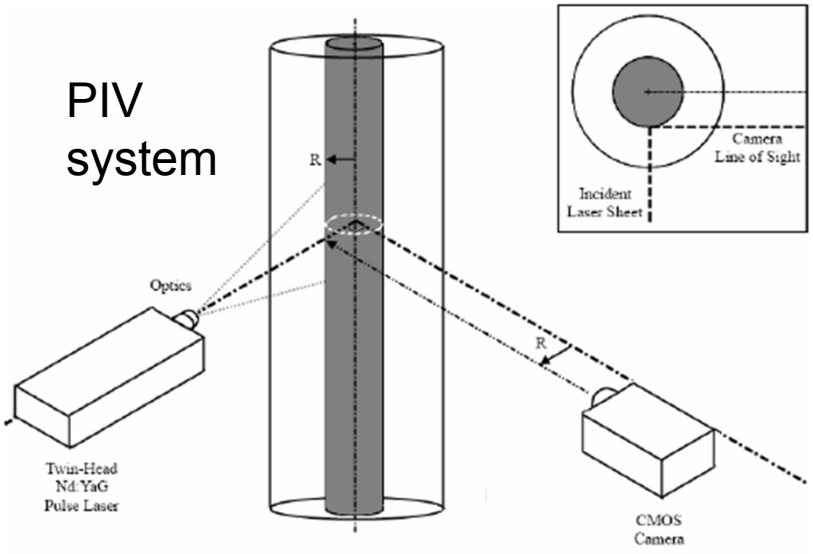
Predictions of RPI model with measured bubble parameters plugged in are in good agreement with measured data

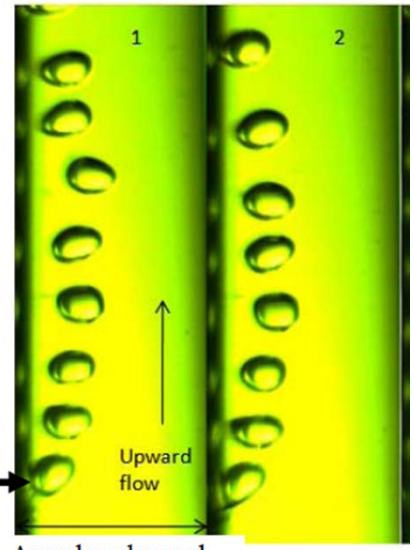


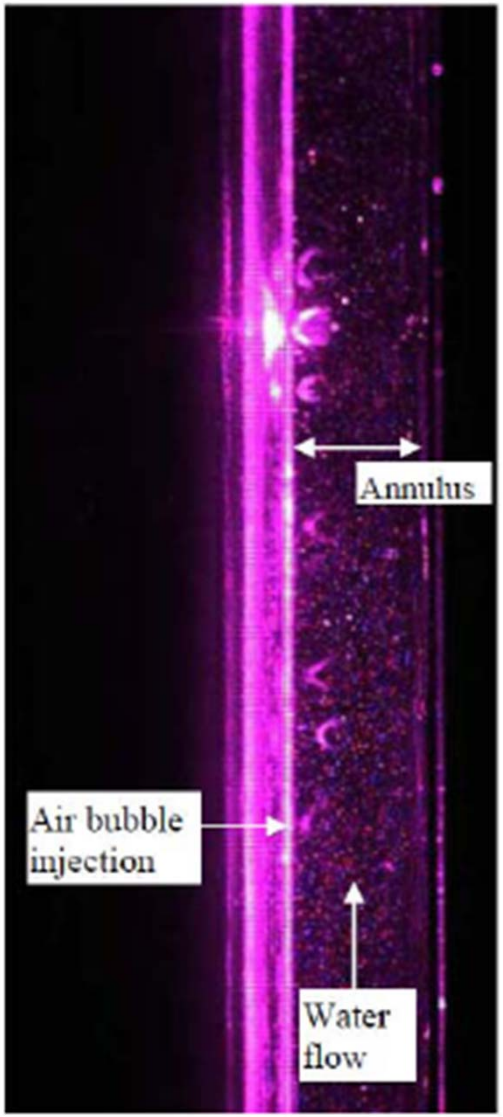
CCNY - Air Bubble Injection Experiments

M. Kawaji, T. Lee and S. Banerjee
The Energy Institute, City College of New York

PIV system







PIV Measurements

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CCNY - Subcooled Flow Boiling Experiments

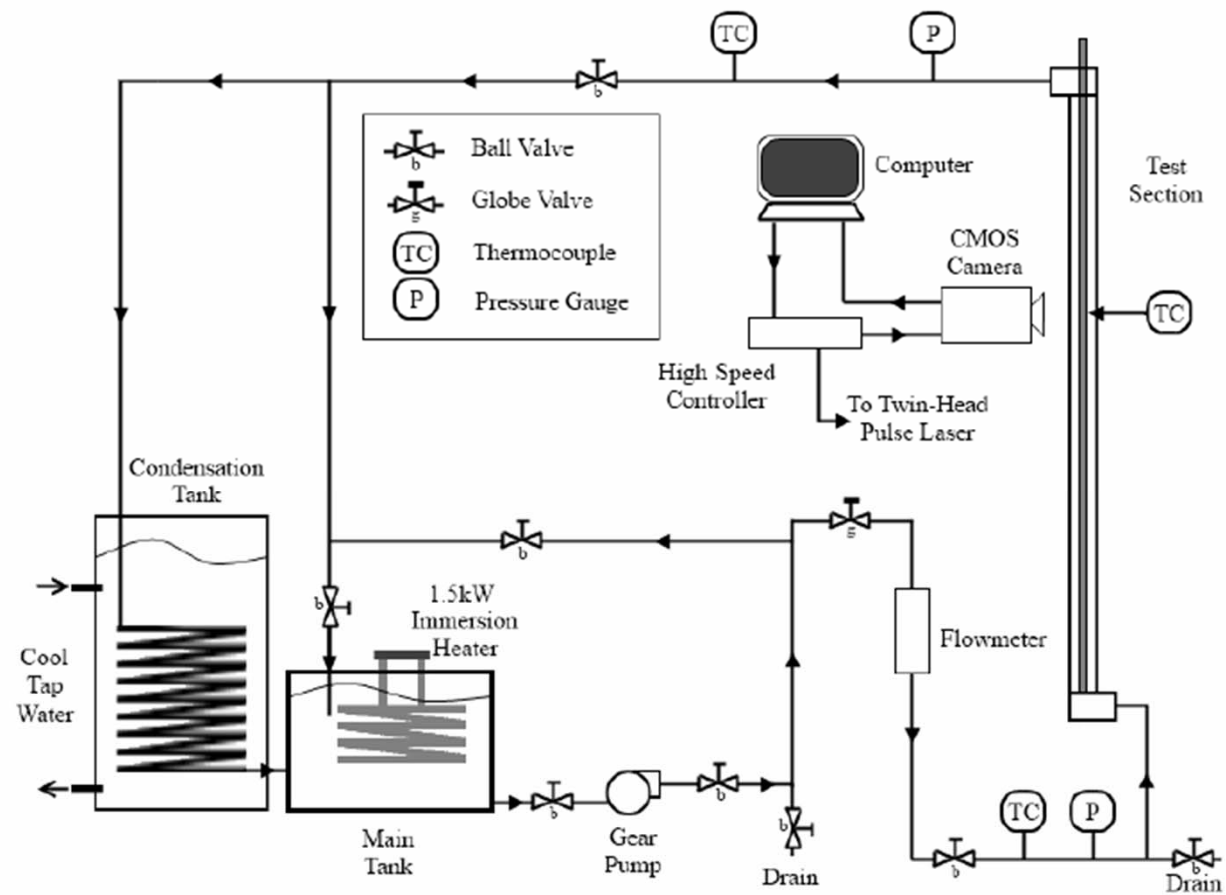
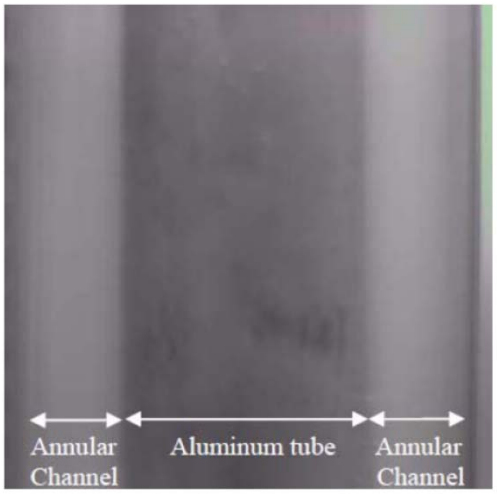
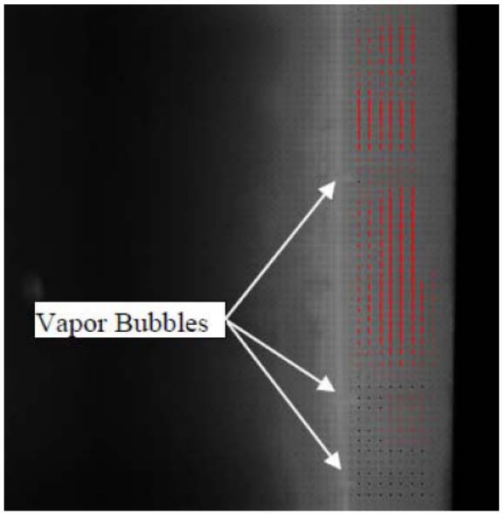


Fig. 1 Subcooled Flow Boiling Loop at CCNY



(a) An annular flow channel around a heated aluminum tube



(b) Velocity vectors obtained from PIV measurements

Timeline for ITM Activities in CASL

- September 2011: finalize definition of test cases
- December 2011: define challenge simulation
- March 2012: finish test case simulations
- June 2012: first runs of challenge simulation
- 2013: complete experimental database for subcooled flow boiling
- 2013: upscale numerical database from ITM challenge simulation to VERA-CFD

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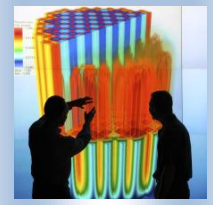
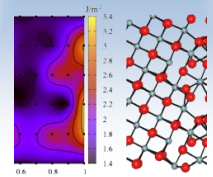




Compute Turbulent CFD Excitation Forces for 3x3 GTRF Problem

THM L3 Milestone: THM.CFD.P2.01

J. Shadid, T. Smith, R. Pawlowski,
E. Cyr, P. Weber, and D. Turner
Sandia National Laboratories

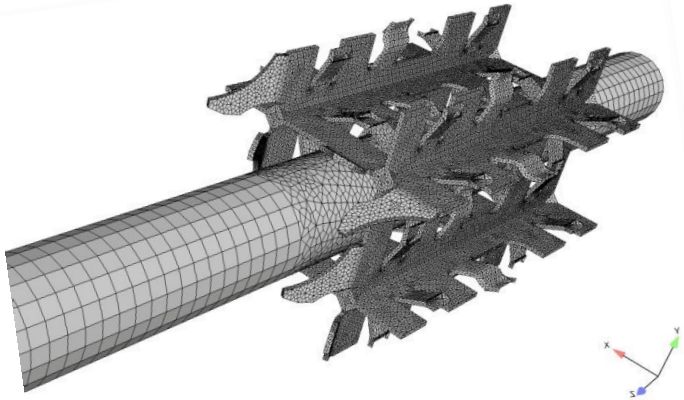
CASL
Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

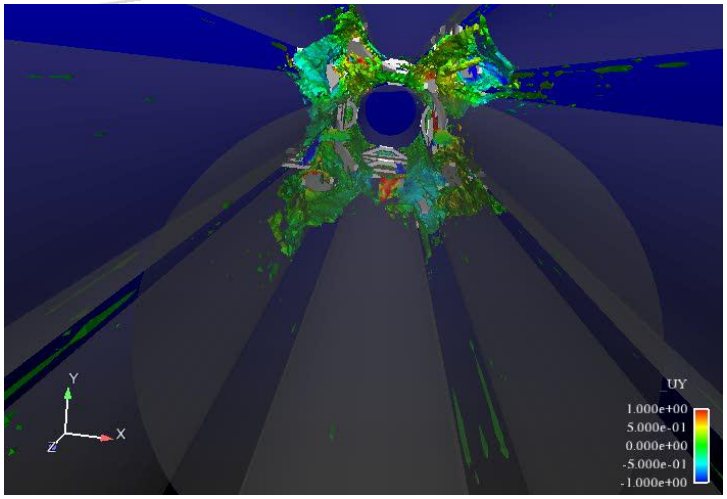
CASL-U-2011-0072-000-R

Background: CASL Relevance

- Targets the Grid-to-Rod Fretting (GTRF) Challenge Problem: Fluid/Structure Vibration Wearing of Pin Cladding.
- WEC Benchmark with experimental data for validation.
- Challenges of simulating 3x3 pin are similar for other important problems (sub-assembly and full core simulations)
- Demonstration of a scalable higher-order accurate CFD 3x3 pin capability will:
  - Help Increase accuracy over current CFD simulations
  - Enable VUQ assessment of CFD and vibration analysis
  - Reduce the margins of uncertainty, allowing for power up-rates, life extensions and future reactor design.
  - Build connections THM – VRI - VUQ and transfer technology within CASL partnership



WEC Grid Spacer



Drekar parallel LES Simulation

CFD plays a critical role in all Y1 Challenge problems

Background: Model & References

- Model:
  - 3x3 Rod bundle, WEC Solid Model with spacer/mixing vane,
  - Iso-thermal Navier-Stokes at 394°K, Re = 2 x 10^5
  - Periodic BCs (x,y) , Inflow specified, outflow zero stress
  - Wall Adaptive Large Eddy (WALE) turbulence model

References

WALE Model:

F. Nicoud, F. Ducros, Subgrid-Scale Stress Modeling on the Square of the Velocity Gradient Tensor, Flow, Turbulence and Combustion 62 (1999) 183–200.

Westinghouse analysis of CFD LES/WALE model using CD-Adaptco STAR-CCM+:

Elmahdi, A.M., Lu, R., Conner, M.E., Karoutas, Z. and Baglietto, E., "Flow Induced Vibration Forces on a Fuel Rod by LES CFD Analysis," The 14th International Topical Meeting on Nuclear Reactor ThermalHydraulics, NURETH-14-365, Toronto, Ontario, Canada, Sept. 25-30, 2011.

Z. Karoutas, Jin Yan, M. Conner and A. Mandour, "Advanced Thermal Hydraulic Method Using 3x3 Pin Modeling," The 14th International Topical Meeting on Nuclear Reactor ThermalHydraulics, NURETH-14-338, Toronto, Ontario, Canada, Sept. 25-30, 2011.

Unstructured FV, Smagorinsky, and SIMPLEC iteration:

Benhamadouche, S., Moussou, P. and Maitre, C. Le, "CFD Estimation of the Flow-Induced Vibrations of a Fuel Rod Downstream a Mixing Grid," Proceedings of the ASME 2009 Pressure Vessels and Piping Division Conference, July 26-30, 2009, Prague, Czech Republic.

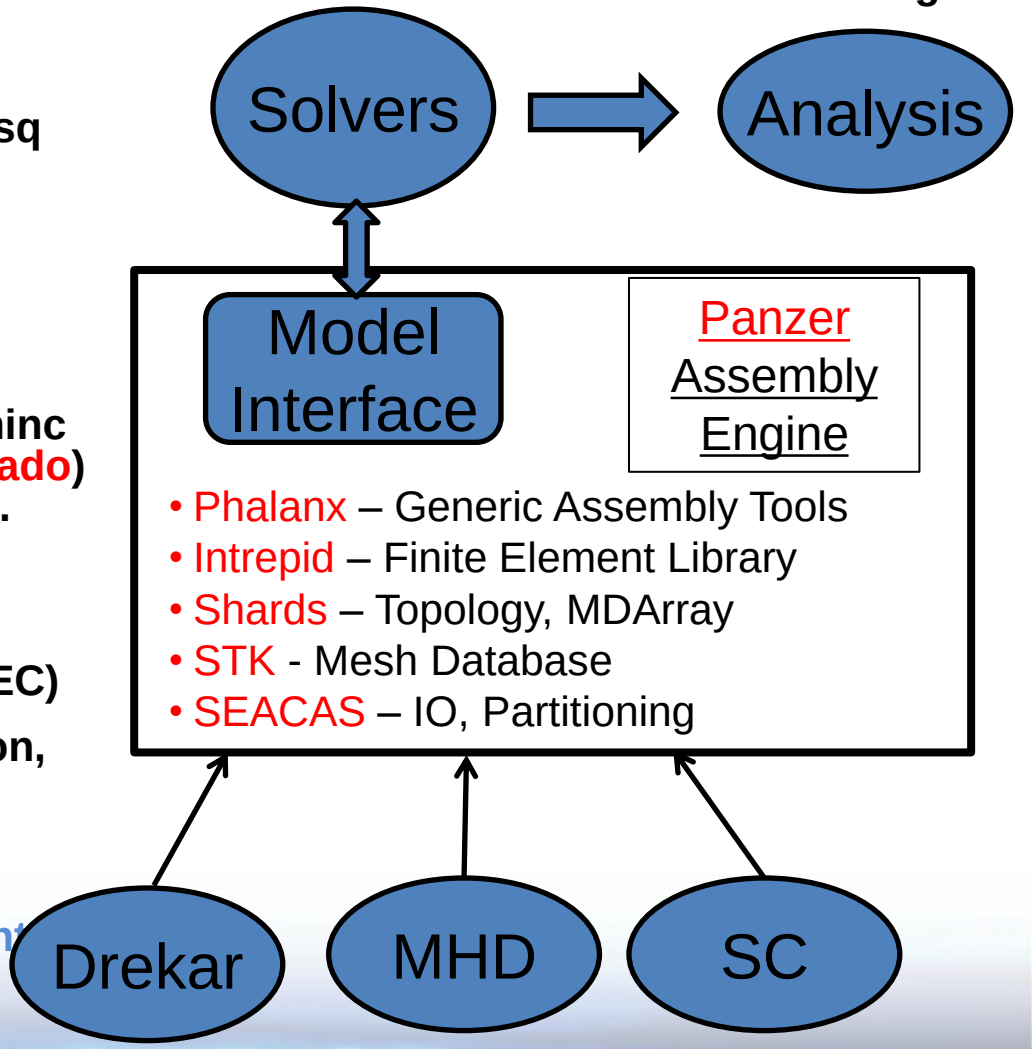
Dynamic Smagorinsky subgrid model:

Abbasian, F., Yu, S.D. and Cao, J., "Large Eddy Simulation of Turbulent Axial Flow Along an Array of Rods," Journal of Fluids Engineering, vol. 132, 2010, pp. 1--11.

Drekar::CFD

- **Massively Parallel: MPI**
- **2D & 3D Unstructured Stabilized FE (currently 2nd order, up to 8th order FE are available.)**
- **Fully-implicit: 1st-5th variable order BDF (Rythmos) & TR**
- **Eq. of State: Constant density; Bousinessq approx.; variable density: low flow Mach number approx., low flow Mach number compressible;**
- **Fully Coupled Globalized Newton-Krylov Solver**
  - **Template-based Generic Programminc with Automatic Differentiation (Sacado) for NK, JFNK, Sensitivities, UQ, etc.**
  - **GMRES (AztecOO, Belos)**
- **Scalable preconditioners: Fully-coupled system AMG, physics-based (e.g. SIMPLEC)**
- **Direct-to-Steady-State (NOX), Continuation, Linear Stability and Bifurcation (LOCA / Anasazi), PDE Constrained Optimization (Moocho)**
- **Future: Adjoints, Edge/face based element high-resolution methods, …**

trilinos.sandia.gov



Why Newton-Krylov Methods?

Newton-Krylov

Direct-to-steady-state

Fully-implicit transient

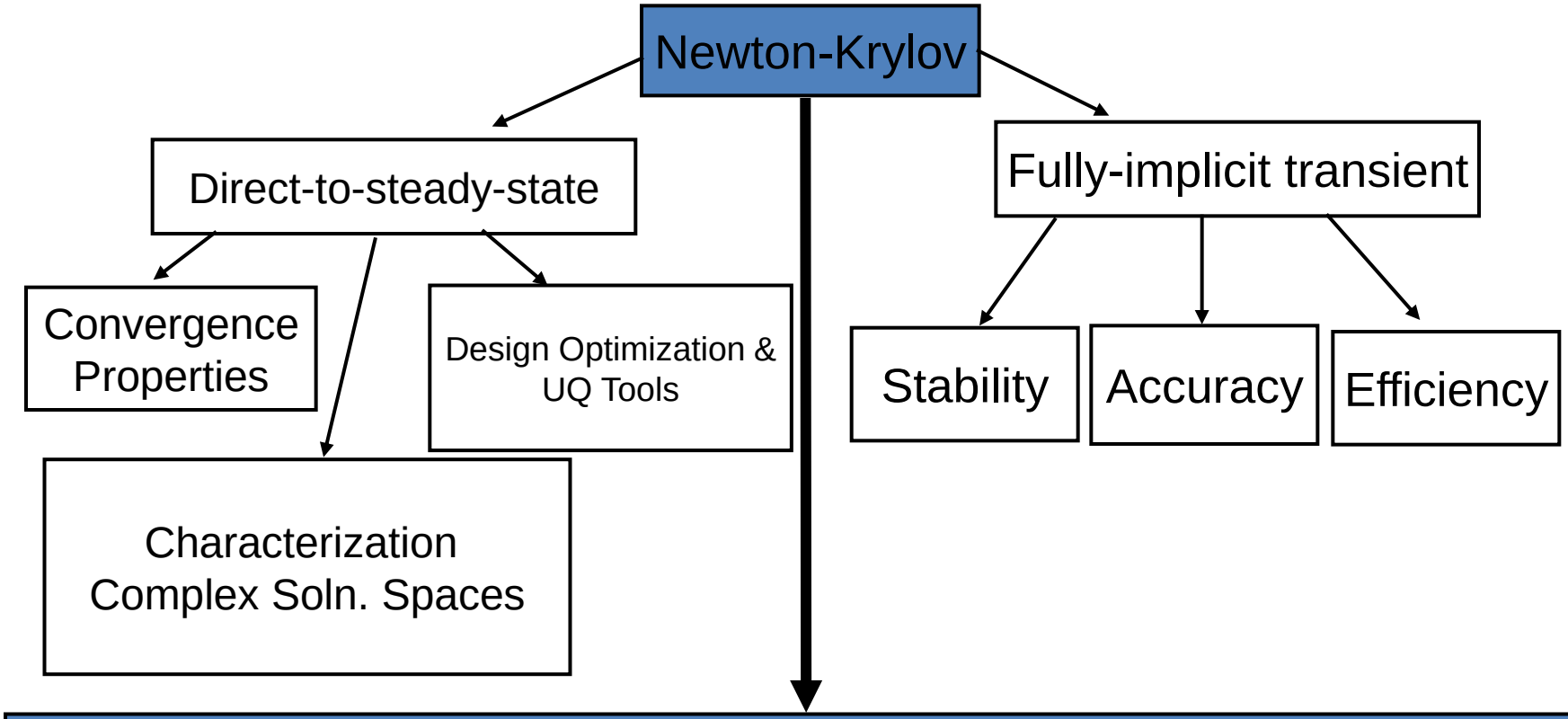
Robustness, Convergence and Flexibility

- Strongly coupled multi-physics often requires a strongly coupled nonlinear solver
- Quadratic convergence near solutions
- Enables bifurcation, stability, optimization, error estimation, sensitivity and UQ

Stability, Accuracy and Efficiency

- Stable (stiff systems)
- High order methods
- Variable order techniques
- Local and global error control possible
- Can be stable, accurate and efficient run at the dynamical time-scale of interest in multiple-time-scale systems (See e.g. Knoll et. al., Brown & Woodward., Chacon and Knoll, S. and Ober, S. and Ropp)

Why Newton-Krylov Methods?

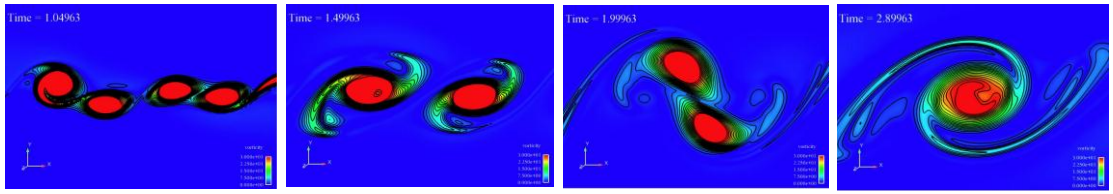


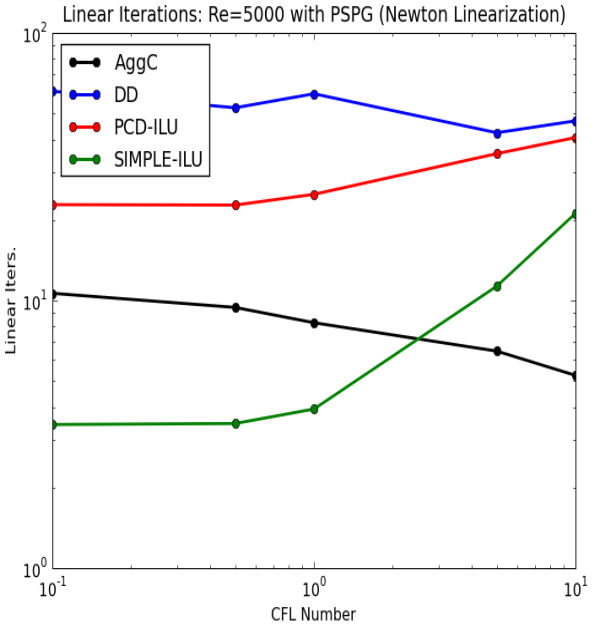
Very Large Problems -> Parallel Iterative Solution of Sub-problems

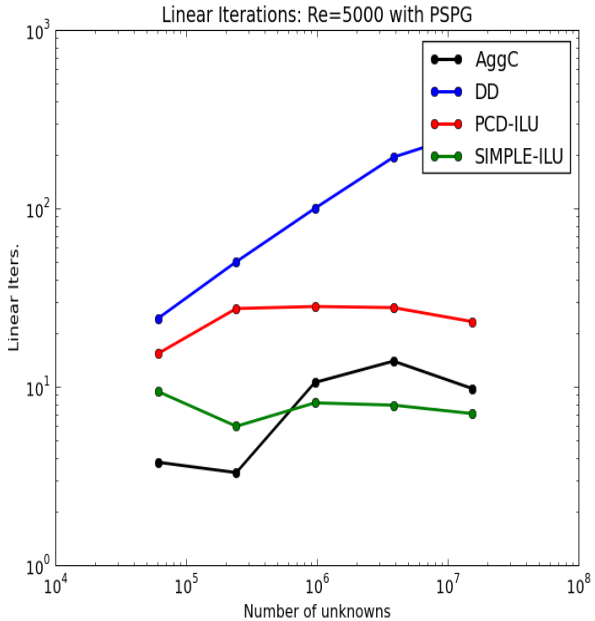
Krylov Methods - Robust, Scalable and Efficient Parallel Preconditioners

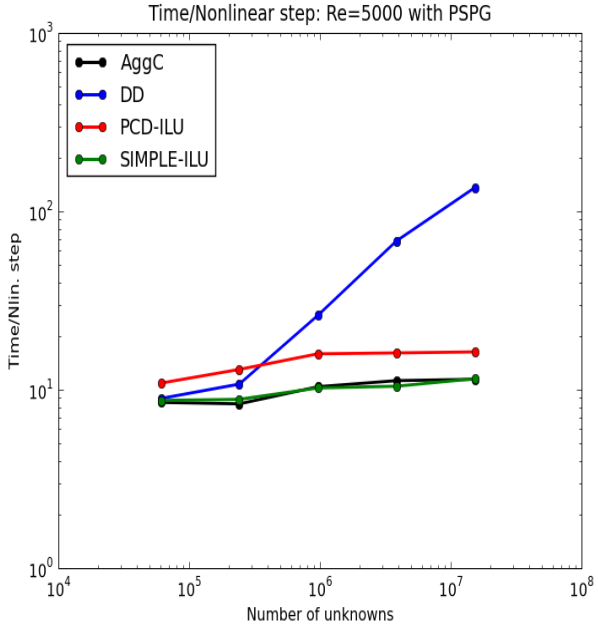
- Approximate Block Factorizations
- Physics-based Preconditioners
- Multi-level solvers for systems and scalar equations

Transient Kelvin-Helmholtz







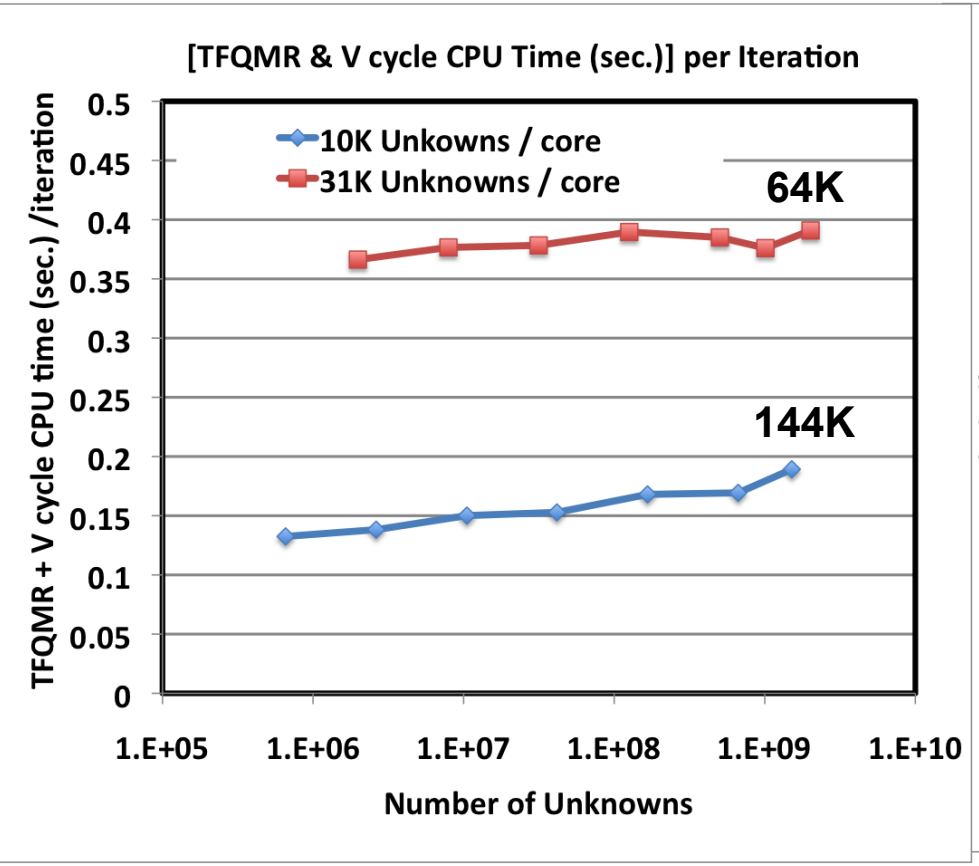


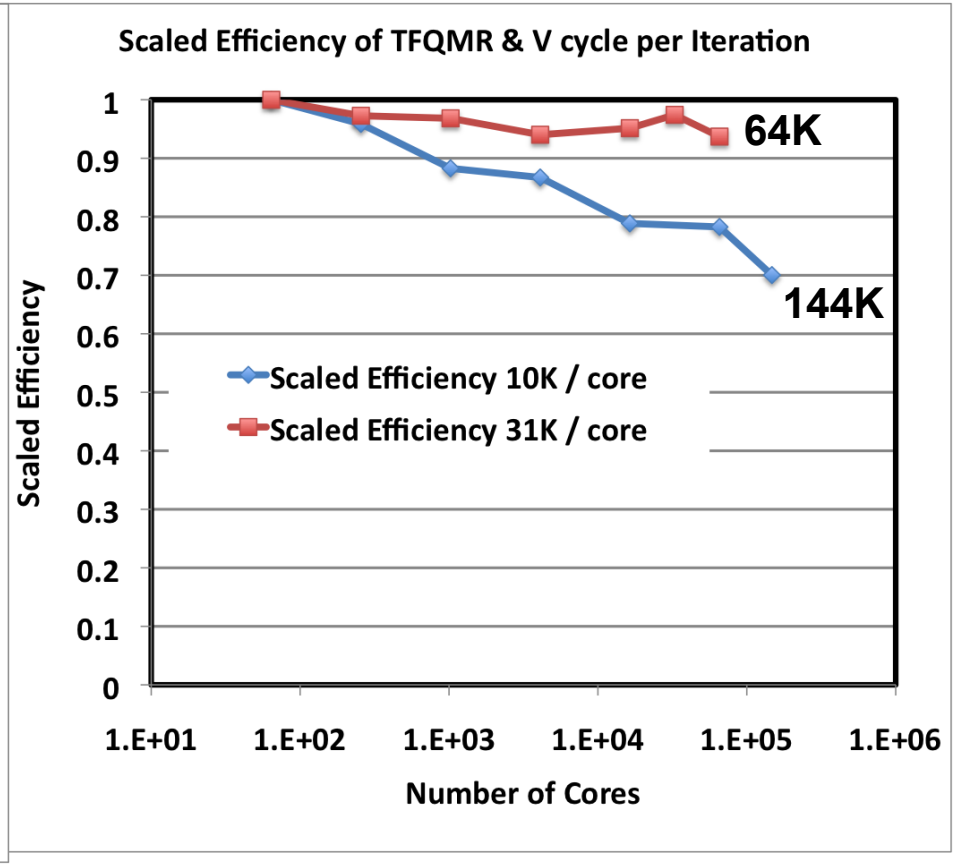
Kelvin Helmholtz: Re=5000, Weak scaling at CFL=2.5

- Run on 1 to 256cores
- Pressure - PSPG, Velocity - SUPG (residual and Jacobian)

1. SIMPLEC strongly dependent on CFL
2. Block methods scale as well as AggC and do not require non-zero C matrix

Weak Scaling Uncoupled Aggregation Scheme: Time/iteration on BlueGene/P (Drift – Diffusion BJT: P. Lin)

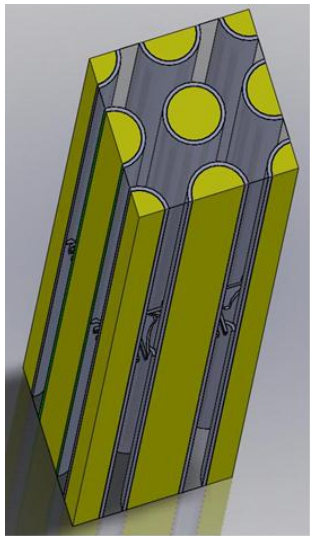


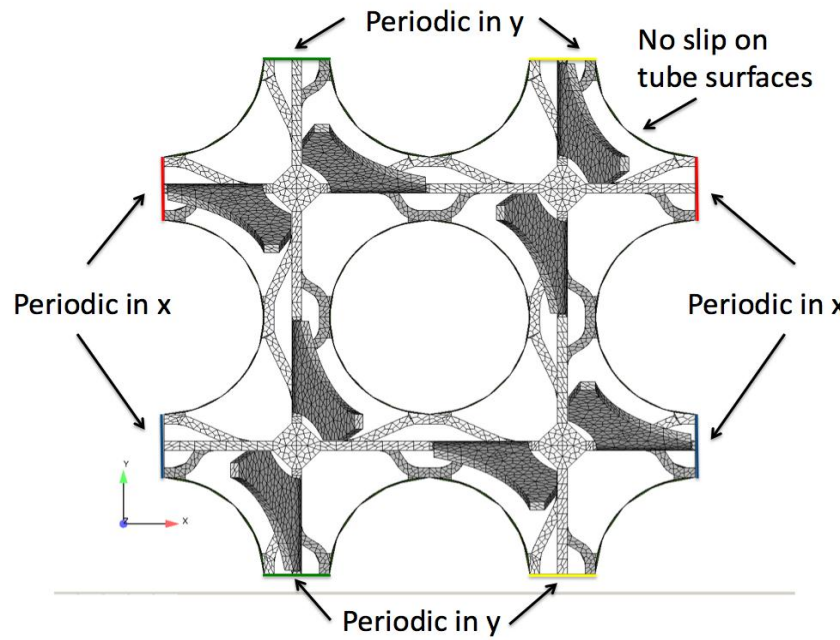


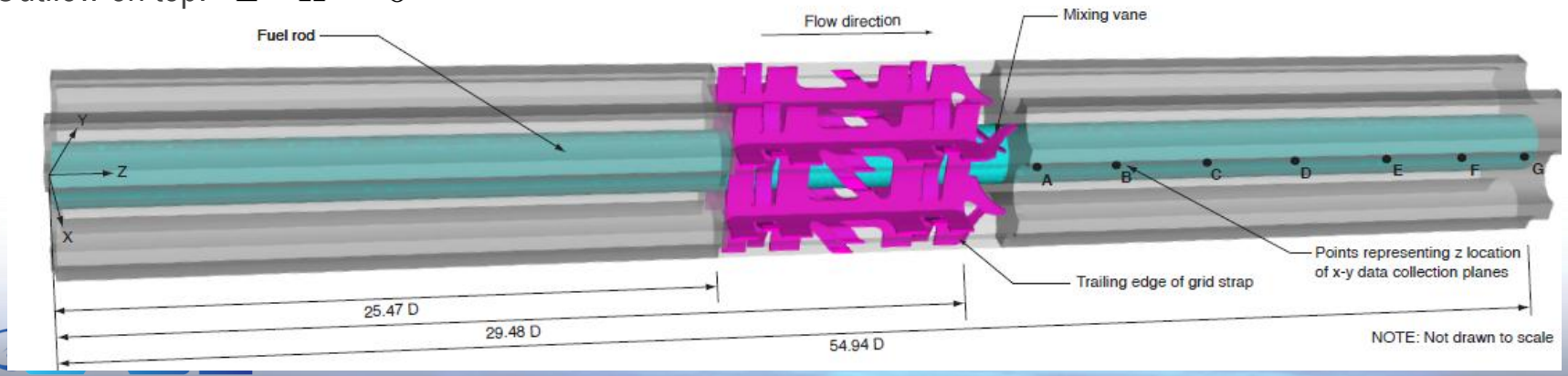
- TFQMR: used to look at time/iteration of multilevel preconditioners.
- W-cyc time/iteration not doing well due to significant increase in work on coarse levels (not shown)
- Good scaled efficiency for large-scale problems on larger core counts for 31K Unknowns / core

Problem Description (3x3 Rod Bundle)

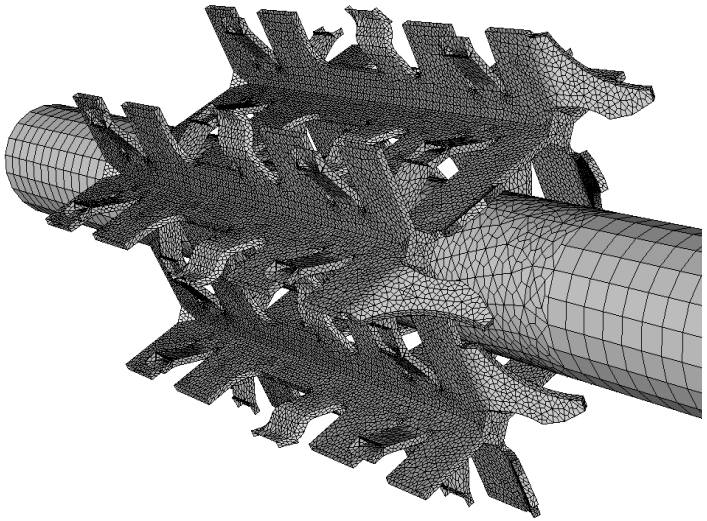
- Isothermal
- Fluid: Water
  - T: 394K
  - Viscosity: 2.32×10^{-4} Pa sec
  - Density: 924 kg/m^3
- Re ~ 2x10^5
- Periodic BCs on sides
- No slip (v=0) on rods
- Inflow on bottom
  - Specified inlet now at 5 m/sec
  - Periodic possible w/set pressure drop
- Outflow on top: $\mathbf{T} \cdot \mathbf{n} = 0$

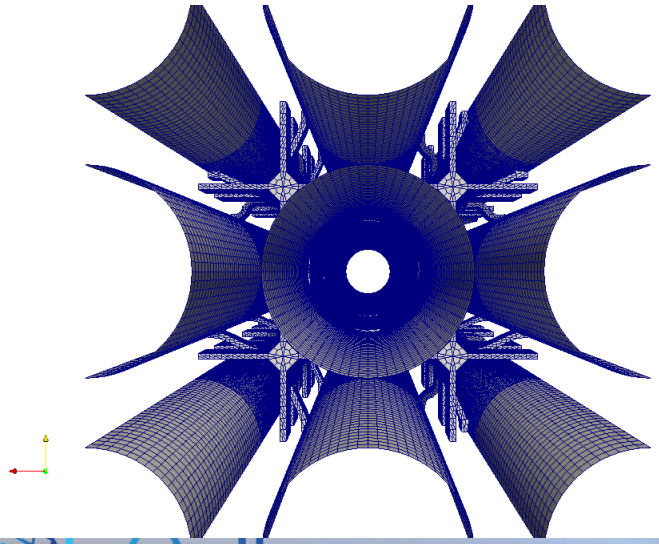


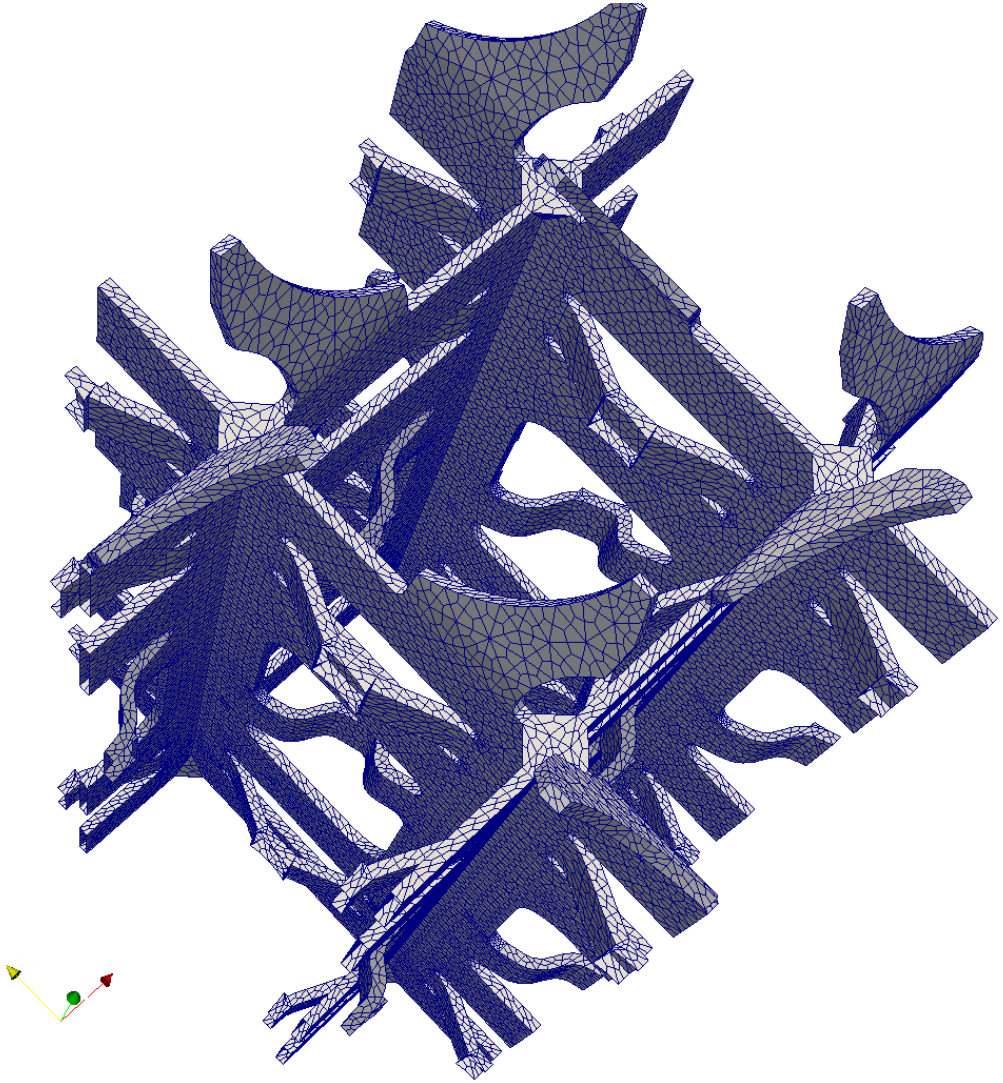




Geometry
(Hexahedral Elements)



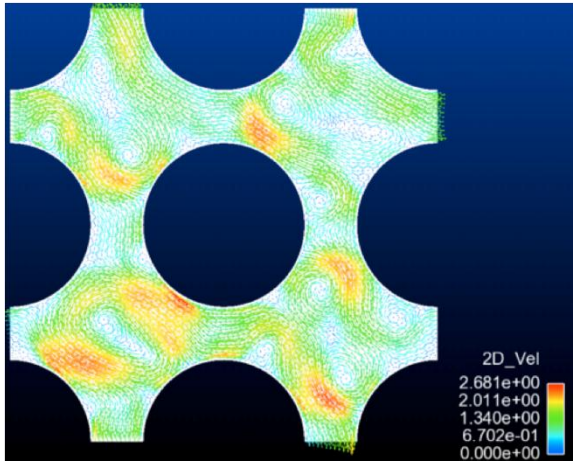


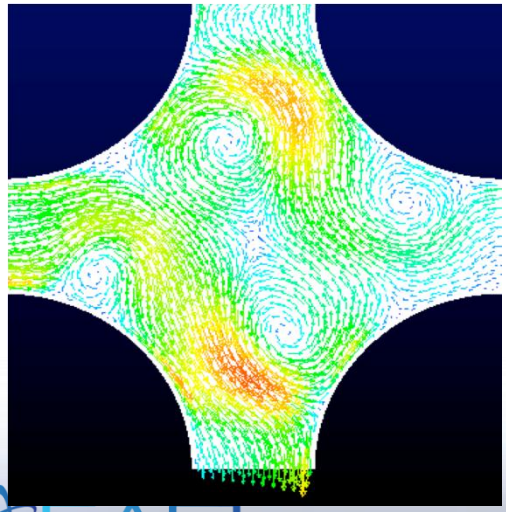


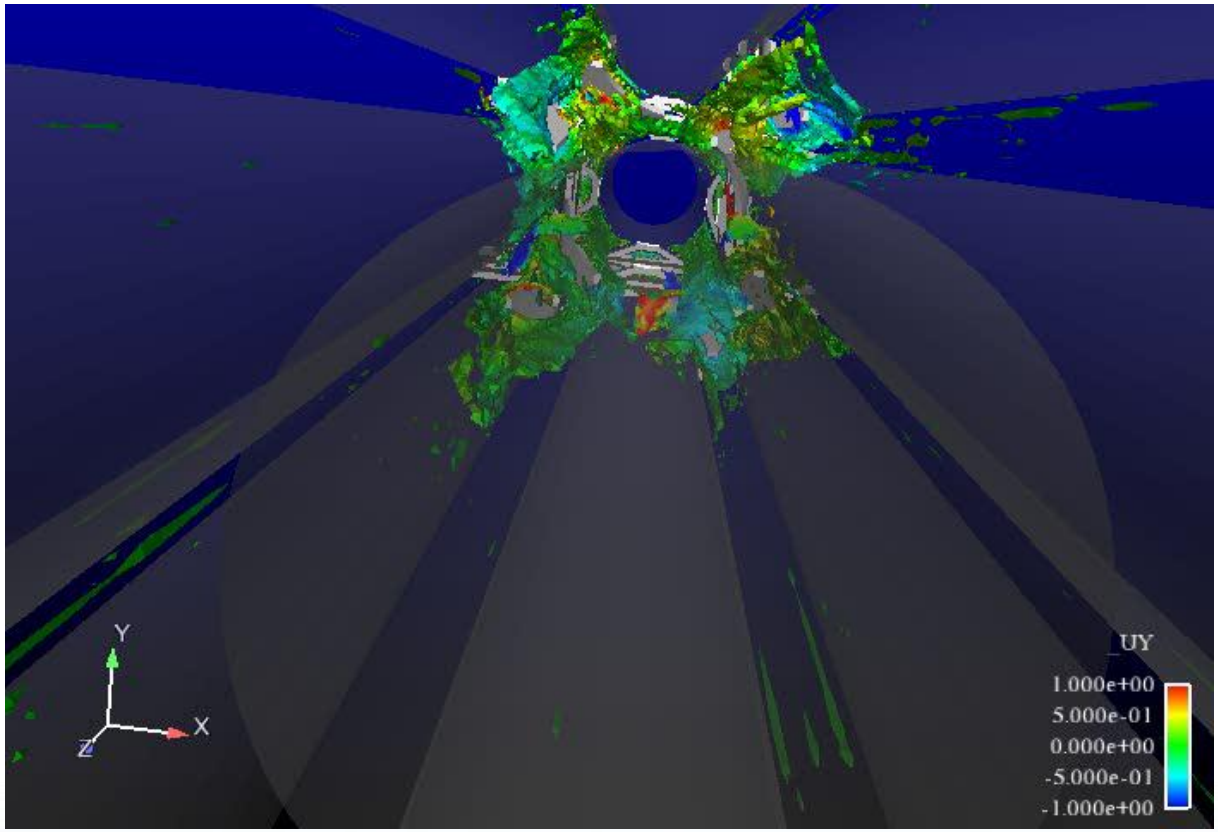
Solution Profiles

- Sandia Redsky platform, 256-1024 cores
- Oak Ridge Jaguar platform, 1200-9600 cores (demo)
- 2nd stabilized FE methods with 2nd order BDF2 time integration

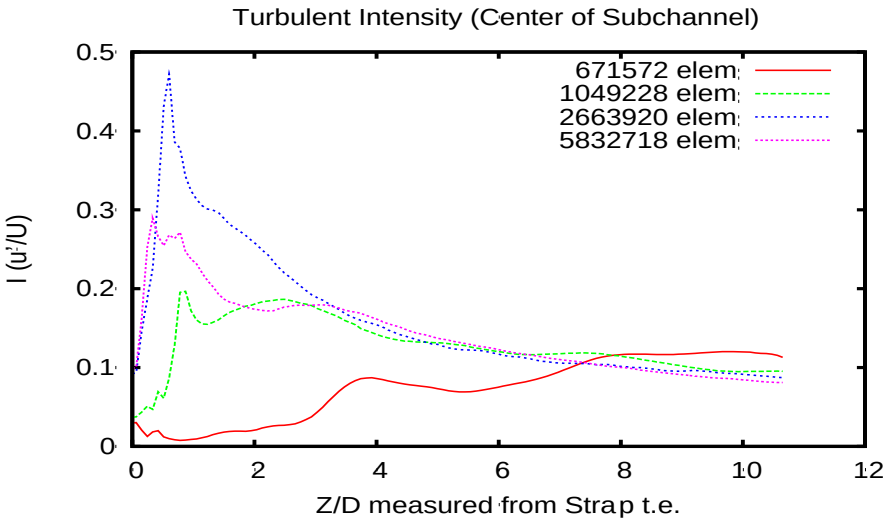
Qualitative correspondence to WEC results – [Elmahdi et al.]

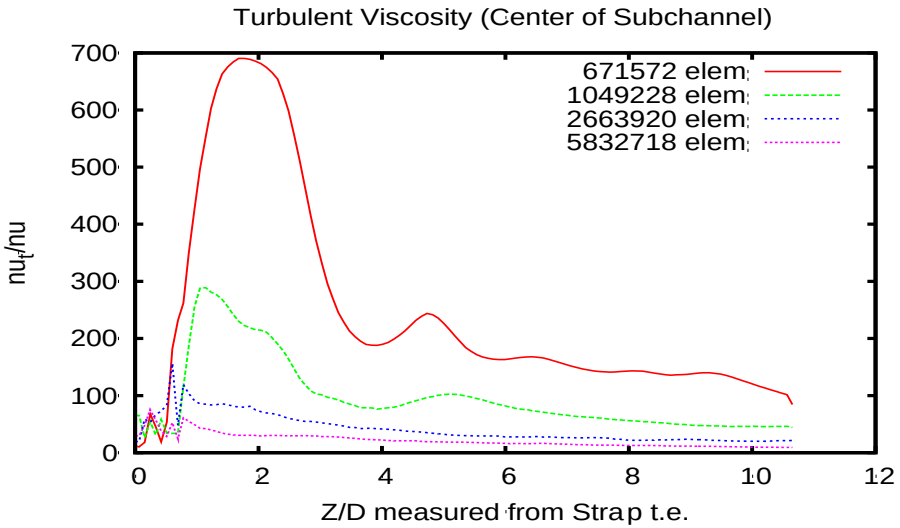






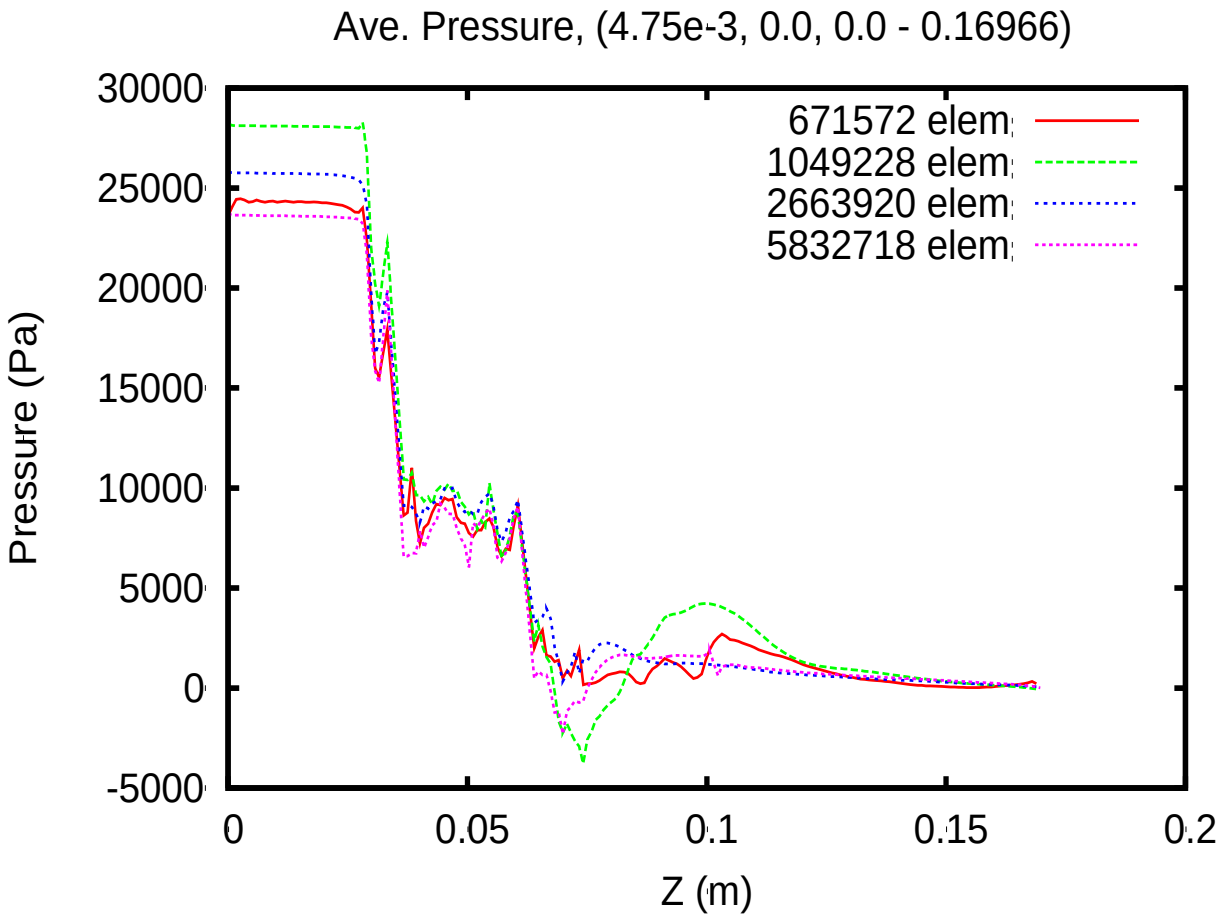
Time-averaged Turbulence Characteristics





- **672K mesh is inadequate to resolve pressure behavior.**
  - **Non-monotonic behavior in turbulent intensity:**
    - **Converges 3 diameters downstream as turbulence subsides**
    - **Suggests under-resolution of mesh near spacer grid**
- **Qualitative Turbulence intensity comparison to Benhamadouche et al. 2009 (slightly different conditions):**
  - **At 3 diameters downstream, Drekar: 18%, Ben.: 11%**
  - **At 10 diameters downstream, Drekar: 10%, Ben.: 8.5%**
- **Monotonic decrease in amount of eddy-viscosity with refined mesh shows correct behavior (reduced contribution of sub-grid model).**

Time Averaged Pressure Profiles Across Spacer Grid

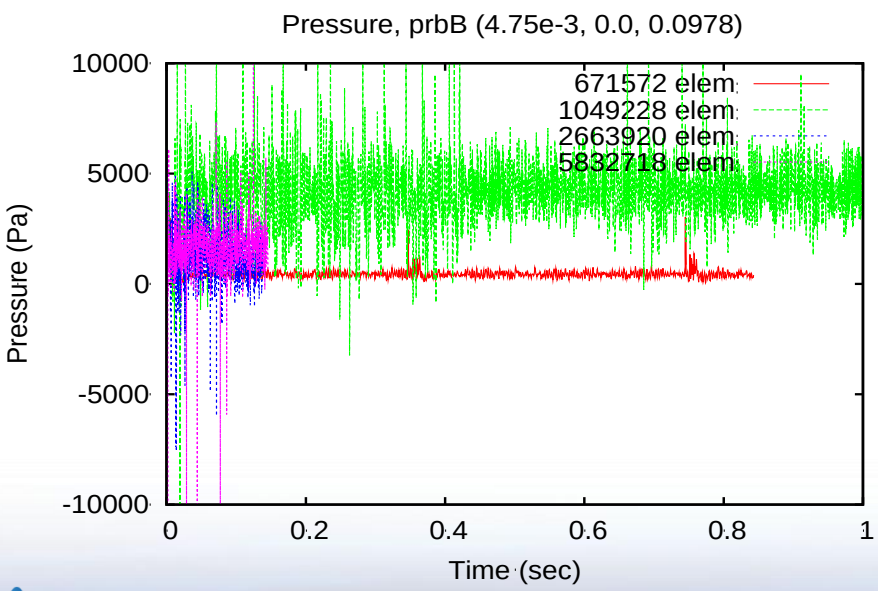


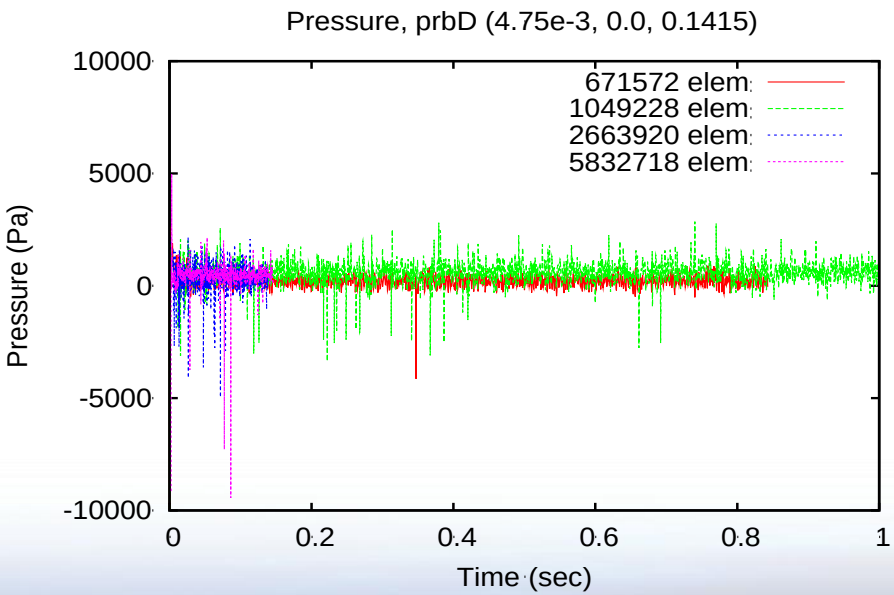
Mesh	Mean Pressure Drop (Pa)
677K	23,400
1M	26,780
3M	23,800
6M	22,042

- 3 finer meshes show signs of convergence
- Reasonable order-of-convergence for preliminary coarse study
- Preliminary Collaborative VUQ study (w/B. Rider) $\Delta P = a + bh^c = 17.42 + 163.7h^{1.234}$

Transient Pressure Profiles

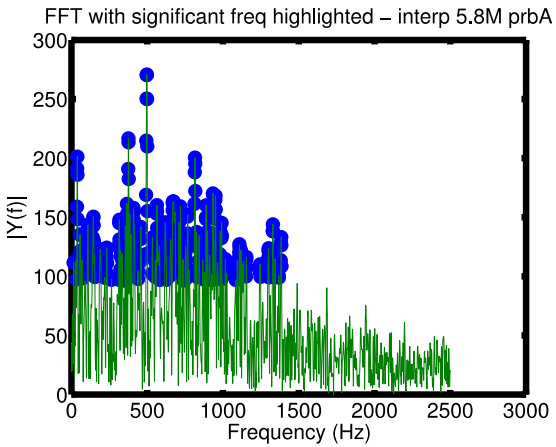
Mesh	# of Elements	Simulated Time (sec.)	Flow through times	Δt	CFL ave. (section1/section3)	Y+ ave.
672K (Red)	671,572	0.88	26	5.0×10^{-5}	9.6/1.3	26
1M (Green)	1,049,288	1.11	33	5.0×10^{-5}	11.1/2.9	19
3M (Blue)	2,663,920	0.2	6	2.0×10^{-5}	5.9/2.1	16
6M (Purple)	5,832,718	0.32	9	2.0×10^{-5}	7.9/2.2	13

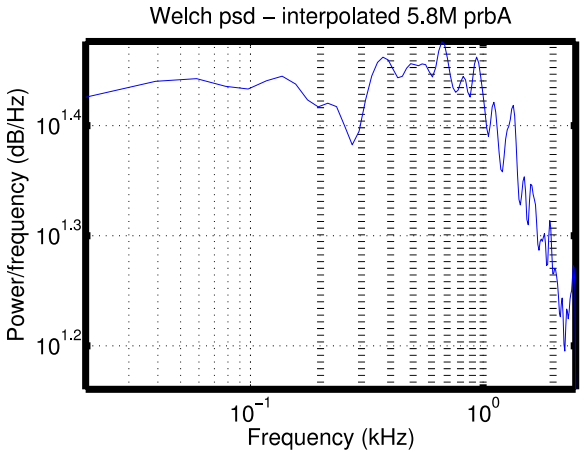




Initial Results: SNL Drekar FE CFD Capability

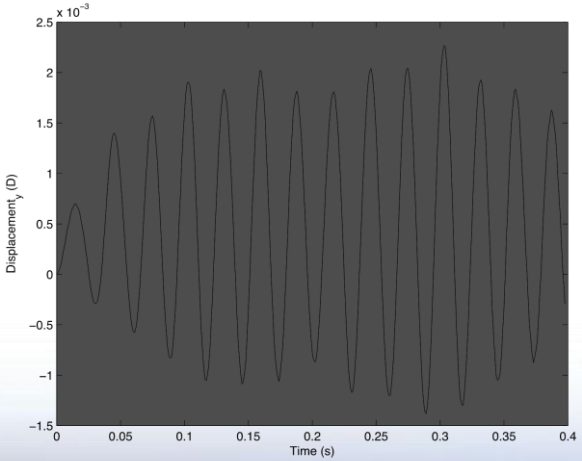
- **Analysis of LES Pressure Field (FFT & PSD)**

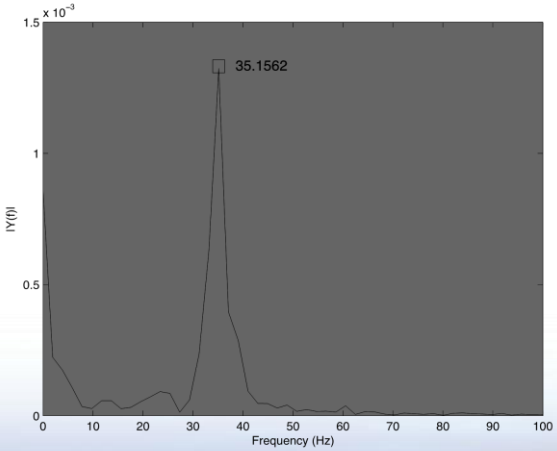




- **Demo of LES Forcing of Structural Vibration (Sierra/Presto). Solid Zircaloy Rod**

Displacement of rod in y-direction from LES forcing





FFT of vibrational response of rod

Next Steps

- Detailed Investigation of temporal and spatial order of accuracy/verification with turbulence on 3x3 model (coordinated with VRI-GTRF & VUQ)
- Demonstrate CFD – Neutronics coupling using Drekar, Denovo and VERA/LIME (coordinated with VRI)
- Demonstrate large-scale parallel conjugate CFD and heat transfer studies
- Additional physics model development (LES/RANS, multiphase-flow models, etc…)
- Carry out optimization and scaling studies on Jaguar (currently run on up to 9600 cores for short time 3x3 simulation)
- Optimize solvers (physics-based preconditioners, one-step Newton, modified Newton, semi-implicit, etc.)
- Demo 5x5, 17x17 sub-assemblies, and ¼ core reactor simulations
- Release Code to CASL Partnership

Extra Slides

Globalized Inexact Newton Method (incomplete citations)

Globalized Newton Methods

- backtracking (line-search)
- trust region (dogleg)
- Dennis-Schnabel 1983

Inexact Newton Methods

- local theory
  Dembo-Eisenstat-Steihaug 1982
- global theory
  Eisenstat-Walker 1994, Brown-Saad 1994
- Linkage to linear solver criteria
  Dembo-Eisenstat-Steihaug 1982, Eisenstat-Walker 1996

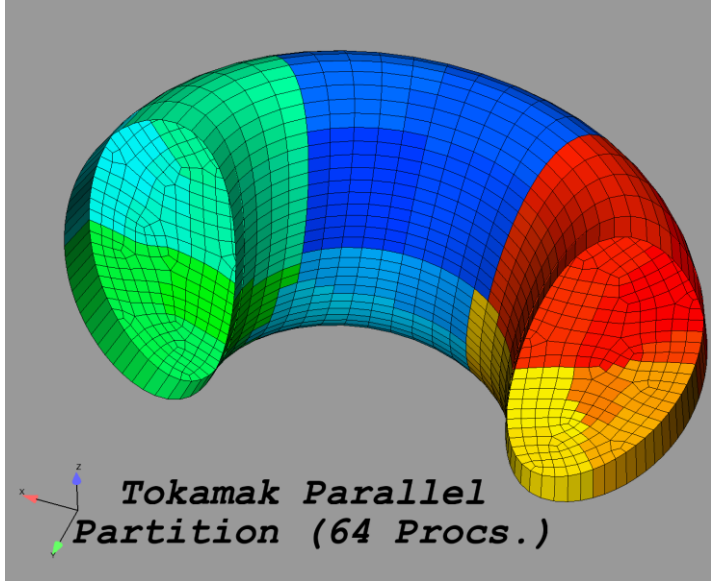
Globalized Newton-Krylov Methods

- Use Krylov solvers to determine inexact Newton steps
- Backtracking and trust region-like globalizations- Robustness
  Brown-Saad 1990, S-Tuminaro-Walker 1997, Pernice-Walker 1998
- Review: Jacobian free Newton methods: Keyes-Knoll, 2003
- Guide: Algorithms and implementation: T. Kelley 2003
- Review: Globalization techniques for Newton-Krylov:
  Pawlowski-S-Simonis-Walker, 2007
- General algorithms and software
  - NKSOL (later KINSOL), Brown-Saad 1990
  - NITSOL, Pernice-Walker 1998
  - PETSc, Balay-Gropp-Curfman McInnes-Smith 2001
  - NOX (Trilinos Solver Framework), Pawlowski-Kolda-Hooper 2002

Preconditioning

Three variants of preconditioning

1. Domain Decomposition (Trilinos/Aztec & IFPack)
   - ILU(k) Factorization on each processor (with overlap)
   - High parallel efficiency, non-optimal algorithmic scalability



2. Multilevel methods: ML Package (Tuminaro, Sala, Hu, Siefert, Gee)

Fully-coupled Algebraic Multilevel methods
- Consistent set of DOF at each node (stabilized FE)
- Aggregation rate chosen to fix coarse grid size
- Jacobi, GS, ILU(k) as smoothers
- Can provide optimal algorithmic scalability

Aggregation based Multigrid:
- Vanek, Mandel, Brezina, 1996
- Vanek, Brezina, Mandel, 2001
- Sala, Formaggia, 2001

3. Approximate Block Factorization / Physics-based (Teko package)
   - Applies to mixed interpolation (FE) or staggered (FV) discretization approaches
   - Applied to systems where AMG is difficult or might fail
   - Can provide optimal algorithmic scalability

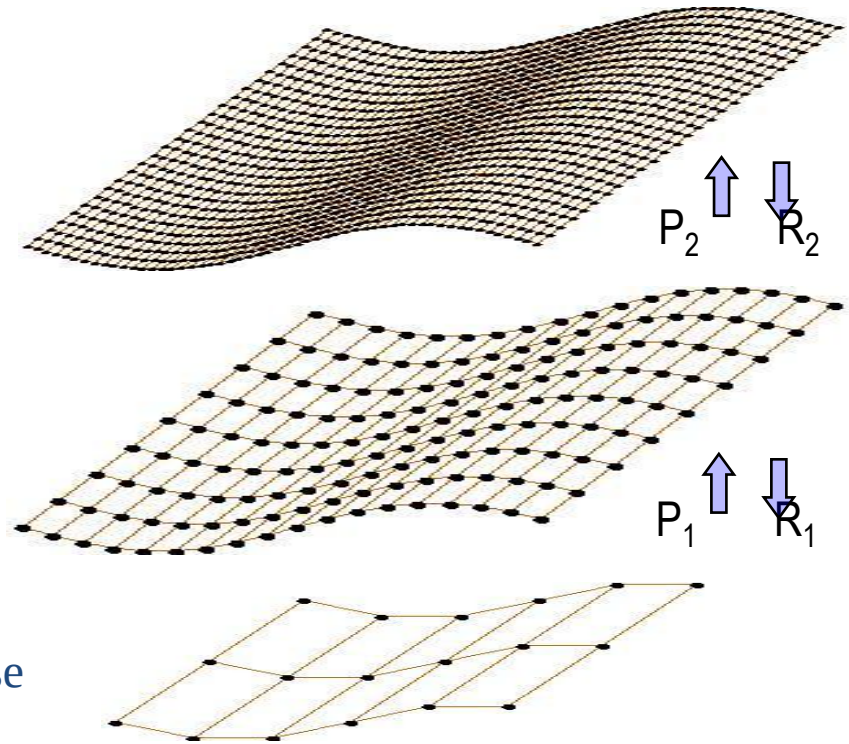
What is Multigrid ?

Modified from
ML Team slides

Solve $A_3 u_3 = f_3$

Basic idea:

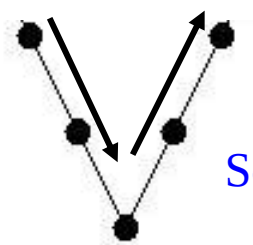
- Develop coarse approximations on multiple levels (e.g discretize)
- Define prolongation P_i and restriction operator R_i (e.g. FE interpolation)
- Accelerate convergence via coarse iterations to efficiently propagate information across domain



Smooth $A_3 u_3 = f_3$. Set $f_2 = R_2 r_3$.

Smooth $A_2 u_2 = f_2$. Set $f_1 = R_1 r_2$.

Solve $A_1 u_1 = f_1$ directly.



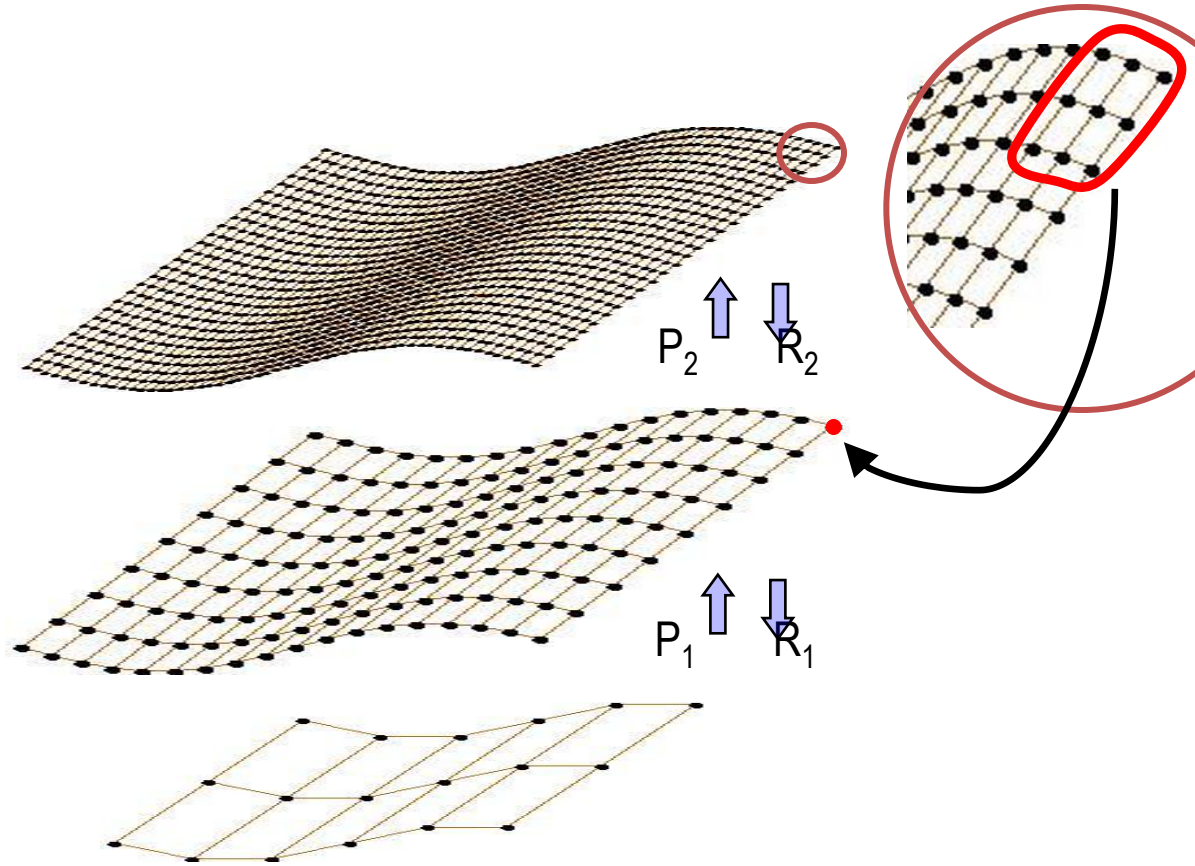
Set $u_3 = u_3 + P_2 u_2$. Smooth $A_3 u_3 = f_3$.

Set $u_2 = u_2 + P_1 u_1$. Smooth $A_2 u_2 = f_2$.

Algebraic What is Multigrid ?

Solve $A_3 u_3 = f_3$

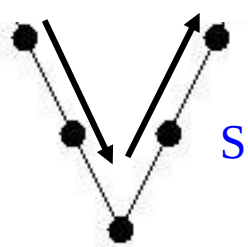
- Construct graph from sparsity pattern of A_{i+1} and partition graph
- Determine P_i & R_i sparsity pattern
- Determine P_i & R_i's coefs (e.g. accurately transfer null space with action of P)
- Project: $A_i = R_i A_{i+1} P_i$ to compute coarse operators



Smooth $A_3 u_3 = f_3$. Set $f_2 = R_2 r_3$.

Smooth $A_2 u_2 = f_2$. Set $f_1 = R_1 r_2$.

Solve $A_1 u_1 = f_1$ directly.



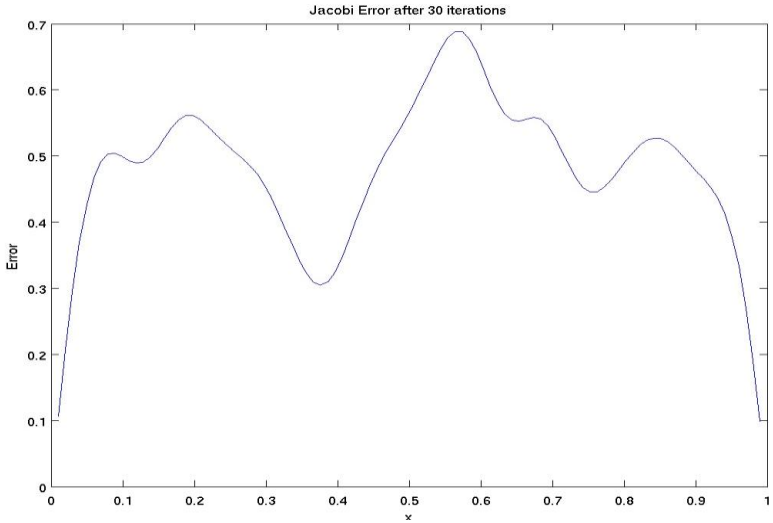
Set $u_3 = u_3 + P_2 u_2$. Smooth $A_3 u_3 = f_3$.

Set $u_2 = u_2 + P_1 u_1$. Smooth $A_2 u_2 = f_2$.

How does it work?

Smoothing and coarse correction complementary!

- Error is smoothed and reduced with increasing Jacobi iterations



Brief Overview of Block Preconditioning Methods for Navier-Stokes: (A Taxonomy based on Approximate Block Factorizations, JCP – 2008)

Discrete N-S	Exact LDU Factorization	Approx. LDU
$\begin{pmatrix} F & B^T \\ \hat{B} & -C \end{pmatrix} \begin{pmatrix} \Delta \mathbf{u}_k \\ \Delta p_k \end{pmatrix} = \begin{pmatrix} \mathbf{g}_u^k \\ g_p^k \end{pmatrix}$	$\begin{pmatrix} I & 0 \\ \hat{B}F^{-1} & I \end{pmatrix} \begin{pmatrix} F & 0 \\ 0 & -S \end{pmatrix} \begin{pmatrix} I & F^{-1}B^T \\ 0 & I \end{pmatrix}$ $S = C + \hat{B}F^{-1}B^T$	$\begin{bmatrix} I & 0 \\ \hat{B}H_1 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & -\hat{S} \end{bmatrix} \begin{bmatrix} I & H_2B^T \\ 0 & I \end{bmatrix}$

Precond. Type	H_1	H_2	$\hat{S}$	References
Pres. Proj; 1st Term Nuemann Series	$\mathbf{F}^{-1}$	$(\Delta \mathbf{t} \mathbf{I})^{-1}$	$\mathbf{C} + \Delta \mathbf{t} \hat{\mathbf{B}} \mathbf{B}^{\mathbf{T}}$	Chorin(1967);Temam (1969); Perot (1993): Quateroni et. al. (2000) as solvers
SIMPLEC	$\mathbf{F}^{-1}$	$(\mathrm{diag}(\sum \lvert \mathbf{F} \rvert))^{-1}$	$\mathbf{C} + \hat{\mathbf{B}}(\mathrm{diag}(\sum \lvert \mathbf{F} \rvert))^{-1}\mathbf{B}^{\mathbf{T}}$	Patankar et. al. (1980) as solvers; Pernice and Tocci (2001) smothers/MG
Pressure Convection / Diffusion	0	$\mathbf{F}^{-1}$	$\mathbf{A_p F_p^{-1}}$	Kay, Loghin, Wathan, Silvester, Elman (1999 - 2006); Elman, Howle, S., Shuttleworth, Tuminaro (2003,2008)

Now use AMG type methods on sub-problems.

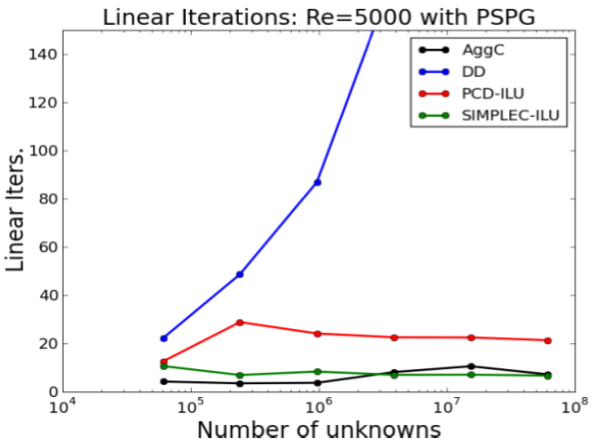
Momentum transient convection-diffusion: $F\Delta \mathbf{u} = \mathbf{r_u}$

Pressure – Poisson type: $-\hat{S}\Delta p = \mathbf{r}_p$

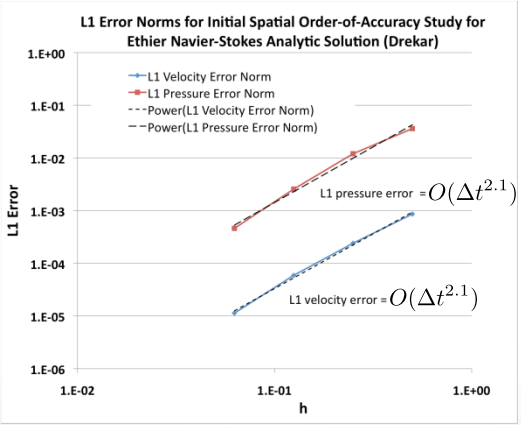
Background: SNL Drekar FE CFD Capability

- Drekar::CFD: Stabilized unstructured FEM CFD. Fully-coupled implicit using scalable physics-based and algebraic multilevel solvers

- Adapt ***scalable*** and higher-order accurate Computational Fluid Dynamics (CFD) simulators
- Goal is to integrate a ***predictive CFD capability*** that scales on leadership class hardware (O(100,000) cores) with rigorous verification and uncertainty quantification.



Parallel Scaling for Kelvin Helmholtz CFD iteration counts vs. No. of unknowns



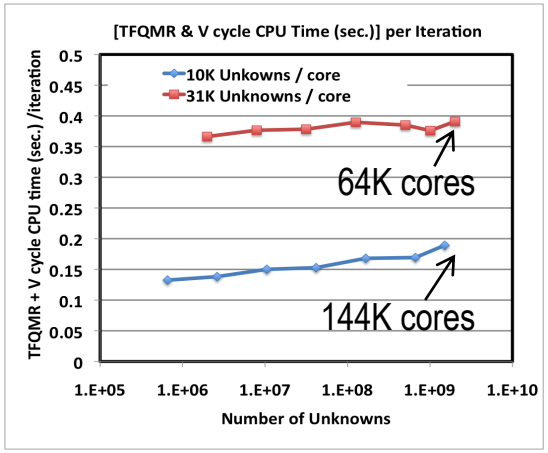
Initial Drekar 2D vortex-shedding frequencies

Method	Experimental Data	Salsa Data	Drekar Data
Re=60	.136 ± .006	0.132	.134 ± .004
Re=100	.164 ± .005	0.163	.163 ± .005
Re=200	.185 ± .007	0.189	.189 ± .004
Re=400	.205 ± .005		.209 ± .005
Re=600	.210 ± .006	0.218	.218 ± .006
Re=1000	.212 ± .006		.222 ± .007
Re=5000	.212 ± .006		.220 ± .010

Initial VUQ Demo Study: Re = 1000

Spatial Order-of-accuracy: $O(\Delta x^{1.9})$

Temporal Order-of-accuracy: $O(\Delta t^{1.6})$

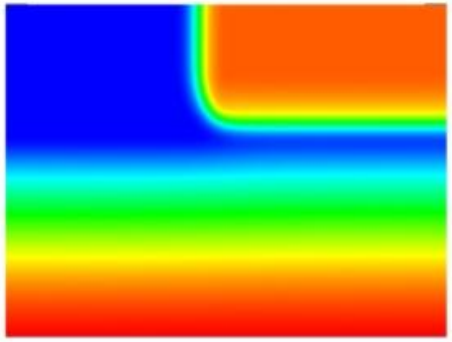


AMG V-cycle CPU time vs. No. of unknowns (Drift-Diff. sys. P. Lin)

Scaling of Jacobian Assembly Times

- Large-scale semiconductor device simulations on IBM Blue Gene platform
- **Generic programming (via AD tools) is applied at the element level, not globally.**
- **Weak scaling to 65k cores and two billion DOF: Jacobian evaluation via AD scales!**
- **Using all four cores per node with MPI process on each core.**

cores	DOF	Jacobian time
256	7.93m	52.19
1024	31.5m	52.28
4096	126m	52.09
8192	253m	52.82
16384	504m	52.74
32768	1.01b	52.96
65536	2.01b	52.94



Governing Equations
(Unsteady Single-phase, Isothermal, Incompressible Flow)

- Navier-Stokes with spatially filtered LES

<u>Momentum</u>

$$R_{\mathbf{u}} = \frac{\partial(\bar{\rho}\bar{\mathbf{u}})}{\partial t} + \nabla \cdot (\bar{\rho}\bar{\mathbf{u}} \otimes \bar{\mathbf{u}} - \mathbf{T})$$

over bar denotes spatial filtering in LES

<u>Continuity</u>

$$R_p = \frac{\partial \bar{\rho}}{\partial t} + \bar{\rho}\nabla \cdot \bar{\mathbf{v}}$$

$$\mathbf{T} = -\bar{P}\mathbf{I} + \mu_{eff}(\nabla\bar{\mathbf{u}} + \nabla\bar{\mathbf{u}}^T)$$

$$\mu_{eff} = \mu + \mu_t$$ (molecular and eddy viscosity)

- Eddy viscosity models unresolved turbulent fluctuations

Turbulence Closure Model

- Wall Adapting Local Eddy-viscosity model (WALE)
  - Nicoud, F. and Ducros, F., “Subgrid-Scale Stress Modelling on the Square of the Velocity Gradient Tensor,” Flow Turbulence and Combustion, Vol. 62, 1999, pp. 183-200.
- Modified Smagorinsky eddy-viscosity model
  - Filter width is based on the square of the deviatoric stress tensor
  - Requires only "local data" to construct.
  - Recovers the proper near-wall scaling for the eddy viscosity so that it inherently decays to zero as the wall is approached without using a dynamic procedure or wall model
- Future work will extend to full VMS-LES models
  - T.J.R. Hughes, L. Mazzei, K.E. Jansen, Large eddy simulation and the variational multiscale method, Comput. Vis. Sci. Vol. 3, 2000, pp. 47-59.

$$\mu_t = \bar{\rho}\nu_t$$

$$\nu_t = (C_w\Delta)^2 \frac{\left(\bar{\mathbf{S}}^d_{ij}\bar{\mathbf{S}}^d_{ij}\right)^{3/2}}{\left(\bar{\mathbf{S}}_{ij}\bar{\mathbf{S}}_{ij}\right)^{5/2} + \left(\bar{\mathbf{S}}^d_{ij}\bar{\mathbf{S}}^d_{ij}\right)^{5/4}}$$

$$\bar{\mathbf{S}}_{ij} = \frac{1}{2}\left(\frac{\partial\bar{\mathbf{u}}_i}{\partial\mathbf{x}_j} + \frac{\partial\bar{\mathbf{u}}_j}{\partial\mathbf{x}_i}\right)$$

$$\bar{\Omega}_{ij} = \frac{1}{2}\left(\frac{\partial\bar{\mathbf{u}}_i}{\partial\mathbf{x}_j} - \frac{\partial\bar{\mathbf{u}}_j}{\partial\mathbf{x}_i}\right)$$

$$\bar{\mathbf{S}}^d_{ij} = \bar{\mathbf{S}}_{ik}\bar{\mathbf{S}}_{kj} + \bar{\Omega}_{ik}\bar{\Omega}_{kj} - \frac{1}{3}\delta_{ij}\left[\bar{\mathbf{S}}_{mn}\bar{\mathbf{S}}_{mn} + \bar{\Omega}_{mn}\bar{\Omega}_{mn}\right]$$

Spatial Discretization

- Stabilized Galerkin Finite Element (2nd-8th order)
- PSPG allows equal order interpolation of velocity and pressure
- SUPG operator to limit oscillations in high grid Re flows.

$$\mathbf{F_{m}}_i = \underbrace{\int_\Omega \Phi R_{u_i} d\Omega}_{\text{Galerkin}} + \underbrace{\sum_e \int_{\Omega_e} \tau_m \left(\bar{\mathbf{u}} \cdot \nabla \Phi\right) R_{u_i} d\Omega}_{\text{SUPG}}$$

$$\mathbf{F_p} = \underbrace{\int_\Omega \Phi R_p d\Omega}_{\text{Galerkin}} + \underbrace{\sum_e \int_{\Omega_e} \bar{\rho} \tau_m \left(\nabla \Phi \cdot R_u\right) d\Omega}_{\text{PSPG}}$$

Mathematical /Computational Motivation: Achieving Scalable Predictive Simulations of Complex Highly Nonlinear Multi-physics PDE Systems

What are multi-physics systems? (A multiple-time-scale perspective)

These systems are characterized by a myriad of complex, interacting, nonlinear multiple time- and length-scale physical mechanisms.

These mechanisms:

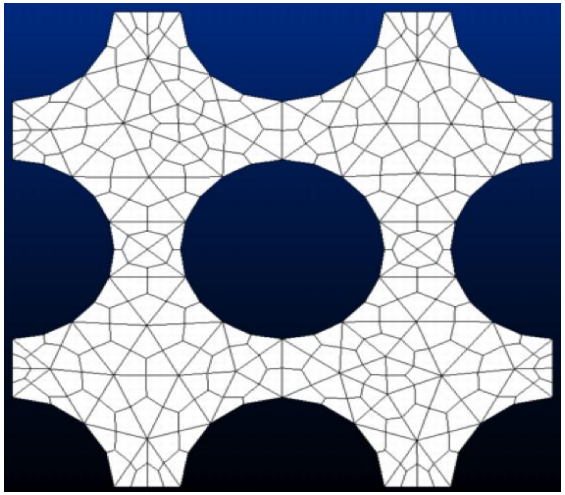
• can be dominated by one, or a few processes, that drive a short dynamical time-scale consistent with these dominating modes,
• consist of a set of widely separated time-scales that produce a stiff system response, • nearly balance to evolve a solution on a dynamical time-scale that is long relative to the component time scales, • or balance to produce steady-state behavior.

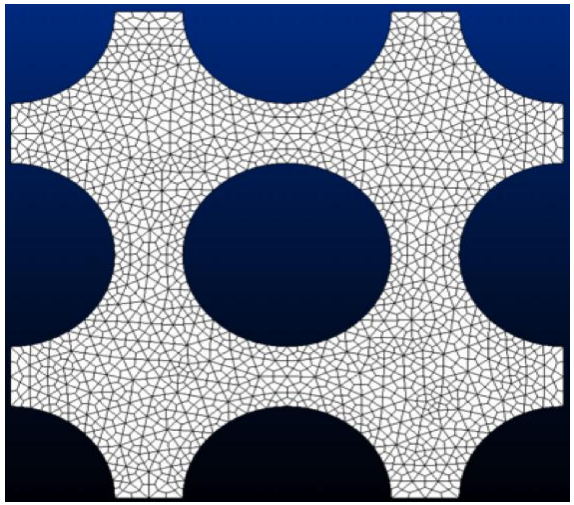
e.g. Nuclear Fission / Fusion Reactors; Conventional /Alternate Energy Systems; High Energy Density Physics; Electro-magnetic Launch; Astrophysics; etc ….

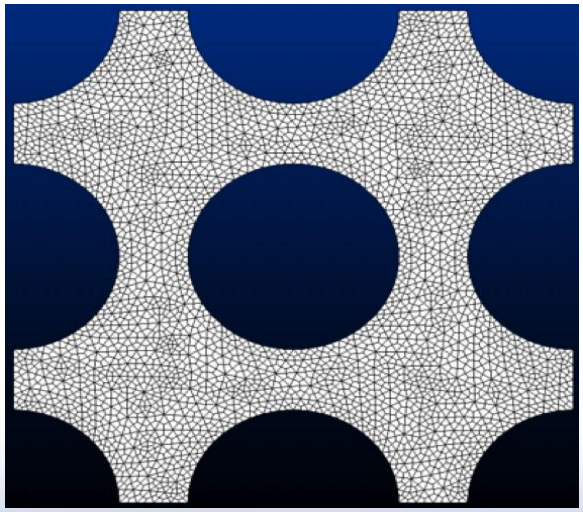
Our approach is to develop:

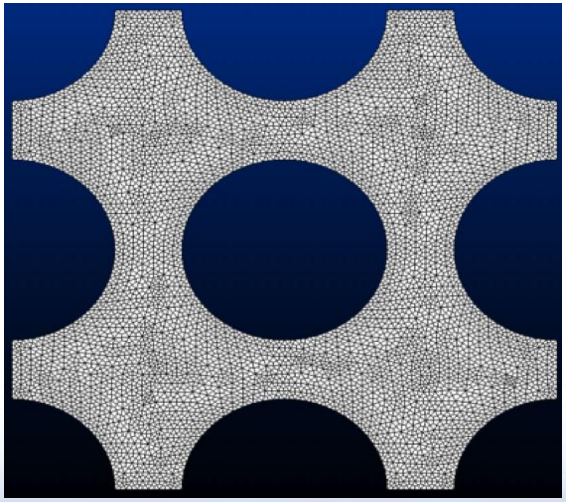
- stable and higher-order accurate implicit formulations and discretizations,
- enabled by robust, scalable and efficient prec. for fully-coupled Newton-Krylov methods,
- with the goal to integrate sensitivity and error-estimation to enable UQ capabilities.

Mesh Refinement for Verification
(Hex mesh ranging from 700K to 6M elements)









INL Multi-Scaled Modeling Approach for Multiphase Flows

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We are interested in multiphase flow models which can serve as a *multi-scale* foundation (single algorithm) to solve multiphase mixtures with multiple velocities as well as solve interface problems while dealing with metastable compressible fluids.

Many applications with gas-liquid interfaces involve a very wide range of Mach number variation, from 10^{-3} to 100 with respect to the mixture sound speed. It is important to build methods free of Mach number restrictions – *all Mach number schemes*.

While most computational approaches consider the two fluids as incompressible, some important efforts have addressed high Mach number flows with material interfaces. A few works deal with incompressible liquid and compressible gas. In many applications gas compressibility is of paramount importance, for example when phase change occurs. In flashing flows, compressibility of all phases is important (liquid phase change occurs due to expansion effects). When liquid-gas mixtures appear, sound propagates with the mixture sound speed which has a non-monotonic variation with respect to volume fraction resulting in very low sound speed, of the order of a few meters per second. Consequently, it is not difficult to reach hypersonic flow conditions with liquid-gas mixtures. Thus it is important to build numerical methods that are able to deal with incompressible flows, transonic flows, <u>and</u> even hypersonic flows in the presence of wave dynamics and material interfaces.

In the past, flows in the low Mach regime have been addressed more by methods developed for incompressible flows. This poses difficulties when wave dynamics are present because incompressible flow solvers are typically not conservative in the compressible flow sense. Also, these methods have difficulties in the presence of large density ratios.

Some Existing Two-Phase Models

Broad review of the available literature on two-phase flows shows that most models can generally be placed into two basic classes of models. Without regard to whether or not multiple velocities are allowed, the first class includes those for which pressure and temperature equilibrium is enforced, while the second class includes those for which the temperatures of the phases are not required to be in equilibrium.

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Pressure and temperature equilibrium models

At least four models belong to this category, which we detail with increasing complexity.

1. The mixture Euler equations with a cubic equation of state such as the *van der Waals* EOS. Loss of hyperbolicity occurs in the spinodal region with such models. Specifically, the squared sound speed may become negative and wave propagation has no physical meaning.

2. Alternatively, the mixture Euler equations can be used with a tabular EOS, or a combination of pure phase equations of state with the assumption of pressure, temperature, and chemical potential (Gibb's energy) equilibrium in the two-phase region. Such models are frequently referred to as *homogeneous equilibrium models*. These models restore the loss of hyperbolicity of the first model type; however, because the mixture is assumed to evolve under thermodynamic equilibrium, there are no metastable states. The model is unable to handle material interfaces separating a liquid and a non-condensable gas. It, therefore, exhibits a restricted domain of application.

3. Sometimes the mixture Euler equations are augmented with a mass fraction evolution equation with a relaxation term (typically referred to in the literature as *homogeneous relaxation models*). Isothermal closure is assumed, which is not compatible with interface conditions (equal pressure and normal velocities, but not temperatures). Therefore it is unable to solve interfaces between a liquid and a non-condensable gas (e.g. water/air). Also, the mass relaxation term can be problematic.

4. The second-gradient theory (Cahn and Hilliard 1958) can be utilized to derive a model in which the interface is described as a diffuse zone with a capillary length scale that has to be resolved. Because this zone length is usually on the order of 1 nanometer, a significant restriction is incurred. As a practical matter, e.g. at the scale of an individual bubble, the interface has to be artificially thickened (Jamet et al. 2001), but such a procedure has important consequences for the model's ability to deal with metastable states. Moreover, interfaces with large density gradients are very difficult to solve, as also are interfaces separating non-condensable fluids such as water and air.

Temperature non-equilibrium models

There are at least four models which belong to this category, which we detail.

1. The traditional, and most common, temperature non-equilibrium model is the ***six-equation model*** obtained with averaging methods (see e.g. Ishii 1975; Delhaye and

Boure 1982). It involves a balance equation of mass, momentum, and energy for each phase or fluid. With this model the mixture evolves with a velocity for each phase, however it has only a single pressure which presents with two options:

a. One of the phases is considered as incompressible with the mixture pressure being that of the gas phase. This does not permit the representation of rarefaction waves in the liquid phase, the presence of which is mandatory in flashing flows.
b. Both phases are compressible, with the closure achieved with assumption of equilibrium pressure.

With either of these options, the six-equation model has a restricted domain of hyperbolicity. This results in a restricted validity, primarily to problems where transient wave propagation is not important. Furthermore, this model cannot solve interface problems, e.g. water/air.

2. The ***seven equation model*** (Baer and Nunziato 1986), and its variants, are unconditionally hyperbolic and are able to deal with a wide range of applications. As with the six equation model, it is composed of a mass, momentum, and energy balance equations for each phase, but with appropriate changes to accommodate physics of separate pressures for each phase. In addition, the model is augmented with an evolution equation for the volume fraction of one of the constituents (for two phases). The seven equation model has been demonstrated to have the ability to solve interface problems as well as fluid mixtures with several velocities, and it has been extended to deal with metastable states, producing, for example (LeMetayer, Massoni, and Saurel 2005), the correct wave propagation dynamics of evaporation fronts in flashing systems.

3. The ***five equation model*** involves a single pressure and velocity and is composed of two mass balance equations, one mixture momentum equation, one mixture energy equation, and a volume fraction evolution equation. It is obtained as an asymptotic reduction of the seven equation model in the mechanical equilibrium limit, and it is unconditionally hyperbolic. It has the ability to solve interface problems with compressible fluids and has been extended to include capillary and viscous effects. Unlike second-gradient type approaches, the interface has no capillary length scale, it can deal with large phasic density ratios, and it employs two pure-phase equations of state instead of a single one. This model can handle metastable states and maintain thermal non-equilibrium. The temperature and chemical potential differences can be used to derive a relaxation model able to deal with phase change fronts – the model can compute evaporation fronts by solving their internal structure (Saurel, Petitpas and

Abgrall 2008) and can dynamically create interfaces were none are initially present (Saurel, Petitpas and Berry 2009).

4. The ***four equation model*** can be viewed either as an extension of the three equation homogeneous equilibrium model or from the non-equilibrium five equation model with a restriction of one of the phases to be always at saturation condition (Berry *in preparation*). This model is a variant of the homogeneous relaxation model. It has a mass balance equation for each phase, one mixture momentum equation, and one mixture energy equation. It can be written in conservative form and is unconditionally hyperbolic (Grillenberger 1976). With this limited non-equilibrium model, one phase has a fully independent thermodynamic state but the other phase is required to be at saturation conditions corresponding to the pressure of the fully independent phase. The saturated phase therefore has a restricted thermodynamic state with reduced dependency, e.g. density and temperature are each functions of pressure only. Therefore, the four equation model is unable to solve interfaces between a liquid and a non-condensable gas (e.g. water/air). Unlike the homogeneous equilibrium model, this model exhibits a continuity of sound speed as the fluid transitions from the single phase (fully independent state) to a two phase mixture.

Diffuse Interface Method (DIM)

Though usually considered as a drawback for a numerical scheme, numerical diffusion is an indispensible feature for capturing discontinuities. In modern computational fluid dynamics (CFD) it facilitates the easy computation of shock and contact discontinuities (as well as predicts their formation) in gas dynamic applications. In the context of flows with interfaces, a numerical scheme that possesses a similar simplicity is sought: a scheme that works on a fixed grid, that allows arbitrarily large interface deformations, that deals easily with inflow and outflow boundary conditions, that uses the same numerical scheme for all computational cells (multiphase mixtures, shocks, interfaces, rarefaction waves, contact surfaces) and that also predicts interface formation. These last *multi-scale* features are most important. Simplicity follows as a result of the scheme and model generality. Interface formation is a very important feature in flashing (cavitation) and boiling flow modeling.

In (Saurel and Abgrall 1986) and (Saurel and LeMetayer 2001) a method based on the compressible multiphase flow equations was proposed for the computation of interfaces. This method is efficient for computing material interfaces separating miscible and non-miscible fluids. It accomplishes this by treating all waves present (interfaces, shocks, expansion waves, contacts) as a numerically diffused zone. The same flow model can be used to solve cavitating and boiling flows. Methods based on the multiphase flow equations, and which consider the

liquid-gas interfaces as diffuse numerical zones (Diffuse Interface Method or DIM, e.g. 5-equation model), have shown several unique advantages:

- The interfaces are handled routinely, i.e. at any point in the flow.
- Allow very general equations of state to be used.
- Are conservative for the mixture, guaranteeing correct wave dynamics in pure fluid zones.
- Able to consider compressibility of all phases.
- Able to account for noncondensible gases; e.g. in many practical situations, the liquid is not a pure liquid and some noncondesible gases are present which strongly influence the mixture compressibility (bubbles expand before reaching the saturation pressure) and modify the mass transfer dynamics.
- Able to model metastable mixtures.
- Able to handle coexisting bubbly flows and flashing (cavitating pockets); e.g. cavitation pockets followed by bubbly flow.
- Allows supercritical states.
- Able to dynamically create (not initially present) and follow interfaces.
- Allows interfaces to separate non-pure fluids (mixtures) on each side of the interface; so called “permeable interface”.
- Able to propagate subsonic and supersonic fronts in multi-dimensions without solving their internal structure.
- Provide accurate internal energies and temperatures at the interface.
- Able to include capillarity (surface tension) effects in a thermodynamically consistent manner; i.e. capillary effects are modeled with the help of a capillary tensor that enters the momentum and energy fluxes conservatively.
- Allows mass transfer in a thermodynamically consistent manner. The entropy is preserved; when phase transition occurs the model guarantees mixture entropy production. It allows mass transfer times to be of the same order as the flow characteristic time.
- Perhaps most importantly, able to model non-equilibrium two-phase flows (bubbles, droplets, annular flows, etc.) as well as flows with interfaces using the same basic equations; even simultaneously.
- Able to deal with a wide range of applications.

This approach obviously has some drawbacks:

- The interfaces can be diffused too much, especially when dealing with long time evolutions. But this is exactly the same drawback as contact discontinuity smearing in

gas dynamic computations, and just as in modern shock capturing CFD methods, there are several ways to reduce its effects: mesh refinement, high-order discretizations, and other strategies. Recent efforts at front sharpening have also been reported.

- Non-conservative equations are present and numerical approximations of non-conservative terms poses difficulties in the presence of shocks.
- The construction of all Mach number methods for this kind of hyperbolic flow model is not an easy task, but efforts are ongoing.

Since the flow model is conservative with regard to the phases' mass equations, mixture momentum, and mixture energy, and because the system is hyperbolic methods developed from compressible flow dynamics should be more tractable. This choice is motivated by the importance of pressure waves present in many nuclear reactor applications as well as the huge density ratios at interfaces that are easier to handle with *"discontinuity capturing"* schemes. For nuclear applications, this is mandatory, as for example with:

- Liquid-gas flows in nozzles and injectors,
- High performance turbo pumps where flashing occurs,
- Flash vaporization.

It is emphasized that the success of this multiphase method relies on:

- Use of an unconditionally hyperbolic model for two-phase compressible mixtures.
- Accurate discretization of the non-conservative terms and equations.
- Use of robust relaxation procedures to restore pressure and velocity interface conditions based on infinite relaxation parameters.

It is important to understand these underlying requirements for the multiphase models that serve as the foundation for this *multi-scale approach*. Traditionally the numerical modeling of two-phase flows utilizes the standard two-fluid model consisting of six governing equations corresponding to balance of mass, momentum, and total energy within each phase. One of the primary problems arising from use of this model, which relies on the single-pressure assumption, is their well known potential loss of hyperbolicity, even for simple sets of initial values. In addition, the maximum principle for the volume fraction does not necessarily hold in general even for smooth solutions of this model, except perhaps in some very special situations. Consequently, these models often contain some ad hoc modifications to the momentum equations (addition of special relative velocity drag, the numerical notion of upwinding, or the use of special fractional step techniques) which attempt to enlarge the hyperbolicity domain. Indeed, though the thought process is still alive and well today, the idea emerged a long time ago that even if the standard two-fluid model may lead in some cases to

an ill-posed initial value problem the negative consequences will never occur because rather course meshes with inherent upwinding behavior will guarantee enough stability to compensate the emerging instability of the PDE set. But with the advent of CFD methods capable of highly resolved details, this argument is spurious. Other researchers have emphasized that some (expected small) interfacial transfer terms in the momentum equation (namely $\beta \cdot \mathrm{grad}(\alpha_g)$) may become predominant in "dangerous" situations (Herard and Hurisse 2005). In reality this term only enlarges the domain of hyperbolicity (Valette and Jayanti 2003), but in such a way that it cannot recover the whole domain including all physically admissible states. Use of well known approximate Riemann solvers which underlie modern computational fluid dynamics requires modifications in order to account for possible entrance into "time-elliptic" regions (Herard and Hurisse 2009) – in brief, "not pretty". This begs the question of whether the lack of hyperbolicity has not been enforced by some failure in physical closure assumptions. The difficulty is closely tied to the assumption of local instantaneous pressure equilibrium. The blow-up of codes using this model may be quite easily postponed, for example, when using upwinding techniques and restricting their use to coarse meshes. Nonetheless, even when drag effects are accounted for, it may be easily checked that this inner stabilization of the latter schemes is no longer sufficient on very fine meshes.

There exists, however, a better alternative that enables the multi-scaled approach with which we began. Some time ago, (Ransom and Schofield 1976) suggested using a two-pressure model based on an eight-equation model. Subsequently, (Baer and Nunziato 1986) and (Nguyen 1981) adopted a similar approach. More recently, their model was extended by (Kapila et al. 1997) and (Gavrilyuk and Saurel 2002). Here the system is composed, for two phases, of seven partial differential equations, two for the mass, two for the momentum, and two for the energy of each fluid and one for the volume fraction (of the gas). In this model so called "interface pressure" and "interface velocity" terms appear; and several definitions for these terms have been given in the references mentioned. As pointed out by (Gallouet and Herard 2004) the closures for the interfacial velocity permits one to obtain a linearly degenerate field associated with the wave which initially separates two mixtures. They also show that the definition of the interfacial pressure is strongly related to the closure of the non-conservative terms; one particular definition enables the system to be complemented with a natural entropy inequality.

(Saurel and Abgrall 1999) and (Saurel and LeMetayer 2001) take basic ideas from the 7-equation model proposed by (Baer and Nunziato 1986) and introduced some slight modifications regarding closure relations and major modifications regarding relaxation parameters to construct a general model able to treat non-equilibrium two-phase flows as well as flows with interfaces. Introducing the notion of infinite relaxation parameters and instantaneous pressure and velocity equilibrium made possible the numerical treatment of

interface problems along with a wider range of applications (interfaces, flashing, and other multiphase systems). With this approach, each phase is considered compressible with its own pressure, temperature, density, and velocity. This guarantees hyperbolicity for all admissible states (i.e. physical states with positive volume fractions, positive mass fractions, and positive internal energies). Recently, reduced forms of this multiphase model have been constructed along with numerical implementations that posses similar features, but which are simpler for certain applications (Massoni et al. 2002), (Murrone and Guillard 2005), and (Saurel, Petitpas, and Berry 2009). This reduced model is also unconditionally hyperbolic.

Perhaps because of the bureaucratic inertia, many workers in the two-fluid community still feel reluctant using these new models. However, in a recent treatise on computational methods for multiphase flow (Prosperetti and Tryggvason 2007), the concluding chapter fairly reflects the current state of traditional multiphase flow modeling:

> "…uncertainties in the correct formulation of the equations and the modeling of source terms may ultimately have a bigger impact on the result than the particular numerical method adopted. Thus, rather than focusing on the numerics alone, it makes sense to try to balance the numerical effort with expected fidelity of the model."
>
> "The formulation of a satisfactory set of average-equations models emerges as the single highest priority in the modeling of complex multiphase flows."

This is the reason that we have embraced the rational *multi-scaled, compressible, unconditionally hyperbolic approach* described above. Moreover, a common framework based on relaxation schemes which unifies both approaches, and which inherits the mathematical properties of the two-pressure closures was espoused in (Herard and Hurisse 2005) and demonstrated in (Berry, Saurel, and LeMetayer 2010). We point out also that this relaxation method also provides a natural approach for coupling models of varying degree of simplification (reduced models).

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Multi-scaled, Two-phase Flow Modeling Directions for Light Water Nuclear Reactors

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August 2011

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Presentation Overview

- ✓ Multi-scaled, multiphase goal
- ✓ Construction of a general 2-phase model
  - Non-equilibrium thermodynamics of two phase non-miscible mixtures
  - Equilibria in two phase mixture
- ✓ Reduced "hyperbolic" models for various equilibrium situations, multiscale, and coupling
  - A hierarchy of "relaxed" or "reduced" models
  - Some examples
  - ✓DEM example
  - ✓DIM advantages and disadvantages for interface capturing
  - ✓INL direction

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Comutational Methods for Multiphase Flow

Edited by Andrea Propseretti and Grétar Tryggvason *(Chapter 11.6)* Cambridge 2007, 2009

- ✓ "…uncertainties in the correct formulation of the equations and the modeling of source terms may ultimately have a bigger impact on the result than the particular numerical method adopted. Thus, rather than focusing on the numerics alone, it makes sense to try to balance the numerical effort with expected fidelity of the model."
- ✓ "The formulation of a satisfactory set of average-equations models emerges as the single highest priority in the modeling of complex multiphase flows."

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Two-Phase Models

- ✓ No general agreement
- ✓ Large # of different models: homogeneous models, mixture models, two-fluid models, drift-flux models
- ✓ Number of variables, definition of the unknowns
- ✓ Number of equations
- ✓ Large # of different approximations
- ✓ Conservative, non-conservative, incompressible vs. compressible techniques
- ✓ Mach number variations of 0.001 to 100 with respect to mixture sound speed; high-speed vs. low-speed, all-speed

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Multiphase Modeling: *Traditional Approach*

- ✓ Most two-phase ***mixture*** algorithms:
  - Use an ill-posed model
  - Use 1st order numerics or less
  - Require at least one phase to be incompressible
- ✓ Most ***phase resolving*** algorithms:
  - Cannot treat interfaces separating pure media and mixtures
  - Cannot treat mass transfer
  - Cannot dynamically create interfaces
- ✓ Neither approach is ***multiscale***

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Modern, high-resolution numerical methods/CFD codes

-- divide the flow space into much finer computational cells.

Therefore they **cannot**:

- ✓ *Utilize traditional multiphase models which are mathematically **ill-posed***
- ✓ *Rely on traditional **"flow regime maps"** used in sub-channel thermal-hydraulic codes to evaluate the interface topology*

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Overarching Goal: Unified Formulation and Numerical Simulation Methodology

- Giving capability to *simultaneous* solve fluid dynamic *interface* problems as well as multiphase *mixtures* arising from:
  - ✓ Boiling
  - ✓ Flashing or Cavitation
  - ✓ Bubble collapse

  in both high- and low-speed (all-speed) LWR flows.
- Provide highly resolved details where necessary, simultaneously lesser resolved large scale vessel/component simulation.
- Using *well-posed, physically meaningful, consistent multi-scale models*:
  - ✓ Resolve interfaces for larger bubbles in DNS-like (direct numerical simulation) manner – ***single velocity***, ***single pressure***
  - ✓ Homogenize or average the two-phase flow field for smaller bubbles – ***two velocities***, ***two pressures***

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General, Averaged Balance Equations (7-eqn.) 1

- Mass

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \vec{u}_k = \Omega_k^{mass}$$

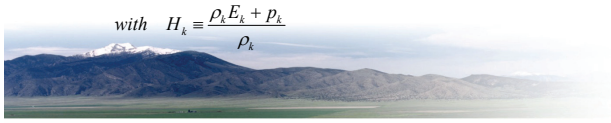
- Momentum

$$\frac{\partial \alpha_k \rho_k \vec{u}_k}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \vec{u}_k \otimes \vec{u}_k \right) + \nabla \alpha_k p_k = p_I \nabla \alpha_k + \vec{u}_I \Omega_k^{mass} + \lambda \left(\vec{u}_m - \vec{u}_k \right)$$

- Energy

$$\frac{\partial \alpha_k \rho_k E_k}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k \vec{u}_k H_k \right) = p_I \vec{u}_I \cdot \nabla \alpha_k + \Omega_k^{mass} E_I + \Omega_k^{energy}$$
$$+ \lambda \left(\vec{u}_m - \vec{u}_k \right) \cdot \vec{u}_I + \mu \left(p_k - p_m \right) p_I$$

$$with \quad H_k \equiv \frac{\rho_k E_k + p_k}{\rho_k}$$



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General, Averaged Balance Equations (7-eqn.)

- Volume Fraction Evolution

$$\frac{\partial \alpha_k}{\partial t} + u_I \cdot \nabla \alpha_k = \mu\left(p_k - p_m\right) + \frac{\Omega^{mass}}{\rho_I}$$

- Interfacial Velocity and Pressure *(for example)*

$$\vec{u}_I = \frac{\sum_{k=1,2} \alpha_k \rho_k \vec{u}_k}{\sum_{k=1,2} \alpha_k \rho_k} \quad \text{and} \quad p_I = \sum_{k=1,2} \alpha_k p_k$$

- Saturation Constraint and Equation of State

$$\alpha_1 + \alpha_2 = 1$$

$$p_k = \left(\gamma_k - 1\right)\rho_k\left(e_k - q_k\right) - \gamma_k p_{k\infty} \qquad \left(stiffened\ gas\right)$$

Summary

✓Two fluid system + volume fraction eq = hyperbolic system

✓This system evolves to a state characterized by

- Pressure equality
- Velocity equality
- Temperature equality
- Chemical potential equality

✓We can control the rate at which these various equilibrium states are reached.

Summary (cont.)

✓Deduce from this system, reduced systems characterized by instantaneous equilibrium (global or local) between

- Pressure *("classical" two-fluid model)*
- Pressure + velocity *(mechanical equilibrium)*
- Pressure + velocity + temperature
- Pressure + velocity + temperature + Gibb's energy

  (thermodynamic equilibrium)

Example: Assume pressure equilibrium -- "classical" two-fluid model

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \nabla \cdot \alpha_1 \rho_1 \vec{u}_1 = 0 \qquad \frac{\partial \alpha_2 \rho_2}{\partial t} + \nabla \cdot \alpha_2 \rho_2 \vec{u}_2 = 0$$

$$\frac{\partial \alpha_1 \rho_1 \vec{u}_1}{\partial t} + \nabla \cdot \left(\alpha_1 \rho_1 \vec{u}_1 \otimes \vec{u}_1\right) + \alpha_1 \nabla p = 0$$

$$\frac{\partial \alpha_2 \rho_2 \vec{u}_2}{\partial t} + \nabla \cdot \left(\alpha_2 \rho_2 \vec{u}_2 \otimes \vec{u}_2\right) + \alpha_2 \nabla p = 0$$

$$\frac{\partial \alpha_1 \rho_1 E_1}{\partial t} + \nabla \cdot \alpha_1 \left(\rho_1 E_1 + p\right) \vec{u}_1 = 0 \qquad \frac{\partial \alpha_2 \rho_2 E_2}{\partial t} + \nabla \cdot \alpha_2 \left(\rho_2 E_2 + p\right) \vec{u}_2 = 0$$

EOS: solve $p_1 = p_2 = p$ for the volume fraction – **Non-hyperbolic !**

- **ill-posed !**

Example: Assume pressure & velocity equilibrium -- 5-equation model (one-pressure, one-velocity)

Stewart-Wendroff 1984, Kapila et al. 1997, Murrone-Guillard 2005

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \nabla \cdot \alpha_1 \rho_1 \vec{u} = 0$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \nabla \cdot \alpha_2 \rho_2 \vec{u} = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} \right) + \nabla p = 0$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left(\rho E + p \right) \vec{u} = 0$$

$$\frac{\partial \alpha_2}{\partial t} + \vec{u} \cdot \nabla \alpha_2 = \alpha_1 \alpha_2 \frac{\rho_1 c_1^2 - \rho_2 c_2^2}{\sum_{k=1}^{2} \alpha_k \cdot \rho_k c_k^2} \nabla \cdot \vec{u}$$

Formally (from the 7-equation model),

- limit $\lambda, \mu \to \infty$,
- while μ / λ remains bounded

Hyperbolic system:

u-c, u+c gnl

u, u, u ld

Entropy satisfying

$$\frac{1}{\rho c_w^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}$$

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Example: Assume pressure, vel., temp., & chem. potential equilibrium – *Homogeneous Equilibrium Model* (HOM)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{u} = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} \right) + \nabla p = 0$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left(\rho E + p \right) \vec{u} = 0$$

Hyperbolic system:

u-c, u+c gnl

u ld

Entropy satisfying

EOS: solve $p_1 = p_2 = p, \quad T_1 = T_2 = T, \quad g_1 = g_2 = g$

$$\frac{1}{\rho c_{eq}^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2} + \left[\frac{\alpha_1 \rho_1}{C_{p,v}} \left(\frac{ds_1}{dp} \right)^2 + \frac{\alpha_2 \rho_2}{C_{p,l}} \left(\frac{ds_2}{dp} \right)^2 \right]$$

Obviously,

$$c_{eq} < c_w$$

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Brief summary:

Model	#eqs	complexity	hyperbolic	conservative	respect contact
total non-equilibrium	7	+++	yes	no	yes
pressure equilibrium	6	+++	no	no	?
pressure & velocity equilibrium	5	++	yes	no	yes
pressure, vel., temp., and chem. pot. equilibrium	3	+	yes	yes	yes

New homogenization method

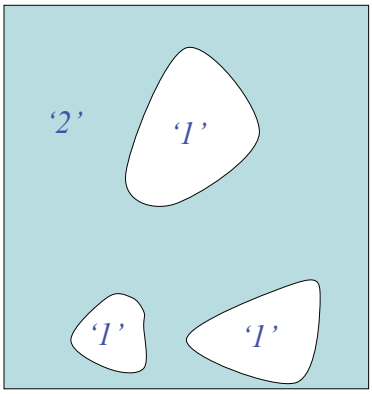
The *Discrete Equation Method* (DEM)

(see Berry, Saurel, LeMetayer, *NED* **240** (2010) 3797-3818 and references therein)

- ✓ Assume topology
- ✓ Discretize subcell
- ✓ Cell (volume) average

→ Accurately compute two-phase fluxes!
→ Solves non-conservative products!

Characteristic function



$$X_k = \begin{cases} 1 & \text{if the point belongs to the phase k} \\ 0 & \text{otherwise} \end{cases}$$

X_k obeys $\dfrac{\partial X_k}{\partial t} + \vec{u}_i.\vec{\nabla} X_k = 0$

$\vec{u}_i$ represents the local interface velocity

We multiply the Euler equations of each phase by this function and then take the average.

The method starts as conventional averaging methods

We start from : $\dfrac{\partial X_k}{\partial t} + u_i \dfrac{\partial X_k}{\partial x} = 0$

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0 \qquad \text{(Euler)}$$

The Euler equations are filtered by the characteristic function X_k and are then averaged (ensemble averaging):

$$\int_{Av} X_k \times Euler = 0$$

→ The seven-equation PDE model

Then during numerical resolution…

Two extra integral operators are used:

$$\int_{time} \int_{space} \underbrace{\int_{Av} X_k \times Euler}_{PDEs} = 0$$

The equations are thus averaged two times !!

Ensemble averages + cell averages

THE NOVELTY : Integrate directly interface problem solutions with cell averages ONLY

$$\int_{time} \int_{space} X_k \times Euler = 0$$

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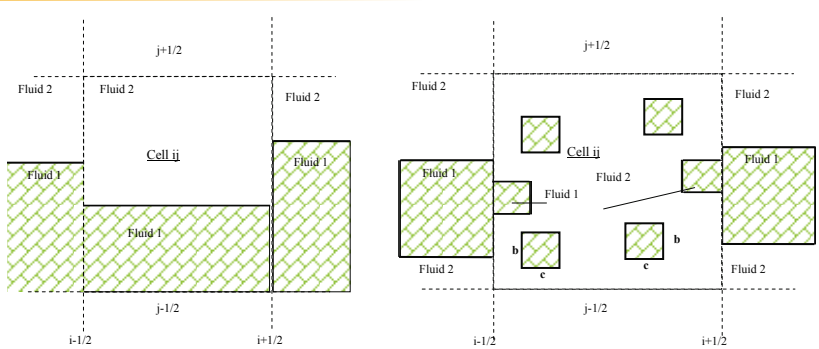
The input of this method is the flow topology



Stratified flow

Bubbly flow

We are going to integrate over space and time the Riemann problem solutions at each interface inside the 2D control volume and at its boundaries

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Fluid selection

Pure fluid system $\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}+\frac{\partial G}{\partial y}=0$

Fluid selection $X_k \times Euler = 0$

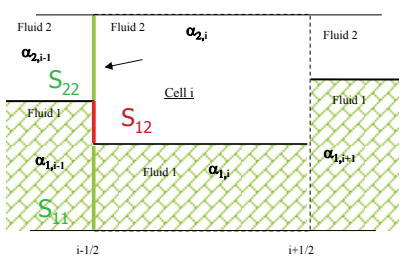
Yields $$\frac{\partial X_k U_k}{\partial t}+\frac{\partial X_k F_k}{\partial x}+\frac{\partial X_k G_k}{\partial y}=(F_k-u_i U_k)\frac{\partial X_k}{\partial x}+(G_k-v_i U_k)\frac{\partial X_k}{\partial y}$$

Integration over the control volume and time step

$$\int_0^{\Delta t}\int_{Ci}\left(\frac{\partial X_k U_k}{\partial t}+\frac{\partial X_k F_k}{\partial x}+\frac{\partial X_k G_k}{\partial y}\right)dxdydt=\int_0^{\Delta t}\int_{Ci}\left((F_k-u_i U_k)\frac{\partial X_k}{\partial x}+(G_k-v_i U_k)\frac{\partial X_k}{\partial y}\right)dxdydt$$

At each cell boundary

- The contact lengths at each pair of fluids are computed



- In this example $S_{11} = H\min(\alpha_{1,i-1},\alpha_{1,i})$, $S_{22} = H\min(\alpha_{2,i-1},\alpha_{2,i})$, $S_{12} = H - S_{11} - S_{22}$

-The fluxes and non-conservative terms are integrated along each contact

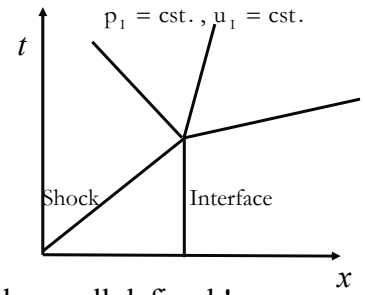
-At each contact (11), (12), (22) the Riemann problem is solved

Example with non conservative terms

We have to compute $\displaystyle\int_0^{\Delta t}\int_{C_{ij}}\left((F-u_i U)\frac{\partial X_k}{\partial x}\right)dxdydt$

- X_k is discontinuous at the interfaces
- But at the interfaces, the Lagrangian flux is precisely constant :

$$F^{Lagrange} = F - u_i U = \begin{pmatrix} 0 \\ p_I \\ p_I u_I \end{pmatrix}$$



The product $(F - u_i W)\dfrac{\partial X}{\partial x}$ is thus well defined !

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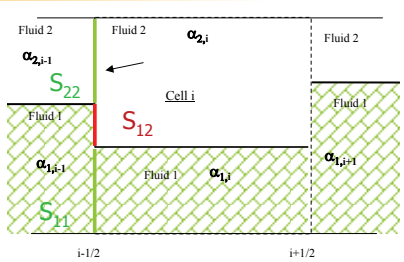
Non-conservative terms are thus integrated easily



$$\int_0^{\Delta t}\int_{C_{ij}}\left((F-u_i U)\frac{\partial X_k}{\partial x}\right)dxdydt = \Delta t\left(S_{11}\left[X^*_{1,11}\right]F_{11}^{*Lagrange} + S_{22}\left[X^*_{1,22}\right]F_{22}^{*Lagrange} + S_{12}\left[X^*_{1,12}\right]F_{12}^{*Lagrange}\right)$$

$$\int_0^{\Delta t}\int_{C_{ij}}\left((F-u_i U)\frac{\partial X_k}{\partial x}\right)dxdydt = \begin{cases} -\Delta t S_{12} F_{12}^{*Lagrange} & \text{if} \quad u^*_{12} > 0 \\ 0 & \text{otherwise} \end{cases}$$

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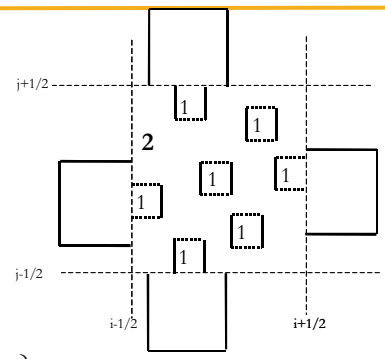
Lagrangian fluxes at internal interfaces



$$\left\{(F-u_i U)\frac{\partial X}{\partial x}\right\}_{\substack{\text{internal}\\ \text{interfaces}}} = \Delta t N a \left(F^{Lag,*}(2,1) - F^{Lag,*}(1,2) \right)_{ij}$$

The differences between interface variables inside the control volume are responsible for ***relaxation effects***.

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The result is a set of discrete equations

$$\frac{\alpha_{i,1}^{n+1}\overline{U}_{i,1}^{n+1} - \alpha_{i,1}^{n}\overline{U}_{i,1}^{n}}{\Delta t} + \frac{\{XF\}_{1,i+1/2} - \{XF\}_{1,i-1/2}}{\Delta x} = \left\{(F-u_1 U)\frac{\partial X}{\partial x}\right\}_{i,1} + \text{Relaxation}$$

with:

$$\{XF\}_{1,i-1/2} = \sum \text{segment length} \times \text{charact. func.} \times \text{Riemann flux})_{\text{cell boundary}}$$

$$\left\{(F-u_i U)\frac{\partial X}{\partial x}\right\}_{i,1} = \sum \text{segment length} \times \text{charact. func. jump} \times \text{Lagrangian Riemann flux})_{\text{cell boundaries}}$$

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Summarizing the two approaches

✓ **Traditional approach:**

Average micro-level PDEs to obtain macro-level PDEs
Simplify by making appropriate (or inappropritate) assumptions for the macro-level PDEs
Determine a phase distribution *topology*
Discretize and solve simplified macro-level PDEs with "standard" numerical methods

✓ **Novel Discrete Equation Method (DEM):**

Set phase *topology* within cell
Discretize within the cell
Average at the cell level
Solve

Remarks

- The methods solves two phase flows with single phase Riemann solvers for the Euler equations.
- The flow topology can be changed: The flux terms are not topology dependent, only relaxation terms change.
- We can determine the continuous system (PDEs) that correspond to these discrete equations.

Seven-Equation Model in 1-D

limit $\Delta x, \Delta t \to 0$, acoustic Riemann, with no mass transfer

$$\frac{\partial \alpha_1}{\partial t} + u_I \frac{\partial \alpha_1}{\partial x} = \mu (p_1 - p_2)$$

$$\frac{\partial (\alpha\rho)_1}{\partial t} + \frac{\partial (\alpha\rho u)_1}{\partial x} = 0$$

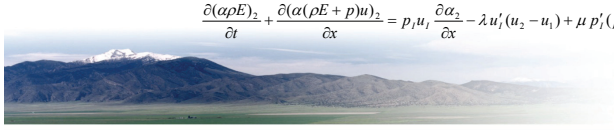
$$\frac{\partial (\alpha\rho u)_1}{\partial t} + \frac{\partial (\alpha\rho u^2 + \alpha p)_1}{\partial x} = p_I \frac{\partial \alpha_1}{\partial x} + \lambda (u_2 - u_1)$$

$$\frac{\partial (\alpha\rho E)_1}{\partial t} + \frac{\partial (\alpha(\rho E + p)u)_1}{\partial x} = p_I u_I \frac{\partial \alpha_1}{\partial x} + \lambda u_I' (u_2 - u_1) - \mu p_I' (p_1 - p_2)$$

$$\frac{\partial (\alpha\rho)_2}{\partial t} + \frac{\partial (\alpha\rho u)_2}{\partial x} = 0$$

$$\frac{\partial (\alpha\rho u)_2}{\partial t} + \frac{\partial (\alpha\rho u^2 + \alpha p)_2}{\partial x} = p_I \frac{\partial \alpha_2}{\partial x} - \lambda (u_2 - u_1)$$

$$\frac{\partial (\alpha\rho E)_2}{\partial t} + \frac{\partial (\alpha(\rho E + p)u)_2}{\partial x} = p_I u_I \frac{\partial \alpha_2}{\partial x} - \lambda u_I' (u_2 - u_1) + \mu p_I' (p_1 - p_2)$$



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Corresponds to previous model, but yields closure relations !

Interfacial variables

$$u_I = \frac{Z_1 u_1 + Z_2 u_2}{Z_1 + Z_2} + \mathrm{sgn}\left(\frac{\partial \alpha_1}{\partial x}\right) \frac{p_2 - p_1}{Z_1 + Z_2} \qquad p_I = \frac{Z_2 p_1 + Z_1 p_2}{Z_1 + Z_2} + \mathrm{sgn}\left(\frac{\partial \alpha_1}{\partial x}\right) \frac{Z_1 Z_2}{Z_1 + Z_2} (u_2 - u_1)$$

Averaged interfacial variables

$$u_I' = \frac{Z_1 u_1 + Z_2 u_2}{Z_1 + Z_2} \qquad p_I' = \frac{Z_2 p_1 + Z_1 p_2}{Z_1 + Z_2}$$

Relaxation parameters

$$\lambda = \frac{1}{2} \mu Z_1 Z_2$$ **(velocity relaxation rate)**

$$\mu = \frac{A_I / V}{Z_1 + Z_2}$$ **(pressure relaxation rate)**

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DEM example (Berry, Saurel, LeMetayer, *NED* **240** (2010) 3797-3818)

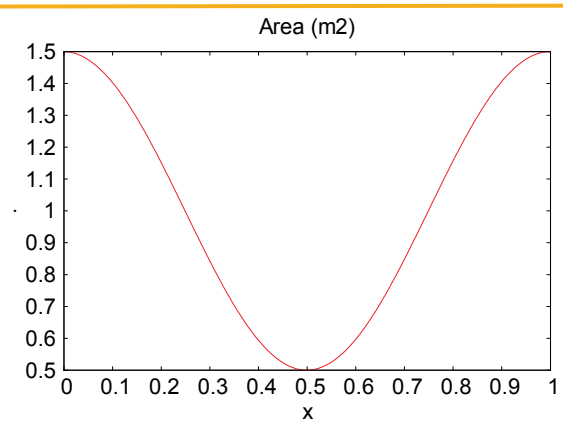
1-D flow in a duct of spatially varying cross-sectional area:

classical converging-diverging nozzle

stagnation (tank conditions) at inlet

static pressure outlet (for subsonic only)

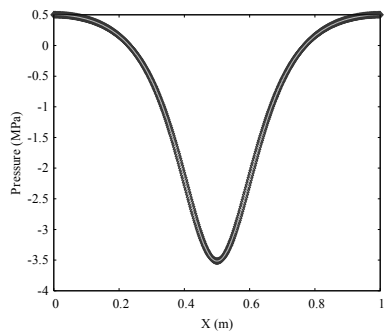
Converging-Diverging Nozzle



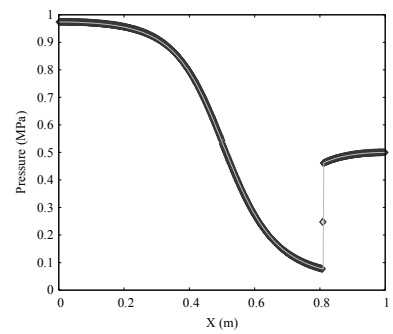
Normalized area distribution for nozzle

BC: Tank conditions left, pressure right

No pressure or velocity relaxation

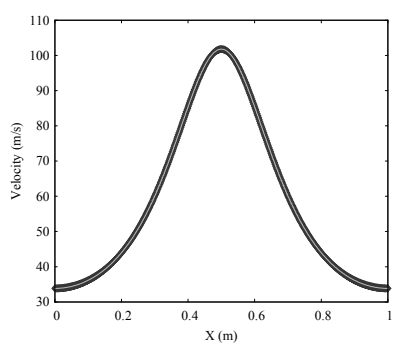


liquid pressure

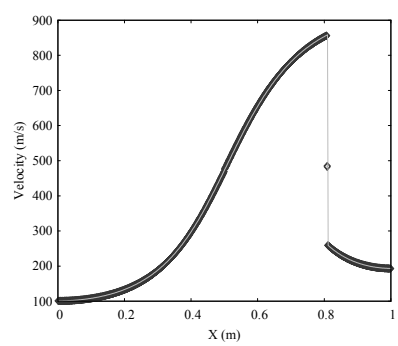


gas pressure

No pressure or velocity relaxation

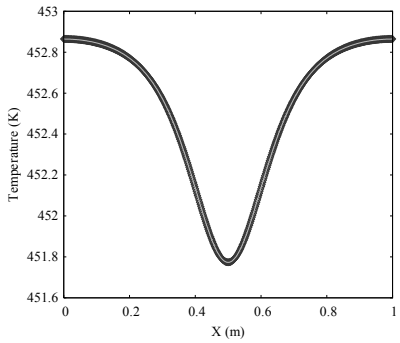


liquid velocity

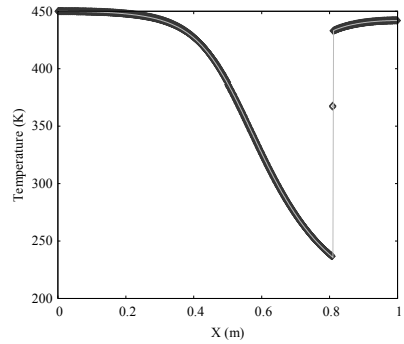


gas velocity

No pressure or velocity relaxation



liquid temperature



gas temperature

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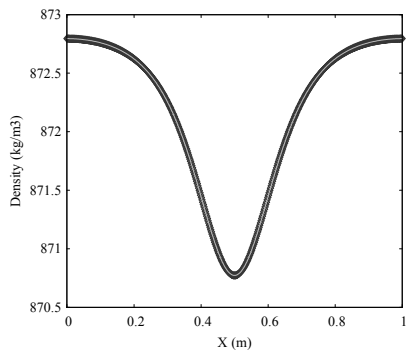
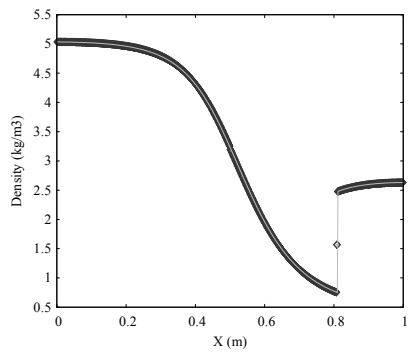
No pressure or velocity relaxation



liquid density



gas density

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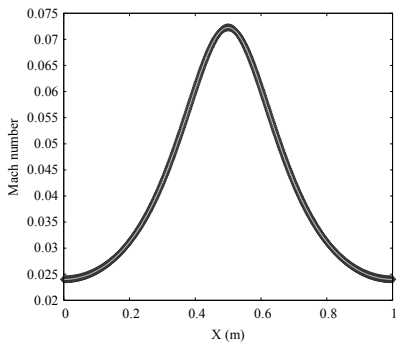
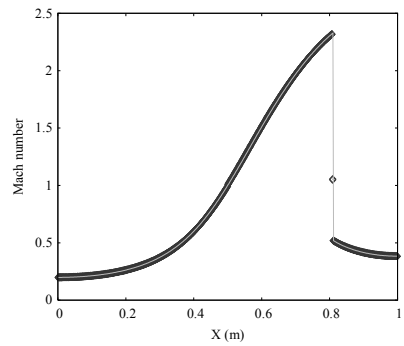
No pressure or velocity relaxation

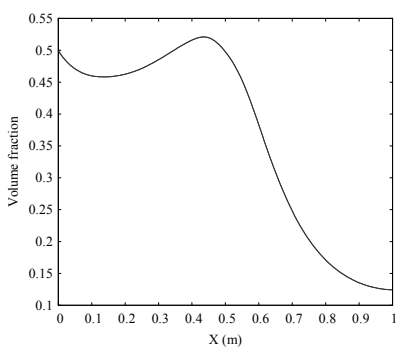


liquid Mach number

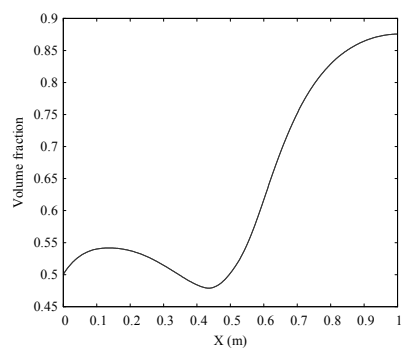


gas Mach number

With pressure relaxation + heat & mass transfer

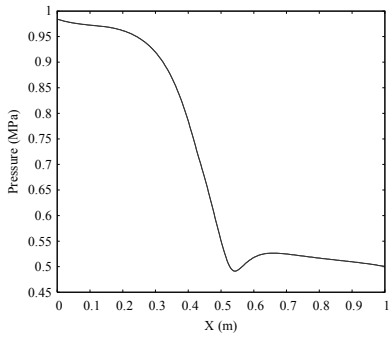


liquid volume fraction

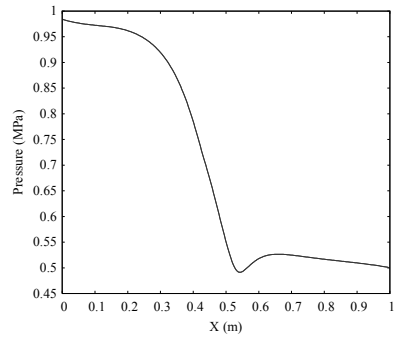


gas volume fraction

With pressure relaxation + heat & mass transfer



liquid pressure



gas pressure

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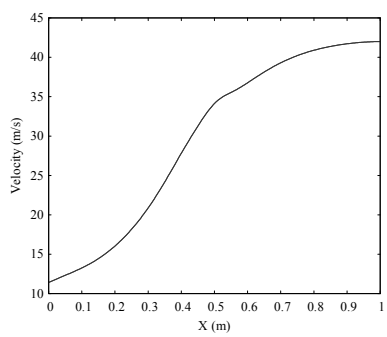
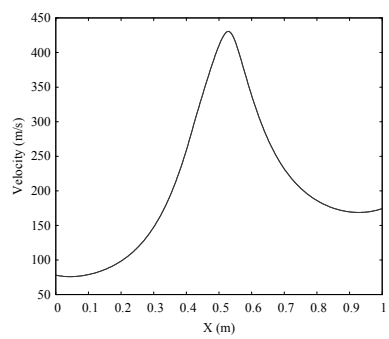
With pressure relaxation + heat & mass transfer



liquid velocity



gas velocity

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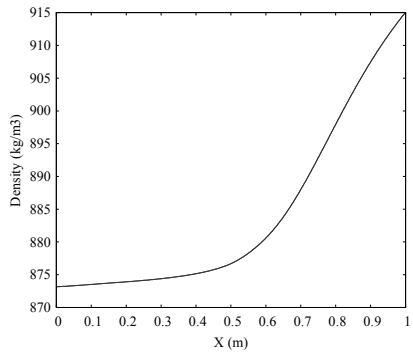
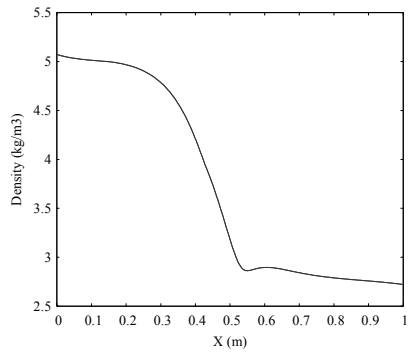
With pressure relaxation + heat & mass transfer

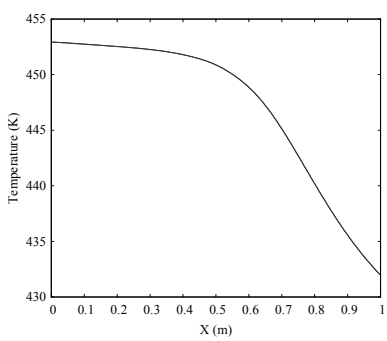


liquid density

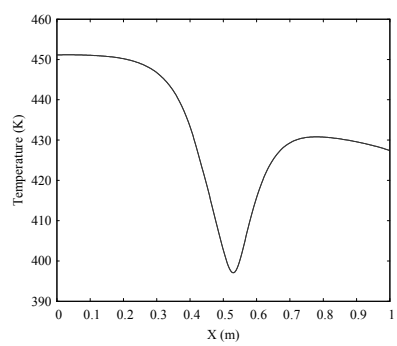


gas density

With pressure relaxation + heat & mass transfer

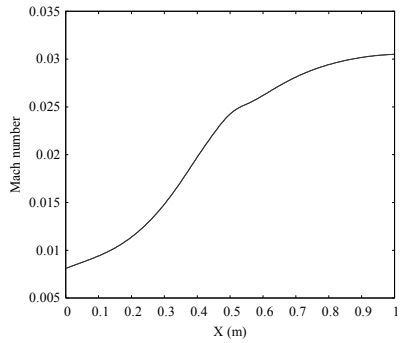


liquid temperature

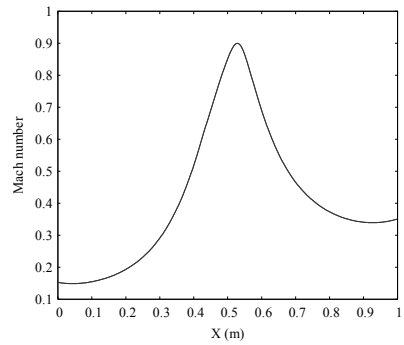


gas temperature

With pressure relaxation + heat & mass transfer



liquid Mach number



gas Mach number

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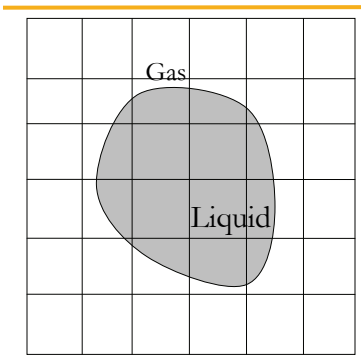
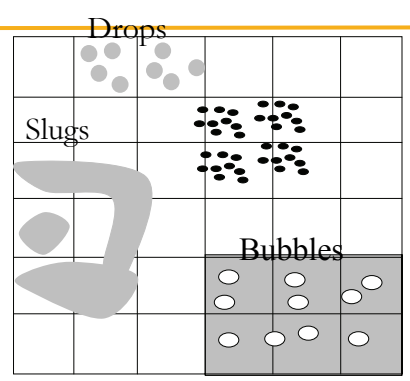
Interfaces vs two-phase mixtures… Disjoined problems ?



Difficulty = mixture cells



Difficulties = model + method

No! It is possible to solve, ***interface problems*** (single velocity) as well as ***multiphase mixtures*** (multiple velocities) with a unique formulation: ***Multi-scale treatment***

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Interface "capturing" vs. interface tracking

- ✓In gas dynamics the debate about shock *tracking* (at that time "shock fitting") versus *capturing* came about 40 years ago. Development of methods with limited artificial viscosity and the increase in computational resources ended the debate in the 1980's with the success of the capturing methods. Indeed, today shock tracking is virtually unheard of – shock capturing is used exclusively.
- ✓This same paradigm can be used with multiphase flow models to eliminate the need for complex interface tracking methods. Though seemingly artificial, this capturing approach permits automatic merging, break-up, coalescence, and extreme deformation of interfaces. The same equations are solved everywhere, and the interface is automatically captured, with some significant added benefits.

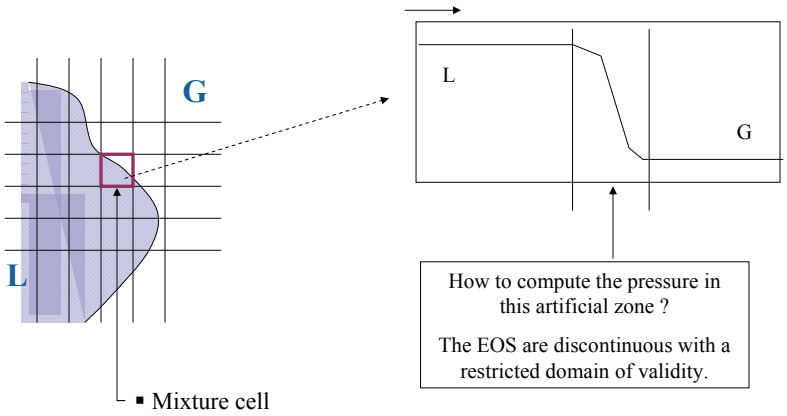
Specialized submodel

Diffuse Interface Method* (DIM)

for resolving an interface

***Saurel, Petitpas, and Berry,** *JCP* **228** (2009) 1678-3818

Diffuse interfaces appear as a consequence of numerical diffusion (cell averages)

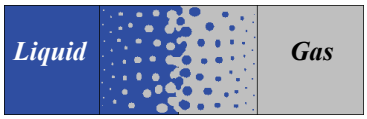


How to compute the pressure in this artificial zone ?

The EOS are discontinuous with a restricted domain of validity.

One way to enforce interface conditions in mixture cells

Interface conditions: **equal normal velocities, pressures, temperatures, and chemical potentials**



$\varepsilon < \alpha_k < 1 - \varepsilon$

'Bubble' expansion/contraction in mixture cells enforces **pressure equilibrium**

$$\frac{\partial \alpha_1}{\partial t} + \bar{u}_i \frac{\partial \alpha_1}{\partial x} = \mu(p_1 - p_2)$$ ***where μ tends to infinity***

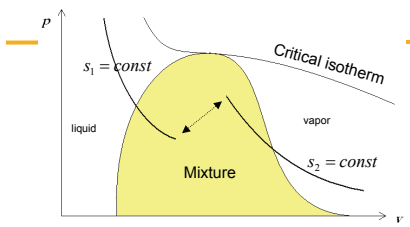
Similar *relaxation terms* are used to guarantee **phasic velocity equality** at the interface

→ ***Stiff mechanical relaxation*** - to fulfill interface conditions

and to guarantee **phasic temperature** and **chemical potential equality** at the interface

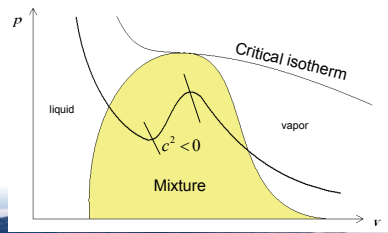
→ ***Stiff thermodynamical relaxation*** - to fulfill interface conditions

Remark: the model involves 2 temperatures and entropies



Hyperbolicity is preserved in the spinodal zone: the connection of the two isentropes is modeled as a **kinetic path**

- ≠ to the Van der Waals model



Mass transfer is modeled as a **thermodynamic path**:

$$c^2 = -v^2 \left.\frac{\partial p}{\partial v}\right)_{s=constant} < 0$$

→ ill-posed model !

Simplifications

For the case where only interfacial resolution is important, it may be advantageous to simplify the DEM method first; by beginning with the mechanically relaxed (one pressure, one velocity) 5-equation model.

This is the minimum model that exhibits complete thermodynamics for each phase.

Saurel, Petitpas, and Berry, *JCP* **228** (2009) 1678-3818

Why the 7- and 5-equation two-phase models?

The success of this multiphase method relies on:

- Use of an unconditionally hyperbolic model for two-phase compressible mixtures
- Accurate discretization of the non-conservative terms and equations
- Use of robust relaxation procedures to restore pressure and velocity interface conditions based on infinite relaxation parameters

Multiphase, DIM advantages

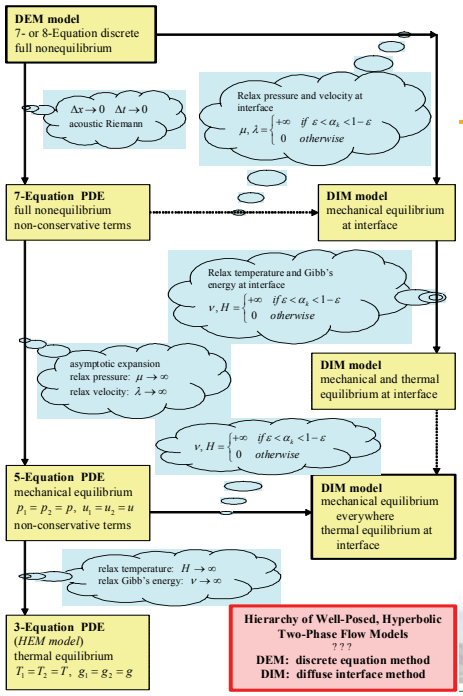
- Interfaces are handled routinely, i.e. at any point in the flow
- Allow very general equations of state and supercritical states
- Conservative for the mixture, guaranteeing correct wave dynamics in pure fluid zones
- Compressibility in all phases
- Able to account for noncondensible gases; e.g. some noncondensible gases in the liquid may strongly influence the mixture compressibility (bubbles expand before reaching the saturation pressure) and modify the mass transfer dynamics
- Provides accurate internal energies and temperatures at the interface
- Able to model metastable mixtures
- Handles coexisting bubbly flows and flashing pockets; e.g. cavitation pockets followed by bubbly flow
- Able to dynamically create (not initially present) and follow interfaces
- Allows interfaces to separate non-pure fluids (mixtures) on each side of the interface; so called “permeable interface”
- Can be use to couple models with variable levels of simplification (consistent reduction or relaxation)
- Able to propagate subsonic and supersonic fronts in multi-dimensions without solving their internal structure

Multiphase, DIM advantages (continued)

- Able to include capillarity (surface tension) effects in a thermodynamically consistent manner, i.e. capillarity tensor that enters the momentum and energy fluxes conservatively
- Allows mass transfer in a thermodynamically consistent manner. The entropy is preserved; when phase transition occurs the model guarantees mixture entropy production. It allows mass transfer times to be of the same order as the flow characteristic time
- Perhaps most importantly, able to model non-equilibrium two-phase flows (bubbles, droplets, annular flows, etc.) as well as interfaces using the same basic equations; even simultaneously ***– multi-scale approach***
- Able to deal with a wide range of applications !

Multiphase, DIM disadvantages

- Interfaces can be diffused too much, especially when dealing with long time evolutions. But this is exactly the same drawback as contact discontinuity smearing in gas dynamic computations, and just as in modern shock capturing CFD methods, there are several ways to reduce its effects: mesh refinement, high-order discretizations, variable remapping, and other strategies. Recent efforts at front sharpening have been reported.
- Non-conservative equations are present and numerical approximation of non-conservative terms poses difficulties in the presence of shocks.
- The construction of all-Mach number methods for this kind of hyperbolic flow model is not an easy task, but progress is being made.



Summary*

Hierarchy of well-posed, hyperbolic, fully compressible two-phase flow models

*R.A. Berry, *Some Specific CASL Requirements for Advanced Multiphase Flow Simulations of Light Water Reactors*, Idaho National Laboratory report INL/EXT-10-20529, December 2010

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INL Direction Summary

We are developing advanced multiphase capability, to include:

- 7- and 5-equation, hyperbolic relaxation models capable of *multi-scale* application
- robust numerical methods for *all-speed* flow
- *coupled implementation* into our fuels behavior and performance package.

Idaho National Laboratory

CASL Industry Perspectives

CASL Roundtable Meeting
August 9 to 11, 2011

Jin Yan

Westinghouse

CASL-U-2011-0072-000-R

Outline

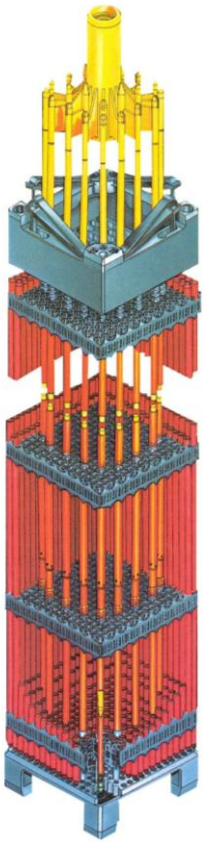
- Engineering Modeling Challenges in A Design Environment
- Geometry & Mesh
- Physics Models
- Documentation and Verification

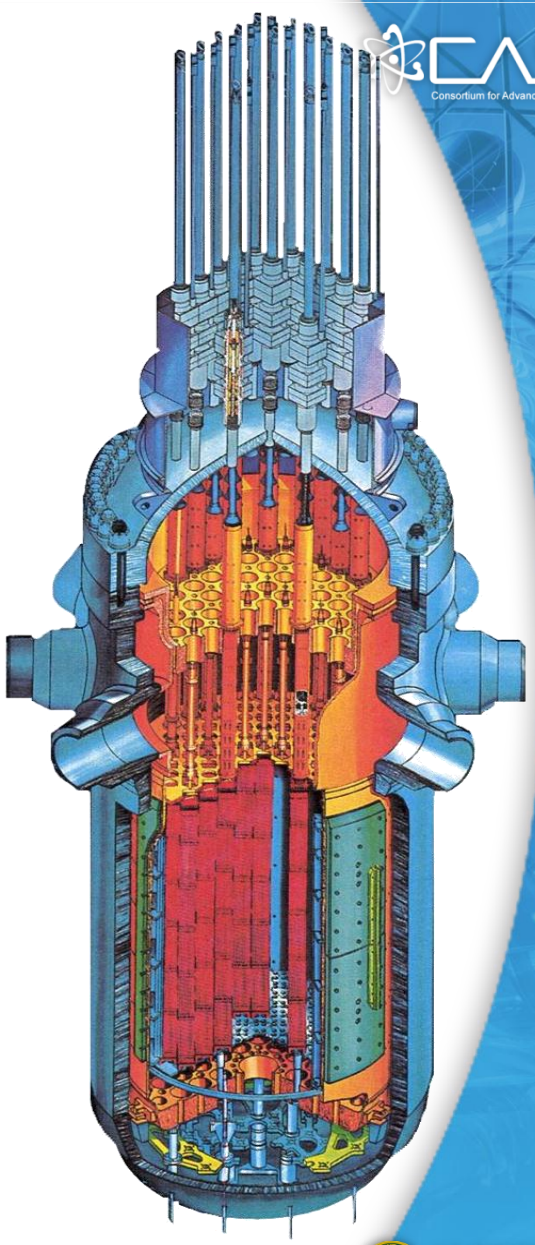
Engineering Modeling Challenges in A Design Environment

- Nuclear engineering design rely more and more on Modeling
- The CFD (TH) and FEA modeling are increasingly seen as bottle necks. The goal in Westinghouse is:
  - Ability to use existing CAD models
  - Overnight meshing
  - Overnight running
  - Build in automatic optimization
  - Easy to use
- Validation becomes more and more important for modeling methodology development

Geometry

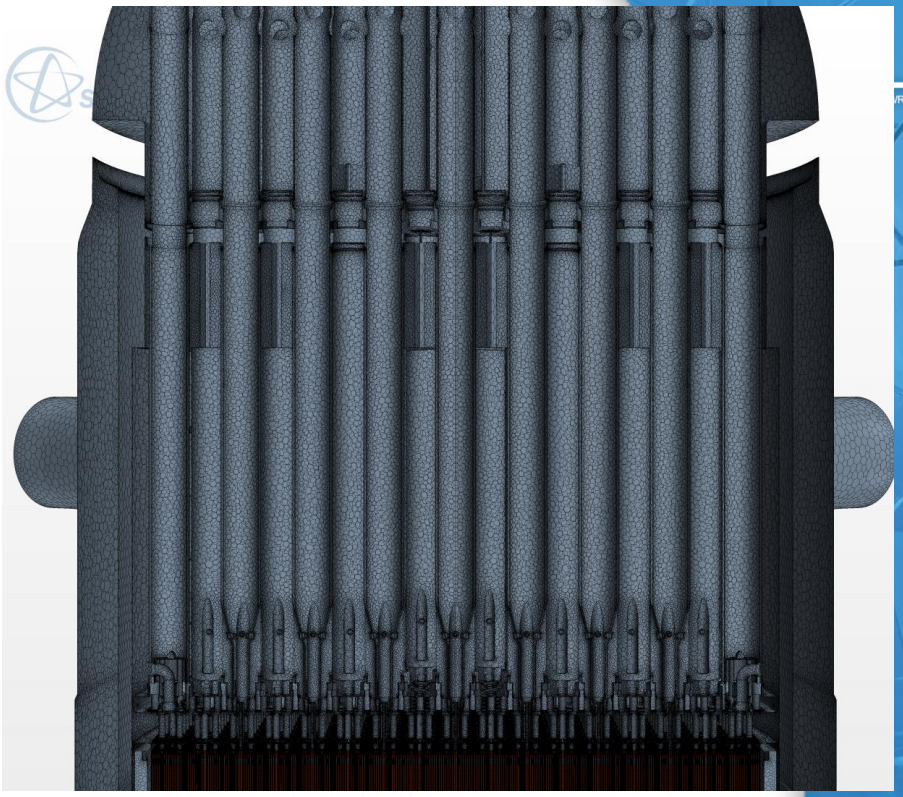
- Nuclear industry have complicated geometries from large scale to small scale.
- One geometry could have 10000 faces.
- The pre-processor needs to be able to handle the geometry.
- 64 bit software is a minimum requirement. Massive parallel geometry manipulation capability is desirable.

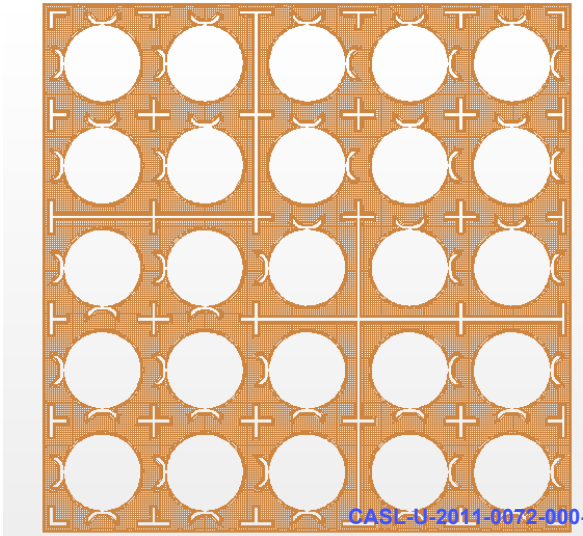


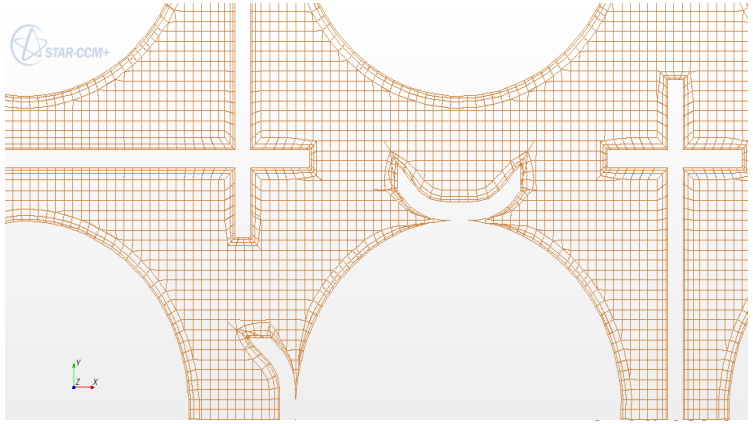


Computational Mesh

- Different cells type have to be used. Hex and Prismatic cells are essential for minimize numerical diffusion.
- Parallel meshing is critical to produce mesh over 1 billion cells.
- The co-existing of the large and small geometry requires flexible mesh refinement ability.







Physics Models

- Nuclear TH Modeling applications involve:
  - Incompressible Flow (Model available and Benchmarked)
  - Heat transfer (Model available, Further benchmark needed)
  - Turbulence (Model available, Further benchmark needed)
  - Radiation (Model available, benchmark needed)
  - Multiphase (No Model yet)
  - Multi-species (Model available, benchmark needed)
  - Supersonic flow (Model available, benchmark needed)
  - Fluid Structure Interaction (FSI) (Model available, benchmark needed)
  - Acoustics

Physics Models

- Multiphase Model Development Dilemma:
  - Many boiling models are being developed in CASL.
  - Different packages, programming languages are used for those models development.
  - Engineers in the industry will not be able to learn all these packages.
- Suggestion
  - Modular based boiling model development focusing on the fundamental physics and mathematical formula.
  - The resulting program will be a highly portable program which can be plug in any CFD software platform.
  - Example: V2F turbulence model from Stanford Univ. has been made portable to CFX, Fluent, Star.

Documentation & Validation

•Need to define a suite of validations cases for CASL

Models	Element Test	Industry Strength Test
Incompressible Flow		V5H test &NESTOR
Heat transfer		V5H & NESTOR
Turbulence		
Radiation		
Multiphase		
Multi-species		
Supersonic flow		
Fluid Structure Interaction (FSI)		
Acoustics		

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Specific ITM Results: Direct Numerical Simulations

Grétar Tryggvason
University of Notre Dame

1st Annual CASL Round Table Meeting
North Carolina State University, Raleigh, NC, August 9-11, 2011

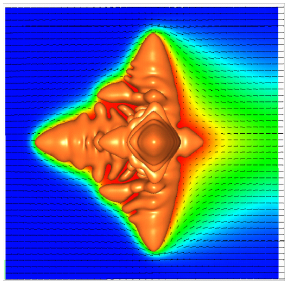
CASL-U-2011-0072-000-R

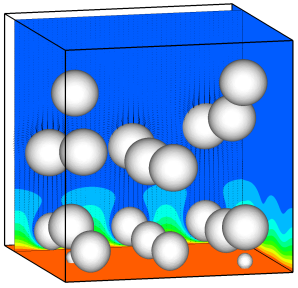
DNS of Multiphase Flows

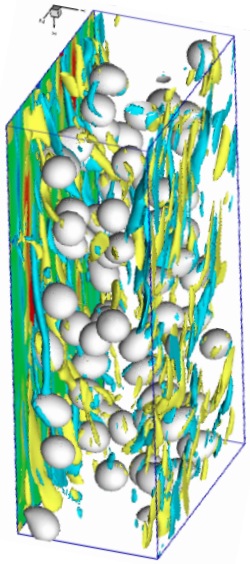
Direct Numerical Simulations (DNS):

Fully resolved and verified (correct and accurate) simulation of a validated (right equations) system of equations that include non-trivial length and time scales

DNS provide “exact” solutions of precisely defined and fully controlled model problems that deliver an understanding of the flow and quantitative inputs for models that describe unresolved processes in computations of industrial size systems



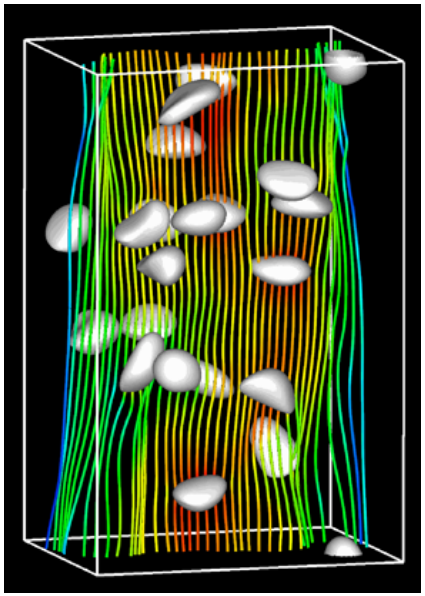


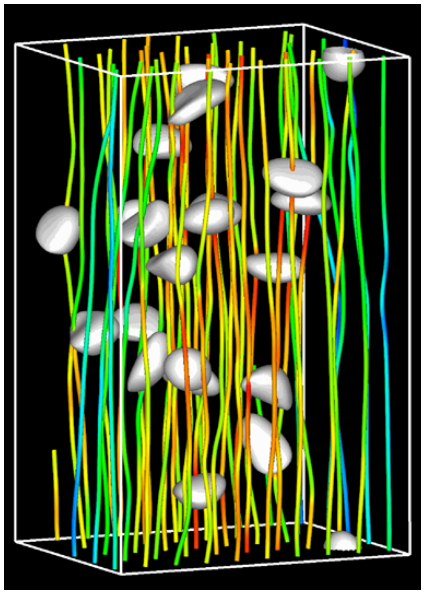


DNS of Multiphase Flows

For CASL, DNS will focus on:

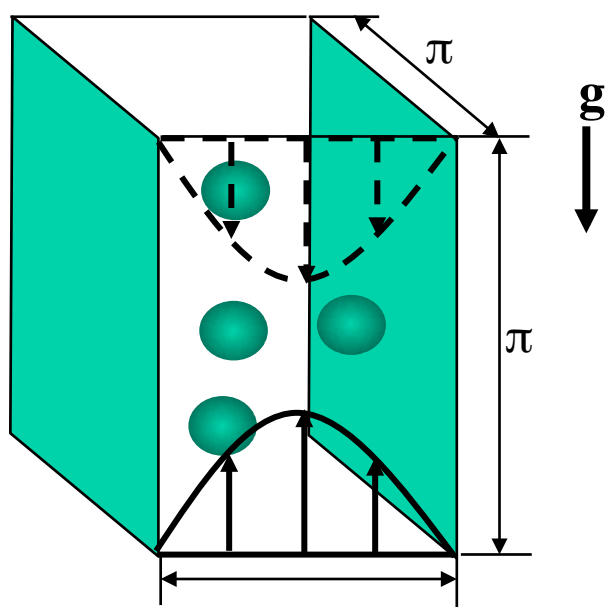
- Bubbly flows in vertical turbulent channels
- Nucleate boiling at vertical walls in turbulent flows
- Multiphase flows undergoing “topology changes” in vertical turbulent channels
- Inclusion of mass transfer and mass deposition in vertical turbulent channels

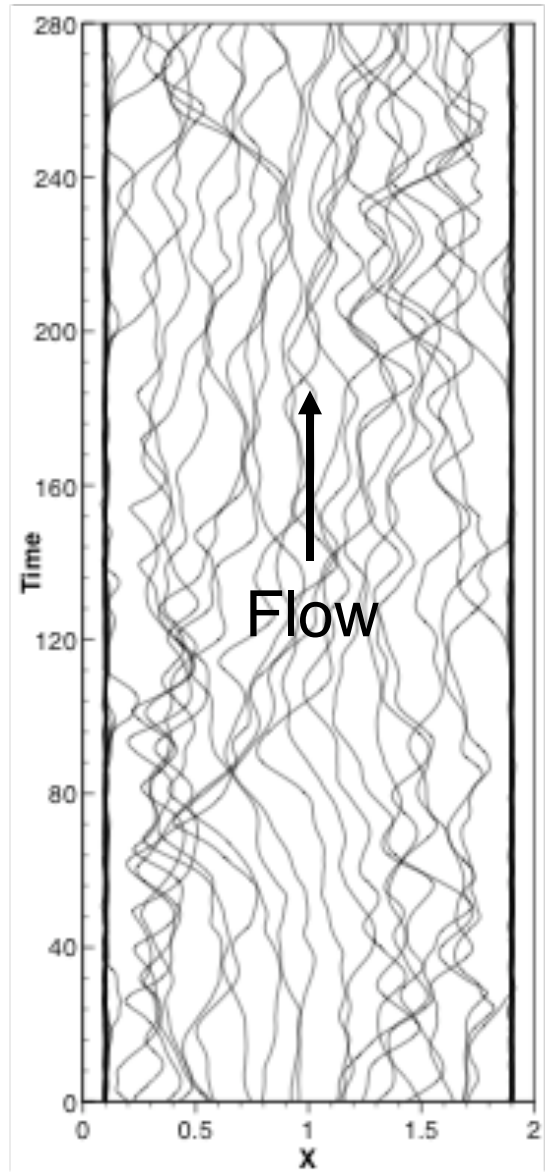


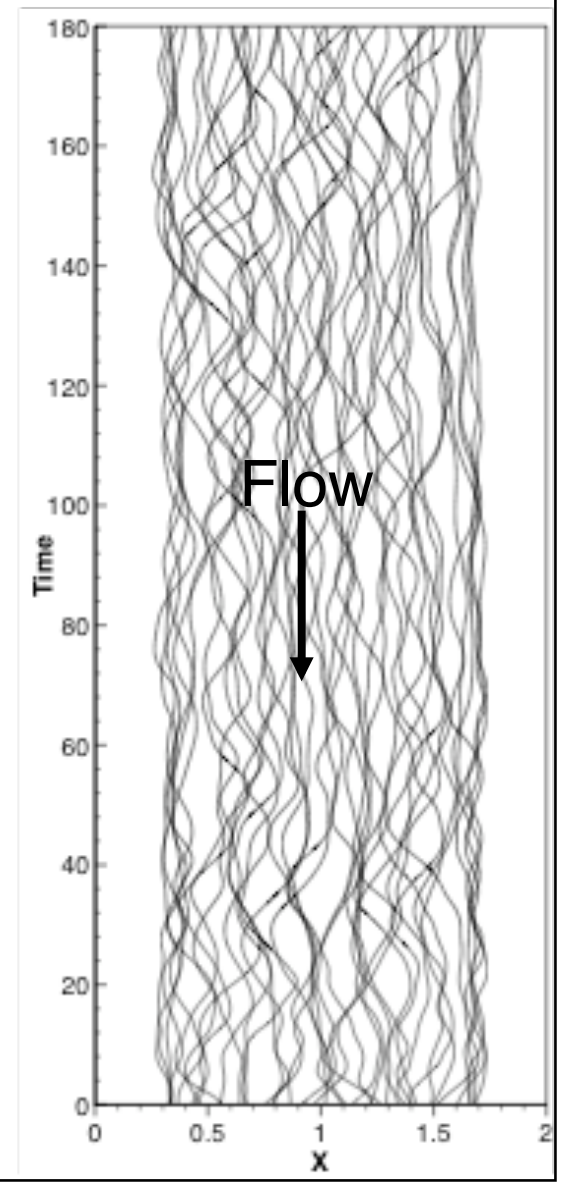


DNS of Multiphase Flows
Bubbles in Vertical Channels

The path of bubbles in laminar flows. The cross-channel coordinate versus time for the upflow (left) and the downflow (right) at approximately steady state.







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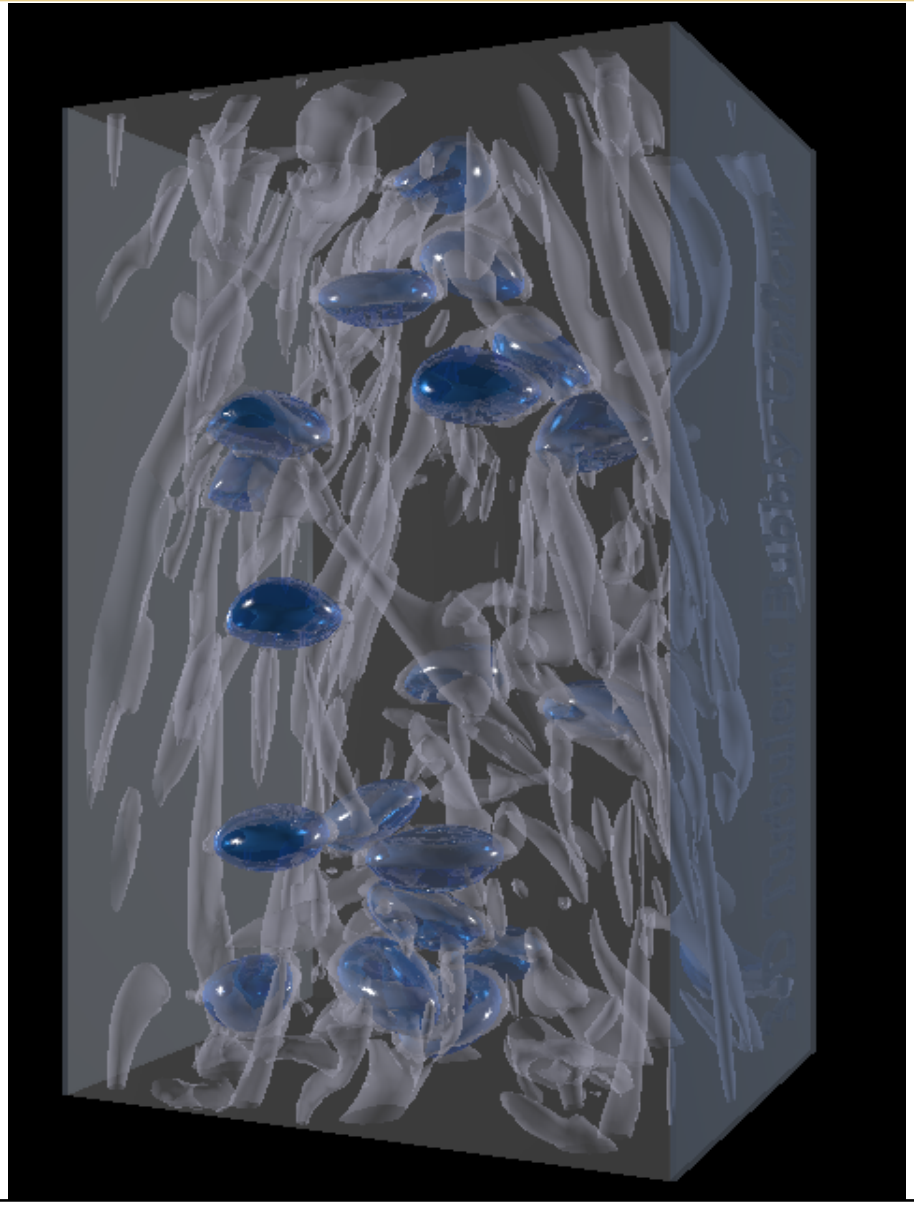
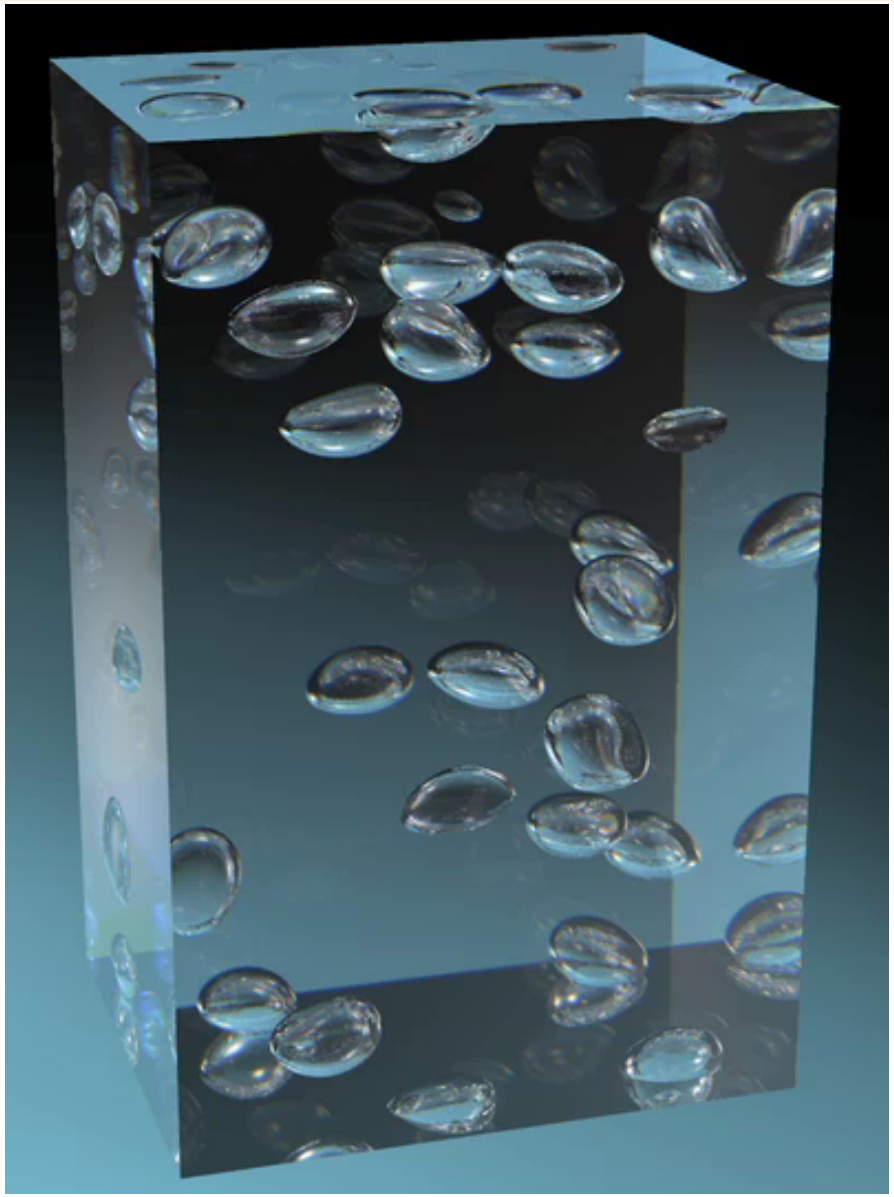
DNS of Multiphase Flows
Bubbles in Vertical Channels





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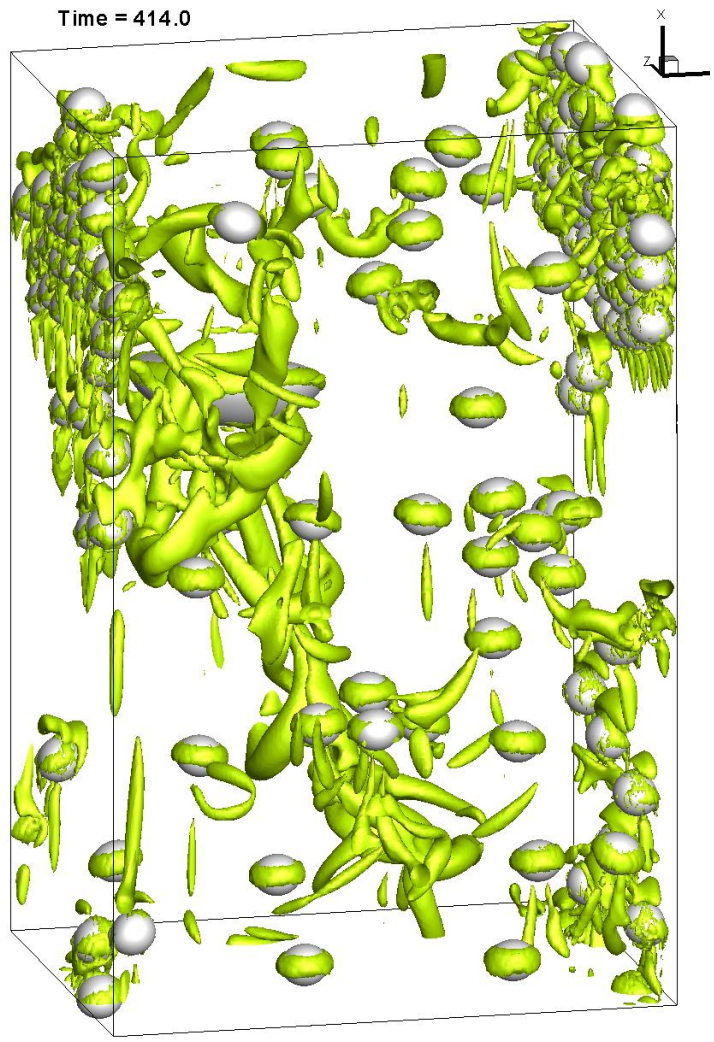
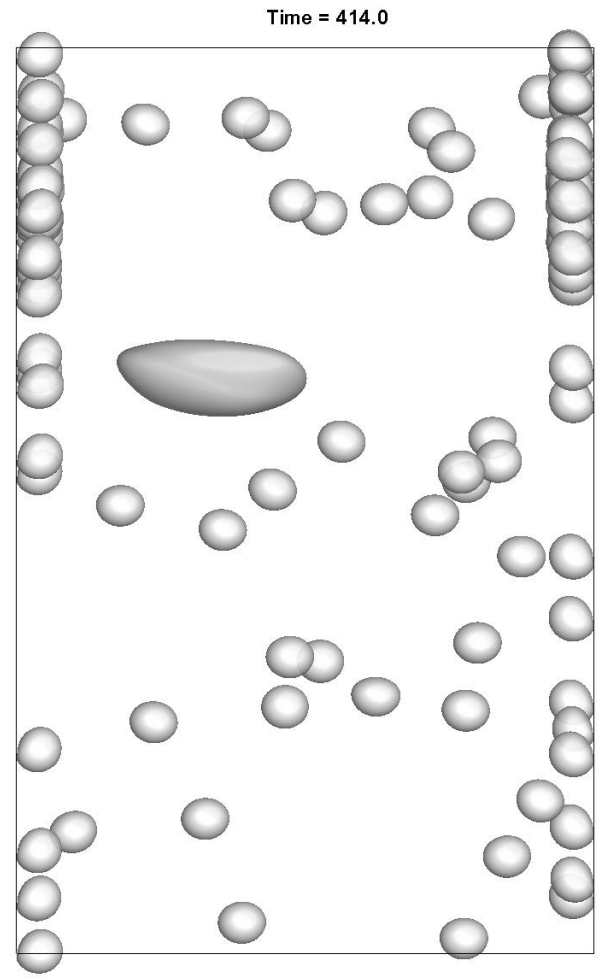
DNS of Multiphase Flows
Bubbles in Vertical Channels

Turbulent Upflow:
Different bubble sizes

512 x 384 x 256 grids, 192 cores)

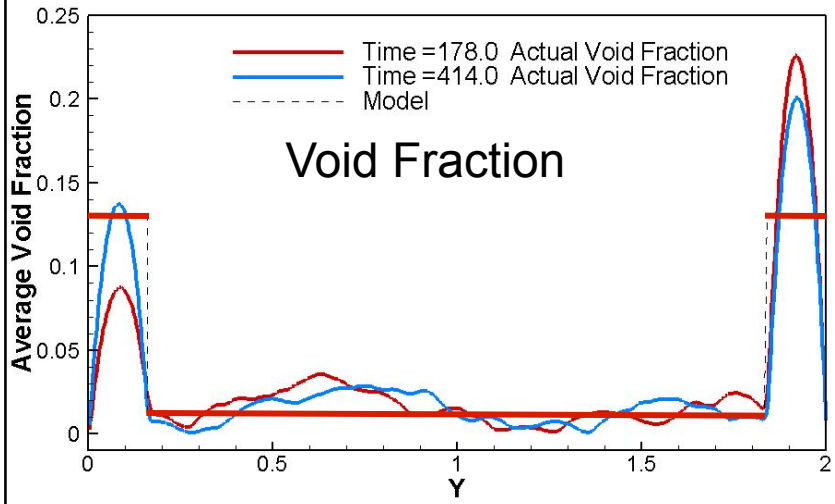
The figures are from a current study of the effect of a large number of bubbles of different sizes in turbulent upflow. Some of the small bubbles hug the wall but the large one stays in the center region. If the bubbles coalesced, the flow rate would eventually increases

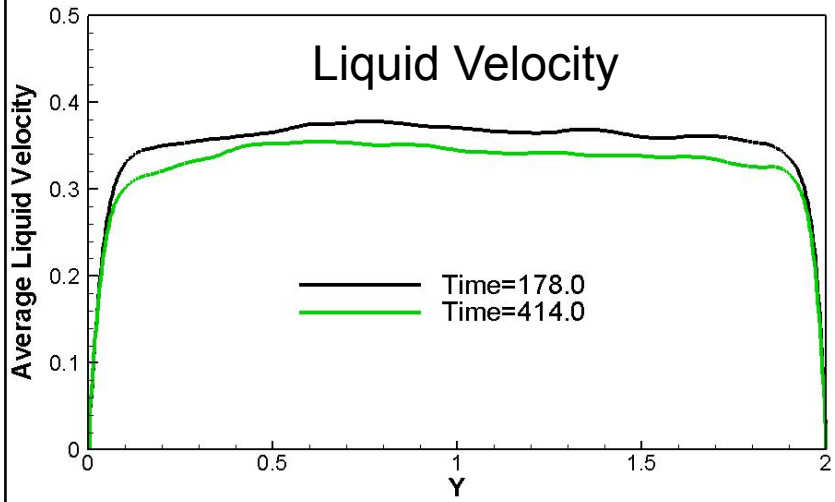


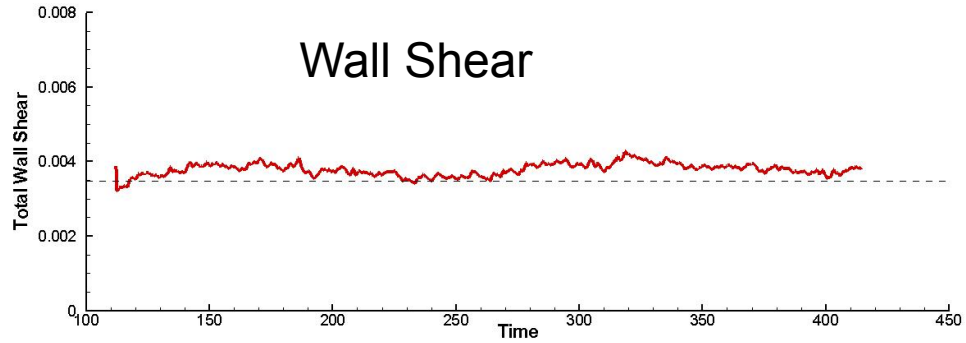


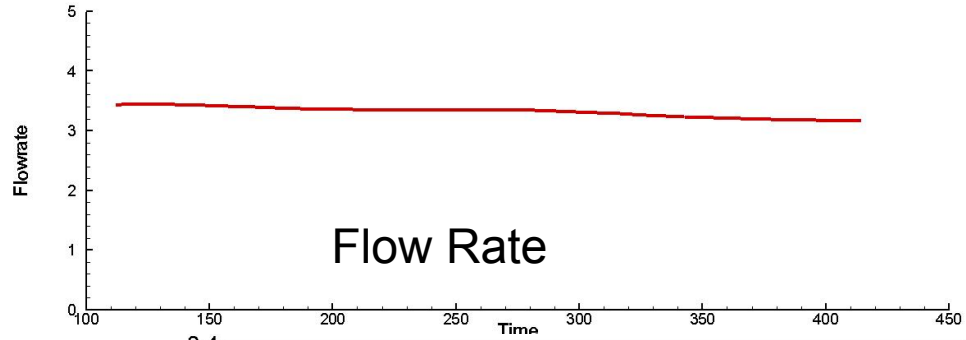
DNS of Multiphase Flows
Bubbles in Vertical Channels

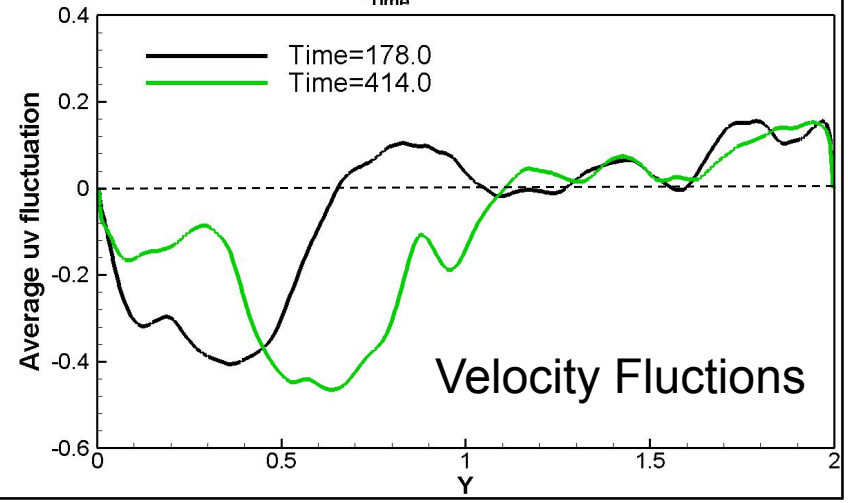
Turbulent Upflow: Different bubble sizes











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DNS of Multiphase Flows
Isothermal Bubbly Flows

- Simulations for bubbles in weakly turbulent flows have shown that the flow has a relatively simple structure for mono-disperse bubble distributions
- This is important for modeling, which should reproduce this structure in the right limits
- Need to understand the effect of a range of bubble sizes
- Need to understand the effect of higher turbulence levels
- Need to understand the effect of a larger range of scales
- A case with several nearly spherical bubbles and one large on has been proposed as Test Case 4
- The results need to find their way into improved models

DNS of Multiphase Flows
Multiscale Issues

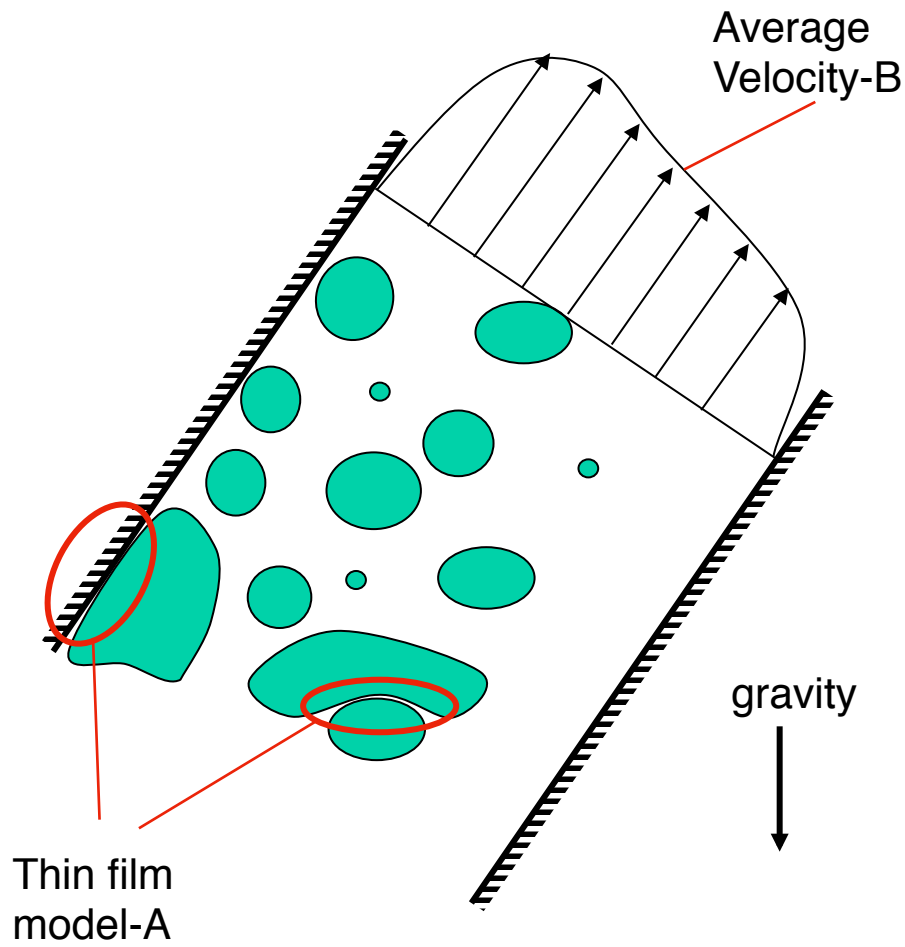
Some communities have defined two types of multi-scale problems.

Type A Problems: Dealing with Isolated Defects

Type B Problems: Constitutive Modeling Based on the Microscopic Models

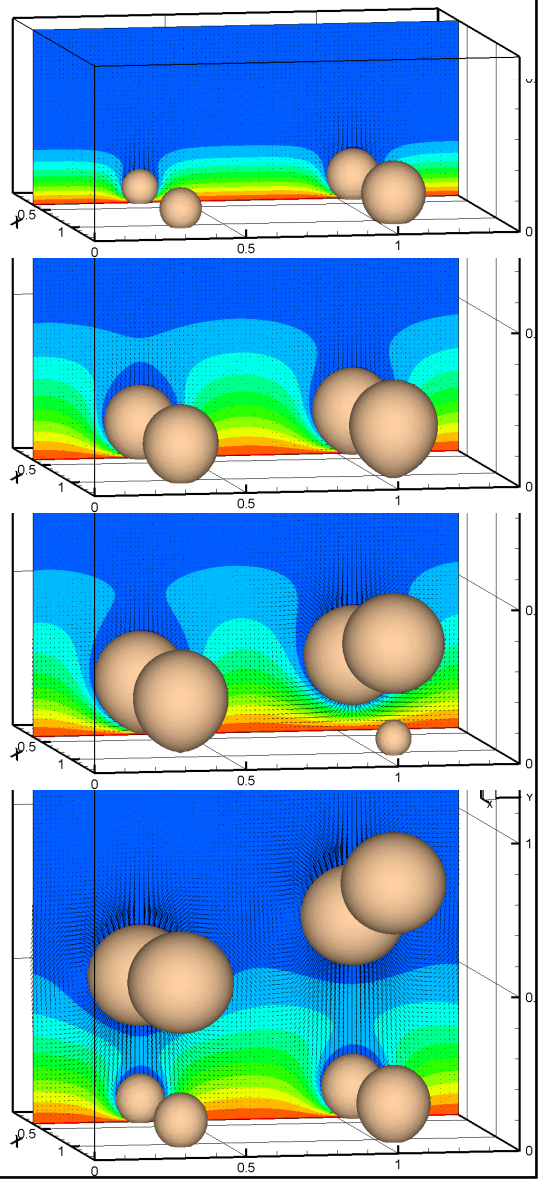
Reference: W. E and B. Enquist, The heterogeneous multiscale methods, *Comm. Math. Sci.* **1** (2003), 87—133.

Buoyant bubbles in an inclined channel flow



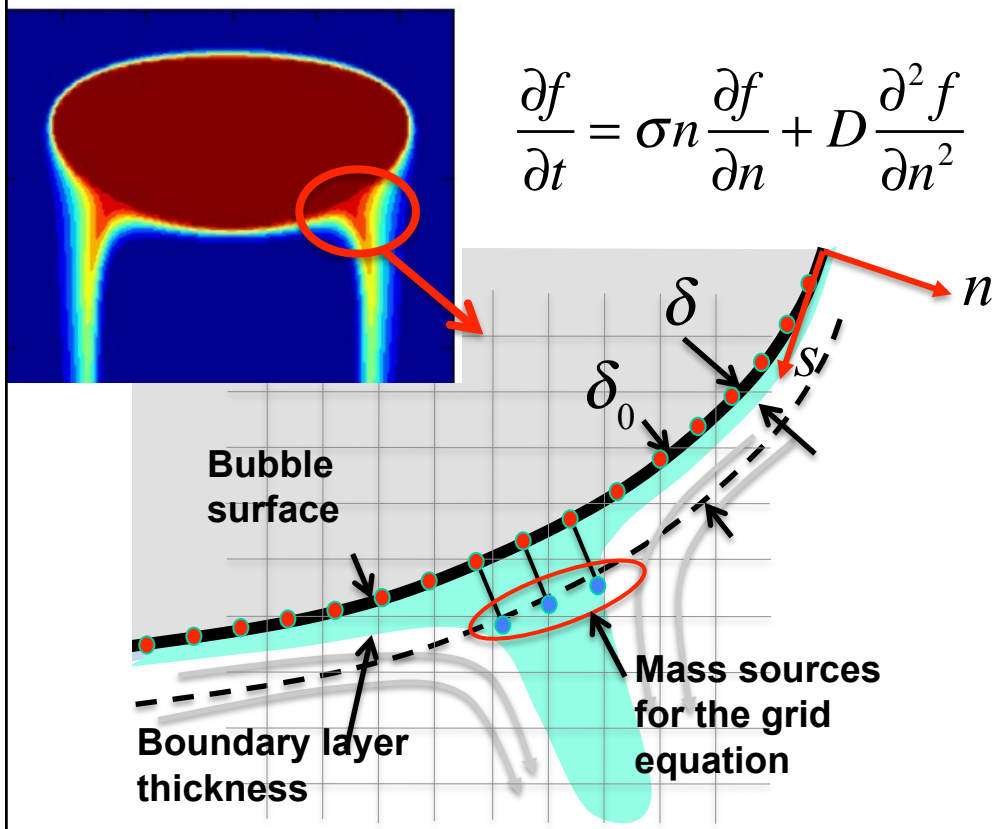
DNS of Multiphase Flows
Nucleate Flow Boiling

- Boiling has been simulated for fairly complex systems away from walls
- Simulations of nucleate boiling is still relatively limited and mostly focused on one nucleation site
- Capturing the full growth of a vapor bubble require modeling the microlayer and the bubble nucleation as well as the temperature distribution in the solid
- Nucleation site distribution needs to be provided
- Extension to nucleate boiling in turbulent flows

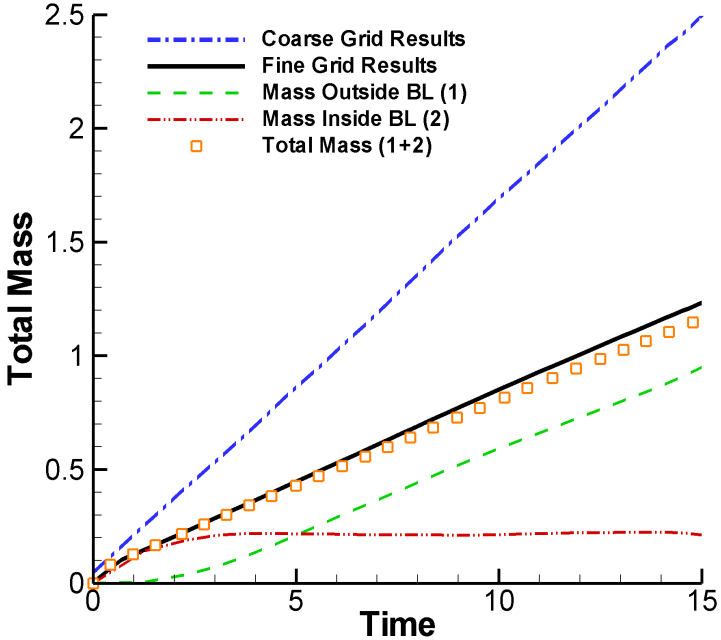


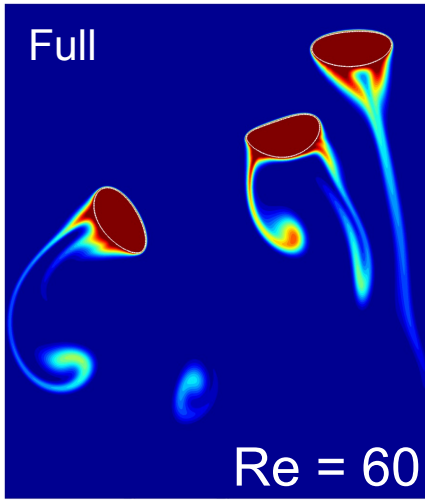
DNS of Multiphase Flows
Mass Transfer in Gas-Liquid Systems

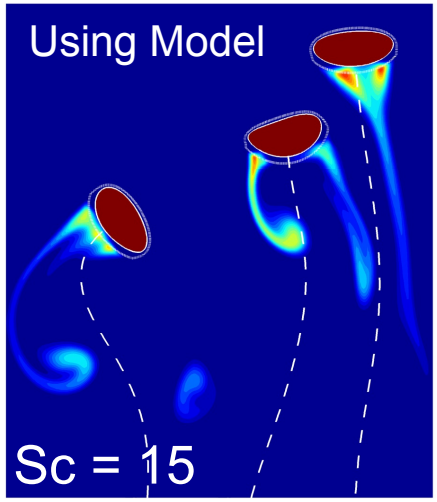
For high Schmidt number flows, mass boundary layers are much thinner than momentum boundary layers, requiring much finer resolution. We are developing a multiscale approach, based on imbedded boundary layer approximations



$$\frac{\partial f}{\partial t} = \sigma n \frac{\partial f}{\partial n} + D \frac{\partial^2 f}{\partial n^2}$$







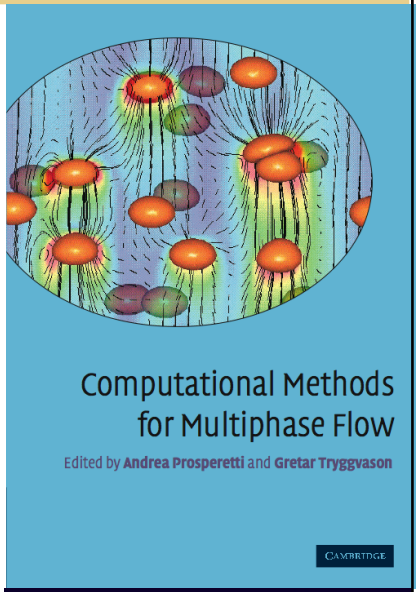
DNS of Multiphase Flows
Now What?

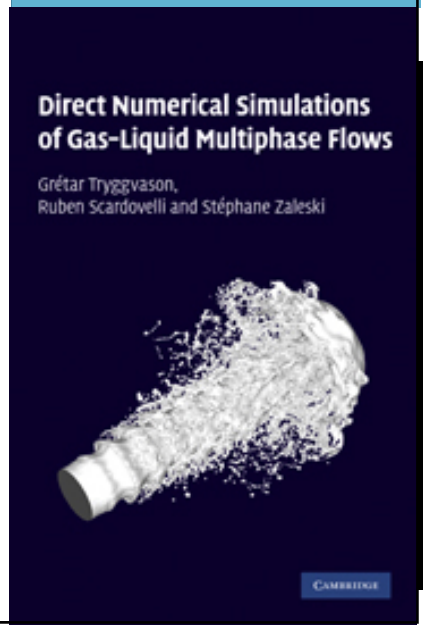
DNS of bubbly flows in turbulent channels have been developed to the point that they should be able to help produce new models for “industrial” simulations

DNS needs to be extended to handle flows with more complex topology and those undergoing flow regime transitions

Complex isothermal flows and flows with phase change and more complex physics, such as mass transfer, need multiscale modeling that must be developed further and put on a rigorous theoretical basis.

DNS data is putting new demands on the modeling of complex multiphase flows. Currently, such modeling relies of fairly basic ideas, first put forward many years ago. DNS should make much more comprehensive models possible





Advanced Modeling Applications (AMA)

Jess Gehin (ORNL)
Steve Hess (EPRI)
Zeses Karoutas (WEC)

CASL Round Table Meeting
NCSU,Raleigh, NC
August 11, 2011

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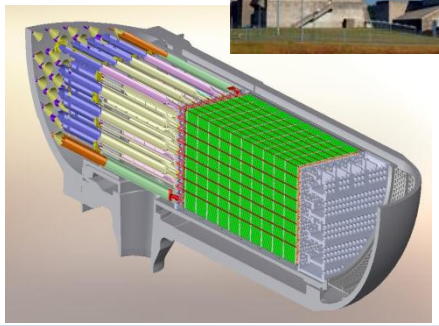
Advanced Modeling Applications

Driving development of VR to support real-world users and applications

Objectives and Strategies

- Ensure that CASL R&D meets user needs and requirements by setting requirements and assessing VR
- Support development of VR that meets user needs by directly engaging users in:
  - Setting VR modeling requirements and assessment
  - Performing VR validation
  - Performing VR application to physical TVA reactors
  - Developing challenge problems and applications
  - Supporting NRC engagement
- Relies on CASL's strong industry and national laboratory engagement



Requirements Drivers

- AMA is the primary connection of the CASL R&D with the problems to be solved.
- To be successful, AMA needs:
  - Industry input and direction on key limitations to power uprates based on experience with physical reactors and challenge problems
  - Capable VR software with robust, accurate physics models that can be applied in an R&D and engineering environment

Outcomes and Impact

- AMA will provide demonstrated applications of CASL capabilities to physical reactors and challenge problems
- Metrics for success include qualification of the CASL capabilities with operational data from TVA reactors and successful application to the CASL challenge problems
- The impact of this activity will be a clear demonstration that the tools can be used to solve problems of interest to the nuclear industry and early deployment through use at the CASL industry partners

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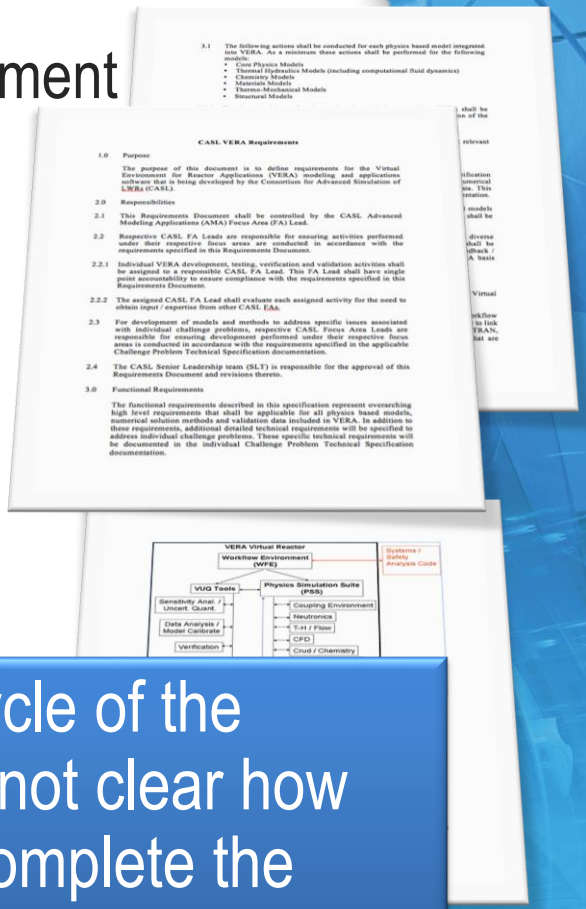
Requirements & Assessment Activities

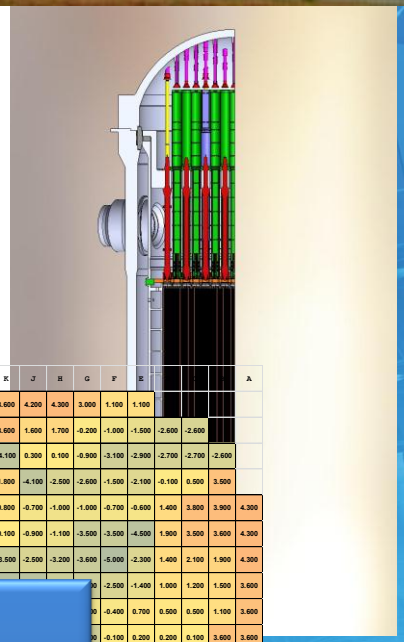
- Purpose: provide AMA priorities for VERA development
  - High level VERA Requirements (SLT approved POR2)
  - Benchmark problems (POR2/POR3)
  - Detailed Technical requirements (POR2/POR3)
- Process for VERA assessment (POR2)
- PCMM approach (POR3 milestone)



We have not performed a complete cycle of the requirements/assessment approach – It's not clear how effective this approach will be until we complete the assessment/feedback phase

Physical Reactor Applications

- Application focus for VERA to ensure that we have a capability to model physical reactors
- Selection of WBN1 for modeling
- Full vessel CFD modeling (CE plant and WBN1)
- ANC/VIPRE models to support CRUD milestone
- Collection of WBN1 data for modeling
- Discussions of additional data plant data needs and potential for additional instrumentation



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2			5.100	5.100	5.100	3.600	1.600	1.700	-0.200	-1.000	-1.500	-2.600	-2.600		
3		2.600	2.500	1.100	1.800	-4.100	0.300	0.100	-0.900	-3.100	-2.900	-2.700	-2.700	-2.600	
4		1.600	1.000	-0.600	1.800	1.800	-4.100	-2.500	-2.600	-1.500	-2.100	-0.100	0.500	3.500	
5	2.500	0.300	0.300	-0.800	0.900	0.800	-0.700	-1.000	-1.000	-0.700	-0.600	1.400	3.800	3.900	4.300
6	-0.300	-0.900	-1.900	-0.700	-0.200	0.100	-0.900	-1.100	-3.500	-3.500	-4.500	1.900	3.500	3.600	4.300
7	1.100	-0.100	-1.700	-2.700	-2.800	-3.500	-2.500	-3.200	-3.600	-5.000	-2.300	1.400	2.100	1.900	4.300
										-2.500	-1.400	1.000	1.200	1.500	3.600
										-0.400	0.700	0.500	0.500	1.100	3.600
										-0.100	0.200	0.200	0.100	3.600	3.600
										-1.800	1.100	1.100	1.600	6.200	3.600
										-1.900	1.600	1.300	4.500	6.200	
										1.000	3.900	2.800	4.000	6.200	
										5.700	4.200	2.700	4.400		
										5.700	4.200				

Modeling physical reactors important for establishing usable capability and providing a connection to industry

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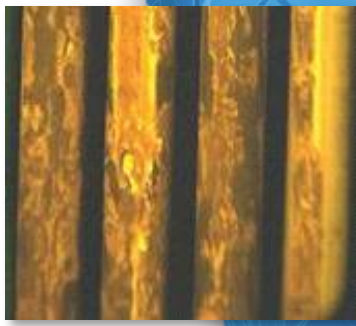
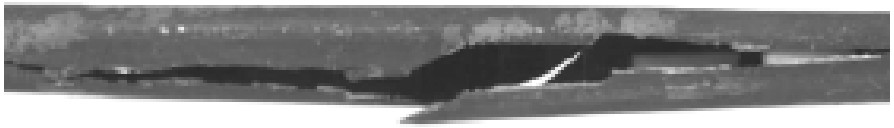
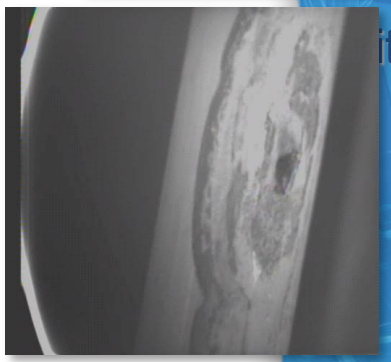
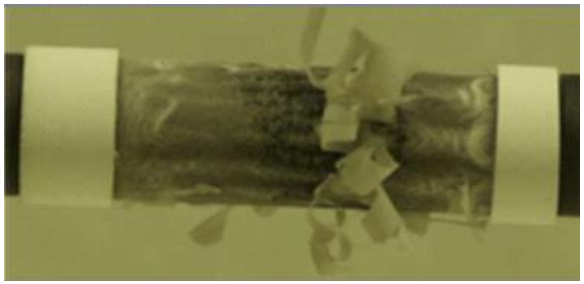
Challenge Problem Applications

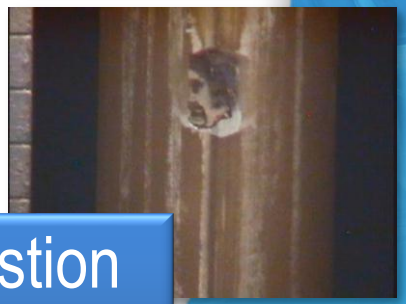
- Specifications of challenge problems (POR1)
- Development of 3x3 problem geometry and models (POR1)
- Coupled CRUD L1 milestone (POR2/3)
- GTRF CFD applications (POR2)







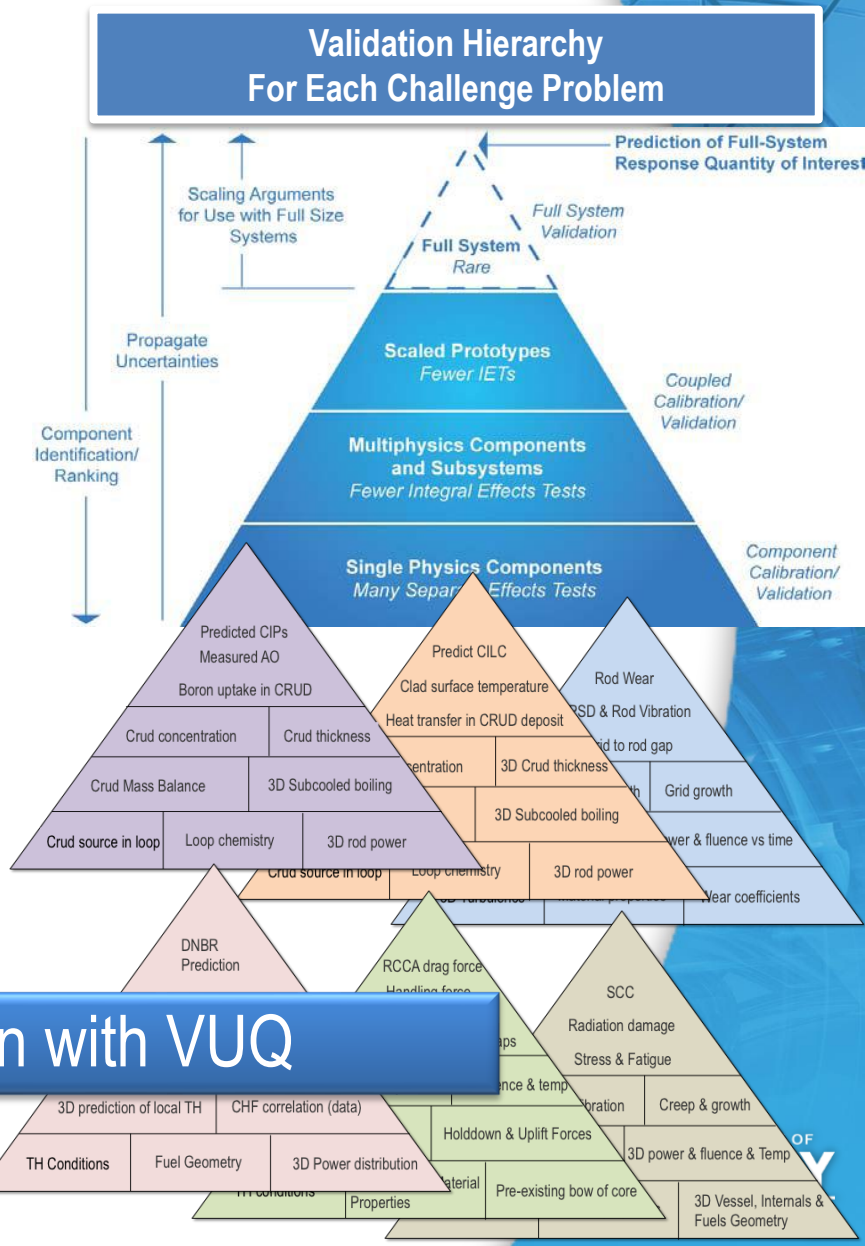




Good interaction across Focus Areas – Question on if we will really address all of the challenge problems in first five years

Validation

- Established an initial validation plan to guide validation methodology and data requirements
- Integral validation against physical reactor operation data
- An approach was proposed for validation for each challenge problem:
  - Define case specification
  - Design and develop database requirements
  - Perform initial qualitative validation
  - Develop quantitative validation
  - Completion of validation with recommendation for application
- Closely connected with validation data needs, also being developed by VUQ



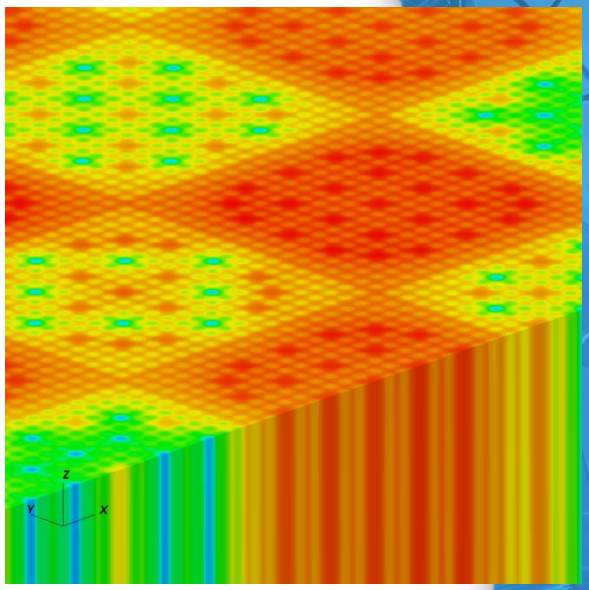
AMA has good connection with VUQ

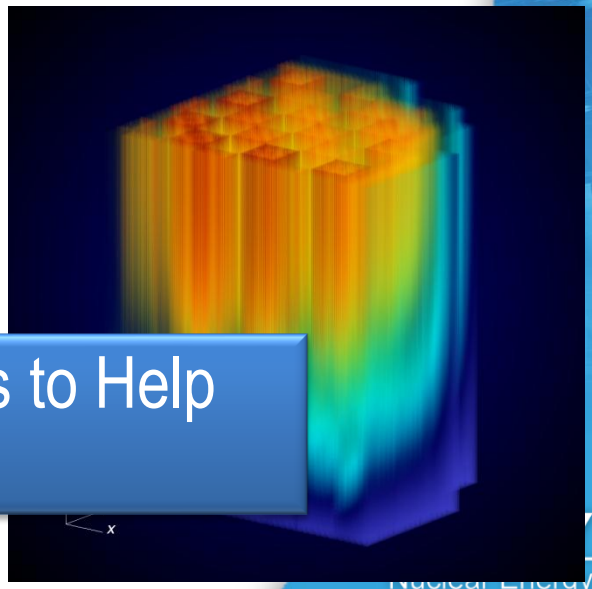
NRC Engagement

- Inform, discuss, and exchange information with NRC Staff on CASL activities, approaches, and developments
  - Familiarize NRC with CASL R&D and use of advanced M&S for nuclear reactors
  - Seek feedback and exchange on scope of work, developments, and approaches
- Approach: Engage with NRC Office of Regulator Research (RES)
  - Interface with RES in development of new M&S capabilities
  - Longer term industry interfaces with NRR in the approval of new M&S capabilities

Additional AMA Activities

- Exercising codes to understand usability, capabilities, etc
  - DENOVO
  - DeCART
  - SCALE
- Development of benchmark progression problems to support demonstration to physical reactor
- Investigation of cross section processing issues and accuracy
- Collaboration with VRI and IC on use case development
- Development of approach for CASL products



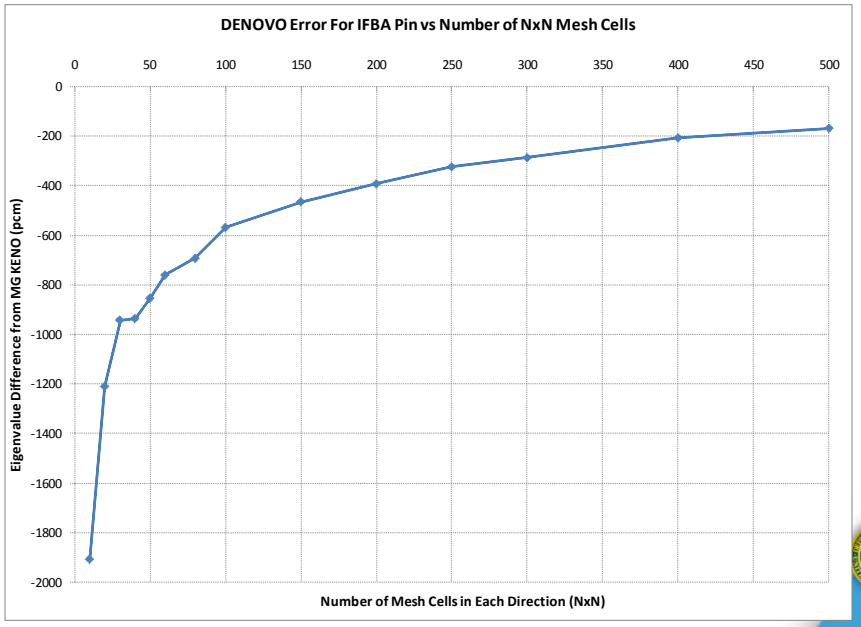


This Work has Highlight Some Issues to Help Guide Decisions

Example: Modeling IFBA with Cartesian Mesh

- IFBA is a very thin coating of ZrB_2 used in many PWRs
  - < 10 micron thickness
  - 50% enriched B-10
- DENOVO uses a Cartesian mesh, typically <10x10 per pin
- To obtain 200 pcm accuracy, DENOVO requires 400x400 mesh
- Fresh UO_2 only - depletion still unaddressed

Code	Groups	k-eff	diff (pcm)
MCNP	CE	0.94913	97
KENO	CE	0.94816	--
	60	0.94829	13
NEWT	999	0.94493	-323
	60	0.94582	-234
DENOVO	60	0.94662	-1909
DECART-AMPX	60	0.94710	-106



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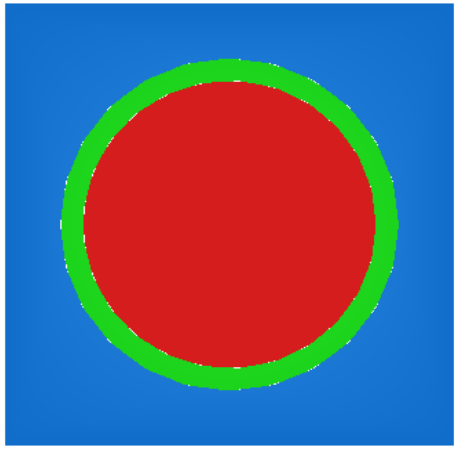
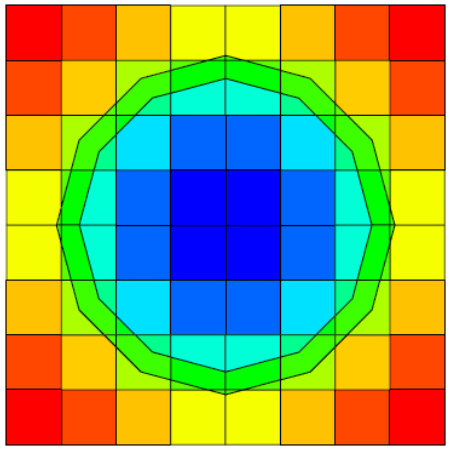
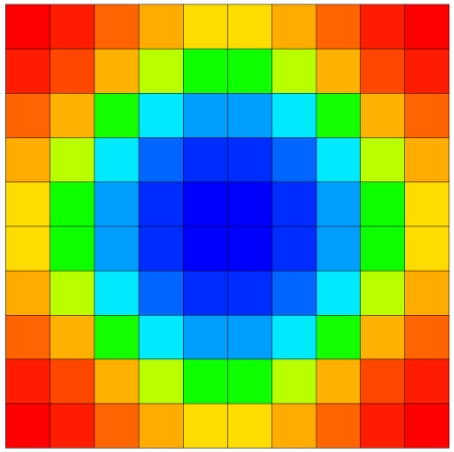
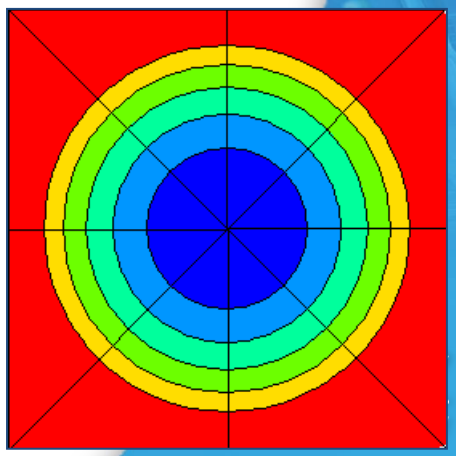
Benchmark Progression to Physical Reactor Modeling

- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #4 HZP 3x3 Assembly CRD Worth
- **#5 Physical Reactor Zero Power Physics Tests (ZPPT)** — Sep 30
- #6 HFP BOL Assembly
- #7 HFP BOC Physical Reactor w/ Xenon
- **#8 Physical Reactor Startup Flux Maps**
- **#9 Physical Reactor Depletion**
- #10 Physical Reactor Refueling
- Challenge Problems Analysis

Problem #1 Results

Code	Energy Groups	ENDF/B-VI Eigenvalue	ENDF/B-VI Diff (pcm)	ENDF/B-VII Eigenvalue	ENDF/B-VII Diff (pcm)
MCNP5†	CE	--	--	1.3283	227
KENO-VI†	***CE***	***1.3221***	***--***	***1.3260***	***--***
	238	1.3181	-406	1.3217	-431
	49	1.3168	-536	1.3214	-457
NEWT	238	1.3178	-437	1.3217	-434
	49	1.3164	-570	1.3209	-507
DENOVO	49	1.3165	-562	1.3211	-494
DECART-AMPX	49	1.3166	-550	1.3211	-494
DECART	47	1.3221	-5	--	--

†All KENO-VI uncertainties are < 21 pcm. MCNP5 uncertainty is 14 pcm.

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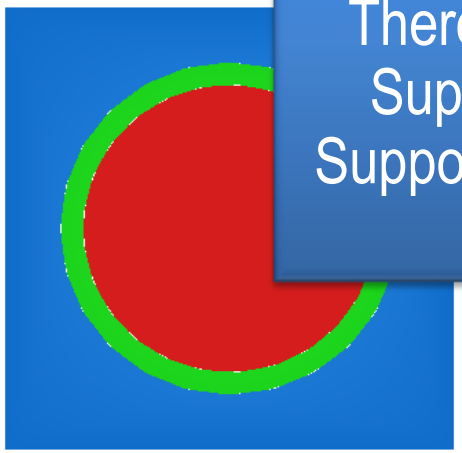
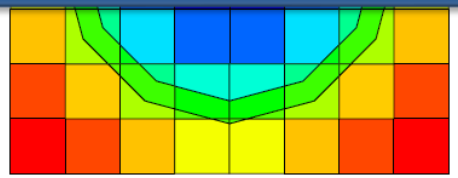
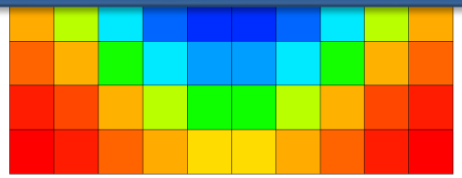
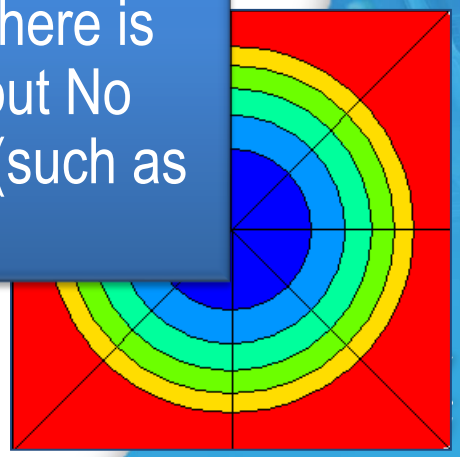
There is a Gap in Cross Section Methods – There is Support under VRI for Software Integration but No Support to Address Methods Accuracy Issues (such as this 500 pcm discrepancy)

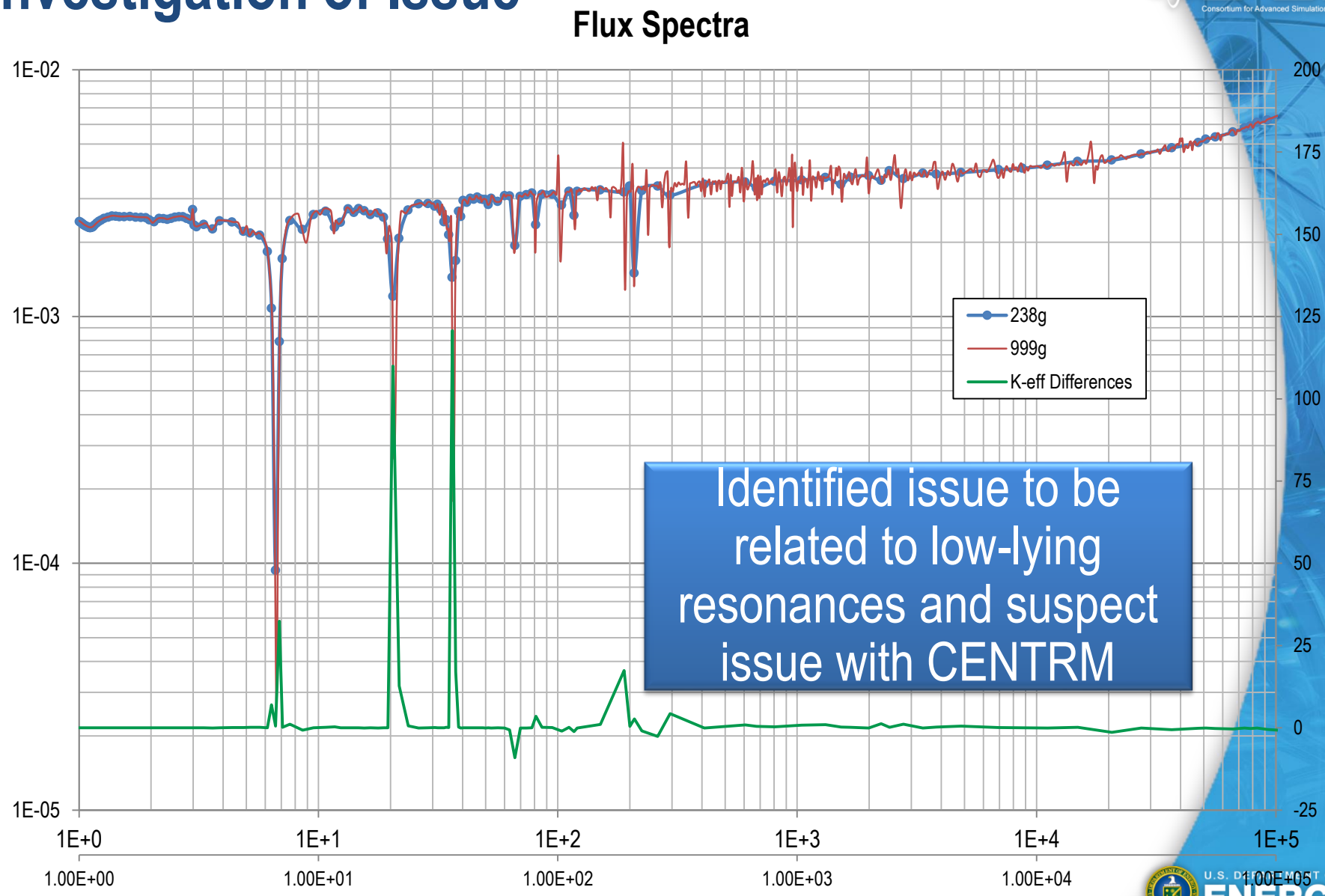








Investigation of Issue



Identified issue to be related to low-lying resonances and suspect issue with CENTRM

Product Focused View of VERA

- Addressing challenge problems is not fully sufficient to provide a useful capability for stakeholders (e.g. industry)
- "Usability" is very important and we have been discussing this with VRI (but it is like the weather)
- Need to distinguish "product development" from "research" (research informs decisions on methods/approaches for the VERA product)
  - Levels of product development need to be considered
  - Near term "product" should focus on a near-term "basic" core simulation capability
  - Allows development of user interfaces (input and output), coupling, provides capabilities to users, and allows research to take it's course
  - Follows a "product life cycle"

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Product Focused View of VERA

- Addres a useful capabil
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  - Level
  - Near apability
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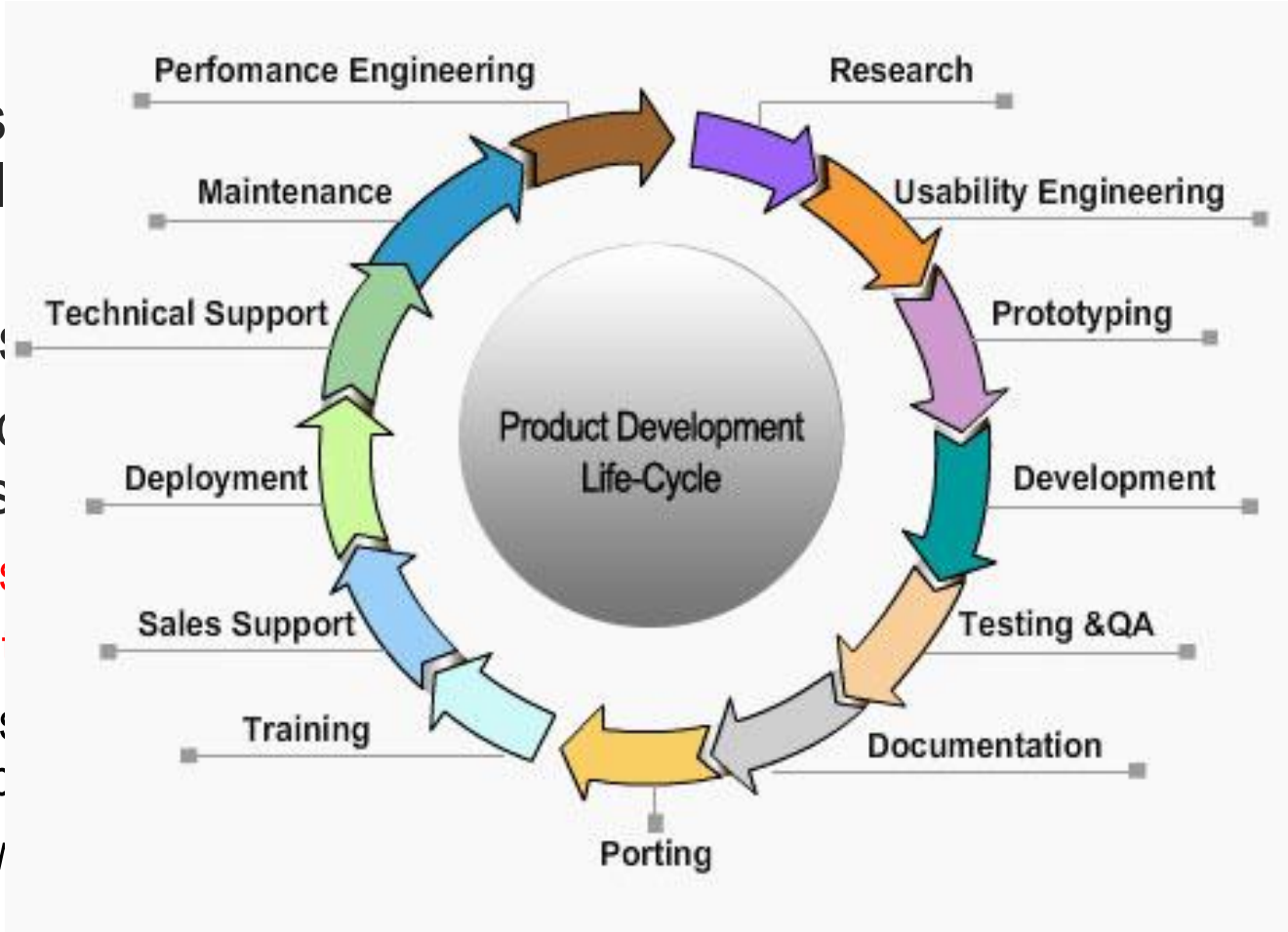

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AMA Discussion Topics

- Development and implementation of PCMM – Steve Hess
- Product Description – Rose Montgomery
- Assessment of Status of Integrated Virtual Reactor Simulation – Scott Palmtag

- Physical reactor data measurements and needs – Rose Montgomery

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Assessment of the Status of Integrated Virtual Reactor Simulation

Scott Palmtag
AMA

CASL Roundtable Meeting

August 9-11, 2011

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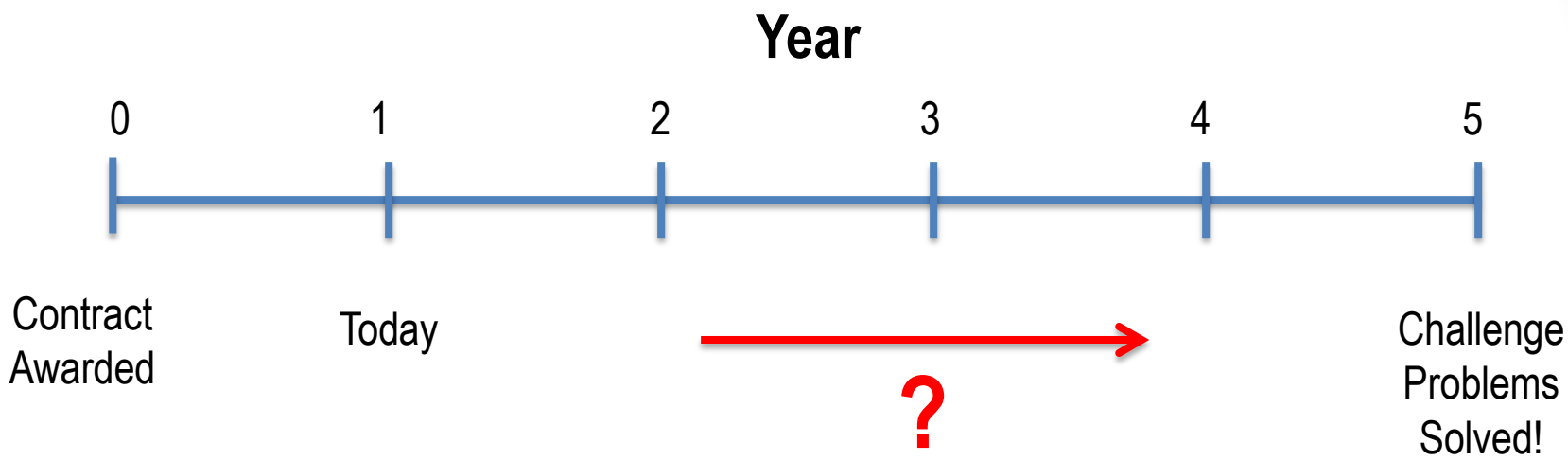
CASL Timeline



How do we get there?

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What do we Need to Solve Challenge Problems?

CIPS/CILC

- CRUD accumulation and depletion
- Steaming Rates
- Chemistry Models

GTRF

- Fluence Accumulation
- Structural Models
- T/H Forces

PCI

- Pin Power History
- Fuel Performance Models

FAD

- Fluence Accumulation
- Structural Models

DNB

- Pin Power
- Local T/H Conditions

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- Local T/H Conditions

Items in Red provided by Core Simulator!

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Basic Core Simulator Components (Integrated Virtual Reactor Simulation)

1. Input processor with common geometry for all codes
2. T/H Solver (Subchannel + CFD)
3. Cross Sections
4. Neutronic Solver
5. Infrastructure (control rod movement, detectors, boron search, etc.)
6. Fuel Performance (Fuel temperatures, Stress/Strain, gap)
7. Depletion (including Xe/Sm)
8. Output processor to calculate peaking factors, DNB margins, etc.

It is much more than just neutronics!

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Development Paths for Core Simulator

- Nodal Methods – ANC/VIPRE/BOA
  - Provides near-term solution
  - Does not provide acceptable pin resolution
  - Limited distribution - composed of proprietary codes
  - Can run on a desktop
- DECART/STAR-CCM+
  - Provides near-term solution
  - May have accuracy issues with the treatment of axial direction
  - Open or Limited Distribution?
  - Can run on medium-sized cluster
- DENOVO/SCALE
  - Needs a lot of development
  - Provide highest fidelity solution needed for Challenge Problems
  - Open Distribution
  - Needs Supercomputer

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DENOVO/SCALE Development Status

1.	Input Processor	Not Started
2.	T/H Solver	Subchannel solver not started
3.	Cross Sections	Accuracy Issues
4.	Neutronic Solver	Accuracy Issues (IFBA/GAD)
5.	Infrastructure	Not Started
6.	Fuel Temperatures	Not Started
7.	Depletion/Xe/Sm	Not Started
8.	Output Processor	Not Started

Needs work!

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Conclusion

- Need to choose development path(s) for CASL and align resources to needs
- Current funding is focused on research problems (CFD, transport methods, high-fidelity fuel performance)
- No funding appears to be spent on basic core simulator functionality
- We need better methods <u>and</u> functionality to solve Challenge Problems!

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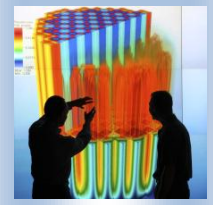

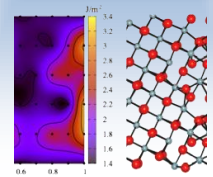

Application of Predictive Capability Maturity Model (PCMM) to VERA

Stephen M. Hess
AMA Deputy FA Lead
CASL Roundtable
North Carolina State University
Raleigh, NC
10 August 2011

Consortium for Advanced Simulation of LWRs

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OAK RIDGE National Laboratory

VERA Capabilities Assessment

- Need: To achieve acceptance of VERA by all stakeholders a formal method to evaluate VERA capabilities and maturity against requirements specified in VRD is required
- During POR-2 a draft procedure / accompanying checklists to achieve this objective were developed by AMA
  - Hosted working meeting to review procedure and assessment checklists during June co-location meeting to obtain input from CASL FAs
  - Developed initial draft procedure to perform and accompanying checklists to document evaluations
    - Validation of Components (VRDCL-C_00)
    - Validation of VERA (VRDCL-V_00)
  - Due to insufficient maturity of VERA 1.0 did NOT apply assessment at this time
- Identified need to develop more formal review / validation of requirements to ensure consistency / accuracy of evaluation
  - PCMM identified as likely candidate to meet this need

Example Checklist Information (1 of 2)

Component Being Assessed

Title: _____

Version: _____ **Date:** _____ **Focus Area:** _____

Short Description: _____

List of Component Documentation

Ref #	Title	Date	Revision	Reference ID
1				
2				

Ownership Record

Prepared By: _____ **Date:** _____

Reviewed By: _____ **Date:** _____

Approved By: _____ **Date:** _____

Record of Revision

Date:	Revision:	Section:	Description:

Example Checklist Information (2 of 2)

1.0 Physical Model VRD Assessment [3.1]

(Note – in this checklist, numbers in brackets (e.g. [X.X]) refer to the corresponding section of the VERA Requirements Document.)

Assessment questions are introduced with a box at the end to enter a grade for how well a requirement is met. For each requirement, assign an assessment graded from 0 to 2.

0 – Not Met,

1 – Partially Met,

2 – Sufficiently Met.

Initial proposal for three levels of evaluation / maturity

After entering a grade, please provide comments on why the requirement was not, partially or sufficiently met.

1.1 Physical models used for this component [3.1]

List all of the physical models and provide references to the theory, formulation, validation and validation data.

Physical Model	**Reference** (*Use page numbers and Ref [#] from List of Component Documentation*)			
	Theory	**Formulation**	**Verification**	**Validation**
<Physical Model A>				
<Physical Model B>				
<Physical Model C>				

The following sections will be repeated and numerically incremented for each physical model identified in the table above.

PCMM Integration into VERA Capability Assessment

- Integrated set of milestone projects to be conducted as joint AMA / VUQ efforts during POR-3 / POR-4
- Investigation to customize PCMM for CASL application (AMA lead / POR-3)
  - Initial working meeting at CASL Roundtable AMA Session (August 2011)
  - Finalize draft PCMM and select first use application by 30 September 2011
- Initial demonstration of PCMM to VERA application (VUQ lead / POR-4)
  - AMA will update VERA evaluation procedure / accompanying checklists to incorporate lessons learned from initial application of PCMM to VERA

PCMM Overview

- PCMM provides a tool for assessing and communicating progress in predictive capability for modeling and simulation.
- Evaluates maturity as matrix of maturity of specific elements
  - M&S elements
  - Maturity levels
  - Assessment criteria
- **Session Objective: Review PCMM constituents for applicability to assess maturity of VERA and its components**

MATURITY / ELEMENT	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and BCs	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built", e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&C) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have an unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive sensitivity analyses conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

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Validation and Uncertainty Quantification (VUQ)

Jim Stewart (SNL)
Dana Kelly (INL)

1st Annual CASL Roundtable Meeting
North Carolina State University
August 9-11, 2011

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VUQ Team: Who we are

- **SNL:** Jim Stewart (VUQ Lead), Brian Adams, Bill Rider, Mike Eldred, Kevin Copps, Jim Kamm, Greg Weirs, others
- **NCSU:** Dan Cacuci, Hany Abdel-Khalik, Ralph Smith, others
- **INL:** Dana Kelly (VUQ Deputy Lead), Nam Dinh, Kim Mousseau, Hongbin Zhang, others
- **LANL:** Brian Williams, others
- Support from many others across CASL

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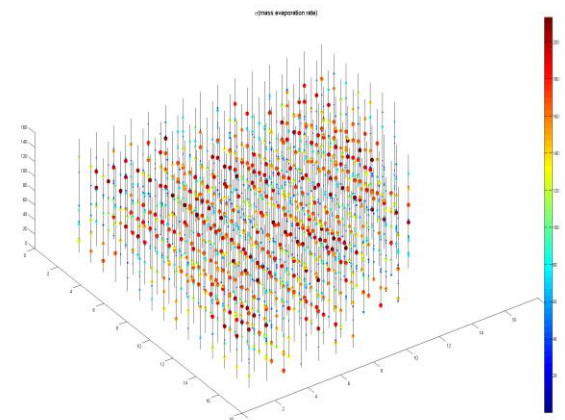
Validation and Uncertainty Quantification (VUQ)

Achieving credible, science-based predictive simulation capabilities

Objectives and Strategies

- VUQ is dedicated to developing overall V&V approach
- VUQ will provide CASL with
  - Best-estimate *predictive capabilities* with reduced uncertainties
  - Capability for quantified *predictive maturity* assessments
- The Sensitivity Analysis & UQ process will guide CASL R&D investments, and aid in designing future experiments



Uncertainty in boiling rate throughout quarter core model

Requirements Drivers

- V&V and UQ methodologies and tools are needed by every Focus Area
- VUQ is the CASL "integrator;" we need:
  - Access to software and underlying math models
  - Validation data (at all physical scales)
  - Partnerships with other Focus Areas to implement uniform VUQ practices

Outcomes and Impact

- Continuous evolution towards *transformational, predictive computational simulation*
- Capability to quantify and reduce uncertainties for the CASL challenge problems
- New ways for experiments and simulations to work together, leading to predictions *with quantified confidence* of scenarios for which experimental data is not directly available

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Validation and Uncertainty Quantification (VUQ)

Jul-Dec 2010 Plan of Record

Activities

- Develop a VUQ case study application
- Integrate DAKOTA as library component in VERA
- Develop initial CASL validation data review
- Implement first-order reduced-order modeling approach based on the Efficient Subspace Method (ESM) into selected neutronics code (Denovo)
- Document CASL verification workflows

Budget

- Project 1 (V&V and Data Assimilation through Model Calibration): $1,481K *(total for Year 1)*
- Project 2 (Sensitivity Analysis and UQ): $1,117K (*total for Year 1)*

Challenges and Risks

- Ability to appropriately define the VUQ case study application (relevance to CASL challenge problem)
- Early readiness of VERA for integration with DAKOTA
- Availability of simulation software (from AMA, VRI, and MNM) required by VUQ to complete its tasks

Milestones

- L2: Integrate DAKOTA into VERA (12/31/10)
  - L3: Develop a verification workflow and toolset requirements
  - L3: Complete initial review of experimental data and plant observations related to CRUD and GTRF challenge problems
  - L4: Quantify contribution of cross-section uncertainties for representative PWR model
  - L4: Report on theoretical applicability of verification to standard TH models and methods

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Validation and Uncertainty Quantification (VUQ)

Jan-Jun 2011 Plan of Record

Activities

- Establish VUQ-led committees
  - Cross-FA Working Group
  - Validation Data Committee
- Complete SA, Calibration, and UQ on VUQ case study application
- Develop VUQ procedures and workflows
- Interface Percept to VERA
- Develop CASL validation data requirements plan

Budget

- Project 1 (V&V and Data Assimilation through Model Calibration): $1,481K *(total for Year 1)*
- Project 2 (Sensitivity Analysis and UQ): $1,117K (*total for Year 1)*

Challenges and Risks

- Availability of required validation data
- Ability to effectively partner with other focus areas to implement V&V practices and integrate VUQ capabilities

Milestones

- L2: Enable statistical sensitivity and UQ demonstrations for VERA (3/31/11)
  - L3: Apply SA and UQ capabilities to VUQ case study application
- L2: Enable generalized data assimilation and model calibration for VERA (6/30/11)
  - L3: Develop mathematical data assimilation framework
  - L3: Develop a VUQ practices document

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The Three "VUQ Thrusts" Emanating from Year 1 of CASL

1. Enabling Sensitivity Analysis, UQ, Data Assimilation and Validation for VERA
2. Enabling Code and Solution Verification for VERA
3. Validation Data Assessments and Requirements

These thrusts are further explored in the next three presentations

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VUQ Thrust 1: Enabling Sensitivity Analysis, UQ, Data Assimilation and Validation for VERA

- CASL Challenge Problem Supported: Crud-Induced Power Shift (CIPS)
- VUQ milestones supporting this work
  - PoR-1: VUQ.P1.01 (Integrate DAKOTA into VERA)
  - PoR-2: VUQ.P2.02 (Enable generalized data assimilation and model calibration…)
  - PoR-2: VUQ.P2.03 (Enable statistical sensitivity analysis and UQ demonstrations…)
  - PoR-2: VUQ.VVDA.P2.03 (Develop a VUQ practices document)
  - PoR-2: VUQ.SAUQ.P2.01 (Apply SA and UQ capabilities to VUQ Case Study…)
- Close collaboration with AMA and VRI Focus Areas
- Key personnel:
  - SNL: Brian Adams and Walt Witkowski
  - LANL: Brian Williams
  - NCSU: Dan Cacuci, Ralph Smith, and Hany Abdel-Khalik

--Westinghouse: Yixing Sung

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VUQ Thrust 2: Enabling Code and Solution Verification for VERA

- CASL Challenge Problem Supported: Grid-to-Rod Fretting (GTRF)
- VUQ milestones supporting this work
  - PoR-1: VUQ.VVDA.P1.04 (Develop a verification workflow and toolset requirements)
  - PoR-2: VUQ.VVDA.P2.03 (Develop a VUQ practices document)
  - PoR-2: VUQ.SAUQ.P2.02 (Develop and document verification guidelines for SA/UQ…)
  - PoR-2: VUQ.VVDA.P2.04 (Integrate Percept into VERA; apply to a verification demo)
  - PoR-2: VUQ.VVDA.P2.05 (Complete assessment of verification applicability of T-H…)
- Close collaboration with VRI, THM, MPO and AMA Focus Areas
- Key Personnel
  - SNL: Bill Rider, Kevin Copps, Jim Kamm, Greg Weirs, Walt Witkowski
  - NCSU: Hany Abdel-Khalik

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VUQ Thrust 3: Validation Data Assessments and Requirements

- CASL Challenge Problems Supported: Crud and GTRF
- VUQ milestones supporting this work
  - PoR-1: VUQ.VVDA.P1.02 (Complete initial review of experimental and plant observations related to Crud and GTRF challenge problems)
  - PoR-2: VUQ.VVDA.P2.02 (Design and develop validation database requirements)
- Close collaboration with AMA Focus Area
- Key Personnel
  - INL: Nam Dinh

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VUQ Path Forward
Thru FY12 (PoR-3, PoR-4, PoR-5)

Themes for FY12

- Challenge problem focus
  - Continue deployment of methods/capabilities for Crud, GTRF; Begin work on PCI
- New algorithm development/deployment
  - UQ/SA: Hybrid stochastic/deterministic methods, new scalable methods, DAKOTA deployment for multiphysics problems, epistemic (model-form) uncertainties
  - Data assimilation: Rubens and DAKOTA; progression of capabilities to nonlinear, multiphysics regimes
  - Verification: Continue emphasis on solution verification, including interface coupling verification
- Validation data
  - Acquisition, qualification, archiving (CASL Validation Data Committee)
- Predictive maturity assessments (PCMM)

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VUQ Path Forward

Thru FY12 (PoR-3, PoR-4, PoR-5)

PoR-3 L3 Milestones

- Uncertainty management hybridization framework
- Scalable UQ algorithm deployment
- Initial UQ roadmap for CASL
- GTRF CFD-to-mechanics data transfer verification
- VUQ Working Group report on predictive-simulation definitions and GTRF VUQ activities

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VUQ Path Forward
Thru FY12 (PoR-3, PoR-4, PoR-5)

Anticipated PoR-4 Milestones *(partial list; planning in progress)*

- Calibration/validation of separate-effects physics for Crud index prediction (e.g., BOA, ANC, VIPRE-W)
- Report on CASL approach for validation data planning
- Initial PCMM assessment for Crud (collaboration with AMA)

Anticipated PoR-5 Milestones *(partial list; planning in progress)*

- Calibration/validation of integral-effects physics for Crud index
- UQ algorithm development for epistemic (model-form) uncertainties
- New data assimilation capabilities accounting for model-form errors and nonlinear effects

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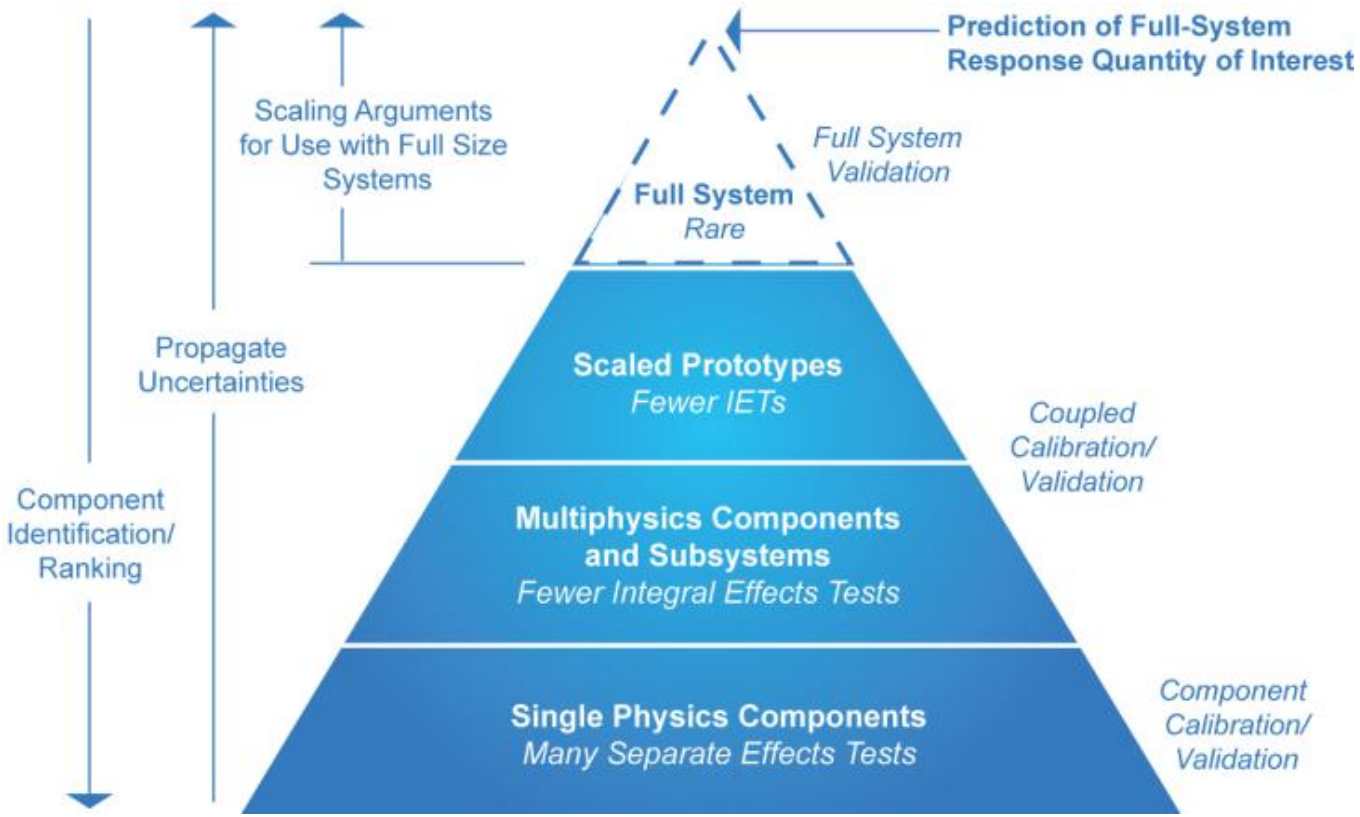
The validation hierarchy integrates all CASL Focus Areas, executed in a bottom-up and top-down way



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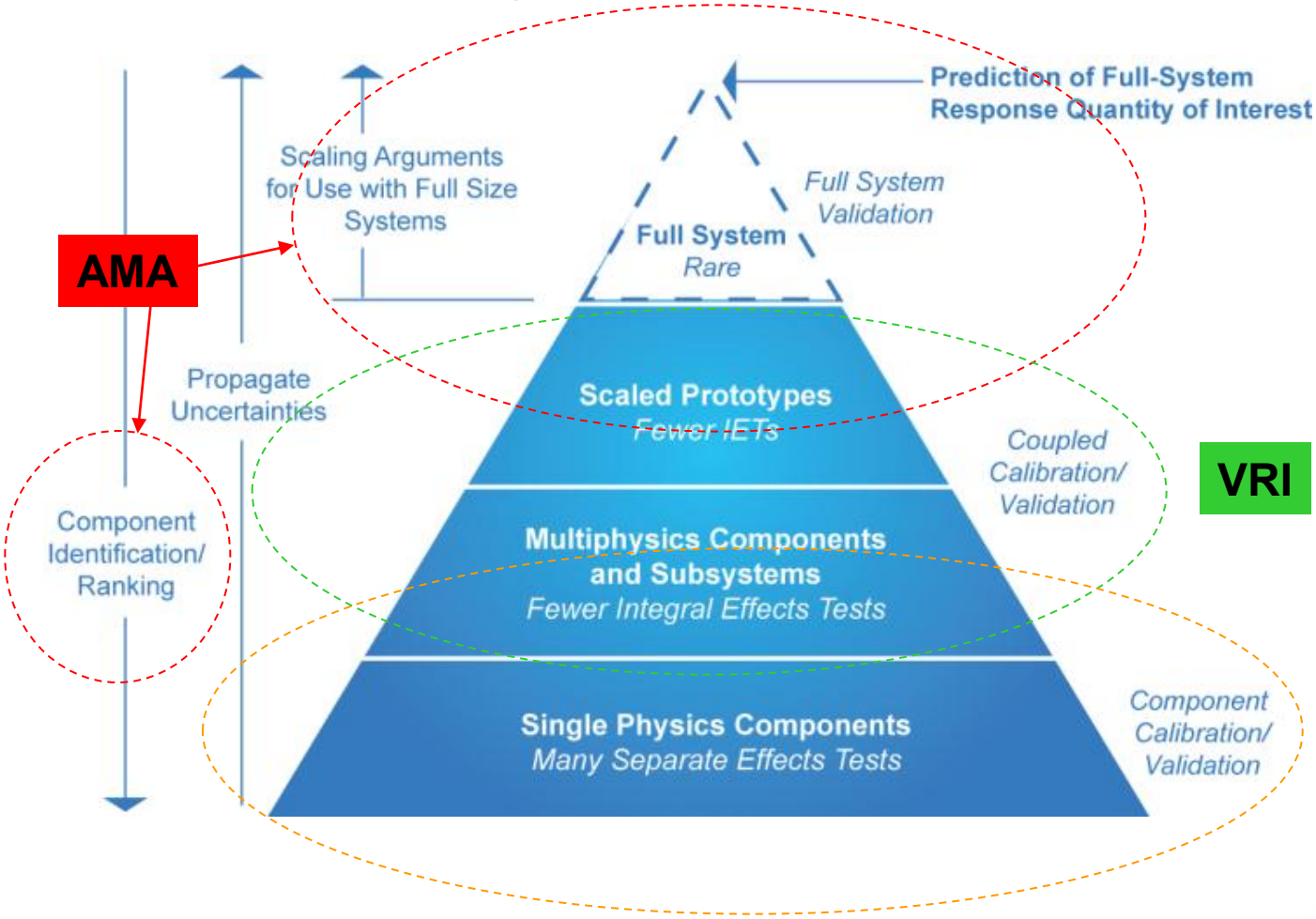

VUQ Activities for CIPS

Brian Adams (VUQ, SNL)
Brian Williams (VUQ, LANL)
Yixing Sung (AMA, Westinghouse)
Jim Stewart (VUQ, SNL)

August 11, 2011

1st Annual CASL Round Table Meeting
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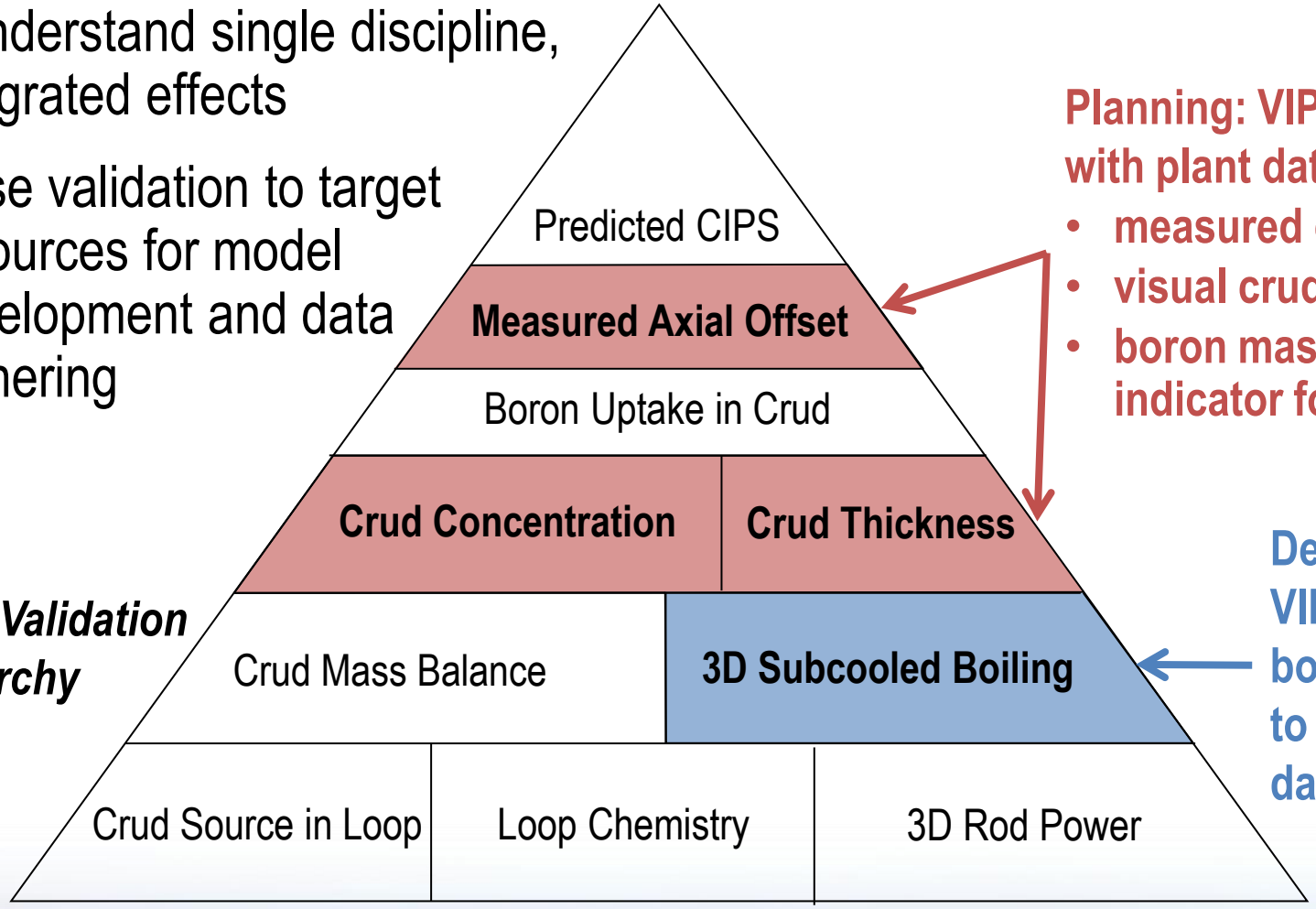
Toward CIPS Predictive Capability: Validated Effects Throughout Hierarchy

- Understand single discipline, integrated effects
- Use validation to target resources for model development and data gathering



CIPS Validation Hierarchy

Planning: VIPRE-W + BOA with plant data for

- **measured crud thickness**
- **visual crud index**
- **boron mass, a direct indicator for CIPS risk**

Demonstrated: VIPRE-W with boiling compared to crud index data

Related VUQ Highlights from Year One (many tracked in cross-FA milestones)

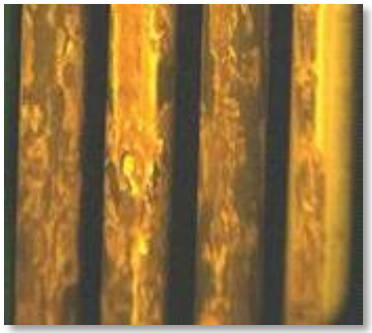
- Evolutionary DAKOTA integration in VERA:
  - Loose (file system) coupling to VIPRE-W
  - Tight LIME coupling for demo multi-physics problem
- RUBENS data assimilation framework
- Verification guidelines for SA and UQ results
- VERA releases, including Westinghouse codes; port software to SNL
- VUQ support/consulting:
  - Engaged Westinghouse (Columbia) on SA/UQ for GTRF and optimization for mixing vein design
  - Engaged SCALE group on DAKOTA for forward SA/UQ analyses

Staged VUQ deployment: simultaneously

- mature software tools and interfaces
- demonstrate on early codes and challenge problem applications
- integrate into VERA

Completed Crud-related VUQ/VIPRE-W Studies: Demo SA, UQ, Calibration, Validation

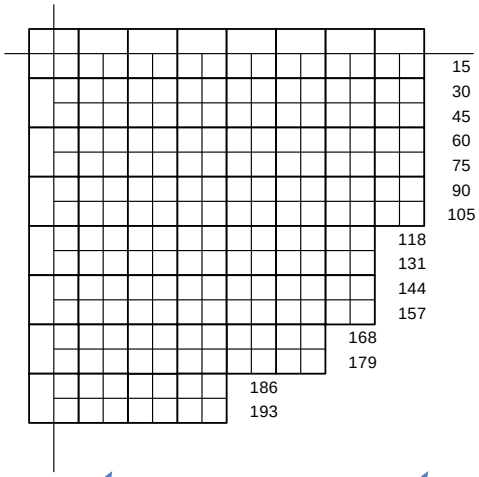
- GOAL: Demonstrate VUQ approaches with VERA components for challenge problem impact; transfer workflow to AMA
- Specifically: study model form and core operating parameters with VIPRE-W prediction of boiling and crud index data
  - Select case study plants and characterize uncertainties
  - Loose-couple DAKOTA and GPMSA with VIPRE-W
  - Select VUQ algorithms
  - Perform iterative studies and analyze results
  - Prepare report; transfer infrastructure to Westinghouse



crud deposits

Demonstration Problems: Westinghouse-designed four-loop PWRs

- "PWR Plant A": AMA-defined reference plant for CASL
- "PWR Plant B": plant with prior CIPS occurrence with available crud-related measurements (validation data)
- Simulate with Westinghouse VIPRE-W T-H
- 193 flow channels (shown) each representing quarter assembly; 93 nodes (50mm nodal spacing) axially (not shown)
- Output of interest: mass evaporation rate "m-dot-e", indicative of localized boiling and predictive of crud



quarter-core geometry and axial layout

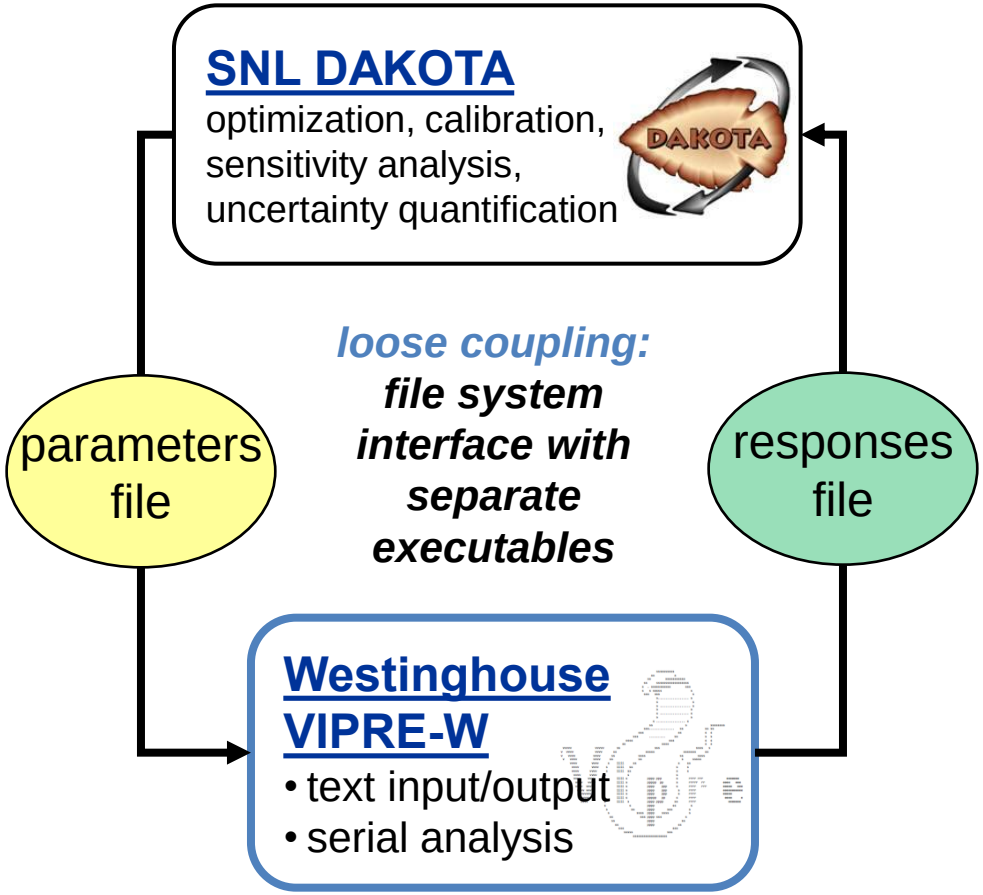
Plausible Uncertainty Specifications are Crucial for UQ and Validation!

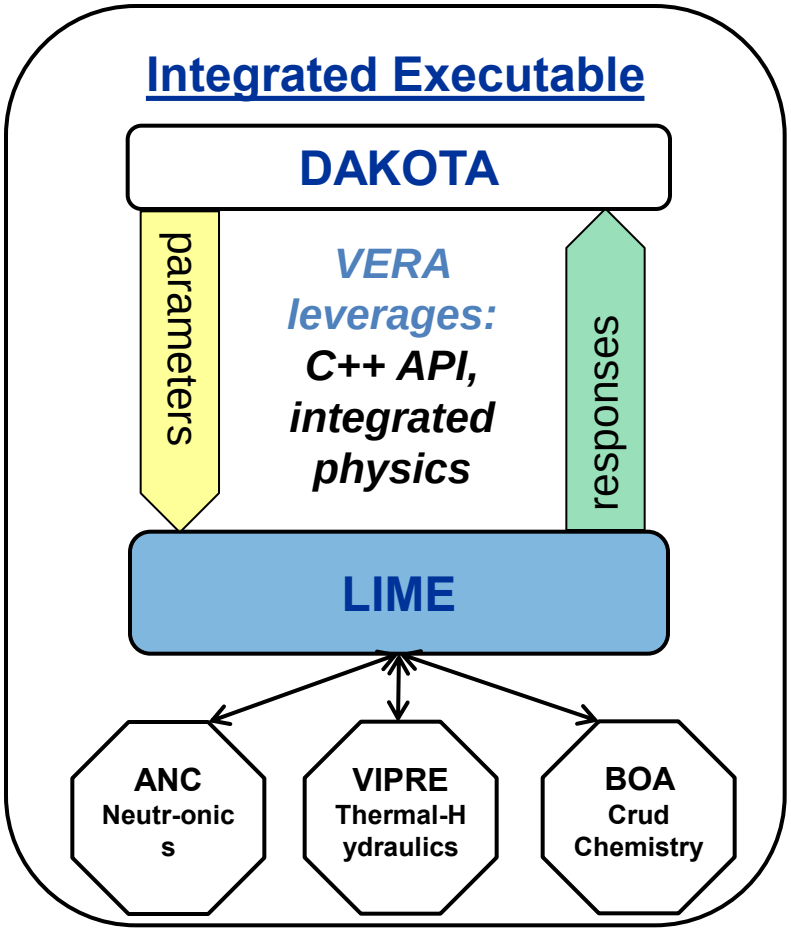
- Characterize plant core operating uncertainty, based on operational limits or expert judgment, e.g.,

Parameter	Mean	Standard Deviation	Lower Bound (truncation)	Upper Bound (truncation)
power	67.88742	0.20366226	67.48009548	68.29474452
flow	15.93387	0.1593387	15.6151926	16.2525474
temperature	556.4	2.5	551.4	561.4
pressure	2270	25	2220.0	2330.0

- Similar for model form parameters (Dittus-Bolter, axial friction, and lateral resistance correlations, grid heat transfer, partial boiling model, subcooled void model, etc.)
- Study derived m-dot-e metrics: {maximum, mean, number nonzero nodes, mean over nonzeroes} of mass evaporation rate

DAKOTA/GPMSA to VIPRE-W Interface Based on Input Templates and Script-based Post-processing





Current → Move from potentially fragile, study-specific script interfaces to a unified, user-friendly capability → *Future*

Demonstrate Various VUQ Algorithms from DAKOTA and GPMSA for AMA

Global sensitivity analysis (SA):

- Latin hypercube sampling: partial correlation coefficients, scatter plots;
- Morris one-at-a-time (MOAT): main, interaction effects
- Polynomial chaos expansions (PCE): analytic Sobol' indices.

Global uncertainty quantification (UQ):

- Latin hypercube sampling: means, standard dev, empirical histograms
- Polynomial chaos expansions: analytic mean and standard deviations.

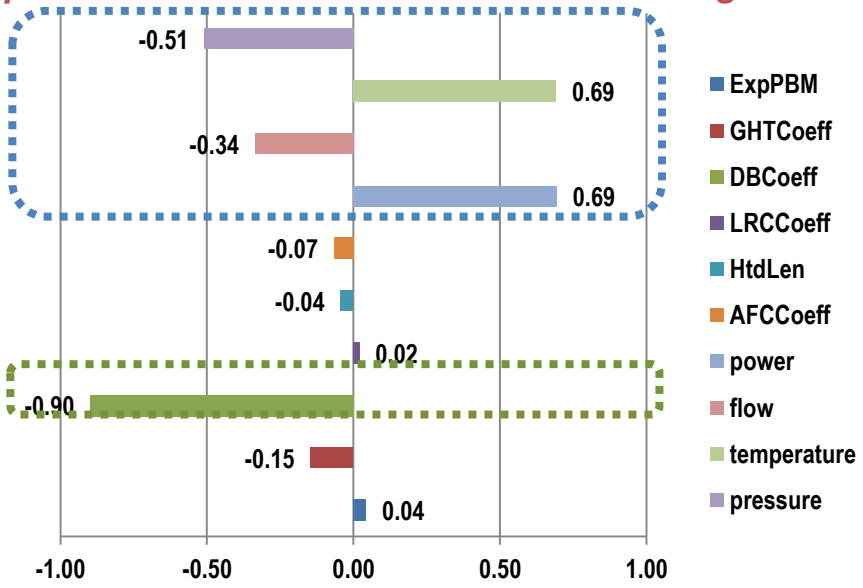
Bayesian Calibration

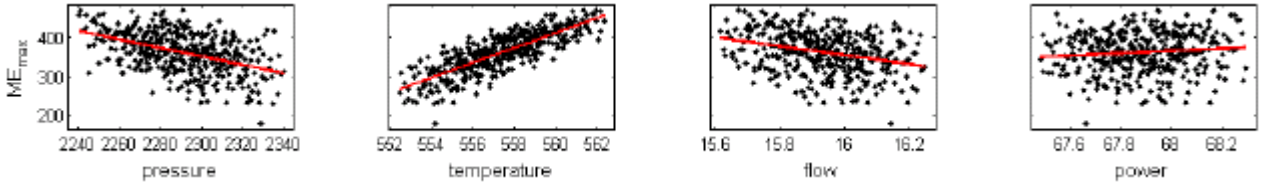
- Direct model evaluation and Gaussian process surrogate approaches
- Calibrate, estimate discrepancy, judge model validity accounting for uncertainties

SA Assesses Parameter Influence on Boiling Rate; Crucial for Screening (Prioritization)

- DAKOTA correlation coefficients: strong influence of core operating parameters (pressure more important than previously thought)
- Dittus-Bolter correlation model may dominate model form sensitivities (also nonlinear effects of ExpPBM)
- Scatter plots help visualize trend in input/output relationships

parameter influence on number of boiling sites



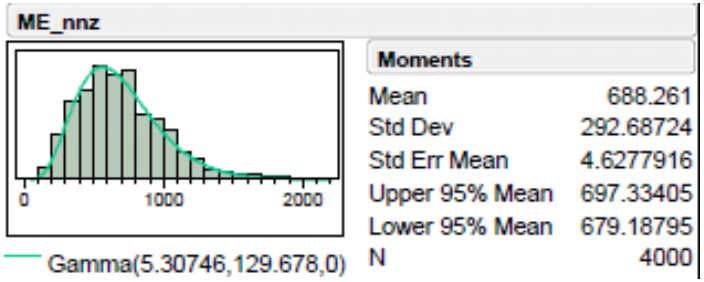


sensitivity of mass evaporation rate (max) to operating parameters

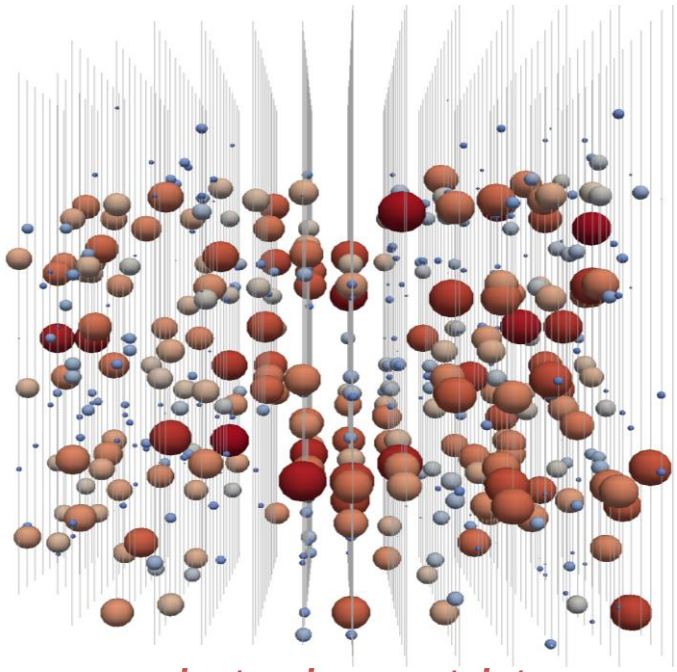
Demonstrate Possible UQ Outcomes

Method	ME_nnz		ME_meannz		ME_max	
	Mean	Std Dev	Mean	Std Dev	Mean	Std Dev
LHS (40)	651.225	297.039	127.836	27.723	361.204	55.862
LHS (400)	647.33	286.146	127.796	25.779	361.581	51.874
LHS (4000)	688.261	292.687	129.175	25.450	364.317	50.884
PCE (Θ(2))	687.875	288.140	129.151	25.7015	364.366	50.315
PCE (Θ (3))	688.083	292.974	129.231	25.3989	364.310	50.869
PCE (Θ (4))	688.099	292.808	129.213	25.4491	364.313	50.872

mean and standard deviation of key metrics



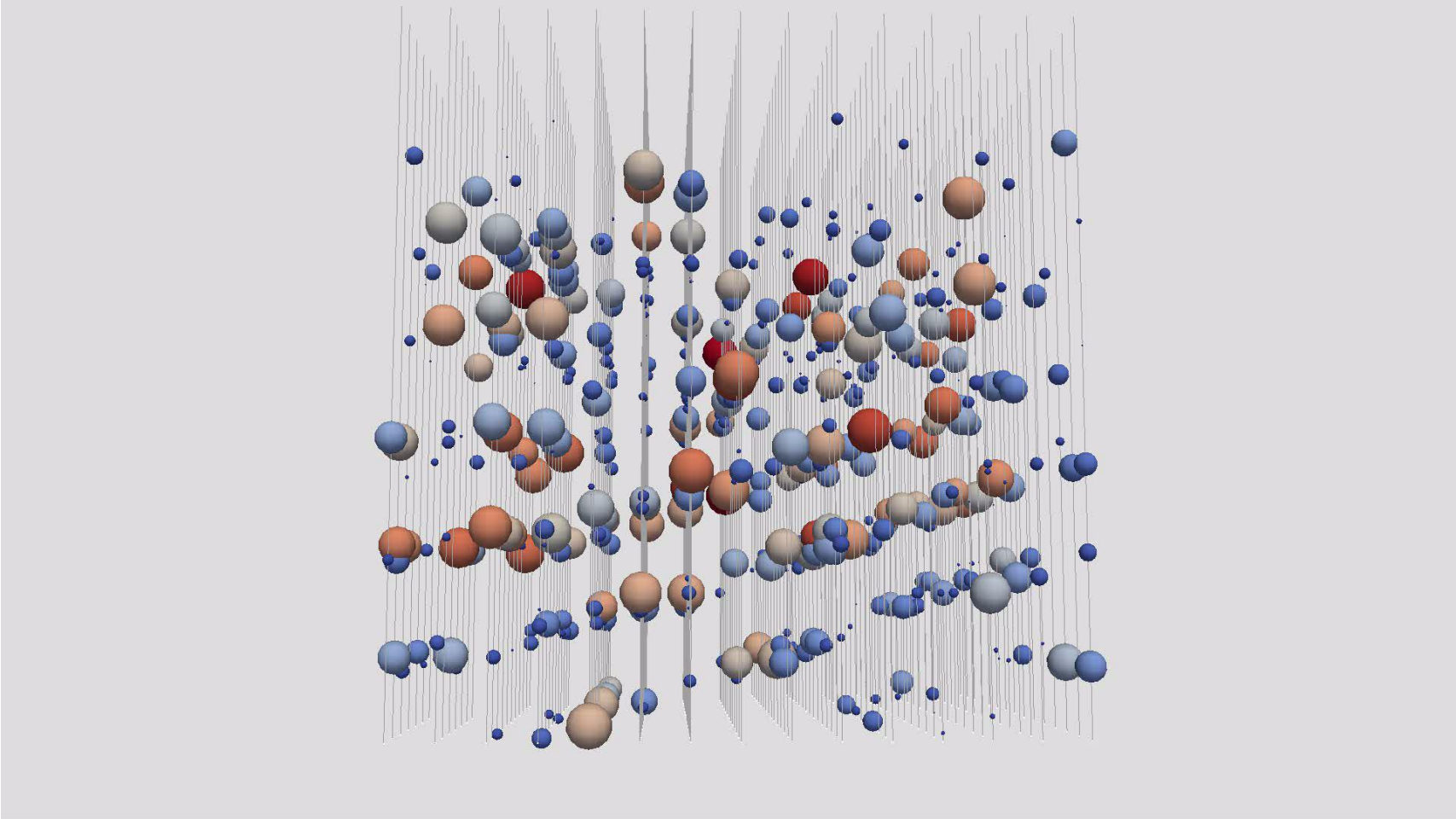
normally distributed inputs need not give rise to normal outputs…



anisotropic uncertainty distribution in boiling rate throughout quarter core model

Not shown: including model form parameters with prescribed ranges results in roughly 50—100% output uncertainty. Need model refinement leveraging available data.

Mass Evaporation Rate in Reactor Quarter Core



mean of boiling rate: 0 97 194 291

size indicates standard deviation of boiling rate ***(lb_m/hr-ft^2)***

Calibrate and Validate VIPRE-W Boiling Rate with Plant B Crud Index Data

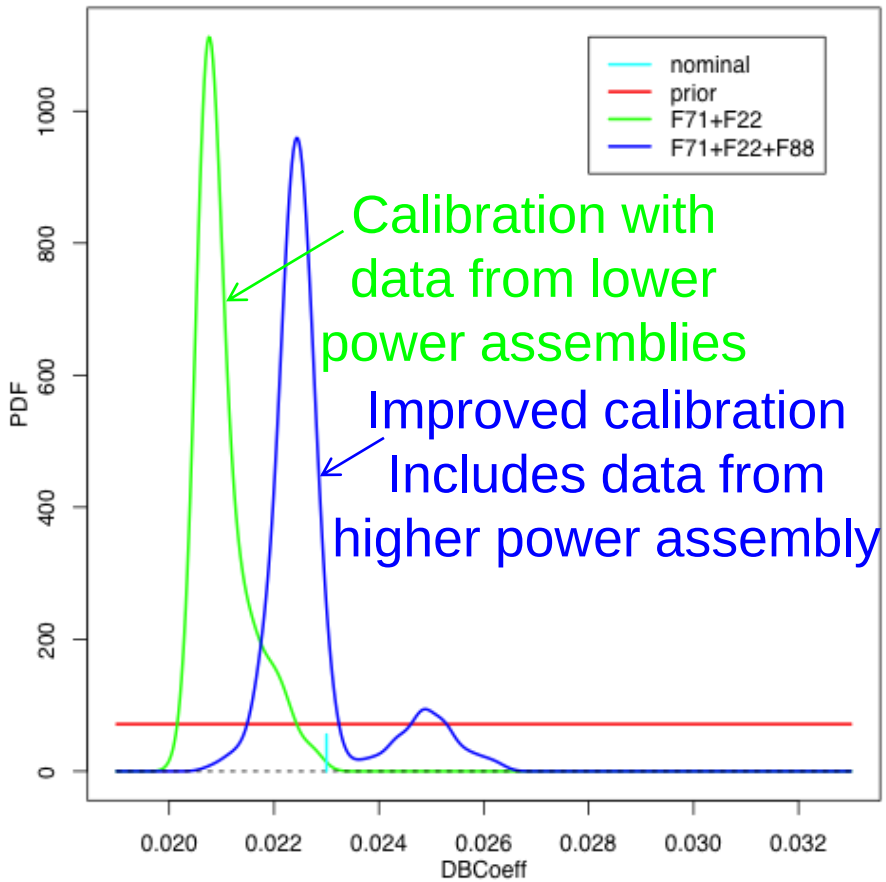
Use probabilistic methodology (GPMSA) to

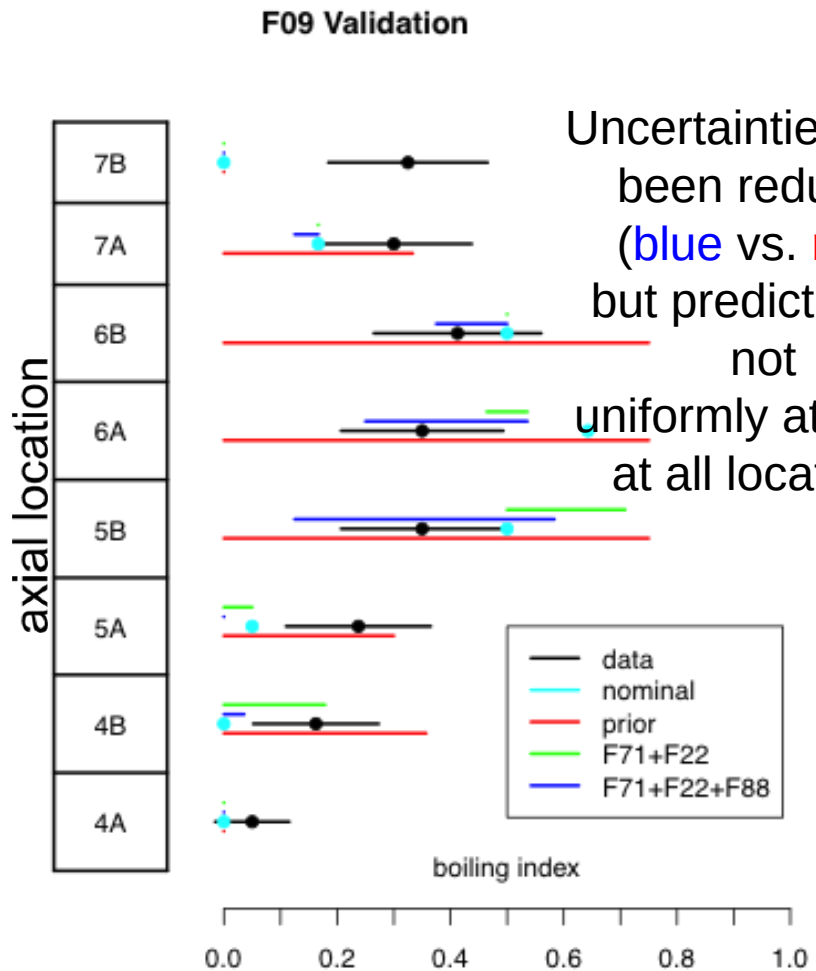
- calibrate VIPRE-W parameters to assemblies F71, F22, and F88

Parameter	Range
Lead coefficient of Dittus-Bolter Correlation (DBCoeff)	0.019 – 0.033
Lead Coefficient of Grid Heat Transfer Model (GHTCoeff)	2 - 6
Axial Friction Correlation Coefficient (AFCCoeff)	0.1 - 0.25
Lateral Resistance Correlation Coefficient (LRCCoeff)	1.5 - 4
Exponent of Partial Boiling Model (ExpPBM)	1 - 4

- validate against with assembly F09 (hold out data)
- assess model discrepancy

VIPRE-W Boiling Index Calibrated to Crud Index





Uncertainties have been reduced (blue vs. red), but predictability not uniformly attained at all locations

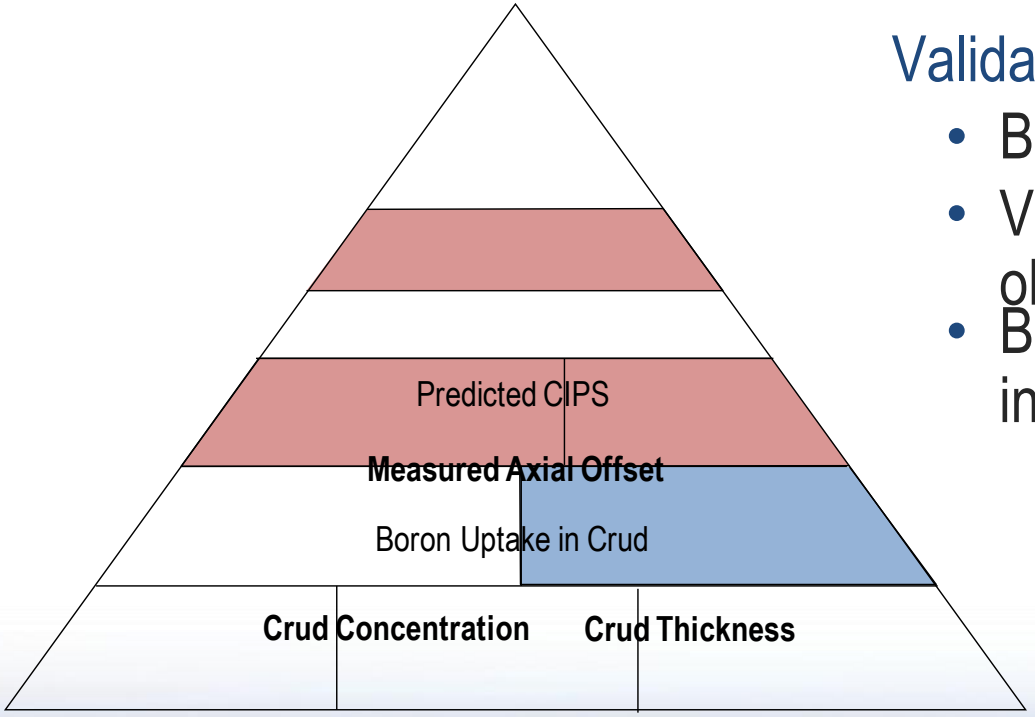
Validation demonstrates that enhanced physics modeling is needed

VUQ Approaches Inform Decision Making, Model Improvements, and Data Gathering

- Demonstrated VUQ workflow applicable to any computational model and that modern algorithms can reduce computational cost
- Enables industry to screen parameters and make risk-informed decisions based on the predicted uncertainty in crud formation, e.g., can fuel be loaded to minimize uncertainty in predicted localized boiling?
- Direct impact on CIPS challenge problem; later impact on others: *established foundation for current calibration and validation studies with VIPRE-W and BOA*.
- *Application of VUQ capabilities such as SA/UQ will drive the CASL R&D investment and data collection priorities. (assessment of discrepancy, e.g.)*

Studies Progressing Now: VIPRE-W + BOA with "Plant C" Data

- Address more of CIPS validation pyramid with similar analyses
- "Plant C" has substantial crud data and models ready
- More realistic validation responses and metrics



Validation comparisons of

- BOA vs. measured crud thickness
- VIPRE-W-derived crud index vs. observed data
- Boron mass which is a direct indicator for CIPS risk

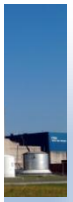
Later: fully coupled ANC/VIPRE/BOA

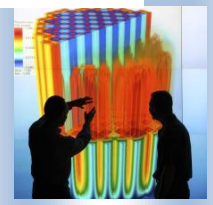
Numerical Error Estimation for LES modeling of GTRF

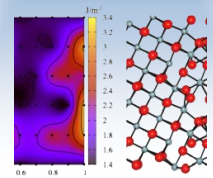
Demonstrating Solution Verification for CFD

Bill Rider (SNL)

Contributions from K. Copps, N. Crane, E. Cyr, R. Garcia, R. Pawlowski, S. Rodriguez, J. Shadid, T. Smith, R. Summers, D. Turner, P Weber, W. Witkowski (SNL), R. Lu and A. Mandour (WEC), S. Sham (ORNL)







Consortium for Advanced Simulation of LWRs

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Talk Outline

- VUQ Overview and Solution Verification's place
- The GTRF Challenge Problem and VUQ's place
- Verification activities within CASL
- The CFD codes used to compute the GTRF problem
  - Fuego
  - Drekar
- Solution verification of the component validation problem used with Drekar
- Solution verification of the GTRF CFD calculations
- Outlook and Recommendations

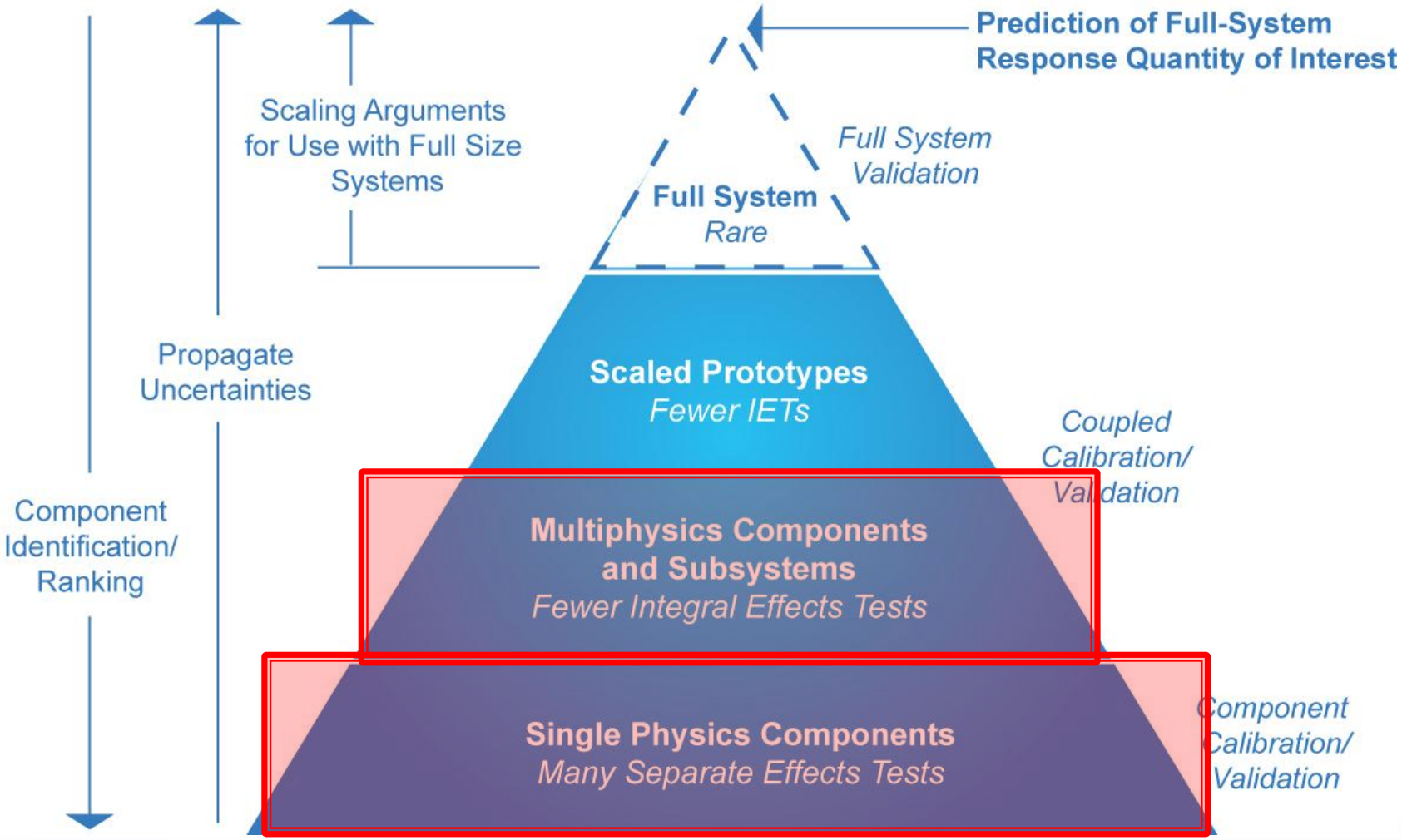
Validation and Uncertainty Quantification (VUQ)

Selected Year-1 Activities	Selected Year-1 Milestones

• Establish VUQ-led committees
  – Cross-FA Working Group
  – Validation Data Committee
• Integrate key software tools into VERA (DAKOTA and Percept)
• Develop VUQ procedures and workflows
• Develop and analyze VUQ case study problems
• Perform verification study on a benchmark T-H problem
• Perform *Predictive Maturity* assessments (PCMM)
• Develop new capabilities for data assimilation, sensitivity analysis, and UQ
• Develop CASL validation data requirements/plan
	• **L2 (12/31/2010): Integrate DAKOTA into VERA**
	• L3 (1/31/2011): Complete initial review of experimental data and plant observations related to CRUD and GTRF challenge problems
	• L3 (3/31/2011): Stand up a VUQ-led Cross-Focus Area Working Group
	• **L2 (6/30/2011): Enable generalized data assimilation and model calibration for VERA**
	• L3 (6/30/2011) Develop mathematical data assimilation framework
	• L3 (3/31/2011) Develop a VUQ practices document
	• L3 (6/30/2011) Validation data requirements
	• **L2 (3/30/2011): Enable statistical sensitivity and UQ demonstrations for VERA**
	• L3 (3/31/2011): Apply SA and UQ capabilities to VUQ case study application

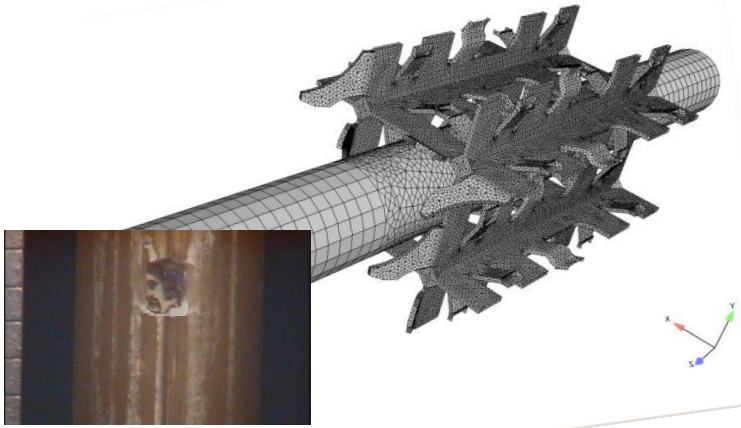
Validation and Uncertainty Quantification (VUQ)

Achieving credible, science-based predictive M&S capabilities

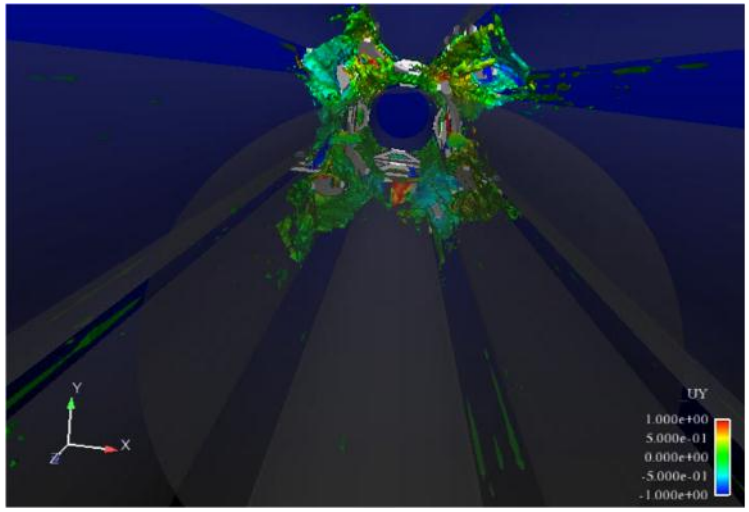


The CASL Relevance of our problem is it's role as one of our "Challenge problems."

- The Grid-to-Rod Fretting (GTRF) Challenge Problem: Fluid/Structure Vibration Wearing of Pin Cladding.
  - WEC Benchmark with experimental data for validation.
- Challenges of simulating 3x3 pin are similar for other important problems we will do later.
- Demonstration of a scalable higher-order accurate CFD 3x3 pin capability will:
  - Help Increase accuracy over current CFD simulations
  - Enable VUQ assessment of CFD and vibration analysis
  - Provide immediate feedback to our codes, models and practices.
  - Reduce the margins of uncertainty, allowing for power up-rates, life extensions and future reactor design.
  - Build connections THM – VRI – VUQ – MPO and transfer technology within CASL partnership



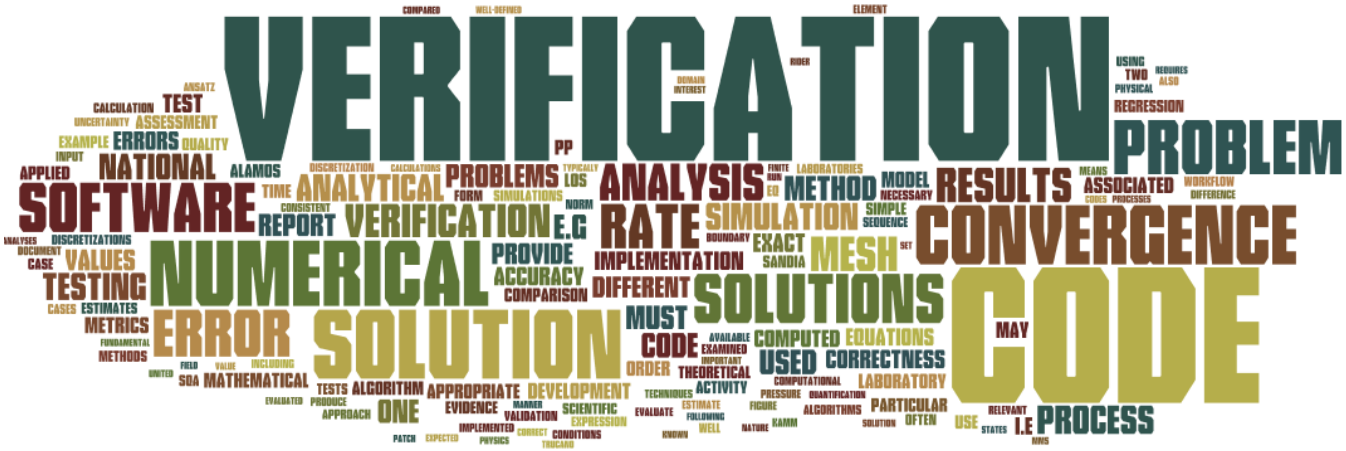
WEC V5H Grid Spacer

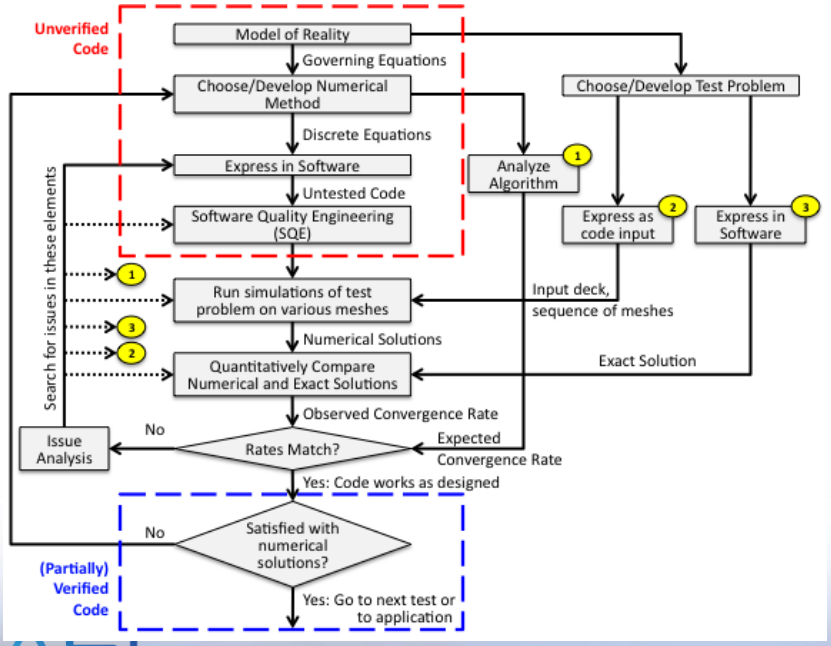


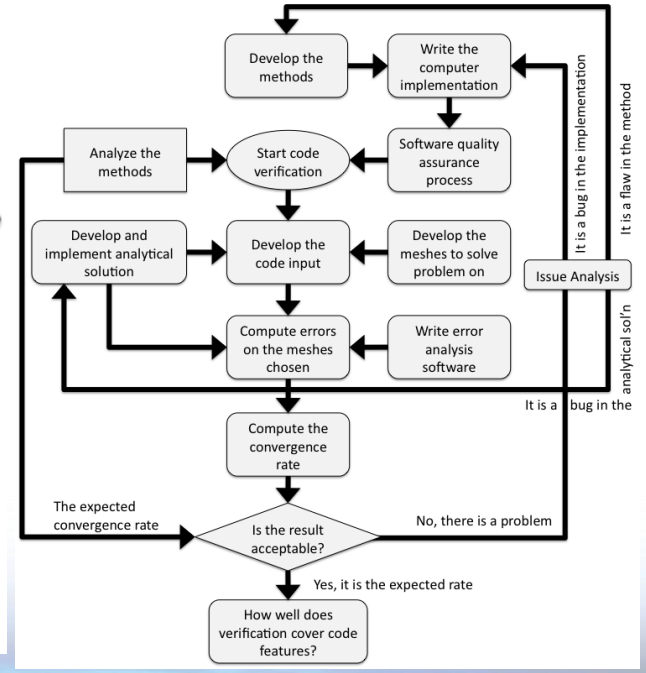
Drekar parallel LES Simulation

CFD plays a critical role in all Y1 Challenge problems

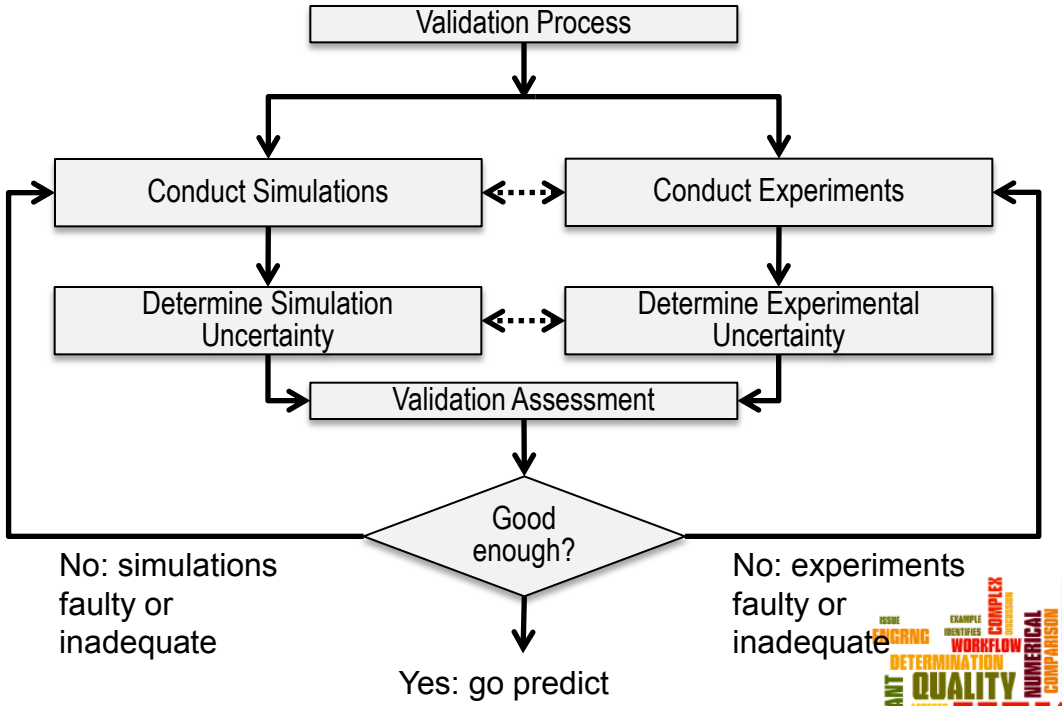
Code Verification Workflow in CASL to be used in code development (VRI)

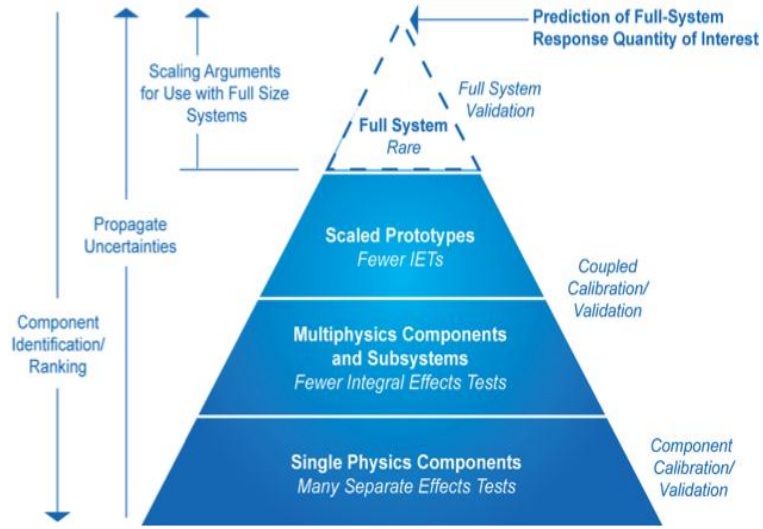


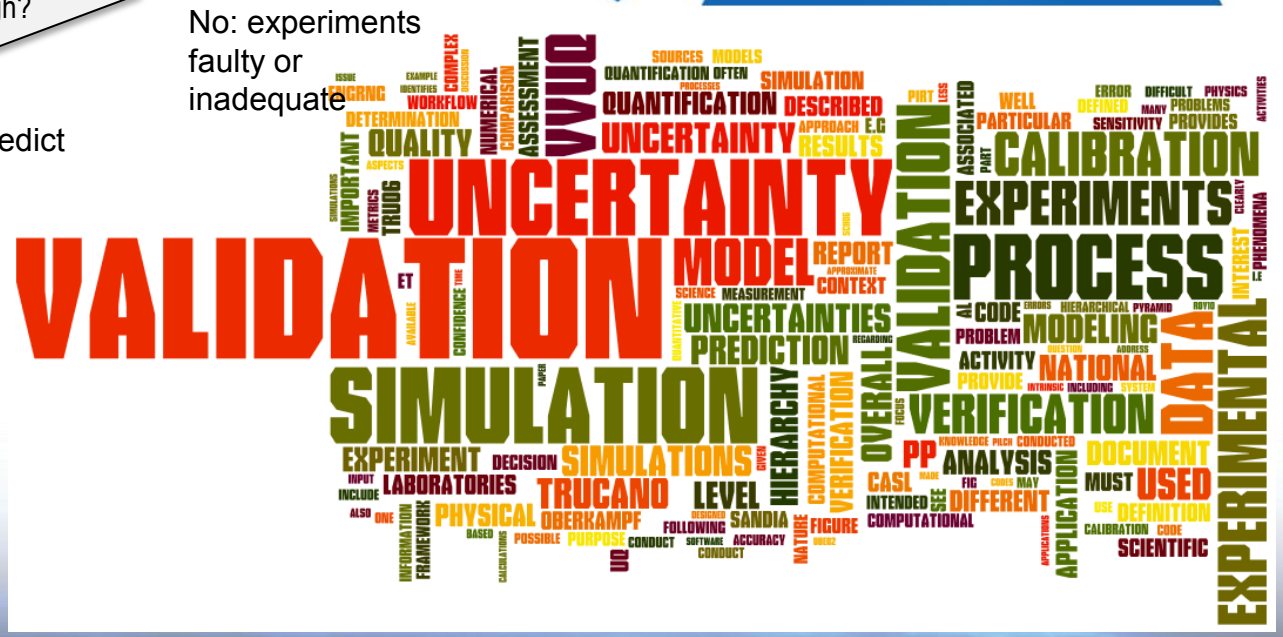




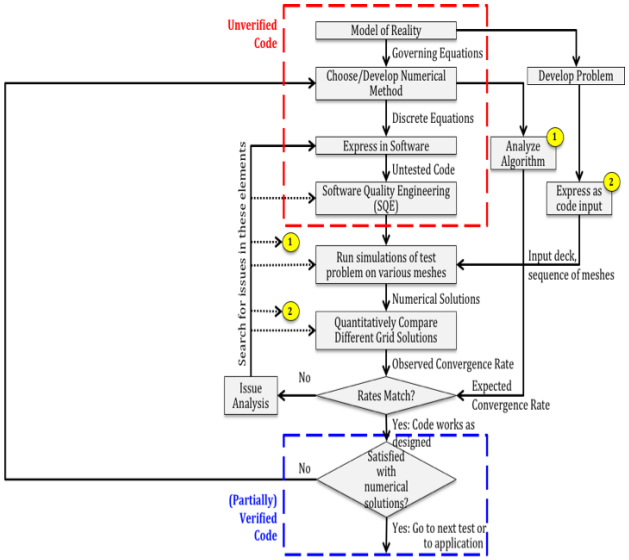
Verification, Validation and Uncertainty Quantification Workflow in CASL (AMA)

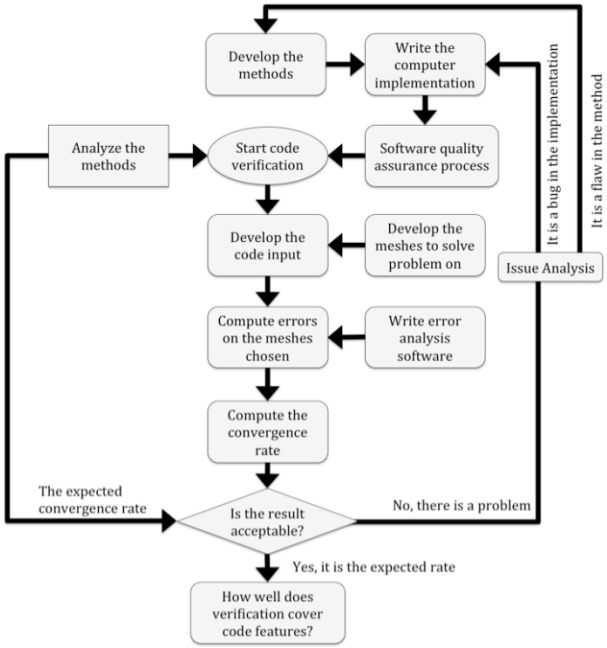


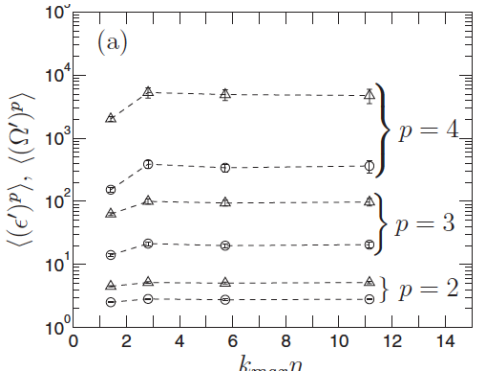


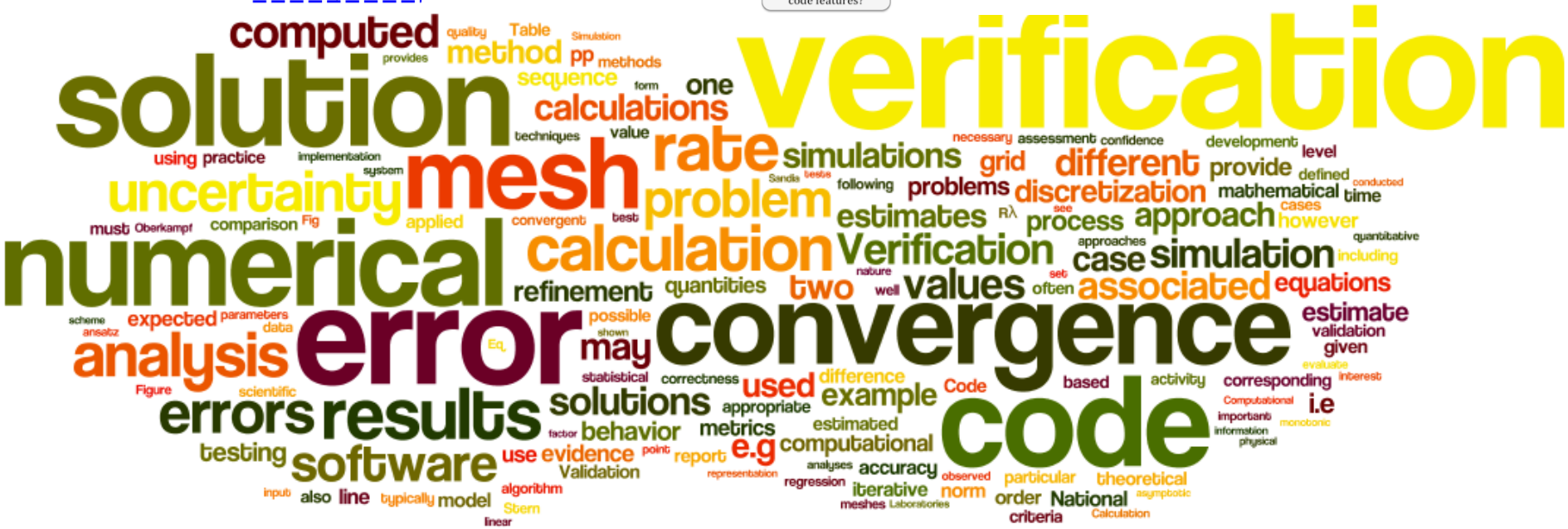


Procedures for Calculation Verification

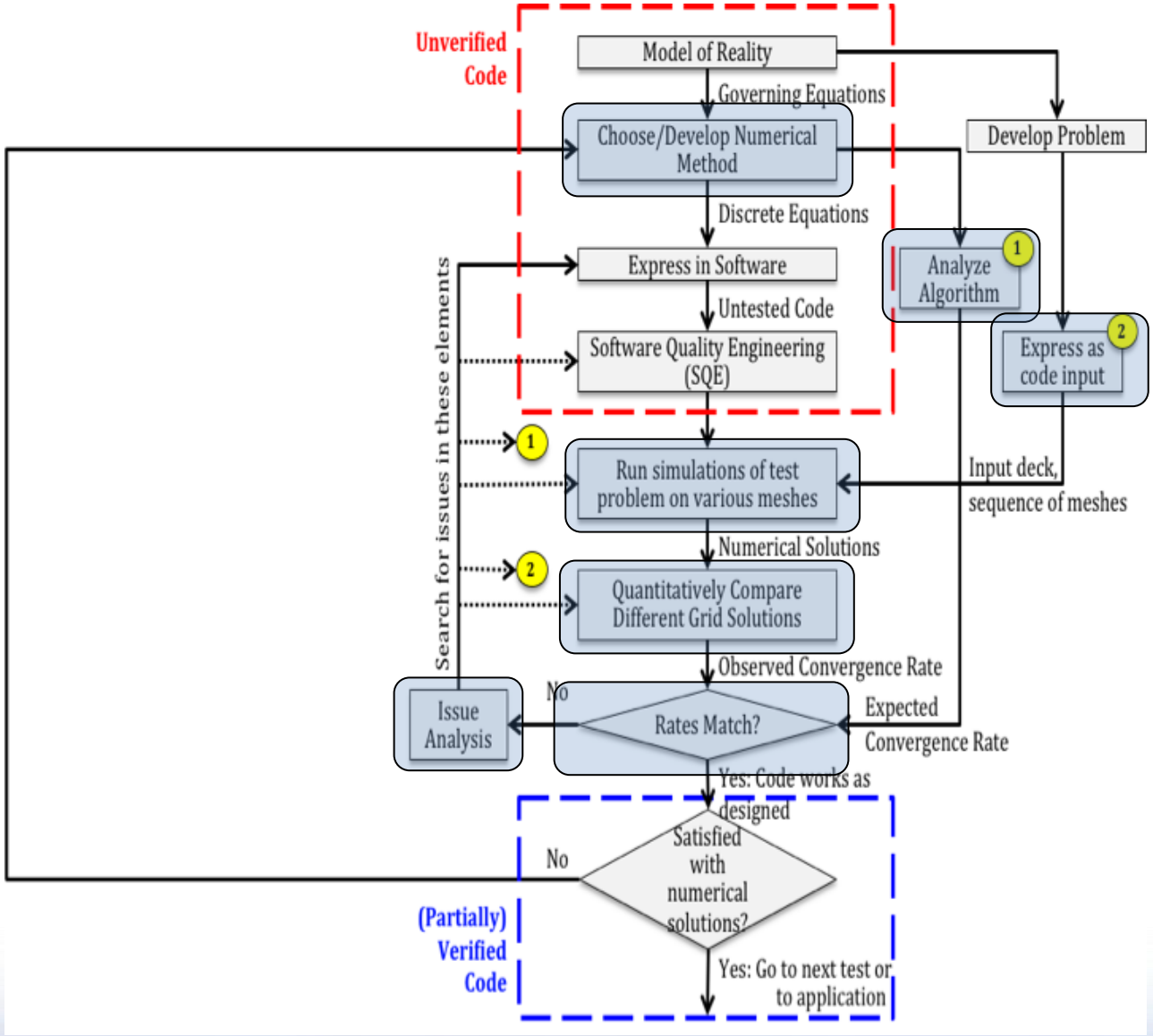








Procedures for Calculation Verification



We focus on the light blue boxes because of the nature of the work considered here.

Basic Descriptions of Drekar and Fuego

- FEM formalism
- WALE LES model and RANS
- Variable order BDF in time
- Second order in space with SUPG
- Discontinuity capturing
- Nonlinearly consistent (N-K)

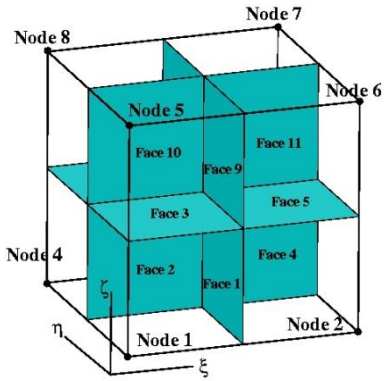
- CV-FEM formalism
- Runs use first-order in time,
- Second-order in space (MUSCL)
- Dynamic Smagorinsky model
- Linearized solution

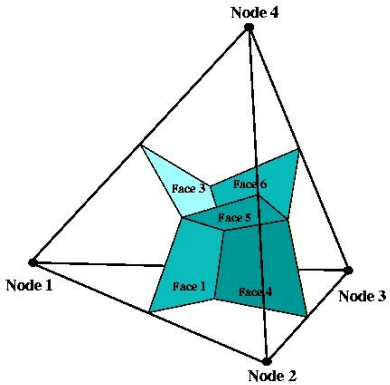
Two similar CFD codes one new, one mature

SIERRA/Fuego/Syrinx/Calore Methodology and Framework

- Common application framework
  - Shared data structure, parser, file I/O, parallel communication, solvers, etc.
- Data exchange for application coupling

- SIERRA/Fuego: Low-Mach turbulent fire
  - Hybrid control volume finite element method (CVFEM)
- SIERRA/Syrinx: Participating media radiation (PMR)
  - Streamwise-upwind Petrov-Galerkin FEM
- SIERRA/Calore: Heat conduction, enclosure radiation
  - Galerkin FEM

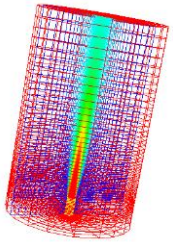


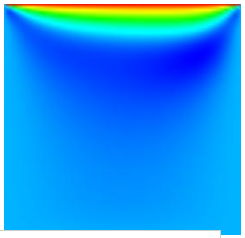


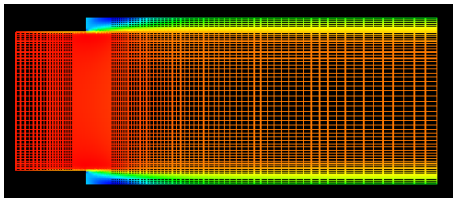
Each code has completed a detailed verification suite!

Fuego has undergone significant code verification testing.

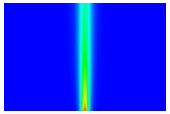
- Single and multi-mechanics verification completed
- Various code comparison metrics ranging from "low" to "high" quality
  - "Code to Code" (not verification)

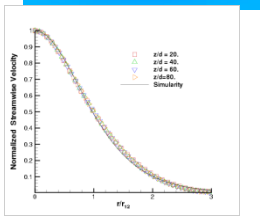


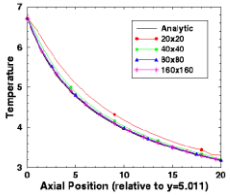




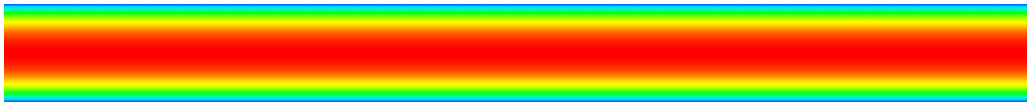
  - Semi-analytical



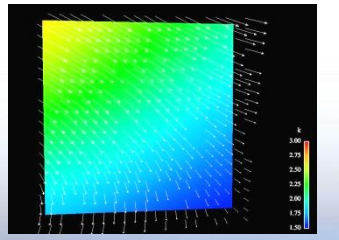


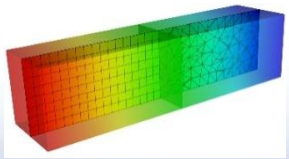


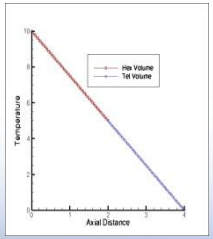
  - Analytical



  - MMS



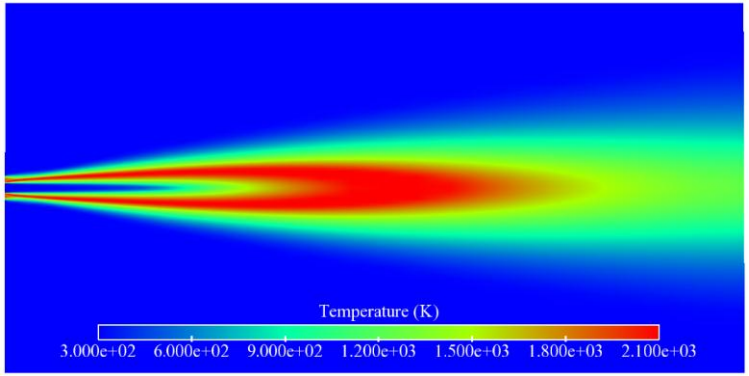




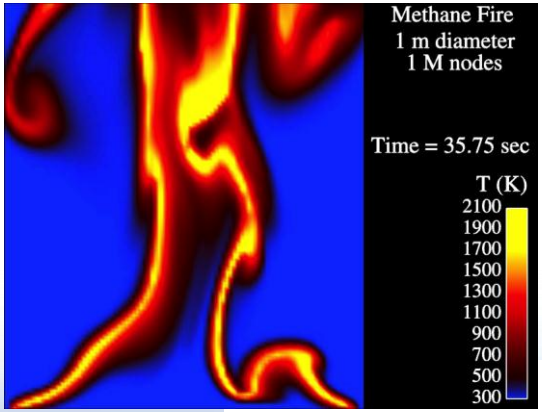
Stronger testing quality

Turbulence Closures

- Several turbulence closures available to satisfy range of affordability and fidelity requirements
  - Laminar flow
  - Reynolds-Averaged Navier-Stokes
    - Low-Re k-e/ω/SST model
    - Standard k-e/ω/SST model
    - RNG k-e model
    - v^2-f model
    - TFNS variable-time-filter model
    - PANS
  - Large Eddy Simulation
    - k_{SGS} one-equation model
    - Standard Smagorinsky model
    - **Germano-Lilly dynamic Smagorinsky model**



Steady Methane Jet

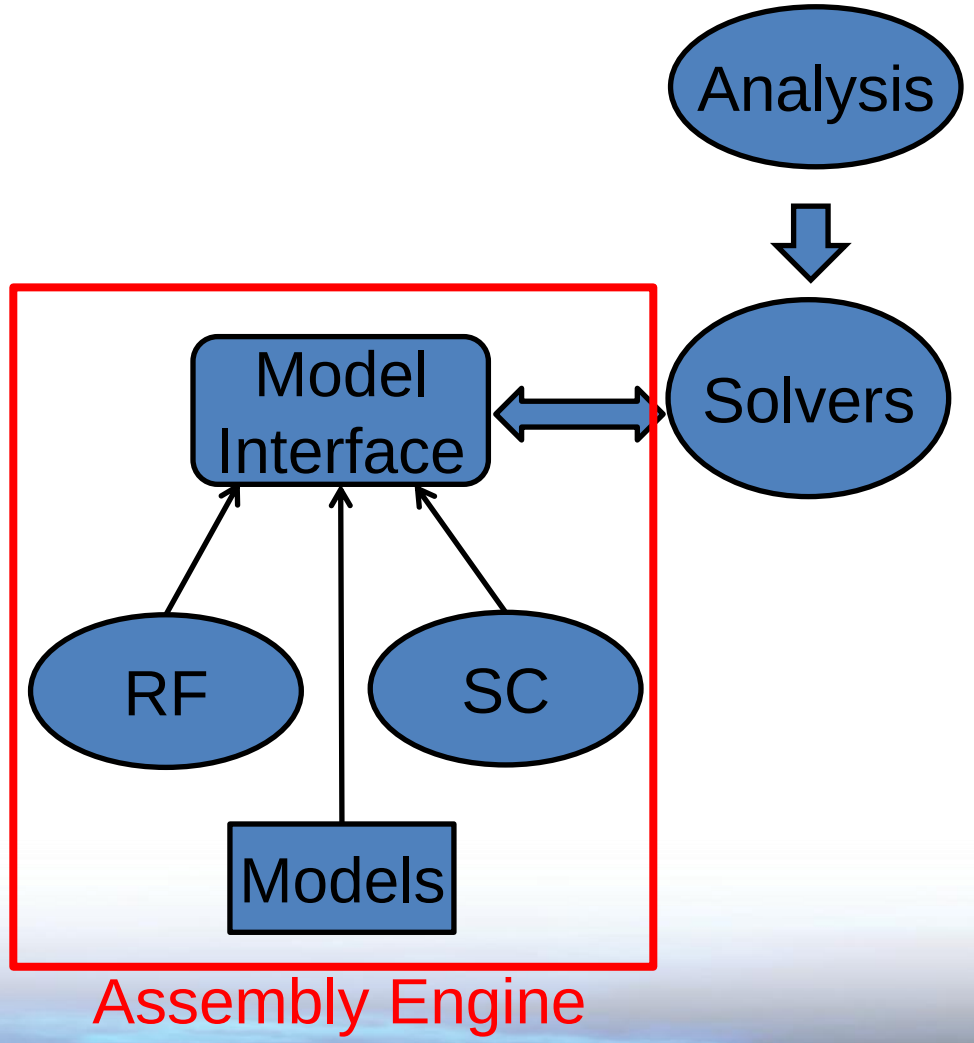


Unsteady Methane Fire

Drekar

trilinos.sandia.gov

- Massively Parallel: MPI
- 2D & 3D Unstructured Stabilized FE
- Fully Coupled Globalized Newton-Krylov solver
  - Sensitivities: Templated C++, Automatic Differentiation (Sacado)
  - GMRES (AztecOO, Belos)
  - Additive Schwarz DD w/ Var. Overlap (Ifpack, AztecOO)
  - Aggressive Coarsening Graph Based Block Multi-level [AMG] for Systems (ML w/Amesos for coarse solve)
  - Physics-based/Block Factorization (Teko)
- Fully-implicit: 1st-5th variable order BDF (Rythmos) & TR
- Direct-to-Steady-State (NOX), Continuation, Linear Stability and Bifurcation (LOCA / Anasazi), PDE Constrained Optimization (Moocho)



Turbulence Closure Model

- **Wall Adapting Local eddy-viscosity model (WALE)**
  - **Nicoud, F. and Ducros, F., "Subgrid-Scale Stress Modelling on the Square of the Velocity Gradient Tensor," Flow Turbulence and Combustion, Vol. 62, 1999, pp. 183-200.**

$$\mu_t = \bar{\rho}\nu_t$$

$$\nu_t = (C_w\Delta)^2 \frac{\left(\bar{\mathbf{S}}^d_{ij}\bar{\mathbf{S}}^d_{ij}\right)^{3/2}}{\left(\bar{\mathbf{S}}_{ij}\bar{\mathbf{S}}_{ij}\right)^{5/2} + \left(\bar{\mathbf{S}}^d_{ij}\bar{\mathbf{S}}^d_{ij}\right)^{5/4}}$$

$$\bar{\mathbf{S}}_{ij} = \frac{1}{2}\left(\frac{\partial\bar{\mathbf{u}}_i}{\partial\mathbf{x}_j} + \frac{\partial\bar{\mathbf{u}}_j}{\partial\mathbf{x}_i}\right)$$

$$\bar{\Omega}_{ij} = \frac{1}{2}\left(\frac{\partial\bar{\mathbf{u}}_i}{\partial\mathbf{x}_j} - \frac{\partial\bar{\mathbf{u}}_j}{\partial\mathbf{x}_i}\right)$$

$$\bar{\mathbf{S}}^d_{ij} = \bar{\mathbf{S}}_{ik}\bar{\mathbf{S}}_{kj} + \bar{\Omega}_{ik}\bar{\Omega}_{kj} - \frac{1}{3}\delta_{ij}\left[\bar{\mathbf{S}}_{mn}\bar{\mathbf{S}}_{mn} + \bar{\Omega}_{mn}\bar{\Omega}_{mn}\right]$$

- Modified Smagorinsky eddy-viscosity model
  - Filter width is based on the square of the deviatoric stress tensor
  - Requires only "local data" to construct.
  - Recovers the proper near-wall scaling for the eddy viscosity so that it inherently decays to zero as the wall is approached without using a dynamic procedure or wall model
- Future work will extend to full VMS-LES models
  - T.J.R. Hughes, L. Mazzei, K.E. Jansen, Large eddy simulation and the variational multiscale method, Comput. Vis. Sci. Vol. 3, 2000, pp. 47-59.

Solution Verification Example using Vortex Shedding to Validate the Drekar Code.

- We are examining the shedding frequency from a cylinder at various Reynolds numbers,

$$\mathrm{Re} = V\ell/\nu$$

  – The data is defined by the Strouhal number,

$$St = f\ell/V$$

- Data is available from classical sources Schlichting ('79)

Flow	Re=60	Re=100	Re=400	Re=1000
St	0.136±0.006	0.164±0.005	0.205±0.005	0.212±0.006

Basic verification assumptions

St=Strouhal number, the object of this part of the work. *a,b,c* are determined by the data.

- We will make the fundamental verification assumption

$$St(h) = a + bh^c$$

  - "a" is the mesh converged result, "c" is the convergence rate.
- Because the data has some fundamental uncertainty, we are extending the assumption,

$$St(h) = \left[a_-, a_+\right] + \left[b_-, b_+\right] h^{\left[c_-, c_+\right]}$$

  - Given statistics we can produce bounds for the results.
  - **This is a new development in verification analysis.**
- If one has the number grids to the number of degrees of freedom in the error model (3), the details of fitting are immaterial to the results.
  - If one has more grids than the minimum, the details are important.

One of the things to understand is the range of results coming from varying quantities.

- We can illustrate the type of results to expect with a set of examples:

Grid	Average	Error Case 1	Error Case 2	Error Case 3	Error Case 4	Error Case 5
4 h	8	± 0	$\pm 1/2$	± 1	± 1	$\pm 1/2$
2 h	6	± 0	$\pm 1/2$	$\pm 1/2$	$\pm 1/2$	± 1
h	5	± 0	$\pm 1/2$	$\pm 1/4$	$\pm 1/16$	$\pm 3/2$

- All the errors will be presented in the following form (the mean tendency of the data:

$$G(\Delta x) = a + b(\Delta x)^c = 4 + \left(\frac{1}{h}\right)(\Delta x)^1$$

- This provides a working example of how idealized data behaves.

The results are simple to develop and compute.

- We summarize the results in the table below:

Case	Lower a	Lower b	Lower c	Upper a	Upper b	Upper c
1	4	1	1	4	1	1
2	3.5	1	1	4.5	1	1
3	4	0.75	1	4	1.25	1
4	3.42857	1.50893	0.62148	4.16000	0.90251	1.2115
5	1.25	2.25	0.73697	6.25	0.25	1.5850

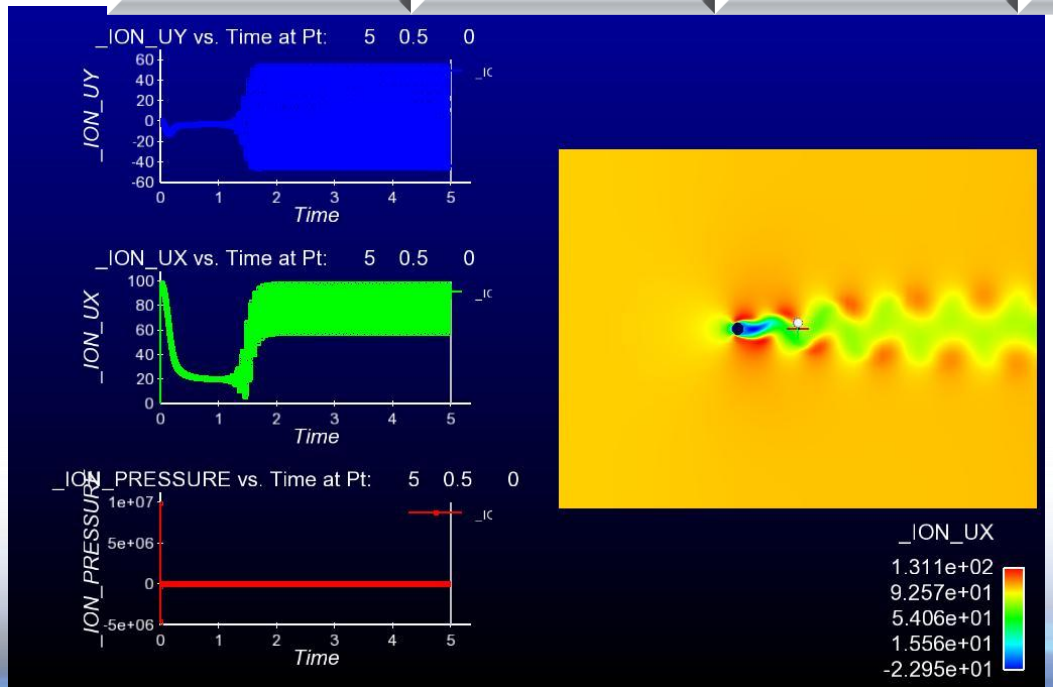
- For the most interesting cases (4 and 5) we can write these as intervals:

$$A(h) = [3.42857, 4.16000] + [0.90251, 1.50893]\, h^{\lfloor 0.62148, 1.2115 \rfloor}$$

$$A(h) = [1.25, 6.25] + [0.25, 2.25]\, h^{\lfloor 0.73697, 1.5850 \rfloor}$$

Drekar Results for Re=100, spatial and temporal resolution study.

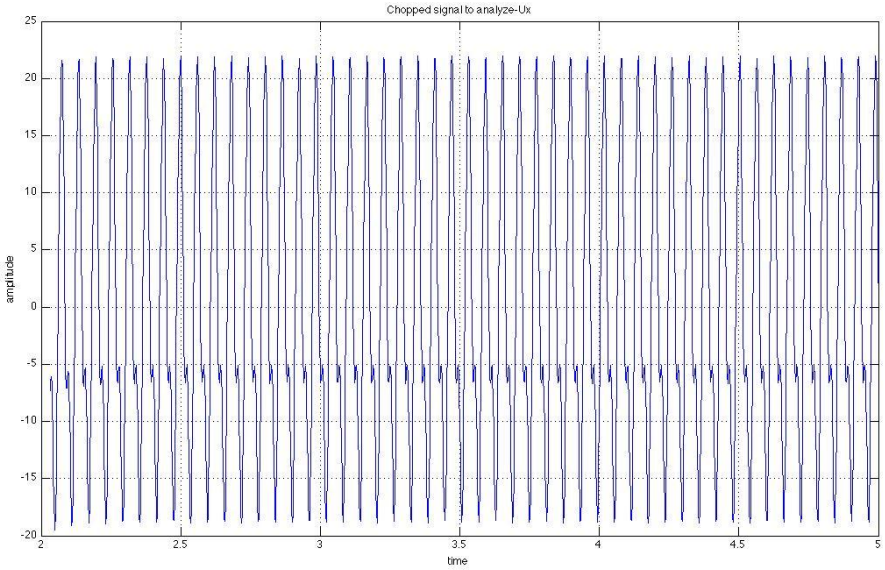
Case	Δt	RMS h	St	Δ(St) 95%
1	0.002	0.054111988	0.110474853	0.001219
2	0.002	0.023801688	0.152492294	0.004537
3	0.002	0.010786082	0.164777976	0.004979
4	0.002	0.005264375	0.165127187	0.004369
5	0.008	0.010786082	0.134265285	0.005306
6	0.004	0.010786082	0.154923058	0.00756
7	0.001	0.010786082	0.165999038	0.00491
8	0.0005	0.010786082	0.1661293	0.005012



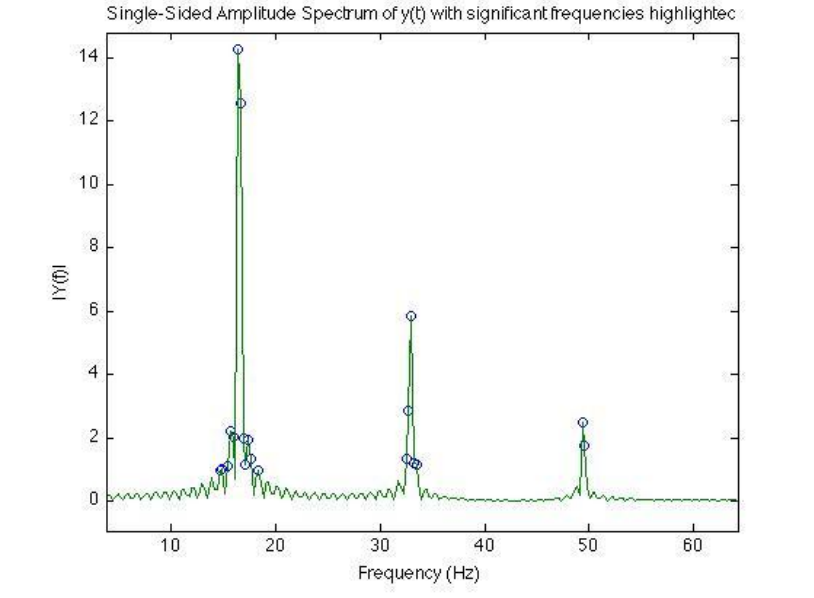
Since the results are obtained at a point, the convergence rates may not be directly related to the theoretically expected rates.

Reducing the data: FFT

- The basic data is defined by th examination of the frequency c vortex shedding for long times and eliminating the startup transient



- The frequency range is reported at the mean and two standard deviations (assuming normal statistics)

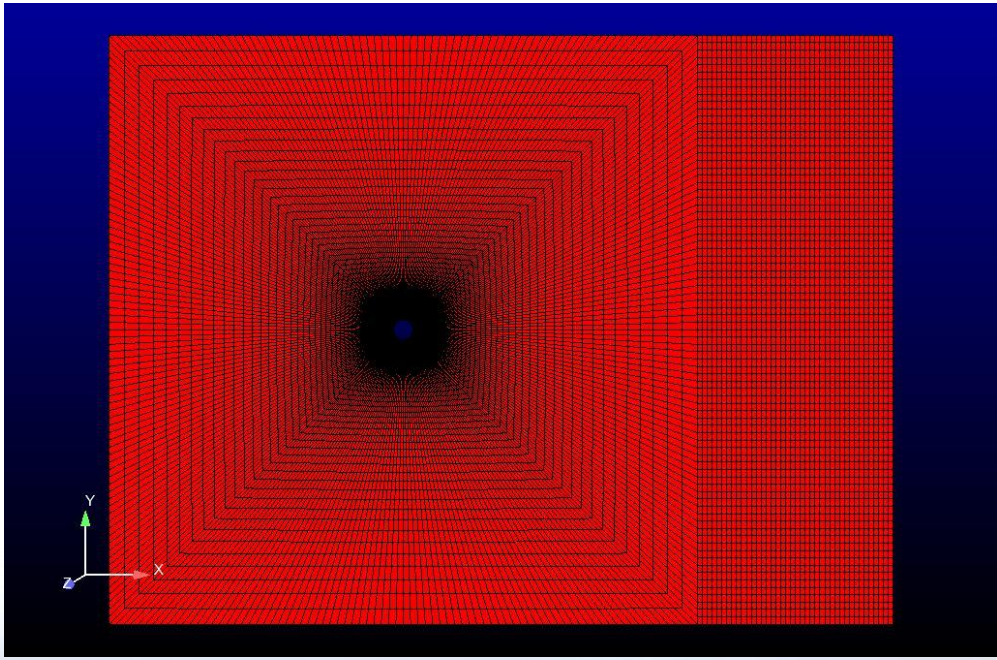


Dealing with the variable meshing

- The mesh is defined by the RMS of the mesh spacing

$$h = \sqrt{(\Delta x)_{\min}^2 + (\Delta y)_{\min}^2}$$

- The assumption is that the minimum mesh spacing is the most important for determining solution accuracy.



The data can be reduced to give a set of error estimates and numerical uncertainties.

- Every thing has the following functional form:

$$St(h,\Delta t) = St_0 + C_h h^a + C_{\Delta t}(\Delta t)^b$$

- The basic results are summarized in these equations:

$$St(h,\Delta t) = 0.167213 - 5.83905h^{1.61558} - 21.7375(\Delta t)^{1.33337} \quad \text{Lower bound}$$

$$St(h,\Delta t) = 0.170935 - 7.94234h^{1.69637} - 47.434(\Delta t)^{1.50502} \quad \text{Mean}$$

$$St(h,\Delta t) = 0.17470 - 10.3214h^{1.76271} - 164.206(\Delta t)^{1.77237} \quad \text{Upper bound}$$

  - 1.8 to 6.5% too high

- If we drop the coarse grids and keep the finest

$$St(h,\Delta t) = 0.162377 - 1726.87h^{3.1575} - 474.21(\Delta t)^{2.0380} \quad \text{Lower bound}$$

$$St(h,\Delta t) = 0.168561 - 190.70h^{2.5584} - 5.7963(\Delta t)^{1.2418} \quad \text{Mean}$$

$$St(h,\Delta t) = 0.171947 - 15428h^{3.7435} - 1774.7(\Delta t)^{2.2061} \quad \text{Upper bound}$$

  - Works out to 0.36%

- The other form of UQ from Xing & Stern yields ΔSt=5.83%

Results for Re=100 accounting for the variability in the results.

- The data is reported with a 95% confidence interval (~2 std. dev.)
- We repeat the analysis for spatial and temporal convergence to define an envelope of solutions.
- The spatial convergence results:

$$St(h) = a + bh^c = [0.1628, 0.1716] - [5.705, 10.54]\, h^{[1.60, 1.77]}$$

- The temporal convergence results:

$$St(t) = a + bt^c = [0.1632, 0.1713] - [14.23, 195.2]\, h^{[1.25, 1.81]}$$

- Combined space time convergence:

$$St(h) = a + bh^c + dt^e = [0.1672, 0.1747] - [5.83, 7.94]\, h^{[1.62, 1.76]} - [21.74, 164.2]\, t^{[1.33, 1.77]}$$

The raw data from Drekar simulations at Re=1000

Case	Δt	RMS h	St	Δ(St) 95%
1	0.002	0.054111988	0.125325559	0.001116
2	0.002	0.023801688	0.19155126	0.00093
3	0.002	0.010786082	0.223538936	0.000943
4	0.002	0.005264375	0.230566339	0.003085
5	0.008	0.010786082	0.168450246	0.001905
6	0.004	0.010786082	0.204941286	0.002198
7	0.001	0.010786082	0.238016281	0.005241
8	0.0005	0.010786082	0.240079932	0.002972

The data reduction yields convergence and error estimates.

- Using all the data gives results of the Strouhal number being 22-29% too high

$$St(h,\Delta t) = 0.259479 - 3.60563h^{1.16818} - 39.2129(\Delta t)^{0.866885}$$ Lower bound

$$St(h,\Delta t) = 0.266514 - 3.26418h^{1.12447} - 26.2295(\Delta t)^{0.805668}$$ Mean

$$St(h,\Delta t) = 0.273924 - 2.97891h^{1.08355} - 18.1265(\Delta t)^{0.748689}$$ Upper bound

  - The uncertainty range is1.97% to 3.57% (Xing & Stern technique)
- We remove the coarse meshes and get better results as before

$$St(h,\Delta t) = 0.251719 - 220.12h^{2.3134} - 285.10(\Delta t)^{1.0562}$$ Lower bound

$$St(h,\Delta t) = 0.252791 - 235.18h^{2.3204} - 12621(\Delta t)^{1.4870}$$ Mean

$$St(h,\Delta t) = 0.256687 - 1196.0h^{2.7508} - 1951.1(\Delta t)^{1.2663}$$ Upper bound

  - The asymptotic value is 19.2% too high at best.

The data reduction yields convergence and error estimates.

- Using all the data gives results of the Strouhal number being 22-29% too high

$$St(h,\Delta t) = [0.259479, 0.273924] - [2.978913]\, h^{[1.08355, 1.16818]} - [18.1265, 39.2129](\Delta t)^{[0.748689, 0.866885]}$$

  – The uncertainty range is1.97% to 3.57% (Xing & Stern technique)

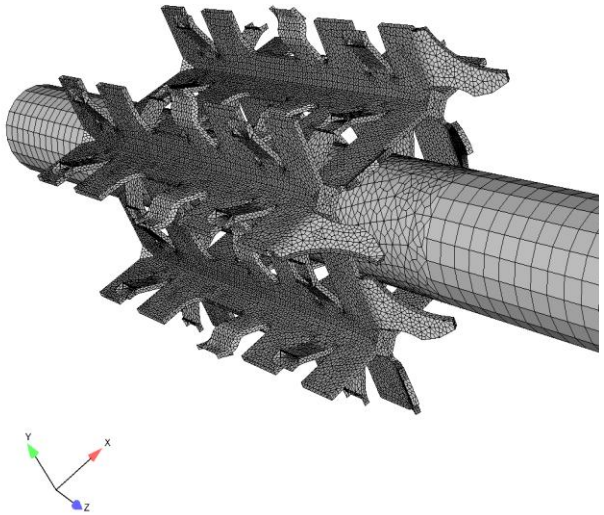
- We remove the coarse meshes and get better results as before

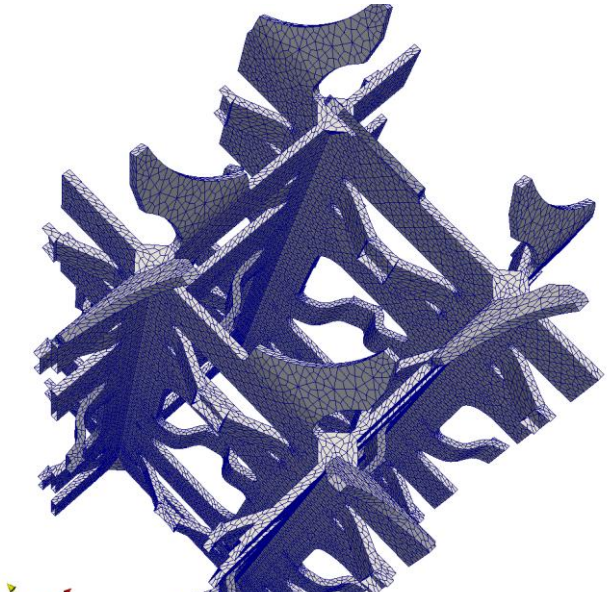
$$St(h,\Delta t) = [0.251719, 0.256687] - [220.12, 1196.0]\, h^{[2.3134, 2.7508]} - [285.10, 12461](\Delta t)^{[1.0562, 1.4870]}$$

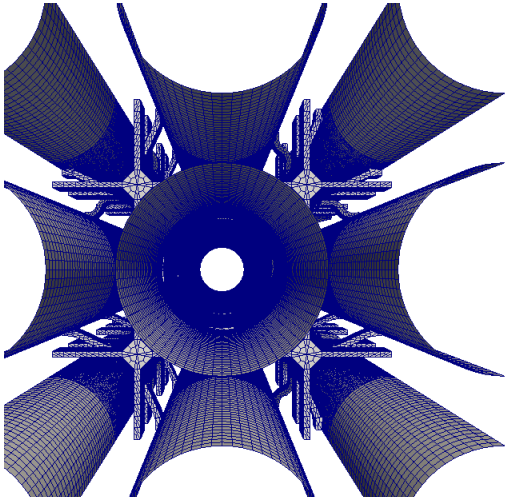
  – The asymptotic value is 19.2% too high at best.

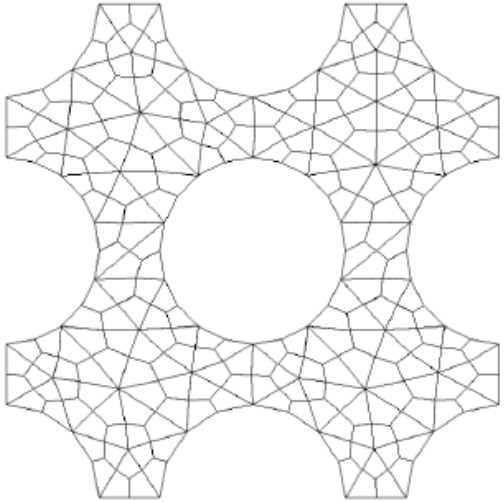
The geometry was meshed with Cubit.

(Complex geometry including mixing vanes, R. Garcia)

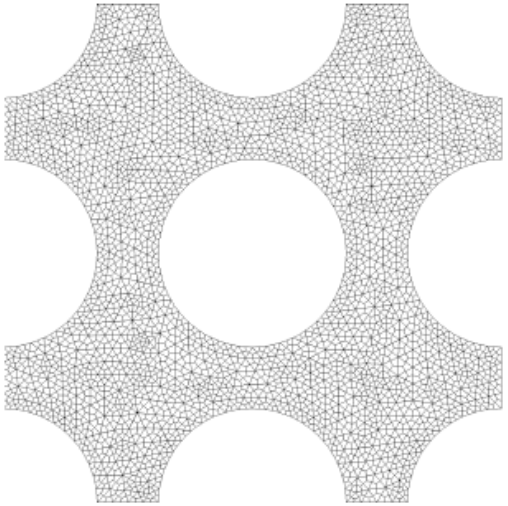




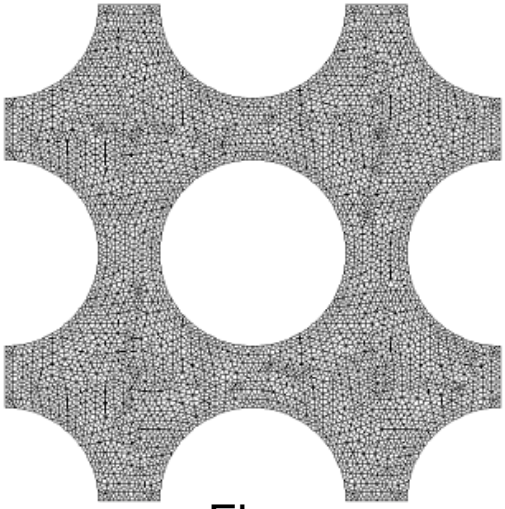




Coarse
664K



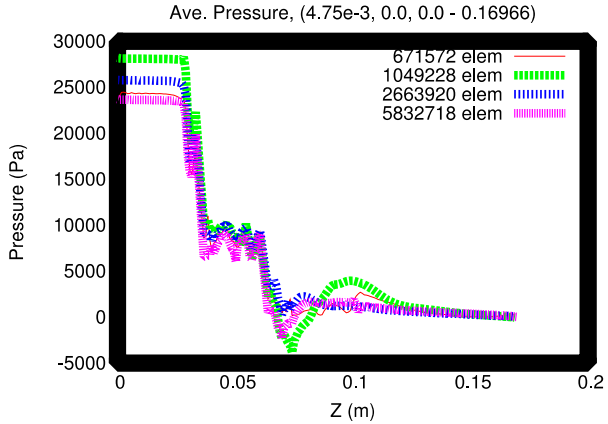
Medium
1912K



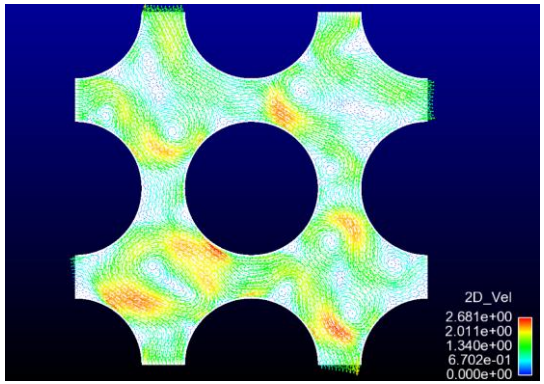
Fine
5280K

Initial Results: SNL Drekar FE LES CFD Capability

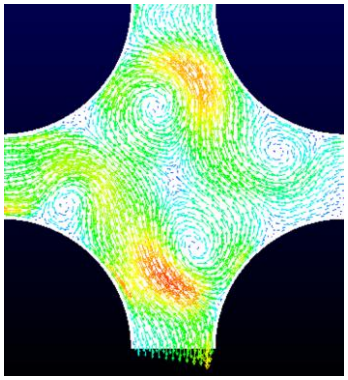
- Time-averaged LES solution



Pressure Drop Profiles Across Mixing Vane

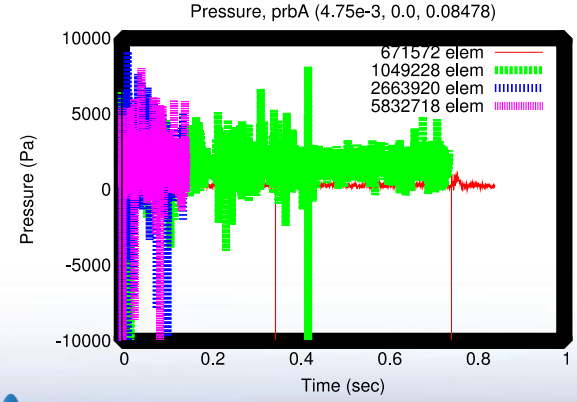


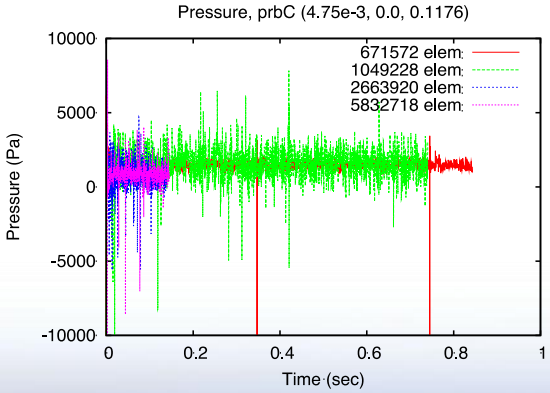
Cut-plane Velocity Vectors Downstream Of Mixing Vane

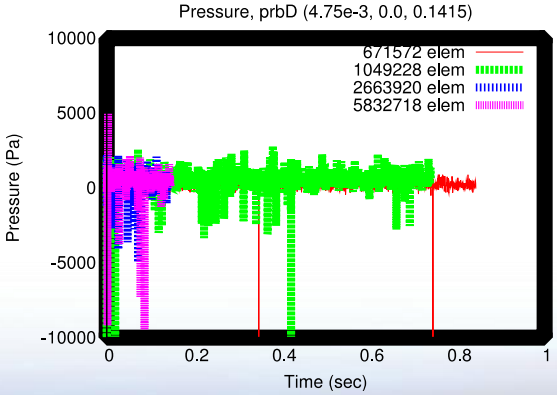


Detail Lower-left Quadrant Velocity Vectors

- Unsteady Pressure Field

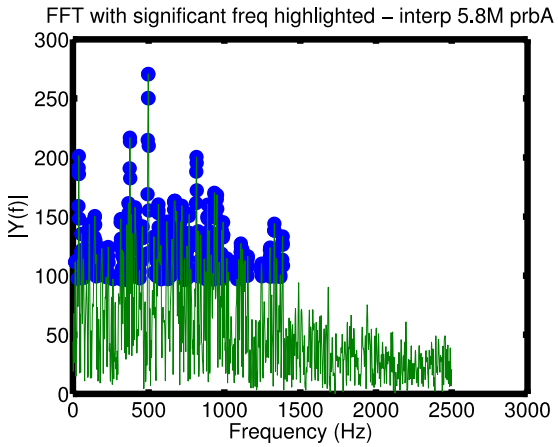


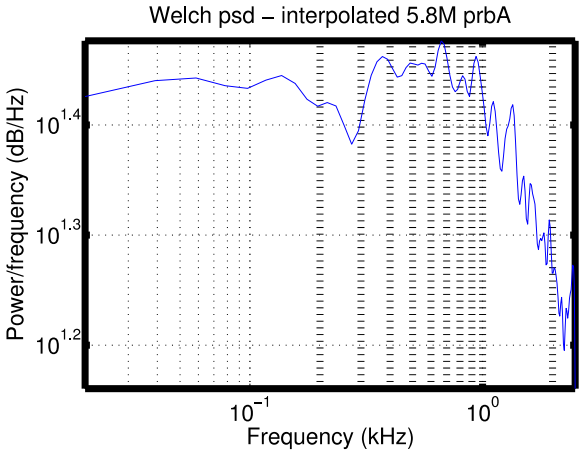




Initial Results: SNL Drekar FE CFD Capability

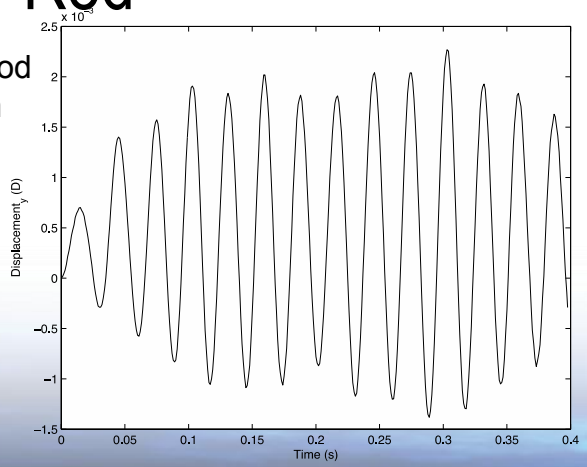
- Analysis of LES Pressure Field (FFT & PSD)

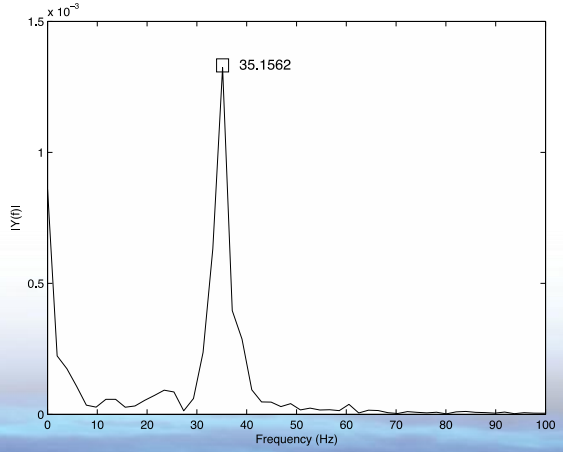




- Demo of Drekar LES Forcing of Structural Vibration (Sierra/Presto). Solid Zircaloy Rod

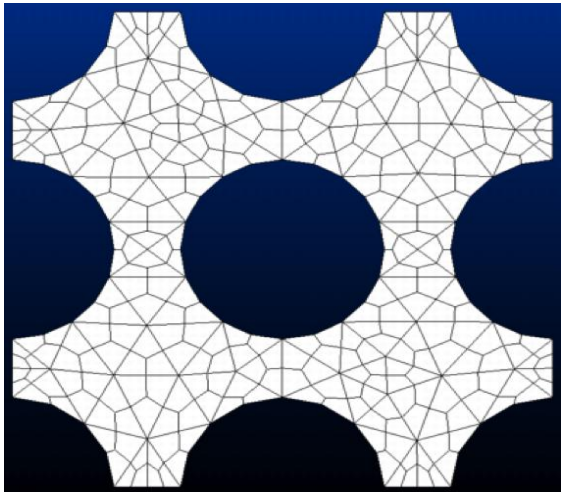
Displacement of rod in y-direction from LES forcing

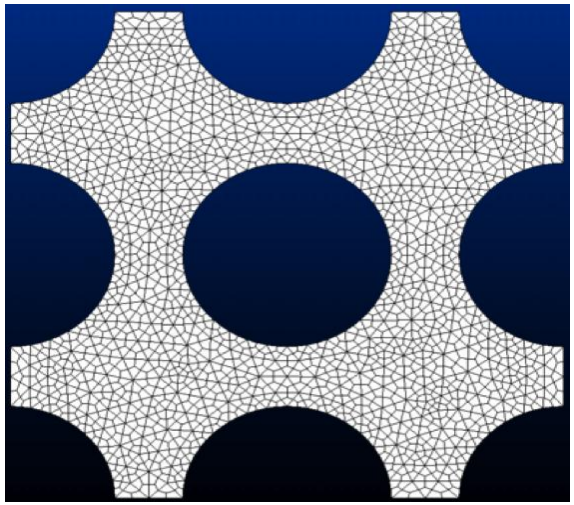


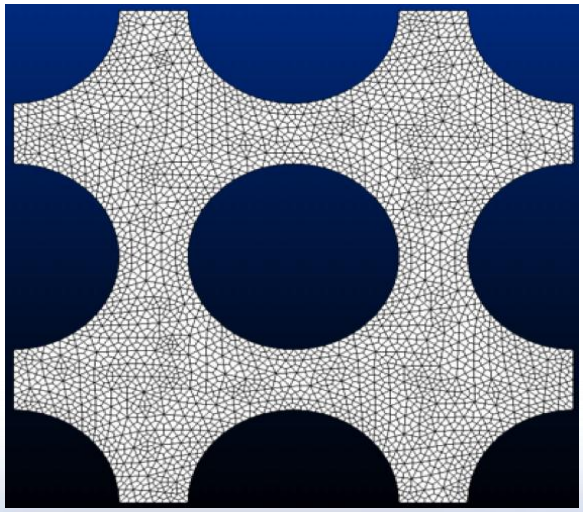


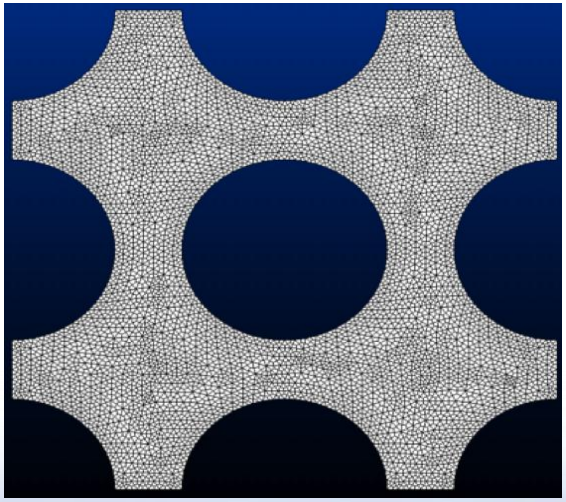
FFT of vibrational response of rod

Mesh Refinement for Verification
(Hex mesh ranging from 700K to 12M elements)

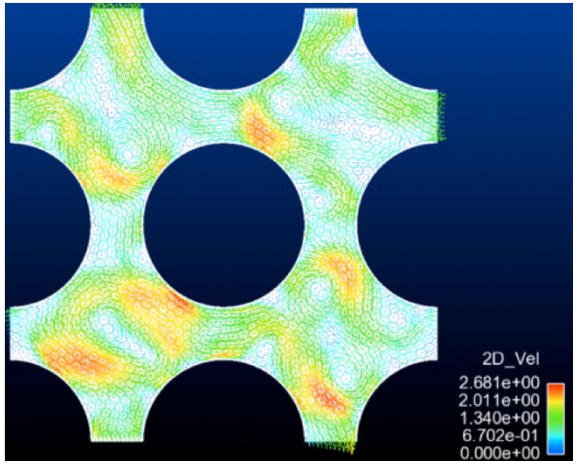


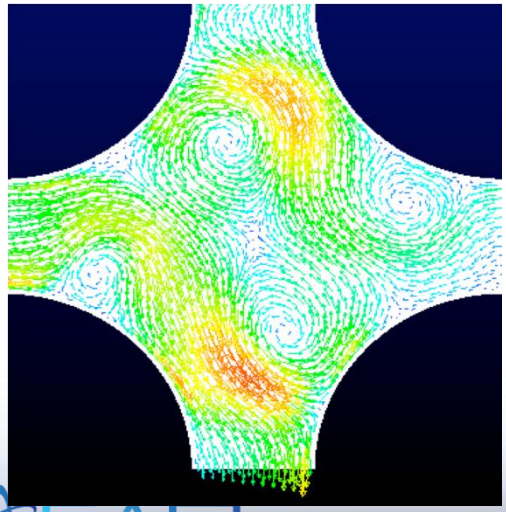




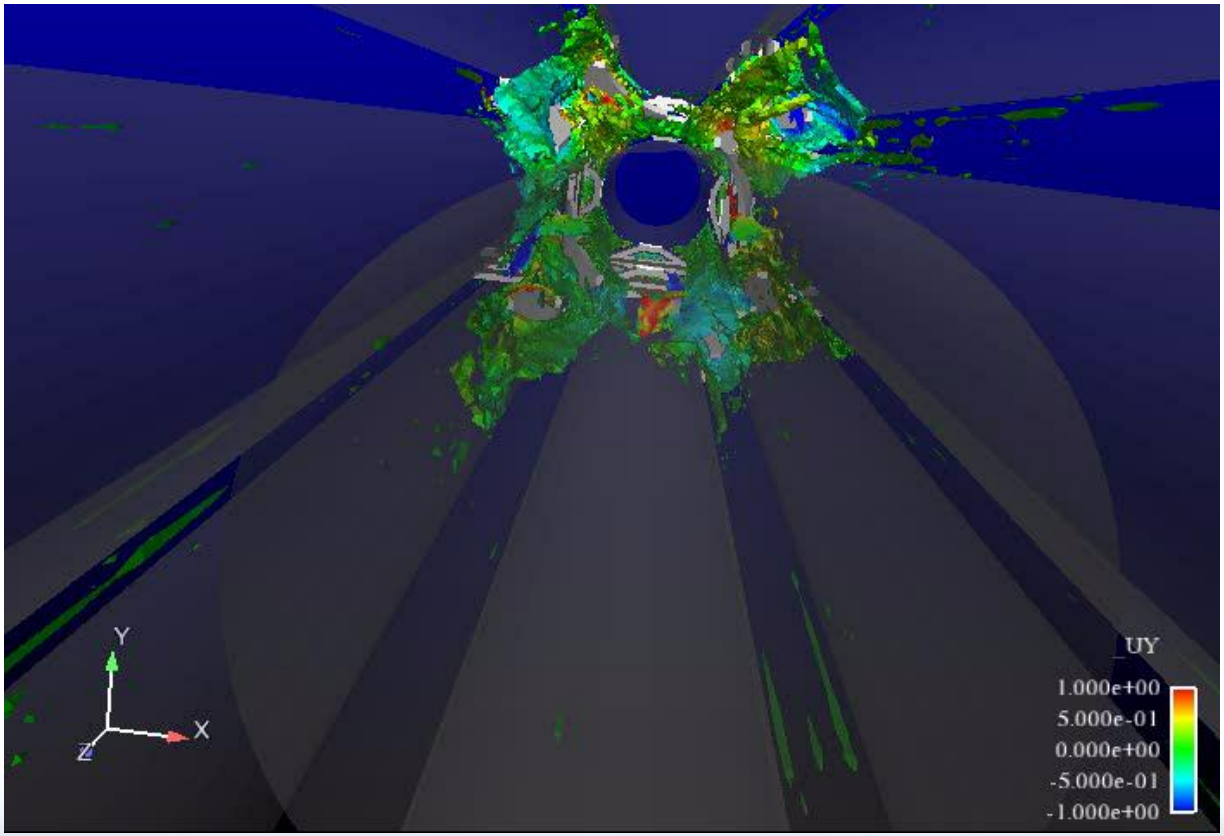


Solution Profiles



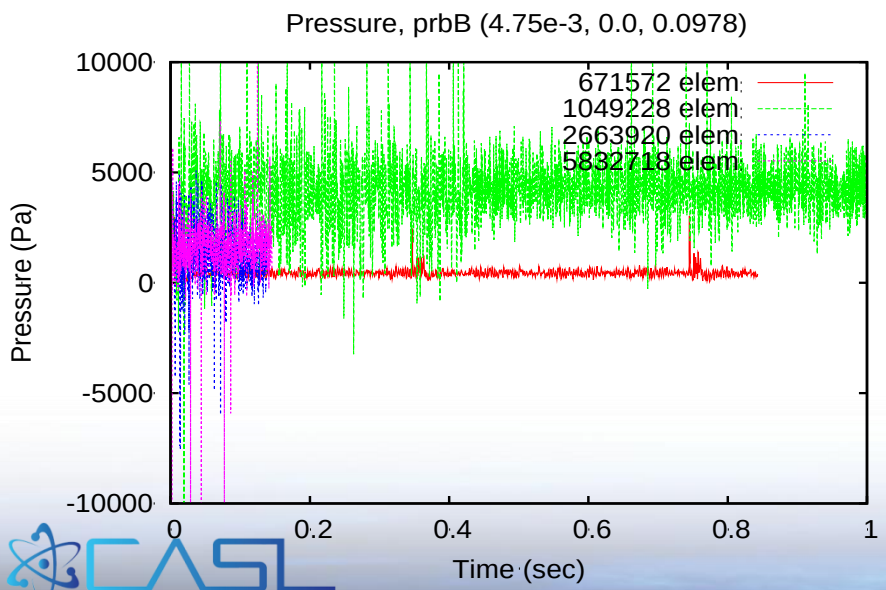


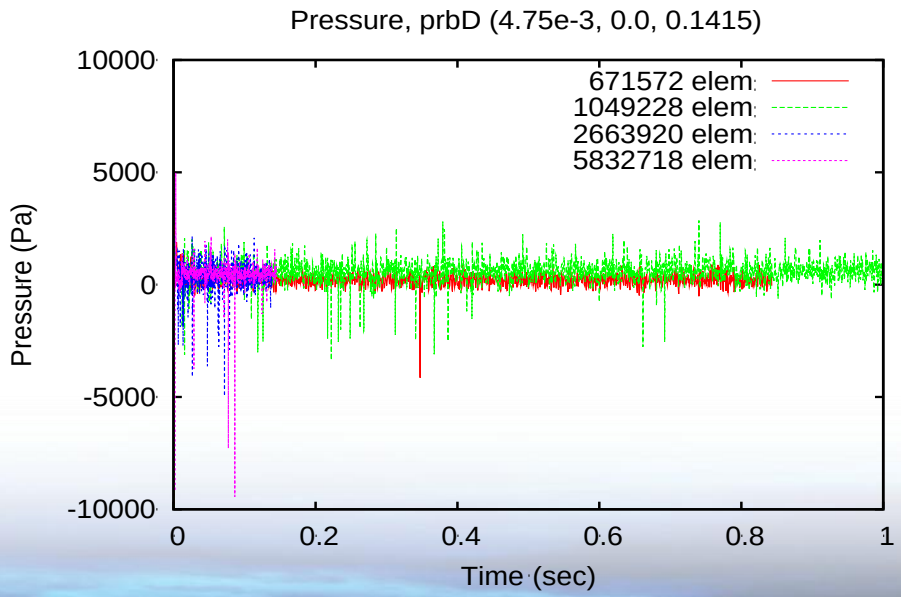
- Sandia Redsky platform, 256-1000 processes
- Oak Ridge Jaguar platform, 1200-9600 processes
- 2nd order BFD time integration
- Linear Lagrange elements (2nd order in space)



Transient Pressure Profiles

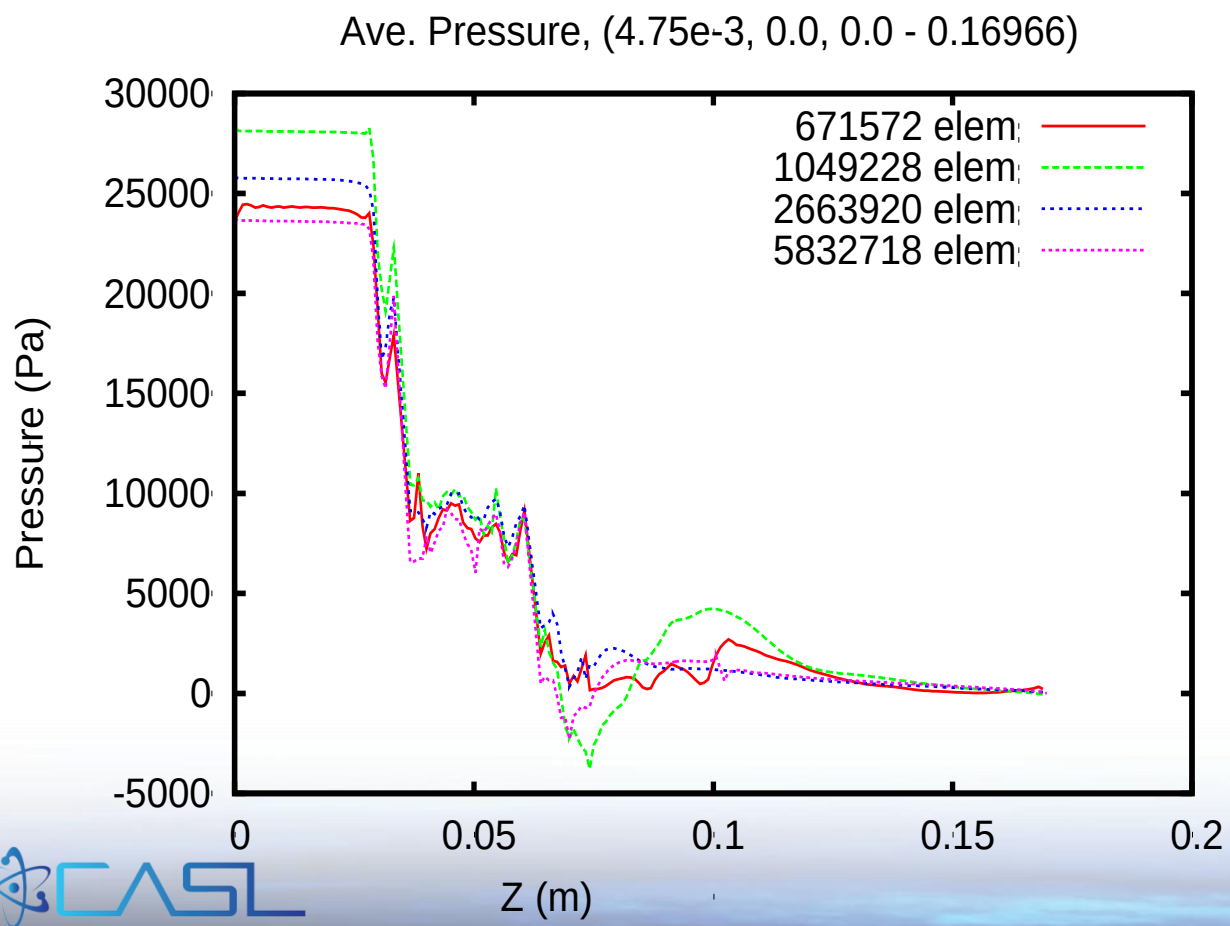
Mesh	# of Elements	Simulated Time (sec.)	Flow through times	Δt	CFL ave. (section1/section3)	Y+ ave.
672K	671,572	0.88	26	5.0×10^{-5}	9.6/1.3	26
1M	1,049,288	1.11	33	5.0×10^{-5}	11.1/2.9	19
3M	2,663,920	0.2	6	2.0×10^{-5}	5.9/2.1	16
6M	5,832,718	0.32	9	2.0×10^{-5}	7.9/2.2	13





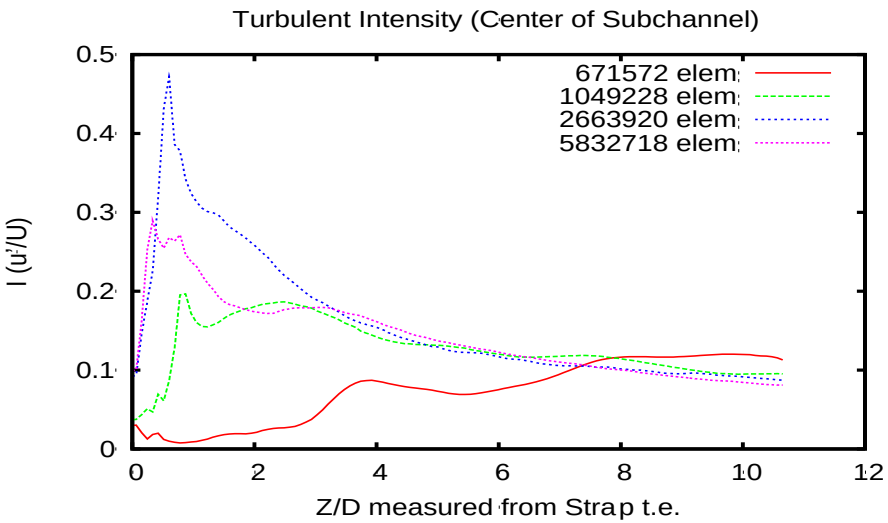
Time Averaged Pressure Profiles Across Spacer Grid

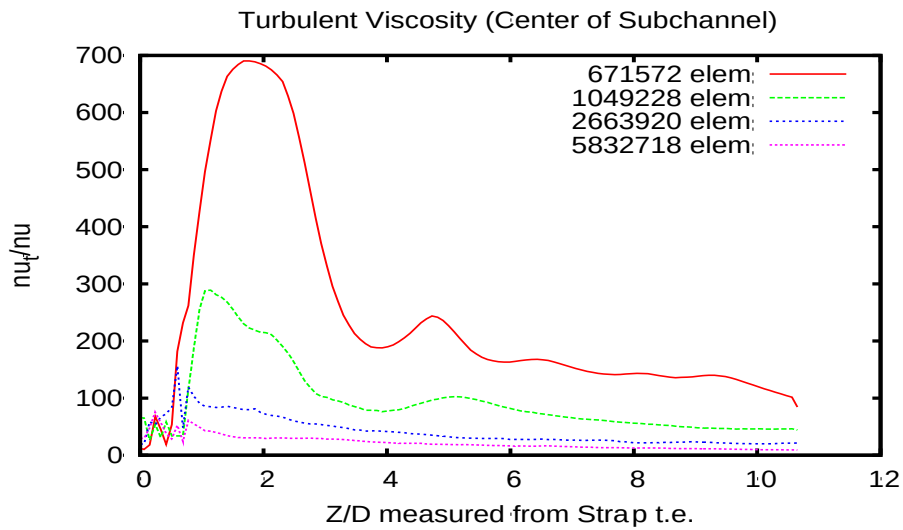
- Coarsest mesh is inadequate for simulation
- 3 finer meshes show signs of convergence



Mesh	Mean Pressure Drop (Pa)
677K	23,400
1M	26,780
3M	23,800
6M	22,042

Turbulence Characteristics



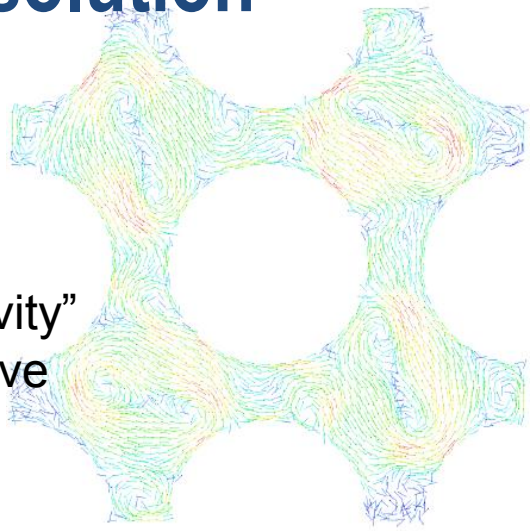


- 672K mesh is inadequate to resolve pressure behavior.
- Non-monotonic behavior in turbulent intensity:
  - Converges 3 diameters downstream as turbulence subsides
  - Suggests under-resolution of mesh near spacer grid
- Turbulent intensity comparison to Benhamadouche *et al.* 2009:
  - At 3 diameters downstream, Drekar: 18%, Ben.: 11%
  - At 10 diameters downstream, Drekar: 10%, Ben.: 8.5%
- Monotonic decrease in amount of eddy-viscosity with refined mesh shows correct behavior (reduced contribution of subgrid model).

Preliminary Verification Results for GTRF CFD with Fuego and Drekar (Δp), just spatial resolution

Mesh	Fuego	Drekar
Coarse	31.8 kPa	26.7 kPa
Medium	24.6 kPa	23.8 kPa
Fine	24.4 kPa	22.0 kPa

A "mesh sensitivity" study would have us stop here!



Fuego

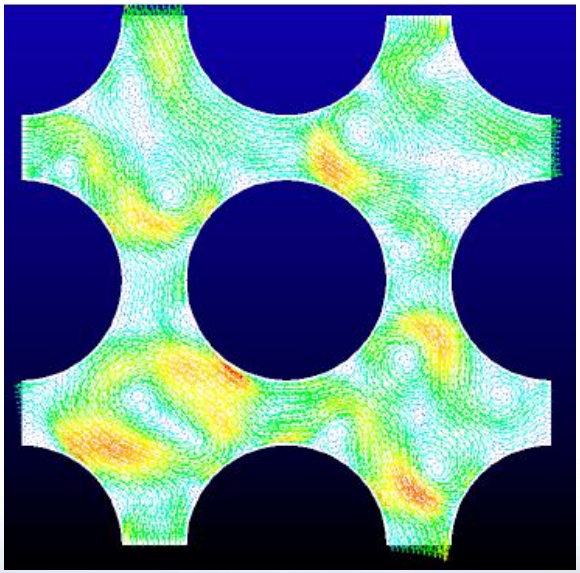
$$\Delta p(h) = 24.34 + 6.10 \acute{} \; 10^{18} h^{15.85}$$

95 % Error Bound -6.5 kPa

Drekar

$$\Delta p(h) = a + bh^{c} = 17.42 - 163.7 h^{1.234}$$

95 % Error Bound -8.9 kPa



Based on the initial results what should we do next?

- More metrics produced from the calculations: velocity, TKE, dissipation, turbulent statistics
- Determine the mesh requirements
- Significant SA/UQ studies of modeling of GTRF, determine the relative importance of various modeling parameters
- Test URANS on GTRF. Our current meshes are too coarse for LES, we have no inertial range resolution
- LES needs signficantly finer meshes, and/or a mesh that more biased towards the boundary layers
- Numerical impact of spatial and temporal integration method
- Impact of the LES model and its parameters
- test the applicability of ILES

CASL Validation Data

Nam Dinh

CASL Roundtable

August 11, 2011

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Validation Data Activity

- "gap analysis":
  - "CASL Validation Data: An Initial Review" (L3M, January, 2011)
  - Gap: multi-physics / multi-scale V&V
- "new experiments":
  - Investigate option with NSUF/ATR, LWR-S (HRP), NEET, FCRD, NEUP
  - New (CASL-guided) experiments
- "database":
  - Validation Database Infrastructure – requirements (L3M, June, 2011)
  - NE-KAMS: Nuclear Energy – Knowledge Base for Advanced Modeling and Simulation
    - Seed funding from CASL-VUQ
    - V&V process document; building / focusing on CFD V&V
    - Database functional requirements, prototyping, demonstration
    - NEAMS VUQ, DOE-NR, NEUP support
- Validation Data Committee (just stand-up)

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Content

- Background (CASL proposal)
- Validation Data Review
- Validation Data Plan
- Path Forward

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The validation hierarchy integrates all CASL Focus Areas, executed in a bottom-up and top-down way

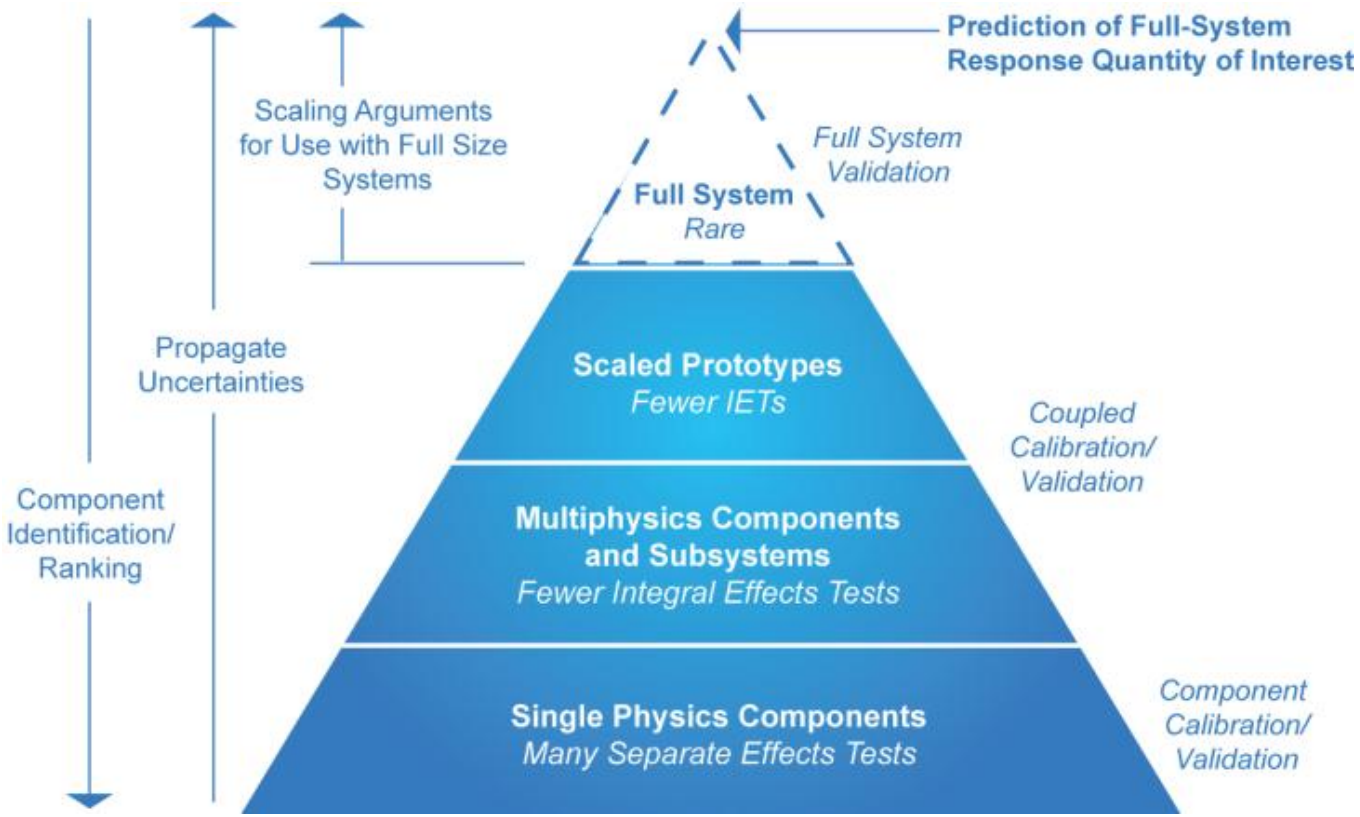

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Table 2-1: CASL Data and Validation Needs

Types of Experiments and Measurements	Phenomena and Regimes	Issues	Focus Area Capability	Measures to Be Taken to Meet Validation Data Needs
Plant and In-Core Diagnostics	Neutronics and T-H data in operational transients	Unable to discern local effects and to reveal relationships of interest for VR validation	Core neutronics, T-H (steady state)	Coordinate with Westinghouse and TVA to plan in-core measurements, and PIE characterization of a used fuel assembly to obtain a complete data set for VR code validation
Fuel Post-Irradiation Examinations of LWR Used fuels	Fuel performance, CRUD, corrosion, fretting wear, and failures	Exhibiting only accumulative effect	Fuel performance, chemistry, fluid-structure interactions	Apply advanced diagnostic techniques to obtain new detailed data on cladding failure modes, oxide layer and CRUD compositions (coordinate with LWR-S Program)
In-Pile and Out-of-Pile Testing of Prototypic Fuels	Fuel behavior under normal, abnormal, transient, and accident conditions	Past tests were conducted with limited diagnostics (main data: post-test characterization)	Assembly dynamics under normal, transient, and accident conditions	Collect and qualify data sets from previous experimental programs (e.g., FLECHT, BFBT, NSSR, CABRI) Coordinate with the planning of fuel tests in OECD Studsvik and Halden Reactor Project and INL's TREAT (under consideration for restarting)
Separate-Effect Tests	T-H– structural mechanics in fuel assembly	Exhibiting only differential relationships under potentially nonprototypic conditions	Multiphase T-H, fluid structure interactions	Coordinate with V&V activity in other DOE-NE programs as well as basic research experiments using advanced diagnostic capabilities at WEC, MIT, TAMU, OSU, and INL
Integral-Effect Tests	System dynamics	Scaling distortions Limited set of scenario and range of test conditions	Coupling to a system code	Coordinate with the INL-led development of database for validation of CFD in nuclear reactor safety applications

CRUD phenomenological decomposition

AOA Prediction: Time- and Space Resolved Core Power over a Fuel Reload Cycle

FA/Fuels/ Rod/Clad	***T-H***	***Neutronics***	***Crud***	***Coolant Chemistry / Material Corrosion***
FALCON	RETRAN/ VIPRE	ANC	BOA	
Support for T-H, and Neutronics	Core-wide T-H coupled with Neutronics	Core power over long operation period	Initial inventory of crud after fuel reloading (e.g., effect of ultra-sound cleansing)	Material corrosion on RCS and heat transfer surfaces
	Plant / Reactor System T-H			Crud detachment in steady-state & transient conditions
Fuel Burnups	Nominal Operation	Core power during transients	Inventory of crud materials in RCS structural and heat-transfer (SG) surfaces	Inventory, transport and distribution of RCS chemicals and corrosion products (incl. particulate materials)
	Operation Transients	T-H feedback		
	Abnormal Transients			
PCI	Rod Bundle T-H (RBHT/RBTH)	Boron effect	Boron distribution (incl. its depletion)	System-level (incl. coolant chemistry regulation sub-system/filters)
	Inlet Flow incl. Temp. & Velocity Fluctuations			
Fuel Rod and Spacer Defor-mation		Hot channel Identified	Effect of grid spacer mixing/ vibration on crud deposition/detach	Core-level (Regional)
	Subchannel Mixing incl. Spacer Effect			Distribution between Rod Bundles
	Turbulence Flow	Pin-by-pin power (heat flux)	Crud character-ristics (thickness, micro-structure, chemical composition)	Within Rod Bundle (Pin Level)
	Subcooled Flow Nucleate Boiling (heat transfer)			Boundary layer concentration profile of different species
Multiphase micro-hydrodynamics that govern crud deposition		Hot spot identified	Physico-chemistry that govern crud characteristics	
Wall bubble layer configuration			Concentration of chemicals (boron, etc.) and particulates at the triple contact line	
Interfacial Instability				
Turbulence-Interface Interactions			Agglomeration, reactions, precipitation in supersaturated solution	
Condensation on bubble dome				
Bubble dynamics in SFB (sliding, coalescence, oscillations)		Fluence Irradiation "aging" effect on cladding and crud stability	Dry-spot synthesis &growth of micro-porous layer (area for further deposition)	
Meniscus / microlayer dynamics			Crud insulation effect on boiling / heat transfer, local temperature, meniscus	
Dynamics of Evaporating Triple Contact Line (Recoil Effect)			Effect (e.g., Maragoni, disjoint pressure) of chemicals and particulates present in coolant on microhydrodynamics of evaporating liquid layer and vapor bubble nucleation	
Effect of surface/crud nano-morphology on micro-hydrodyn.				
Nucleation (energy barrier)				

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GTRF model integration

"Fret Map": GTRF-prone domain boundaries				
GTRF wearing rate (at sensitive locations)				
Forcing at GTR Contact			Wear Rate	
Rod-Grid Vibration Analysis			Tribology	
Pressure/stress field	GTR Gap	Spring Relaxation Spacer Expansion		
Flow Turbulence Power Spectral Density (PSD)	Spring Dynamics Rod bending	Irradiation-Induced Grid Spacer Expansion	Cladding Properties	Grid Spacer Properties
Fuel Rod-Grid System ***Identify sensitive FRGS***		***Aging Effect***	**Materials Properties (Degradation)**	
Subcooled Boiling	FA Bowing	FA shuffling / Contact Reset	Contact area relocation	Fluence
Sub-channel Mixing	Friction Forces	Power transients,	Cladding Deformation	Pin-by-pin Power
Fuel Assembly ***Identify sensitive FAs***		Secondary side transients	Pellet-Cladding Interactions	Effect of Control Rod FSI
In-vessel flow mixing in downcomer & lower plenum	FA-to-structures couplings (incl. loose, float) FA-to-FA couplings	Pump transients, Pump asymmetry		Structural Feedback on Neutronics
System Thermal-Hydraulics	Core barrel Core support plates	Effect of Heat Axial Distribution on Subcooled boiling		Thermal-hydraulic Feedback on Power
Core-wide Structural Dynamics[1]		Plant Operation & Abnormal Transient	**Core-Wide Thermal-Hydraulics**	
Stresses	Mechanics	Heat Flux	Fuel Burnups	Core Power
Fluid Flow	**Structures**	**Thermal**	**Fuels**	**Neutronics**

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Validation Data Support of CASL Objectives

The success of CASL effort is to be demonstrated through "predictive capability maturity" measured in VERA applications to challenge problems .

> The measured maturity demonstrates that CASL-generated VERA-based capability constitutes a significant step forwards in "predictive capability" for the respective challenge problem (shown by uncertainty reduction in challenge problem's FOM).

Validation-grade data are instrumental in this demonstration, both at the stage of model calibration, and at the stage of maturity assessment, including validation of the capability for the intended application.

High priority is given to data and databases to support validation of VERA multi-physics simulation / coupled-code capability.

Validation Data Plan – Top-Down Drive

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Factors Affecting Validation Data Planning

- Challenge problem specification (mission and success criteria)
- Problem solution framework and approach (which and how simulation codes are used and their applicability assessed)
- Status of required capabilities in available and selected analysis tools
- VUQ techniques and method for assessment of predictive capability
- Types, quality, availability, and accessibility of existing data
- Projected time and resources for generating new data
- Decision model that integrates information from (i) through (vi) and prioritizes data activities, based on cost-benefit analysis of possible activities.

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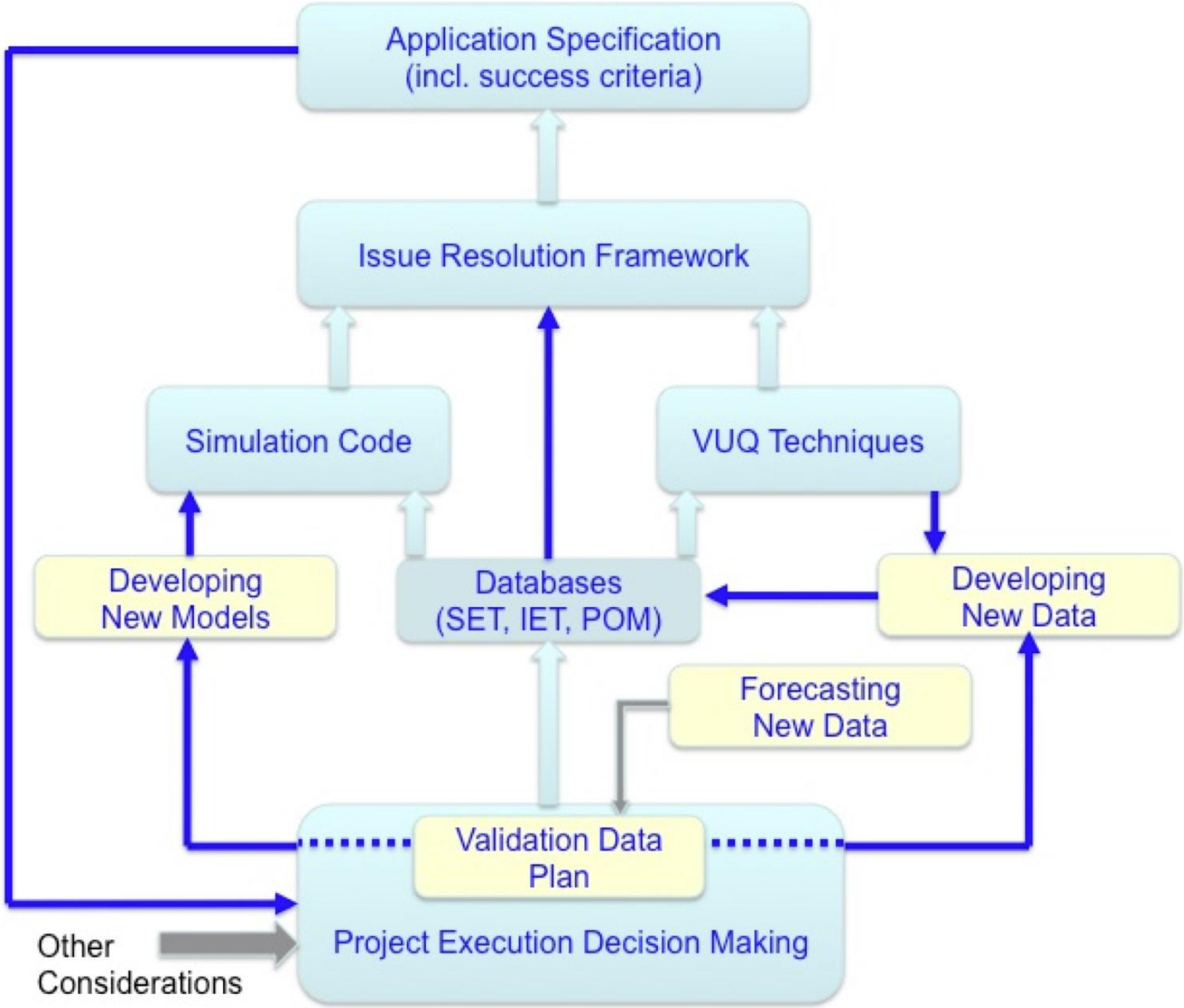
Application Specification
(incl. success criteria)
Issue Resolution Framework
Simulation Code
VUQ Techniques
Developing
New Models
Databases
(SET, IET, POM)
Developing
New Data
Forecasting
New Data
Validation Data
Plan
Project Execution Decision Making
Other
Considerations

Validation Data Plan

- Validation Data Plan (VDP) is a ***dynamic planning*** instrument to guide (potentially, optimize) activities on data production (e.g., new experiments or plant measurements), collection, management (i.e., analysis, qualification, archiving), and usage so that they enable effective support for development, assessment and application of simulation tools intended for a challenge problem

- VDP development must build on insights derived from substantial tasks of
  - identification of data gaps (data needs), including specification of required characteristics of data that would fill the gaps;
  - evaluation of means, time and resources needed to acquire the data identified / specified;
  - selection and prioritization of data (production, collection, analysis) tasks that most cost-effectively and timely fill the gaps.

Validation Data Plan – Sufficiency

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Validation Data Plan

Activity Thrusts

Validation Database

Collect Deem-Relevant Experimental & Plant Data

Analyze, Qualify and Characterize Data

Process ("Fit") and Archive Data for VUQ Tasks

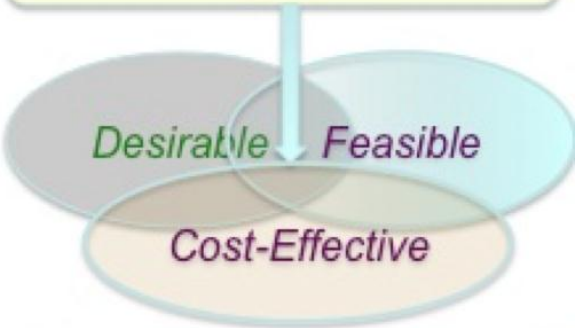
Identification & Assessment of Data Needs (Gaps)

Separate-Effect Tests (MPO, MNM)

Multi-physics and Integral-Effect Tests

Plant Measurements and Observations (AMA)

Getting New Data



Stimulate and guide the development of advanced diagnostics & experiments

Support design of new plant tests & observations

NE-CAMS

Q-PIRT

PCM

Develop and Apply Infrastructure to Support VDP Implementation

Develop and Apply Techniques to Support VDP DM

Validation Data Review

- Characterization by Data Sources
  - Physics Tested
  - Modes of Experimentation
  - Data producer and ownership
  - Data format, storage, maintenance, and accessibility
- Characterization by Data Usage
  - Quality of Information
    - Relevance, Scalability, and Uncertainty
  - Usability of Information
    - Model development, calibration, code validation/UQ
  - Compatibility with VUQ (VUQ friendliness)
    - Comprehensiveness, completeness and consistence with implementation of VUQ

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Validation Data Sources

Plant & In-Core Diagnostics

TVA: Plant operational data
EPRI: Fleet-wise fuel reliability and failure data
Westinghouse: fuel manufacturing, properties, testing

PIE of Used Fuels

ORNL: PIE of used fuel cladding
INL: PIE, crud characterization
EPRI: industry database

In- & Out-of-Pile Testing of Prototypic Fuels

INL: ATR National Scientific User facility
INL: TREAT (transient fuel testing – TBD)
INL: Halden Reactor Project Tests (via LWR-SP)
Studsvik Clad Integrity Project (SCIP)

Separate-Effect Tests

MIT Boiling heat transfer
TAMU Crud deposition
TAMU PIV flow imaging in subcooled boiling
INL corrosion (LWR-SP)
CFD databases (NE-KAMS)

Integral Effect Tests

Westinghouse Fuel Assembly Mockups
OrSU: APEX test facility for system dynamics (LWRSP)
Halden Reactor Project (AOA tests)

Formulate tasks on underlying physics that govern uncertainties

DOE-BES
DOE-ERFC
DOE-NE, LWR-S, NEUP
DOE-NR

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Assessment of Validation Data Sets for CRUD and GTRF Challenge Problems

- ✧ Plant and in-pile testing data
  - ✧ Database on Nuclear Fuel Performance
    - ✧ International Fuel Performance Experiments
    - ✧ ***Studsvik Cladding Integrity Project (SCIP)***
  - ✧ Individual Plant data
  - ✧ Halden Reactor Project (HRP)
    - ✧ ***Axial Offset Anomaly (CRUD) tests***

- ✧ Out-of-pile integral-effect tests
  - ✧ ***Industry Programs (WALT, NESTOR)***

- ✧ Separate-effect tests
  - ✧ Rod Bundle Heat Transfer
    - ✧ ***PFBT benchmark***
  - ✧ Subcooled Flow Boiling
  - ✧ Fuel Rod Vibration

- ✧ Advanced Diagnostics

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Data Realism

- Data (non)representativity
  - Issues in experimental conditions, design, procedure, diagnostics, processing
  - Relevance
  - Scaling
- Data quality… not "UQ-perfect" experiments
  - Past (pre-VUQ) experiments
  - Quality of data (in UQ grade)
- Not all experiment "born equal"
  - Over-kill model calibration by aligning with certain SETs
- Even within an experiment, not all data "born equal"
  - Measuring devices
  - Relevance of that parameters to FOM
    - P, T, VF, velocity…

Data Heterogeneity

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Table 3.1. Grading of experimental or plant test data by their VUQ quality.

VUQ Quality	Grade				
	4	**3**	**2**	**1**	**0**
Relevance [R]	Very High (direct)	High	Medium	Low	N/A
Scaling [S]	Prototypic (full-scale)	Adequately scaled	Medium	Inadequately scaled (large distortions)	N/A
Uncertainty [U]	Well-Character-ized	Character-ized	Medium	Poorly-Characterized	N/A

Validation Data Review

- Quantity and quality of experimental data potentially accessible for use in CASL challenge problems are (far) coarser and integrated (in time and space) than the level of fidelity characteristic of advanced modeling and simulation, and VUQ methods and tools available for, and developed in, CASL (MPO/MNM,VUQ)

- Within the CASL time frame (5-7 years), the situation with validation data (content) is not expected to significantly improve
  - Long lead time and large resources required for development of advanced diagnostics, advanced experiments

- With advent of ModSim, data support will inevitably remain the weakest link, *potentially* limiting quality of CASL (as well as other complex and new nuclear engineering) applications

- Path forward is to cope with data realism, while minimizing potential of R&D process being misguided by deficient data or illusion of "advanced models"

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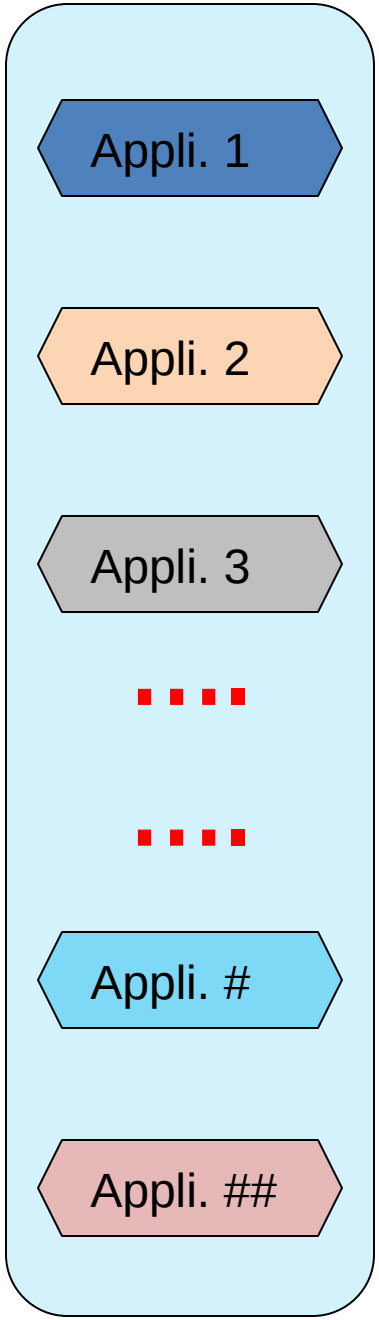
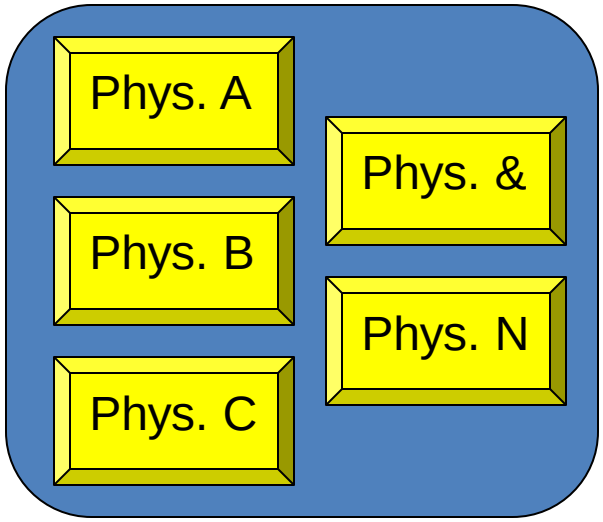
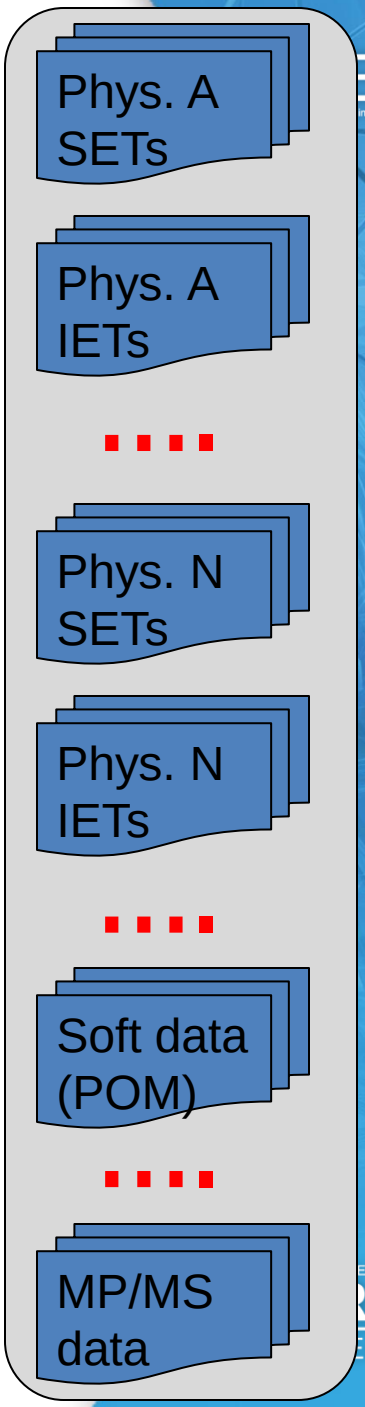
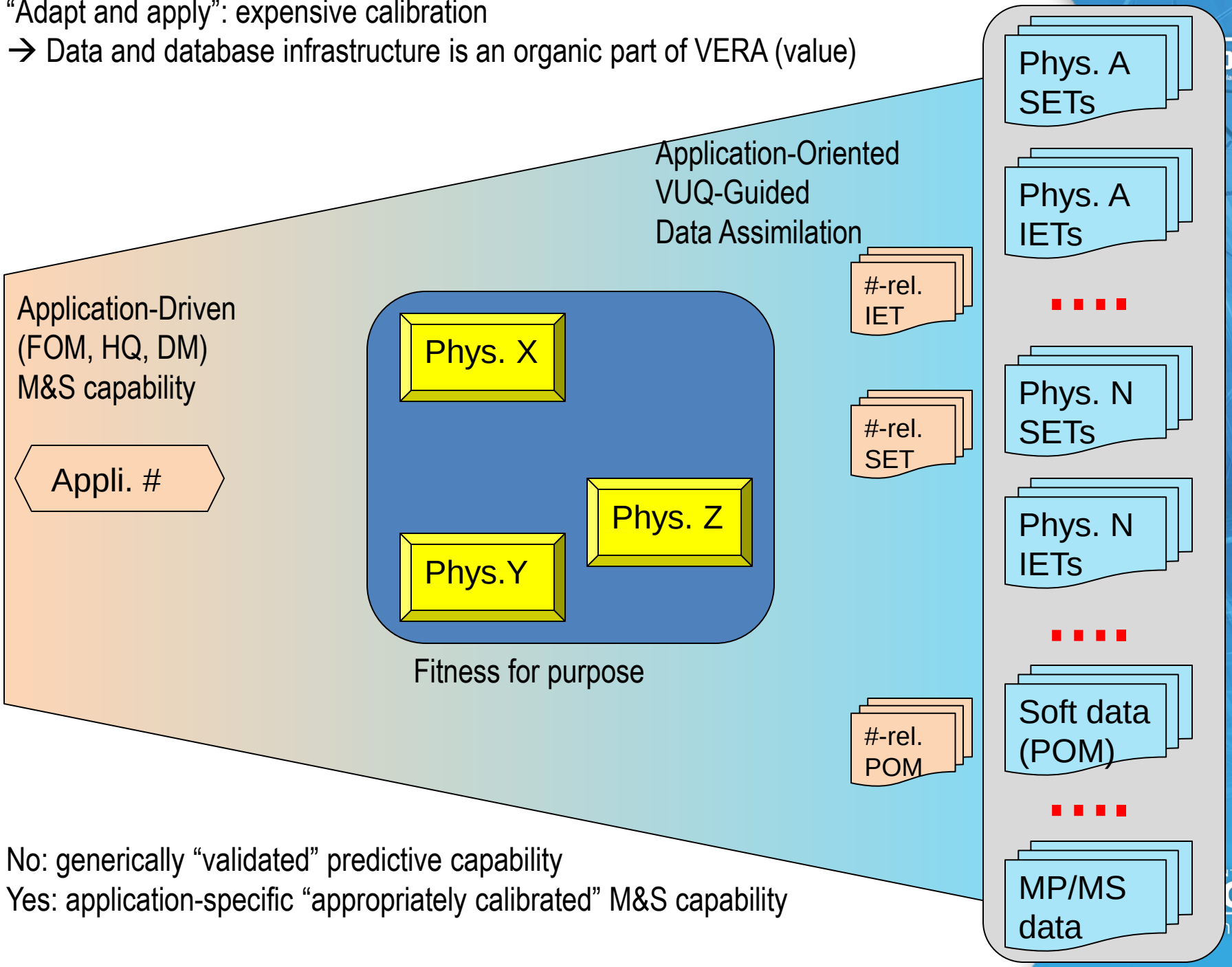

Appli. 1
Appli. 2
Appli. 3
Appli. #
Appli. ##


Phys. A
Phys. B
Phys. C
Phys. &
Phys. N


Phys. A SETs
Phys. A IETs
Phys. N SETs
Phys. N IETs
Soft data (POM)
MP/MS data

“Adapt and apply”: expensive calibration

→ Data and database infrastructure is an organic part of VERA (value)



No: generically “validated” predictive capability

Yes: application-specific “appropriately calibrated” M&S capability

Validation Data Plan: "*With the end in mind*"

How CASL products are going to be used?	Validation Requirements
Mode 1. [Codes at all levels in hierarchy] Gain insights into governing physics and mechanistic understanding of phenomena of importance / relevance.	Qualitative comparison with multifaceted evidences from used fuels observations, measurements, and data obtained under relevant conditions in various experiments.
Mode 2. Use high-resolution models / codes to develop constitutive correlations to be used as closure laws in coarsened-grain (lower resolution) models.	A set of measured data that are complete (i.e. with sufficiently specified operating / boundary / geometry / materials / etc. conditions) for problem definition, over the range of (high-resolution model / code) applicability.
Mode 3. Quantification of uncertainties of models / correlations used in codes that are to be used in design, safety analysis and licensing.	Extensive set of data with specification of uncertainties / sensitivities in test conditions and measurements.

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Validation Data Plan: *Where and When Do Data Come from?*

How CASL products are going to be used?

Validation Requirements

Mode 1. [Codes at all levels in hierarchy] Gain insights into governing physics and mechanistic understanding of

Legacy data from
- past R&D/ literature, industry observations

Trend data from
- TVA Plant Operational Data
- Westinghouse Fuel Test Data

Qualitative comparison with multifaceted evidences from used fuels observations, measurements, and data obtained under relevant conditions in various experiments.

Mode 2. Use high-resolution models / codes to develop constitutive correlations to be used as closure laws in co

Evaluated data from
- CASL Data Center (evaluated data from past relevant experiments and PIE)
- TVA Operational Plant Data (quality set)

A set of measured data that are complete (i.e. with sufficiently specified operating / boundary / geometry / materials / etc. conditions) for problem definition, over the range of (high-resolution model / code) applicability.

Mode 3. Quantification of uncertainties of models / co de

CASL-driven and designed test data from
-Westinghouse Fuel Assembly Mockups
- Experiments performed under LWR-S, NSUF & other DOE/ EPRI/ NRC programs

Extensive set of data with specification of uncertainties / sensitivities in test conditions and measurements.

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A Multi-Faceted, Complementary Approach

(necessitated by short term data needs *vs.* longevity of new experiments)

CRUD

Industry (Plant, Fuel) Data

+ Plant power measurements
- *Coarse, super-assembly level*

+ Used fuels (cladding)
- *Visual observation, limited material characterization*
- *Only "end-cycle" information*
- *Poorly characterized local RP / TH / CC conditions*

Legacy (R&D) Data

+ Crud characterization and analysis
- *Only "end-cycle", accumulative information*

+ Physics of boiling of solvent
- *Not in prototypic reactor coolant chemistry / irradiation / flow / thermal conditions*

CASL Data Center Evaluated Data

+ TVA Plant Data
- *Enhanced control of local conditions*

New Experiments (Separate Effects)

+ CASL-coordinated experiments performed by LWR-S, NSUF / NEUP, other EPRI / NRC projects
- *Controlled conditions, with sensitivity / uncertainty*

CASL-Driven Data (CASL-Initiated Tests)

+ Westinghouse Fuel Assembly Mockups Test
- *Controlled conditions, with sensitivity / uncertainty*

Trend Data

Model Calibration Data

Validation & UQ Data

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A Multi-Faceted, Complementary Approach

(necessitated by short term data needs *vs.* longevity of new experiments)

CRUD

Industry (Plant, Fuel) Data

Legacy (R&D) Data

CASL Data Center Evaluated Data

New Experiments (Separate Effects)

CASL-Driven Data (CASL-Initiated Tests)

+ Plant power measurements
- Coarse, sup

+ Used fuels
- Visual o
- Only "end-cy
- Poorly characterized local conditions

+ Crud characterization and analysis
- Only "end-cycle", acc

+ Physics of boil
- Not in pr / flow / *thermal co*

+ TVA Plant Data
- Enhanced control of local conditions

+ CASL-coordinated expe LWR-S, NSUF / NEUP, other EPR
- Controll

+ Westinghouse
- Controlled conditions, wi uncertainty

Aiding a basic understanding of physico-chemical mechanisms that need to be modeled in VRI

Useful for specifying parameter ranges in closure models

Predicting deposition, composition, characteristics of crud in plant conditions

Requiring a MP/MS Data Assimilation M&T To Make Effective Use of Heterogeneous, Non-Statistical & Variable-Quality Evidences

Trend Data

Validation & UQ Data

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Validation Data Path Forward

- Instead of longing for magical appearance of "VUQ-grade" data, CASL is expected to demonstrate that VERA capability can be used intelligently to generate added values in engineering practice (and in doing so, spearheading the way of applying modern M&S in data-deficient world).

This can be achieved by:

- Recognizing that lack of "VUQ-grade" data is, and will remain, a practical constraint, common to all significant problems (issues) in nuclear engineering
- Recognizing data realism and potential synergistic value of data (and models) of different quality and origins
- Recognizing potential synergistic value of assimilating application-***relevant*** data with consistent M&S capability

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Validation Data Path Forward

- **Validation data plan includes three objectives**

  (a) "database" – to maximize value of existing and available data for VUQ needs,

  (b) "gap analysis" – to identify missing information and cost-effective way to acquire it (or compensate for its effect); and

  (c) "new experiments" – to plan new experiments and plant tests, maximizing their VUQ value under constraints.

- **VUQ Methods and Tools**
  - To enable the three activity thrusts achieving their objectives
  - Reducing barrier to VERA (streamline calibration)… "usability".

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Validation Data Path Forward

- "Database":
  - Should be part of VERA (adding value, streamlining calibration… "usability", A&A)
  - CASL-specific requirements on validation database infrastructure
  - NE-KAMS vs CASL Data Center (to decide)
- "Gap analysis":
  - Data: multi-physics / multi-scale V&V
  - Methods and tools for Data Assimilation for MP/MS problems with "data realism"
- "New experiments":
  - New (CASL-guided) experiments are unlikely in Phase 1
  - Potential of NSUF/ATR, LWR-S (HRP), NEET, FCRD, NEUP
- "VUQ M&T":
  - Data Assimilation for MP/MS problems with "data realism"
- Validation Data Committee

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VUQ Risks and Challenges

Jim Stewart (SNL)
Dana Kelly (INL)

1st Annual CASL Roundtable Meeting
North Carolina State University
August 9-11, 2011

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VUQ Risks and Challenges *(Nontechnical)*

- Ability to appropriately define the VUQ case study application (relevance to CASL challenge problem)
  - *Status: Year-1 schedule delays; finally addressed in collaboration with AMA (Crud boiling index simulation using VIPRE-W). Similar Year-2 challenges remain.*
- Early readiness of VERA for integration with DAKOTA
  - Status: DAKOTA successfully integrated in loose-coupling mode. Challenges still remain in tighter LIME-based coupling in Year 2. Coordination with VRI critical.
- Availability of simulation software (from AMA, VRI, and MNM) required by VUQ to complete its tasks
  - Status: SNL/LANL access to codes has been adequate; lack of NCSU access to Westinghouse codes due to NDA issues continues to be an impediment to progress.
- Ability to effectively partner with other focus areas to implement V&V practices and integrate VUQ capabilities
  - Status: Some successes (AMA, VRI, THM); more effort needed in Year 2 with RTM and MPO, as well as in execution of the VUQ-led committees/working groups.

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VUQ Risks and Challenges *(Technical)*

- Calibration/validation data is unavailable and/or of poor quality
  - *Mitigation: Use "expert judgment" to conceive and construct "worst-case", "possible-case" and "best-case" data (nominal values and uncertainties). Prioritize efforts with outside partners to seek or generate better data.*
  - *Status: Year-1 milestones (L3:VUQ.VVDA.P1.02 and L3:VUQ.VVDA.P2.02) delivered validation data review and requirements/path forward. One conclusion: Situation with integrated-effects data worse than previously thought. Path forward: CASL Validation Data Committee; leverage (NEAMS VU) NE-KAMS project. This remains one of our largest resource risks!*
- Use of legacy software physics models and codes: Inadequate access to source code and/or poor software design leads to inability to implement intrusive (e.g., adjoint-based) capabilities for error estimation, sensitivity analysis, reduced-order modeling, uncertainty quantification, and/or optimization.
  - *Mitigation: Resort to non-intrusive methodologies (e.g., use DAKOTA and "brute-force"); Replace with new physics capabilities developed within CASL.*
  - *Status: Ongoing; we will continue to work with other FA's to address these issues.*

VUQ Risks and Challenges *(Technical)*

- Use of legacy software physics models and codes: Poor parallel scalability limits the computational efficiency of our algorithms.
  - *Mitigation: Invest in new algorithm technology that minimizes the effects of poor scalability. Alternatively, replace with parallel scalable physics capabilities developed within CASL.*
  - Status: Ongoing; scalability has yet not surfaced as a primary driver of priorities.
- Use of legacy software physics models and codes: Mathematically inconsistent behavior under mesh refinement leads to inadequate verification
  - *Mitigation: Develop innovative ways to fix or control mesh sizes locally where necessary; develop capability for verifying solutions in the presence of these mesh-dependent models. Preferred path: Remove offending models and/or codes and replace with mathematically consistent, mesh-independent models.*
  - *Status: PoR-2 Milestones L3:VUQ.VVDA.P2.04 and L3:VUQ.VVDA.P2.05 have addressed verification issues for GTRF. Non-legacy CFD and mechanics codes were considered. Work will continue beyond PoR-2.*

CASL Consortium for Advanced Simulation of LWRs
U.S. DEPARTMENT OF ENERGY Nuclear Energy

VUQ Risks and Challenges *(Technical)*

- Extreme ***high-dimensionality*** and ***nonlinearity*** of the fully-coupled VR poses difficulties for scalable, efficient error estimation, data assimilation, sensitivity analysis, and UQ.
  - *Mitigation: Increase investments in new algorithm developments; Leverage existing advanced software tools where possible, including DAKOTA and Trilinos.*
  - *Status: PoR-3 Milestones L3:VUQ.SAUQ.P3.01 (Uncertainty Management Hybridization Framework) and L3:VUQ.SAUQ.P3.02 (Scalable UQ Algorithm Deployment) will begin to address this issue.*

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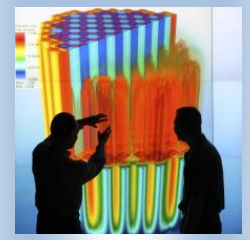
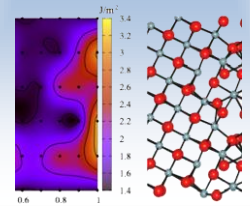




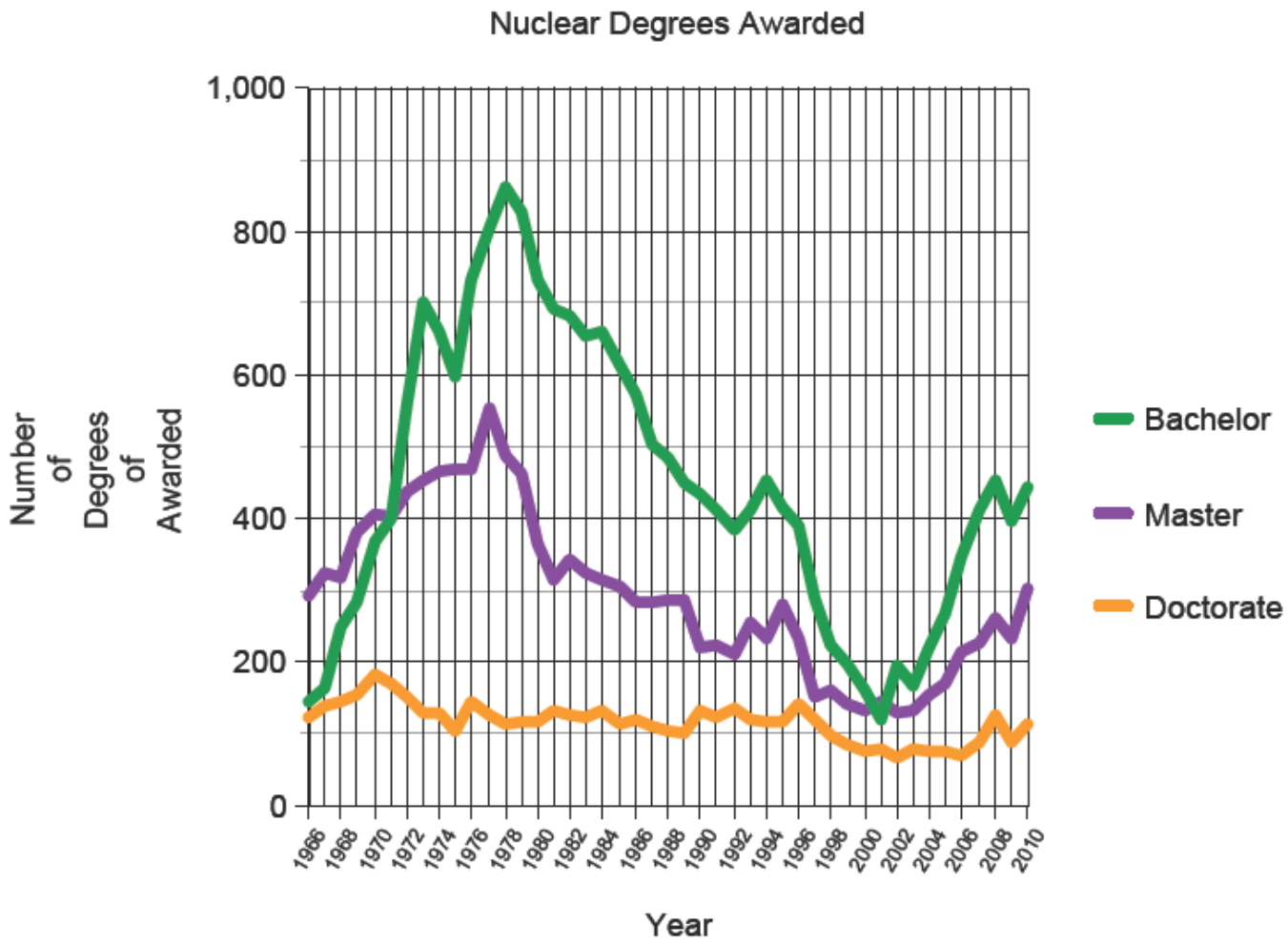
Education Council Activities

Consortium for Advanced Simulation of Light Water Reactors

John Gilligan
Professor of Nuclear Engineering
North Carolina State University
Chair CASL Education Council

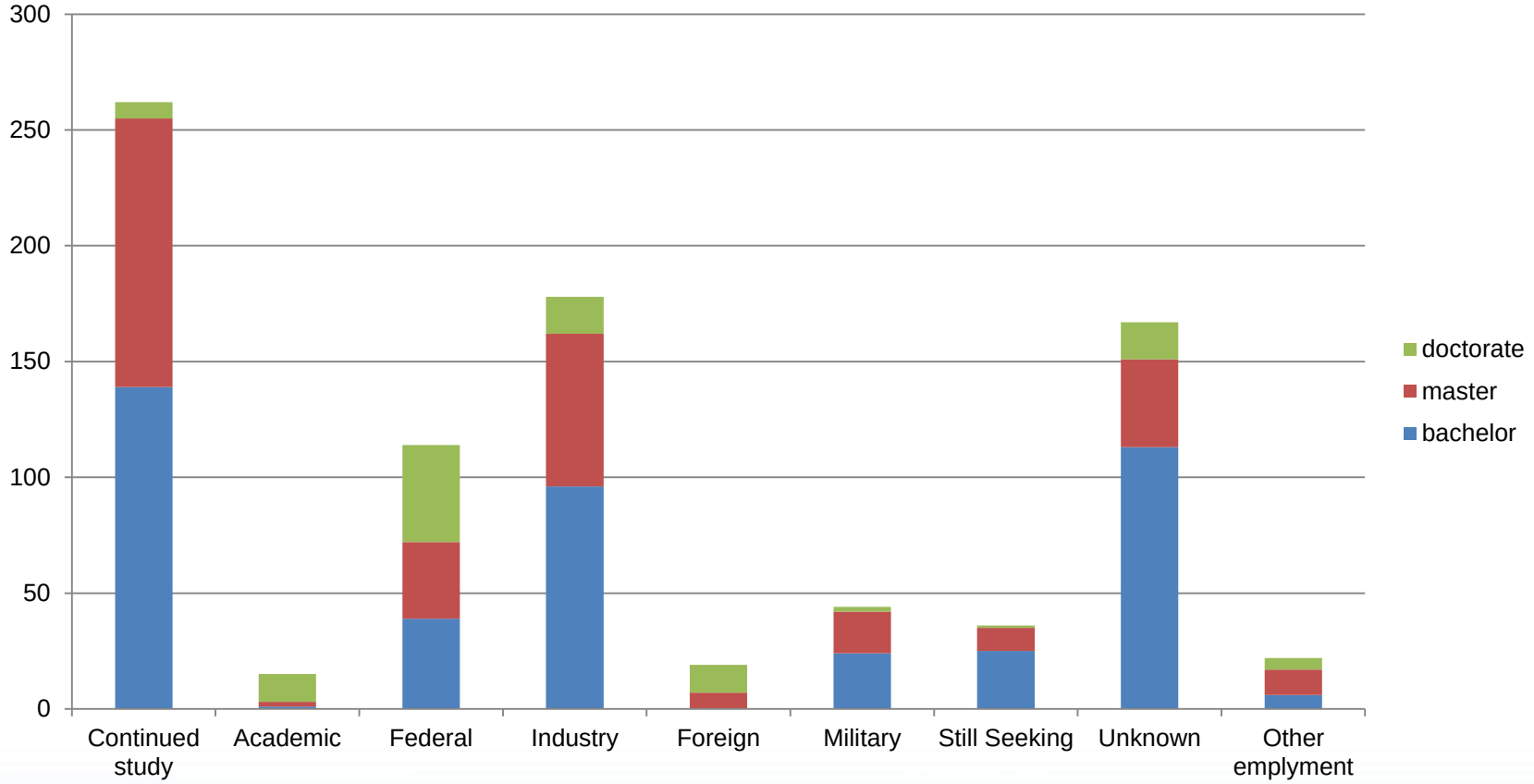
Consortium for Advanced Simulation of LWRs

The Nuclear Renaissance is Apparent to Students



Oak Ridge Institute of Science and Education

Where Graduates Go 2010



CASL Education Council

Creating a new generation of LWR designers, Scientists, and Nuclear Power Professionals

Council Charter:

- Assure that results are integrated into undergraduate, and graduate curricula and transferred to industry users
- Encourage diversity of participation in CASL activities
- Advise Chair on educational development activities
- Review and recommend education curricula and programs

Council Activities:

- Nuclear Education Center of Excellence (GoNERI) Presentation, Dec. 7 2010, Tokyo, Japan
- CONTE Conference Paper, Feb. 2011, Jacksonville, FL
- Meetings via conference calls and at ANS meetings

Council Members:

Push and Pull Philosophy

John Gilligan, Chair, Professor, North Carolina State University

- **Ken Canavan**, Manager, EPRI
- **Ben Forget**, Asst. Professor, MIT
- **John Goossen**, Director, Westinghouse
- **James Holloway**, Professor and Assc. Dean, Univ. of Michigan
- **Ivan Maldonado**, Assc. Professor, Univ. of Tennessee/ORNL
- **Rose Montgomery**, Manager, TVA
- **Ken Okafor**, Assc. Professor, South Carolina State Univ.

Education Council Status

- Council charter and milestones have been established
- First conference call was in August 2010, support started Feb.-April 2011
- Plans for PoR 1-3
  - Develop diversity and recruiting plan
  - Map CASL challenge problems into curricula
  - Develop prototype course modules
  - Develop transfer plan to industry and post docs
  - Develop framework for use of Virtual Design Tools in curricula
- Challenge for education programs will be to integrate the many multidisciplinary programs for Virtual Design Tools

Education Challenge: Bridge Interdisciplinary Academic Cultures

Leverage

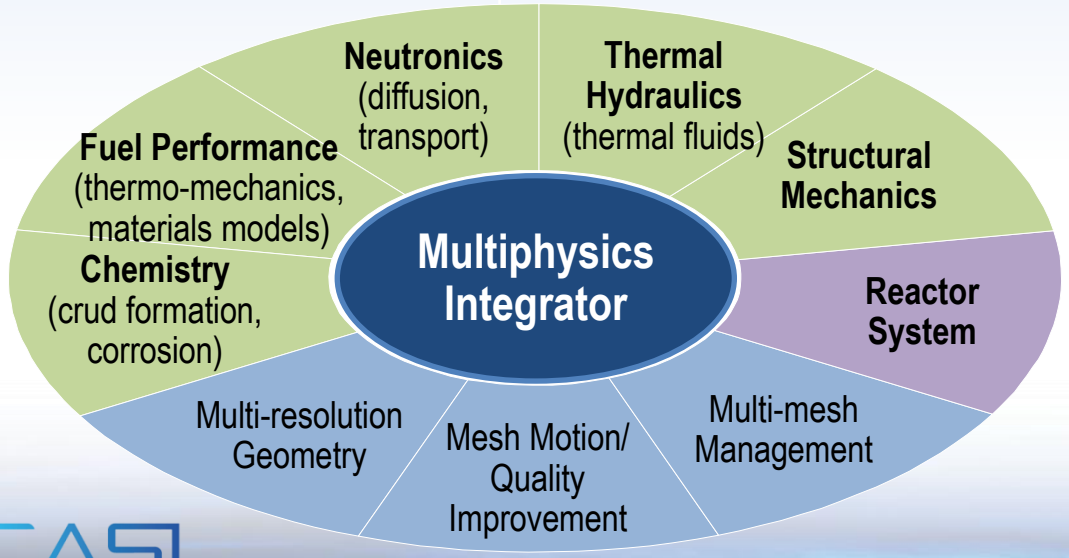
- Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications
- Existing systems and safety analysis simulation tools

Develop

- New requirements-driven physical models
- Efficient, tightly-coupled multi-scale/multi-physics algorithms and software with quantifiable accuracy
- Improved systems and safety analysis tools
- UQ framework

Deliver

- An unprecedented predictive simulation tool for simulation of physical reactors
- Architected for platform portability ranging from desktops to DOE's leadership-class and advanced architecture systems (large user base)
- Validation basis against 60% of existing U.S. reactor fleet (PWRs), using data from TVA reactors
- Base M&S LWR capability



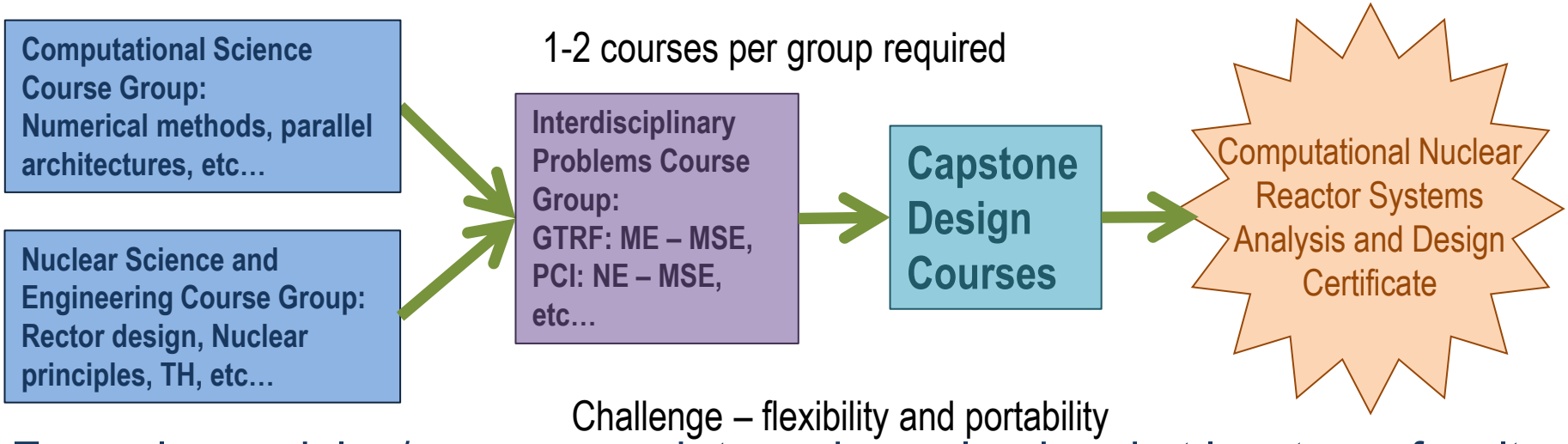
Education Challenge: Bridge Interdisciplinary Academic Cultures

Leverage	Develop	Deliver
• Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications • Existing systems and safety analysis simulation tools	• New requirements-driven physical models • Efficient, tightly-coupled multi-scale/multi-physics algorithms and software with quantifiable accuracy • Improved systems and safety analysis tools • UQ framework	• An unprecedented predictive simulation tool for simulation of physical reactors • Architected for platform portability ranging from desktops to DOE's leadership-class and advanced architecture systems (large user base) • Validation basis against 60% of existing U.S. reactor fleet (PWRs), using data from TVA reactors • Base M&S LWR capability

Education Opportunity: Interdisciplinary Courses Focused on Challenge Problems and Spanning Nanoscale to Macroscale

Academic Certificate for Nuclear Reactor Design

Implementation of CASL Discoveries in Nuclear Engineering Curricula



Example: modules/courses, each team has a lead and at least one faculty member

- Grid to Rod Fretting – ME, MSE, CS
- Crud Induced Localized Corrosion – MSE, Chem, CS, NE (Ballinger, MIT)
- Pellet Clad Interaction – MSE, ME, NE, CS (Eapen, NCSU)
- Crud Induced Power Shift – NE, ME, CS (Abdel Khalik, NCSU)
- Departure from Nucleate Boiling – ME, NE (Annalisa Manera, Michigan)
- Fuel Assembly Distortion – ME, NE, MSE
- Capstone course on VRD (Maldonado, UTK, Okafor, SCSU)

NE- Nuclear Engr., ME – Mechanical Engr., CS- Computational Science, MSE-Materials Science/Engr., Chem – Chemistry/Engr.

Workforce Development and Diversity Activities

Recruiting and developing a new generation of LWR designers, Scientists, and Nuclear Power Professionals

Current Progress:

- Developed recruitment materials
- Participated in ANS Student Meeting, Atlanta GA April 14-16
- Large response at both undergraduate and graduate level

Added Personnel:

- Added program coordinator and associate to facilitate curriculum development and program logistics

Next Steps:

- Implement newly developed undergraduate scholarship program
- Conduct student workshops – July 11-13, ORNL
- CASL Roundtable Student Poster Session- Aug 9-11, NC State Univ.
- Establish mentoring programs
- Internship programs at labs and industry
- Leverage national and local STEM programs- NEUP, NRC, NSF and professional organizations, WISE, SHPE, NSBE, …

2011 Summer Student Workshop

First annual workshop for graduate students held at ORNL July 10-12

Program:

Give students perspectives on CASL mission

- Networking and team building exercises
- Presentations by FA leaders and industrial partners
- Tours of CASL Facilities

Participation:

Transfer knowledge from leaders to students

- 35+ students, mostly graduate, from partner institutions
- CASL leadership, FA representatives, and industry leaders

Progress:

Enhance student contributions

- Students took away a greater understanding of their role in CASL
- Students were thoroughly engaged in workshop and provided thoughtful feedback to CASL leadership