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

ANS MC2015 - Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) Plenary Presentation

Nashville, Tennessee

Jess C. Gehin, PhD
Director, Consortium for Advanced Simulation of Light Water Reactors

April 20, 2015
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ANS M&C + SNA + MC 2015
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**CASL’s Mission is to Provide Leading-Edge M&S Capabilities to Improve the Performance of Operating LWRs**

<table>
<thead>
<tr>
<th>Vision</th>
<th>Predict, with confidence, the performance and assured safety of nuclear reactors, through comprehensive, science-based M&amp;S technology deployed and applied broadly by the U.S. nuclear energy industry</th>
</tr>
</thead>
</table>
| Goals  | • Develop and effectively apply modern virtual reactor technology  
• Provide more understanding of safety margins while addressing operational and design challenges  
• Engage the nuclear energy community through M&S  
• Deploy new partnership and collaboration paradigms |
CASL Phase 1 Is Nearing Completion
Five Year Award Period Ends June 30, 2015

✓ Year 1: Build the foundation by evaluating component options for challenge problem investigation
✓ Year 2: Advance the science basis of the M&S technology components
✓ Year 3: Assess, refine, down-selection of components. Begin integration within the multi-physics Virtual Reactor environment
✓ Year 4: Focus on coupling components for challenge problems, improve efficiency, being applications to reactor operations and assess for improvement
✓ Year 5: Continue maturation of the multi-physics Virtual Reactor technology and show applications to challenge problems

Scientific Output in Phase 1

• Virtual Reactor M&S technology integrated, under active development and assessment, and deployed for beta testing
• 113 journal articles
• 362 conference papers
• 219 technical reports
• 118 invited talks
• 493 milestone reports
• 216 programmatic reports
Phase 2 Application Approved by DOE on Jan 30, 2015 – Five Year, up to $121.5M Award

In support of the President’s call during his State of the Union Address to advance an all-of-the-above energy strategy, the U.S. Department of Energy announced on Jan 30, 2015 it would renew funding for CASL, an Energy Innovation Hub established in 2010 to develop advanced computing capabilities that serve as a virtual version of existing, operating nuclear reactors.

“As President Obama made clear during his State of the Union address, reducing carbon pollution and protecting the climate has to be a top priority. CASL’s work to help further our understanding of nuclear reactors, improving safety while also making them more efficient, will help the transition to a low carbon economy.”

- Energy Secretary Ernest Moniz

“The work being done at the Energy Innovation Hub at Oak Ridge National Laboratory is an important part of our country’s ability to innovate and safely maintain our nuclear reactor fleet. I’m glad to see the Consortium for the Advanced Simulation of Light Water Reactors remains a priority as we rely on nuclear power to provide the clean, cheap, reliable energy we need to power our 21st-century.”

- Senator Lamar Alexander
CASL is a National Laboratory, Industry, University Partnership

CASL Contributing Partners

CASL-NERI International Partners
Our Challenge Problems are Focused on Key Industry Reactor Performance Areas

**Core Operation Environment**
Conditions for fuel rod depletion over operating cycle
*Neutronics, Thermal-Hydraulics, Fuel Performance*

- **Pellet-Clad Interaction**
  - Predict Core Wide PCI Margin and Missing Pellet Surface PCI
  - *Neutronics, Thermal-hydraulics, Fuel/Cladding Performance*

- **CRUD**
  - Predict CRUD Thickness Boron Uptake and Impact on Core Power Distribution (CIPS) and Cladding Corrosion (CILC)
  - *Neutronics, Thermal-hydraulics/Fluid Flow, Chemistry*

- **Cladding Integrity**
  - Reactivity Insertion Accident
  - Predict Pellet-Clad Mechanical Interaction
  - *Reactor kinetics, Transient fuel/cladding Performance*

- **Cladding Integrity**
  - Loss of Coolant Accident
  - Predict Peak Clad Temperature and Oxidation Margin given Thermal-Hydraulic Conditions
  - *Fuel/cladding performance*

- **Departure from Nucleate Boiling**
  - Predict DNB Margin for Steam Line Break and RIA and Predict Mixing & DNB
  - *Neutronics, Thermal-hydraulics/Fluid Flow*

- **Grid-to-Rod Fretting**
  - Predict Fluid-Structure Excitation Forces, Grid Gap, and Cladding Wear
  - *Fluid flow, Fuel/Clad Performance, Materials Performance*
CASL is developing a high-fidelity virtual environment for reactor applications (VERA)

Interoperability with External Components

Industry Codes
Reactor System
Commercial CFD

Geometry / Mesh / Solution Transfer

Common Input / Output
front-end & back-end (workflow / analysis)

VERA

Solvers / Coupling / SA / UQ

Neutronics
Insilico
Shift

MPACT

Thermal-Hydraulics
COBRA-TF
Hydra-TH

Fuel Performance
Bison-CASL

Chemistry
MAMBA

Trilinos
libMesh
STK
DTK
DAKOTA
MOOSE
PETSc
VERA Core Simulator Couples Components for Simulating Steady State Operation

Interoperability with External Components

Industry Codes
Reactor System
Commercial CFD

Geometry / Mesh / Solution Transfer

VERA Core Simulator

Neutronics
- Insilico
- Shift

Thermal-Hydraulics
- COBRA-TF
- Hydra-TH

Fuel Performance
- Bison-CASL

Solvers / Coupling / SA / UQ

Chemistry
- MAMBA

Common Input / Output
front-end & back-end (workflow / analysis)
VERA for CRUD Induced Power Shift Component Coupling

Interoperability with External Components

- Industry Codes
- Reactor System
- Commercial CFD

VERA for CRUD Induced Power Shift Component Coupling

CIPS

Geometry / Mesh / Solution Transfer
- DAKOTA
- MOOSE
- Trilinos
- PETSc

Solvers / Coupling / SA / UQ

Neutronics
- Insilico
- Shift
- MPACT

Thermal-Hydraulics
- COBRA-TF
- Hydra-TH

Fuel Performance
- Bison-CASL

Chemistry
- MAMBA

Common Input / Output
front-end & back-end (workflow / analysis)
VERA for CRUD Induced Localized Corrosion – Component Coupling

Interoperability with External Components

- Industry Codes
- Reactor System
- Commercial CFD

Geometry / Mesh / Solution Transfer

- DTK
- libMesh
- STK

Solvers / Coupling / SA / UQ

- DAKOTA
- MOOSE
- Trilinos
- PETSc

Common Input / Output

- front-end & back-end (workflow / analysis)

CILC

Neutronics

- Insilico
- Shift
- MPACT

Thermal-Hydraulics

- COBRA-TF
- Hydra-TH

Fuel Performance

- Bison-CASL

Chemistry

- MAMBA
VERA for Pellet Clad Interaction Component Coupling

Interoperability with External Components

Industry Codes
Reactor System
Commercial CFD
VERA for LOCA Cladding Integrity
Component Coupling

Interoperability with External Components

Industry Codes
Reactor System
Commercial CFD

Geometry / Mesh / Solution Transfer

DAKOTA
MOOSE
Trilinos
PETSc

Solvers / Coupling / SA / UQ

Neutronics
Insilico
Shift
MPACT

Thermal-Hydraulics
Cobra-TF
Hydra-TH

Fuel Performance
Bison-CASL

Chemistry
MAMBA

Common Input / Output
front-end & back-end (workflow / analysis)
Progress on Core Simulator Development

- Multiple routes were originally pursued
  - DECART used for early exploratory work
  - Early results with Sn and SPn (SCALE/Insilco)
  - "Pin Resolved" 2D MOC/1D Low order transport (MPACT)
  - Effort on Monte Carlo development to provide high-fidelity reference solutions

- Current focus is on Pin-Resolved approach
  - Provides more detail needed for challenge problems
  - 2D/1D approach proving to be accurate and efficient

- Completing initial development phase to support multi-cycle depletion

- Verification and Validation is underway
  - Critical experiments
  - BEAVRS, Watts Bar Unit 1, Krsko plant data comparison
  - High fidelity Monte Carlo comparisons

Paper 198 on MPACT by Brendan Kochunas on Monday Afternoon
Current Approach is focused on 2D/1D Methods Implemented in MPACT

- University of Michigan and ORNL team developing advanced core simulator

- Provides pin-resolved capability to support CASL challenge problem needs
  - 2D radial methods of characteristics + 1D axial lower-order transport
  - Sub-group and embedded self-shielding method cross section processing
  - ORIGEN-based isotopic depletion

- Leverages ORNL expertise in cross sections, transport, depletion and validation

- CASL supported research:
  - Convergence stability of 2D/1D method
  - Methods for improved sub-pin resonance shielding methods
  - Physics coupling and performance optimization

Paper 253 on Multigroup Library by Keog Seog Kim on Wednesday Morning
COBRA-TF Subchannel T/H Provides Pin-Resolved Capability

- Core simulator T/H provided by subchannel T/H using COBRA-TF (CTF) code being jointly developed by Penn St. and ORNL
- CTF is a two fluid, three-field model (liquid, droplets, vapor)
- Several developments required to support full core pin-cell level resolution:
  - Optimization of COBRA-TF solvers to reduce memory and execution time
  - Spatial decomposition parallelism to reduce run time
  - Preprocessor to automate input development from VERA common input
A Series of “Progression Problems” Developed to Support Development

- Provides a definition of problems to be progressively addressed to achieve needed capability
- Remains as a useful resource for testing and benchmarking codes

- #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
- #6 HFP BOL Assembly
- #7 HFP BOC Physical Reactor w/ Xenon
- #8 Physical Reactor Startup Flux Maps
- #9 Physical Reactor Depletion
- #10 Physical Reactor Refueling

Specifications available on www.casl.gov
**Watts Bar Unit 1 Cycles 1 and 2**

**Progression problems 9 & 10**

- Benchmark Spec provides data for WBN1 zero power physics tests (problem 5), first cycle operation (problem 9) and second cycle shuffle (problem 10)

- Watts Bar Unit 1, Cycle 2 BOC
  - 4 new fuel assembly types
  - include different IFBA loadings
  - Tritium Producing Burnable Poison Rods (TPBARS)
CASL is also Analyzing BEAVRS Benchmark

• Benchmark for Evaluation and Validation of Reactor Simulations
  – Four loop Westinghouse Design
  – Specs prepared by MIT
• Provides 2 cycles of data
  – Detailed assembly designs and core loading
  – Daily power history

Paper 302 on BEAVRS by Ben Collins on Tuesday Afternoon
Cycle 1 Results for Boron Let Down and Flux Map Comparison completed

Boron Let Down

- Calculated CBC
- Measured CBC
- Flux Map CBC

Effective Full Power Days

Critical Boron Concentration [ppm]

Flux Maps

- 2D RMS
- 3D RMS
- Outages
- Power

Effective Full Power Days

Detector Comparisons [%]

Critical Boron Concentration

[Measured - Predicted]
Westinghouse Application of VERA-CS to AP1000 First Core

- **Advanced Core design**
  - Heterogeneous core
  - 5 Fuel Regions
  - IFBA and part-length WABA inserts

<table>
<thead>
<tr>
<th>Region</th>
<th>Fuel Type</th>
<th>Description</th>
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<tr>
<td>A</td>
<td>IFBA</td>
<td>No BA</td>
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<tr>
<td>B</td>
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<td>Short WABA</td>
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<td>D</td>
<td>IFBA</td>
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<tr>
<td>E</td>
<td>IFBA</td>
<td>Intermediate WABA</td>
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<td>F</td>
<td>8-in Solid Blanket</td>
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<tr>
<td>G</td>
<td>8-in Solid Blanket</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>8-in Annular Blanket</td>
<td></td>
</tr>
</tbody>
</table>

**Paper 205 on MPACT Improvements for Modeling AP1000® by Shane Stimpson on Tuesday Afternoon**
Massively Parallel Monte Carlo Capability Provides High Value Reference Solutions

- Monte Carlo research performed by University of Michigan, MIT and ORNL

- VERA Shift Monte Carlo capability combined with Titan supercomputer is being used to provide high fidelity neutronics solutions

- Applied by Westinghouse to generate reference solutions for AP1000® startup
  - Awarded 60 million core-hours on Titan as part of Early Science program
  - AP1000® model created and results generated for reactor criticality, rod worth, and reactivity coefficients

- Large Monte Carlo reactor calculation, 1 trillion particles completed using 230,000 cores

- On-going research to support Doppler Broadening to provide broader range of reference solutions

Paper 180 on Shift by Tara Pandya on Tuesday Afternoon
Poster 6 on Shift at MC Poster Session
Fission Rate Distribution: MPACT Excellent Agreement vs SHIFT Monte Carlo

3D Core x100 Delta Power
MPACT vs. SHIFT (>1.5% dP)

3D Core x100 Delta Power
MPACT vs. SHIFT (Slices)

AO AIC/Plug Transition
MD W/SS Transition
MC W/SS Transition
BISON-CASL: Advanced Fuel Rod Modeling Capability for LWRs

- Purpose is to enhance the modeling of thermal, mechanical, and chemical behavior of LWR fuel using multi-physics and multi-scale methods to reduce uncertainties in performance and safety margins.

- Based on the MOOSE finite element computational framework and leverages the INL BISON nuclear fuel modeling environment.

- Focuses on specific functionality to model the behavior of LWR fuel.

- CASL Research and Development:
  - Advanced material properties and constitutive relationships.
  - Challenge problem specific analysis methodologies.
  - Benchmark and validation efforts working in parallel with development activities.
  - Improved Mechanistic Models of Cladding Deformation.
VERA Computational Fluid Dynamics

• Goal is to provide high-fidelity, scalable fluid flow simulation through complex geometries

• Computational Fluid Dynamics: Deliver scalable, verified and validated CFD tools focusing on LANL Hydra-TH code

• Closure Modeling (CLS): Exploit micro-scale simulation results and experimental data for CFD closure models and validation based on new physical understanding

• CASL research is extending CFD capabilities to provide multi-phase flow
We Are Now Focusing on Advanced Multi-Physics Capabilities:
MAMBA capability Integrated with COBRA-TF For CIPS Challenge Problem

CASL-U-2015-0137-000
CILC Requires Coupling Local Flow Conditions with CRUD Deposition

Investigations performed with coupling of MAMBA and Star-CCM+

- First high-fidelity, two-way coupled CFD/CRUD simulation of a plant cycle
- Axial and azimuthal thermal hydraulic effects dramatically affect CRUD deposition patterns
- Axial and azimuthal CRUD deposition patterns were consistent with plant data

Now Integrating MAMBA as subgrid Model in Hydra-TH

- CRUD deposition simulated directly on fuel rod surfaces.
- Will be applied for subregion of core using CIPS calculation of power history

Paper 31 on CRUD Layer Modeling in MOC by Dan Walter on Wednesday Afternoon
Multi-Physics Coupling For DNB Challenge Problem: Low Flow Steamline Break

**Input Flow Distribution**

**COBRA-TF Enthalpy**

**VERA-CS Power Distribution**

- PWR DNB event - steamline break without offsite power
- Cobra-TF ~45000 channels x 151 axial nodes = ~6.8M control volumes
- Simulation of DNB limiting time step (low pressure/low flow)
- High void predictions in hot channels without VERA neutronic coupling (Center)
- Coupled Neutronics/TH VERA-CS calculations (right)

Paper 176 on CTF Parallelization and Application to DNB by Vefa Kucukboyaci on Wednesday Afternoon
Multi-Physics Coupling to Support PCI Challenge Problem is Under Development

COBRA-TF

Clad heat flux
Clad Surface Temperature

Fluid Temperature
Fluid Density

Power
Fuel Temperature

BISON-CASL

Paper 59 on TIAMAT Development for PCI by Kevin Clarno on Wednesday Afternoon
Paper 244 on Solution Transfer by Stuart Slattery on Thursday Morning
Paper 280 on Anderson Acceleration of Coupling by Alex Toth on Thursday Morning
Plans for CASL Phase 2

- Expand capabilities for PWR Challenge Problems
- Extend and apply capabilities to SMRs (iPWRs)
  - Natural circulation
  - DNB in low-flow conditions
  - CRUD for long-cycle operations
- Extend capabilities to BWR challenge problems
  - Thermal-hydraulic flow regimes
  - Core simulation (sub regions and potentially full core)
  - Fuel performance – PCI, cladding integrity
  - Convective and solute flows and mixing
- Continued releases and deployment to potential end users

Five-year renewal extends CASL into 2020
Thank You for Your Attention!