Virtual Environment for Reactor Applications (VERA) Workshop

Session 1: Physics and Methods

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The Tennessee Valley Authority

April 1, 2015
The Virtual Environment for Reactor Applications (VERA)

Session 1: Physics and Methods

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April 1, 2015
Hilton Head, SC
# Overview of CASL

**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*

<table>
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<th>Goals</th>
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<td>• Develop and effectively apply modern virtual reactor technology</td>
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<tr>
<td>• Provide more understanding of safety margins while addressing operational and design challenges</td>
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<td>• Engage the nuclear energy community through M&amp;S</td>
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<td>• Deploy new partnership and collaboration paradigms</td>
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**CASL Mission:** provide leading-edge M&S capabilities to improve the performance of operating LWRs
CASL Founding Partners
Simulation Capability Development Focus

VERA: Virtual Environment for Reactor Applications

Interoperability
- Commercial CFD
- Reactor System (RELAP-5, RELAP-7)
- Industry Codes

Chemistry
- Chemistry (MAMBA, MAMBA-BDM)
- CRUD Deposition (MAMBA, MAMBA-BDM)

Thermo-Mechanics
- Fuel Performance (BISON-CASL)

Thermal-Hydraulics
- Subchannel Thermal-Hydraulics (CTF)
- CFD (Hydra-TH)
- VERA-CS

Neutronics
- Neutron Transport (MPACT, Insilico, Shift)
- Isotopics (ORIGEN)
- Cross Sections (AMPX/SCALE)

Geometry / Mesh / Solution Transfer (DTK)

Physics Coupling / Solvers / UQ (MOOSE, Trilinos, PETSc, DAKOTA)

Input / Output (VERAin)

PWRs
VERA Subcomponent Contributions

- **Oak Ridge National Laboratory**
  - Depletion, Cross sections (SCALE/Origen/AMPX)
  - Sn Neutronics (Insilico)
  - Monte Carlo Neutronics (Shift)
  - Solution platforms and coupling (DTK)
  - MOC Neutronics (MPACT)
  - Subchannel Thermal-Hydraulics (CTF)

- **Idaho National Laboratory**
  - Fuel performance (Peregrine/CASL-Bison)
  - Solution platforms (MOOSE)

- **Los Alamos National Laboratory**
  - Computational Fluid Dynamics (Hydra-TH)
  - Coolant Chemistry (MAMBA/MAMBA-BDM)
  - Solution platforms and coupling (PETsc)

- **Penn State University**
  - Subchannel Thermal-Hydraulics (CTF)

- **Core Physics, Inc**
  - VERA-CS code integration and VERAin

- **Sandia National Laboratory**
  - Solution platforms and coupling (Trilinos)

- **University of Michigan**
  - MOC Neutronics (MPACT)

VERA utilizes many software resources; these are the primary physics and infrastructure components used in VERA3.3
Industry Challenge Problems
VERA products and use cases

**Fuel Performance**
- Predict Core Wide PCI Margin using 2D model, then zoom in and Predict MPS PCI fuel failure with 3D single rod model

**CRUD**
- Predict Boron Uptake with a subgrid model for CIPS and predict Crud thickness & corrosion with a subgrid model for CILC

**Cladding Integrity (RIA)**
- Predict PCMI Margin using coupled neutronics and 2D models

**Cladding Integrity (LOCA)**
- Predict PCT – Fuel rod oxidation Margin using 2D core wide fuel performance models coupled with a systems code

**DNB**
- Predict DNB Margin for RIA with coupled 3D neutronics and subchannel T-H, and predict Mixing & DNB threshold with CFD

**GTRF**
- Predict Minimum GTRF Margin core wide using 2D fuel performance models and CFD-predicted excitation forces
Important Modeling Attribute
Multi-Physics Coupling

With rigorous representation of physics feedback, simulations yield higher confidence predictions of core performance.
• Best Estimate + Uncertainty is the current norm
• Moving toward predictions of fuel integrity - versus using a conservative surrogate such as experiencing DNB - will require probability density function predictions
Potential Benefits of Advanced Simulation

• Greater freedom in loading pattern determination
  – Reduction of feed region size

• Improved core product designs
  – Enhanced mixing vane design
  – Crud resistant fuel designs

• Increased operating flexibility
  – Improved load follow capability
  – Power uprates

• Addressing NRC safety concerns
  – Recent LOCA and RIA issues
Example: Flexible Operations

- Load follow is routine at international plants; some domestic utilities are considering the use of load following.
- VERA designed to estimate fuel performance margins in load following conditions:
  - Assess high-risk rods core-wide (2D r-z fuel rod model)
  - Further assess limiting rods (high risk rods using 3D fuel rod model)
  - Inform licensed codes that calculate the specific risk
Example: Optimizing Fuel Design

- Effects of mechanical changes on performance
  - Able to predict relative changes among designs
  - Minimal tuning
  - Allows inclusion of proprietary models

- CIPS
  - VERA tools provide direct method for CIPS evaluation
    - Improved crud/chemistry model
    - Advanced chemical thermodynamics
    - Accurately treat assemblies with power gradients or Gad BAs
    - Fully coupled feedback

- CILC
  - Drill down to predict CRUD-induced accelerated corrosion

CASL tools help optimize designs, minimize costly testing and introduce new products to market faster
Example: Core and Accident Analysis

Full core pin-resolved neutron transport and Monte Carlo benchmark

- **Simplicity**
  - Single deck to run simulator neutronics and T-H
  - Quick to setup (<2hr for a new core) and easy to verify

- **Accuracy**
  - Direct full-core transport calculation
  - Many group cross-sections
  - Coupled physics
  - Pin-resolved results

- **Robustness**
  - Eliminates: Two-step (i.e. lattice physics + nodal diffusion) approach; Pin-power reconstruction; Diffusion theory

Consolidates workflow tasks while achieving more reliable core behavior prediction capabilities
CASL Goals for VERA

- Rigorous physics treatment
  - First principles
  - Multi-physics
- Broader applicability
  - New and old nuclear fuel and core designs
- Higher accuracy
  - Reliable predictions
- Higher Resolution
  - Detailed reactor response
- Convenience of Use
  - Practical computation times
  - Practical input structure
- Leverages High Performance Computing Platforms
  - Cope with large computational burden

CASL Mission: provide leading-edge M&S capabilities to improve the performance of operating LWRs
The VERA Core Simulator
VERA-CS is a specific subset of VERA
## VERA-CS vs. Industry Core Simulators

<table>
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<tr>
<th>Physics Model</th>
<th>Industry Practice</th>
<th>CASL (VERA-CS)</th>
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</thead>
<tbody>
<tr>
<td>Neutron Transport</td>
<td>3-D diffusion (core) 2 energy groups (core) 2-D transport on single assy</td>
<td>3-D transport 47+ energy groups</td>
</tr>
<tr>
<td>Power Distribution</td>
<td>nodal average with pin-power reconstruction methods</td>
<td>explicit pin-by-pin</td>
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<tr>
<td>Thermal-Hydraulics</td>
<td>1-D assembly-averaged</td>
<td>subchannel (w/crossflow)</td>
</tr>
<tr>
<td>Fuel Temperatures</td>
<td>nodal average</td>
<td>pin-by-pin 2-D or 3-D</td>
</tr>
<tr>
<td>Fuel Performance</td>
<td>Empirically-based models for key performance phenomena</td>
<td>Science-based models for key performance phenomena</td>
</tr>
<tr>
<td>Xenon/Samarium</td>
<td>nodal average w/correction</td>
<td>pin-by-pin</td>
</tr>
<tr>
<td>Depletion</td>
<td>infinite-medium cross sections quadratic burnup correction history corrections spectral corrections reconstructed pin exposures</td>
<td>pin-by-pin with actual core conditions</td>
</tr>
<tr>
<td>Reflector Models</td>
<td>1-D cross section models</td>
<td>actual 3-D geometry</td>
</tr>
<tr>
<td>Target Platforms</td>
<td>workstation (single-core)</td>
<td>1,000 – 100,000 cores</td>
</tr>
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VERA Transport Methods

• 3D $S_N$ Discrete Ordinates
  – 3D Transport equation is solved using the method of Discrete Ordinates ($S_N$)
  – $S_N$ solver uses the KBA implementation which solves the problem on a Cartesian grid in a method that can scale efficiently to over 100,000 processors

• Method of Characteristics (MOC)
  – 2D: Transport equation is solved for multiple 2D planes
  – 3D: axial transport problem solved with diffusion approximation using pin-by-pin “nodal” equations
  – VERA’s workhorse; Provides ability to run on smaller clusters (order 5,000 cores).

• Monte Carlo
  – method of particle transport is most rigorous with fewest approximations but requires significant computational resources
Thermal-Hydraulics

• Subchannel methods provide the ability to closely monitor the core coolant
  – 3 field representation (liquid, vapor, droplets)
  – allows for future applications to BWR’s and transient problems

• Simulations can be run without T-H feedback or using subchannel coupling

• CFD is available within VERA
  – The core simulator module doesn’t incorporate CFD at this time
Fuel Performance

• VERA’s fuel performance subcomponent includes faster-running 2-D r-z models of each fuel pin in the core with the core simulator
  – VERA-CS is used to pinpoint areas of interest for sub-region calculations

• VERA’s fuel performance subcomponent also includes the capability for higher fidelity 3D single pin simulations
  – Full 3D with ability to model missing pellet surfaces, cladding flaws, or other specific boundary conditions

Note: the core simulator module includes simplified fuel conduction models for neutronics calculations; these models are not used for fuel performance calculations

Accurate pin-by-pin conditions
Multi-physics Coupling: 2 physics 2-way

• Neutronics + Thermal-Hydraulics

- T-H models internal to the neutronics component
- Coupling with the subchannel T-H component

Both utilize simplified fuel performance models to evaluate fuel and gap thermal conductance
Multi-Physics Coupling
3 physics 2-way
VERA Common ASCII Input

- Simple, intuitive interface to build complex models
- One input for multiple physics codes (cross sections, transport, thermal-hydraulics, fuel performance)
- Free format, minimum characters, and symmetry options

[ASSEMBLY]

```
title "Westinghouse 17x17"
npin 17
ppitch 1.260
```

fuel U21 10.257 94.5 / 2.110
fuel U26 10.257 94.5 / 2.619
fuel U31 10.257 94.5 / 3.100

- cell 1 0.4096 0.418 0.475 / U21 he zirc
- cell 2 0.4096 0.418 0.475 / U26 he zirc
- cell 3 0.4096 0.418 0.475 / U31 he zirc
- cell 4 0.561 0.602 / mod zirc
- cell 5 0.418 0.475 / he zirc

lattice LAT21

```
4
1 1 1 1 4
1 1 1 1 1
1 1 1 1 1
4 1 1 4 1
1 1 1 1 1
1 1 1 1 1
1 1 1 1 1
1 1 1 1 1
```

[CORE]

```
size 15
rated 3411 131.68
apitch 21.5
height 406.337
```

assm_map

```
 1 2 1 1 2 1 2 1 1 2 2
 2 1 2 1 2 1 2 1 2 3
 3 3 3 3 3 3 3 3 3 3
```

crd_bank

```
D - A - D - C -
- - - - - - - -
A - C - - - - B -
- - - - A - SC -
D - - - - - - - -
- SB - SD - - - -
- SB - SD - - - -
C - B - SA - - - -
- - - - - - - -
```
VERA HDF5

- Standardized hierarchical binary format for output
- Accessible by many languages such as FORTRAN, C/C+, Java
- Free utilities available for data viewing, manipulation, post-processing, and visualization

Images created using Visit: [https://visit.llnl.gov/](https://visit.llnl.gov/)
VERA Multi-physics Simulation of PWR Fuel Assembly

- Coupled multi-physics simulation of Westinghouse PWR fuel assembly
  - Neutron transport to calculate power distribution (Sn)
  - Thermal-Hydraulics in coolant (subchannel T-H)
  - Heat conduction in fuel rods (subchannel T-H)
  - Neutron cross sections as function of temperature and density

Lower boron level is more bottom peaked (more negative moderator temp. coeff.)

<table>
<thead>
<tr>
<th>Boron (ppm)</th>
<th>Iters</th>
<th>K-eff</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>11</td>
<td>1.31286</td>
</tr>
<tr>
<td>600</td>
<td>11</td>
<td>1.23344</td>
</tr>
<tr>
<td>1300</td>
<td>11</td>
<td>1.15336</td>
</tr>
</tbody>
</table>

~8 pcm/ppm worth

Grid Depressions

Fast, Epithermal, and Thermal Flux Profiles
VERA was used to simulate startup tests for an advanced reactor design and the results were compared with the reactor vendor’s in-house predictions.

- All figures of merit that were compared were within acceptable limits.
- VERA provided a reduced uncertainty in the rod worths that enabled more flexibility in setting loading patterns.

VERA provides more confidence in startup and cycle predictions.
Results: Fuel Performance coupled with Neutronics and Thermal-hydraulics

Data for a selected rod

- Rod Temperature Distribution
- Cladding Temperature Distribution
- Average Fuel Temperature
- Fission Rate
Questions?
VERA Neutronics
Traditional Industrial Neutronics Method

Pin Powers are reconstructed

Intra-nodal flux shape reconstruction

Pin factors applied

\[ PF_s(r) \equiv \frac{\phi_s(r)}{\phi_s} \]
VERA Transport Methods

- **3D $S_N$ Discrete Ordinates**
  - 3D Transport equation is solved using the method of Discrete Ordinates ($S_N$).
  - $S_N$ solver uses the KBA implementation which solves the problem on a Cartesian grid in a method that can scale efficiently to over 100,000 processors.

- **Method of Characteristics (MOC)**
  - 2D: Transport equation is solved for multiple 2D planes.
  - VERA’s workhorse; Provides ability to run on smaller clusters (order 5,000 cores).

**Monte Carlo**
- method of particle transport is most rigorous with fewest approximations but requires significant computational resources.
Method of Characteristics (MOC)

- MOC has become the most popular transport method within the industry for routine 2-D assembly level analysis.
- MOC enables the solution of the steady-state Boltzmann neutron transport equation in “characteristic” directions, i.e., along rays.
- CMFD acceleration is used for the whole core transport calculation.
- The mesh used is a pin cell much coarser than that used for MOC.
- The effectiveness of the CMFD formulation is in the homogenization of pin cell group constants.
VERA’s 2D/1D Method

• MOC transport physics in radial directions
  - Space is discretized into flat source regions
  - Angle is discretized into predefined directions
  - Equidistant parallel lines are overlaid on the spatial grid and the segment lengths are calculated for each angle

• Uses nodal transport / diffusion in axial direction

More accurate than nodal methods, but less computationally expensive than explicit 3D transport
Monte Carlo Neutronics in VERA

- Integrated depletion
- Fully operational in multiple parallel modes
  - Domain replication
  - Domain decomposition w/overlap
  - Multiple sets
  - Nearest-neighbor, scalable fission bank communication
- Benchmarking validation against B&W experiments and Watts Bar startup data

VERA MC simulation of Westinghouse AP1000 core
Depletion Methodology

\[
\frac{dX_i(t)}{dt} = \sum_{j=1}^{N} \ell_{ij} \lambda_j X_j + \bar{\varphi} \sum_{k=1}^{N} f_{ik} \sigma_k X_k - (\lambda_i + \sigma_i \bar{\varphi}) X_i
\]

\[
\tilde{X}(t) = \exp(At) \cdot \tilde{X}(0)
\]

- Exponential matrix is broken into two components; short lived and long lived
- Nuclides are tracked on a different mesh than transport

Obtain Normalized Region Spectrum and Collapse cross sections to 1 group

Construct Transition Matrix, Eq. (1)

Iterate to next Nuclide, \( X_i \)

Long-lived nuclide? Eq. (5)

Find the chains consisted of short-lived precursors of nuclide, \( X_i \)

Apply Batemen Correction to chains, Eq. (10)

Store transition coefficient in reduced Matrix \( A' \)

More Nuclides?

Yes

Series Solution of Matrix Exponential Method for long-lived nuclides, Eq. (4)

No

Iterate to next Nuclide, \( X_i \)

Long-lived nuclide? Eq. (5)

No

Update the short-lived PND Eq. (8)

More Nuclides?

Yes

No

Converged? Max(|1 - \( X_i^{(l+1)} / X_i^{(l)} \)|) < \( \varepsilon \)

Transport Mesh

Depletion Mesh

No

End
Cross Section and Depletion Libraries

- ENDF-B/VII basic nuclear data library
  - Collapsed to a multi-group library
- Subgroup Self Shielding
- Embedded Self Shielding Method (ESSM) was developed as an alternative self-shielding calculation
- Depletion library included
- Additional Xe/Sm model provides tighter feedback of fission products during iterations
  - equilibrium Xe/Sm
  - peak Xe
  - deplete Xe/Sm
Questions?
VERA Work Shop: Thermal-Hydraulics

April 1, 2015
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VERA has two thermal-hydraulics (T-H) tools
- A computational fluid dynamics (CFD) tool
- A subchannel T-H tool

VERA’s subchannel tool is set up and run using the VERA common input; the CFD tool is not.
VERA-CFD Toolkit

- Hybrid finite-element/finite-volume code built using the CFD toolkit specifically to attack a broad class of incompressible / low-Mach, viscous fluid dynamics problems
- Supports multiple discretization techniques
- Provides I/O interfaces for reading/writing multiple file formats
- Provides run-time parallel domain decomposition
- Linear algebra handled virtually

✓ Lagrangian Hydrodynamics
✓ FVM-FEM Hybrid Navier-Stokes
✓ Rigid Body Dynamics
✓ FEM/FVM Heat Conduction
CASL uses a combined experimental, theoretical, and computational approach

- Integrating Research from 11 Institutions (> 33 Researchers)

VERA - CFD

Experiments
- Fundamental Understanding
- Code Validation
- Multiphase Closure Models

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

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

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

2-phase flow past a V5H spacer grid in a 3x3 rod-bundle showing the central rod, and volume fraction isosurfaces of the bubbly phase
• Repeatable flow patterns are generated by the mixing vanes on the spacer grids of a PWR fuel assembly. These are revealed through CFD flow simulation. Low-pressure regions (the dark blue spots) indicate stable vortices in two of the flow sub-channels; the associated instantaneous velocity vectors shown indicate the presence of swirl in the region downstream of the spacer grid and mixing vanes.
VERA Subchannel T-H

- Subchannel is the primary T-H workhorse for coupled simulations (as opposed to CFD)

- Simplified fuel rod models are included in the subchannel T-H to calculate fuel temperature for neutronics calculations (not used when coupled fuel performance is utilized)
VERA Subchannel T-H

- 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)
- Internal pin conduction model and material properties for reactivity calculations
- Spacer grid terms included
- Parallel Solution (one assembly/processor)
• Quasi-steady state option is used to simulate Normal Conditions of Operation
  - “Quasi” because $\frac{\partial}{\partial t}$ terms are not set to zero

• Convergence criteria for quasi steady state:
  1. Amount of Energy stored in the Fluid
  2. Amount of Energy stored in the Solids
  3. Amount of Mass stored in the system
  4. Global Energy balance
  5. Global Mass balance
Subchannel Discretization

Two sets of meshes

1. Scalar mesh (holds scalar variables)
2. Momentum mesh (holds fluid velocity field)
The subchannel component models conduction inside fuel rods / heated solids / un-heated solid using simplified models.
Equations of State

• Delivers fluid properties (e.g., thermal conductivity, specific heat, viscosity, etc.) to constitutive models and governing equations for:
  – Saturated Liquid / Vapor
  – Superheated Vapor
  – Subcooled Liquid

• Two sources available:
  – IAPWS-IF97
  – ASME 1968
Constitutive Models

- Flow-regime dependent constitutive models for:
  - Inter-phase friction
  - Inter-phase heat and mass transfer
  - Two-phase wall drag
  - Two-phase wall heat transfer

- Flow regimes:
  - $\alpha < 0.2$
  - $0.2 \leq \alpha < 0.5$
  - $0.5 \leq \alpha < \alpha_{crit}$
  - $\alpha_{crit} \leq \alpha$
VERA Accident Analysis
Subchannel Models

- Includes advanced models for accident analysis
  - Expansive flow / heat transfer regimes
  - Radiative heat transfer
  - Grid droplet breakup
  - Grid re-wet
  - Rod re-meshing
  - Non-condensable gases
Simulation of DNB limiting time step for PWR DNB event steamline break without offsite power
Questions?
VERA Work Shop:
Coolant Chemistry / CRUD Capabilities

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Hilton Head, SC
CASL Chemistry Tools

- Simulate three-dimensional crud growth along the surface of a single fuel rod
VERA Chemistry Subcomponent Capabilities

- Models fluid transport within the crud layer and the chemistry/thermodynamics required to treat the coolant chemistry, and several ionic species) including the rate of CRUD precipitation

- Chemistry models include:
  - coolant/crud soluble Li-B-H equilibrium chemistry
  - nickel ferrite (NiFe$_2$O$_4$) deposition/precipitation
  - lithium tetraborate (Li$_2$B$_4$O$_7$) precipitation
VERA Chemistry Physics Approach

- Crud layer is modeled using an adaptive 3D grid in (r, θ, z)
  - Crud surface deposition is enhanced by boiling induced flow into crud layer
  - Time dependent microstructure (porosity) due to NiFe$_2$O$_4$ and Li$_2$B$_4$O$_7$ deposition/precipitation within the pores of the crud

- General non-linear, time-dependent 3D heat transport equation is solved to determine internal crud temperature distribution at each time step
  - Boundary conditions are the rod heat flux and crud surface temperature (or a crud/coolant heat transfer coefficient)
  - Includes internal “heat sinks” due to chimney boiling (vaporization)
  - Includes microstructure (porosity) dependent thermal conductivity

- Mass transport models include:
  - Convective transport of soluble species via boiling induced flow within the crud layer
  - Diffusion of soluble species due to concentration gradients
  - Vaporization due to boiling
  - Models the erosion of the CRUD’s surface due to the turbulent flow of coolant along the surface of the CRUD
VERA Chemistry application: full length pin

Crud temperature (2D profile)

Crud porosity (2D profile)

"Hot Spot" (red) increased CILC risk

Boron (blue) increased CIPS risk

Flow

NiFe$_2$O$_4$

Li$_2$B$_4$O$_7$
Boiling heat power density (W/cm³)

Boiling region moves away from cladding surface as the crud’s pores fill with NiFe₂O₄ and Li₂B₄O₇.

Boron Concentration (mg/cm³)

Boric acid concentrates near cladding surface due to boiling induced Darcy flow.
Coupled Subchannel/CRUD

- CRUD capability has been coupled to subchannel T-H
- Demonstration performed by modeling quarter-symmetry Watts Bar Unit 1 for 360 day cycle
- Power distribution obtained from coupled neutronics / T-H simulation

BOL, no CRUD
Coupled Subchannel/CRUD
Coupled Subchannel/CRUD
Coupled Subchannel/CRUD

CRUD deposited in upper spans on higher powered assemblies
Coupled Subchannel/CRUD

Calculated Steaming Rates
Questions?
Advanced Fuel Rod Modeling Capability for LWRs

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

• Provide physics-based materials models of fuel/clad/internals property evolution to enable predictive modeling of CRUD, GTRF and PCI within 3D, multi-physics, virtual reactor simulator
• Improved physics and chemistry insight delivered via constitutive relations

Leveraging lower length scale models for higher fidelity predictive capability
Fuel behavior is a combination of complex interactions: multiple modeling approaches are required.

Requirements
- Produce Thermal Energy
- Retain Fission Products
- Maintain Structural Integrity

Performance Indicators
- Temperature
- Stress and Strain

Behavioral Mechanisms
- Power, Burnup
- Corrosion, Fission Gas Release
- Swelling, Thermal Expansion, Creep, Irradiation Growth, Cracking, etc.

Atomistic Processes
- Atomic Fission, Lattice Impurities
- Atom Diffusion, Defect Formation and Annihilation, Chemical Reactions, etc.
Geometric Representations: 2D R-Z and full 3D

2-D R-Z model with smeared fuel column

3-D model with discrete pellets

Two Levels of Fuel Performance Predictions for Versatile Applications
Fuel Rod Geometric Representation: R-Θ (Planar)

Simulation of discrete cracks using 180-degree and 90-degree geometric representations

Capability to explicitly model Missing Pellet Surface
Extensive Comparisons with Experimental Data and Comparable Industry tools

- Results comparable to industry codes
- Accommodates burnup effects
- Solver able to support complex power vs. time functions
- Models capture both long-term and instantaneous cladding deformations
- Zr creep and growth constitutive law is functional
- Work is ongoing

Very good progress; more work needed
PCMI - Missing Pellet Surface Analysis

- High resolution 3D calculation (250,000 elements, 1.1x10^6 dof)
- Simulation from fresh fuel state with a typical power history, followed by a late-life power ramp
Results: Missing Pellet Surface

displacements magnified 25x
Transient Fuel Behavior: Reactivity Insertion Accidents

Modeling must be supported by experimental observations

Phase 1
- Pellet Thermal Expansion
  - Pellet-Cladding Contact
  - PCMI Loading
- Cladding Failure by Hydrogen-Induced Embrittlement

Phase 2
- Heat Conduction to the Cladding
  - Increase Cladding Temperature
  - Initiate DNB
  - Decrease Cladding Strength
- Grain Boundary Cracking and Fission Gas Release
  - Increase Rod Internal Pressure
  - Additional Radial Deformation
RIA Fuel Behavior Is Function of Prior Irradiation and Event Conditions

Improved multi-physics and multi-scale modeling methods are necessary to understand:
- Non-uniform power deposition on failure modes
- Cracking and spalling of the corrosion layer under rapid loading conditions
- Tighter coupling between void volume pressure and structural deformations
- Cladding to coolant heat transfer and high temperature material behavior
Transient Modeling
RIA Demo

Pellet Burnup - 75 GWd/tU
Deposited Enthalpy ~120 cal/gm

Radial Temperature Distribution at 0.5 secs
Fast Fluence ~ $1.2 \times 10^{23} \text{n/cm}^2\text{-s}$

Fuel Rod Average Linear Power
Time History

Cladding Stress and Strain Response

Temperature Contour at 0.5 seconds
HALDEN IFA-432 Rod 1 Experiment

He fill gas (1 atm)

UO₂ fuel

Zr-2 clad

114.3 µm gap

radius expanded 5x

Temperature at 7 days

upper TC

lower TC

0.58 m
Halden IFA-432 Rod 1 – BOL Comparison

- BOL comparisons validate power generation, thermal conductivity, thermal expansion, gap closure and heat transfer, and fuel fracture models
- Highly empirical relocation models result in very good comparison, as expected
- Smeared fuel cracking models provide a portion of the “relocation effect” but are more mechanistic-based

Active development ongoing
Lower Length Scale Modeling—Important for Transients

- High temperature thermal creep and creep rupture
- Water side corrosion kinetics for oxide layer crystallography, morphology, and thickness
- Hydrogen uptake, hydride formation, and redistribution
- Xenon diffusion and bubble growth behavior in irradiated UO2 material
VERA Work Shop: Uncertainty Quantification

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The Predictive Code Maturity Model (PCMM) is the process being employed in CASL to measure software quality and maturity. This is an iterative process where one continually works on increasing the lower scores.
VERA-VUQ Subcomponent

- VERA includes a tool for uncertainty quantification and calibration (data assimilation)
- Provides broader and deeper perspective for analysts and decision makers
  - Enhances understanding of risk by quantifying margins and uncertainties (QMU)
  - Improves products through simulation-based design
  - Assess simulation credibility through verification and validation
- Enables QMU and design with simulations in manner analogous to experiment-based QMU and physical design/test cycles – Complements experimental-based QMU

Tailors code iterations to efficiently solve VUQ problems
VERA-VUQ Subcomponent Capabilities

- Parameter studies for basic exploration
- Global sensitivity analysis for parameter ranking/screening
- Design of experiments (supporting SA and surrogate builds)
- Calibration: Bayesian deterministic & stochastic (BE parameter values & joint PDFs)
- Dimensional reduction to address multi-parameter calibration & biased Monte Carlo sampling for UQ
- Automated surrogate (e.g. response surface model) construction
- Recognizing multiphysics filtering effects
- Tailored surrogated-based versions of methods above
- Non-deterministic analysis, e.g., reliability-based design
- Epistemic uncertainty methods

Wide variety of tools for broad applications
The VUQ Tool perturbs the VERA input and runs necessary cases to define uncertainty for parameters of interest.
VUQ Analysis of VERA Subchannel Parameters

- Simulation of a single PWR assembly
  - Hot Full Power, T/H feedback
  - Boron concentration of 1300 ppm, 100% power
  - Power supplied by neutronics held constant
- Quantity of Interest is maximum fuel temperature
- We have three parameters distributions to construct
  - Expert opinion
  - Marginal (independent)
  - Joint distribution

\[ Nu = 0.023 \, Re^{0.8} \, Pr^{0.4} = \theta_1 \, Re^{\theta_2} \, Pr^{\theta_3} \]

Single phase heat transfer
Illustration:
VUQ Analysis of VERA Subchannel Parameters (2)

Bayesian Calibration Reveals Parameter Interactions

Experts assume independent
Illustration: VUQ Analysis of VERA Subchannel Parameters (3)

Capturing the joint distribution

Dittus-Boelter
Results: Coupled Neutronics / Thermal-Hydraulics Studies

• Uncertainties in Dittus-Boelter and McAdams parameters inferred from data with Bayesian calibration
• Neutronics sampled from 100 cross section libraries
Example: Validation Pyramid for CRUD

Macro-scale
- CRUD core-wide distribution
- CRUD mass, composition, and morphology

Meso-scale
- Boron, additive B/Add transport
- Corrosion product CP transport
- B/Add near-wall
- CP near-wall
- Crud temp./dryout
- Microfluid transport
- Precipitation/deposition
- Microstructure

Micro-scale
- Activation energy
- Solubilities
- Diffusion Coeff.
- Rate Coeff.
- Ni-Fe-Zn-Cr-Co-B-O... chemistry/Thermodynamics
- Coolant chemistry, CRUD
VERA Validation Activities

- Each subcomponent is evaluated individually
- VERA coupled subcomponents are evaluated as a group
- Challenge problem applications are evaluated based on a validation pyramid

Example: fuel rod temperature with CRUD deposition

**FUEL**
- Density
- Heat capacity
- Specific heat
- Convection
- Radiation

**THERMAL HYDRAULICS**
- Cross flow
- Single phase heat trans.
- Surface effects
- Bubble drag

**NEUTRONICS**
- Subcooled boiling
- Fission heat
- Moderator density
- Boron density
- Energy per fission

**VERA Validation Activities**
- Gap cond.
- Heat removal
- Gap cond.
Challenge Problem VUQ

- Challenge problem are addressed from the top of the validation pyramid
  - These are integral effects experiments
  - Many physics and a few codes coupled together to produce the solution
  - The following steps need to be done:
    - documentation,
    - solution verification,
    - IET validation,
    - uncertainty quantification.

- PIRTs are used to select parameters of interest for VUQ
- CASL will provide limited VUQ; the user group is expected to fill the gap

VUQ is complex and judicious selection of parameters of interest is key
CASL Validation Examples

- Watts Bar cycle 1
  - Zero power physics tests
  - Progression problem results vs. Monte Carlo

- BEAVRS
  - Zero power physics tests
  - Flux mapping
  - Cycle 1 depletion

- KRISCO
  - Zero power physics tests

- Subchannel
  - Forced convection
  - Turbulent mixing and void drift
  - Single and two phase heat transfer / pressure drop
  - Natural circulation

- Fuel Performance
  - Comparisons with similar industry codes
Questions?
Workshop Participants: Lunch is provided in the Edisto Room