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

Technical Society Meeting of Knoxville

Jess C. Gehin
Oak Ridge National Laboratory

March 3, 2014
The Consortium for Advanced Simulation of Light Water Reactors
A DOE Energy Innovation Hub

Jess C. Gehin
Oak Ridge National Laboratory

Technical Society Meeting of Knoxville
March 3, 2014
CASL
A DOE Energy Innovation Hub in the Office of Nuclear Energy

• First Introduced by Former Energy Secretary Chu 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”

Mission
Provide leading edge modeling and simulation 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 modeling and simulation technology that is deployed and applied broadly within the U.S. nuclear energy industry

Goals
1. Develop and Effectively Apply Modern Virtual Reactor Technology
2. Provide More Understanding of Safety Margins While Addressing Operational and Design Challenges
3. Engage the Nuclear Energy Community Through Modeling and Simulation
4. Deploy New Partnership and Collaboration Paradigms
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
CASL Organization
A diverse multi-institutional leadership team leads to informed decision making
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 ($S_p$, $S_n$, & MOC) and stochastic (MC) models capable of full core analysis with pin-homogenized or pin-resolved detail.
CASL Innovations

**Validation & Uncertainty Quantification**
- Integrating and evolving a state-of-the-art uncertainty quantification, sensitivity, and data assimilation tool into engineering workflows
- Bringing together local ("physical") and geographically distributed ("virtual") contributors in a meaningful and productive way

**Materials Performance and Optimization**
- 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
CASL Scope: Develop and apply a “Virtual Reactor” to assess fuel design, operation, and safety criteria

• Deliver improved predictive simulation of PWR core, internals, and vessel
  – Couple Virtual Reactor to evolving out-of-vessel simulation capability
  – Maintain applicability to other NPP types

• Execute work in six technical focus areas to:
  – Equip the Virtual Reactor with necessary physical models and multiphysics integrators
  – Build the Virtual Reactor with a comprehensive, usable, and extensible software system
  – Validate and assess the Virtual Reactor models with self-consistent quantified uncertainties

Focus on Addressing Challenge Problems to Drive Development and Demonstration
CASL Challenge Problems
Key safety-relevant reactor phenomena that limit performance

CASL is committed to delivering simulation capabilities for

- Advancing the understanding of key reactor phenomena
- Improving performance in today’s commercial power reactors
- Evaluating new fuel designs to further enhance safety margin

Safety Related Challenge Problems

Operational Challenge Problems
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)
VERA Core Simulator (VERA-CS)

- Simulate steady-state reactor operation during depletion
- Contains only neutronics (transport, cross sections, depletion), thermal-hydraulics and fuel rod temperature components
## VERA-CS vs. Industry Core Simulators

<table>
<thead>
<tr>
<th>Physics Model</th>
<th>Industry Practice</th>
<th>VERA-CS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutron Transport</td>
<td>3-D diffusion (core)</td>
<td>Transport-based</td>
</tr>
<tr>
<td></td>
<td>2 energy groups (core)</td>
<td>23+ energy groups</td>
</tr>
<tr>
<td></td>
<td>2-D transport on single assy</td>
<td></td>
</tr>
<tr>
<td>Power Distribution</td>
<td>nodal average with pin-power reconstruction methods</td>
<td>explicit pin-by-pin(†)</td>
</tr>
<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>Xenon/Samarium</td>
<td>nodal average w/correction</td>
<td>pin-by-pin(†)</td>
</tr>
<tr>
<td>Depletion</td>
<td>infinite-medium cross sections</td>
<td>pin-by-pin(†) with actual</td>
</tr>
<tr>
<td></td>
<td>quadratic burnup correction</td>
<td>core conditions</td>
</tr>
<tr>
<td></td>
<td>history corrections</td>
<td></td>
</tr>
<tr>
<td></td>
<td>spectral corrections</td>
<td></td>
</tr>
<tr>
<td></td>
<td>reconstructed pin exposures</td>
<td></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 – 300,000 cores</td>
</tr>
</tbody>
</table>

(†) pin-homogenized or pin-resolved depending on application
Core Simulator Progression Problems Status

**FY11**
- SCALE cross-section processing for DENOVO in VERA
- DENOVO pin cell capability with SCALE in VERA
- #1 2D HZP Pin Cell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #4 HZP 3x3 Assembly CRD Worth
- #5 Physical Reactor Zero Power Physics Tests (ZPPT)
- #6 HFP BOL Assembly (begin Challenge Problem coupling)
- #7 HFP BOC Physical Reactor
- #8 Physical Reactor Startup Flux Maps
- #9 Physical Reactor Depletion
- #10 Physical Reactor Refueling

* Bold text signifies ability to compare to measured plant data*
Problem #5: VERA Modeling Comparisons to Plant Measurements: Zero Power Physics Tests

- TVA’s Watts Bar Nuclear Unit 1 is CASL’s “physical” reactor
- Recently modeled the zero power physics tests performed at start up of the reactor (Cycle 1)
- Zero Power Physics Tests are performed at the startup of each operation cycle to confirm the the core had been loaded correctly and that control rod worth meets safety requirements
- Goal of analysis is to predict critical configurations, control rod worth, differential boron absorber worth and isothermal temperature coefficients.
Neutronics – Insilico

- Part of the Exnihilo environment
- Transport solver is $S_N$ (pin-resolved) or $S_N$ (pin-homogenized)
- Built in cross section processing with XSProc
- $S_N$ uses the KBA implementation which solves the problem on a Cartesian grid and can scale efficiently to over 100,000 processors

Efficient Scaling to Large 3D Problems
Three-Dimensional Core/Vessel Neutronics Model
Fission Distribution for Initial Critical Configuration

Radial Fissions – Initial Criticality

3D Fissions – Initial Criticality
Fission Distribution for Two Different Inserted Control Rod Bank Configurations

Radial Fissions – Bank D Fully Inserted

Radial Fissions – Bank SB Swap
VERA Results for WBN1 Startup Critical Configurations

<table>
<thead>
<tr>
<th>Critical Configuration</th>
<th>VERA k-eff</th>
<th>Difference (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial</td>
<td>1.00122</td>
<td>122</td>
</tr>
<tr>
<td>ARO</td>
<td>1.00157</td>
<td>157</td>
</tr>
<tr>
<td>Bank D In</td>
<td>1.00084</td>
<td>84</td>
</tr>
<tr>
<td>Bank C In</td>
<td>1.00094</td>
<td>94</td>
</tr>
<tr>
<td>Bank B In</td>
<td>1.00081</td>
<td>81</td>
</tr>
<tr>
<td>Bank A In</td>
<td>1.00092</td>
<td>92</td>
</tr>
<tr>
<td>Bank SD In*</td>
<td>1.00073</td>
<td>73</td>
</tr>
<tr>
<td>Bank SC In*</td>
<td>1.00071</td>
<td>71</td>
</tr>
<tr>
<td>Bank SB In</td>
<td>1.00100</td>
<td>100</td>
</tr>
<tr>
<td>Bank SA In</td>
<td>1.00070</td>
<td>70</td>
</tr>
<tr>
<td>Average</td>
<td>1.00094</td>
<td>94</td>
</tr>
<tr>
<td>St. Deviation</td>
<td>0.00027</td>
<td>27</td>
</tr>
</tbody>
</table>

Excellent Agreement with Plant Conditions (keff = 1)
## Control Bank Worth Results

<table>
<thead>
<tr>
<th>Bank</th>
<th>Original Measured Worth (pcm)</th>
<th>Original Measured Worth (pcm)</th>
<th>Worth Difference (pcm)</th>
<th>Worth Difference (pcm)</th>
<th>Relative Worth Error (%)</th>
<th>Relative Worth Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>WBN1</td>
<td>KENO</td>
<td>VERA</td>
<td>KENO</td>
<td>3.3%</td>
<td>4.3%</td>
</tr>
<tr>
<td>D</td>
<td>1342</td>
<td>45</td>
<td>58</td>
<td>3.3%</td>
<td>4.3%</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>940</td>
<td>20</td>
<td>37</td>
<td>2.1%</td>
<td>3.9%</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>871</td>
<td>-1</td>
<td>-11</td>
<td>-0.1%</td>
<td>-1.3%</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>830</td>
<td>44</td>
<td>64</td>
<td>5.1%</td>
<td>7.5%</td>
<td></td>
</tr>
<tr>
<td>SD</td>
<td>495</td>
<td>9</td>
<td>14</td>
<td>2.0%</td>
<td>3.0%</td>
<td></td>
</tr>
<tr>
<td>SC</td>
<td>494</td>
<td>14</td>
<td>16</td>
<td>2.9%</td>
<td>3.4%</td>
<td></td>
</tr>
<tr>
<td>SB</td>
<td>1048</td>
<td>7</td>
<td>10</td>
<td>0.6%</td>
<td>1.0%</td>
<td></td>
</tr>
<tr>
<td>SA</td>
<td>431</td>
<td>22</td>
<td>7</td>
<td>5.2%</td>
<td>1.7%</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>6451</td>
<td>160</td>
<td>196</td>
<td>2.5%</td>
<td>3.0%</td>
<td></td>
</tr>
</tbody>
</table>

✅ Very Good Agreement

†Typical acceptance criteria = 10-15%
Problem 6 – PWR Single Assembly

17x17 Westinghouse Fuel Assembly
Watts Bar Unit 1 Cycle 1

Hot Full Power (HFP)
Beginning of Life (BOL) – no depletion

- Fuel Pins
- Plenum
- End Plugs
- Cladding
- Guide Tubes
- Spacer Grids
- Nozzles
- No Control Rods
Coupling of neutronics and thermal-hydraulics components for hot full-power beginning of life assy.

- Progression problem 6
  - neutronics (cross sections + neutron transport)
  - thermal-hydraulics (fluid flow and fuel/clad temperatures)

- Coupling becomes more complicated with more codes, but we’ve done it.
- Challenges are related more to data transfer than “framework”.

**Diagram:**

- Neutronics (Insilico)
  - Power
  - Fuel/Clad/Fluid Temperature
  - Fluid Density

- Thermal-Hydraulics (COBRA-TF)
  - Power
  - Fuel/Clad/Fluid Temperature
  - Fluid Density
Thermal Hydraulics – COBRA-TF

• COBRA-TF (CTF) subchannel code from Penn. State Univ.
• 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
• Since bringing in for CASL / VERA:
  – dramatically reduced memory usage
  – dramatically increased performance
  – dramatically expanded test coverage
  – implementing parallel version for further reduction in run-times
Coupled Results – Different Boron Concentrations

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

Grid Depressions

<table>
<thead>
<tr>
<th>Boron</th>
<th>Iters</th>
<th>K-eff</th>
</tr>
</thead>
<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

Insilico $S_N$
- 23 energy groups
- 4x4 mesh per pin
- $P_0$ scattering
- QR 4x4 quadrature
- Titan: 1156 cores
VERA Simulation of Hot Full Power Assembly
(neutronics with fluid / moderator temp. feedback)

0 ppmB

1300 ppmB
Coupled Results – Power Level

Higher power level is more bottom-peaked

Grid Depressions

<table>
<thead>
<tr>
<th>Power</th>
<th>Iters</th>
<th>K-eff</th>
</tr>
</thead>
<tbody>
<tr>
<td>70%</td>
<td>11</td>
<td>1.24012</td>
</tr>
<tr>
<td>100%</td>
<td>11</td>
<td>1.23344</td>
</tr>
<tr>
<td>130%</td>
<td>15</td>
<td>1.22643</td>
</tr>
</tbody>
</table>

Insilico $S_N$
- 23 energy groups
- 4x4 mesh per pin
- $P_0$ scattering
- QR 4x4 quadrature
- Titan: 1156 cores
Problem 7: VERA Analysis of Watts Bar 1 Hot Full Power Simulation

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)
- SPN 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 14.5 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

Goal: reduce required memory footprint by 3x and compute runtime by 5x
VERA-CS results for Watts Bar Cycle 1 at startup and full power (no measured results)

Mid-plane Thermal Flux

Exit Coolant Enthalpy
Pin-Resolved Results with Depletion for Watts Bar Cycle 1 at Mid-plane

**Purpose**

- Provide capability to model depletion of reactor core in the Michigan Parallel Characteristics (MPACT) capability
- Track isotopic number densities throughout the core during operation

**Execution**

- Implement depletion methodology into MPACT
- Comparison to experimental and computational benchmarks show very good comparison
- Comparison of 2D core critical boron concentration agrees well with Westinghouse (WEC) methods

![Boron Concentration vs. Effective Full Power Days](chart)

![Images of core at different stages](beginning, middle, end)
VERA Status Summary and 2014 plans

• Accomplishments and Status
  – Build/test infrastructure in place
  – Individual code components integrated
  – Common input defined and implemented for neutronics and subchannel thermal-hydraulics
  – Initial physics coupling (focus on core simulator)
  – Benchmark progression problems 1 – 7
  – Initial comparisons with operational plant data
  – VERA components deployed to WEC for analysis of AP1000

• 2014 Plans
  – Continue individual component development
  – Continue core simulator development including, pin resolved methods of characteristics transport and depletion (complete through problem 10)
  – Continue component integration and coupling (VERA-CS with Peregrine, MAMBA)
  – Validation and Uncertainty Quantification integration
  – Development of common output
Questions?
www.casl.gov or info@casl.gov