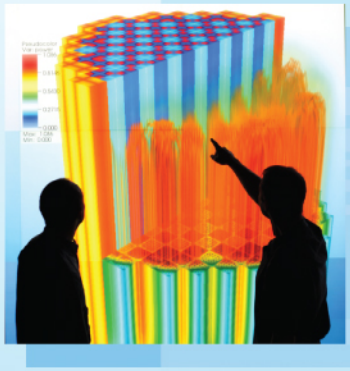
Power uprates
and plant life extension

CASL-U-2014-0354-000

Consortium for Advanced Simulation of LWRs



Engineering design
and analysis

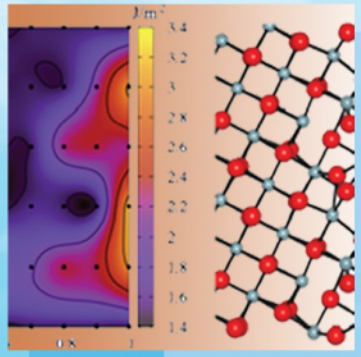
CASL: The Consortium for Advanced Simulation of Light Water Reactors - A DOE Energy Innovation Hub

Science-enabling
high performance
computing

Douglas Kothe

Oak Ridge National Laboratory

February 18, 2014



Fundamental science

Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub

Douglas B. Kothe
Oak Ridge National Laboratory
Director, CASL

University of Notre Dame
Notre Dame, IN
Feb 18, 2014

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

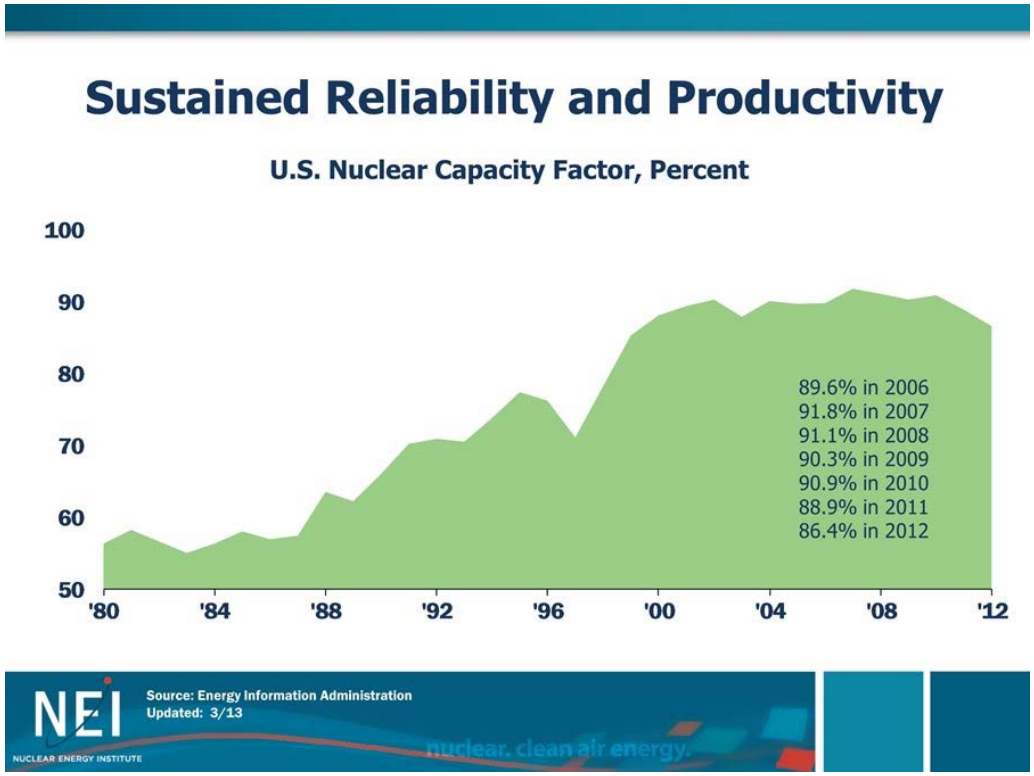
CASL
Consortium for Advanced Simulation of LWRs

CASL-U-2014-0354-000

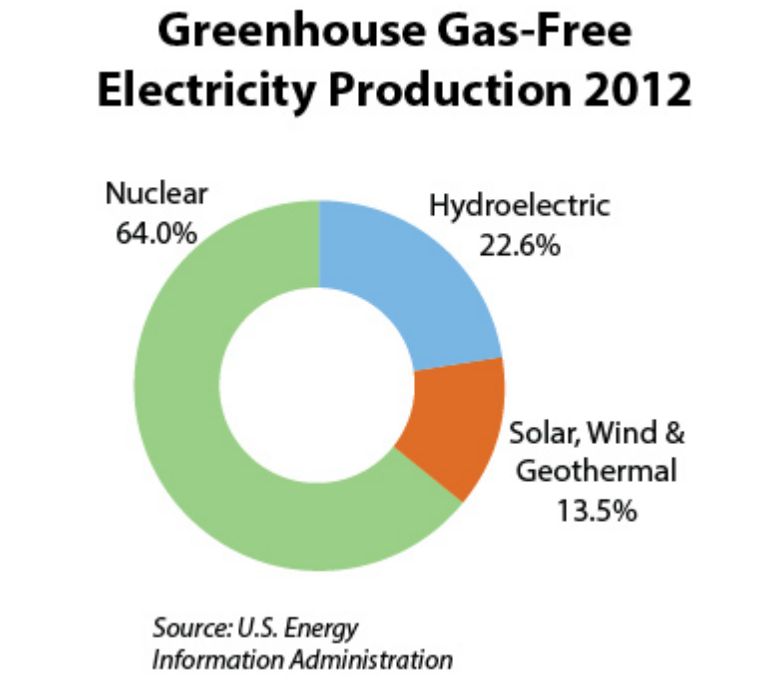
Nuclear Energy Overview

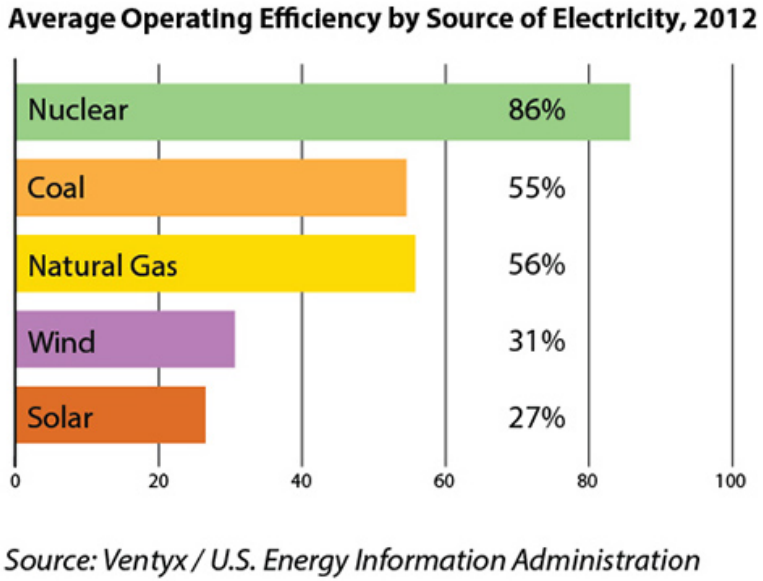
Source: Nuclear Energy Institute (NEI)

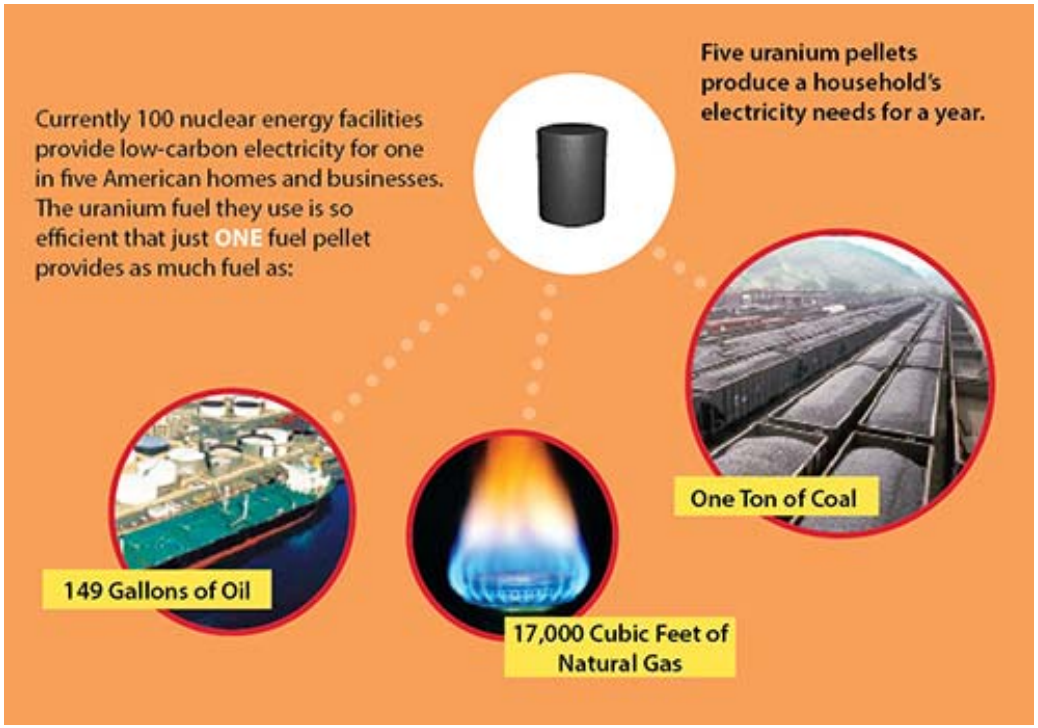
- World nuclear power generating capacity
  - 436 plants (U.S. - 100 plants in 31 states)
  - U.S. electricity generation (2012): nuclear is 0.77 out of 4.05 TWh
  - 72 nuclear plants under construction in 15 countries (5 in U.S.!)
- Electricity from nuclear: 19.0% in U.S. (12.3% worldwide)
- U.S. electricity demand projected to grow 25% by 2030
  - 2007: 3.99 TWh
  - 2030: 4.97 TWh
- Nuclear accounts for 64% of emission-free electricity in U.S.



Nuclear Energy Overview







More info at nei.org (Nuclear Energy Institute)

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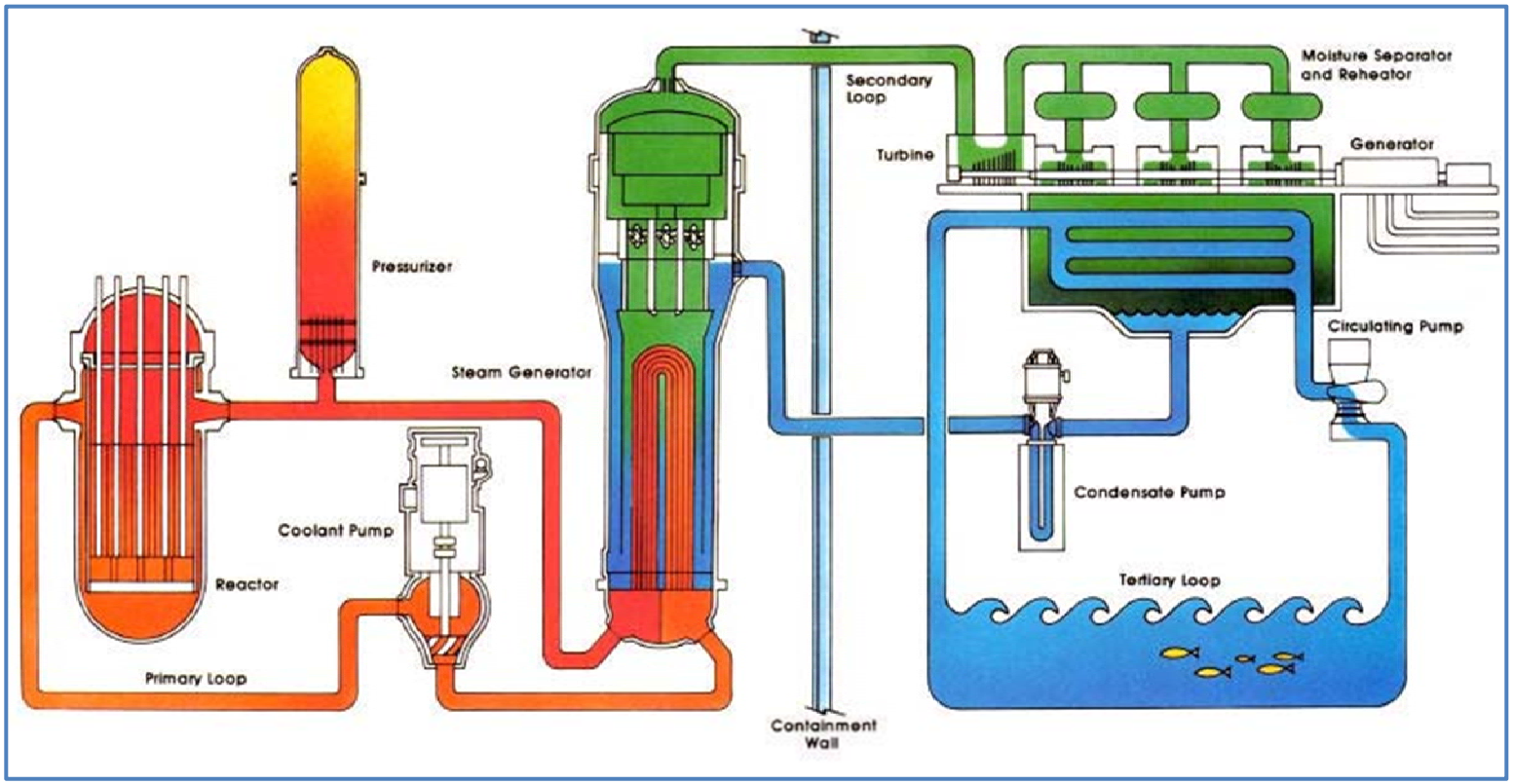
Anatomy of a Nuclear Reactor

Example: Westinghouse 4-Loop Pressurized Water Reactor (PWR)



Power: ~1170 MWe (~3400 MWth)

Core: 11.1' diameter x 12' high, 193 fuel assemblies, 107.7 tons of UO_2

Coolant: pressurized water (2250 psia), T_{in} ~ 545°F, T_{out} ~ 610°F, 134M lb/h (4 pumps)

Pressure Vessel: 14.4' diameter x 41.3' high x 0.72' thick alloy steel

Containment Building: 115' diameter x 156' high steel / concrete

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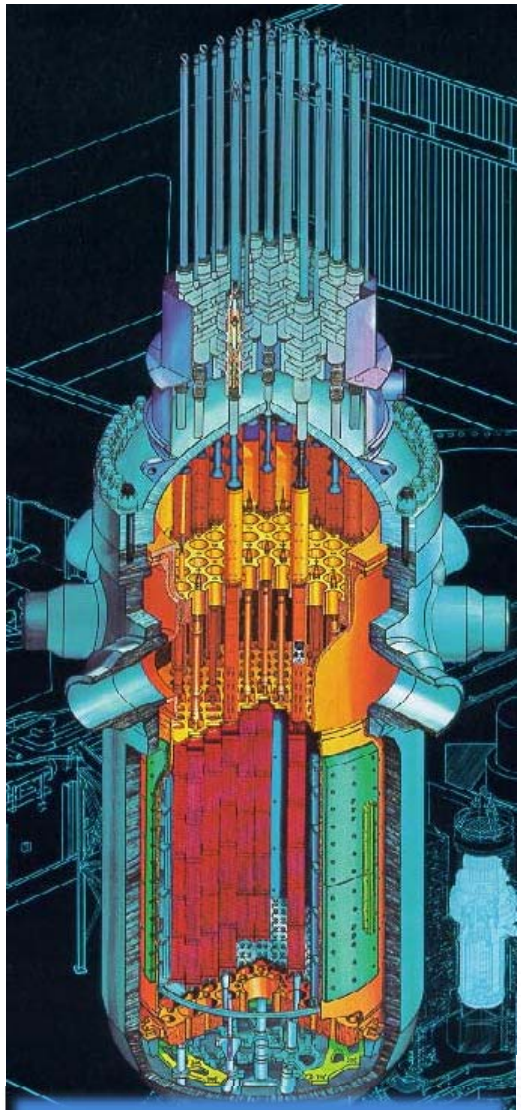
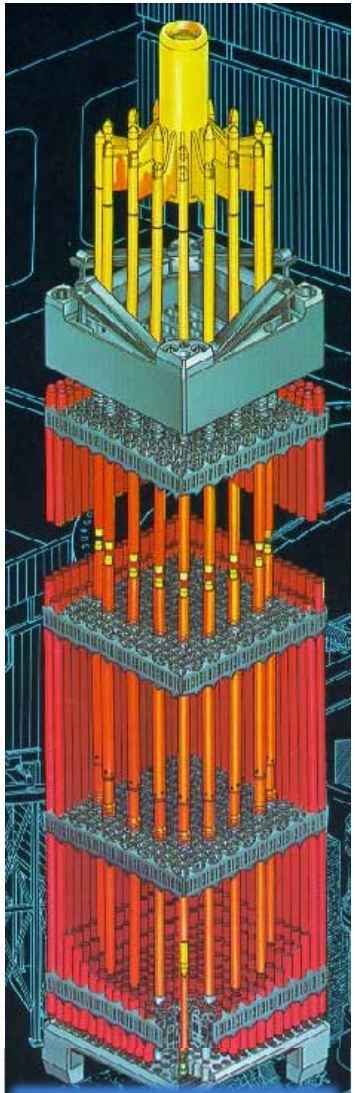
Anatomy of a Nuclear Reactor

Example: Westinghouse 4-Loop Pressurized Water Reactor (PWR)



reactor vessel and internals



17x17 fuel assembly

Core

- 11.1' diameter x 12' high
- 193 fuel assemblies
- 107.7 tons of UO_2 (~3-5% U_{235})

Fuel Assemblies

- 17x17 pin lattice (14.3 mm pitch)
- 204 pins per assembly

Fuel Pins

- ~300-400 pellets stacked within 12' high x 0.61 mm thick Zr-4 cladding tube

Fuel Pellets

- 9.29 mm diameter x ~10.0 mm high

Fuel Temperatures

- 4140° F (max centerline)
- 657° F (max clad surface)

~51,000 fuel pins and over 16M fuel pellets in the core of a PWR!

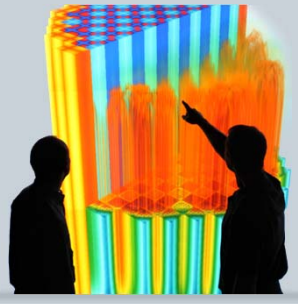
CASL Consortium for Advanced Simulation of LWRs

CASL-U-2014-0354-000

CASL's Charter

Provide leading-edge modeling and simulation (M&S) capabilities to improve the performance of currently operating light water reactors

Vision	*Predict, with confidence, the performance and assured safety of nuclear reactors, through comprehensive, science-based M&S technology deployed and applied broadly by the U.S. nuclear energy industry*
Goals	• Develop and effectively apply modern virtual reactor technology • Provide more understanding of safety margins while addressing operational and design challenges • Engage the nuclear energy community through M&S • Deploy new partnership and collaboration paradigms
Strategies	• Virtual Environment for Reactor Applications (VERA) • Industry Challenge Problems • Technology Delivery • Targeted, Enabling R&D • Education and Training • Collaboration and Ideation



Scope

- Address, through new insights afforded by advanced M&S technology, key nuclear energy industry challenges
  - ✓ furthering power uprates
  - ✓ higher fuel burnup
  - ✓ lifetime extension

  while providing higher confidence in enhanced nuclear safety
- Focus on performance of pressurized water reactor core, vessel, and in-vessel components to provide greatest impact within 5 years

CASL Components

US team with a remarkable set of assets – Address tough industry challenges that matter – Urgent and compelling plan

Collaborate creatively – Target and foster innovation - Deliver industry solutions with predictive simulation

Consortium for Advanced Simulation of LWRs

CASL Background

- What is CASL doing?
  - *Create* an advanced coupled multi-physics "virtual reactor" technology by adapting existing and developing new modeling and simulation (M&S) tools
  - *Effectively apply* the virtual reactor technology to provide more understanding of safety margins while addressing selected operational and design challenges of operational light water reactors
- Why?
  - Improve the performance and energy output of existing nuclear reactors by focusing on important industry defined challenge problems
  - M&S technology has long been a mainstay in the nuclear industry (vendors, owner/operators), helping to inform consequential operational and safety decisions codes daily. Current nuclear industry M&S technology, though continuously improved, has failed to capitalize on the benefits that more precise predictive capability and fundamental understanding offer (from leader to follower)
- Why do this in the Hub R&D business model?
  - Solution requires clear deliverables & products promoted by Hub R&D approach ("fierce sense of urgency")
  - Public-private partnership essential for adaptation, application, and "useful and usable" deployment of advanced M&S technologies under development at DOE national labs and universities to nuclear enterprise
- What is working?
  - Several elements have proven effective: partnerships, industry pull, technology deployment, clear deliverables and plans, effective and agile project management, 5-year time horizon, S&T guidance/review

Strong Dependency on Modeling and Simulation

Need to assure nuclear safety but limited by inability to perform full-scale experimental mockups due to cost, safety & feasibility [1% power derating translates to $(5-10)M annual loss of revenue for 1 GWe unit]

Need to minimize economic uncertainty associated with new product introduction (e.g. fuel) by employing precise predictions [1% error in core reactivity has $4M annual fuel cycle cost impact for 1 GWe unit]

CASL Consortium for Advanced Simulation of LWRs

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The CASL Team

Core partners

Oak Ridge National Laboratory

Electric Power Research Institute

Idaho National Laboratory

Los Alamos National Laboratory

Massachusetts Institute of Technology

North Carolina State University

Sandia National Laboratories

Tennessee Valley Authority

University of Michigan

Westinghouse Electric Company

Contributing Partners

ASCOMP GmbH
CD-adapco
City College of New York
Florida State University
Imperial College London
Rensselaer Polytechnic Institute
Texas A&M University
Pennsylvania State University
University of Florida
University of Tennessee – Knoxville
University of Wisconsin
University of Notre Dame
Anatech Corporation
Core Physics Inc.
Pacific Northwest National Laboratory
G S Nuclear Consulting, LLC
University of Texas at Austin
University of Texas at Dallas

First Introduced by Secretary in the President's FY2010 Budget

A Different Approach

- "Multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges" – *Steven Chu*
- "Create a research atmosphere with a fierce sense of urgency to deliver solutions." – *Kristina Johnson*
- Characteristics
  - Leadership – Outstanding, independent, scientific leadership
  - Management – "Light" federal touch
  - Focus – Deliver technologies that can change the U.S. "energy game"

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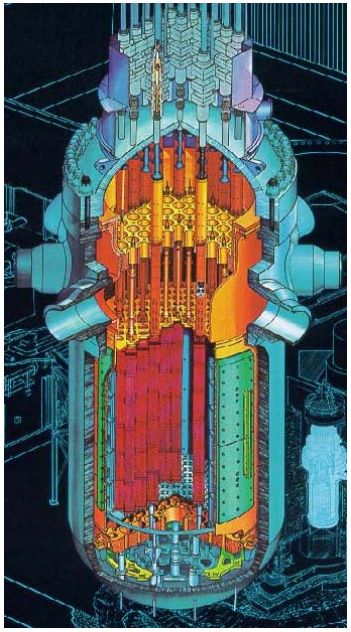
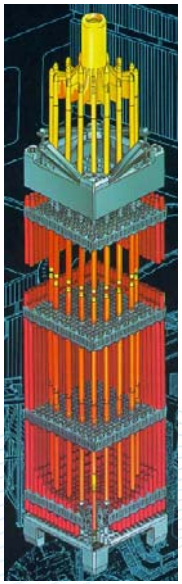
Nuclear Energy Drivers and Payoffs for M&S technology



- Extend licenses of existing fleet (to 60 years and beyond)
  - Understand material degradation to reduce inspection & replacements
- Up-rate power of existing fleet (strive for another 5-10 GWe)
  - Address power-limiting operational & design basis accident scenarios
- Inform flexible nuclear power plant operations
  - Load follow maneuvering & coolant chemistry to enhance reliability
- Design and deploy accident tolerant fuel (integrity of cladding)
  - Concept refinement, test planning, assessment of safety margins
- Margin quantification, recovery, tradeoff
  - Plant parameters, fuel hardware, reload flexibility, regulatory changes
- Resolve advanced reactor design & regulatory challenges
  - Support Gen III+ reactors under construction (AP1000), refine SMR designs
- Fuel cycle cost savings
  - More economical core loadings and fuel designs
- Used fuel disposition
  - Inform spent fuel pools, interim storage, and repository decisions



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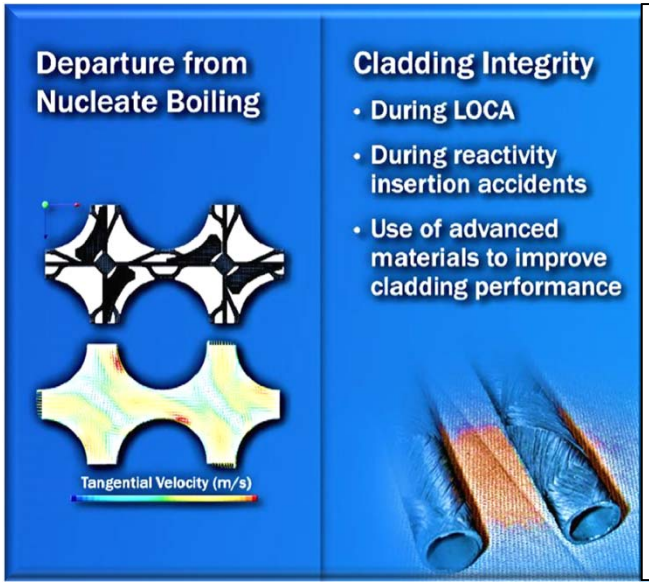
CASL Challenge Problems

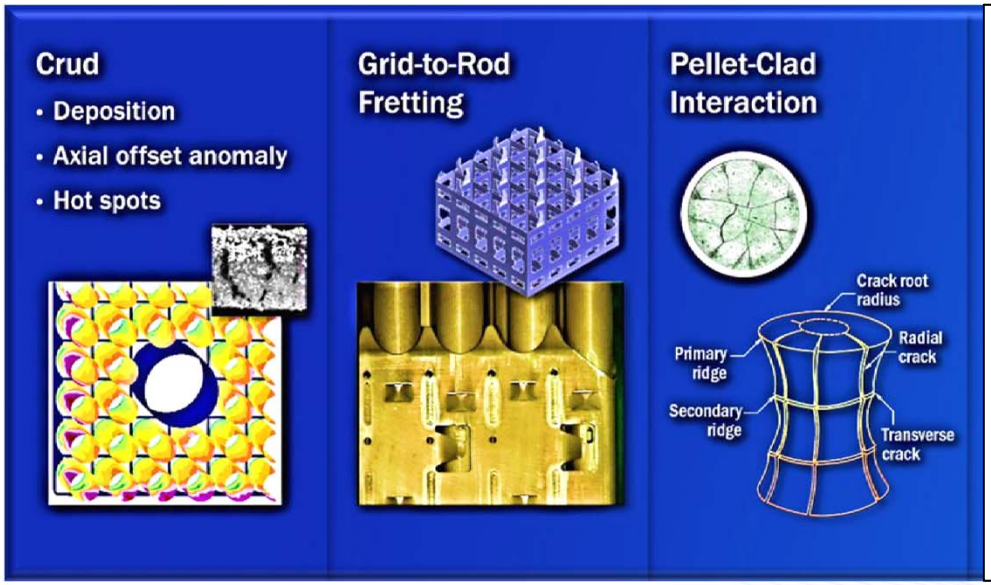
Key safety-relevant reactor phenomena that limit performance



Safety Related Challenge Problems

CASL Challenge Problems

- Are relevant industry problems whose solutions remain elusive
- Are amenable to insight afforded by advanced M&S
- Help to direct RD&D activities on CASL M&S technology
- Help to establish clear performance metrics



Operational Challenge Problems

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Power Uprates

Source: Heather Feldman (EPRI)

- Measurement uncertainty recapture (MUR)
  - Ex: Feed water flow rate (<2%)
- Stretch Power Up-rate (SPU)
  - Ex: Instrument set points (2% to 7%)
- Extended Power Up-rate (EPU)
  - Ex: Design changes (7% to 20%)
- Ultra Power Up-rate (UPU)
  - Ex: Extensive fuel and BOP changes (> 20%)
  - None have been performed
- Equivalent to ~6 large nuclear power plants (6,440 Mwe) added to the grid thru uprates
  - 143 power up-rates approved since 1977
- About 6,000 MWe remains available for EPU
  - 17 applications currently under review (9 MURs, 8 EPUs)
  - 15 new applications are expected in the next 5 years (8 MURs, 7 EPUs)

Westinghouse Experience

MUR COMPLETED
- 25 Americas PWRs
- 5 European PWRs
- 2 Asian PWRs

SPU COMPLETED
- 10 Americas PWRs
- 0 European PWRs
- 4 Asian PWRs

EPU COMPLETED
- 7 Americas PWRs
- 5 European PWRs
- 0 Asian PWRs
- Completed/planned: 5 of 6 2-loops, 4 of 13 3-loops, 0 of 30 4-loops, 5 of 14 CE Design

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Where is NRC's Focus on Up-rates?

- Japan Event Follow-up
- GSI -191 Post-LOCA Debris Effects
- Containment Accident Pressure (CAP)
- Thermal Conductivity Degradation (TCD)
- Boron Precipitation/Long Term Cooling
- Gas Accumulation
- LOCA Analysis
- Spent Fuel Pool Issues
- Digital I&C
- Alternate Source Term
- Steam Dryers
- Steam Generator Issues
- Single Failure Concerns
- High Energy Line Break
- Licensing Amendment Issues
- Licensing Conditions and Commitments

More at: http://www.nrc.gov/reactors/operating/licensing/power-uprates.html

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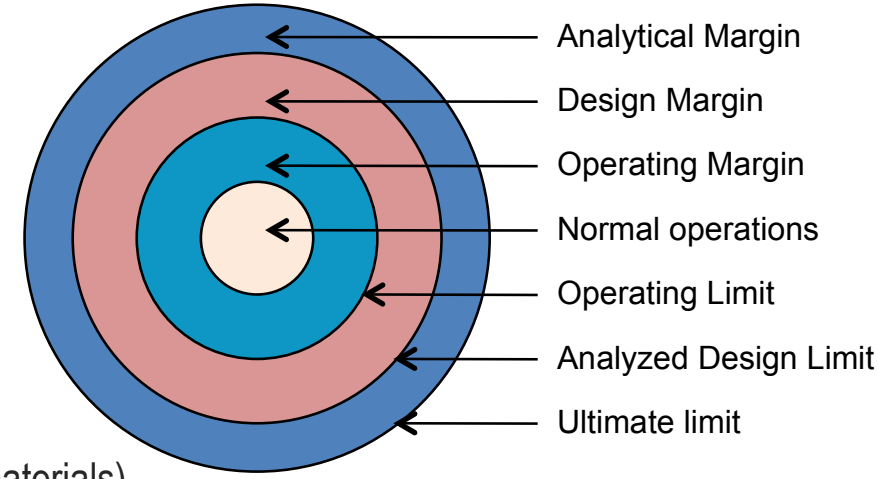
Margin Management

Source: Sumit Ray (Westinghouse)



- Requires a strategic approach
  - 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
- Margins can be "recovered"
  - 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

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.)

One of the strategic targets for the CASL VERA toolkit is to provide enhanced insights in the area of critical reactor margins

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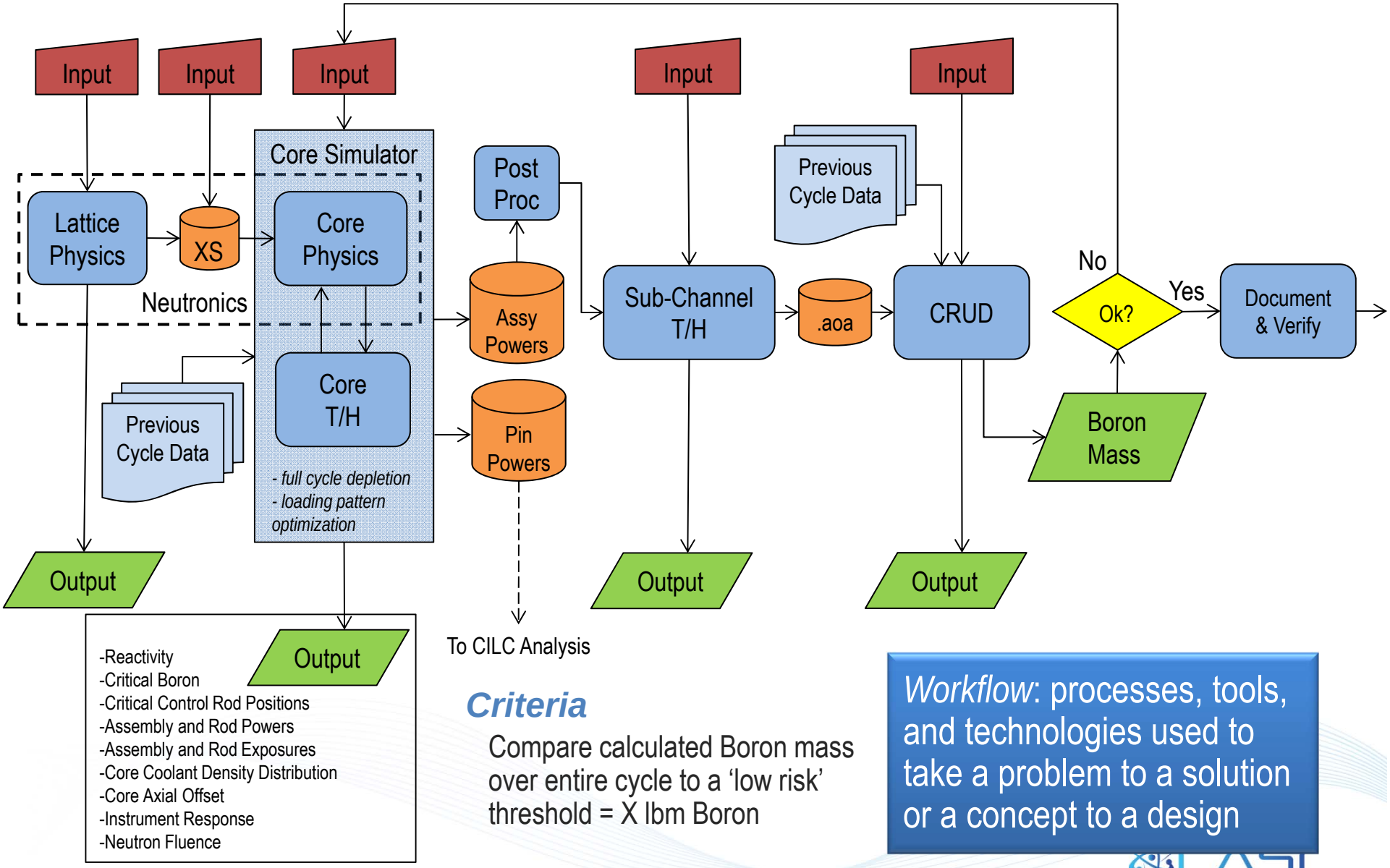
An Example Nuclear Industry M&S Workflow

Crud Induced Power Shift Risk Evaluation



Criteria

Compare calculated Boron mass over entire cycle to a 'low risk' threshold = X lbm Boron

Workflow: processes, tools, and technologies used to take a problem to a solution or a concept to a design

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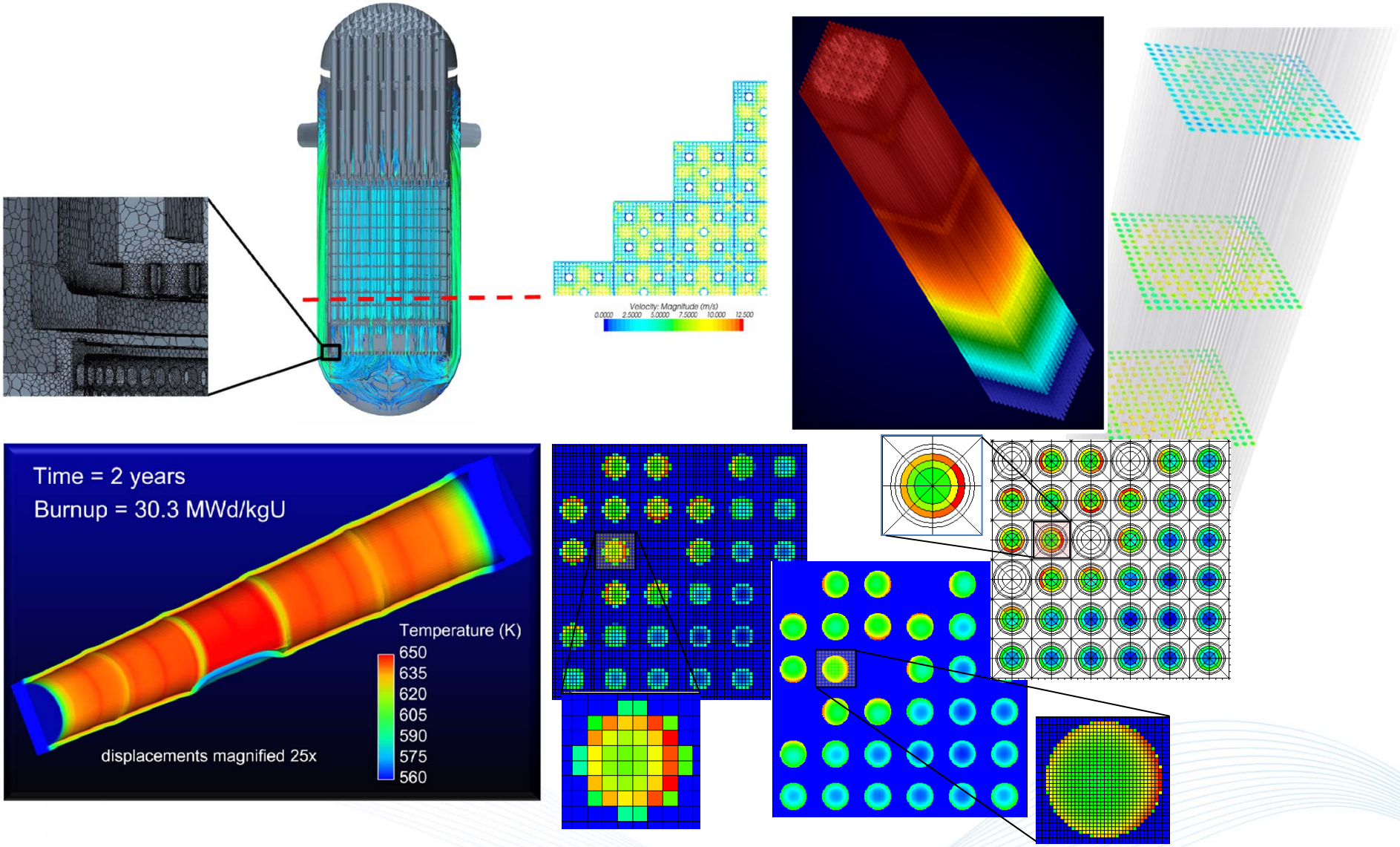
CASL Targets the Multi-Scale Challenge of Predictively Simulating a Reactor Core



From full core to fuel assembly to fuel subassembly to fuel pin/pellet

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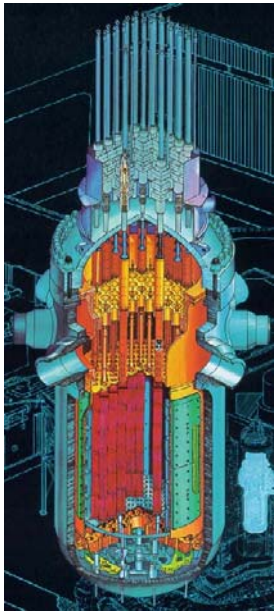
Creating a Virtual Reactor

Enable assessment of fuel design, operation, and safety criteria

Deliver improved predictive simulation of PWR core, internals, and vessel	• Couple Virtual Reactor (VR) to evolving out-of-vessel simulation capability • Maintain applicability to other nuclear power plant (NPP) types
Execute work in 6 technical focus areas	• Equip VR with necessary physical models and multiphysics integrators • Build VR with a comprehensive, usable, and extensible software system • Validate and assess the VR models with self-consistent quantified uncertainties



MPO	RTM	THM	VUQ	PHI	AMA
Materials performance and optimization	Radiation transport methods	Thermal hydraulics methods	Validation and uncertainty quantification	Physics integration	Advanced modeling applications

Integrated and interdependent projects span the range from basic science to application

Consortium for Advanced Simulation of LWRs

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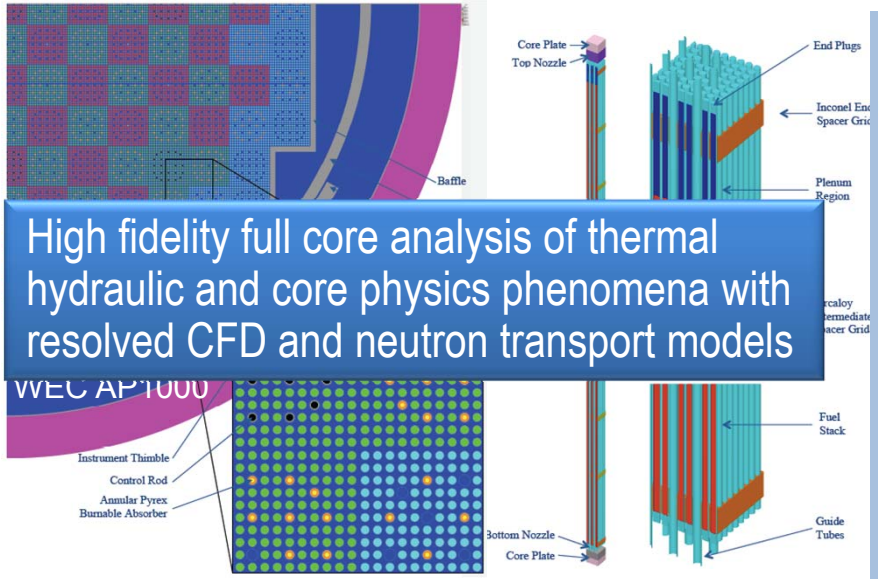
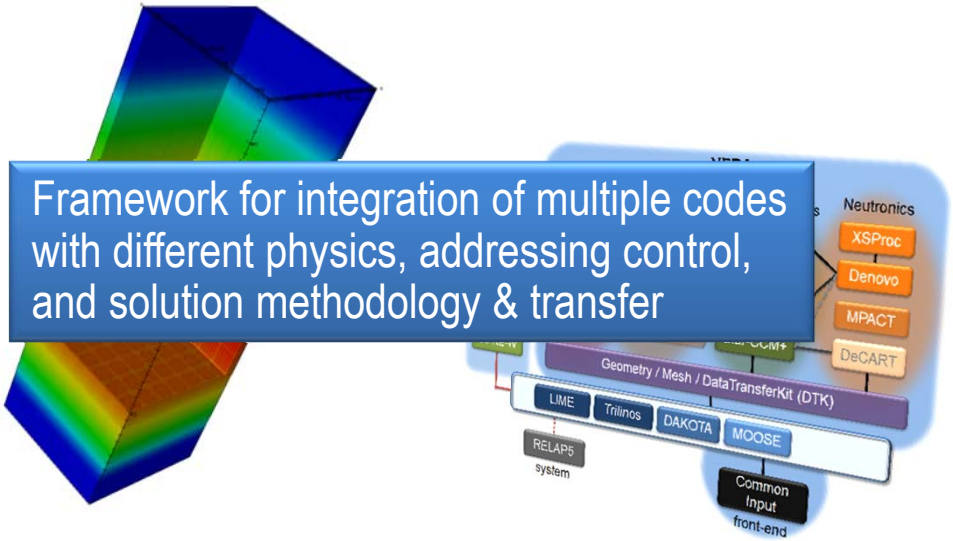
CASL Innovations

Advanced Modeling Applications



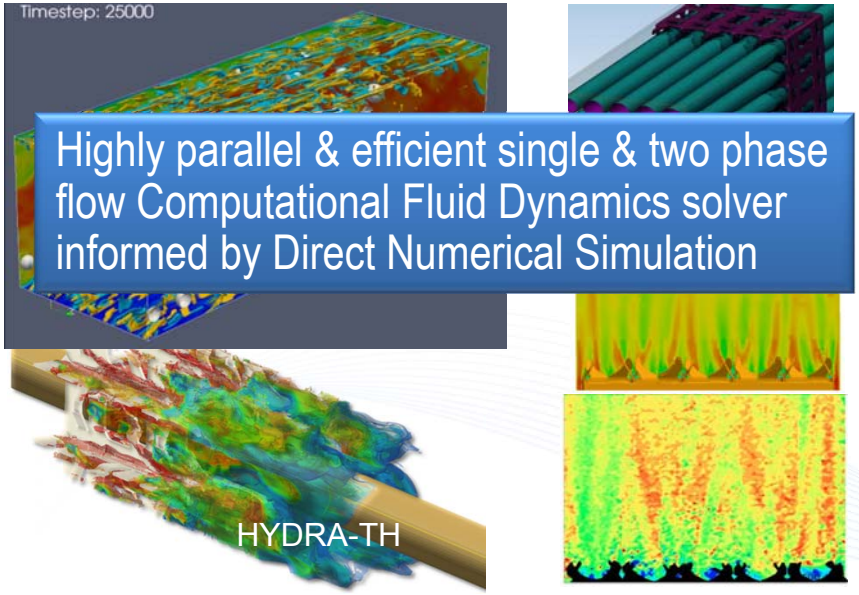
High fidelity full core analysis of thermal hydraulic and core physics phenomena with resolved CFD and neutron transport models

Physics Integration



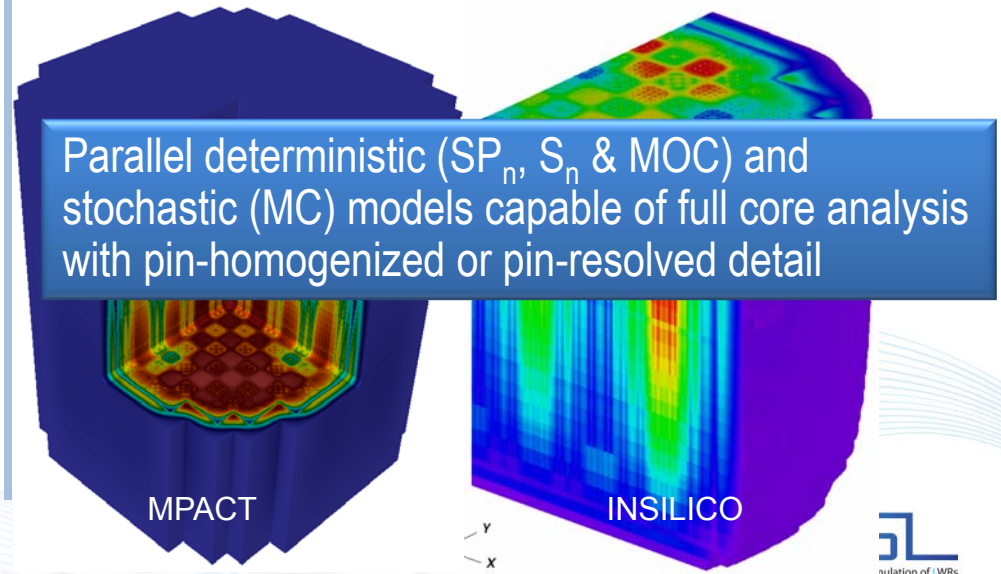
Framework for integration of multiple codes with different physics, addressing control, and solution methodology & transfer

Thermal Hydraulic Methods



Highly parallel & efficient single & two phase flow Computational Fluid Dynamics solver informed by Direct Numerical Simulation

Radiation Transport Methods



Parallel deterministic (SP_n, S_n & MOC) and stochastic (MC) models capable of full core analysis with pin-homogenized or pin-resolved detail

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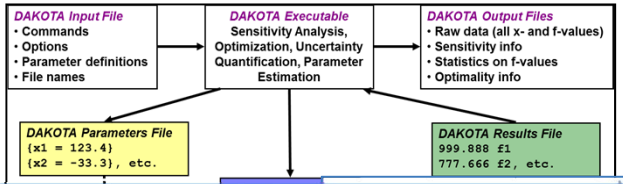
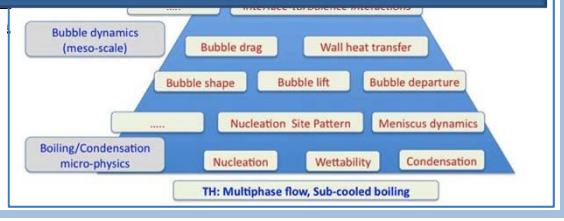
CASL Innovations

Validation & Uncertainty Quantification



Integrating and evolving a state-of-the-art uncertainty quantification, sensitivity, and data assimilation tool into engineering workflows

DAKOTA



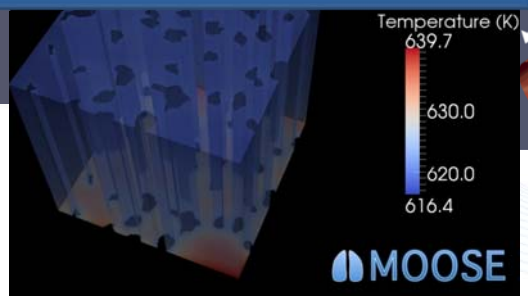
VOCC

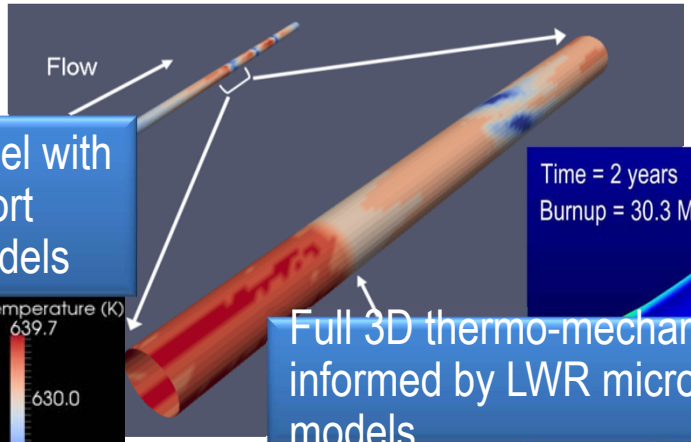
Bringing together local ("physical") and geographically distributed ("virtual") contributors in a meaningful and productive way

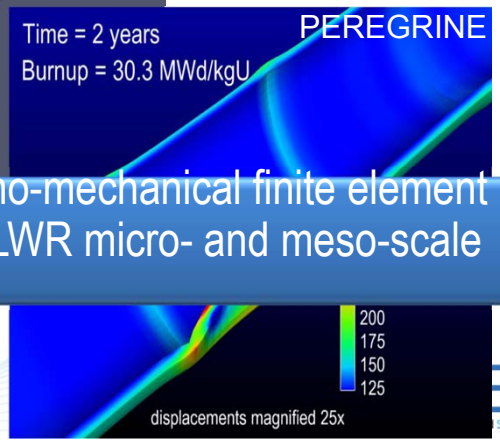
Materials Performance and Optimization

MAMBA

CRUD growth and boron retention model with enhanced thermodynamics and transport treatments informed by micro-scale models



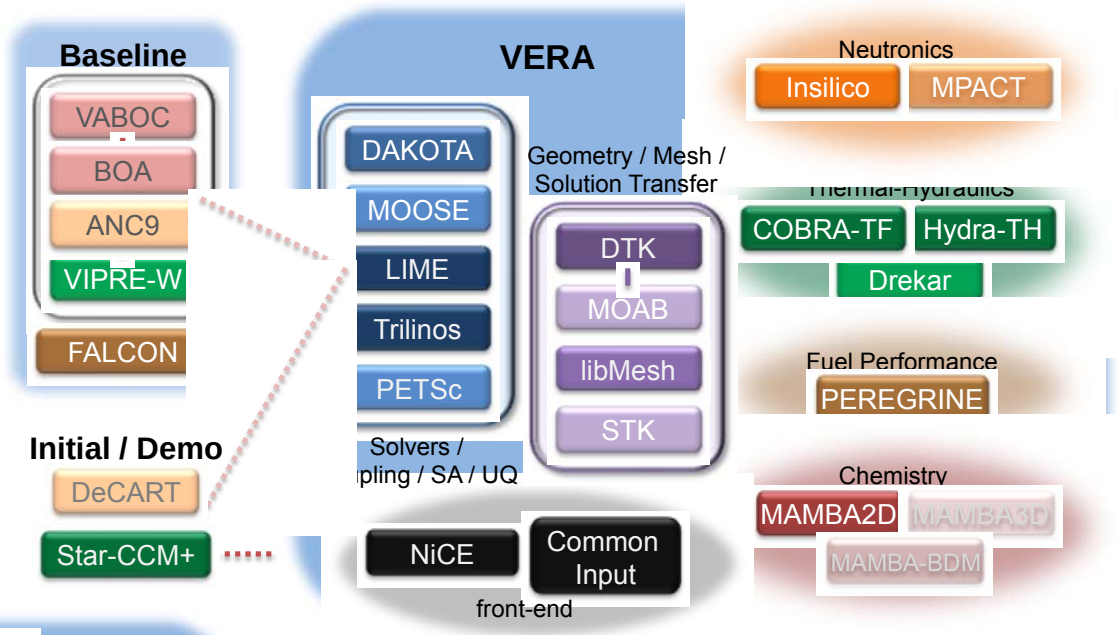




Full 3D thermo-mechanical finite element model informed by LWR micro- and meso-scale models

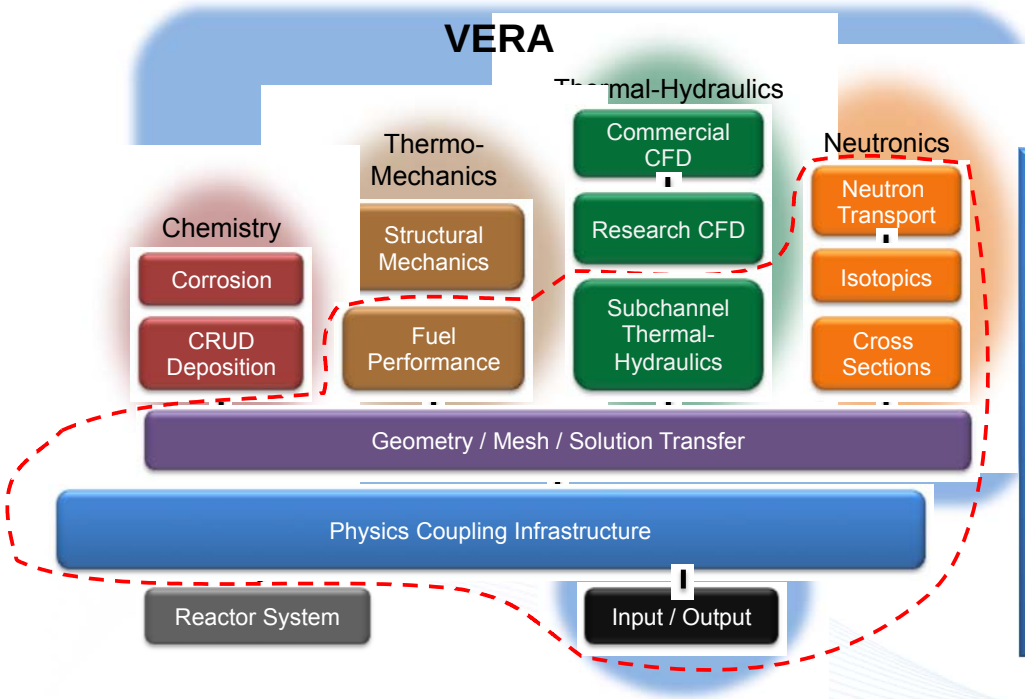
VERA: Virtual Environment for Reactor Applications

CASL's evolving virtual reactor for in-vessel LWR phenomena



VERA as of Aug 2013 (Version 3.1)

Required functional capabilities



CASL has 3 M&S technology products

1. VERA-CS as the fast running core simulator, which has value both standalone and for providing power histories, etc for more detailed codes
2. Engineering suite of standalone codes with ability to couple 2 or more within VERA or in other environments
3. Leadership suite of high fidelity codes used to drive improvements in 1 and 2

CASL Consortium for Advanced Simulation of LWRs

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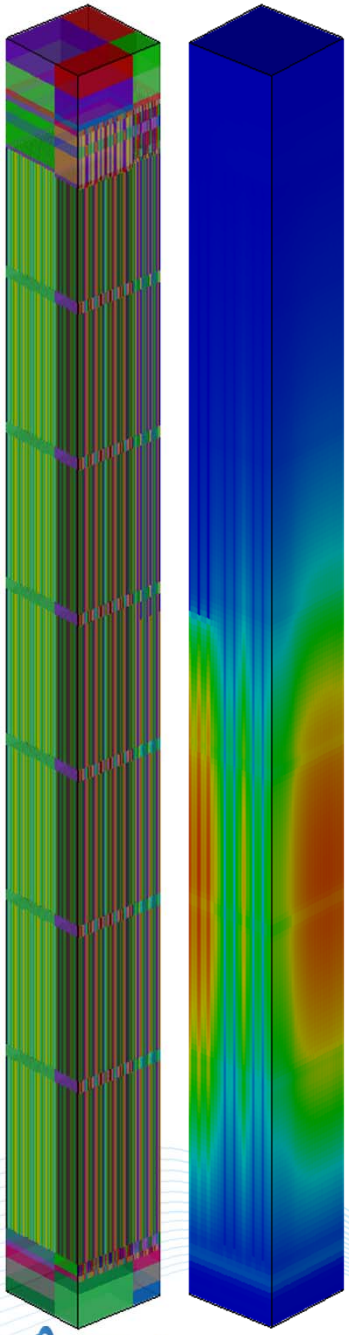
CASL Innovations

CASL vs. Industry Core Simulators

Physics Model	Industry Practice	CASL (VERA-CS)
Neutron Transport	3-D diffusion (core) 2 energy groups (core) 2-D transport on single assy	3-D transport 23+ energy groups
Power Distribution	nodal average with pin-power reconstruction methods	explicit pin-by-pin
Thermal-Hydraulics	1-D assembly-averaged	subchannel (w/crossflow)
Fuel Temperatures	nodal average	pin-by-pin 2-D or 3-D
Xenon/Samarium	nodal average w/correction	pin-by-pin
Depletion	infinite-medium cross sections quadratic burnup correction history corrections spectral corrections reconstructed pin exposures	pin-by-pin with actual core conditions
Reflector Models	1-D cross section models	actual 3-D geometry
Target Platforms	workstation (single-core)	1,000 – 300,000 cores



CASL current and planned capabilities will leapfrog calibrated industry core simulators that use lumped homogenization and correlation-based closures

Consortium for Advanced Simulation of LWRs

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Industry Role and Impact in CASL

Industry Council: Assure that CASL solutions are "used and useful" by industry and that CASL provides effective leadership advancing the M&S state-of-the-art.

Industry Council Objectives and Strategies

- Early, continuous, and frequent interface and engagement of end-users and technology providers
- Critical review of CASL plans and products
- Deployment and applications of periodic VERA releases
- Identification of strategic collaborations between industry and CASL for access to data and technical information, testing and evaluation, regulatory interface, or targeted RD&D

Outcomes and Impact

- Industrial technology-providers and end-users benefit by influencing VERA and its development process to be compatible with expected applications
- They also prepare their business and technical processes to make early use of CASL products

Industry Council Members

Owner/ Operators of Nuclear Plants	Fuel and/or SMR Vendors	Engineering Design, Service Providers, R&D	Independent Software Vendor	Computer Technology Companies	Ex-Officio
Dominion	AREVA	Battelle	ANSYS	Cray	BOD
Duke Energy	GNF	Bettis /NNPP	CD-adapco	IBM	DOE
EDF	mPower	EPRI	GSE Systems	NVIDIA	
Exelon	NuScale	Rolls Royce			
TVA	WEC	Studsvik Scandpower			

CASL Core Industry Partners Represent 3 Pillars of Nuclear Industry

- EPRI: *R&D arm* of industry as driven by near-term utility (owner/operator) needs
  - Power uprates, license extensions, new fuel designs
- TVA: *owner/operator* of 6 nuclear reactors – also brings operational reactor data for validation
  - Address power-limiting operating scenarios
- Westinghouse: *vendor* - designer and seller of commercial fuel and integrated reactor designs
  - Enhanced insights in critical reactor margins

Consortium for Advanced Simulation of LWRs

CASL-U-2014-0354-000

Nuclear Applications Must Support a Wide Range of Spatial and Temporal Scales

- Nuclear fuel behavior and performance
  - Spatial scale: fuel pellet to fuel pin to fuel sub-assembly (3x3 pins)
    - From dislocations/voids/cracks (< 1 μm) to grains (<100 μm) to clad (<1 mm) to pellet (<5 cm) to pins (<4 m)
- Single-phase thermal hydraulics
  - Spatial scale: fuel sub-assembly (3x3 pins) to fuel assembly (17x17 pins)
    - From mixing vanes (<1 mm) to boundary layers (<1 cm) to turbulent structures (<10 cm) to assemblies (5 m)
- Multi-phase thermal hydraulics
  - Spatial scale: fuel assembly (17x17 pins) to full core (193 assemblies or >51K pins)
    - Same as single phase except now add bubbles (<1 mm to 1 cm) and full core (<10 m)
- Neutron transport
  - Spatial scale: fuel pellet to fuel pin to fuel assembly to full core; also 2D lattice
    - From burnable absorber layers (<1 mm) to pellet (< 1 cm) to lattice (<1 m) to full core (< 10 m)
- Coolant chemistry and CRUD deposition/buildup
  - Spatial scale: fuel pellet to fuel pin to fuel subassembly(?)
    - From oxide/hydride layers (<10 μm) to CRUD layers (< 0.1 mm) to pellets (<5 cm) to pins (<4 m)

Operational time scales: hours to days to years to decades
Safety time scales: sec to min to hours to days

Consortium for Advanced Simulation of LWRs

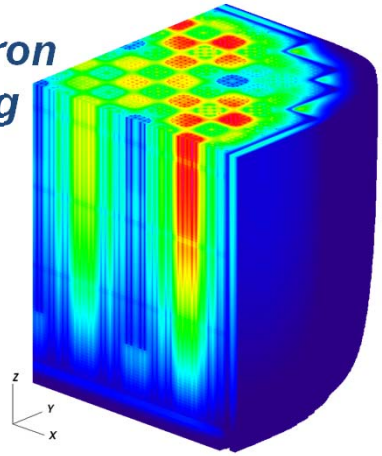
CASL-U-2014-0354-000

Solutions Realizeable at the Petascale

A Step Change in Technology

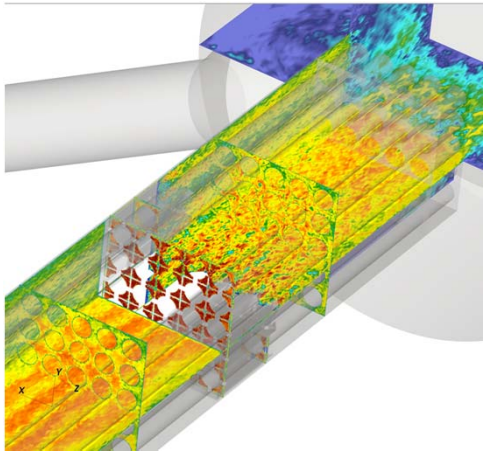
Predictive full core neutron state points for operating reactors

- Consistent method for 3D pin-resolved deterministic and Monte Carlo transport



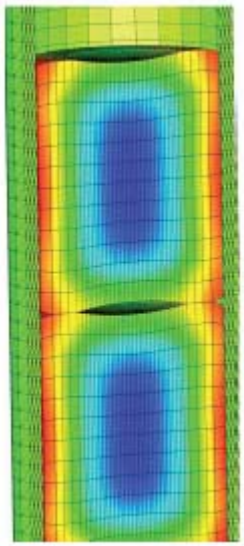
Calibrated CFD of full core turbulent multi-phase flows

- With boiling and upscaled closure models, mechanistic DNB assessment



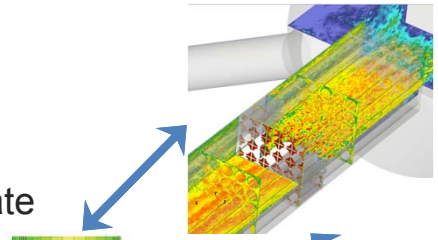
Reliable 3D assessment of nuclear fuel performance

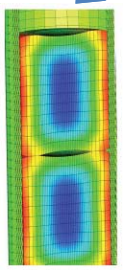
- Inform assessments of operational risks & identify solutions (PCI,CRUD)
- Functional capability for fuel response in reactor transients (RIA, LOCA)

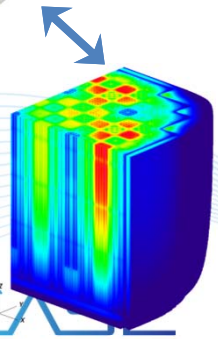


Identify vulnerabilities to operational & safety performance-limiting reactor phenomena

- Tightly-coupled multi-physics assessment of system performance
- Understand best-estimate system response and associated uncertainties upset events







Leapfrogs calibrated industry core simulators that use lumped homogenization & correlation based closures

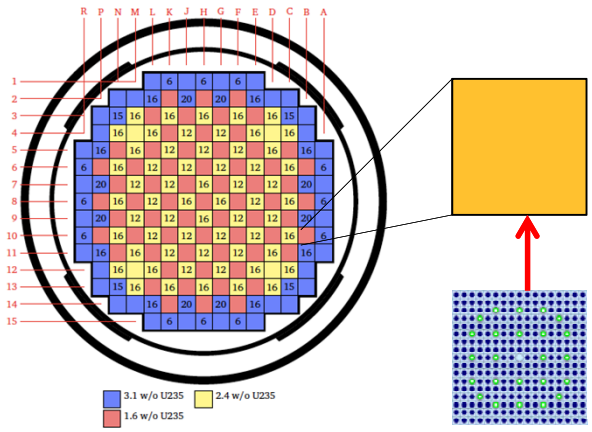
Consortium for Advanced Simulation of LWRs

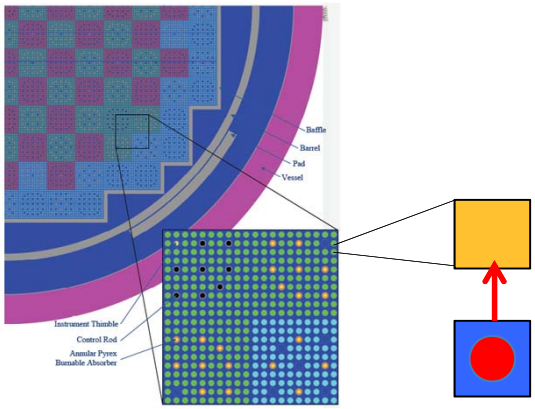
CASL-U-2014-0354-000

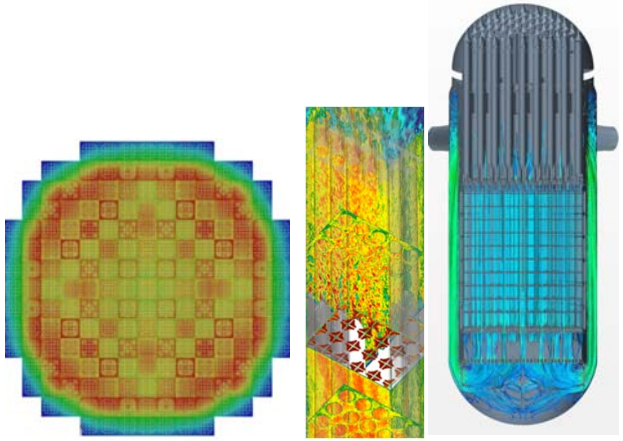
Coupled-Physics Core Simulations

HPC provides opportunities for predictive maturity

Terascale	Petascale	Exascale
Engineering Analysis	*High-Fidelity Core Analysis*	*Extreme-Fidelity Analysis*
• Criticality and safety set-points • Core power predictions • Cycle fuel depletions • Transient safety analysis • Core loading optimization • Operator-assist predictions • Real-time operator training simulators	• Criticality and safety set-points • Core pin power predictions • Cycle isotopic fuel depletions • Localized sub-channel feedback • Assembly or full core structural models	• Azimuthal/radial intra-pellet isotopics • Rim effects in high burnup fuel pins • Localized CRUD deposition//corrosion • Fluid/structure vibrations/wear • Physics-based DNBR predictions • Vessel flow asymmetry and instabilities • Fully coupled TH/structural full core



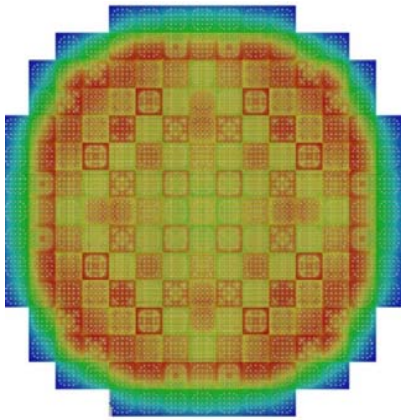
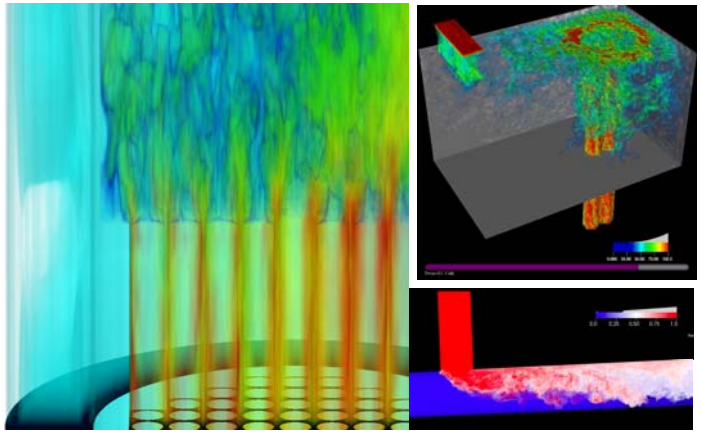
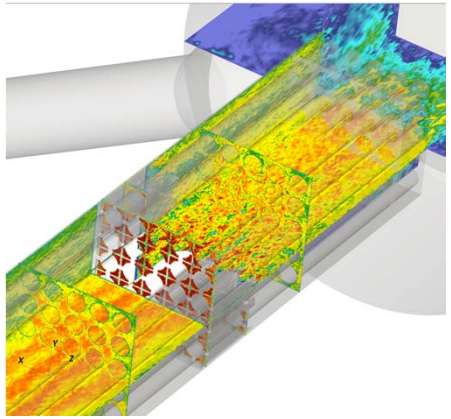




Homogenized Fuel Assemblies	*Homogenized Fuel Pin-Cells*	*Explicit Fuel/Clad/Fluids &Vessel*
• Pre-computed assembly data tables • Few-group nodal diffusion neutronics • Characteristic-channel fuel pin • Characteristic-channel thermal fluids • Macroscopic fuel assembly depletion • Lumped-parameter closure relations	• Pre-computed pin-cell data tables • Multi-group transport neutronics • Simplified explicit-pin fuel mechanics • Sub-channel and CFD thermal fluids • Microscopic fuel pin depletion • Simplified-physics closure relations	• No pre-computed data tables • Continuous-energy Monte Carlo • Meso/macro fuel pin mechanics • CFD and DNS thermal fluids • Intra-pellet isotopics in fuel depletion • Physics-based closure relations

Thermal Hydraulics

HPC provides opportunities for predictive maturity

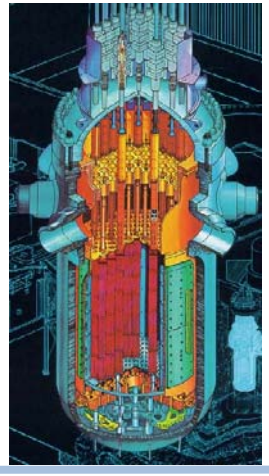
Terascale	Petascale	Exascale
Lumped parameter models for full reactor core ▪ Calibrated subchannel models capture large scale axial flow effects - estimate transverse flow	*High-fidelity telescoping* of localized regions ▪ Large-Eddy Simulations locally: sub-assembly, steam generator, upper plenum	*High-fidelity full core* simulations ▪ Large-eddy simulations over entire reactor core
		
▪ Experiments required to calibrate simplified physics methods and closure models ▪ Thermal, multiphase, and boiling effects modeled – not resolved	• Reveal complicated heat transfer physics + mechanism for instabilities difficult to attain with experiments	• Experimental “data sets” of whole core effects. • Enable virtual prototyping.

CASL-U-2014-0354-000

Solutions Expected at the Exascale

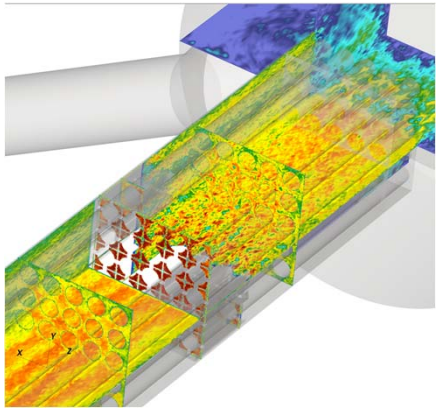
Reactor Core Physics

- **Predictive load-follow simulation for feedback to operational reactors for plant maneuvering and upset event recovery**
  - Core-wide multi-physics: radiation transport, fluids, fuels, chemistry, material, local wear and contacts, full core structural response
- **Expand to entire power plant**



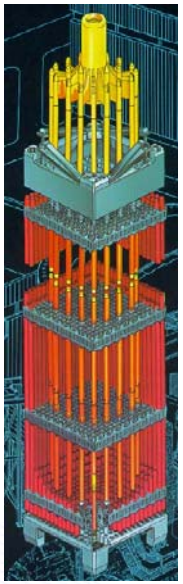
Thermal Hydraulics

- **Enhanced heat transfer from fuel to coolant within quantified safety margins**
  - Core-wide multi-scale fluids performance with two-way DNS-to-LES CFD coupling



Nuclear Fuels

- **Investigation and suppression of barriers to higher fuel burnup**
  - Micro-scale informed fuel behavior and transient transport
- **Reliable, targeted fuel designs outside of principal test base**
  - Multi-scale fuel performance (active two-way coupling micro to meso to macro)
- **Fuel failure prediction**
  - Move from empirical failure thresholds to mechanistic models of actual failure



V&V, Data Assimilation & UQ

- **Execution of quality virtual experiments to fill validation data gaps**
  - Computational (pseudo experimental) data generated by full resolution core simulator used for data assimilation & UQ of design tools
- **Optimum experimental design & usage**
  - Integrated data assimilation, UQ & mathematical optimization to design experiments & process resulting data to recover margins to safety & operational limits

Underpinned by enabling science-based engineering models

CASL Consortium for Advanced Simulation of LWRs

CASL-U-2014-0354-000

Demonstration of a New High Fidelity Multi-Physics Simulation Model of PWR Reactor

Purpose

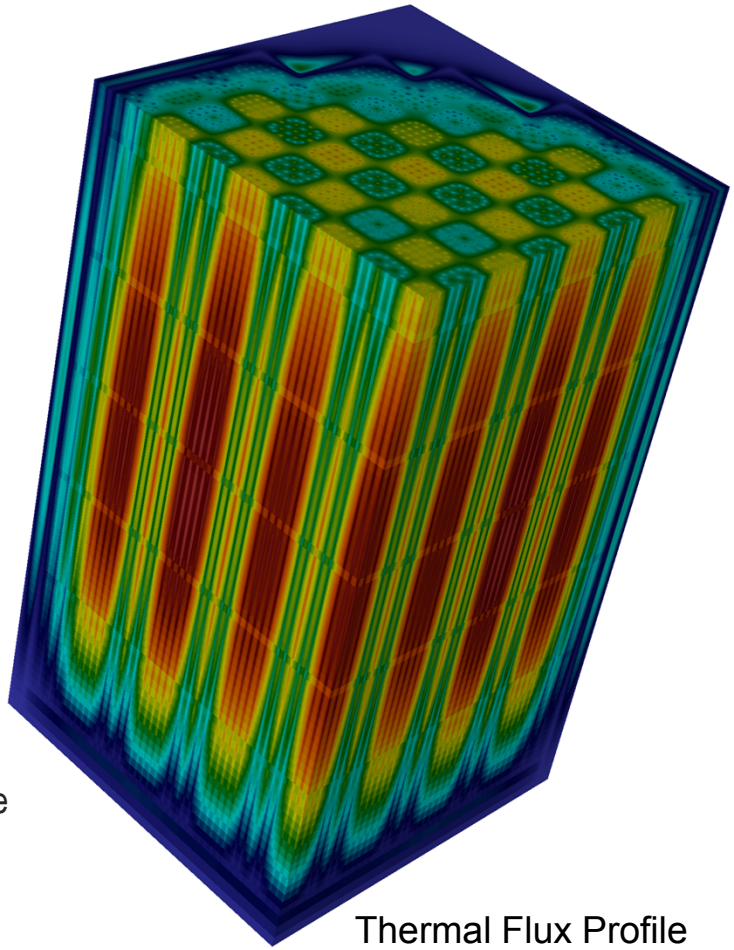
- First large-scale coupled multi-physics model of operating PWR reactor using Components of CASL's Virtual Environment for Reactor Applications (VERA)
- Features resolved are based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1: geometry for fuel, burnable absorbers, spacer grids, nozzles, and core baffle

Execution

- Common input used to drive all physics codes
- Multigroup neutron cross sections calculated as function of temperature and density (SCALE/XSPROC)
- SP_N neutron transport used to calculate power distribution (DENOVO)
- Subchannel thermal-hydraulics in coolant (COBRA-TF)
- Rod-by-Rod heat conduction in fuel rods (COBRA-TF)
- Simulation ran in 17.5 hours on Titan using 18,769 cores – over 1M unique material (fuel/coolant/internals) regions resolved

Next Steps

- Add fuel depletion and core shuffling
- Compare results to plant measured data



Thermal Flux Profile in Reactor Core

"Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using VERA," CASL-U-2013-0196-000, Dec 2013.

CASL-U-2014-0354-000

Evaluate New VERA Continuous-Energy Monte Carlo Capability (Shift) – Quarter-Core Zero Power Physics Test

Goals

- Compare fidelity and performance of Shift against Keno, SP_N, and S_N (Denovo)
- Generate high-fidelity neutronics solution for code comparison of solutions for predicting reactor startup and physics testing

Contributors

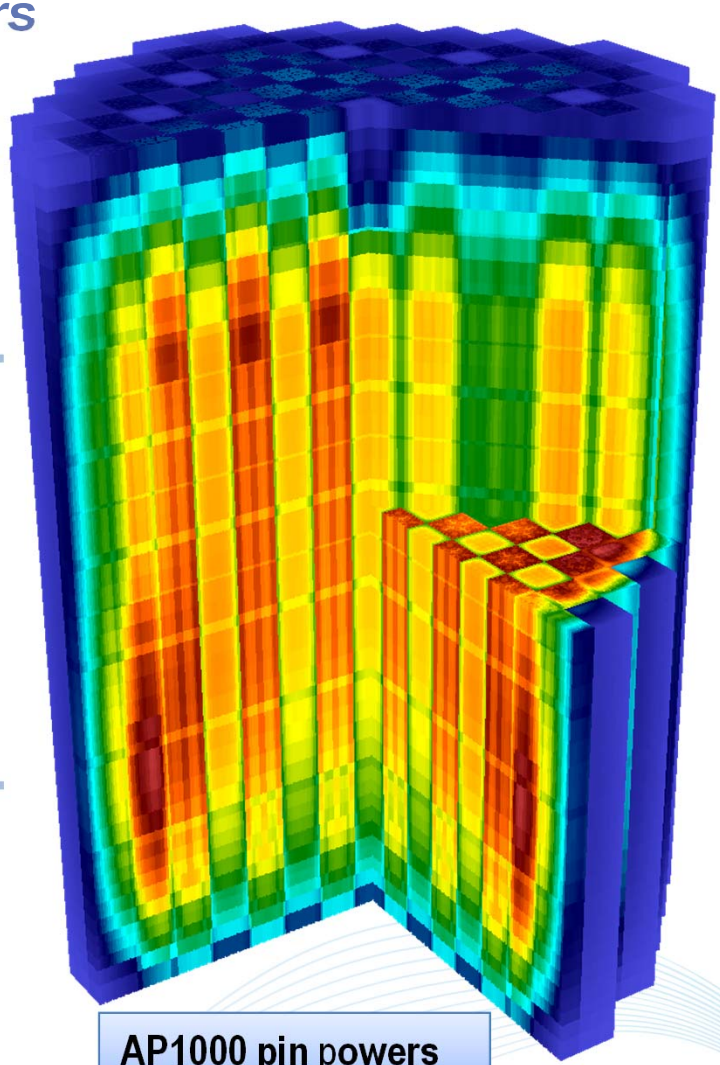
Tom Evans
Fausto Franceschini
Andrew Godfrey
Steve Hamilton
Wayne Joubert
John Turner

Execution

- Proposal submitted to OLCF as part of Titan Early Science program
- Awarded 60 million core-hours on Titan (worth >$2M)
- AP1000 model created and results generated for reactor criticality, rod worth, and reactivity coefficients
- Identical VERA Input models used for Shift, SP_N, and S_N
  - dramatically simpler than KENO-VI input model

Results

- Some of the largest Monte Carlo calculations ever performed (1 trillion particles) have been completed
  - runs use 230,000 cores of Titan or more
- Excellent agreement with KENO-VI
- Extremely fine-mesh S_N calculations, which leverage Titan's GPU accelerators, are under way



AP1000 pin powers

CASL-U-2014-0354-000

CASL "Test Stand" at Westinghouse

- VERA-CS deployed at Westinghouse to simulate the AP1000® PWR Zero Power Physics Tests
- Results in excellent agreement with KENO reference solutions
  - Full Public Report Available
  - Some differences in ITC & MTC

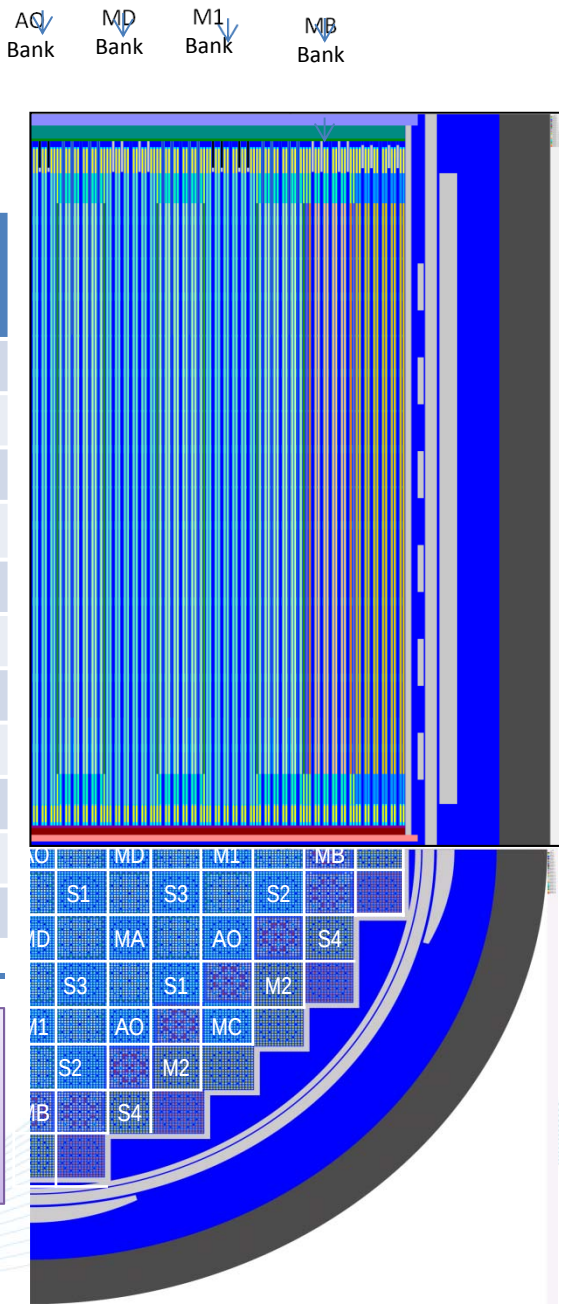
Start-up Boron and Reactivity Coefficients

	KENO	VERA
Critical Boron (ppm)	1314	1311
Isothermal Temperature Coefficient (pcm/F)	-2.7	-3.2
Doppler Temperature Coefficient	-1.6	-1.7
Moderator Temp. Coeff.	-1.1	-1.5

Control Rod Worth

	KENO	VERA-KENO (pcm)	VERA-KENO (%)
MA	258	-1	-0.5
MB	217	-5	-2.1
MC	188	-2	-1.1
MD	234	0	0.0
M1	651	-4	-0.6
M2	887	3	0.4
AO	1635	-4	-0.3
S1	1079	0	0.0
S2	1096	-9	-0.8
S3	1124	0	0.0
S4	580	-3	-0.4

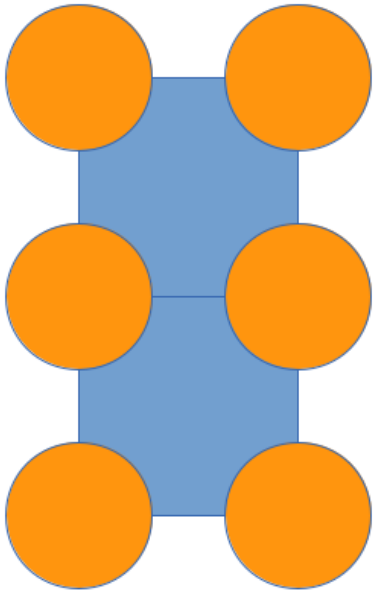
AP1000 Core KENO Model



CASL technology deployed at the industry proves beneficial for challenging simulation scenarios

Main Contributors: F. Franceschini (Westinghouse) and A. Godfrey (ORNL)

Subchannel Modeling Approach

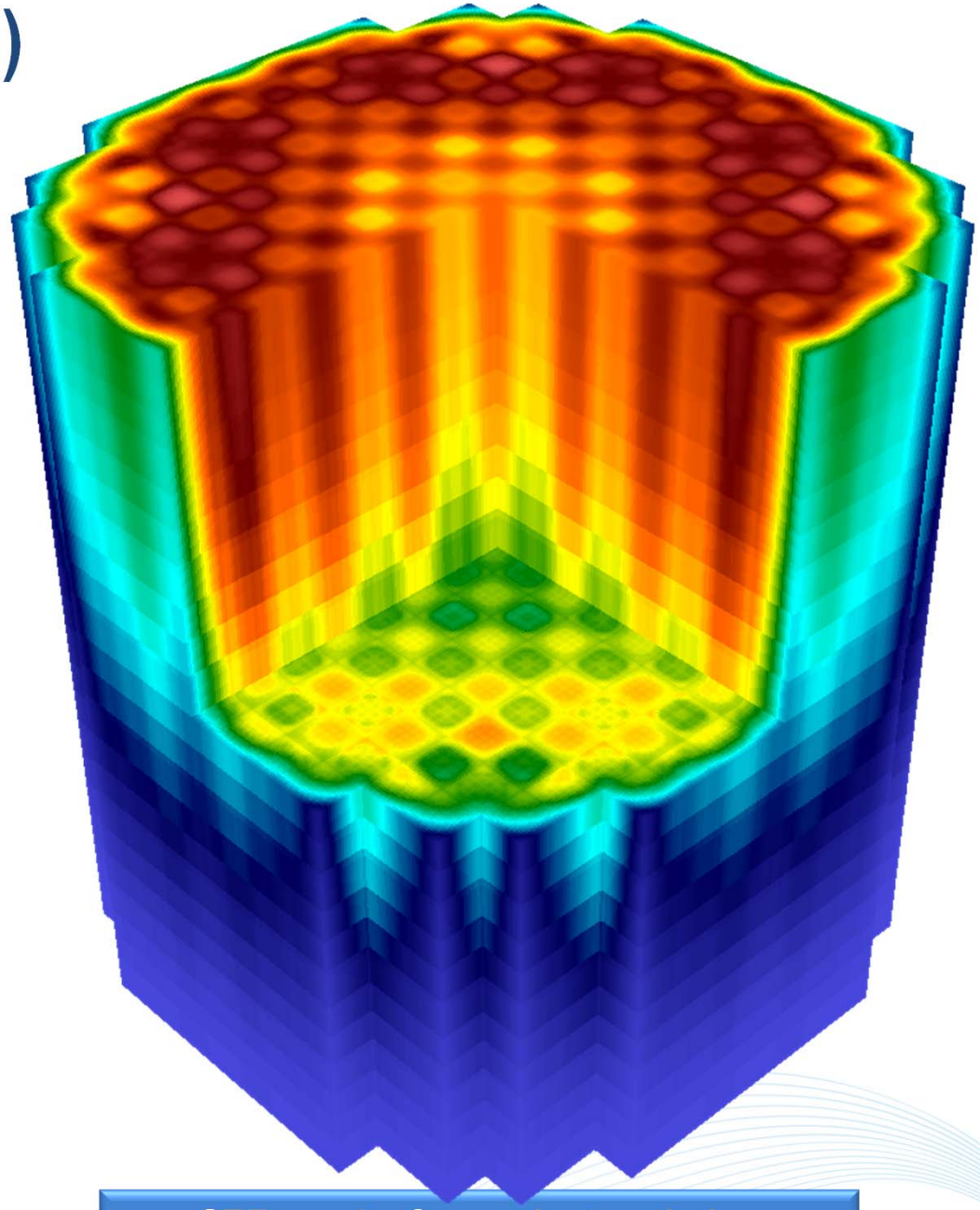


- Method for discretizing the model
- Volumes constrained by adjacent fuel rods
- Navier-Stokes equations averaged over these volumes
  - Simplifications typically made
- Size of volumes same as scale of bundle subchannels
- Volumes connect in lateral direction via “gaps”
  - Flow “loses” its direction after passing through the gap
  - Transverse gradients cannot be resolved
- Due to equation simplifications and mesh coarseness:
  - Fast-running simulations are possible
  - Certain details (e.g. turbulent structures) are not captured

CASL-U-2014-0354-000

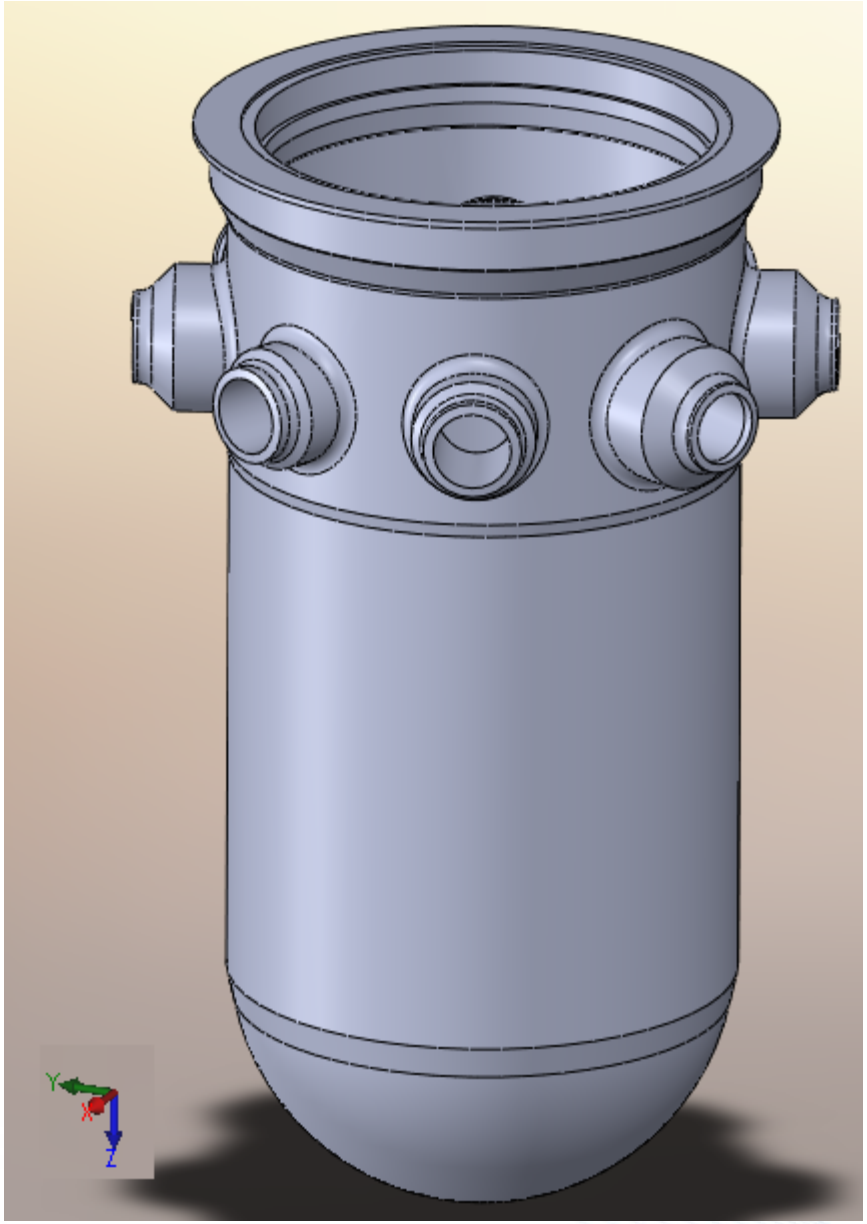
Thermal-Hydraulics (T-H)

- Subchannel run-times
  - Few minutes for single assembly
  - Scalable to full core (>62,000 subchannels) using one assembly per compute core
- CFD can provide higher fidelity for smaller assembly-sized problems
  - HYDRA and STAR-CCM
  - Currently impractical for full-core depletion calculations

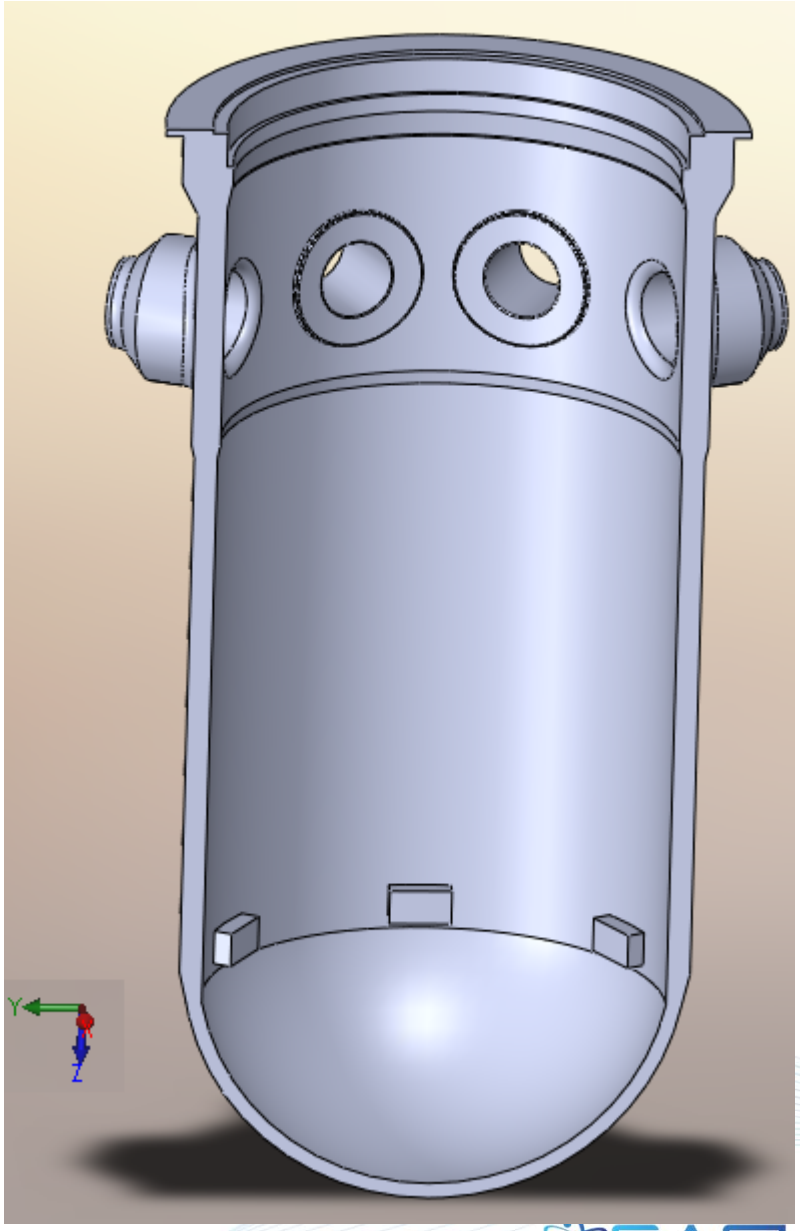


CTF results for coolant enthalpy in quarter-core Watts Bar model

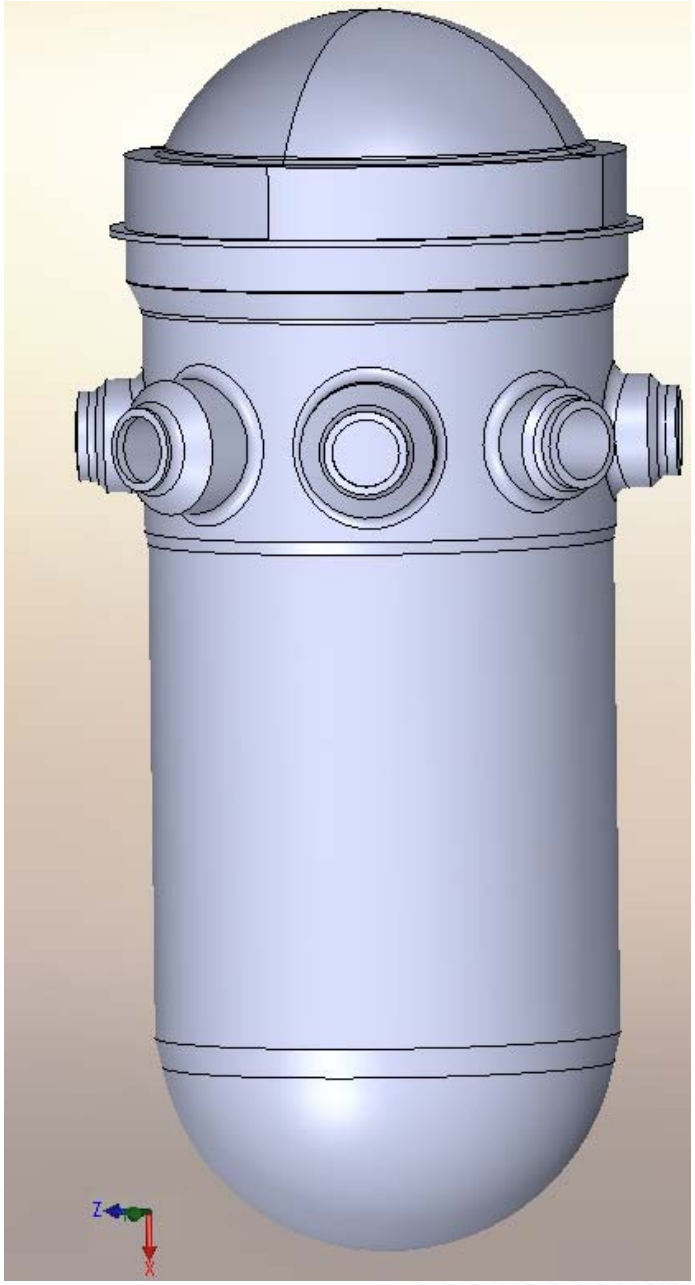
CASL-U-2014-0354-000



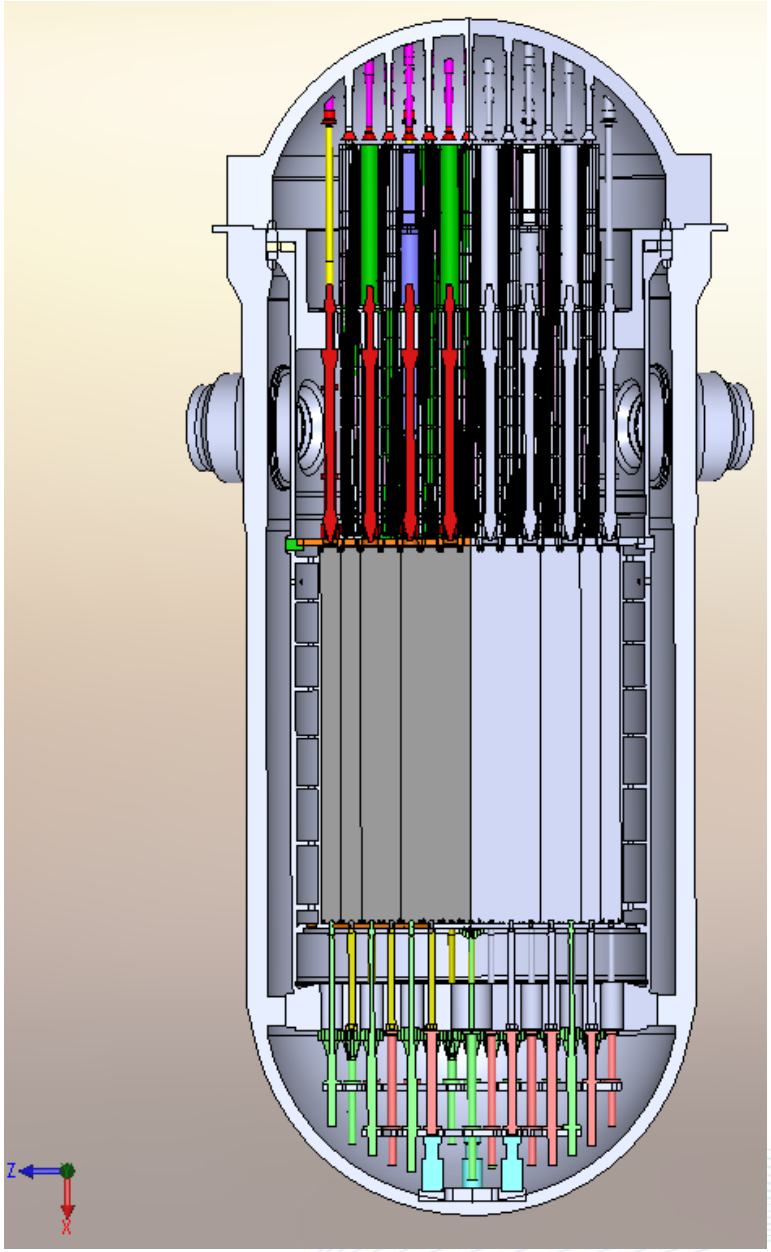
Reactor Vessel



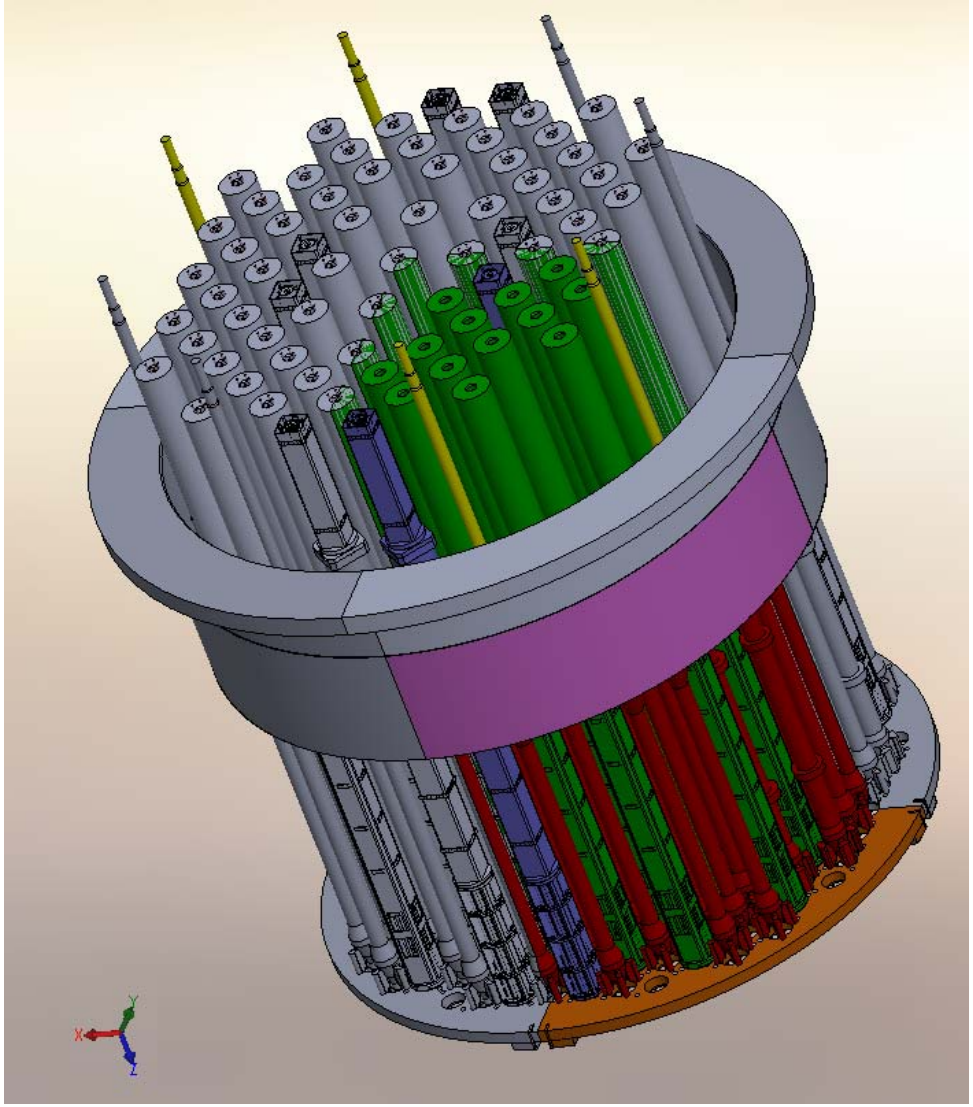
Reactor Vessel (cut view)

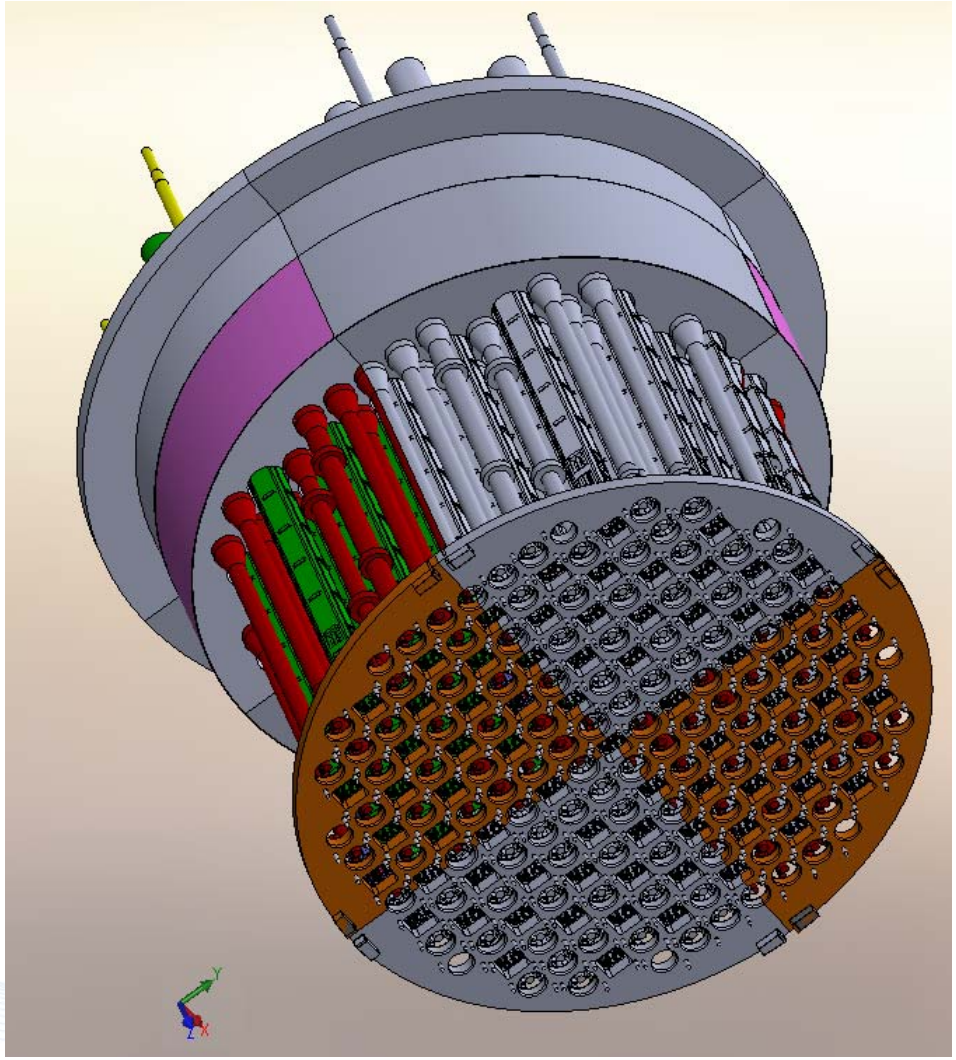


Reactor Solid Model

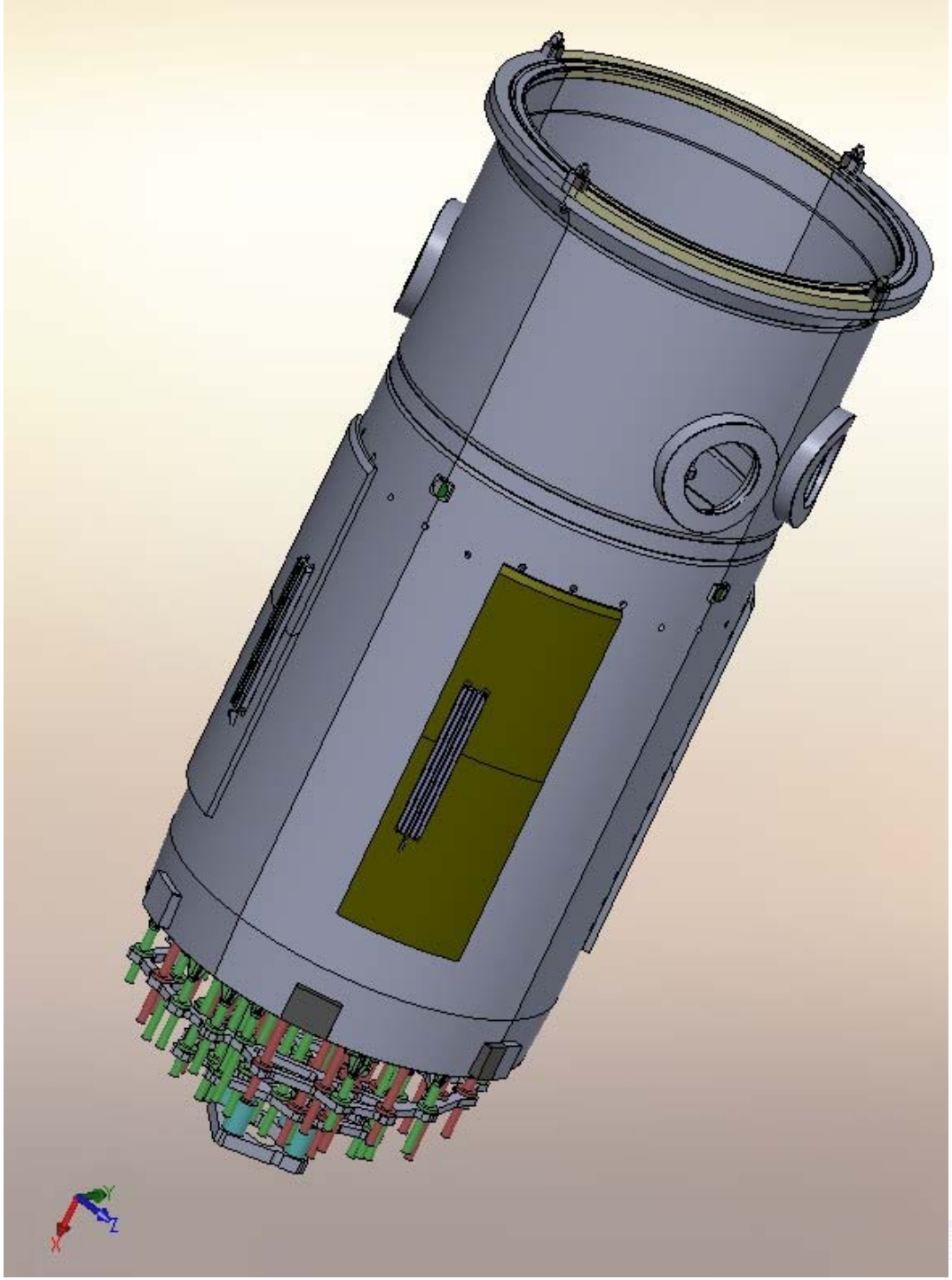


Reactor Solid Model (Cut Plane View)

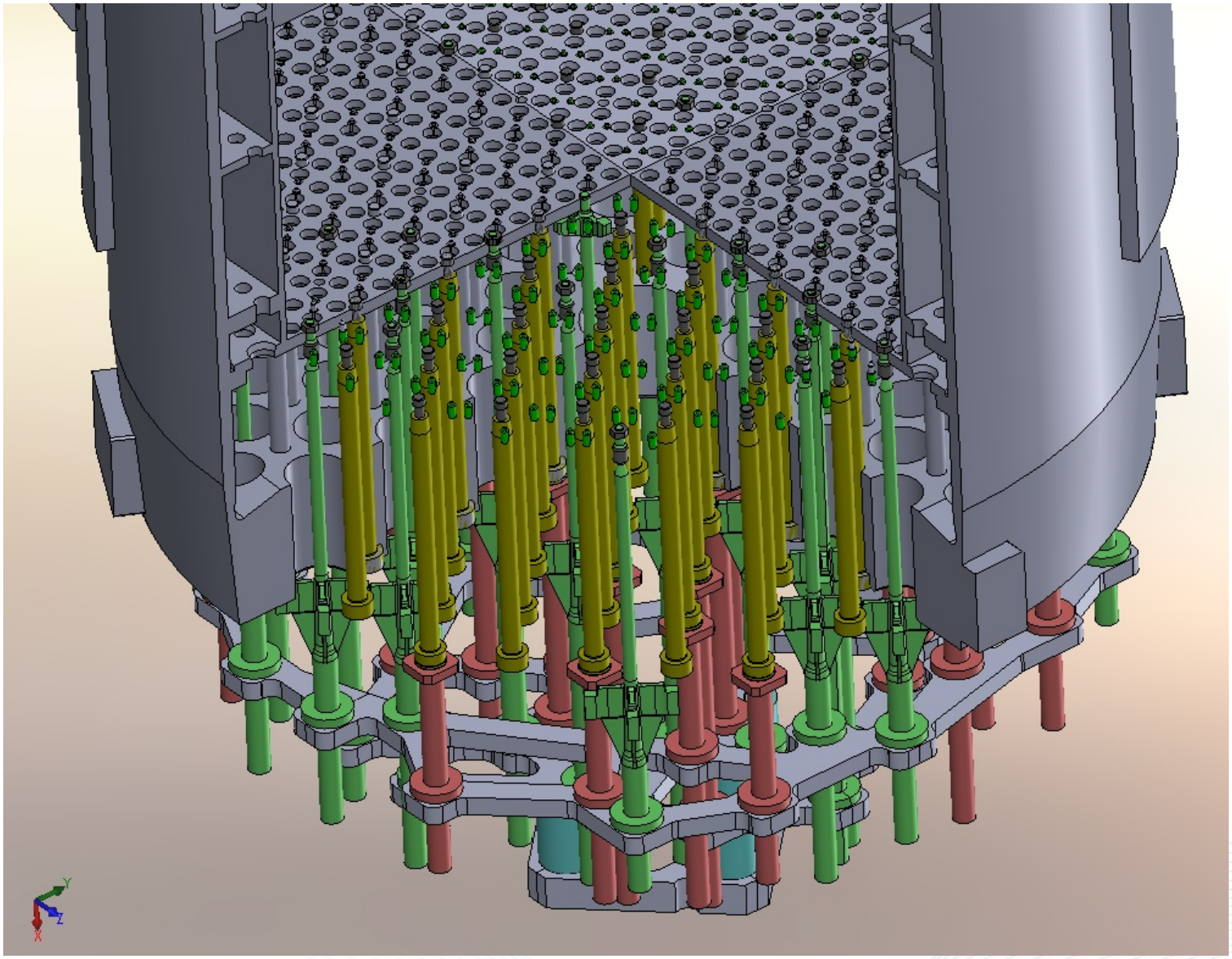




Upper Internal Assembly



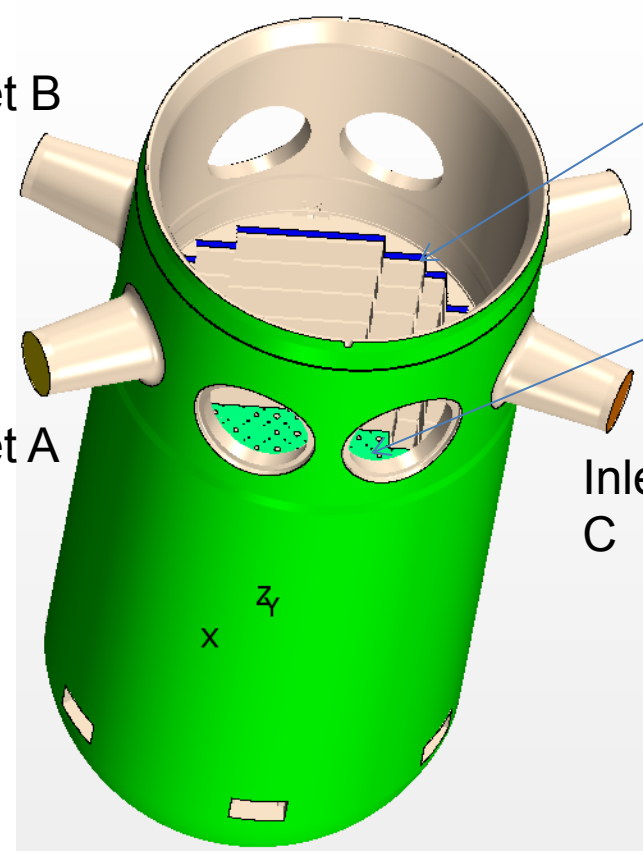
Lower Internal Assembly

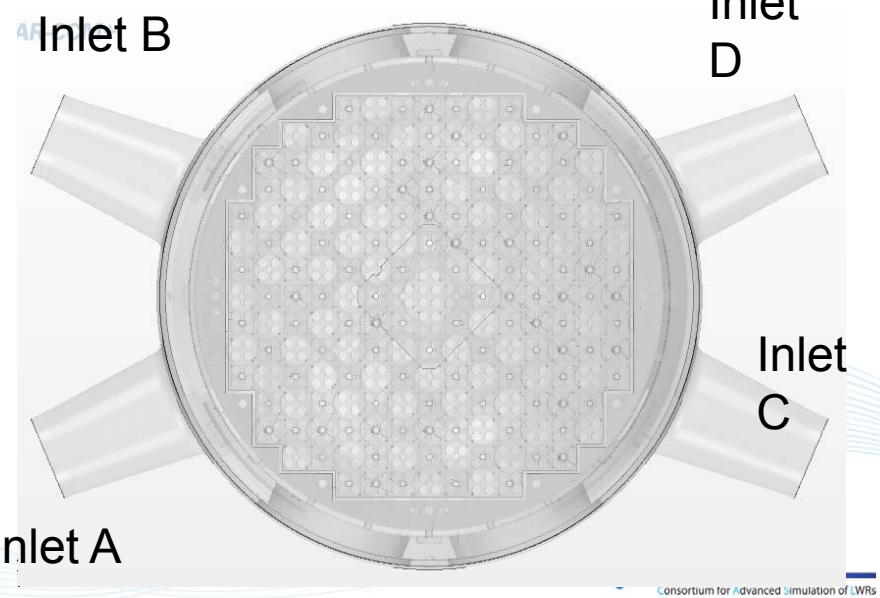


Lower Internal Assembly (a closer look with several components removed)

CFD Domain

Reactor vessel surface mesh

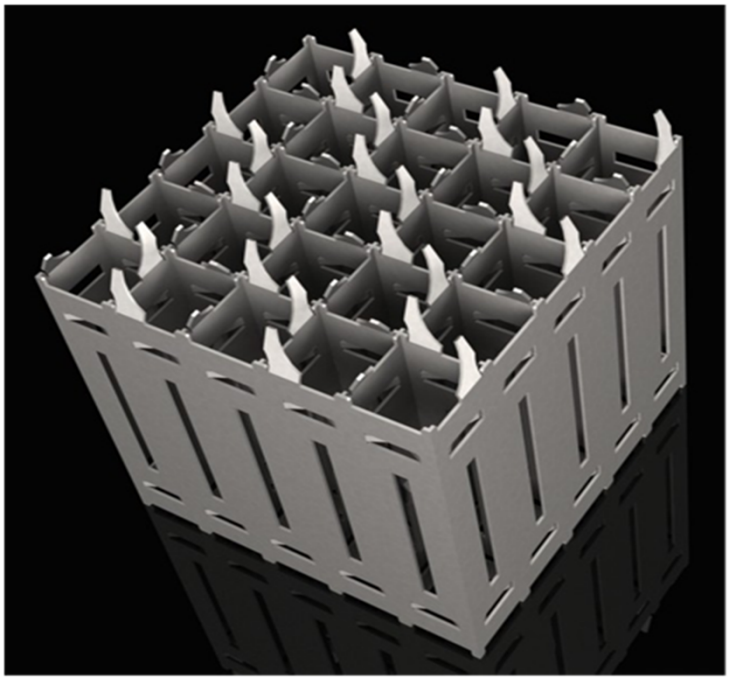


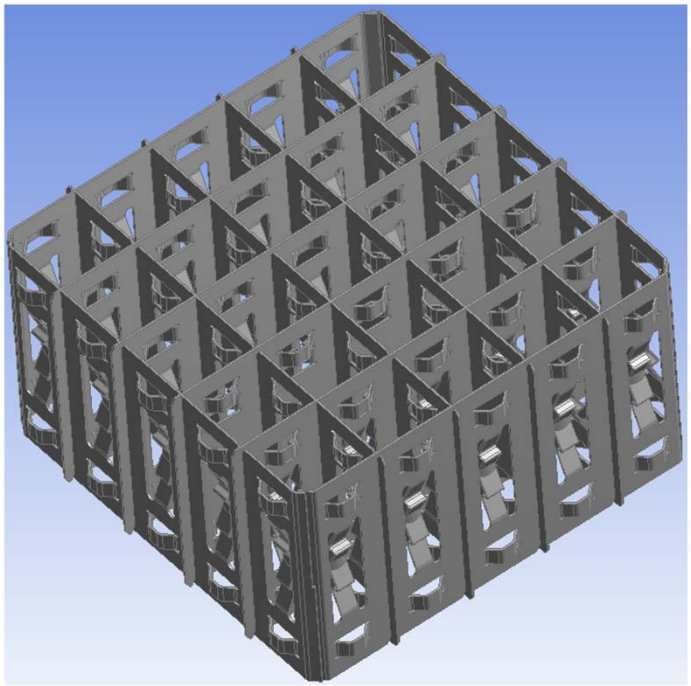


Current practice is to approximate regions of complex geometry as porous media to model pressure drop, etc.

CASL-U-2014-0354-000

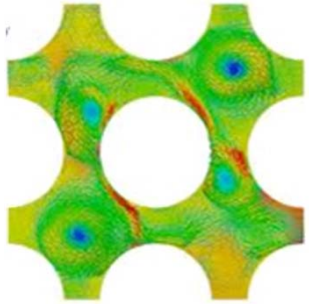
PWR Fuel Assembly Grid Spacers

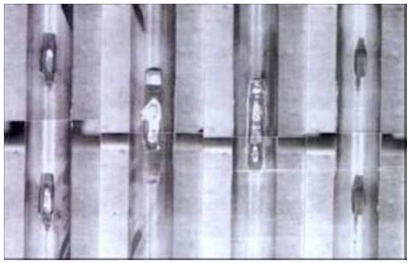




CASL Thermal-Hydraulics applications range from FSI to reacting chemistry, and multiphase flows

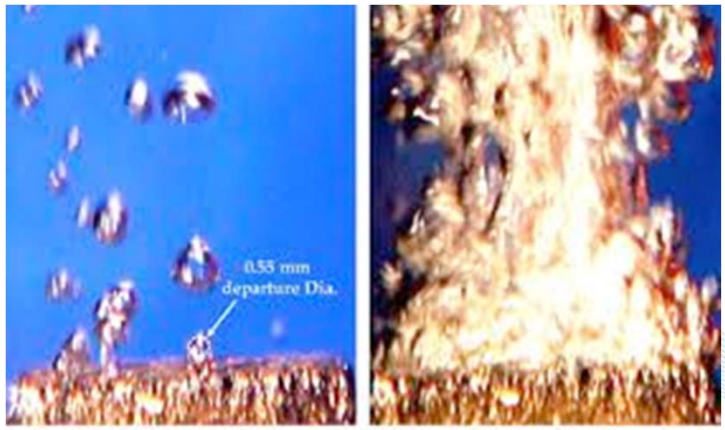
- CRUD-Induced Power Shift (CIPS)
- CRUD-Induced Localized Corrosion (CILC)
- Grid-To-Rod Fretting (GTRF)
- Departure from Nucleate Boiling (DNB)





A largely metaborite 7.5 cm "rock" found in a reactor residual heat removal system

DNB: The point at which the heat transfer from a fuel rod rapidly decreases due to the insulating effect of a steam blanket that forms on the rod surface with a concomitant temperature increase.



(a) 0.2 W/cm^2, ΔT_{sat} = 0.8 K (b) 10.0 W/cm^2, ΔT_{sat} = 7.9 K

CASL-U-2014-0354-000

Demonstration and Assessment of Advanced Modeling Capabilities for Pressurized Water Reactor Thermal Hydraulics: Multiphase Flow with Subcooled Boiling

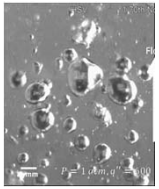
Mark Christon (LANL)
Emilio Baglietto (MIT)

A 'tour de force' coordinated and integrated research effort among the broad and diverse set of researchers in CASL Thermal Hydraulics Methods Focus Area

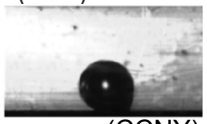
- Development of a new computational framework (Hydra-TH) to be deployed with CASL's Virtual Environment for Reactor Applications (VERA)
- Deployment of hardened theoretical models and numerical methods for subcooled flow boiling
- Construction of an integrated multiphase computational fluid dynamics (CFD) closure algorithm

(LANL, ORNL)

(LANL, INL)



(MIT)



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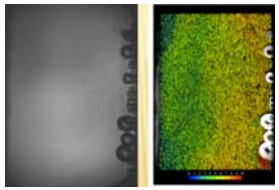
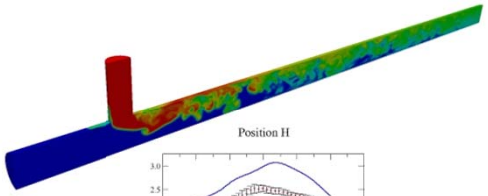
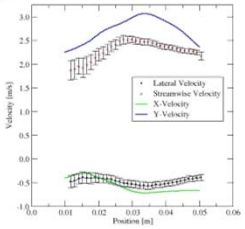


(TAMU)



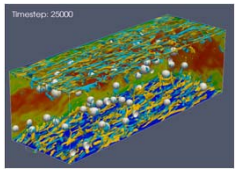
(LANL, UM, SNL)



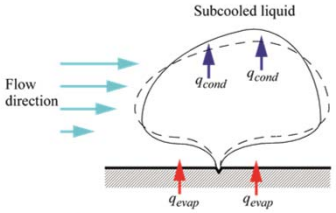
Experiments
- Fundamental Understanding
- Code Validation
- Multiphase Closure Models

Algorithms & Architectures
- Advanced CFD Algorithms
- Multiphase Solution Methods
- Advanced Architectures – NVIDIA nvAMG Library

V&V, Uncertainty Quantification
- Intrusive VUQ Algorithms
- Multiphase Model Sensitivities
- CFD Verification



(NCSU)

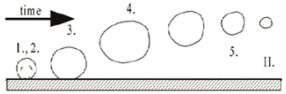


(Notre Dame)

DNS - Interface Tracking
- Fundamental Understanding
- Multiphase Closure Models
- Code Validation

VERA -CFD (Hydra-TH)

Multiphase Closure Models
- Mechanistic Subcooled Boiling
- Refined momentum closures
- Integrated lift/drag forces



(MIT, ORNL, UM, NCSU, Notre Dame, RPI)

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Hydra-TH Development Path

Mark Christon (LANL)
Emilio Baglietto (MIT)

FY2011 - 2012

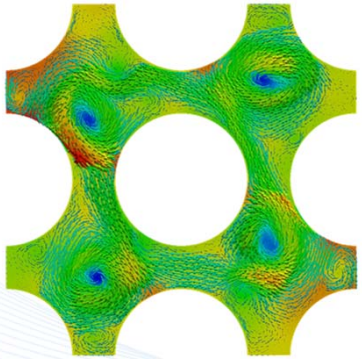
- Hybrid Parallel Meshing of V5H. 3x3 and 5x5 V5H meshes up to 192M cells
- Development of a priori mesh assessment based on y+
- Runtime turbulence statistics
- Parallel Visualization (ParaView)
- L1 Milestone: Determine sensitivity of structural response to GTRF RMS forces
- Investigate sensitivity of GTRF forces to URANS and LES models
- Validation LES calculations with 5x5 V5H TAMU Data
- Direct integration of Hydra-TH forces using WEC VITRAN code. Less than 1.7% difference compared to STAR-CCM+ "gold standard"
- Development of Hydra-TH Multiphase development roadmap

FY2013

- Hydra-TH Assessment on THM Benchmark Problems
- Development of Hydra-TH V&V/Benchmark Problems and Documents
- General-purpose Steam Property Library (IAPWS-95/97)
- Fully-implicit single-phase
- Initial (anelastic) multiphase flow demonstration
- Integration of asymmetry preserving drag model
- Enthalpy and Internal Energy form of Energy Equation
- Enhanced surface/statistics output
- Direct nightly code integration into VERA
- Addition of ~ 50 licensed users

FY2014

- Expose Native CHT Capabilities
- Release porous drag for simplified meshing
- Single-phase validation for fuel applications
- Improved parallel linear algebra
- Enhanced turbulence single/multiphase turbulence models
- Fully-implicit multiphase
- Boiling closure models
- Single/multiphase V&V
- Hydra-Mamba direct coupling
- Expanded "open" Hydra development model



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The Phasic, Ensemble-Averaged Equations

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Mass:

$$\frac{\partial \alpha_k \bar{\rho}_k}{\partial t} + \nabla \cdot \left(\alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k\right) = \boxed{\Gamma_k}$$

Momentum:

$$\frac{\partial \alpha_k \bar{\rho}_k \tilde{\mathbf{v}}_k}{\partial t} + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{\mathbf{v}}_k \otimes \tilde{\mathbf{v}}_k + \bar{p}_k\right]\right) = \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \nabla \alpha_k + \boxed{\mathbf{M}_k'} +$$

$$+ \nabla \cdot \left(\alpha_k \left[\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}_k^{Re}}\right]\right) + \alpha_k \bar{\rho}_k \boxed{\tilde{\mathbf{b}}_k} + \boxed{\mathbf{v}_{ki}^m} \boxed{\Gamma_k}$$

Total energy:

$$\frac{\partial}{\partial_t}\left(\alpha_k \bar{\rho}_k \tilde{e}_k\right) + \nabla \cdot \left(\alpha_k \left[\bar{\rho}_k \tilde{e}_k + \bar{p}_k\right] \tilde{\mathbf{v}}_k\right) = \boxed{\mathbf{M}_k'} \cdot \tilde{\mathbf{v}}_k + \left(\boxed{p_{ki}} - \boxed{\tau_{ki}}\right) \tilde{\mathbf{v}}_k \cdot \nabla \alpha_k +$$

$$+ \nabla \cdot \left(\alpha_k \left[\tilde{\mathbf{v}}_k \left(\boxed{\bar{\tau}_k} + \boxed{\mathbf{T}_k^{Re}}\right) - \boxed{\bar{\mathbf{q}}_k} - \boxed{\mathbf{q}_k^{Re}}\right]\right) +$$

$$+ \alpha_k \bar{\rho}_k \left(\boxed{\tilde{r}_k} + \boxed{\tilde{\mathbf{b}}_k} \cdot \tilde{\mathbf{v}}_k\right) + \boxed{\Gamma_k} \left(\boxed{u_{ki}} + \frac{\left(\boxed{v_{ki}^e}\right)^2}{2}\right) + \boxed{E_k} + \boxed{W_k'}$$

+ Turbulence equations

Closures:

+ N equations of state, $\bar{p}_k\left(\bar{\rho}_k, \tilde{u}_k\right)$
+ Constitutive physics (for terms in boxes $\boxed{}$)
+ Compatibility condition, $\sum_k \alpha_k = 1$
+ Bulk pressure difference models, $\Delta \bar{p}_{(ij)}\left(\mathbf{U}\right),\ i \neq j,\ (i,j) = 0, \ldots, N-1$

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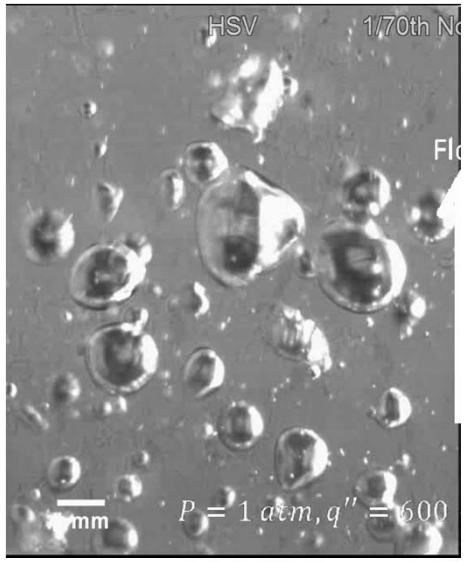
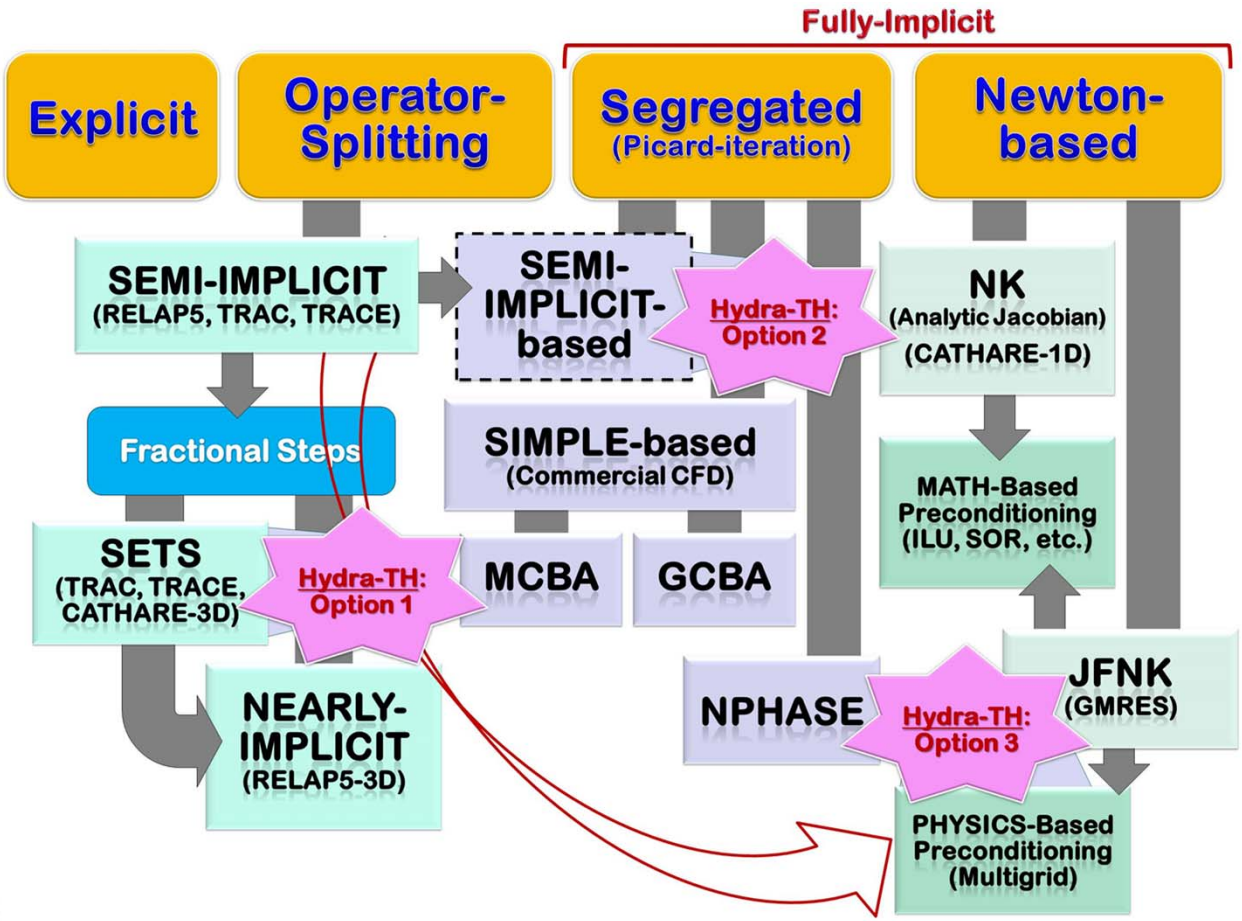
Multiphase flow algorithms and the Hydra multiphase flow strategy/roadmap

Mark Christon (LANL)
Emilio Baglietto (MIT)

- "Option 1" with momentum transfer (drag)
- "Option 2" - Picard (for single field) exercised





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Designing Hydra's flow solvers

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Emilio Baglietto (MIT)

Advection is one of the most critical algorithmic components because it determines the ability to treat PDE's that require bounded variables, e.g., turbulence, species and volume fractions

Some Desirable Attributes in an Advection Scheme:

- Consistency: discretization recovers the PDE as $\Delta x \to 0,\ \Delta t \to 0$
- Stability: $\left\| u^{n+1} \right\| \le \left\| u^{n} \right\|$, e.g., stable for all Δt and insensitive to roundoff
- Convergence: numerical solutions approach the PDE solution as $\Delta x \to 0,\ \Delta t \to 0$
  - For linear problems, automatic given stability & consistency via Lax's equivalence theorem
- Conservation: 0th-moment should be globally conserved (at a minimum)
- Non-dispersive: all wavelengths propagate at the 'true' advective speed
- Non-dissipative: there should be no 'numerical diffusion'
- Shape-preserving: positivity, monotonicity, lack of spurious oscillations
- Compact operators: local 'stencils' for the 'difference' operators
- Computationally efficient: reasonable memory and CPU requirements

Baptista, Adams, Gresho, "Benchmarks for the transport equation: the convection-diffusion forum and beyond", QSACOM, V47, 1995.

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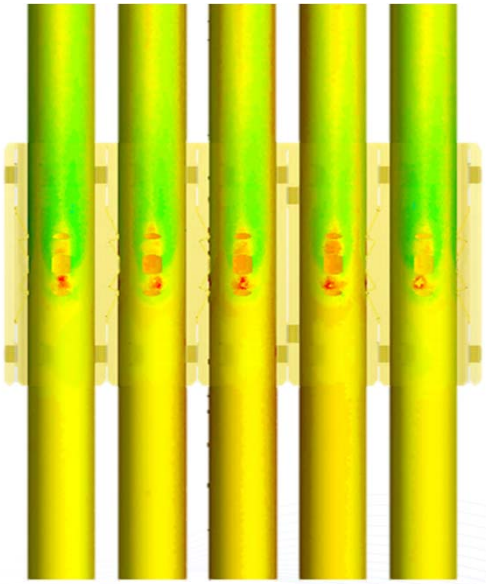
The targets: PWR first!

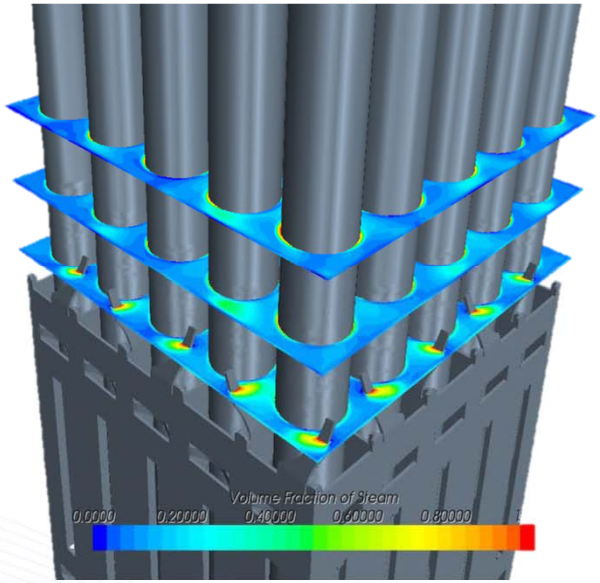
Mark Christon (LANL)
Emilio Baglietto (MIT)

Multiphase, multispecies, poly-dispersed, all-regimes model?

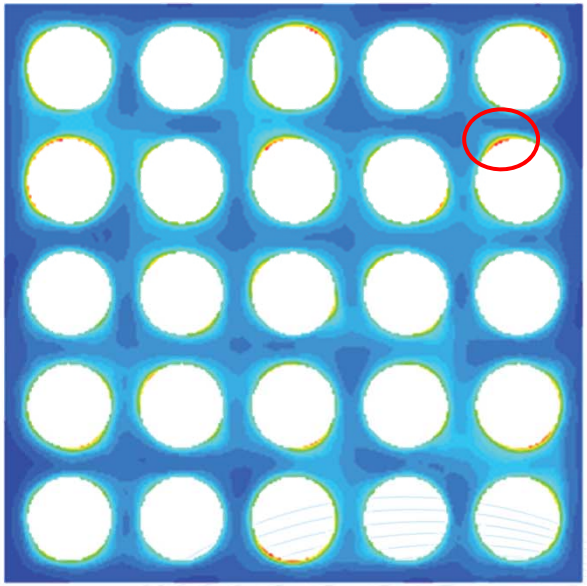
- First aim is PWR operational conditions, leverages well known subcooled flow regime, small channels, incompressible, “mono-dispersed”
- Framework should be designed for all-regimes: provides increased robustness, supports future applications
- Well defined short term targets: boiling heat transfer, void fractions, DNB.



boiling heat transfer



void fraction



DNB

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The approach: Physics-Based, Robust, and Assessable

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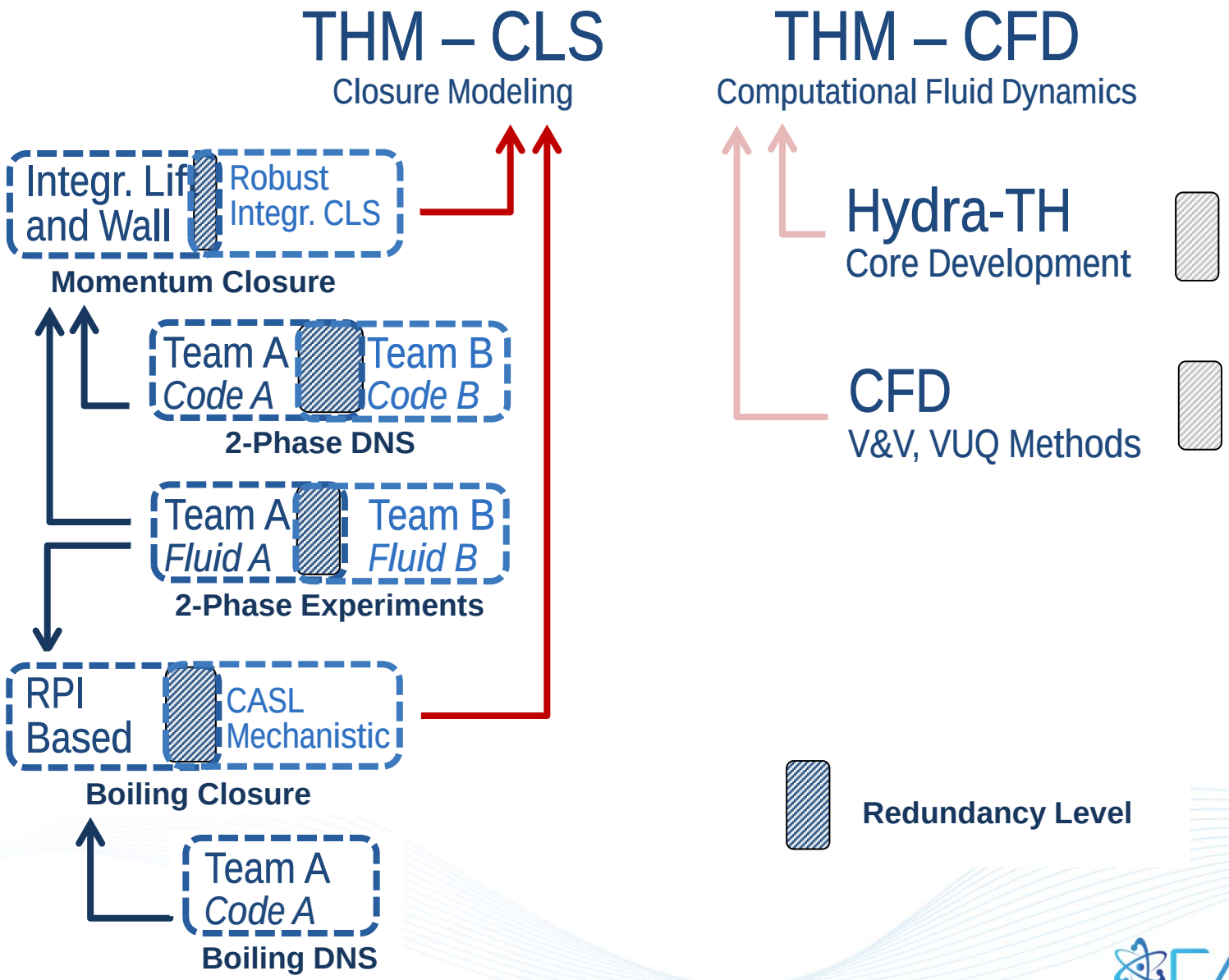

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Deliverables

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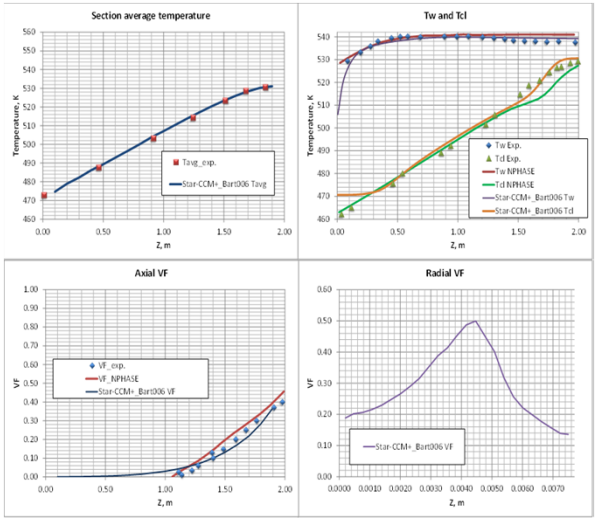
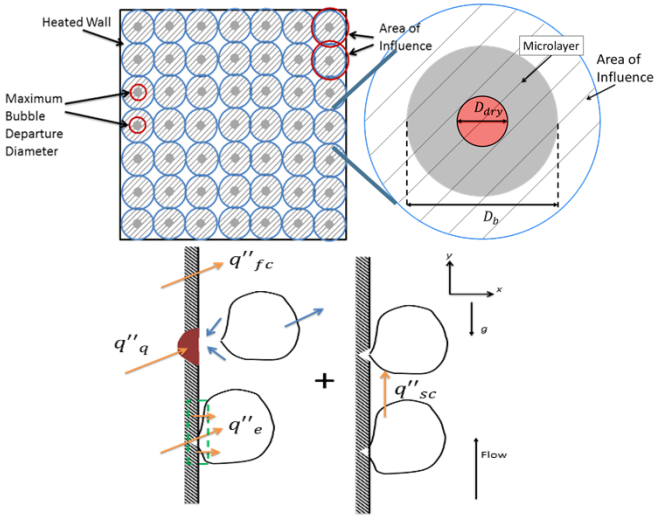
Emilio Baglietto (MIT)

Robust Baseline Closure



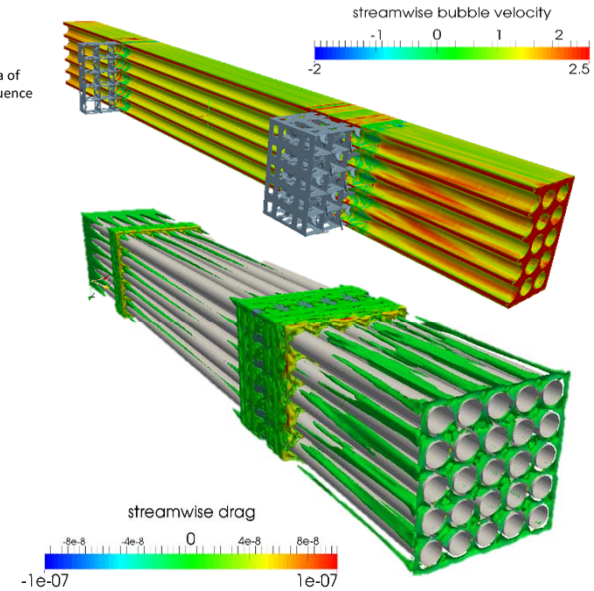
- First Generation Closure in Hydra-TH should leverage existing experience
- Implementation of baseline closure in STAR-CCM+ allows direct comparison to CD-adapco baseline closure results (platform independent)
- Sensitivity of model parameters should confirm PoR-3 studies

Innovative GEN-II Closure



- Second Generation Closure should incorporate new physical understanding
- Increased synergy with experimental "micro" measurements
- Extended applicability (lower/ higher vapor generation)
- Include modeling toward limiting behavior (CHF)

New M-CFD Platform



- Hydra-TH baseline multiphase capabilities first shakedown
- Hydra-TH Mupltiphase implementation should target enhanced applicability towards transient simulations (including fast transients)

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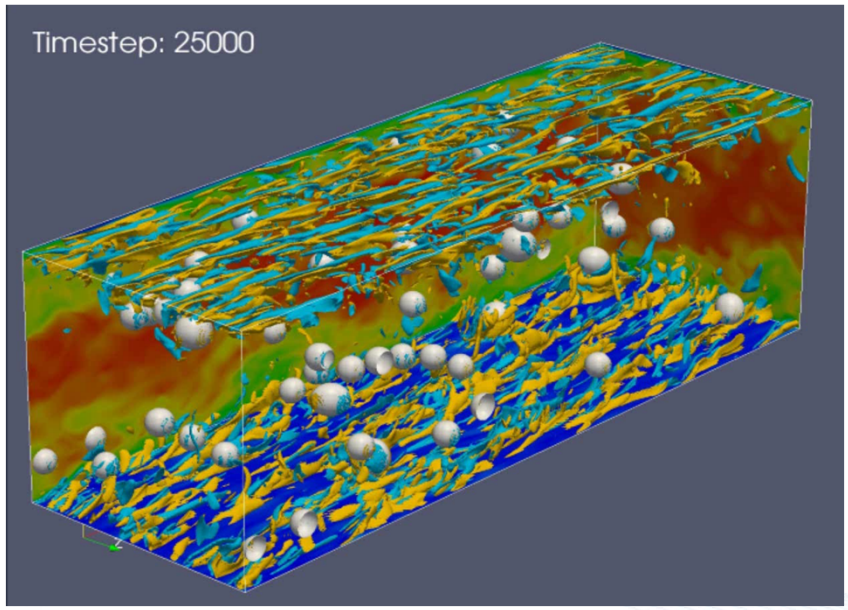
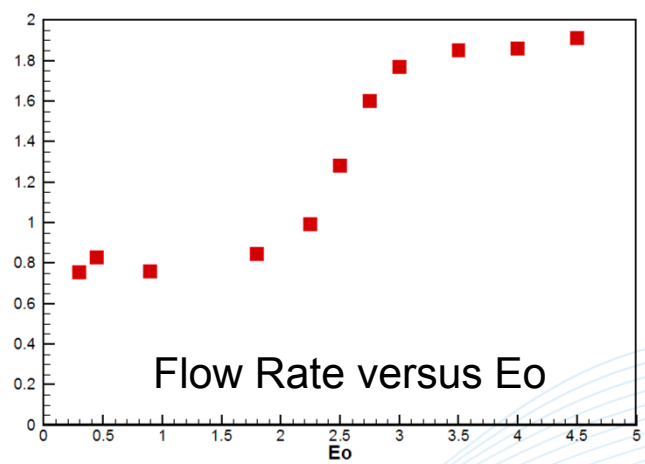
ITM/DNS Data Changes Closure Model Development in a Fundamental Way

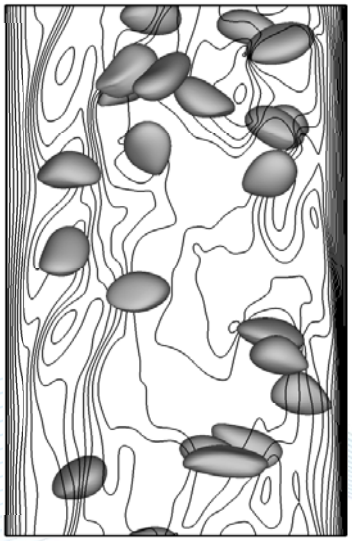
- Permits direct computation of modeled terms at given points in space/time and to assess their mean and fluctuation components
- Approach in single-phase flows has led to significant advances in understanding and developing closure models
- Provides the foundations for more complete multiphase CFD turbulence modeling
- Developing a DNS lift/drag database for integral momentum closure model



Bubble Deformability Effects



High Eo



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Questions?

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

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CASL Status and Looking Forward

- ✓ Year 1: Build the foundation
- ✓ Year 2: Advance the science basis of the M&S technology components
  - ◆ Guided by challenge problem requirements baselined against industry capabilities
- ✓ Year 3: Assess, refine, integrate, and beta test the M&S technology components within the multi-physics Virtual Reactor environment
  - ◆ Perform initial verification and validation (V&V), sensitivity analysis (SA), and uncertainty quantification (UQ) analyses
- ✓ Year 4: Harden for robustness & efficiency and deploy & apply the coupled multi-physics Virtual Reactor technology for broader assessment and continuous improvement
  - ◆ Prepare for possible 5-year renewal that leverages development to date
- ✓ Year 5: Continue maturation of the multi-physics Virtual Reactor technology thru increased breadth and depth of testing and application offered by a general release
  - ◆ Self-sustaining technology deployment (release/support) and evolution plan in place

Scientific Output thru Year 3

- Virtual Reactor M&S technology integrated, under active development and assessment, and deployed for beta testing
- 81+ journal articles
- 328 conference papers
- 28 technical reports
- 51+ invited talks
- 382 milestone reports
- 216 programmatic reports

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Supplemental Material

CASL Innovations

Challenge Problems

Product Integrators are in place and driving metrics, products, and plans

CP	Description and Impact	Simulations Gaps and Drivers
Crud-induced power shift; crud-induced localized corrosion	High uncertainties in crud source, thickness, boiling surface area, and margin to fuel leakage affect fuel management and thermal margin in many plants, limiting power uprates	More accurate, higher resolution models for boiling surface area, crud deposition, boron uptake and cladding oxidation rate for each rod in core, with boron feedback in neutronics
Grid-to-rod fretting	Rod growth changes, flow induced vibration, irradiation-induced grid growth and spring relaxation affect wear, especially for fuel near the core shroud	Reliable predictions of grid to rod gap, turbulent flow excitation, and resulting rod vibration and wear at any location in core
Pellet-clad interaction	Cladding creep-down onto pellets, followed by pellet expansion, creates local cladding stresses at pellet imperfections, resulting in clad failure sometimes assisted by SCC	Sufficient 3D geometric detail of fuel rod material property changes; pellet growth, cracking and fission product release; cladding stresses, creep, fracture and SCC attach; fuel-cladding binding; and coupling to neutronics and T-H
Fuel assembly distortion	Forces from radiation-induced growth and fluid flow may cause distortion and alter power distributions, challenge fuel handling, retard control rod insertion, and restrict plant operation	Fully 3D structural models of fuel assemblies accounting for material property changes, growth and creep; coupled with neutronics and TH
Reactor vessel and internals integrity over reactor lifetime	Damage from radiation results in increased temperature for onset of brittle failure and higher failure probability due to thermal shock stresses with safety injection for RV, and damage from radiation, thermal & mechanical fatigue render upper internal package more susceptible to distortion under blow-down or seismic loads.	3D prediction of temperature, force, stress, fluence and resulting material property changes of reactor internal structures and vessel; and solid mechanics prediction of vessel fracture and internals distortion
Departure from nucleate boiling	Local clad surface dryout, affected by detailed flow patterns and mixing, cause dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow) leading to high cladding temperatures	3D subchannel and CFD tools to model detailed flow patterns downstream of mixing grids for single and two-phase flow, coupled to detailed pin-resolved radiation transport and fuel performance models for application to DNB transients (e.g., RIA, Loss of Flow)
Cladding integrity during a reactivity insertion accident and loss of coolant accident	Physical changes during transient (e.g., swelling and burst, oxidation mechanics), leading to clad failure followed by fuel dispersal	Enhanced fuel rod models, with improved predictive capability for normal operations to obtain fuel initial conditions at initiation of accident simulation, and transient fuel rod behavior

- FAD: Defer until mechanics plan and capability in place thru GTRF execution
- Lifetime Extension (integrity): Leverage scope in LWR Sustainability Program

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Path Forward to Address Challenge Problems

CP	Simulation Capability Targets	Path Forward
CIPS	Validated, predictive tools that reduce uncertainty for simulating CIPS and increase flexibility in incore fuel management	▪ Couple models for consistent feedback between neutronics, T-H, crud/chemistry accounting for boron and crud feedback ▪ Calculate 3D pin resolved transport neutronics, subchannel TH and crud deposits ▪ Calculate erosion of crud and crud chemistry ▪ Calculate 3D mass of boron deposited in crud and CIPS throughout life
CILC	Validated, predictive tools that reduce uncertainty for simulating CILC and increase flexibility in incore fuel management	▪ Zoom in to limiting region of core for crud deposition based on CIPS analysis ▪ Provide azimuthal variation of heat transfer downstream of spacer grids ▪ Predict 3D crud deposits, crud chemistry and clad temperature around limiting rods ▪ Predict CILC and margin to leaker
GTRF	Validated, predictive tools for simulating wear of any rod in core and to evaluate impact of spacer grid design features	▪ Predict turbulent excitation force at any location in core using 3D CFD modeling tools. ▪ Predict fuel rod and spacer grid structural material behavior as function of fast fluence ▪ Predict fuel rod and spacer grid corrosion material behavior as function of fast fluence ▪ Predict gap between grid cell support structures and the fuel rod versus time in core ▪ Develop wear model that takes into consideration of contact type and material condition ▪ Perform structure-dynamic simulation to translate hydraulic forces to rod vibration ▪ Predict rod wear margin for any location in core
PCI	Validated, predictive models for 3D fuel rod behavior that increase flexibility in plant power maneuvering	▪ Couple fuel rod model (2-D) to core simulator (core-wide power/TH calculations) to calculate performance indicator throughout entire core ▪ Develop method to couple full-length fuel rod model to local effects stress and failure potential simulation (3-D effects) ▪ Develop fuel rod model to calculate fuel rod conditions during operation for full-length rods ▪ Develop 3-D local effects (few pellets) modeling methods to evaluate conditions leading to PCI failure

Path Forward to Address Challenge Problems

CP	Simulation Capability Targets	Path Forward
FAD	Validated, predictive tools for fuel assembly distortion to evaluate impact of assembly skeleton design features	• Build 3D structural models for fuel in core • Couple structural model with neutronics and TH
DNB	Validated tools to predict DNB using more advanced methods to evaluate safety margin, enhance understanding, and evaluate impact of spacer grid design features	• Couple neutronics and subchannel thermal hydraulic tools to better predict DNB for transients such as RIA • Implement and validate two-phase models in CFD tools for predicting DNB • Predict DNB with improved CFD tools and validate to available data
RIA	Validated modeling improvements to more accurately assess fuel performance during RIA and LOCA and evaluate impact of Accident Tolerant Fuel features	• Implement pin-resolved modeling of the transient neutronics for RIA including the effects of local temperature reactivity feedback • Develop advanced transient fuel rod thermal-mechanical tools capable of modeling all of the characteristics of the initial and transient conditions and behaviors of the fuel rod such as fuel pellet cracking and relocation, fuel-to-pellet contact and binding, and cladding outer diameter oxidation due to normal in-service corrosion and hydrogen pickup. • Couple tools to simulate RIA and predict PCMI and margin to failure
LOCA	Validated modeling improvements to more accurately assess fuel performance during RIA and LOCA and evaluate impact of Accident Tolerant Fuel features	• Perform same tasks as RIA but apply to LOCA transient • Utilize boundary conditions from RELAP5 System Code for LOCA • Evaluate maximum PCT and oxidation margin • Investigate benefits of ATF
RV & Internals Integrity	Validated, predictive tools for vessel performance during cold leg injection and for internal performance during hot leg blow down	• 3D prediction of temperature, stress, fluence, and growth of fuel and reactor internal structures and vessel • Predict any component vibration • LWRS Scope: Predict fatigue, SCC and radiation damage

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High Level CASL Plan to Address Challenge Problems

PCI*

- Predict Core Wide PCI Margin with **PEREGRINE2D** - Plant data
- Zoom in and Predict MPS PCI leaker with **PEREGRINE3D** -Hot Cell, Halden, & Plant data

CRUD*

- **CIPS:** Predict Boron Uptake with **MAMBA2D** -Plant CIPS data
- **CILC**: Predict Crud thk & corrosion with **MAMBA3D** use STAR/HYDRA-TH single phase heat transfer multipliers -WALT loop,& Seabrook CILC data

RIA*

• Predict PCMI Margin using **PEREGRINE2D** –CABRI & NSRR data, Apply to Reactor core

VERA-CS*

Insilico-MPACT/ COBRA-TF/PEREGRINE
(full depletion for all rods in core)
Watts Bar 1 Physics Data, etc

LOCA*

•Predict PCT – Oxidation Margin using **PEREGRINE2D** & System Code **RELAP5** –FLECHT,APEX, Halden, Studsvik Data, Apply to Reactor Core

DNB*

- Predict DNB Margin for RIA – Apply to Core
- Predict Mixing & DNB with CFD using **STAR/HYDRA-TH** 1 and 2 phase flow - PIV,LDV, boiling, T/C mixing & DNB data

GTRF*

- Predict Minimum GTRF Margin in Core using **PEREGRINE2D** –gap, **STAR/HYDRA-TH**-excitation force, **BEAM** tool –vibration/wear –PIV, LDV, Vibration, Wear, Plant PIE wear data

*** For Each Challenge Problem Apply DAKOTA using Coupled Tools for UQ**

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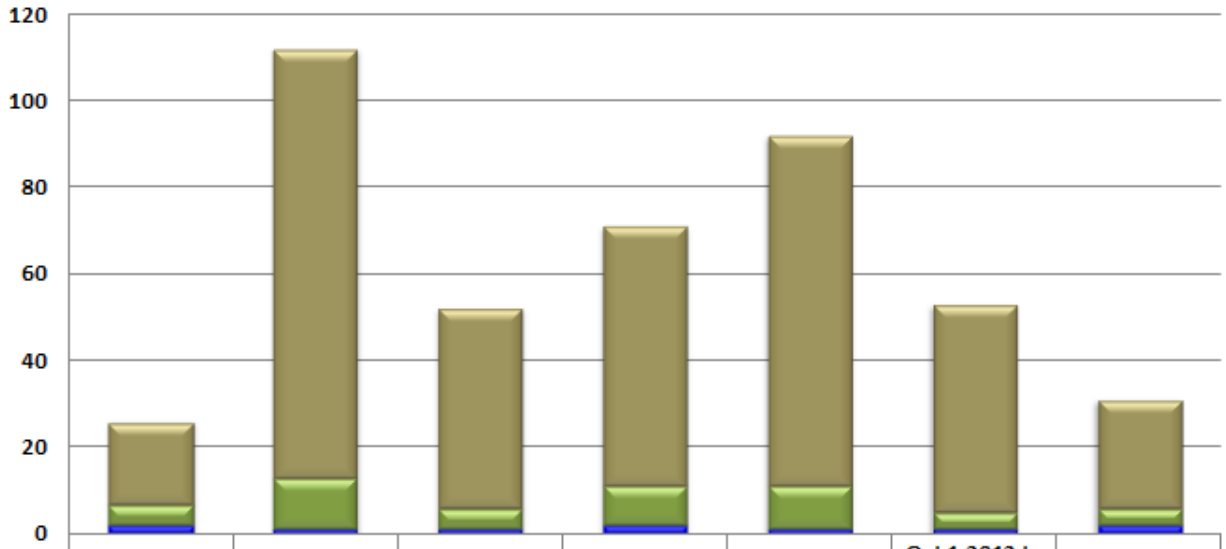
CASL Milestone Statistics

Milestones delivered since CASL start (Jul 2010)



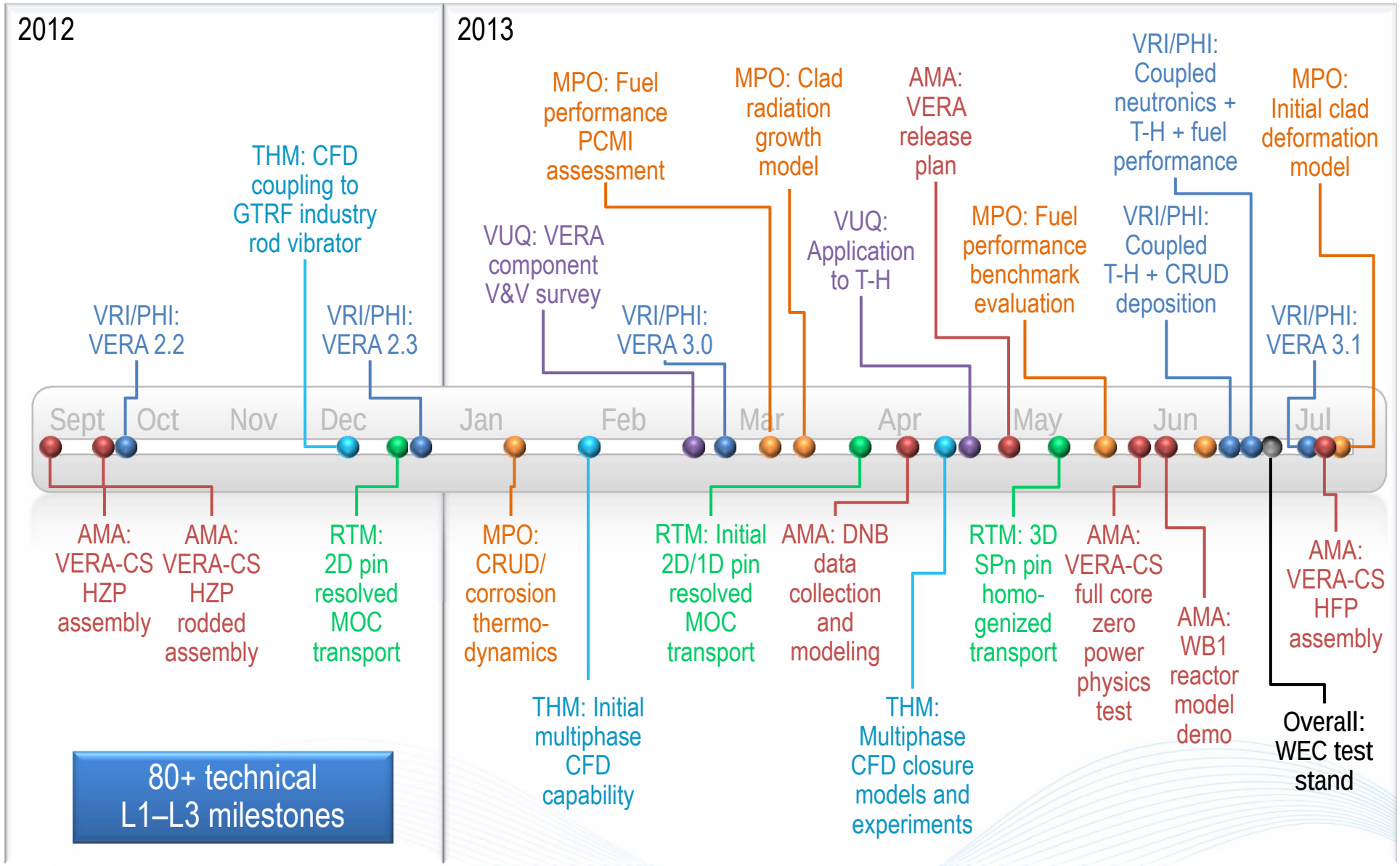
	July 1 to Dec 31 2010 (P1)	Jan 1 to June 30 2011 (P2)	July 1 to Sept 30 2011 (P3)	Oct 1 to Mar 31 2012 (P4)	Apr 1 to Sept 30 2012 (P5)	Oct 1 2012 to Mar 30 2013 (P6)	Apr 1 to Sept 2013 (P7)
L3	19	99	46	60	81	48	25
L2	5	12	5	9	10	4	4
L1	2	1	1	2	1	1	2
total delivered	26	112	52	71	92	53	31

Milestone count: 10 L1s, 49 L2s, 378 L3s

382 milestone documents in the CASL records management system

CASL Consortium for Advanced Simulation of LWRs

Selected Accomplishments (Milestones) in FY13



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Technical Execution in FY13: Summary

Focus Areas

- AMA: WB1 zero power physics test demo; VERA-CS core physics benchmarks; first DNB application; THM early adoption; operational reactor data identification and transfer
- VRI/PHI: Multiple snapshot releases, multi-physics coupling gaining pace; VERA-CS steadily evolving, users growing; responsive subchannel T-H integration and development
- VUQ: VERA component SQA & code verification survey; VUQ applied to T-H; DAKOTA integration into VUQ; identify and prioritize validation data needs; surrogate model & data assimilation methodologies
- RTM: Pin-resolved transport pace lags planned pace but capability promising, pin-homogenized transport delivers, hybrid MC ready for end use, resonance treatment still a challenge
- THM: Novel multi-phase solution algorithm and initial demo realized, coordinated closure model theory & experimental work delivering; meshing analysis illuminating; GTRF application demo
- MPO: Fuel performance model on par with commercial & positioned for new FG/clad models and PCI CP; crud development & CFD coupling continues; revised GTRF modal/beam prototype proving helpful; micro/macro balance achieved

Challenge Problems

- CIPS: Mamba evolution and VERA-CS integration; sub- & full-assembly coupled applications; full core demonstration (target)
- CILC: Mamba/BDM evolution and CFD coupling; sub-assembly coupled application and assessment against plant data (target); enhanced thermochemical understanding & data base
- GTRF: Wear & radiation growth/creep model evolution; CFD turbulent forcing; rod modal/beam prototype & path forward
- PCI: Fuel performance thermal/PCMI models on par with industry standard; initial FG release and VPSC-based cladding deformation models; initial coupling of fuel performance into VERA-CS
- DNB: DNB test data identified and collected; baseline subchannel & CFD assessment on DNB tests; learning of VERA subchannel & CFD tools
- RIA: Validation data identification; VERA-CS neutronics + T-H + fuel performance coupling, transient pin-resolved transport development
- LOCA: Fuel performance development; aligns well with DNB and RIA CPs
- All: CP charters and implementation plans defined and evolving; VERA products defined

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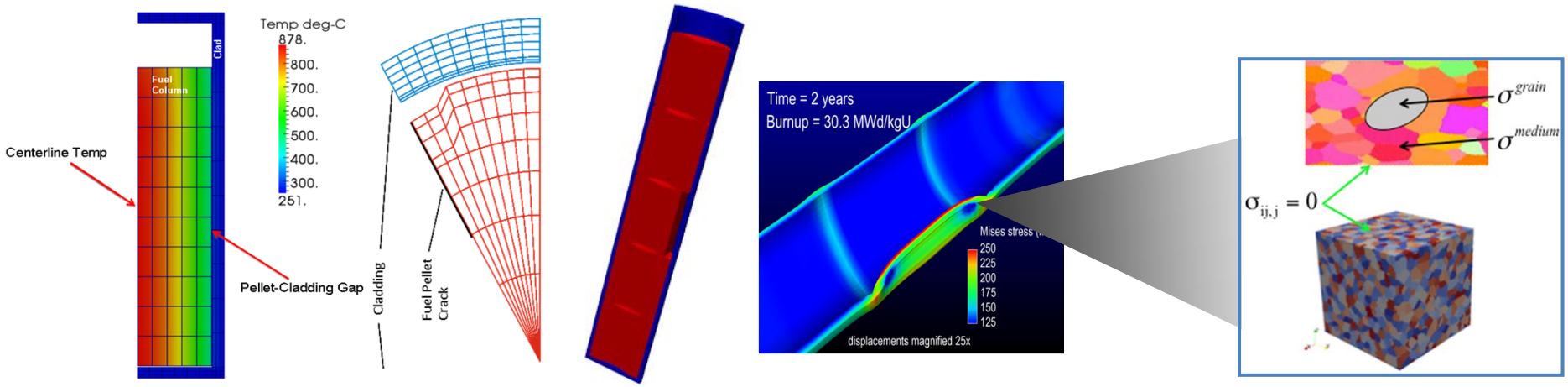
Nuclear Power Reactors

Fuel performance

Terascale	Petascale	Exascale
Limited assessment of fuel pellet cladding interaction	*Capture 3D failure modes for fuel and cladding*	*Virtual test reactor for advanced fuels*
▪ Fuel type and conditions pinned to experimental database	▪ Additional experimental data on 3D effects required	▪ Requires separate effects experiments for validation



▪ 2D finite element analysis of fuel thermo-mechanics ▪ Empirical material property and response models calibrated in 2D to experimental data	▪ 3D finite element analysis ▪ Reformulation of material models calibrated in 2D ▪ Selected upscaling of microscale phenomena (crack propagation, fission product release)	▪ Physics-based fuel performance ▪ Replacement of empirical material property and response models ▪ Expand applicability outside of test database

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What enhanced capabilities over current practices will CASL provide?

Predictive capabilities

- Utilization of more science based models
- Utilization of micro and mesa scale models to increase understanding and provide closure relationships

Phase-space resolution

- Space, time, energy and angle
- Pin-resolved detail

VUQ practices

- Verification & validation
- Data assimilation
- Uncertainty quantification

Computational resource utilization

- Hardware: multiprocessor, multicore & GPUs
- Software: object oriented, I/O standards, third-party software (modern solvers)

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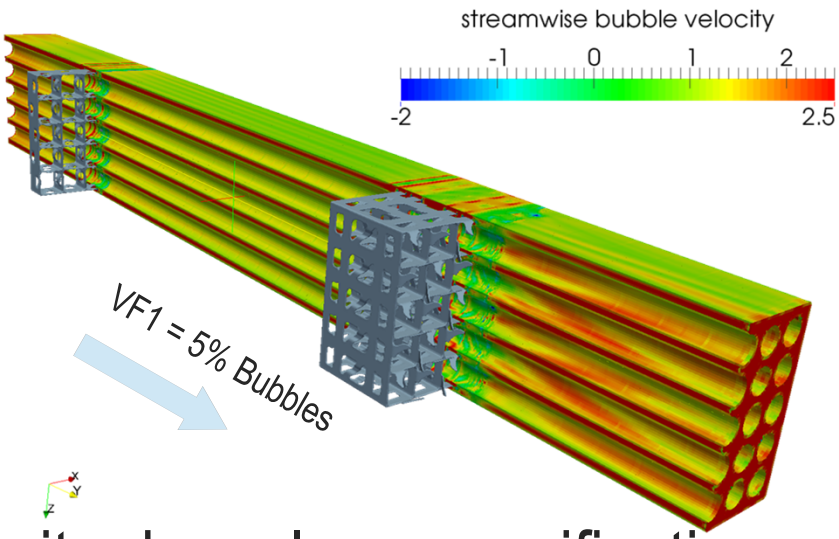
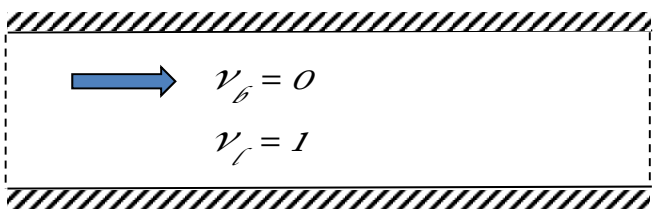
MultiPhase Flow in 5x5 Rod-Bundle



- "Option-1" Calculation w. Drag
- V5H 5x5 Spacer – 14M Cells
- Re=28,000 (TAMU Exp. Cond.)
- 100:1 water/air density ratio

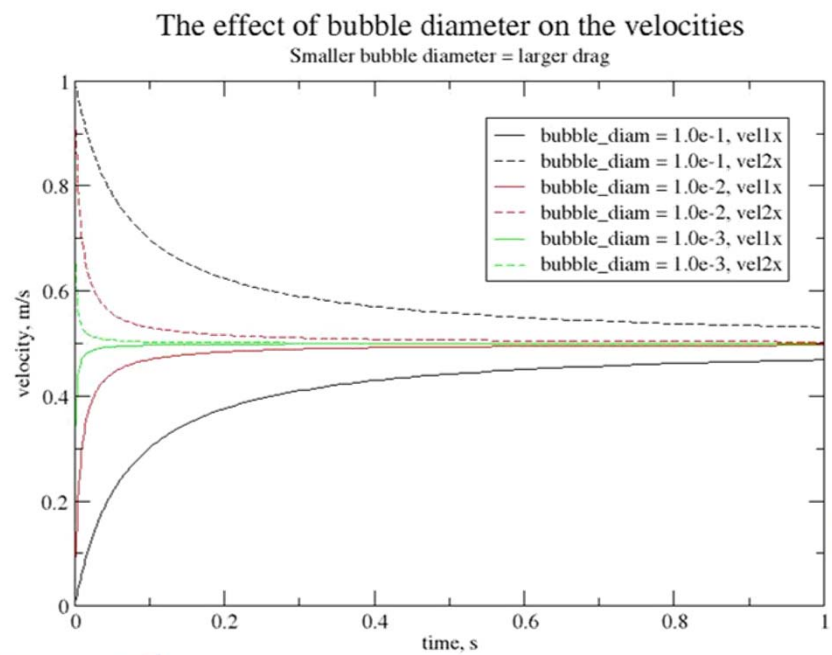
Verifies force anti-symmetry and momentum conservation!!

- In-situ drag closure verification



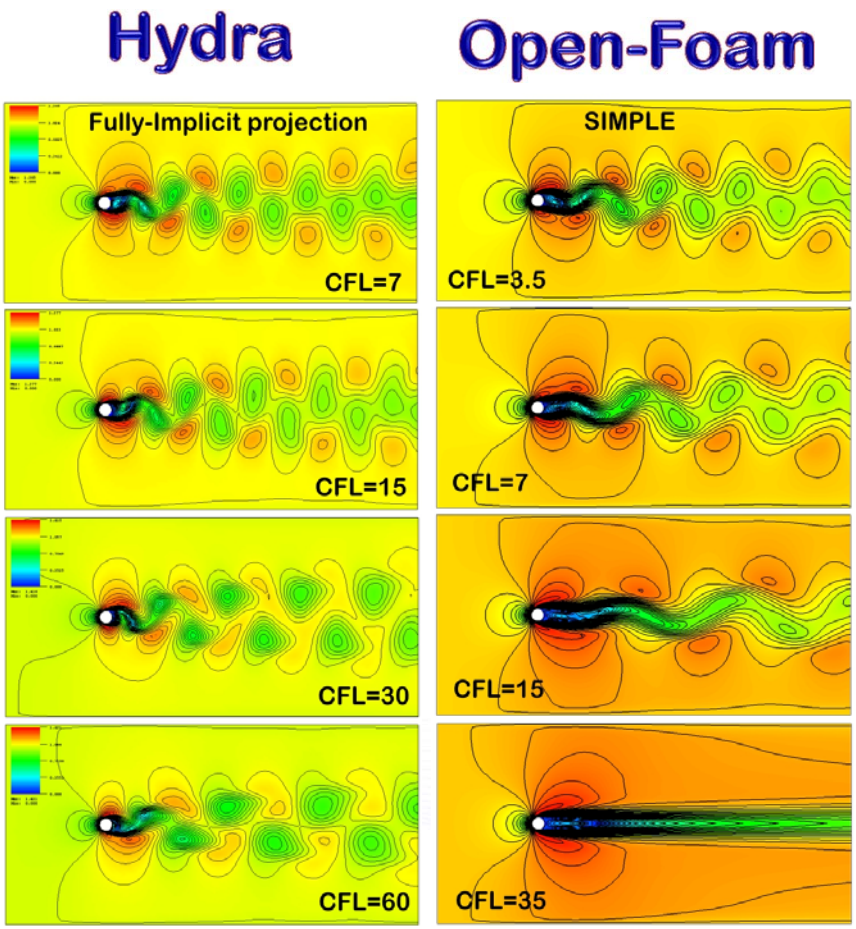
$$\mathcal{F}_D = -\frac{3}{4}\frac{C_D}{D_b}\alpha_f \rho_f \left\| v_b - v_f \right\| \left(v_b - v_f \right)$$

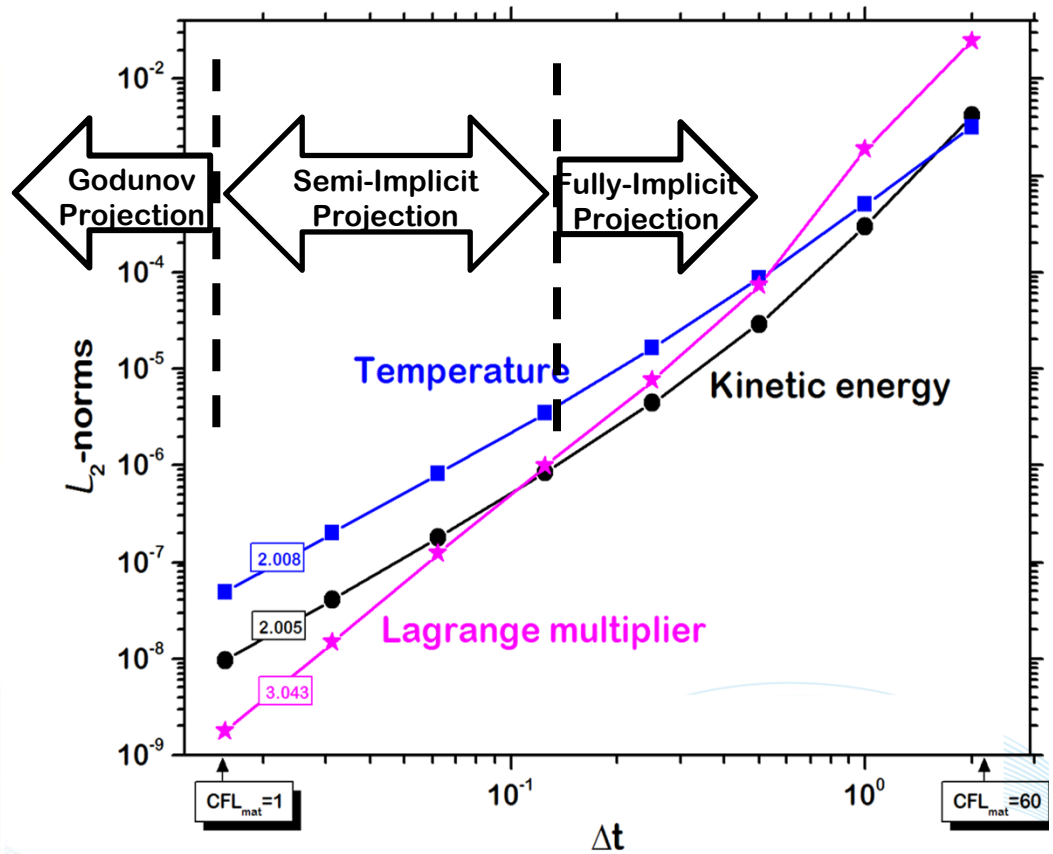
$$C_D = \begin{cases} \frac{24}{Re_b}\left[1 + 0.15\, Re_b^{0.687}\right] & 0 < Re_b \le 1000 \\ 0.44 & Re_b > 1000 \end{cases}$$



Fully-Implicit Algorithms based on Projection Methods

- Projection method acts a physically-based preconditioner providing an approximate factorization of the discrete Navier-Stokes Equations





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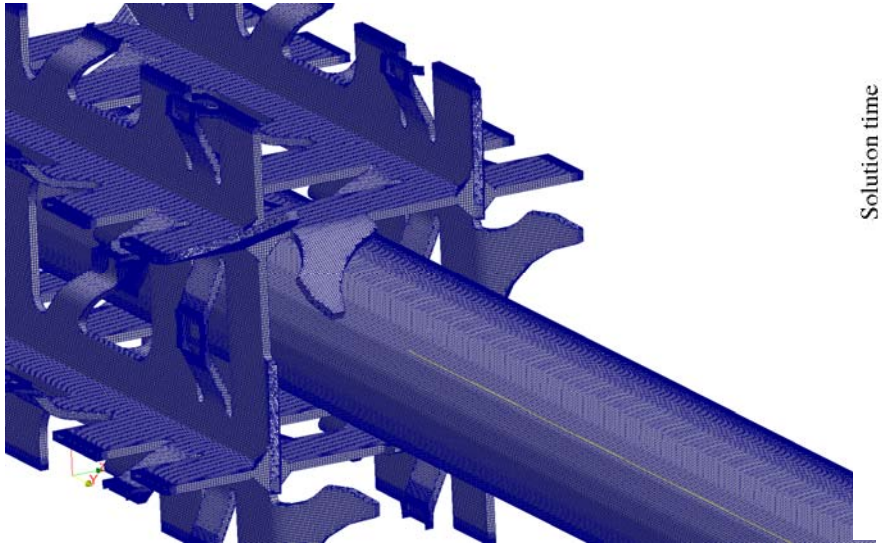
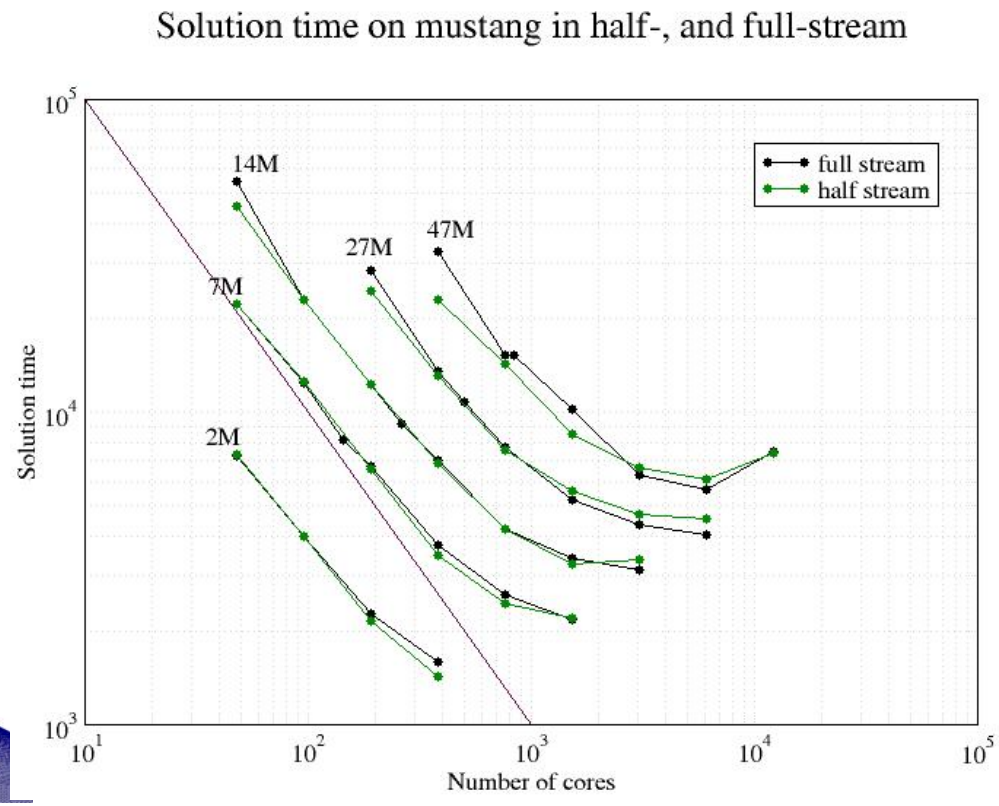
Some performance numbers using the V5H 3x3 rod bundle

- Mustang – AMD 6176 Opteron 24 cores per node





Titan early profiling studies

- 1024 nodes, 8 FP cores ea.
- 1.8 – 3.2% of peak FLOPs rate for AMD's

CASL L3 Milestone: Computational Performance Assessment of Hydra-TH

- *NVIDIA Tesla K20s delivered to LANL & ORNL*
- *Beginning to work with NVAMG library*

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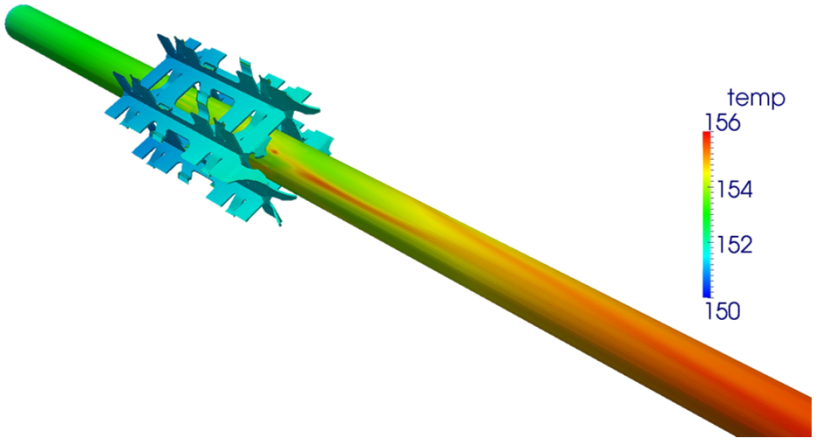
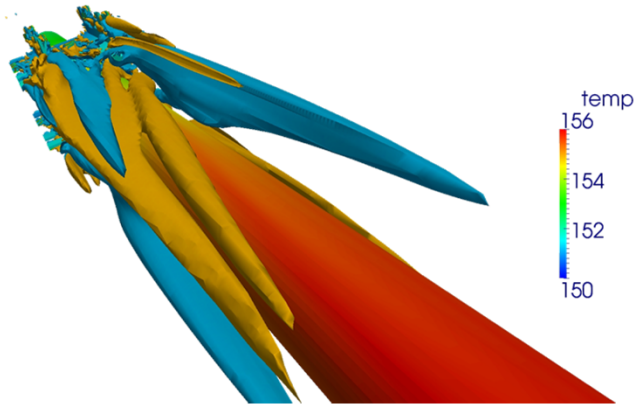
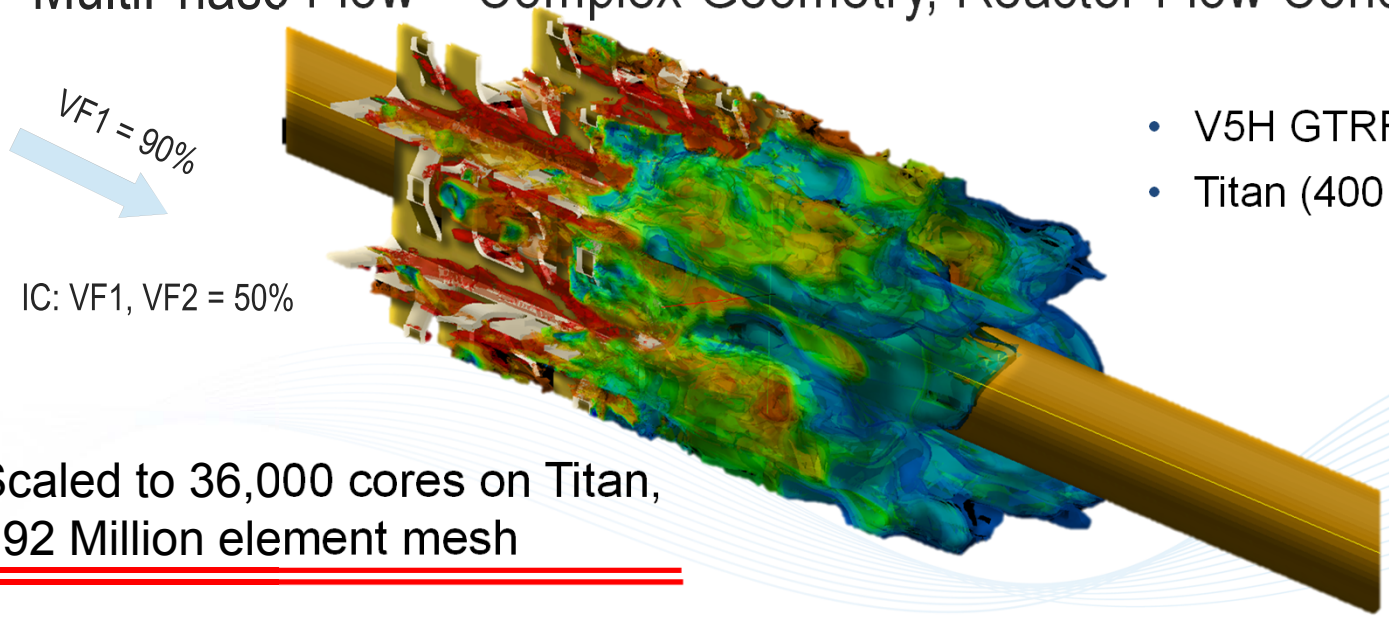
Some Sample Calculations for FY2013/14 Milestones

- Fully-implicit projection, RNG k-e model, Re ~ 4.0×10^5, $q_w = 10^6$ W/m^2
  - 2.4M elements, ~18M DoF, ~ 4.75 hours on 16-core Intel Xeon desktop





- MultiPhase Flow – Complex Geometry, Reactor Flow Conditions



- V5H GTRF 3x3 2M cells
- Titan (400 CPU cores)

Scaled to 36,000 cores on Titan,
192 Million element mesh

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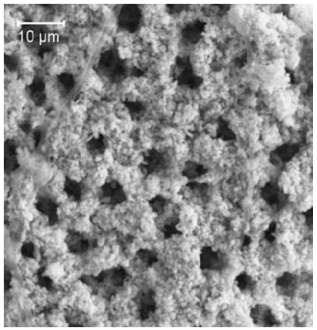
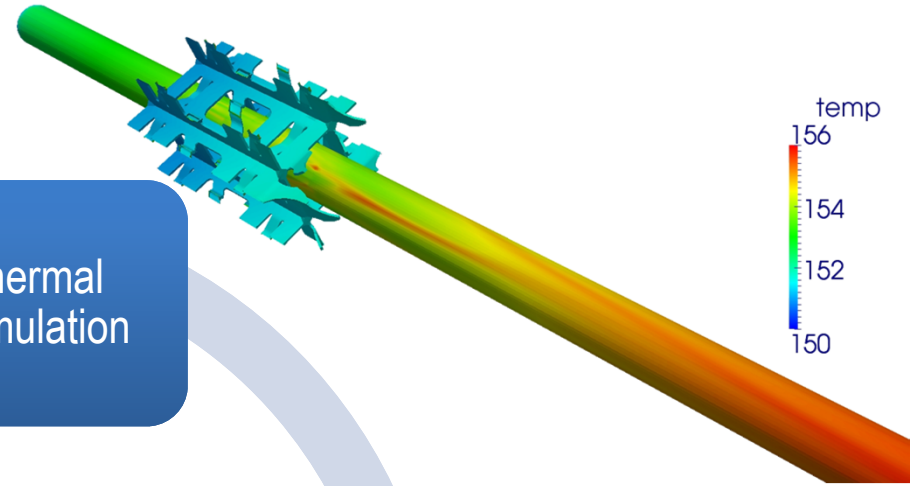
Hydra-TH <-> Mamba Coupling for CRUD Deposition

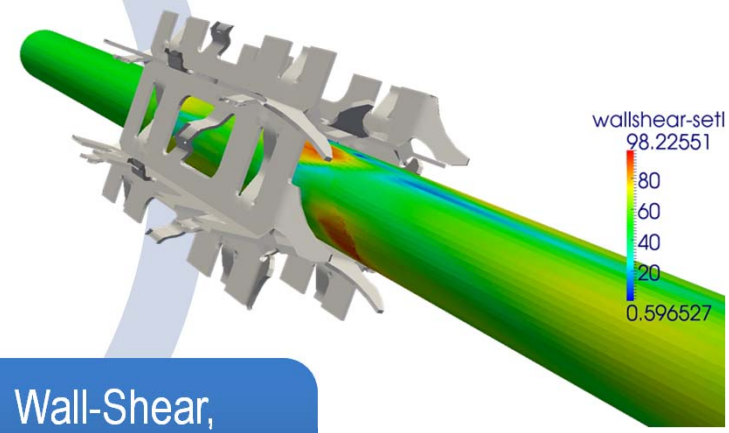


- Local CRUD Chemistry
- Boiling, chimney formation
- CRUD deposition
- Thermal resistance

Hydra-TH Thermal Hydraulics Simulation



- **CRUD Induced Power Shift**
- **CRUD Induced Localized Corrosion**



Wall-Shear, Temperature, Heat Flux

MAMBA Sub-Grid Scale Model

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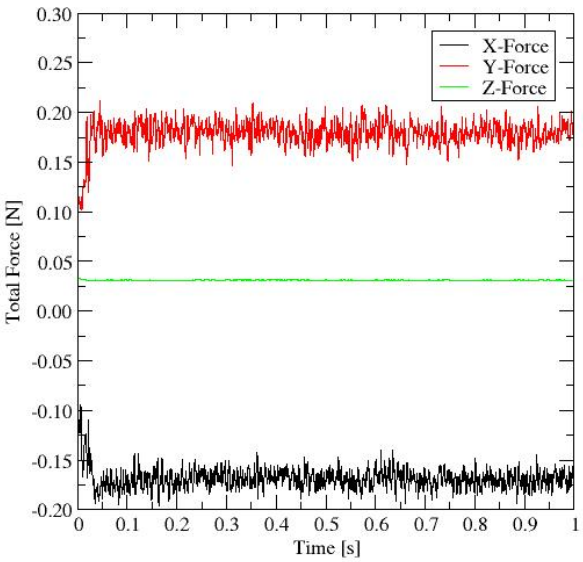
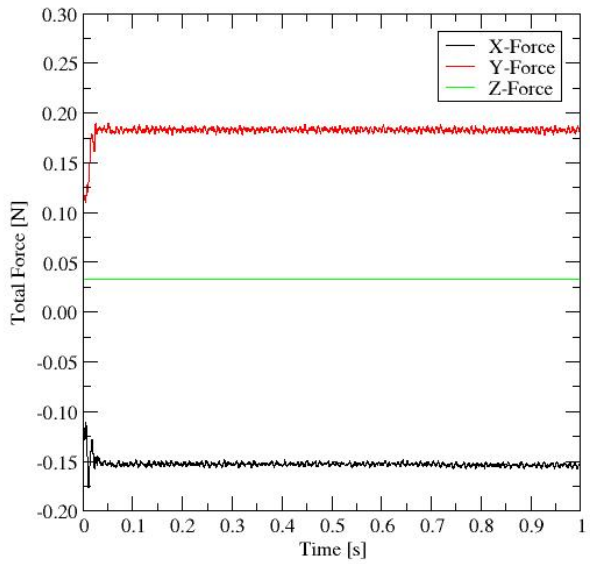
However, current RANS models do not accurately predict the RMS forces

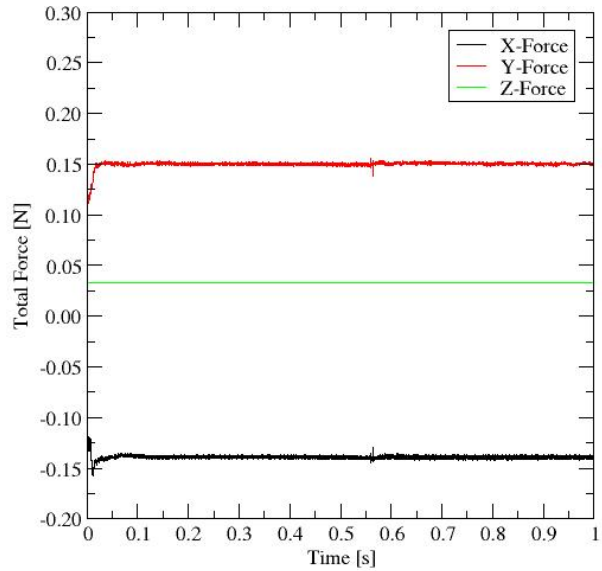
- Spalart-Allmars URANS shows decreased RMS and Mean forces
- DES may require better boundary layer meshes to achieve larger RMS forces



Implicit
Large-Eddy Simulation



Detached-Eddy
Simulation



Spalart-Allmaras
RANS

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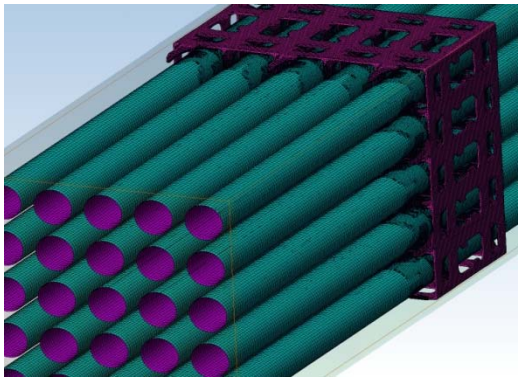
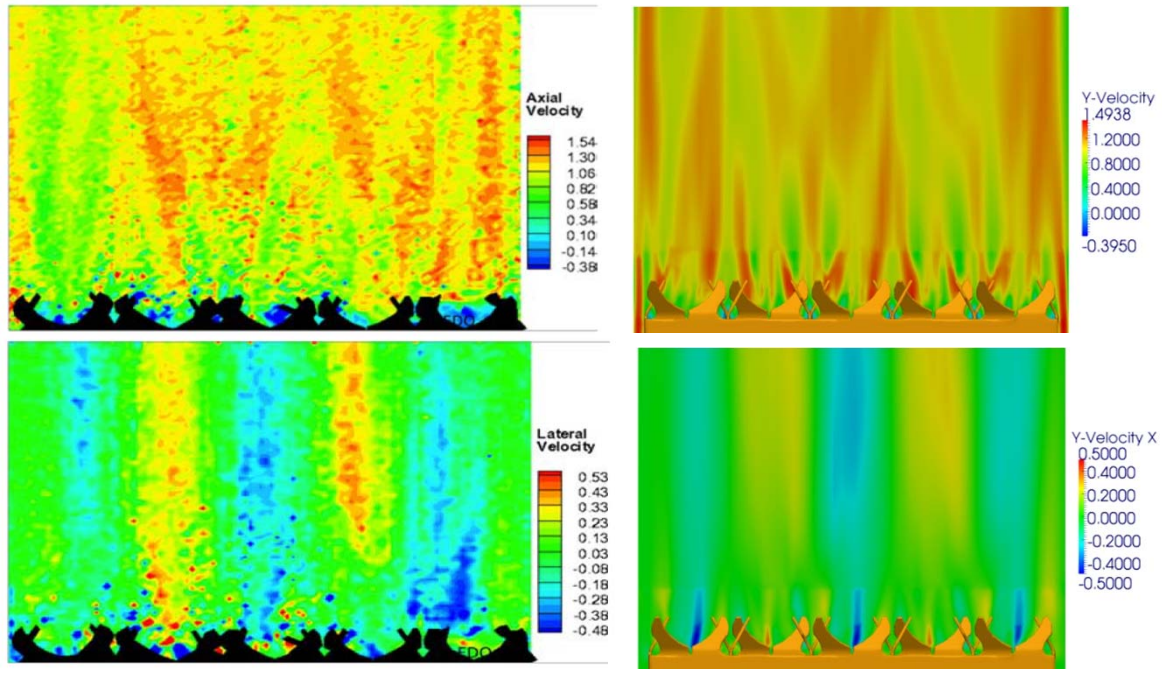
5x5 V5H study shows good agreement with experimental data



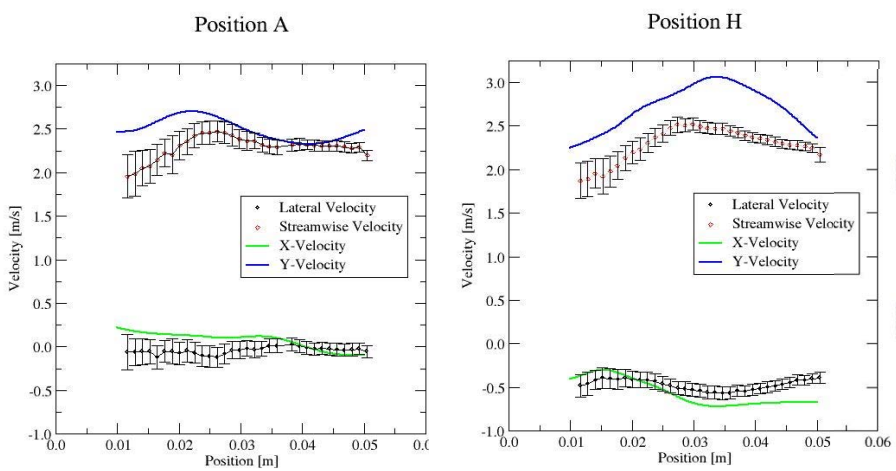
- Predicted mean peak velocities within 5% of experiments

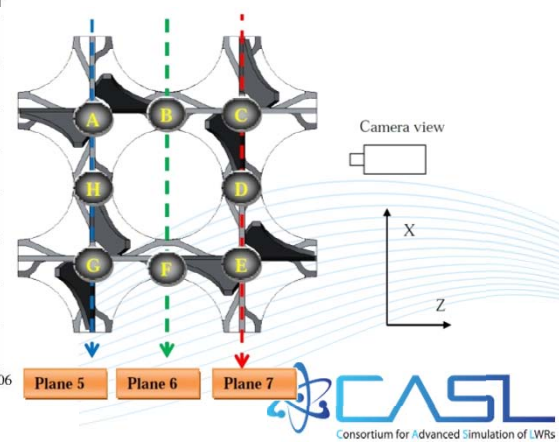


Texas A&M experiments

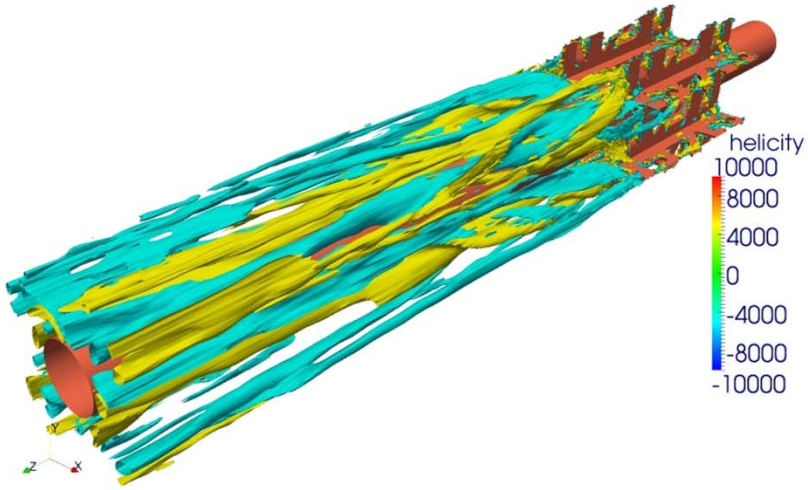
Hydra-TH calculations

- Time-averaged velocity profiles downstream of mixing vanes (96M mesh)

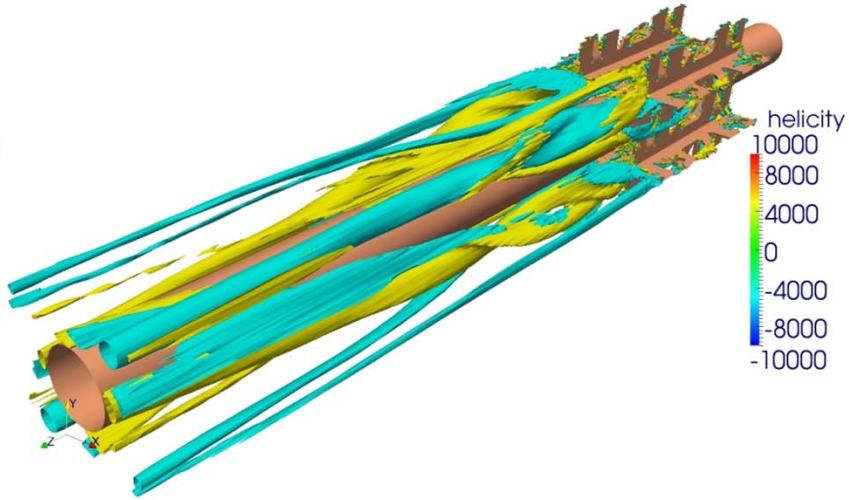




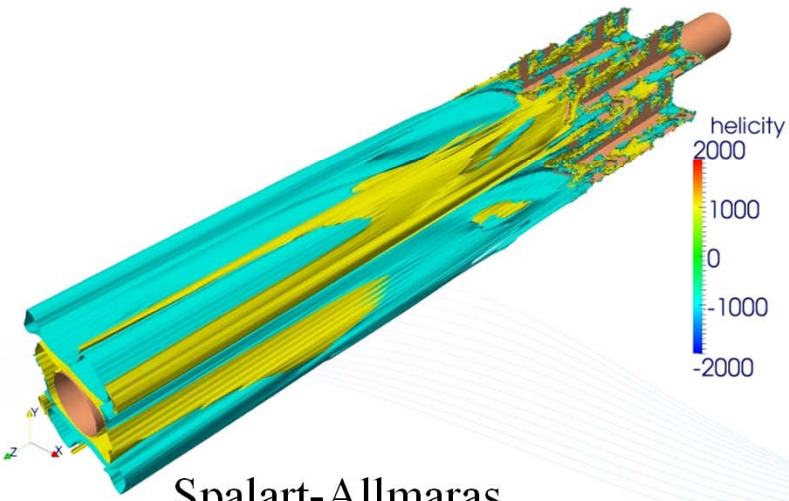
The ILES, DES and Spalart-Allmaras models capture the swirl to some degree …



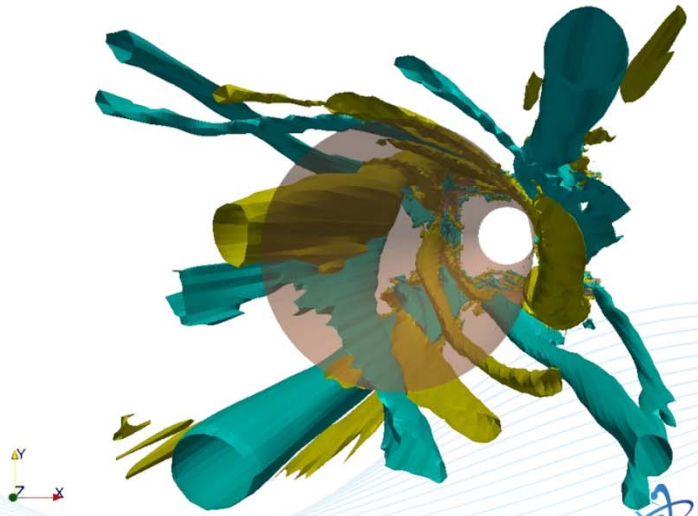
ILES



DES



Spalart-Allmaras



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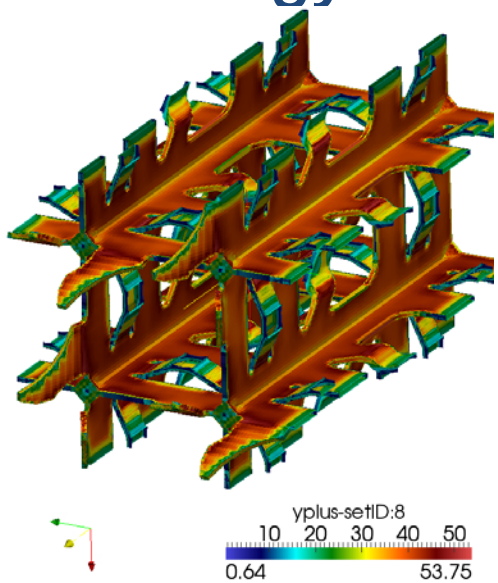
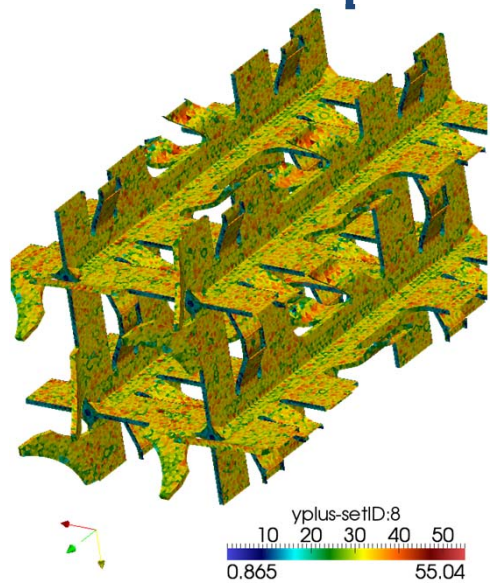
A Quantitative "A Priori" Mesh Assessment Methodology has been Developed for GTRF



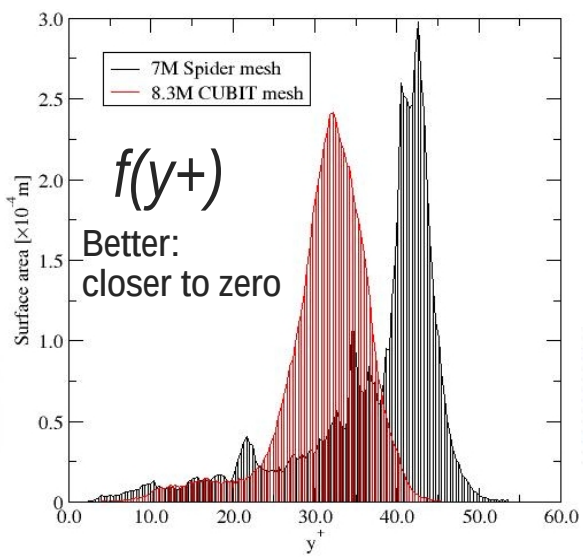
y+ 7M Spider mesh

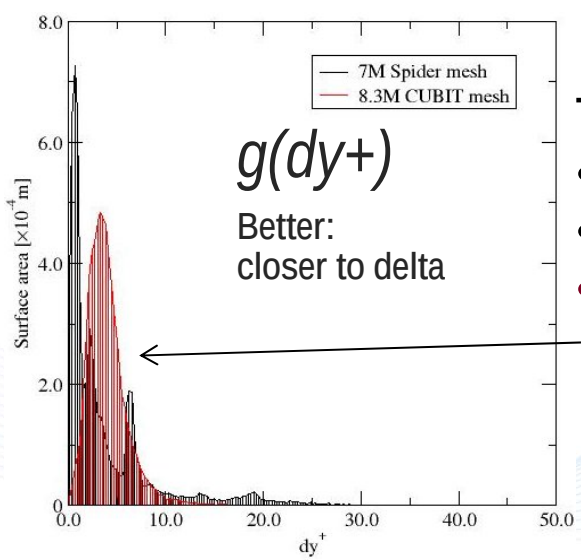


y+ 8.3M Cubit mesh

$$y^+ = \frac{y}{\nu}\sqrt{\frac{\tau_w}{\rho}}$$

- *How well is the boundary layer resolved?*
- *How good is the mesh quality at walls?*





Total Variation Metric

- Cubit spike shifted to right
- Poor uniformity near walls
- May lead to unphysically perturbed boundary layers

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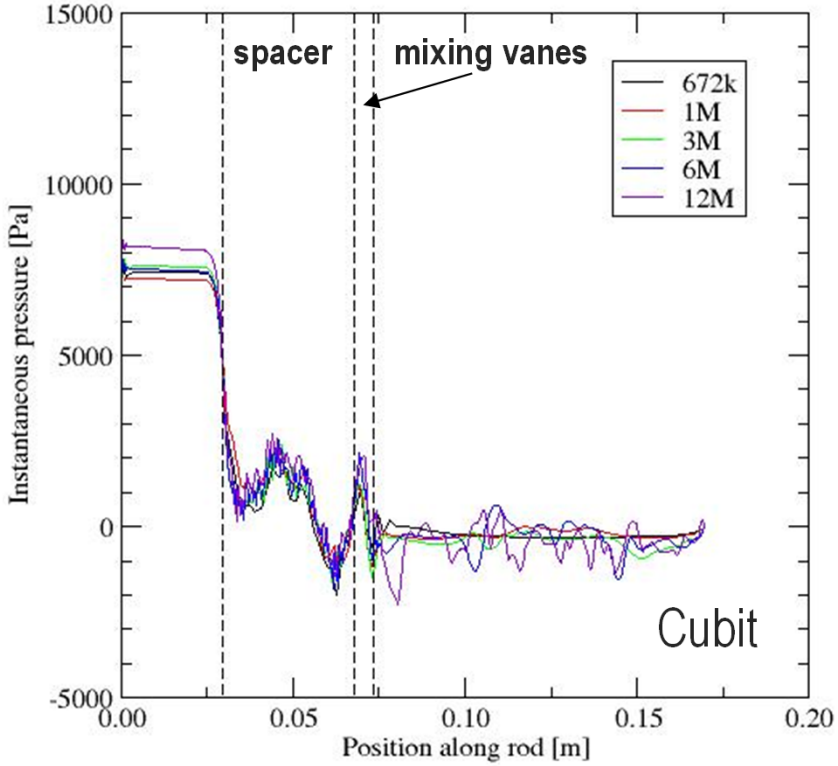
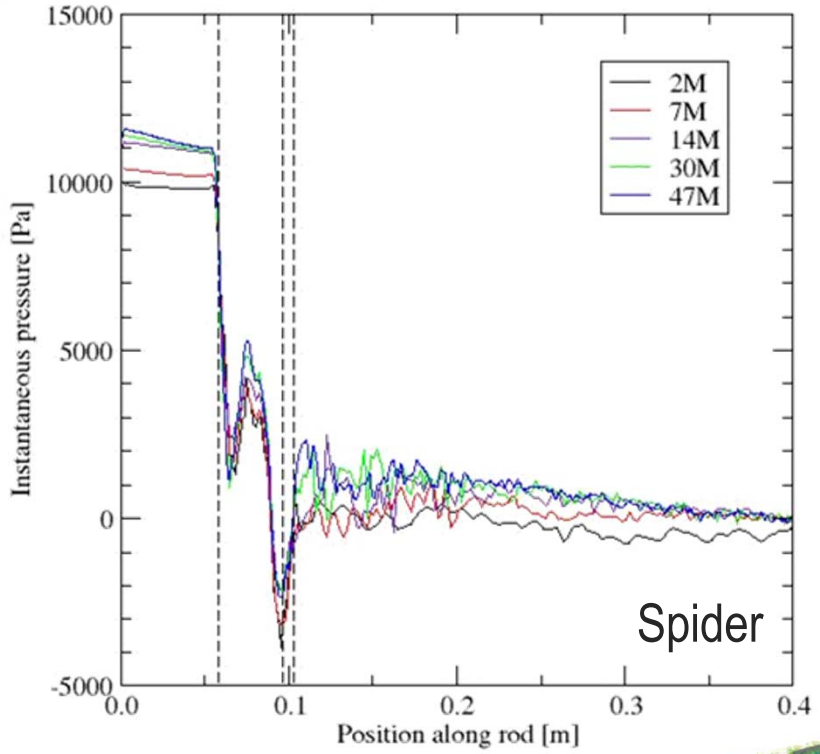
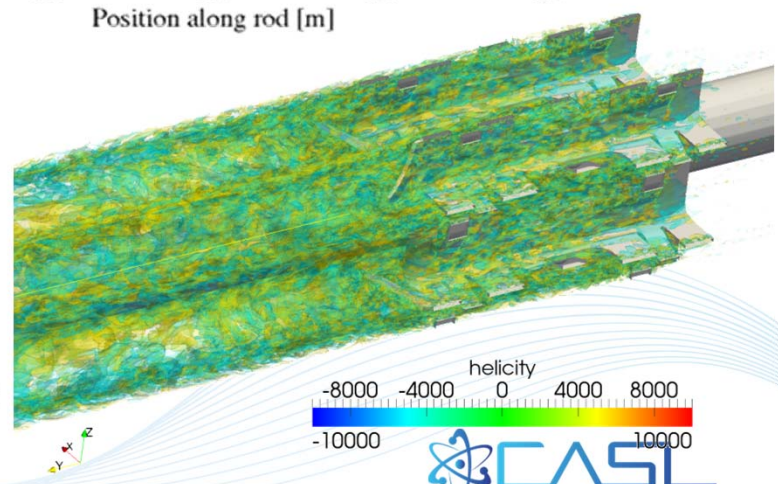
Main findings based on the 3x3 rod bundle

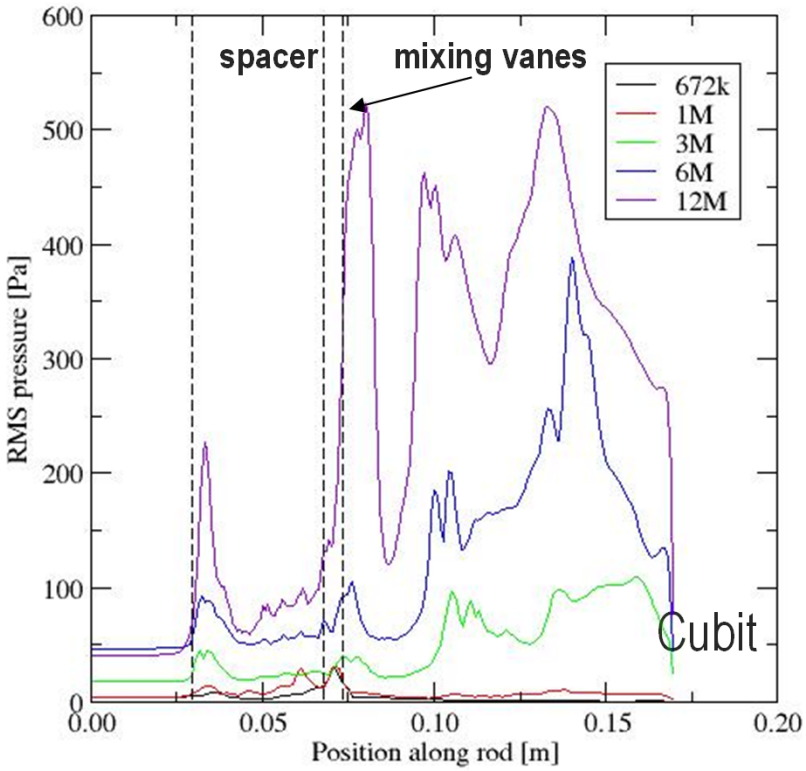


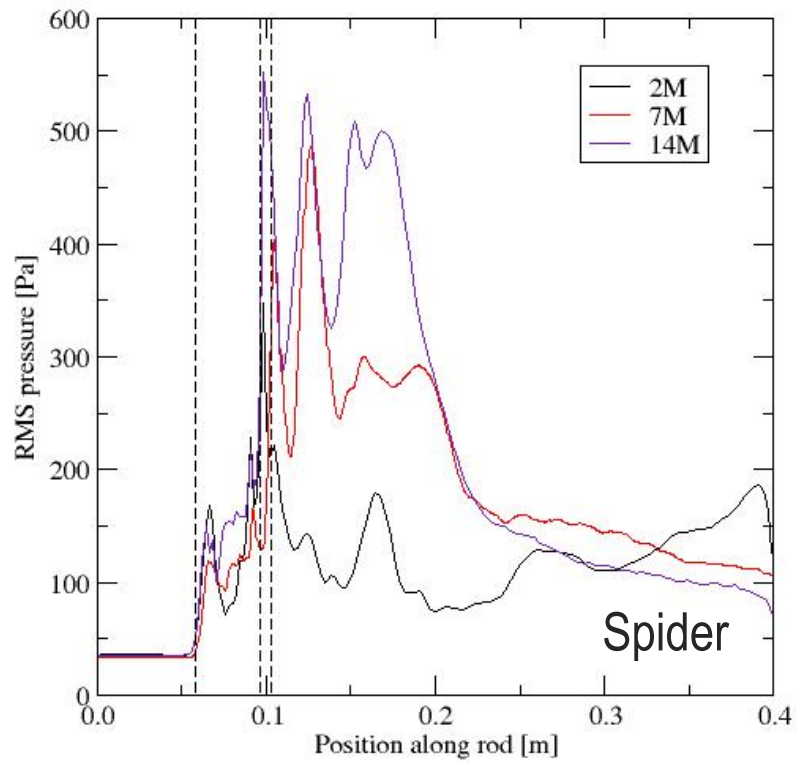


- Pressure profiles significantly different between Spider and Cubit
  - Different mesh generation technology
  - ~50% shorter domain length for Cubit meshes
  - Inadequate wall mesh resolution for Cubit meshes
  - Lack of pressure drop at inlet for Cubit meshes



Main findings based on 3x3 – RMS Pressures





- RMS pressure profiles significantly different between Spider and Cubit
  - TKE (and RMS pressure) should peak at mixing vanes
  - Cubit RMS pressures peak far downstream, and increase with refinement
  - Coarsest Spider mesh (2M) also presents a non-physical pressure variance

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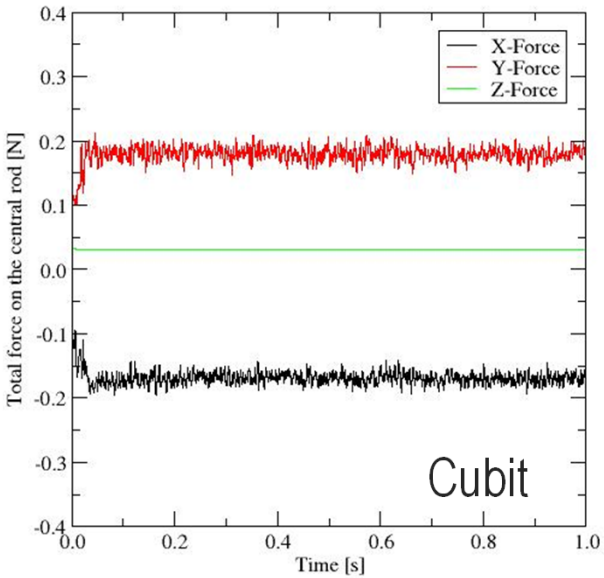
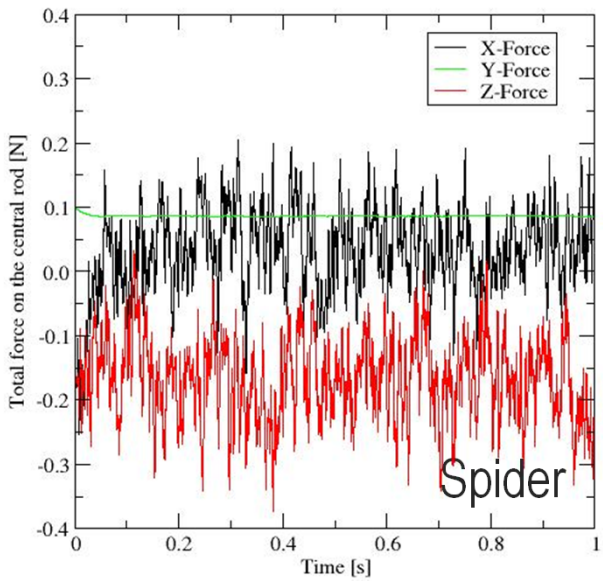
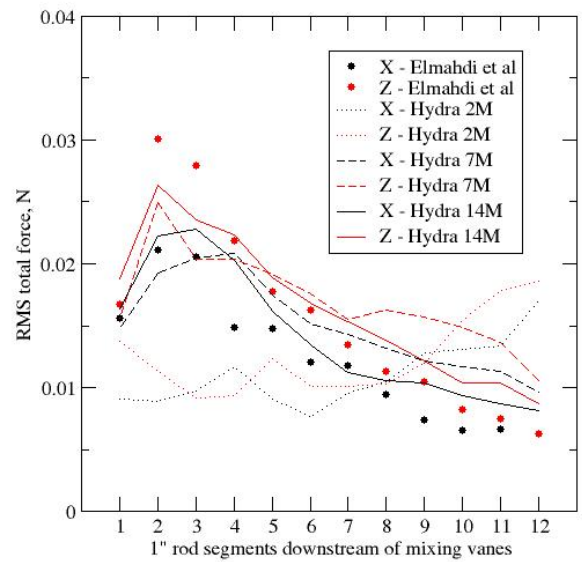
Main findings based on 3x3 – Rod Forces







- RMS forces differ by an order of magnitude between Spider and Cubit
  - Increased force amplitudes appear to be due to better wall-resolution
  - 14M force distribution along the rod agrees well with STAR-CCM+ results despite 3X coarser mesh
  - 2M force distribution displays pathological behavior associated with under-resolved LES as indicated previously by RMS pressures

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Gen-1: Robust Baseline Closure

- Leverage extraordinary experience at RPI
- Evaluate a reference closure without code effect
- Provide a GEN-1 closure for Hydra-TH
- Testing in STAR-CCM+ for immediate accessibility and platform independent evaluation

RPI MODEL

BUBBLE FORCES

Drag force

(1) $\vec{F_D} = -\frac{3}{4}\frac{C_D}{D_b}\alpha\rho_l|\vec{u}_v - \vec{u}_l|(\vec{u}_v - \vec{u}_l)$ — Eq. (1) in Ref. [1]; Eq. (4) in Ref. [2]

(2) $C_D = \frac{24}{Re_b}\left(1 + 0.092Re_b^{0.78}\right)$ — Eq. (2) in Ref. [1]

(3) — Eq. (5) in Ref. [2]

(4) $C_D = \frac{24}{Re_b}(1 + 0.1Re_b)^{0.75}$ — Slide (9) in Ref. [3]

(5) $Re_b = \frac{\rho_l|\vec{u}_v - \vec{u}_l|D_b}{\mu_b}$ — Eq. (3) in Ref. [1]

(6) $F_D = -\frac{3}{4}\frac{C_D}{d_b}\alpha\rho_l u_r^2$ — Slide (4) in Ref. [3]

Lift force

(7) $\vec{F_L} = -C_L\alpha\rho_l|\vec{u}_v - \vec{u}_l| \times (\vec{\nabla} \times \vec{u}_l)$ — Eq. (5) in Ref. [1]

with $C_L = 0.03$ — Ref. [3]

The lift force is acting in the axial direction and takes the form:

(8) $F_L = -C_L\alpha\rho_l u_r \frac{du_r}{dr}$ — Slide (5) in Ref. [3]

Turbulent dispersion force

(9) $\vec{F}_{TD} = -C_{TD}\alpha\rho_l\bar{\bar{k}}_l\nabla\alpha$ — Eq. (6) in Ref. [1]

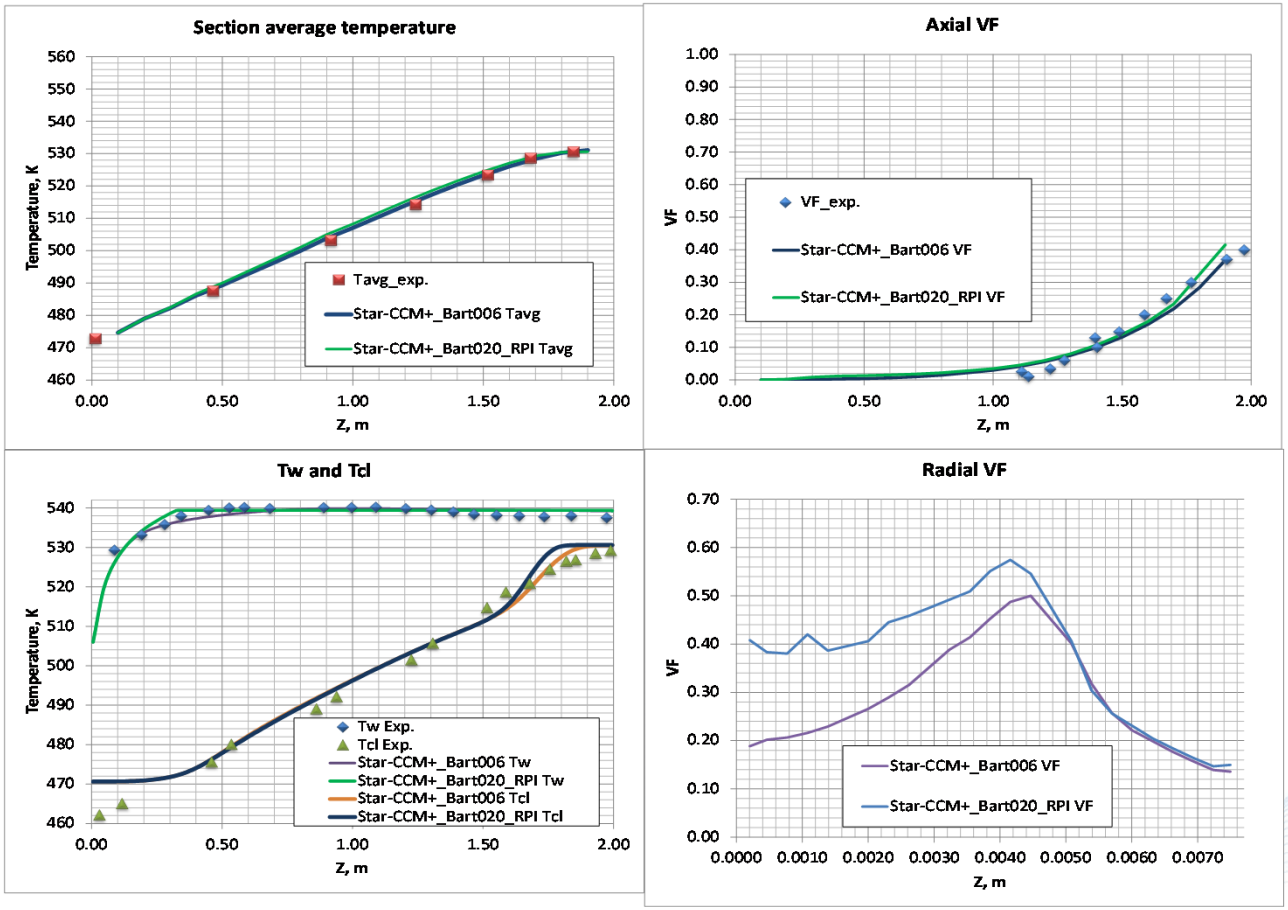
The turbulent dispersion force is acting in the radial direction. After some manipulations, it becomes:

(10) $F_{TD} = -C_{TD}\alpha\rho_l\frac{d}{dr}[k(1-\alpha)]$ — Slide (5) in Ref. [3]

Gen-1: Robust Baseline Closure

Delivery and preliminary testing (implementation in STAR-CCM+)

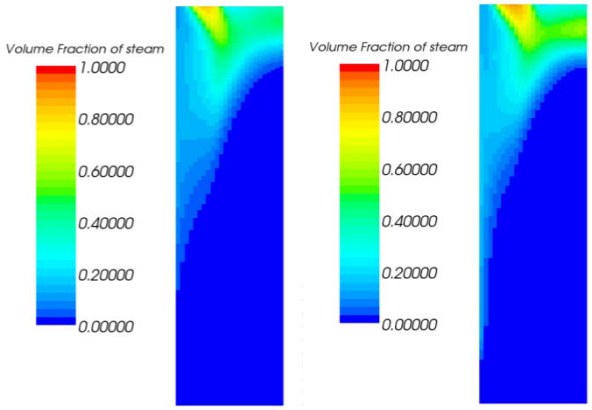
- Comparisons show that the two model perform equally well.
- The only significant difference is observed in the radial void fraction distribution, for which (unfortunately!) no experimental data are available.
- The wall temperature seems to be only affected by the bubble nucleation site density model (confirming expected behavior)



run Bart006 = STAR-CCM+ reference model

Run Bart020_RPI = CASL GEN-I Model

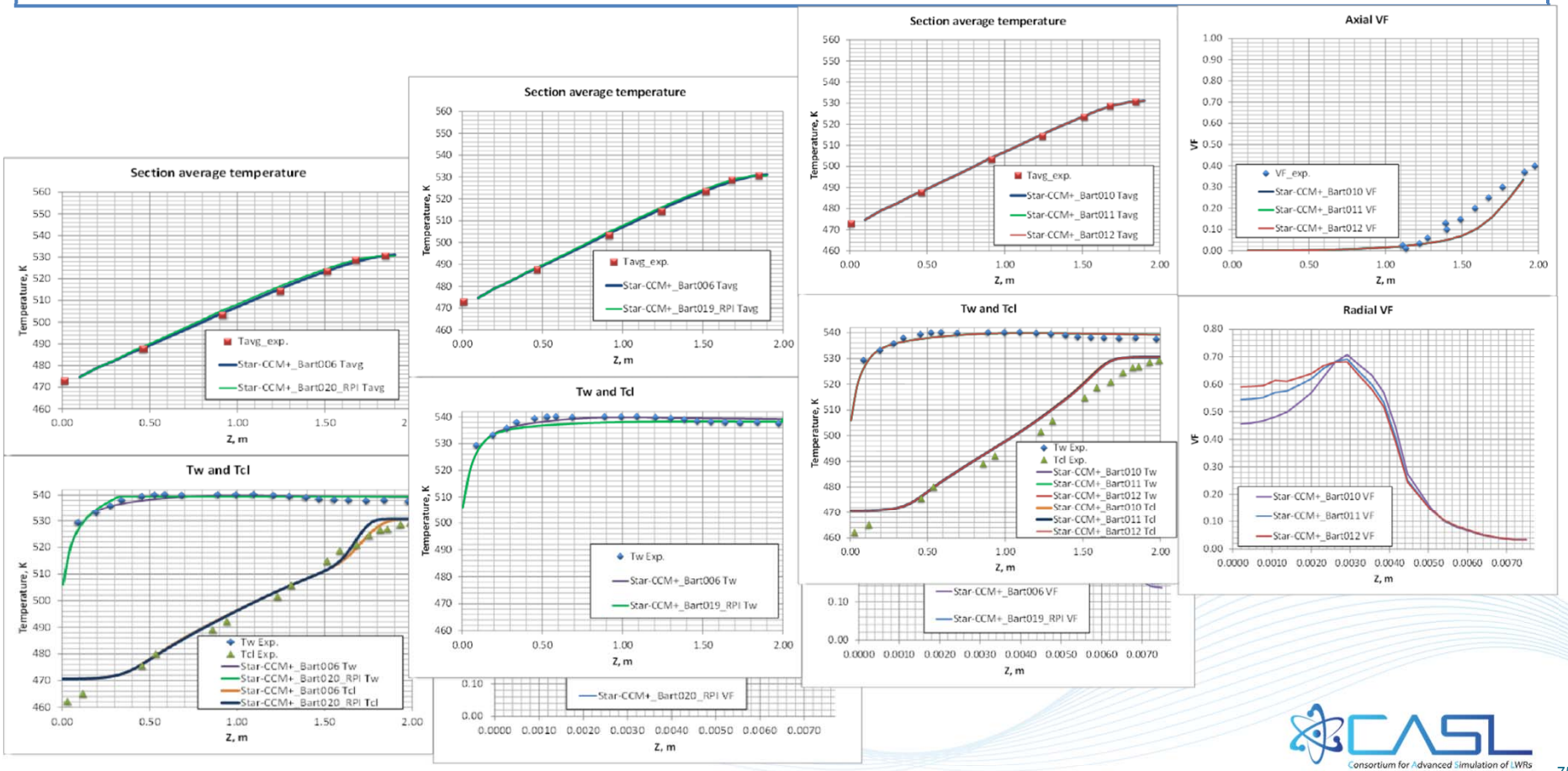
Reference model **CASL GEN-I**



Gen-1: Robust Baseline Closure

Sensitivity Analysis

- Confirms the findings from PoR-3 V&V Study (Fidkowski)
- Bubble departure diameter and Nucleation Site density correlaction drive the Wall temperature effect
- Hydrodynamic closure has limited effect on wall temperatures, but more understanding necessary for regions of void accumulation



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GEN-2: Advanced CASL Closure
Brief version of an extensive effort

Specific Model Components

- Redesigned Partitioning Heat Flux Model
- Built-in DNB capturing approach

Sharable Model Components

- Improved Mechanistic Departure Diameter and frequency
- Hardened Hydrodynamics Closure
- Condensation

Coming up

- Interfacial Area Quantification

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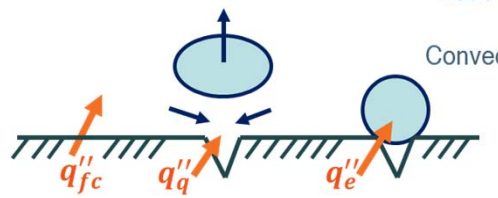
GEN-2: Advanced CASL Closure
New Physics Based Heat Partitioning

$$q''_{tot} = q''_{fc} + q''_q + q''_e$$

Convective Quenching Evaporation



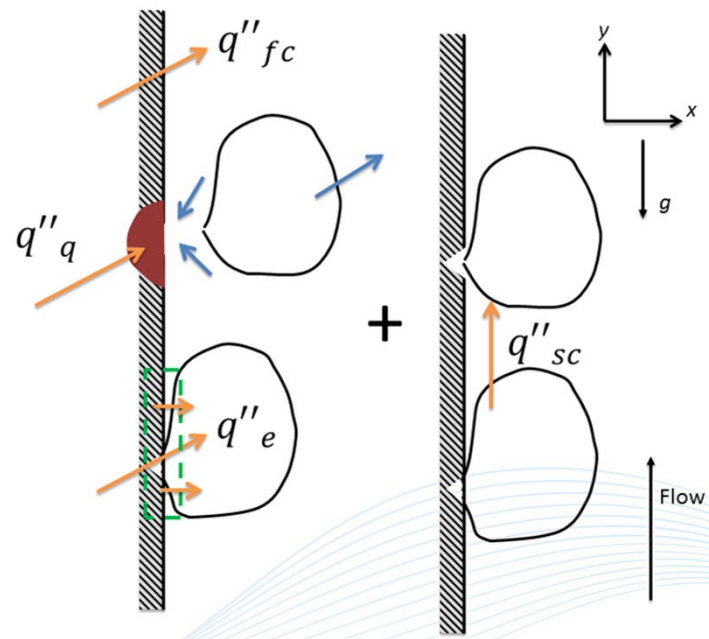
Classic RPI Approach

- Flexible model
- Proven application record

So why a new model? (start addressing Nam's fundamental question: "how do we use all these experimental findings?")

- There are a few too many components but listing some fundamental ones:
- Increased synergy with experimental "micro" measurements
- Extended applicability (lower/ higher vapor generation)
- Include modeling toward limiting behavior (CHF)

$$q''_{tot} = q''_{fc} + q''_e + q''_q + q''_{sc}$$



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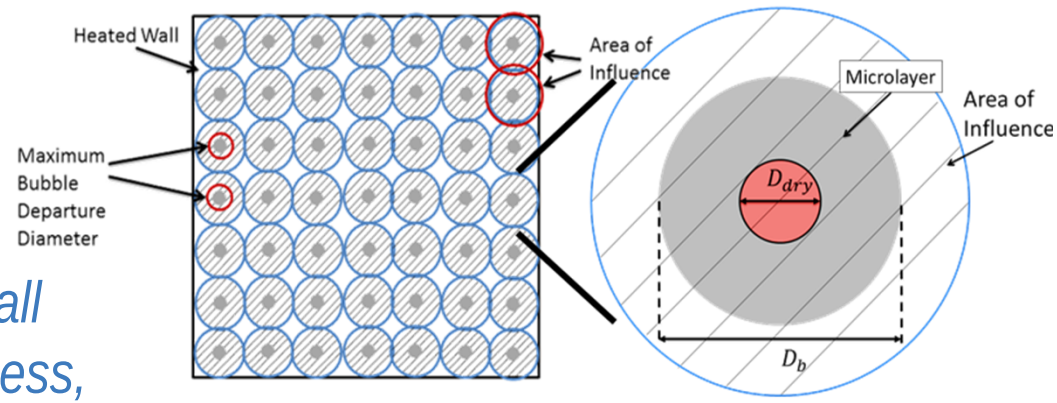
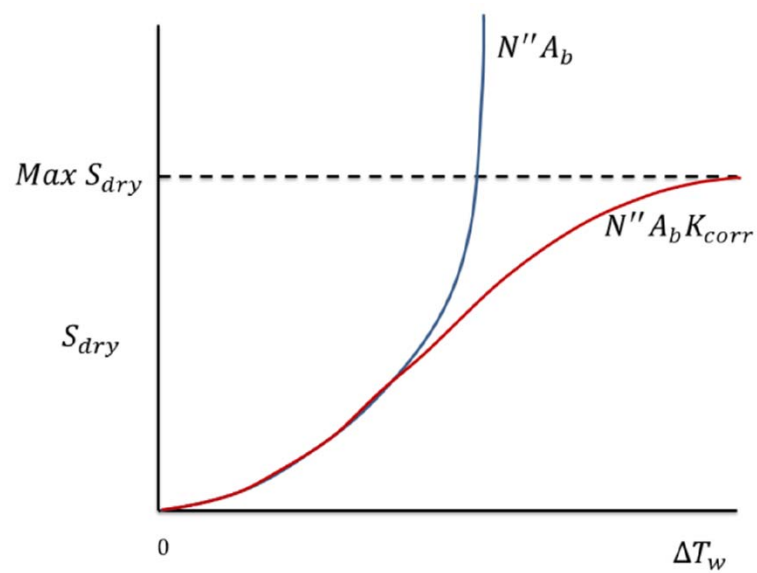
GEN-2: Advanced CASL Closure
Developments towards High Heat Flux/DNB



Key features:

- Includes Fundamental Physical Description: *dry-wetted surface, bubble crowding, bubble sliding, wall quenching, bubble induced roughness, surface conditions (corrosion, CRUD)*
- Includes physics based limiting behavior (eliminates the need for experienced based limiters)
- Synergy with experimental measurements allows validation of separate modeling components
- DNB can be expressed as the limit of dry surface area

- ***Allows tracking physical limits***



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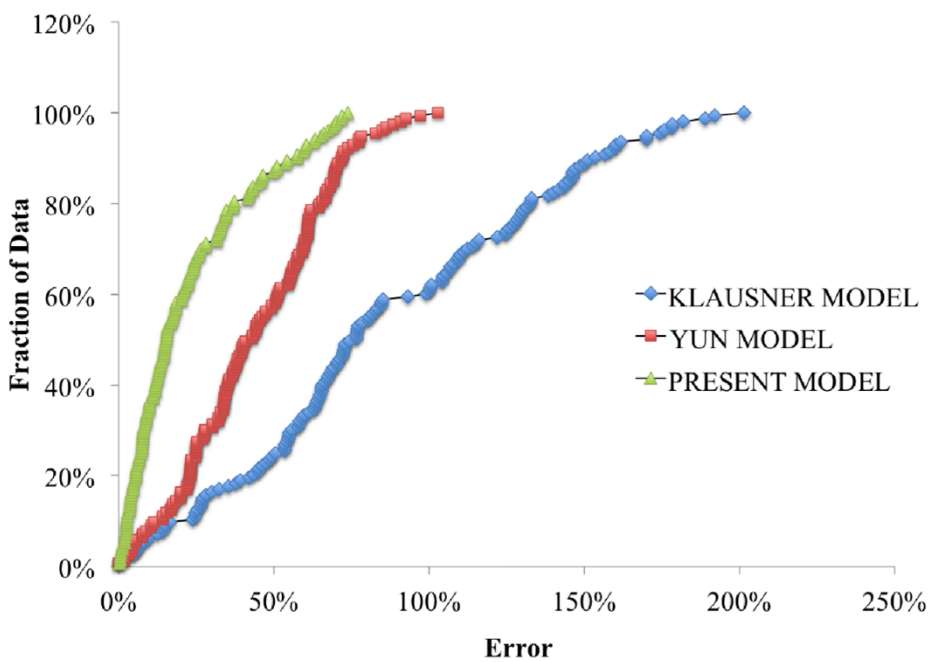
GEN-2: Advanced CASL Closure

Shared Model Components

Key example:

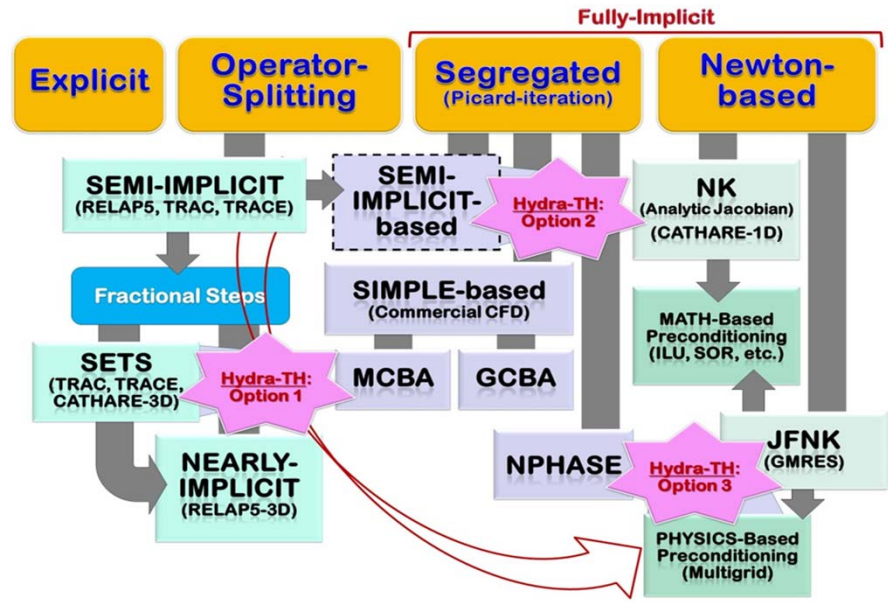
- Advanced Mechanistic Bubble Departure Model (à la Klausner)
- Includes new MIT database Dd
- Considerably improved model performance




```
/*****************************************************************************
**
 * userBubbleDiameter(bubbleVolumeFraction).
*****************************************************************************
/

void userBubbleDiameter(
  Real*        result,
  int          size,
  CoordReal*   SurfaceTensionPhaseInteraction,
  Real*        DensityLiquid,
  Real*        DensityVapor,
  CoordReal*   DynamicViscosityLiquid,
  CoordReal*   UstarLiquid,
  CoordReal*   Alpha,
  CoordReal*   SpecificHeatLiquid,
 // CoordReal* ThermalDiffusivity,
  CoordReal*   BoundaryHeatFluxLiquid,
  CoordReal*   Beta,
  CoordReal*   theta,
  CoordReal*   ThermalConductivityLiquid,
  //CoordReal* Tau_wall,
  CoordReal*   TemperatureLiquid,
  CoordReal*   TemperaturePhaseInteraction,
  CoordReal*   LatentHeatPhaseInteraction

) {

  /* [0] declarations */
// Defining Constants in the Bubble Departure Model //

// Surface Tension Force //

double pi       =       3.1416;                 // Defining the constant pi; This may already be
defined in C by using
//double alpha   = 90.63*(pi/180);  // Advancing contact angle in Rosie's Experiment [rad] //
//double beta =          8.03*(pi/180); // Receding contact angle in Rosie's Experiment [rad] //

// Buoyancy Force //

double g =              9.81; // Gravitational Constant [m/s^2] //
double v_l =            0.4174;          // Bulk Fluid Velocity [m/s] //


// Quasi-Steady Drag Force //

double Kappa = 0.4;   // Constant provided by Klausner //
double Chi =   11;       // Constant Provided by Klausner //
double c =              7.4;  // Constant Provided by Klausner //
double n =              0.65; // Constant Provided by Klausner //

// Unsteady Force //

double b = 1.56;         // Constant provided by Zuber //
int          s = 2;          // Constant Provided by Yun //
double phi = pi/18; // Inclination angle of the growing bubble; Provided by Klausner //
double C_s = 1;                  // Variable constant in the model; Yun uses C_s=1 //

  /* [1] record user model activation and run parameters */
```

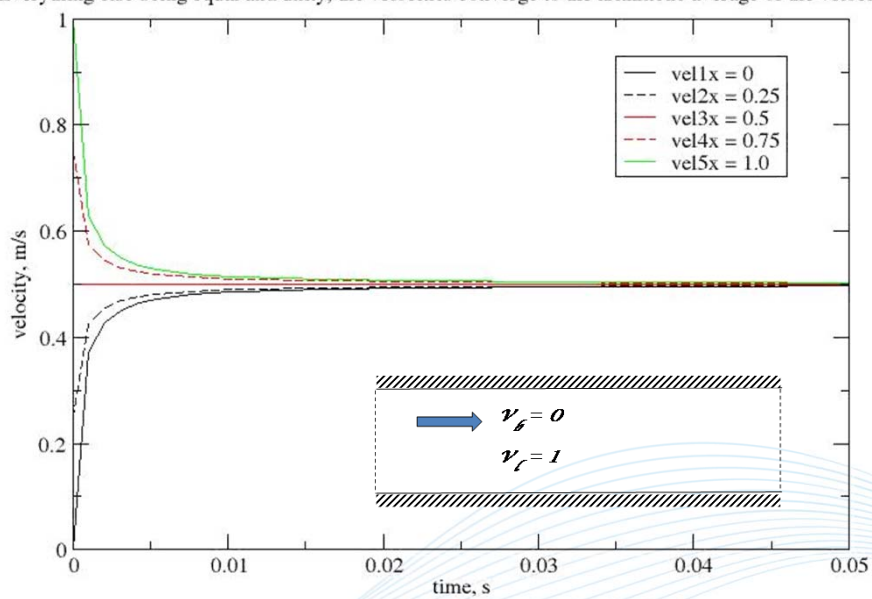
New M-CFD Platform
Robust Algorithms

- Multi-stage implementation of multiphase solution algorithms
- Inelastic formulation ($\nabla \cdot \rho v = 0$) that admits weak compressibility in the overall multiphase mixture, e.g., compressibility due to the presence of bubbles
- This algorithm admits the treatment of large density differences, e.g., 1000:1 for water and air, while retaining a simple form of the pressure-Poisson equation.
- Fully-Coupled Momentum Exchange critical to faithfully simulating the physics involved in multiphase flow.



Drag force among 5 fields with different but constant volume fractions (0.2)

Everything else being equal and unity, the velocities converge to the arithmetic average of the velocity ICs



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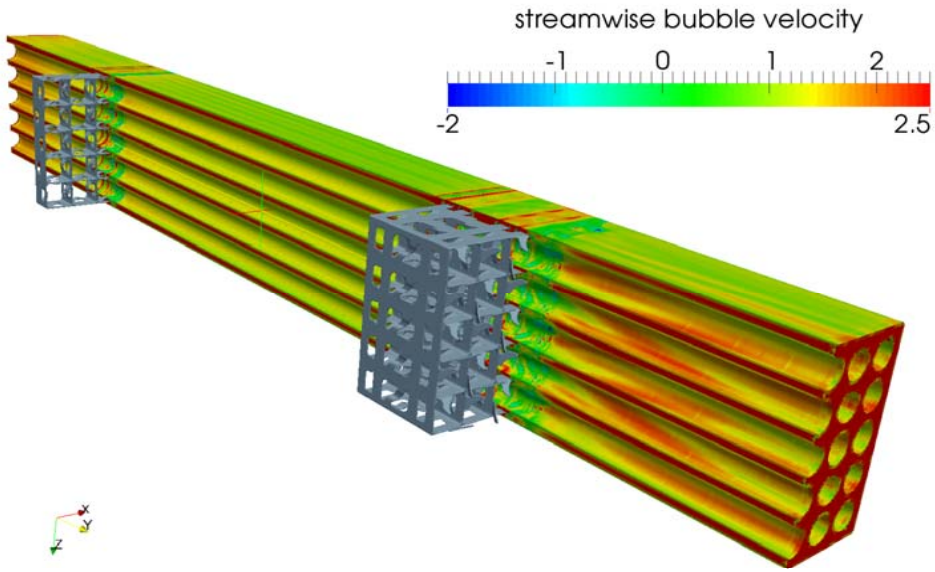
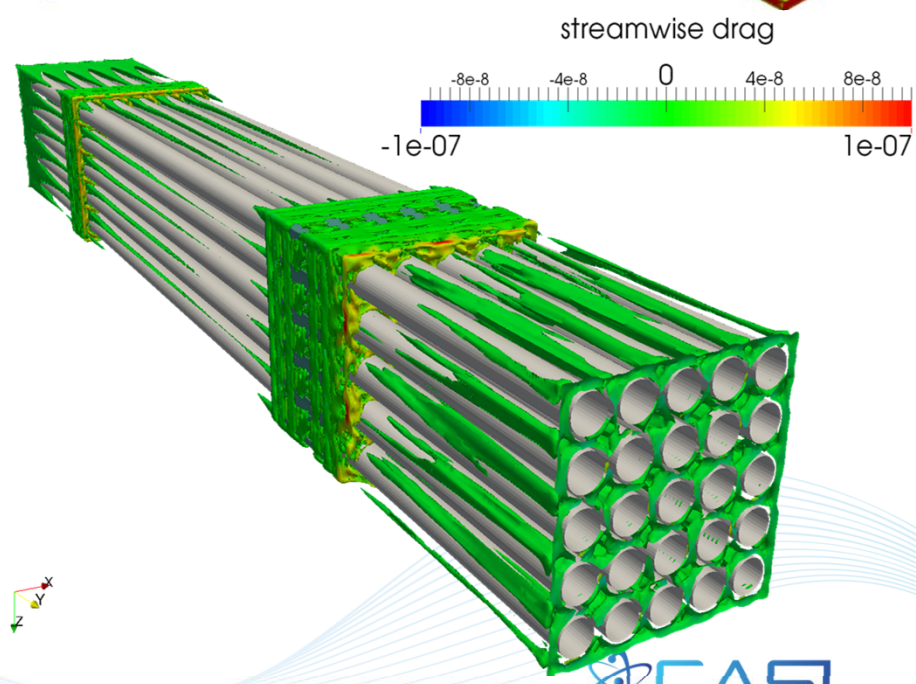
New M-CFD Platform
Multiphase Framework Shakedown

- Multiphase ILES calculations for the 5x5 fuel rod bundle
- Differential gas and liquid inlet velocity at the inlet to test fully-coupled momentum exchange
- Quick convergence shows promising robustness of framework
- Framework shows robust behavior for transient multiphase, currently Achilles'heel of M-CFD codes.





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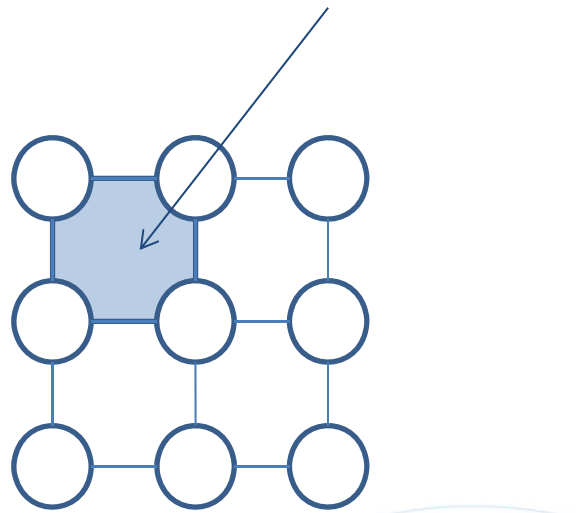
Thermal Hydraulics – COBRA-TF

- COBRA-TF (CTF) subchannel code from PSU
- Two-fluid, three-field representation of the two-phase flow
  - Continuous vapor (mass, momentum and energy)
  - Continuous liquid (mass, momentum and energy)
  - Entrained liquid drops (mass and momentum)
  - Non-condensable gas mixture (mass)
- Spacer grid models
- Pin conduction model
- Built-in material properties



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Thermal Hydraulics – CTF Equations

Three Phases:
- Liquid
- Vapor
- Droplets

Conservation of Momentum:

$$\frac{\partial}{\partial t}\left(\alpha_k \rho_k \vec{U}_k\right) + \nabla \cdot \left(\alpha_k \rho_k \vec{U}_k \vec{U}_k\right) =$$

$$\alpha_k \rho_k g - \alpha_k \nabla P - \underline{\tau}'''_{wall,k} - \underline{\tau}'''_{i,k} + \left(\Gamma''' \vec{U}_k\right) + M_k^T$$

Additional Mass Equation for non-condensible gases

Conservation of Mass:

$$\frac{\partial}{\partial t}\left(\alpha_k \rho_k\right) + \nabla \cdot \left(\alpha_k \rho_k \vec{U}_k\right) = \Gamma_k + W_k^T$$

Liquid drops are assumed to be in thermal equilibrium with vapor

Conservation of Energy:

$$\frac{\partial}{\partial t}\left(\alpha_k \rho_k h_k\right) + \nabla \cdot \left(\alpha_k \rho_k h_k \vec{U}_k\right) =$$

$$-\nabla \cdot \alpha_k \underline{Q}_k + \Gamma_k h_k^i + q'''_{i,k} + \alpha_k \frac{\partial P}{\partial t} + Q_k^T$$

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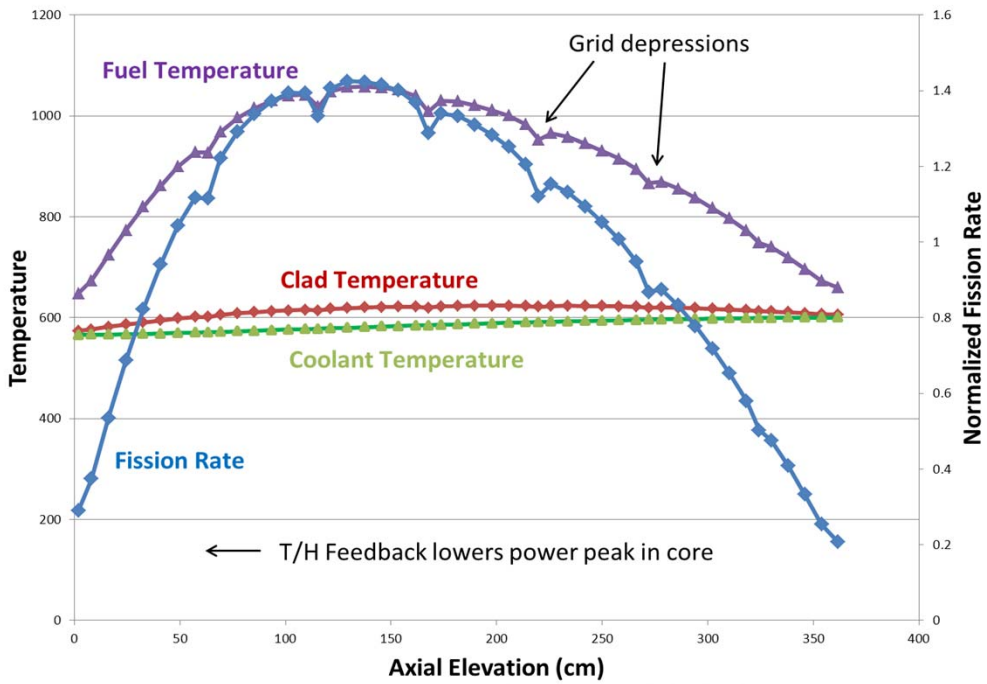
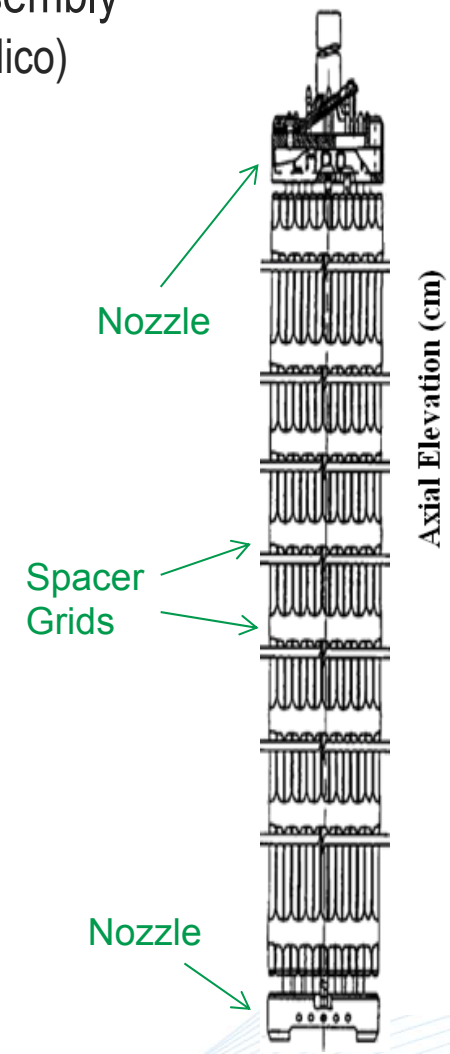
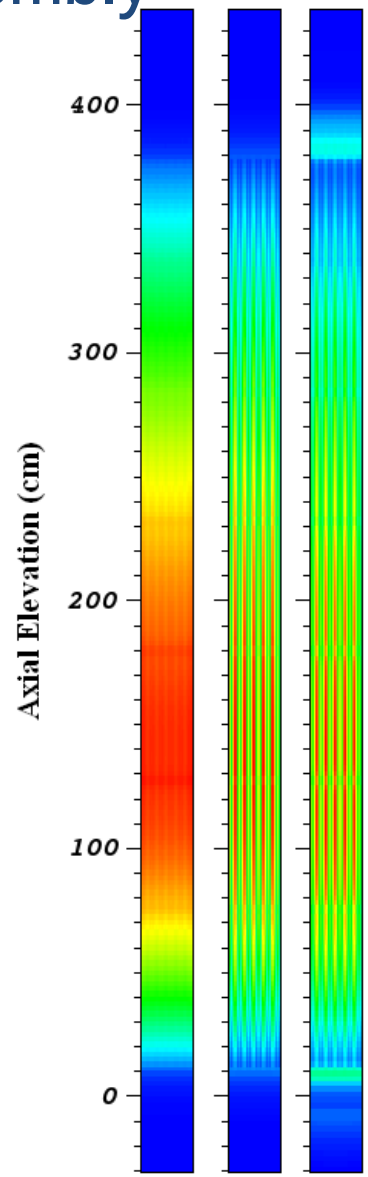
VERA Multi-physics Simulation of PWR Fuel Assembly
- Base for adding Challenge Problems Physics

- Coupled multiphysics model of WEC PWR fuel assembly
  - Neutron transport to calculate power distribution (Insilico)
  - Thermal-Hydraulics in coolant (COBRA-TF)
  - Heat conduction in fuel rods (COBRA-TF)
  - Neutron cross sections as function of temperature and density (XSProc)







Fast, Epithermal, and Thermal Flux Profiles

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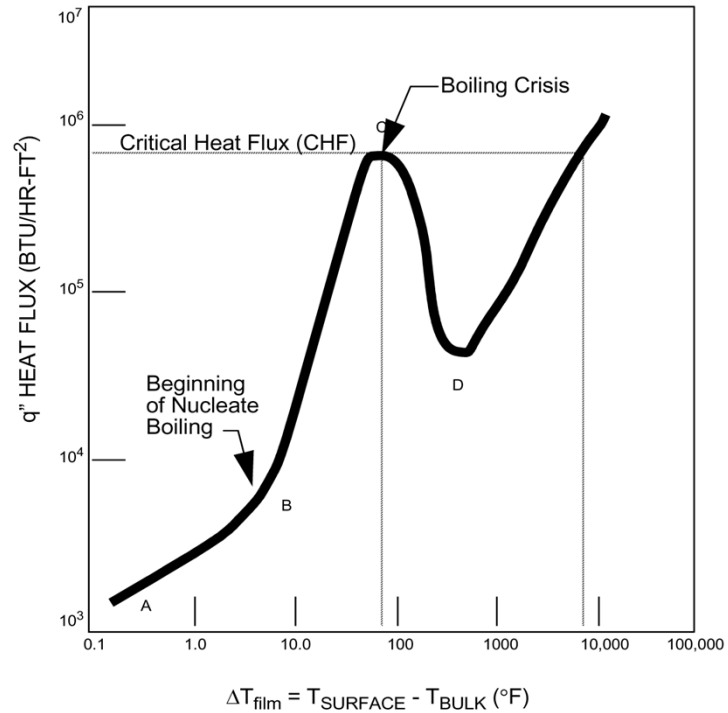
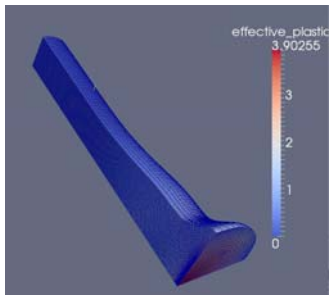
Departure from nucleate boiling (DNB)

- Local clad surface dryout causes dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow)
- Problem statements
  - Current DNB predictions limited by subchannel code, steady state test data from small scale of rod bundles (e.g., 5x5), and an empirical correlation
  - Lack of understanding on DNB occurrence and effects of reactor core features and conditions
  - lack of predictive capability of transient DNB or fuel failure mechanism
  - Requires conservative and sometimes unrealistic DNBR predictions in safety analysis and regulatory licensing

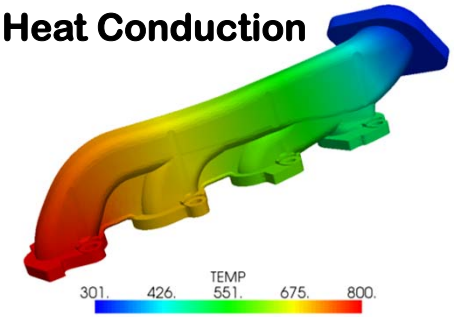


The Hydra Toolkit for Multi-Physics

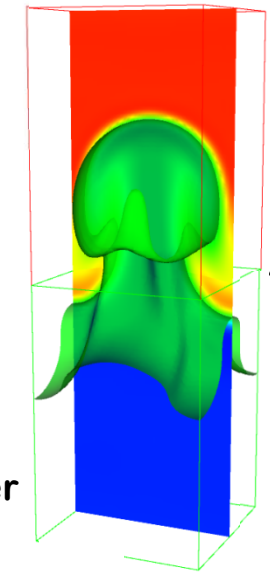
Lagrangian Hydrodynamics



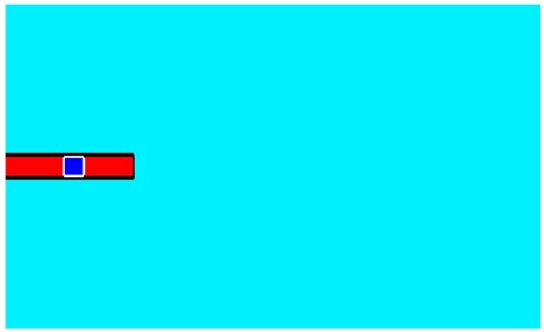
FEM/FVM Heat Conduction



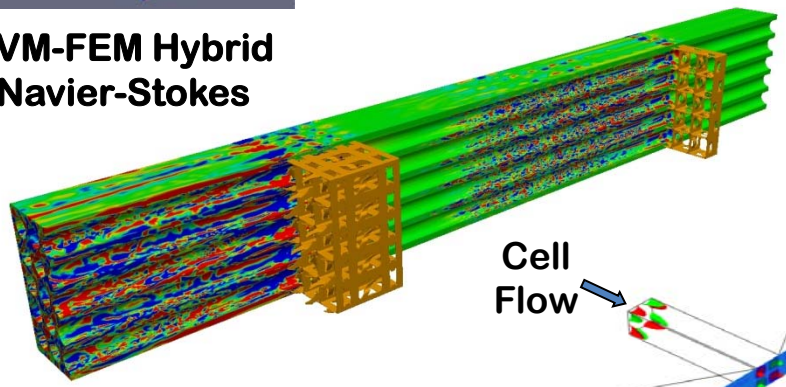
FVM Compressible w. Front-Tracking



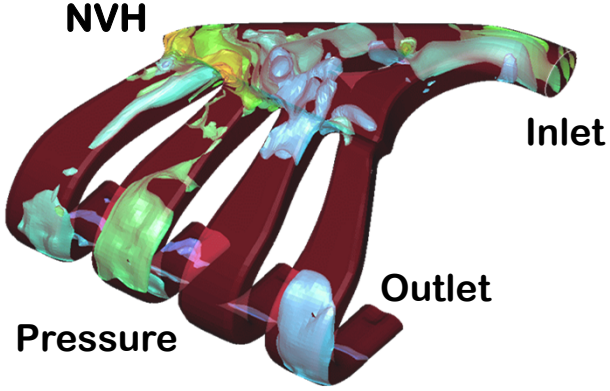
FVM Compressible w. Level Sets



FVM-FEM Hybrid Navier-Stokes

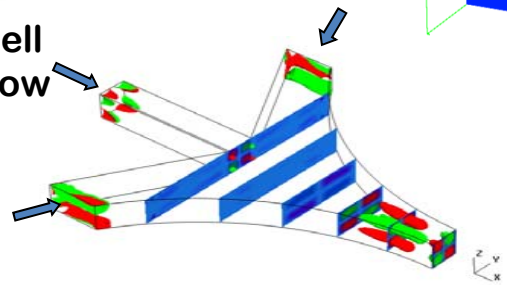


Automotive NVH

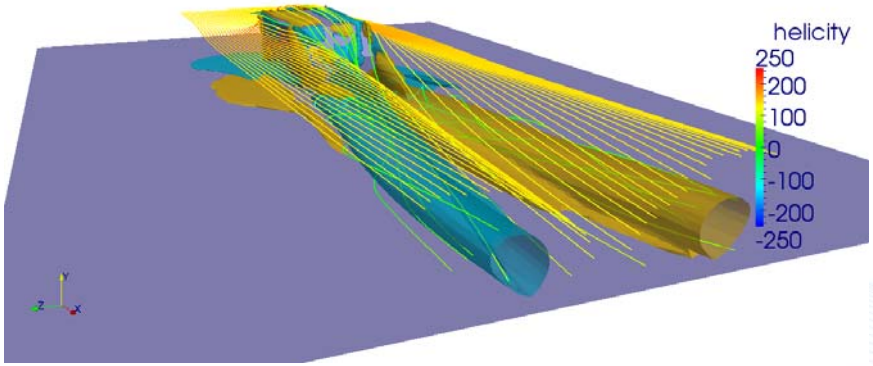


Carrier

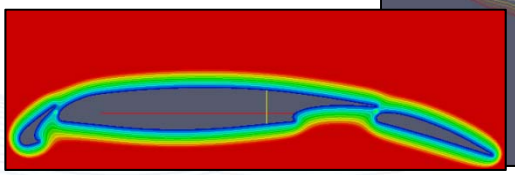
Cell Flow

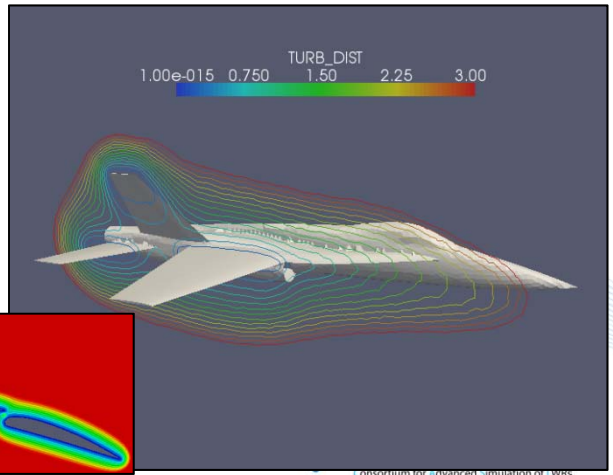


Rigid-Body Dynamics



Flow Cytometry





The well-posed incompressible Navier-Stokes flow problem satisfies "solvability"

- $\rho\left\{\frac{\partial v}{\partial t}+v\cdot\nabla v\right\}=-\nabla p+\mu\nabla^2 v+\boldsymbol{f}$

  $\nabla\cdot v=0$

- BC's: $v(\boldsymbol{x},t)=\hat{v}(\boldsymbol{x},t)\ on\ \Gamma_1$

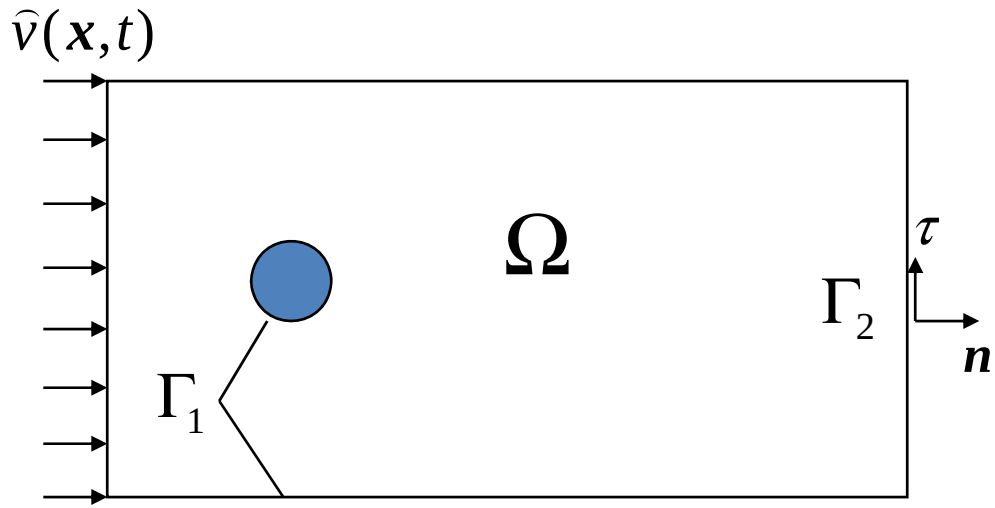
  $$\left.\begin{aligned}-p+\mu\frac{\partial v_n}{\partial n}&=f_n\\ \mu\frac{\partial v_\tau}{\partial \tau}&=f_\tau\end{aligned}\right\}\ on\ \Gamma_2$$

- IC's: $v(\boldsymbol{x},0)=v^0(\boldsymbol{x})$

- Constraints:

  $$\left.\begin{aligned}&\boldsymbol{n}\cdot v^0=\boldsymbol{n}\cdot\hat{v}\ on\ \Gamma_1\\ &\nabla\cdot v^0=0\ in\ \Omega\\ &\int_{\Gamma_1}\boldsymbol{n}\cdot\hat{v}=0\ \ if\ \ \Gamma_2=0\end{aligned}\right\}$$

  "Solvability" for a well-posed incompressible N-S problem



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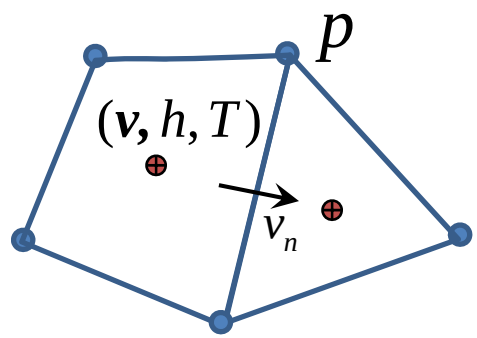
Spatial discretization produces DAE's -- ODE's with constraints



- Discretize domain and form a weighted residual

$$\int_{\Omega_e} \rho \dot{\mathbf{v}} + \int_{\Gamma_e} (\rho \mathbf{v}) \mathbf{v} \cdot n - \int_{\Gamma_e} (\mu \nabla \mathbf{v} \cdot n)\Big|_{\Gamma_e} + \int_{\Omega_e} \nabla p = \int_{\Omega_e} \boldsymbol{f}$$

$$\int_{\Gamma_e} v_n = 0$$

- Index-2 DAE's are solved *fully-coupled*

$$M\,\dot{\mathbf{v}} + A(\rho, \mathbf{v})\mathbf{v} + K\mathbf{v} + \mathbf{G}p = \boldsymbol{F}$$

$$\boxed{\mathbf{D}\mathbf{v} = g}$$

- Index-1 DAE's are *segregated*

$$M\,\dot{\mathbf{v}} + A(\rho, \mathbf{v})\mathbf{v} + K\mathbf{v} + \mathbf{G}p = \boldsymbol{F}$$

$$\boxed{Lp = \mathbf{D}M^{-1}\{\boldsymbol{F} - K\mathbf{v} - A(\rho, \mathbf{v})\mathbf{v}\} - \dot{g}}$$

M – *mass matrix*
$A(\mathbf{v})$ – *advective terms*
K – *viscous terms*
G – *gradient*
D – *divergence*
L – *pressure – Poisson*

If the solvability conditions are satisfied, then the Index-1 DAE's deliver the same velocity-pressure solution as the Index-2 DAE's!!!

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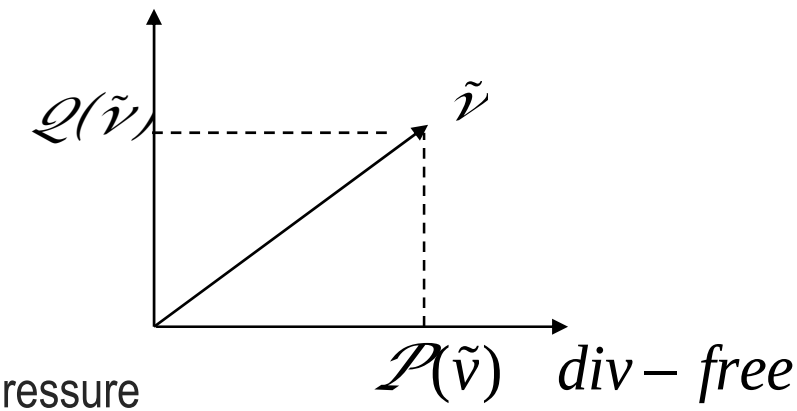
The approximate, incremental projection algorithm is "realized" by a velocity decomposition

- Decompose the velocity into div-free and curl-free parts, a Helmholtz decomposition

$$\rho\tilde{\boldsymbol{v}} = \rho\boldsymbol{v} + \nabla\lambda$$

$$\nabla\cdot\boldsymbol{v} = 0,\ and\ \ \nabla\times\nabla\lambda = 0$$



- Uses physical BC's
- Attempts to "legitimately" decouple the velocity and pressure
- Preserves a discretely div-free velocity field at each time step
- Use div-constraint and solve via Galerkin FEM

$$\left.\begin{aligned}\nabla\cdot\left(\frac{1}{\rho}\nabla\lambda\right) &= \nabla\cdot\tilde{\boldsymbol{v}}\\ \boldsymbol{v} &= \tilde{\boldsymbol{v}} - \frac{1}{\rho}\nabla\lambda\end{aligned}\right\} \Rightarrow \left\{\begin{aligned}&\int_\Omega \nabla w\cdot\left(\frac{1}{\rho}\nabla\lambda\right) = \int_{\Gamma_N} w\left(\frac{1}{\rho}\frac{\partial\lambda}{\partial n}\right)\\ &\qquad -\int_{\Gamma_D} w\left(\tilde{\boldsymbol{v}}\cdot\boldsymbol{n}\right)\Big|_{\Gamma_D} + \int_\Omega \tilde{\boldsymbol{v}}\cdot\nabla w\end{aligned}\right.$$

$$L\lambda = b$$

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Projection methods admit semi-implicit and fully-implicit time integration methods

- The kernel of the projection algorithm

Non-Sharp Stability Est.

$$CFL = \frac{\|v\|\Delta t}{h}$$

$$CFL \le O(10)$$

1. $$\left[M - \theta\Delta t\left[K - A(\rho,\mathbf{v})\right]\right]\tilde{\mathbf{v}} = \left[M + (1-\theta)\Delta t\left[K - A(\rho,\mathbf{v})\right]\right]\mathbf{v}^n + \Delta t\left\{\theta\mathbf{F}^n + (1-\theta)\mathbf{F}^{n+1} - \mathbf{B}p^n\right\}$$

2. $$L\lambda = b(\tilde{\mathbf{v}}) - b(\mathbf{v}^n)$$

- "Project the difference" for steady-state (Gresho, et al., IJNMF, 1995)
- Solve with Multigrid-preconditioned CG

3. $$\mathbf{v}^{n+1} = \tilde{\mathbf{v}} - M^{-1}\mathbf{B}\lambda$$

4. $$\mathbf{v}^{n+1}\Big|_{\Gamma_e} = \tilde{\mathbf{v}}\Big|_{\Gamma_e} - \left(M^{-1}\mathbf{B}\lambda\cdot\mathbf{n}\right)\Big|_{\Gamma_e}$$

$\mathbf{B}p^n$; $\mathbf{B}\lambda$ computed using FEM shape functions and nodal data

5. $$p^{n+1} = p^n + \frac{\lambda}{\theta\Delta t}, \quad where \quad \lambda = \theta\Delta t\left(p^{n+1} - p^n\right)$$

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Using the projection method to build a fully-implicit flow solver with physics-based preconditioning

- Interpretation of projection as a block LU factorization first presented by Perot in 1993
- Discrete momentum + div constraint

$$\left[M-\theta\Delta t\left[K-A\left(\rho,\mathbf{v}\right)\right]\right]\mathbf{v}^{n+1}=\left[M+(1-\theta)\Delta t\left[K-A\left(\rho,\mathbf{v}\right)\right]\right]\mathbf{v}^{n}$$
$$+\Delta t\left\{\theta\boldsymbol{F}^{n}+(1-\theta)\boldsymbol{F}^{n+1}-\boldsymbol{B}p^{n}-\boldsymbol{B}\lambda^{n+1}\right\}$$

$$Dv^{n+1}=0,\quad and\quad \lambda=\theta\Delta t\left(p^{n+1}-p^{n}\right)$$

- In block form,

$$\begin{bmatrix} Q & QM^{-1}B \\ D & 0 \end{bmatrix}\begin{Bmatrix} v^{n+1} \\ \lambda^{n+1} \end{Bmatrix}=\begin{Bmatrix} r-\Delta t\left(QE\right)Bp^{n}-\boxed{\Delta t\theta\left[K-A\left(\rho,v\right)\right]M^{-1}B\lambda^{n+1}} \\ 0 \end{Bmatrix}$$

$$Q=M-\Delta t\theta\left[K-A\left(\rho,v\right)\right]$$

$$r=\left[M+\left(1-\theta\right)\left[K-A\left(\rho,v\right)\right]\right]v^{n}+\Delta t\left\{\theta F^{n}+\left(1-\theta\right)F^{n+1}\right\}$$

Dropped in typical projection methods

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The fully-implicit projection method based on a block LU decomposition (cont.)

- $$\begin{bmatrix} Q & QM^{-1}B \\ D & 0 \end{bmatrix} \begin{Bmatrix} v^{n+1} \\ \lambda^{n+1} \end{Bmatrix} = \begin{Bmatrix} r - \Delta t(QE)Bp^n - \Delta t\theta\left[K - A(\rho, v)\right]M^{-1}B\lambda^{n+1} \\ 0 \end{Bmatrix}$$
  - For SIMPLE algorithm, $E \approx Q^{-1}$, is approximated by various discretization choices
  - $E = Q^{-1}$ corresponds to Uzawa's algorithm in velocity-pressure
  - For fully-coupled projection: $E = Q^{-1}$
- The factored operator: $$\begin{bmatrix} Q & QM^{-1}B \\ D & 0 \end{bmatrix} = \begin{bmatrix} Q & 0 \\ D & -DM^{-1}B \end{bmatrix} \cdot \begin{bmatrix} I & M^{-1}B \\ 0 & I \end{bmatrix}$$

Iterate on k

1. Solve for the approximate velocity, Lagrange multiplier (forward elimination)

$$\begin{bmatrix} Q & 0 \\ D & -DM^{-1}B \end{bmatrix} \begin{Bmatrix} v^{*} \\ \lambda^{k+1} \end{Bmatrix} = \begin{Bmatrix} r - \Delta t Bp^{n+1} - \Delta t\theta\left[K - A(\rho, v)\right]M^{-1}B\lambda^{k} \\ 0 \end{Bmatrix}$$

1. Projection (back substitution): $$\begin{bmatrix} I & M^{-1}B \\ 0 & I \end{bmatrix} \begin{Bmatrix} v^{k+1} \\ \lambda^{k+1} \end{Bmatrix} = \begin{Bmatrix} v^{*} \\ \lambda^{k+1} \end{Bmatrix}$$

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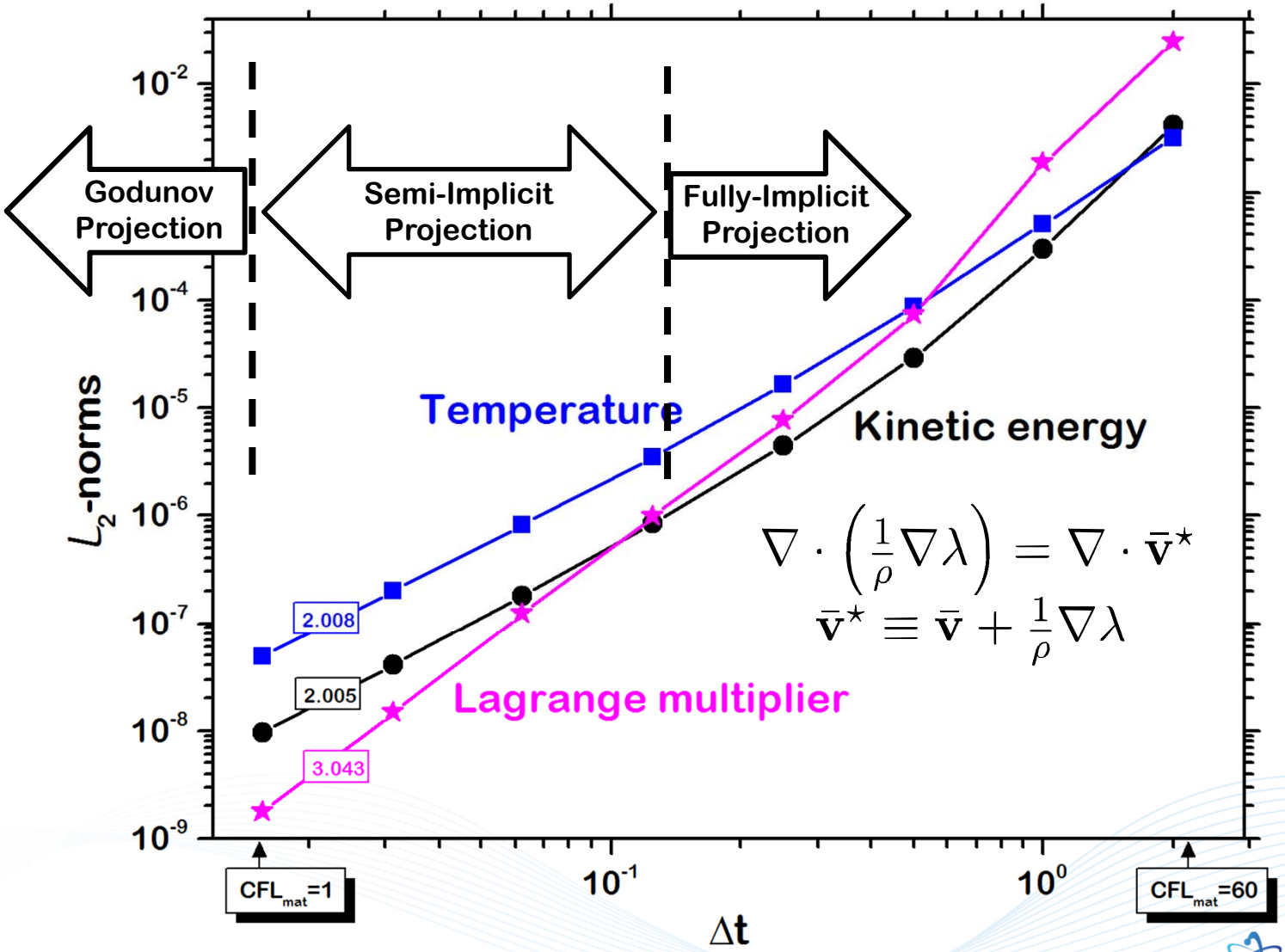
Fully-Implicit Algorithms – Accuracy, Robustness & Efficiency (cont.)



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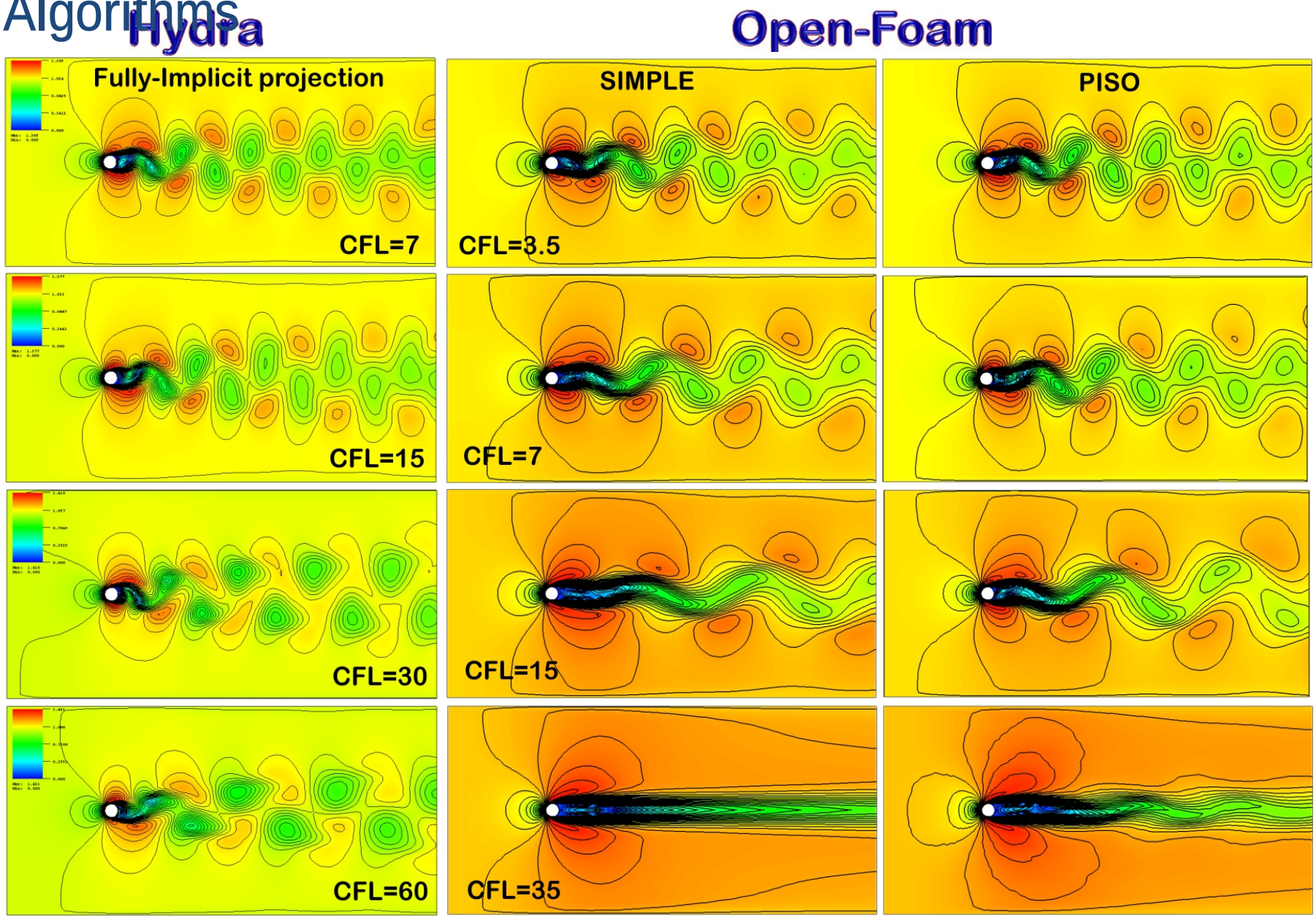
Fully-Implicit Projection vs. SIMPLE vs. PISO Algorithms

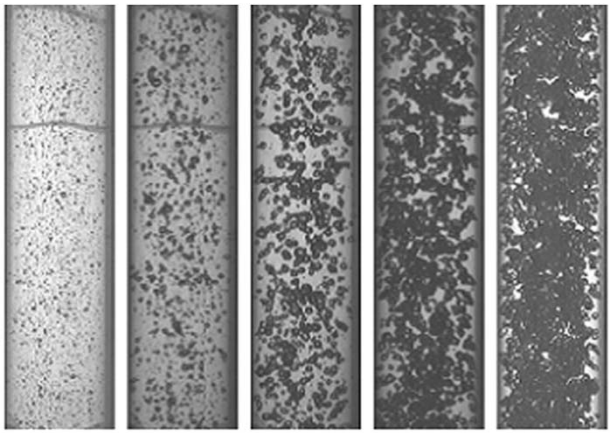


A "Multiphase Flow" Taxonomy: Multifluid, Multiphase and Multispecies Flows

Multimaterial/Multifluid

- Materials are immiscible
- Modest number of sharp interfaces are represented numerically
- Typically relies on "mean-strain" approximation -- can be extended to partition deviatoric strain
- Each material has a unique stress and energy
- Sub-cell level pressure equilibrium can be enforced, but it can be expensive to do so exactly
- Incorporates treatment of void

(Eulerian) Multiphase



- Large number of small material domains that are not resolved by a single element
- Too many interfaces to treat individually
- Relies on spatially-averaged mixture approximations, i.e., homogenized equations
- Multiphase fluid formulations may be used in the multimaterial limit, but still a research area with few production-level codes

Multispecies

- Components are completely miscible from a continuum view
- Typically applied to gases or materials at high temperatures, i.e., plasmas
- Use pressure-temperature equilibrium, i.e., Amagat model for gases
- Extensible to a carrier material with stress deviator and advective transport of multiple species
- Frequently incorporates reaction chemistry

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The Ensemble Averaging Process for "Eulerian" Multiphase Flows

- Characteristic function: $\mathrm{X}_k(x,t;\mu) = \begin{cases} 1 \text{ if } x \in k \text{ in realization } \mu \\ 0 \text{ otherwise} \end{cases}$
  - Ex.: 1 in bubbles, 0 in liquid phase

- Multiply phasic conservation equations by X_k, and perform ensemble averaging over multiple realizations
  - Average: $\bar{f} = \int_{\mathcal{E}} f(x,t;\mu)\,d\mu$
  - Averaging follows Reynolds rules, e.g., for products, etc.
- Ex.: Continuity Eq.

$$\int_{\mathcal{E}} \mathrm{X}_k \left\{ \frac{\partial \rho_k}{\partial t} + \nabla \cdot \left(\rho_k v_k \right) \right\} = 0$$

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \left(\alpha_k \rho_k v_k \right) = \Gamma_k$$

$$\alpha_k = \overline{\mathrm{X}}_k; \quad \Gamma_k = \overline{\rho_k \left(v_k - v_{k_I} \right) \cdot \nabla \mathrm{X}_k}$$

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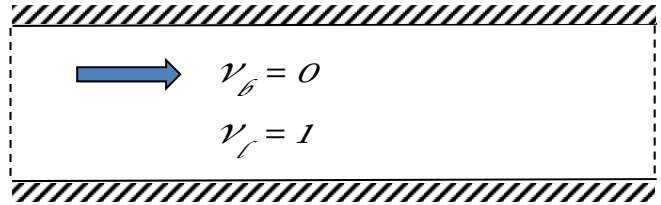
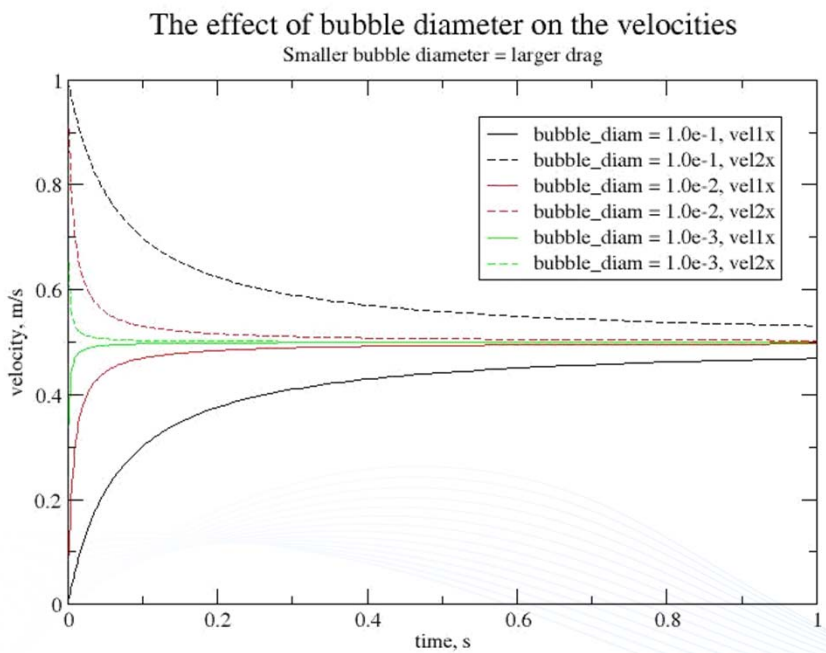
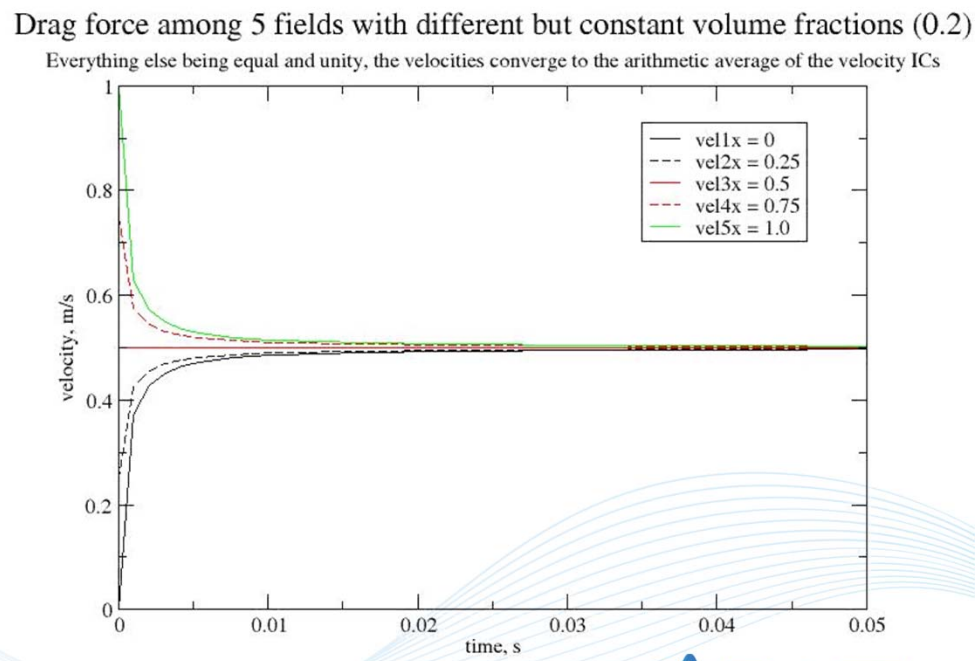
A prototypical drag closure relationship & in-situ verification during development

- $\mathcal{F}_{\mathcal{D}} = -\frac{3}{4}\frac{C_{\mathcal{D}}}{\mathcal{D}_b}\alpha_\ell \rho_\ell \left\| v_b - v_\ell \right\| \left(v_b - v_\ell \right)$

$$C_{\mathcal{D}} = \begin{cases} \frac{24}{\mathcal{R}e_b}\left[1 + 0.15\,\mathcal{R}e_b^{0.687}\right] & 0 < \mathcal{R}e_b \le 1000 \\ 0.44 & \mathcal{R}e_b > 1000 \end{cases}$$



Verifies force anti-symmetry and momentum conservation!!