CASL Industry Council Meetings
January 11, 2011 – Oak Ridge, TN
February 8, 2011 – Charlotte, NC

Minutes

The second meeting of the Industry Council (IC) for the Consortium for Advanced Simulation of Light Water Reactors (CASL) was held in two parts on January 11, 2011 at Oak Ridge National Laboratories (ORNL), Oak Ridge, TN; and on February 8, 2011, at the facilities of the Electric Power Research Institute (EPRI) in Charlotte, NC. Both meetings were chaired by John Gaertner of EPRI.

Two meetings were necessary because of inclement weather which prohibited travel to the January 11 session by many members. The agenda content was the same for both meetings. The agendas including meeting attendees are included as Attachment 1 to these minutes.

Attendance was by invitation only. Representatives from 18 organizations, not including CASL staff members, were invited. All sent representatives except Battelle Columbus, Cray Computing, Bettis Laboratories, and Swanson Analysis Services. In addition, many members of the CASL project team participated in the meetings.

After the introduction of each participant, John Gaertner previewed the agenda and presented the objectives of the meeting: 1) update the members on the CASL project status, 2) address actions from the September 9, 2010 meeting, 3) review the VERA Requirements Document, 4) discuss non-VERA deliverables planned by CASL, 5) report on response to September 9 Robin Comments to CASL, and 6) address several IC emergent issues.

The CASL staff presented an update of CASL activities. Doug Kothe, CASL Director, offered a "refresher" on the CASL project. He reviewed the Challenge Problems which will drive the advances in technology, development of the virtual reactor, and applications of the technology. He reviewed the organization of CASL which is structured around the five technical Focus Areas and the external Councils. He discussed the elements of the project which establish its cadence – six month Periods of Record with clear milestones and deliverables, regularly scheduled and frequent releases of virtual reactor software (VERA), and collaborations and partnerships throughout the development process. He spoke of features of the project designed to promote collaboration and innovation. Finally, he reviewed significant achievements in the first six months of CASL and the challenges which will be addressed in the next six months. His presentation is included as Attachment 2 to these minutes.

Leads from each of the Focus Areas then summarized their Focus Area objectives and significant milestones during the first year of the project. At the January meeting, Focus Area Leads made the presentations as indicated below except for the Materials Performance Optimization area – Chris Stanek did not attend due to flight cancellations; so his area, Material Performance Optimization, was presented by Paul Turinsky, CASL Chief Scientist. At the February meeting, due to schedule conflicts, all presentations were given by Paul Turinsky and Jess Gehin, Area Lead for Advanced Modeling Applications. The presenters for the January and the February meeting, respectively, are shown below.

P. Turinsky/Paul Turinsky	Material Performance Optimization (MPO)
Bill Martin/Paul Turinsky	Models and Numerical Methods (MNM)
John Turner/P. Turinsky	Virtual Reactor Integration (VRI)
Jim Stewart/Jess Gehin	Validation and Uncertainty Quantification (VUQ)
Jess Gehin/Jess Gehin	Advanced Modeling Applications (AMA)

Discussion among IC members and CASL staff occurred throughout these presentations. All actions that were created during these discussions are included in the Action Items section of these minutes below. The presentations are included as Attachment 3 to these minutes.

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John Gaertner summarized the proceedings of the September 9, 2010, meeting and asked for any revisions or comments on the minutes. There were no recommended revisions or comments, and the minutes were approved at the February meeting. He then summarized the proposed IC Charter. The draft charter had been changed to remove the IC Steering Committee – CASL management and DOE management preferred to have only a single category of IC membership, so the Steering Committee was not included as part of the IC structure. The Charter was approved at the February Meeting. He then reviewed the progress on Action Items from the September meeting, and the IC members concurred at the February meeting that all Action Items had been closed.

Steve Hess then led a discussion of the Draft VERA Requirements Document that had been distributed to all IC Members for review prior to the meeting. At both meetings, many comments and suggestions were offered by IC members and were discussed among IC members and CASL staff. This meeting session was extended at both meetings to accommodate the discussions. All actions that were created during these discussions are included in the Action Items section of these minutes below. The presentation is included as Attachment 4 to these minutes.

The next agenda item called for leads from each of the Focus Areas to present examples of "Technology Solutions", in addition to the VERA software product, that are expected to result from the work within their focus areas in the near term. This session was in response to a clear message from the IC in the September 9, 2010, meeting that end users would benefit from CASL results delivered through papers, reports, and other technology transfer that could be used directly, even though these results might be also embedded in the VERA product.

At the January meeting, Focus Area Leads made the presentations as indicated below.

- Brian Wirth — Material Performance Optimization (MPO)
- Bill Martin — Models and Numerical Methods (MNM)
- John Turner — Virtual Reactor Integration (VRI)
- Jim Stewart — Validation and Uncertainty Quantification (VUQ)
- Jess Gehin — Advanced Modeling Applications (AMA)

The presentation referred, in each case, to the last slide in each Focus Area presentation of Attachment 3. Discussion among IC members and CASL staff ensued from these presentations.

At the February meeting, these presentations were not made – IC members agreed that these Technology Solutions were pointed out and discussed in earlier agenda items, so the time would be spent better on other issues.

All actions that were created during these discussions of Technology Solutions are included in the Action Items section of these minutes below.

John Gaertner then presented the report on "Themes" for IC activities. These themes are a roll-up of issues identified by the IC in the September meeting. The CASL project responded to the issues. In some cases changes were made in CASL plans to address recommendations or concerns of the IC. In other cases, the CASL project recommended ongoing IC involvement to advise the project. The CASL responses are included as Attachment 5 to these minutes. This version was used for the February meeting, which reflects some IC recommendations made in the January meeting. All actions that were created during these discussions of Themes are included in the Action Items section of these minutes below.

Finally, John Gaertner led discussion of several issues before the Council.

- The IC considered the appropriate response to the comments sent by email to the IC by John Swanson and his subsequent resignation from the IC. It was agreed that his comments deserved consideration and a response by CASL and the Council. It was agreed that his perspective was valuable and his continuation on the IC was desirable. Finally, it was agreed that John Gaertner

would draft a response to John Swanson on behalf of the IC. After IC concurrence, this response would be sent to Mr. Swanson.

- The IC considered whether to add members representing Small Modular LWR Reactors (SMR) onto the IC. The IC saw no need to add this category of user to the IC at this time, given the necessary focus of CASL on current reactors. However, the IC agreed to remain open to such opportunities in the future.
- The IC considered a role to sponsor IC member participation in CASL activities such as providing problems and datasets; and performing reviews, tests, and applications of CASL products. It was agreed that this is an appropriate and important function of the IC.
- The IC considered the potential to establish sub-committees to address resolution of issues identified in the earlier discussion of IC Themes. It was agreed to consider sub-committees in 3 areas:
  - Computer platforms for CASL applications and releases
  - Collaborative applications of VERA
  - Ensuring CASL Problem Solutions beyond VERA
- The IC considered options for the next IC meeting including 1) a webcast meeting, and 2) postponing until the CASL Innovation Fair in August. It was agreed that the next meeting should be face-to-face at ORNL, and that coordination with the ribbon-cutting in Mid May was desirable.

The following Action items were identified as a result of this meeting:

1. VRI to send Industry Council more information on the LIME integration environment and on the decision to use LIME versus options for "heavier" integration options.
2. IC Chairman to investigate sending the report on CASL validation data requirements, by Nam Dinh, to the IC members.
3. AMA to arrange for Industry Council to have access to technical specifications for Challenge Problems for better understanding of VERA requirements.
4. VRI to consider a larger context for specifying "Workflow Management" than currently in the VRI focus area plan. Define necessary interfaces with other systems of the end-users. These workflows will vary for different "use types" (see next action).
5. CASL to create a catalog of likely VERA "use-case types" and define the attributes that will require differences in the VERA physics simulation suite or the workflow environment. Consider two pathways – R&D applications and design simulations.
6. IC sees mesh generation strategy as an important factor in VERA usability and versatility. VRI to investigate potential collaboration with EDF and Rolls-Royce on this issue.

7. MNM to investigate potential use and collaboration on open-source or otherwise accessible turbulent flow models, particularly at EDF and Imperial College of London.
8. IC Chairman to define proposed IC subcommittees and participation in other CASL councils based on Industry Council discussions.
9. CASL to develop report to IC on VERA Requirements Document: consolidating IC comments and addressing them.
10. IC Chairman to draft a response to John Swanson on behalf of the IC.

The meeting was adjourned at approximately 4:30 pm.

Prepared: March 3, 2011
By John Gaertner

Attachment 1

CASL Industry Council Meeting Minutes

Agenda
January 11, 2011
Location: ORNL, Conference Center
Building 5200 Room 214

Tuesday, January 11

8:00	Registration and Coffee
8:30	Welcome and Introductions, *John Gaertner*
8:40	Update CASL Activities/Plans since September, *CASL Management Team*
9:40	Report on CASL Actions from Last IC Meeting, *John Gaertner*
10:30	Review VERA Requirements Document, *Steve Hess*
12:00	Lunch, ORNL Cafeteria
1:00	CASL as a Resource for Technical Solutions, *CASL Technical Team*
2:00	Prioritize Industry Council Themes for 2011, *IC Members*
3:30	Identify Specific IC member Activities and Participant Commitments, *IC Members*
4:15	Summary of Action Items, *John Gaertner*
4:30	Adjourn

CASL Industry Council Attendees*

1. John Gaertner, (EPRI) jgaertner@epri.com
2. Jean-Yves Berthou, (EDF) jy.berthou@edf.fr
3. David Modeen, (EPRI) dmodeen@epri.com
4. Kord Smith, (STUD) kord.smith@studsvik.com
5. Alan Copestake, (RR) alan.copestake@rolls-royce.com

* Because the meeting was held during co-location week for the CASL Project, many CASL staff attended or participated in portions of the meeting. CASL staff who contributed to agenda items are noted in the meeting minutes.

Rescheduled Meeting Agenda
February 8, 2011
Electric Power Research Institute
1300 West W.T. Harris Blvd
Building 1, Room 305
Charlotte, NC 28262

Tuesday, February 8

8:00	Registration and Coffee
8:30	Welcome and Introductions, *John Gaertner*
8:40	Update CASL Activities/Plans since September, *CASL Management Team*
9:40	Report on CASL Actions from Last IC Meeting, *John Gaertner*
10:30	Review VERA Requirements Document, *Steve Hess*
12:00	Lunch
1:00	CASL as a Resource for Technical Solutions, *CASL Technical Team*
2:00	Prioritize Industry Council Themes for 2011, *IC Members*
3:30	Identify Specific IC member Activities and Participant Commitments, *IC Members*
4:15	Summary of Action Items, *John Gaertner*
4:30	Adjourn

Attendees List

1. John Gaertner, (EPRI) jgaertner@epri.com
2. George Chiu, (IBM) gchiu@us.ibm.com
3. John Harrell, (DMN) john.harrell@dom.com
4. Sumit Ray, (WSTS) rays@westinghouse.com
5. Russell Stachowski, (GE) russell.stachowski@gnf.com
6. Scott Thomas, (DUKE) scott.thomas@duke-energy.com
7. Thomas Weaver, (BOEING) thomas.l.weaver@boeing.com
8. Alan Copestake, (RR) alan.copestake@rolls-royce.com
9. Rose Montgomery, (TVA) rmontgomery@tva.gov
10. Doug Kothe, (ORNL) kothe@ornl.gov
11. Mario Carelli, (WES) carellmd@westinghouse.com
12. Ronaldo Szilard, (INL) ronaldo.szilard@inl.gov
13. Paul Turinsky, (NCSU) turinsky@ncsu.edu
14. Steve Hess, (EPRI) shess@epri.com
15. Jeff Banta, (ORNL) bantaj@ornl.gov
16. Jess Gehin, (ORNL) gehinjc@ornl.gov
17. Christopher Lewis, (AREVA) christopher.lewis@areva.com
18. Sal Golub, (DOE) sal.golub@hq.doe.gov
19. Zeses Karoutas, (WES) KaroutZE@westinghouse.com

<u>Attachment 2</u>
CASL Industry Council Meeting Minutes
CASL Refresher and Overview

<u>Attachment 3</u>
CASL Industry Council Meeting Minutes
Focus Area Status Reports and Technology Solutions

<u>Attachment 4</u>
CASL Industry Council Meeting Minutes
Review of VERA Requirements Document

<u>Attachment 5</u>
CASL Industry Council Meeting Minutes
CASL Response to Industry Council Themes

CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

Douglas B. Kothe

Director, CASL
Oak Ridge National Laboratory

CASL
Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Challenge Problems: Key phenomena limiting PWR reactor performance

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

CASL scope: Develop and apply the "Virtual Reactor" to assess fuel design, operation, and safety criteria

Near-term priorities (years 1–5)

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

Longer-term priorities (years 6–10)

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

Focus on challenge problem solutions

CASL's technical focus areas are executing the plan

MPO
Materials Performance and Optimization
Chris Stanek, Lead
Sid Yip, Deputy
Brian Wirth, Deputy

- VERA Integration
- Fuel microstructure
- Clad/internals microstructure
- Corrosion
- CRUD deposition
- GFRF

MNM
Models and Numerical Methods
Bill Martin, Lead
Rob Lowrie, Deputy

- Radiation transport
- Thermal hydraulics

VRI
Virtual Reactor Integration
John Turner, Lead
Randy Summers,
Rich Martineau, Deputiy

- Coupled multi- physics environment
- VR simulation suite
- Challenge Problem Integration

VUQ
Validation and Uncertainty Quantification
Jim Stewart, Lead
Dan Cacuci, Deputy

- V&V and calibration through data assimilation
- Sensitivity analysis and uncertainty quantification

AMA
Advanced Modeling Applications
Jess Gehin, Lead
Zeses Karoutas, Deputy
Stephen Hess, Deputy

- VR requirements
- VR physical reactor qualification
- Challenge problem application
- VR validation
- NRC engagement

18 integrated and interdependent projects

Overall CASL Cadence

- CASL will execute per 6-month *Plan of Record (PoR)* tasks, deliverables, and milestones
  - We have just started our second PoR (PoR-2: Jan-Jun 2011)
  - Imposes (we believe) more agility and flexibility in our plan and actions
- We plan to release our virtual reactor (VERA) regularly (e.g., at least bi-annually) and follow an evolutionary delivery life cycle
  - Place our M&S products into hands of users early and often
  - Follow quarterly "treadmills": science delivery, release, assessment, solution
- We encourage & need evolving collaborations and partnerships to succeed
  - This is too hard of a problem; our partnerships (formal and informal) will likely change as we encounter new problems and solve old ones

CASL sees the Industry Council as instrumental to our success

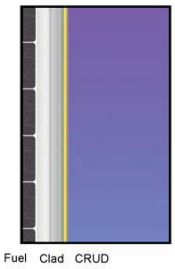
Virtual Reactor (VERA) Capability Roadmap

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

CRUD Nucleation and Growth Affects Localized Fuel and Overall Reactor Performance*

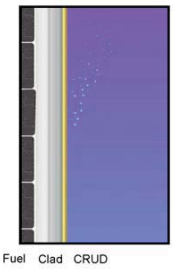
A complicated, localized phenomenon that has global whole-core effects

Step 0 – Normal Operation



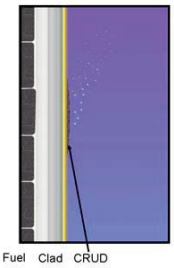
- Minimal sub-nucleate boiling
- Normal clad temperature
  - No serious fuel/clad contact yet

Step 1 - Nucleation



- Initiating event causes local clad temperature to rise
  - Could be PCI, etc.
- Induces more sub-nucleate boiling
  - This causes local supersaturations of Ni,Fe ions
  - If they can't diffuse away fast enough, they can precipitate out on the clad

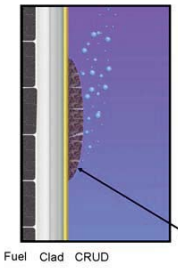
Step 1 - Nucleation



- Sub-nucleate boiling nucleates CRUD
  - Supersaturates ions at boiling surface[1]
  - These ions (mostly Fe, Ni) crystallize out, forming CRUD[1]
- Little boron accumulation
- Slight temperature rise in clad

[1]Secker, J. R. "BOA Theory and Methods." Presentation to MPO, 9/2010.

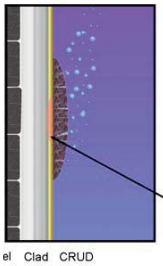
Step 2 - Growth



- CRUD nuclei cause local rise in temperature
- Induces more sub-nucleate boiling, more CRUD deposition
- Layer increases in thickness

$Ni(Ni,Fe)O_{3-4}$ – "Tenacious CRUD"

Step 3 - CILC

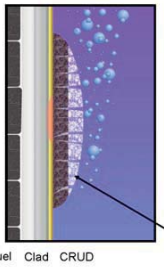


- CRUD creates the environment for CILC
  - Temperature rises beneath CRUD
  - High concentrations of ions are trapped in CRUD capillaries
  - Radiolysis, LiOH cause localized high pH[3]
  - Li ions could also migrate into ZrO_2 as interstitials and release Zr^{+2} ions
- Starts to dissolve Zr^{+2} ions from ZrO_2
  - Henshaw model does not account for Zr, but acknowledges it[2]
  - Non-trivial amount of ZrO_2 observed in some CRUD scrapes[3]
- These ions have to go somewhere…

CILC-affected cladding

[2]Henshaw, J. et al. "A model of chemistry and thermal hydraulics in PWR fuel crud deposits." *J. Nuc. Mat.* 353 (2006), pp. 1-11
[3]Deshon, J. "PWR Axial Offset Anomaly (AOA) Guidelines, Revision 1." EPRI Report 1008102, 6/2004

Step 3 - CILC

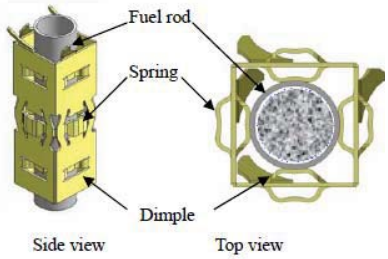


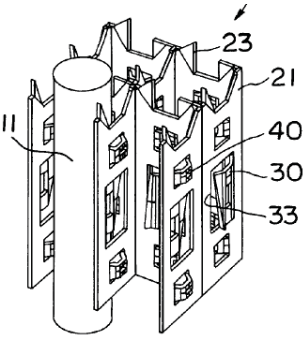
- … so they plate out on the CRUD
  - Outer CRUD layer is lower in pH, temperature
    - Zr^{+2}, O^{-2} ions restabilize & crystallize in less harsh environment, lower temp., lower pH
      - Also hypothesized by Deshon[3]
- CRUD gets thicker, more insulating

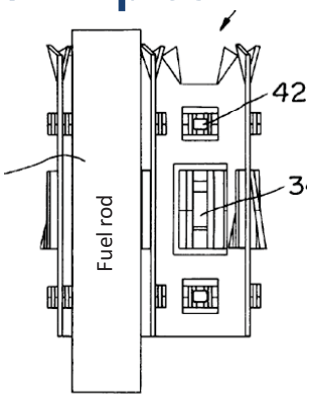
ZrO_2-rich CRUD

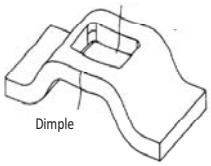
*figures courtesy of Mike Short (MIT)

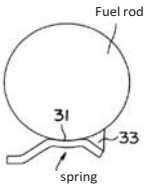
GTRF: Spacer Grid with Springs/Dimples

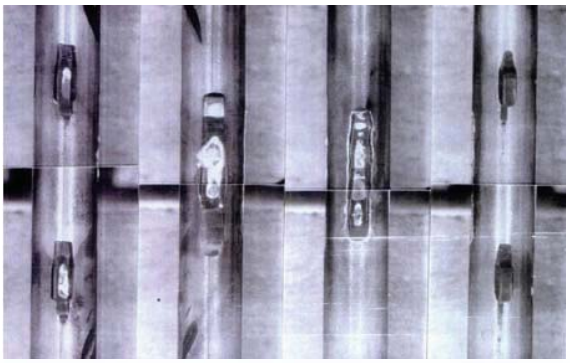






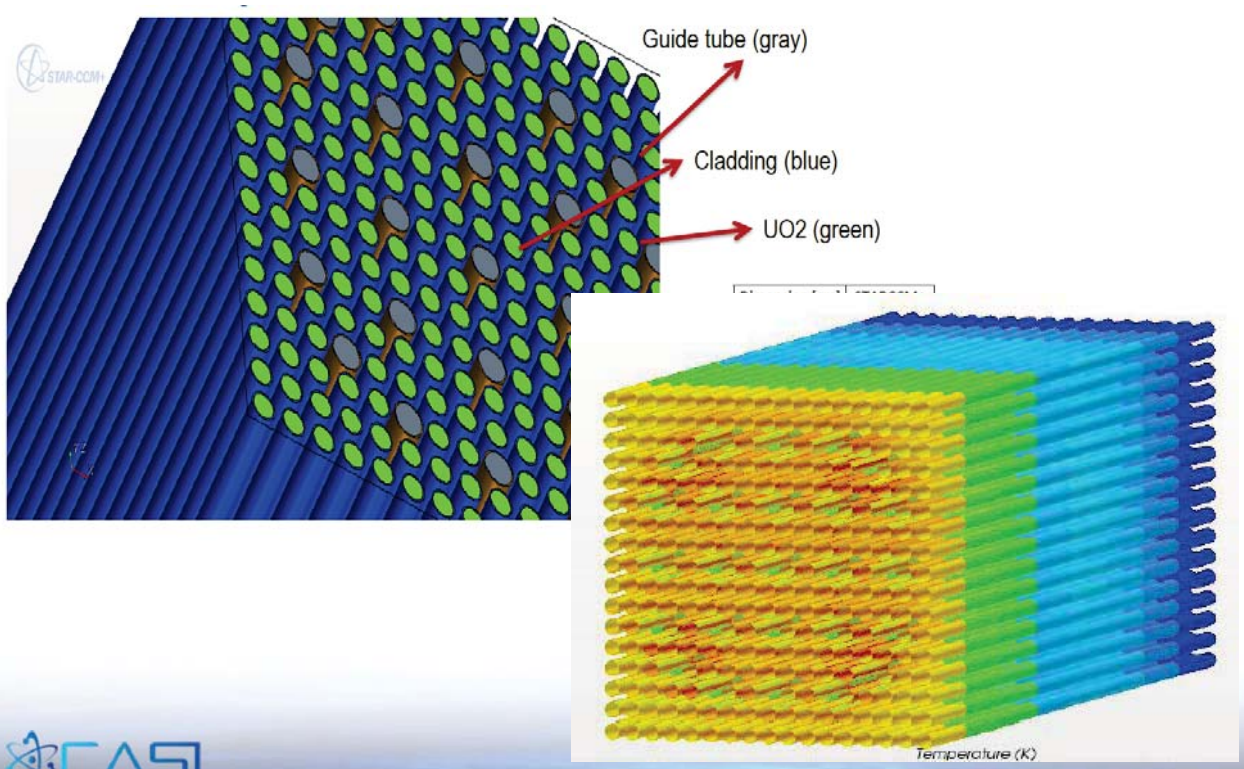






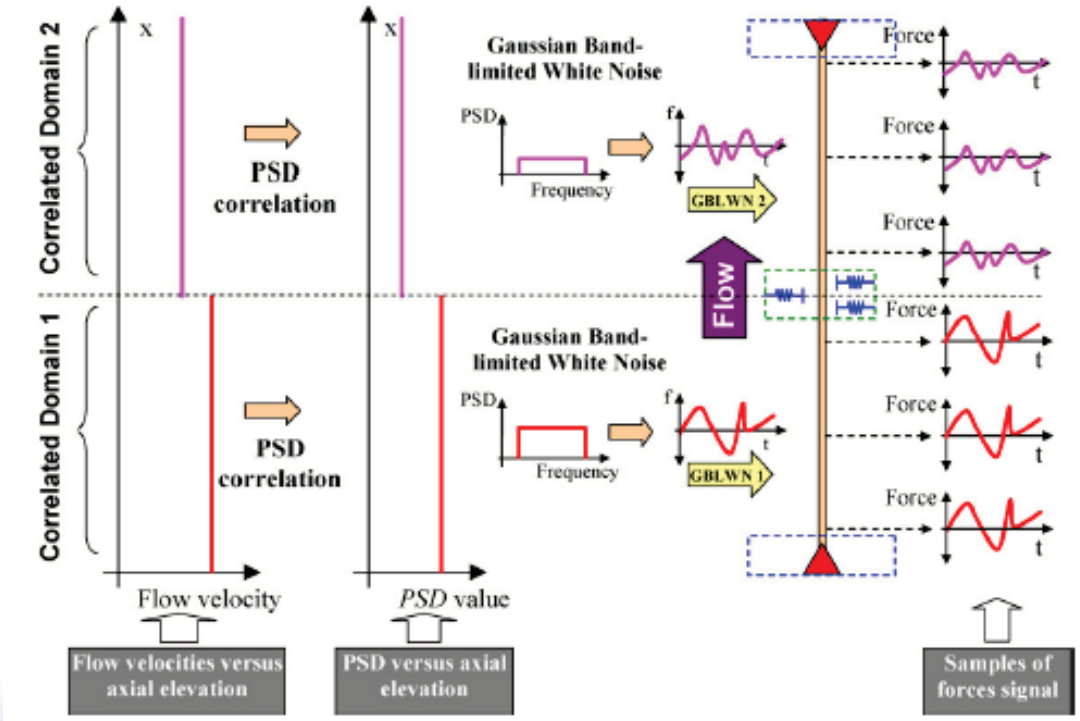
16x16 KOFA fuel rods (Kim, 2010)

17x17 Assembly Model



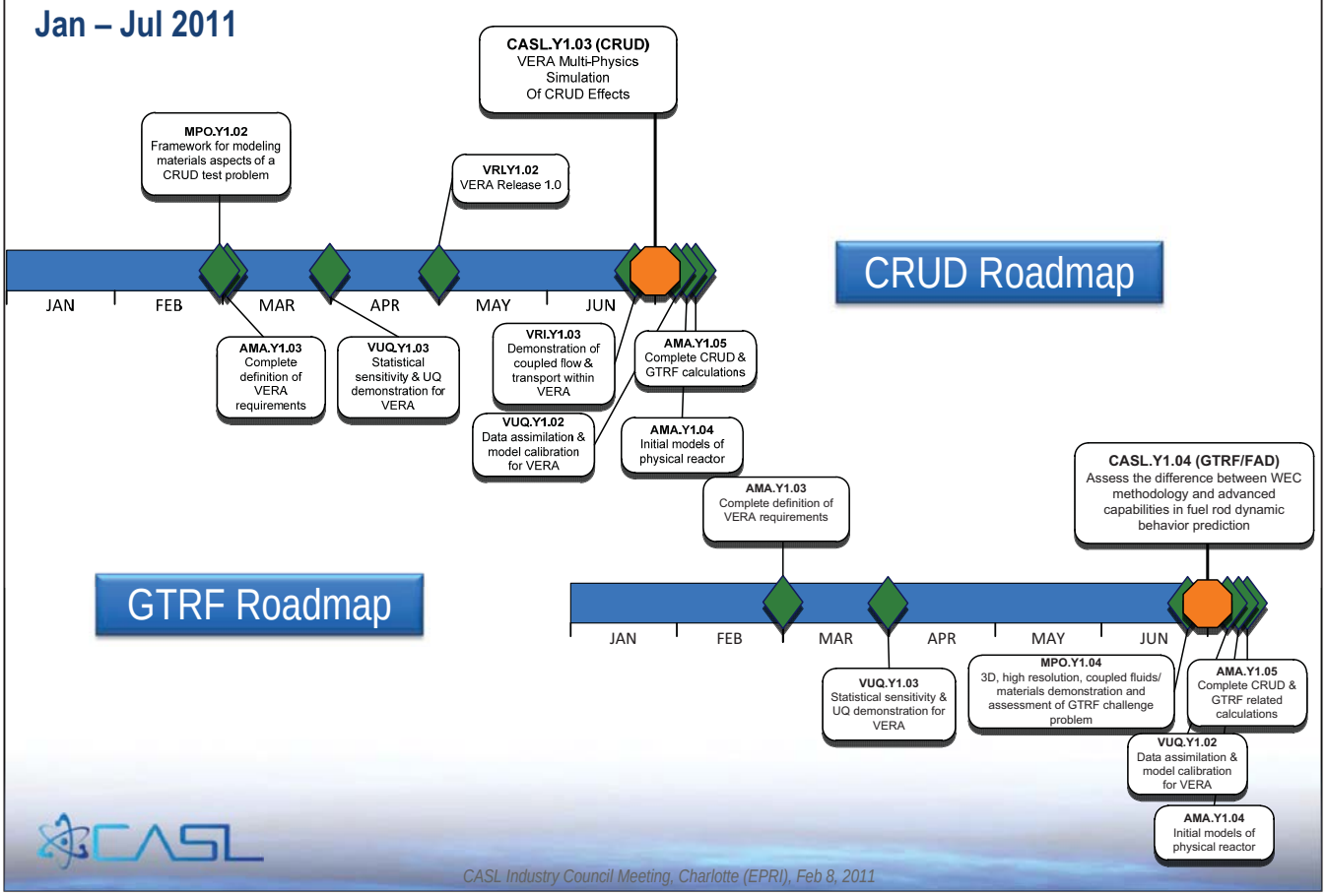
GTRF Baseline Workflow

WEC VITRAN application (Rubiolo and Young, 2009)



Period 2 Plan of Record L1/L2 Milestones

Jan – Jul 2011



PoR-2 Milestone Roadmap

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

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

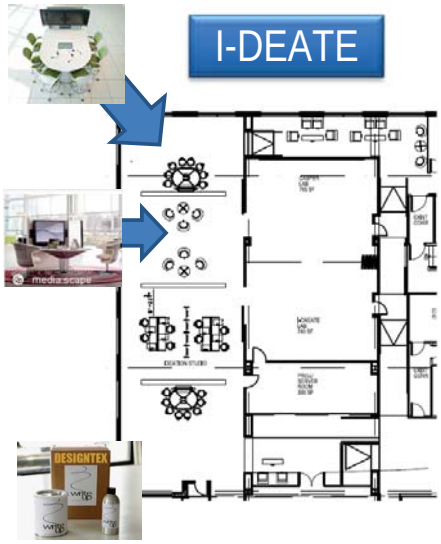
Collaboration and Ideation (C&I)

- Create a state-of-the-art scientific collaboration space, a space that will support the cognitive convergence of the best LWR scientists, engineers, and industrialists available under “one-virtual-roof”
- Understand CASL’s C&I needs, evaluate existing and new tools and capabilities, make recommendations, identify paths for research and development of technology gaps, and take on responsibility of overseeing the implementation, including testing and validation.
- Virtual one-roof efforts
  - *Synchronous Communication*: Immersive Telepresence & video desktop collaboration
  - *Online collaboration tools*: Webex, ReadyTalk, EVO, Live Meeting
  - *Sharing data (viz) between electronic venues*: Conduit, CAVELIB, Chromium, Visit, etc.
  - *Connectivity to HPC resources*: democratization to all CASL partners
  - *Assist in HCI design for CASL end user*: standardize design and interaction

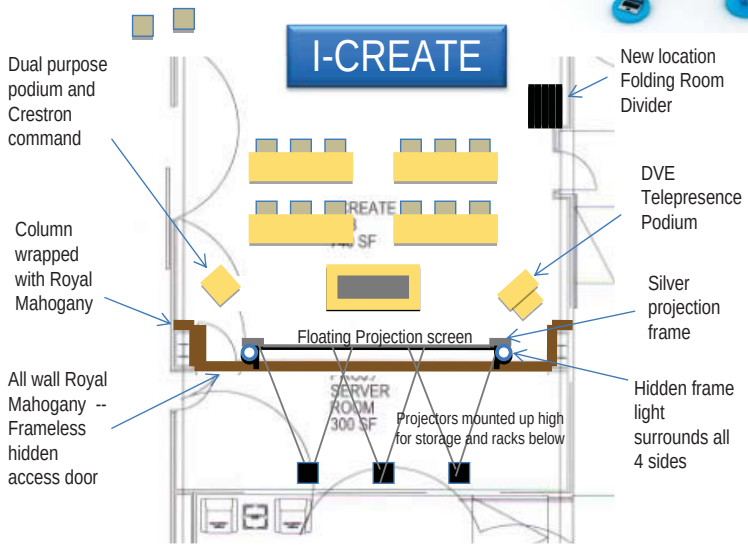
Problem solving at the speed of human insight

Collaboration & Ideation Venues

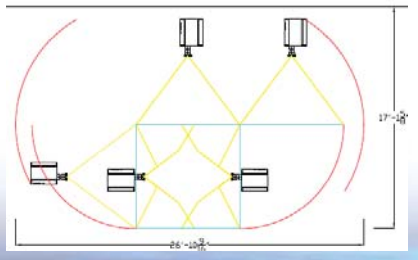
I-DEATE



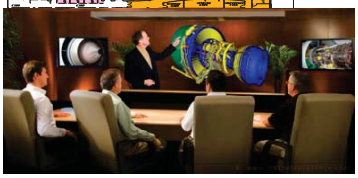
I-CREATE



I-VAC



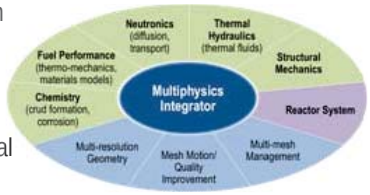
Achievements the First 6 Months



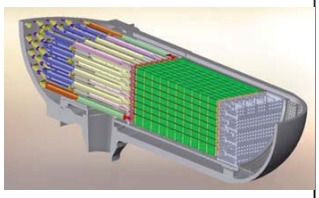
◆Operational Achievements

- ❑ Building out HQ Facility: 5600/5700 redesign with HQ & partner virtual collaboration (I-DEATE/I-CREATE) & design (IVAC) centers
- ❑ Bringing up operations and operational team
- ❑ Stood up Board of Directors, Councils, best-practice program management processes

◆Technical Achievements

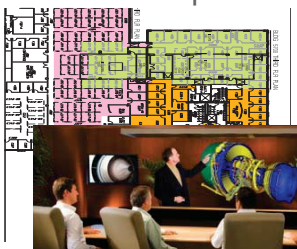


- ❑ Successfully met all major technical milestones in first five months of execution
- ❑ Established the CASL virtual reactor "software repository" known as VERA (Virtual Environment for Reactor Analysis) and integrated 8 different computational capabilities from CASL partners (including 2 WEC codes and 1 commercial code) into the common VERA software environment
- ❑ First release of Version 0.5 of VERA to CASL partners
- ❑ Application of advanced radiation transport and computational fluid dynamics in VERA virtual reactor to a operational PWR sub-core scenario to demonstrate feedback coupling and contrast predictions with Westinghouse coupled tool predictions.
- ❑ State-of-the-art sensitivity and optimization capability integrated within VERA to support uncertainty analysis of nuclear reactor operational and safety scenarios
- ❑ Development of requirements and validation plan to support and guide CASL virtual reactor development
- ❑ Comprehensive plan developed for upscaling fundamental and improved fuel, materials science, and coolant chemistry research efforts into operational reactor analysis and design workflows with VERA

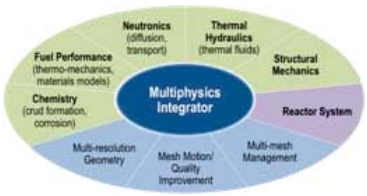


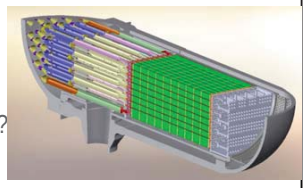
Outstanding Challenges

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



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





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

Focus Area Status Reports

Industry Council Meeting
February 8, 2011

Doug Kothe
Director, CASL

Paul Turinsky
Chief Scientist, CASL

Jess Gehin
Advanced Modeling Applications Lead

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

OAK RIDGE National Laboratory

Materials Performance and Optimization (MPO)

Chris Stanek
MPO Lead, CASL
Los Alamos National Laboratory
Brian Wirth
MPO Deputy Lead, CASL
University of Tennessee
Sidney Yip
MPO Deputy Lead, CASL
Massachusetts Institute of Technology

CASL PoR-2 Plans
January – July 2011

OAK RIDGE National Laboratory

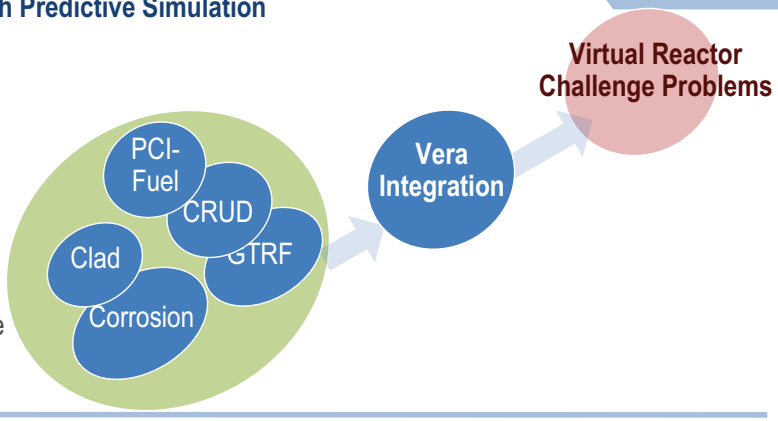
Materials Performance Optimization (MPO)

Chris Stanek
Brian Wirth
Sid Yip

Enabling Improved Fuel Performance through Predictive Simulation

Objectives and Strategies

- Provide physics-based materials models of CRUD, GTRF and PCI for 3D, multi-physics, virtual reactor simulator
- Improved physics and chemistry insight delivered via constitutive relations
- MPO is comprised a diverse group of computational materials scientists with a wide range of capabilities



Requirements Drivers

- MPO enables solutions to CASL challenge problems by delivering a multiphysics, multiscale materials M&S capability to the CASL virtual reactor
- What does MPO need to be successful?
  - Industrial guidance for problem definition
  - Experimental data, both full scale reactor tests and unit mechanisms
  - External program leverage, e.g. EFRCs, FCRD, etc.

Outcomes and Impact

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

Materials Performance Optimization (MPO)

Selected Year-1 Activities	Selected Year-1 Milestones
• Familiarization of current industry knowledge to establish CRUD, GTRF and PCI test problems, including acquiring the supporting validation database	3x L3 11/30-12/31/2010: Assess available experimental data and define test problem for CRUD, GTRF and CRUD
• Delivery of initial high-resolution, 3-D, coupled physics modeling framework for all three challenge problems, and identification of initial materials/chemistry constitutive relationships	3x L2 12/31-4/29/2011: Deliver a structural mechanics (or materials) framework for a GTRF, CRUD and PCI challenge problems to VRI
• Initiation of supporting microscale chemistry and physics activities for all three challenge problems, to improve fidelity of fuel performance models.	L2 7/01/11: Conduct 3-D, high resolution, coupled fluids/materials demonstration and assessment of GTRF challenge problem (co-owned by VRI)

Models and Numerical Methods (MNM)

Methods Development for Transport, T-H, and Multiphysics Coupling

Bill Martin (Michigan)
Rob Lowrie (LANL)

CASL PoR-2 Plans

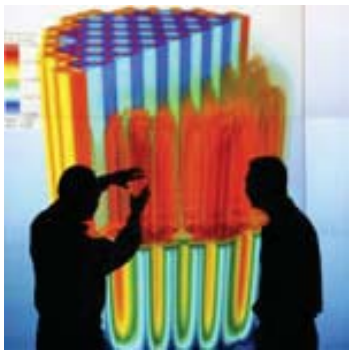
January – July 2011

Models and Numerical Methods (MNM)

Developing the transport, T-H, and multiphysics models for VERA

Objectives and Strategies

- MNM will deliver radiation transport and T-H component models for integration into VERA.
- Two projects combine to form the MNM focus area:
  - Radiation transport
  - Thermal-hydraulics
- These projects include (or enable) multiphysics coupling



Outcomes and Impact

- MNM will deliver state-of-the-art radiation transport and T-H models, including coupled multiphysics models, for integration into VERA.
- MNM success can be measured by
  - Successful implementation into VERA and application to Challenge Problems
  - MNM models chosen for use in VERA (versus existing industry solutions)
- MNM success will transform industry analysis, enabling tightly-coupled, high-fidelity simulation for Challenge Problems as well as routine reactor analysis.

Models and Numerical Methods (MNM)

Selected Year-1 Activities	Selected Year-1 Milestones
• Define MNM benchmark suite for transport, T-H, and multiphysics • Coupled neutronic/T-H simulation of full core PWR (DeCART and Star) • Development of scalable, multilevel energy-space-angle eigensolver for 3D Sn transport code on Jaguar • Development of hybrid Monte Carlo capability with CMFD acceleration • Evaluation of existing codes and algorithms for further development into VERA-CFD • State-of-the art turbulent flow calculations for GTRF • Development plan for non-proprietary T-H code (VERA-CFD)	• L1 (12/31/2010): Coupled DeCART/Star for PWR sub-core scenario with W predictions • L2 (6/30/2011): Full-core 3D MOC transport with single phase T-H coupling • L2 (6/30/2011): Benchmark test suite for CFD, ITM, transport, and coupled physics analysis • L3 (6/30/2011): Determine development plan for Monte Carlo and hybrid transport capability • L3 (1/31/2011) Document implementation plan for next-generation flow simulation capability (VERA-CFD) • L3 (6/30/2011) Compute turbulent excitation forces on 3x3 GTRF problem with various turbulence models • L3 (6/30/2011) Evaluate NPHASE-CMFD code on a leadership computer system

Virtual Reactor Integration (VRI)

Code Development and Integration
Software Process and Quality

John A. Turner (ORNL)
Randy Summers (SNL)
Rich Martineau (INL)

CASL PoR-2 Plans

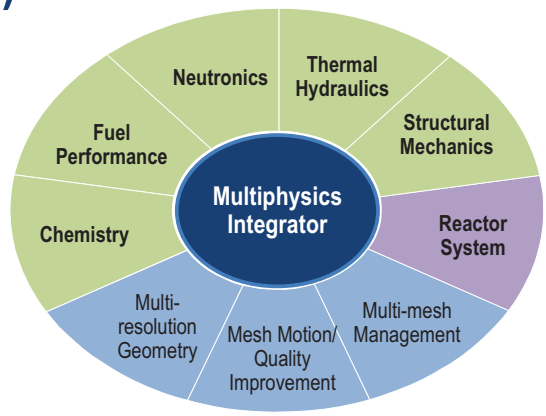
January – July 2011

Virtual Reactor Integration (VRI)

Bridging the gap between research and engineering.

Objectives and Strategies

- VRI will deliver a suite of robust, verified, and usable tools within a common multi-physics environment for the design and analysis of nuclear reactor cores, with quantified uncertainties.
- Three projects combine to form the VRI focus area:
  - VERA: Virtual Environment for Reactor Applications
  - VERA Physics Simulation Suite (PSS)
  - Challenge Problem Integration



Outcomes and Impact

- VRI will deliver the environment described above, portions of which will be openly-available.
- VRI success can be measured by
  - downloads of the open portion(s) of VERA
  - measurable use of VERA by industry partners in understanding and mitigating key issues
- VRI success will transform industry analysis, bringing tightly-coupled, high-fidelity simulation into daily engineering workflows.

Virtual Reactor Integration (VRI)

Selected Year-1 Activities	Selected Year-1 Milestones

• Establishment of Agile software development processes
• Deployment of integrating software environment (LIME)
• Integration of initial physics components for challenge problems
• Assessment of mesh management options and integrate initial capability
• Coupling of selected initial physics components
• Integration of DAKOTA into VERA for UQ and optimization
• Workflow analysis and design
	• L3 (10/29/2010): LIME Release
	• **L2 (12/17/2010): VERA Release 0.5**
	  – **integration of existing physics components**
	• L3 (2/28/2011): RAVE components fully integrated
	• **L2 (3/31/2011): VERA Release 1.0**
	  – **initial coupling of existing physics components**
	• L3 (3/31/2011): Initial mesh interpolation capability
	• L3 (5/31/2011): Workflow design specification
	• **L2 (6/30/2011): Initial demo of tightly-coupled flow/heat transport and neutronics**

Validation and Uncertainty Quantification (VUQ)

Methods and Software for Achieving Credible, Predictive M&S Capabilities

Jim Stewart (SNL)
Dan Cacuci (NCSU)

CASL PoR-2 Plans

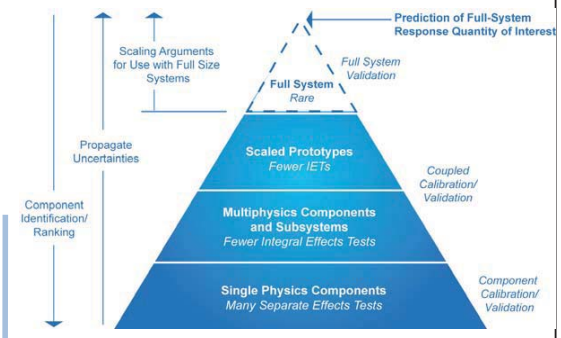
January – July 2011

Validation and Uncertainty Quantification (VUQ)

Achieving credible, science-based predictive M&S capabilities

Objectives and Strategies

- VUQ is dedicated to developing overall V&V approach
- We will develop new methods for the VUQ *capability areas*
  - Project 1: Verification, Validation, and Data Assimilation
  - Project 2: Sensitivity Analysis and UQ
- VUQ is the CASL "integrator" – V&V and UQ methods and tools are needed by every Focus Area



Outcomes and Impact

- VUQ will deliver continuous evolution towards transformational, predictive M&S
- VUQ success can be measured by the ability to quantify and reduce uncertainties for the CASL challenge problems
- VUQ success will transform the way experiments and simulations work together, leading to new capabilities for predictions, *with confidence*, of scenarios for which experimental data is not directly available

Models and Numerical Methods (MNM)

Selected Year-1 Activities	Selected Year-1 Milestones
• Establish VUQ-led committees – Cross-FA Working Group – Validation Data Committee • Integrate key software tools into VERA (DAKOTA and Percept) • Develop VUQ procedures and workflows • Develop and analyze VUQ case study problems • Perform verification study on a benchmark T-H problem • Perform *Predictive Maturity* assessments (PCMM) • Develop new capabilities for data assimilation, sensitivity analysis, and UQ	• **L2 (12/31/2010): Integrate DAKOTA into VERA** • L3 (1/31/2011): Complete initial review of experimental data and plant observations related to CRUD and GTRF challenge problems • L3 (3/31/2011): Stand up a VUQ-led Cross-Focus Area Working Group • **L2 (6/30/2011): Enable generalized data assimilation and model calibration for VERA** • L3 (6/30/2011) Develop mathematical data assimilation framework • L3 (3/31/2011) Develop a VUQ practices document • **L2 (6/30/2011): Enable statistical sensitivity and UQ demonstrations for VERA** • L3 (3/31/2011): Apply SA and UQ capabilities to VUQ case study application

Advanced Modeling Applications (AMA)

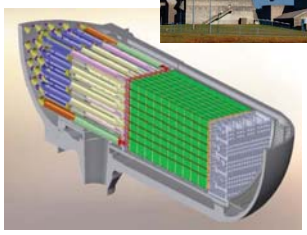
Jess Gehin (ORNL)
Steve Hess (EPRI)
Zeses Karoutas (Westinghouse)

CASL PoR-2 Plans

January – July 2011

Advanced Modeling Applications (AMA)

Driving development of VR to support real-world users and applications



Objectives and Strategies

- Ensure that CASL R&D meets user needs and requirements
- Applications of VERA and CASL tools through AMA projects:
  - Supporting validation of VERA
  - Performing modeling of physical reactors (WB1 & WB2)
  - Analyzing challenge problems

Outcomes and Impact

- AMA will provide demonstrated applications of CASL capabilities to physical reactors and challenge problems
- Metrics for success include qualification of the CASL capabilities with operational data from TVA reactors and successful application to the CASL challenge problems
- The impact of this activity will be a clear demonstration that the tools can be used to solve problems of interest to the nuclear industry and early deployment through use at the CASL industry partners

Advanced Modeling Applications (AMA)

Selected Year-1 Activities	Selected Year-1 Milestones
• Define functional and user requirements for VERA • Development of VERA models of WB1 • Development of challenge problem specifications, testing problems, validation data sets • Perform analysis of CRUD and GTRF challenge problems • Development of initial validation plan (working with VUQ) • Initiate engagement with NRC • Assessment of VERA version 1.0 against requirements	• L1 (6/30/2011): Analysis of CRUD problem with coupled VIPRE/ANC/BOA • L2 (12/31/2010): Initial Validation Plan • L2 (2/28/2011): Complete VERA Requirements • L2 (6/30/2011): Complete coupled CRUD and GTRF related calculations • L3 (6/30/2011) Complete models and analysis of physical reactor with VERA • L3 (3/30/2011) Complete initial model development of CRUD challenge problem (neutronics/TH) • L3 (3/30/2100) Complete initial model development of GTRF challenge problem (CFD) • L3 (6/30/2011) Complete validation hierarchy with VUQ for CRUD, GTRF, and PC

CASL as a Resource for Technical Solutions

Materials Performance Optimization (MPO)

Technology Solutions

A multiphysics capability to address materials performance issues critical to CASL challenge problems CRUD, GTRF and PCI

- Framework receptive to improved physics and chemistry models
- Multiphysics coupling, e.g. using CFD to generate high res PSD for wear/fatigue models for GTRF
- Multiscale materials modeling and simulations, state-of-the-art and beyond
- Integration of UQ, verification, and optimization
- Potential for science-based innovation (life extension)

Models and Numerical Methods (MNM)
Technology Solutions

- Full-core, pin-resolved transport capability with tightly-coupled T-H, structural, and materials response
- Validation test suite for transport, T-H, and coupled multiphysics
- Production hybrid/Monte Carlo capability for routine design/analysis
- Deployment of VERA-CFD: Non-proprietary (open to collaboration), scalable, verified and validated T-H tool that complements capabilities of existing commercial codes
- Generate microscale T-H simulation results and experimental data for T-H closure models and validation, including for multiphase flow and boiling models

Virtual Reactor Integration (VRI)
Technology Solutions

- **Agile software development process lessons-learned**
  - application to a multi-institutional, geographically-distributed, goal-driven, scientific research program
- **software and numerical approaches for component-based coupled-physics simulations**
  - integration of components of varying heritage
  - managing intellectual property issues
  - integration of UQ, verification, and optimization
  - numerical challenges, including mesh mapping
- **transforming an established design/analysis workflow**

Validation and Uncertainty Quantification (VUQ)
Technology Solutions

- New, state-of-the-art data assimilation capabilities
  - Accounting for modeling errors, nonlinear effects, and experimental uncertainties
- Validation data requirements and specifications for validation database
- New capabilities for *robust and efficient* sensitivity analysis and UQ
  - Handling all sources of uncertainties including discretization errors, integrated with robust verification procedures
- Best-estimate predictive capabilities with quantified predictive maturity assessments

Advanced Modeling Applications (AMA)
Technology Solutions

- Coupled physics analysis of physical reactors (WB1/WB2) using state-of-the-art VERA tool set
  - Analysis performed with near-term/existing tools (VIPRE/ANC)
  - Analysis performed with advanced tools (CFD/DECART-DENOVO)
- Analysis of challenge problems using VERA tool set
  - Coupled physics models to provide more insight into challenge problem physical phenomenon to support understanding of drivers
  - Analysis of challenge problem experiments provides data for validation of VERA
  - Analysis in support of CASL goals related to power uprate, life extension
- Development of “test-stand” concept to demonstrate how the advanced mod/sim tools can be integrated into engineering environment

VERA Requirements Document

Stephen M. Hess (EPRI)
AMA Deputy Lead

CASL Industry Council
12 January 2011

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

OAK RIDGE National Laboratory

Presentation Purpose

Provide information to CASL Industry Council on VERA Requirements Document and Obtain Feedback / Suggestions for Consideration

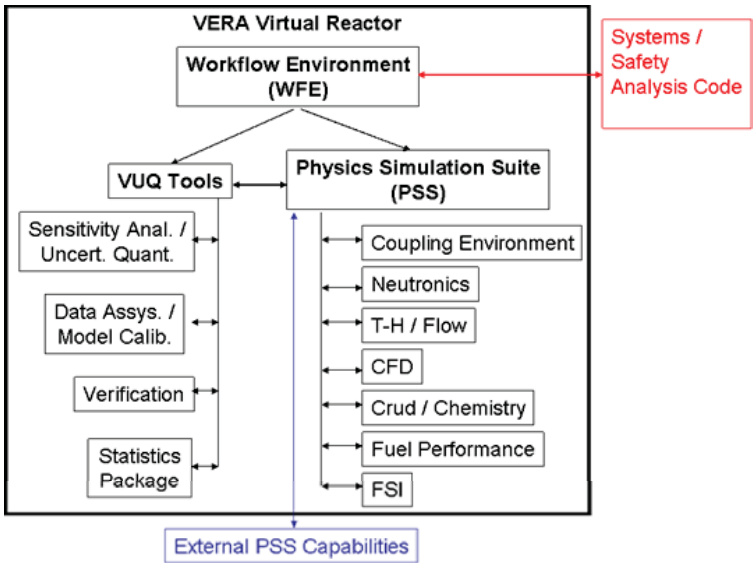
Presentation intended to support discussion to identify improvements / enhancements to VERA Requirements Document from perspective of industry end users

Purpose and Responsibilities

- Purpose: define requirements for VERA modeling and applications software
- Responsibilities:
  - Setting of requirements owned by AMA FA Lead
  - Individual FA Leads responsible for managing development / testing performed under their respective FAs
  - SLT responsible for approval of requirements and changes to them

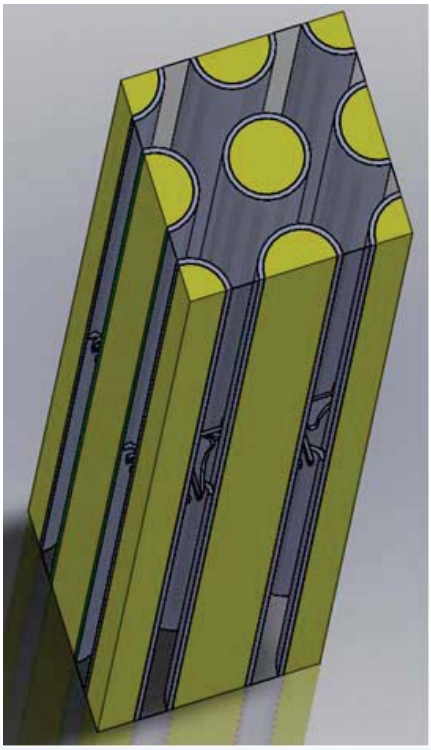
Functional Requirements

- Models and Couplings
- Workflow Environment
- Meshing
- Technical Capabilities
- Modularity



Challenge Problems

- Challenge Problems represent framework within which VERA will be developed and validated
- Separate Challenge Problem Technical Specifications provide detailed requirements necessary to address technical aspects of each challenge problem
- Suggested scale-up sequence
  - Reduced 3x3 pin geometry array standard test bench
  - Full 5x5 pin geometry array
  - 17x17 pin fuel assembly
  - 3x3 fuel assembly array
  - ¼ core geometry
  - Full core geometry (which may include asymmetries)



End User Capabilities / Data Management

- End User Instructions / Capabilities
  - Select / setup / link / modify models
  - Execute application simulation on selected computational platform
- Data Management
  - Visualize and analyze data and results
  - Manipulate / edit / store / transfer simulation output data
  - End user capability to add user specified / proprietary information

Quality Assurance / V&V-UQ

- VERA will NOT be developed to conform to 10CFR50 App B requirements BUT will be developed with sufficient QA to permit upgrading at time when applications / regulatory interface would require it
- Basic QA Plan
  - Conform to ASME NQA-1 to greatest extent practicable
  - Written software testing plans (approved / controlled under responsibility of VRI FA Lead with concurrence of AMA FA Lead)
  - Acceptance of test results approved by the SLT
  - Documentation and Records
  - Forums for user support and training
- V&V-UQ: Validate VERA predictions for each challenge problem:
  - Quantification of key modeling parameters and their uncertainties
  - Verify uncertainties are properly propagated through intermediate calculations
  - Verify predictions obtained and their uncertainties correspond to available operational or testing data that representative of phenomena modeled

CASL Industry Council

Report on Themes for Industry Council Activities

John Gaertner

February 8, 2011

Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

OAK RIDGE National Laboratory

Themes and CASL Interfaces

1. IP, Licensing and Distribution of VERA and Ancillary Products
2. Technical Content and Configuration of VERA – interim versions, modularity, generic vs W-4 loop, extent of coupling, including un-validated modules, …
3. Specifying Functional Requirements – IC review, ordering of priorities, fix what's broken first, define data needs, importance of uncertainty, simulation function
4. Computer Platforms for Development, Testing, and Release
5. Scope of Applications to Support beyond W-4 loop: new plants, BWRs, ex-vessel apps, next fuel problem identification
6. CASL as Center of Excellence; e.g., DARPA, Bell Labs – delivering methods vs tools, problem solving vs code development, publishing results and papers
7. Quality Assurance, Verification, Documentation – NRC interface and eventual acceptance, technical tool vs licensing tool
8. Communications Plan – dynamic two way interface at all times

Themes and CASL Interfaces

1. **IP, Licensing and Distribution of VERA and Ancillary Products**
   - CASL Intends to transfer the new tools "early and often" into the current and future culture of nuclear engineers and produce a multi-physics environment to be used by a wide range of practitioners to conduct predictive simulations.
   - CASL will develop a Commercialization Plan Document. IC will review.
   - ***Interface with Commercialization Council through Jeff Cornett.***
2. **Technical Content and Configuration of VERA – interim versions, modularity, generic vs W-4 loop, extent of coupling, including un-validated modules, …**
   - Strategy established to provide evolution of VERA from a loosely coupled integration of existing codes to a tightly coupled multi-physics environment.
   - Intent is to provide maximum modularity and generic functionality of released versions.
   - Partially validated or unvalidated modules that may result from this project will be available as research products.
   - ***Interface with the VRI Focus Area through John Turner and the Science Council through Paul Turinsky.***

Themes and CASL Interfaces

3. **Specifying Functional Requirements – IC review, ordering of priorities, fix what's broken first, define data needs, importance of uncertainty, simulation functions**
   - The Industry Council will review the VERA Functional Requirements Document prior to release.
   - ***Interface through Steve Hess to the AMA Focus Area. CASL will make a formal written response to IC.***
4. **Computer Platforms for Development, Testing, and Release**
   - CASL will employ high power computer capabilities of the National Laboratories as needed to develop a high performance M&S product and solutions to the challenge problems.
   - CASL intends to provide access to high power versions of VERA for testing and application at ORNL or at "Test Stands" at EPRI, Westinghouse, and TVA.
   - Versions of VERA on more accessible platforms will be produced for applications and release to licensees.
   - ***Interface with the AMA and VRI Focus Areas.***

Themes and CASL Interfaces

5. **Scope of Applications to Support beyond W-4 loop: new plants, BWRs, ex-vessel apps, next fuel problem identification**
   - In order to meet requirements to DOE, CASL will focus on capabilities necessary for the W-4 loop challenge problems within the first five years.
   - CASL will anticipate the use of VERA and CASL technology for other PWRs, BWRs and SMRs and allow for modifications necessary for such applications.
   - CASL will seek funding or collaborations for application and validation of VERA and CASL technology by IC members – data and case studies of existing challenge problems and new problems will be considered.
   - ***Identify collaborations with individual IC members in coordination with the CASL Senior Management Team.***
6. **CASL as Center of Excellence; e.g., DARPA, Bell Labs – delivering methods vs tools, problem solving vs code development, publishing results and papers**
   - CASL will immediately engage the Industry Council to develop a strategy to deliver technical solutions through and in addition to the formal VERA releases and challenge problem applications.
   - ***CASL IC will make formal written recommendations to CASL Senior Management Team***

Themes and CASL Interfaces

7. **Quality Assurance, Verification, Documentation – NRC interface and eventual acceptance, technical tool vs licensing tool**
   - CASL has defined its quality assurance plan as part of the VERA Requirements Document.
   - CASL has no plans to secure regulatory approval within its current scope; but the QA, verification, and documentation will anticipate supporting such efforts.
   - CASL has already engaged U.S. NRC to ensure their early and continuing familiarity with CASL technical developments.
   - ***Interface through Jess Gehin of the AMA Focus Area***
8. **Communications Plan – dynamic two way interface at all times**
   - CASL recognizes the need for a formal communications plan.
   - ***Interface through Ken Nemeth and the Communications, Policy, and Economic Development Council. That council will develop a communications plan.***