CASL: The Consortium for Advanced Simulation of Light Water Reactors
A U.S. Department of Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

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What is a DOE Innovation Hub?

- **04/06/2009**: Secretary Chu proposes 8 Energy Innovation Hubs (idea pre-dates Chu)
  - modeled after research entities like the Manhattan Project (nuclear weapons), Lincoln Lab at MIT (radar), and AT&T Bell Labs (transistor)
  - highly-integrated & collaborative teams - solve priority technology challenges to national climate and energy goals
  - problems that have proven the most resistant to solution via the normal R&D enterprise
  - focused, spanning spectrum from basic research through engineering development to partnering with industry in commercialization
  - bring together expertise across the R&D enterprise (gov, academia, industry, non-profits)
  - $25M per yr for 5 years, with possible 5-yr extension

- **06/25/2009**: House bill did not approve any of the proposed Hubs
  - $35M in Basic Energy Sciences for the Secretary to select one Hub

- **07/09/2009**: Senate approves 3 of the proposed hubs, but at $22M
  - Fuels from sunlight (in EERE)
  - Energy efficient building systems (in EERE)
  - Modeling and simulation for nuclear energy systems (in NE)

- **10/01/2009**: Final bill out of conference matches Senate bill

- **01/20/2010**: FOA released, proposals due 03/08/2010

- **05/27/2010**: CASL selected, first funding arrived 07/01/2010
The Consortium for Advanced Simulation of Light Water Reactors (CASL)
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Core partners
Oak Ridge National Laboratory
Idaho National Laboratory
Sandia National Laboratories
Los Alamos National Laboratory
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North Carolina State University
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Electric Power Research Institute
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Challenges
- High visibility
- Geographically-dispersed
- Diversity of experience
- Wide range of motivation / priorities
- Proprietary codes and data
- Role of commercial codes
- Export control
Nuclear Energy Overview
Source: Nuclear Energy Institute (NEI)

- World nuclear power generating capacity
  - 439 plants (U.S.- 104 plants in 31 states)
  - 373 GWe (U.S.- 100.7 GWe, 798.7 TWh in 2009)
  - ~90% capacity factor (>6 GWe added to grid)

- U.S. electricity from nuclear: 20.2%
  - One uranium fuel pellet provides as much energy as:
    - one ton of coal
    - 149 gallons of oil
    - 17,000 cubic feet of natural gas

- U.S. electricity demand projected to grow 25% by 2030
  - 2007: 3.99 TWh
  - 2030: 4.97 TWh

- Nuclear accounts for 73% of emission-free electricity in US
Anatomy of a Nuclear Reactor

Power: ~1170 MWe (~3400 MWth)

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

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

Coolant: pressurized water (2250 psia), $T_{\text{in}} \sim 545^\circ \text{F}$, $T_{\text{out}} \sim 610^\circ \text{F}$, 134M lb/h (4 pumps)

Example: Westinghouse 4-Loop Pressurized Water Reactor (PWR)
Anatomy of a Nuclear Reactor

Core
- 11.1' diameter x 12' high
- 193 fuel assemblies
- 107.7 tons of UO$_2$ (~3-5% U$_{235}$)

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

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

Fuel Pellets
- 9.29 mm diameter x ~10.0 mm high

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

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

~51,000 fuel pins and over 16M fuel pellets in the core of a PWR
# CASL mission is to improve reactor performance (initially currently-operating LWRs)

## Power uprates
- 5–7 GWe delivered at ~20% of new reactor cost
- Advances in M&S needed to enable further uprates (up to 20 GWe)
- **Key concerns:**
  - Damage to structures, systems, and components (SSC)
  - Fuel and steam generator integrity
  - Violation of safety limits

## Lifetime extension
- Reduces cost of electricity
- Essentially expands existing nuclear power fleet
- Requires ability to predict structures, systems, and components aging and life-cycle management
- **Key concerns:**
  - Effects of increased radiation and aging on integrity of reactor vessel and internals
  - Ex-vessel performance (effects of aging on containment and piping)
  - Significant financial decisions to support operation beyond 60 years must be made in ~5 yrs

## Higher burnup
- Supports reduction in amount of used nuclear fuel
- Supports uprates by avoiding need for additional fuel
- **Key concerns:**
  - Cladding integrity
  - Fretting
  - Corrosion/CRUD
  - Hydriding
  - Creep
  - Fuel-cladding mechanical interactions
Fuel failure modes provide motivation for CASL activities

Summary of US fuel failure mechanisms (2000-2008)

* Edsinger, Stanek, Wirth, JOM 63, no. 8 (2011)
Grid-to-Rod-Fretting (GTRF)
CRUD-induced power shift (CIPS)

• deviation in axial power shape
  – Cause: boron uptake in CRUD deposits in high power density regions with subcooled boiling
  – affects fuel management and thermal margin in many plants
• power uprates will increase potential for CRUD growth

Need: Multi-physics chemistry, flow, and neutronics model to predict CRUD growth
Virtual Environment for Reactor Applications (VERA)
A suite of tools for scalable simulation of nuclear reactor core behavior

- Flexible coupling of physics components
  - Toolkit of components
    - Not a single executable
    - Both legacy and new capability
    - Both proprietary and distributable
- Attention to usability
  - Rigorous software processes
  - Fundamental focus on V&V and UQ
- Development guided by relevant challenge problems
  - Broad applicability

- Scalable from high-end workstations to existing and future HPC platforms
  - Diversity of models, approximations, algorithms
  - Architecture-aware implementations

**VERA: Virtual Environment for Reactor Applications**
A suite of tools for scalable simulation of nuclear reactor core behavior
Lightweight Integrating Multiphysics Environment (LIME)

Base LIME software

Input File(s)

Input Files (xml)

Problem Manager

Multi-Physics Driver

Physics Component A
Model Evaluator
Physics Component B
Model Evaluator
Physics Component C
Model Evaluator

Dakota Sensitivity, UQ

Trilinos, NOX Solver Library

“Plug and Play!”

https://sourceforge.net/projects/lime1/
Writing software is easy

• “Writing songs is easy. Writing great songs is hard.”
  – Bono (? couldn’t verify)

• Writing software is easy. Writing great software is hard.

Easier

- single author
- self
- research / exploration
- serial

Harder

- collocated team
- targeted
- prototype
- shared-memory parallel

developers

- geographically-dispersed team
- users
- production
- distributed-memory parallel

platform(s)

- broad community
- regulatory environment
- heterogeneous

CASL
CFD is required for several challenge problems (GTRF, CRUD/CIPS) - remainder of presentation focuses on neutronics...
Discrete Ordinates Methods for Neutron Behavior

- We solve the first-order form of the transport equation:
  - Eigenvalue form for multiplying media (fission):
    \[ \hat{\Omega} \cdot \nabla \psi(r, \Omega, E) + \Sigma(r, E, T)\psi(r, \Omega, E) = \]
    \[ \int dE' \int_{4\pi} d\Omega' \Sigma_s(r, \hat{\Omega} \cdot \hat{\Omega}, E' \rightarrow E, T)\psi(r, \Omega', E') + \]
    \[ \frac{1}{k} \chi(E) \int dE' \int_{4\pi} d\Omega' \nu \Sigma_f(r, E', T)\psi(r, \Omega', E') \]
  - T-H coupling comes through the temperature-dependent material cross sections
- Total number of unknowns in solve:
  - unknowns = \( N_g \times N_c \times N_u \times N_a \times N_m \)
- An ideal (conservative) estimate.
  - (238) x (1 \times 10^9) x (4) x (288) x (16)

\[ \text{unknowns} > 4 \times 10^{15} \]
Current State-of-the-Art in Reactor Neutronics

Pin cell (single fuel pin)
- 0/1-D transport
- high energy fidelity ($10^{2-5}$ unknowns)
- approximate state and BCs

Lattice cell (single assembly)
- 2-D transport
- moderate energy fidelity (7-102 groups)
- approximate state and BCs
- depletion with spectral corrections
- space-energy homogenization

Full core
- 3-D diffusion
- low energy fidelity (2-4 groups)
- homogeneous lattice cells
- heterogeneous flux reconstruction
- coupled physics
Can we approach resolution/fidelity of current 2D analysis in 3D for full core analysis?
PWR-900 Whole-Core Reactor Problem

- 2 and 44-group, homogenized fuel pins
- $2 \times 2$ spatial discretization per fuel pin
- $17 \times 17$ fuel pins per assembly
- 289 assemblies
  - 157 fuel, 132 reflector
  - high, med, low enrichments
- Space-angle unknowns:
  - 233,858,800 cells
  - 128 angles (1 moment)
  - 1 spatial unknown per cell
Performance at scaling on ORNL Titan (Cray XK6)

- full partitioning scales well to 275K cores
- improved interconnect + reduce-scatter have dramatically reduced global reduction cost
- upscatter partitioning more efficient at lower set counts
- roll-over occurs between 4 and 11 sets (5 and 2 groups per set) where serial work in GS solver dominates

- Constant number of blocks = 12,544
- 44 total groups/22 coupled groups
What does this mean?

<table>
<thead>
<tr>
<th>Where we want to be…</th>
<th>Where we are…</th>
</tr>
</thead>
<tbody>
<tr>
<td>• reproduce fidelity of 2D calculations using consistent 3D methods</td>
<td>• assuming 2% peak, we can solve $1.7 \times 10^{13}$ unknowns/hour (XT5)</td>
</tr>
<tr>
<td>• produce all state-points for an 18-month depletion cycle in $O(8 \text{ hours})$</td>
<td>• we can solve a reduced 3D problem ($O(10^{15})$ unknowns) in 175 hours</td>
</tr>
<tr>
<td>• $O(72)$ state points per cycle (1 week steps)</td>
<td>– assumes status quo on a 1 PF/s XT5 machine</td>
</tr>
<tr>
<td>• steady-state, coupled neutronics simulation with T-H feedback = $O(10^{19})$ unknowns</td>
<td></td>
</tr>
</tbody>
</table>

So…

• to reach 2D fidelity at 3D we need to solve $\sim 10^4 \times$ more unknowns
• to run all state points in one day at this fidelity using existing code and methods would require $\sim 140 \text{ EF/s}$
Is it hopeless?

- according to industry partners, a fully-consistent 3D calculation in 1 week would be acceptable
  - factor of 7 (20 EF/s)
- valuable insight possible without reproducing full 2D fidelity
  - factor of 150-200 (100 PF/s)
- utilize GPUs
  - if current projections hold, we can potentially get a factor of 3x-4x improvement by executing sweep kernels on the GPU
- further solver research (multigrid-in-energy) shows promise for reducing iteration counts as well

A 30-40 PF/s machine could allow fully-consistent, 3-D neutronics simulations
GPU Sweep Kernel

- Krylov multigroup solvers allow space-angle sweeps to be performed over all groups concurrently
- ideal for exploiting thread-based concurrency on GPUs
- space-angle sweep for all groups on GPU

<table>
<thead>
<tr>
<th>Performance Improvement factors</th>
<th>GPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>CPU</td>
<td></td>
</tr>
<tr>
<td>XK6 / Interlagos</td>
<td>3.5</td>
</tr>
<tr>
<td>XE6 / dual Interlagos</td>
<td>3.3</td>
</tr>
</tbody>
</table>

Sweep Performance

- CPU/XK6
- CPU/XE6 (actual - hera)
- GPU/TitanDev
Future large-scale systems present challenges for applications

- Dramatic increases in node parallelism
  - 10 to 100× by 2015
  - 100 to 1000× by 2018
- Increase in system size contributes to lower mean time to interrupt (MTTI)
- Dealing with multiple additional levels of memory hierarchy
  - Algorithms and implementations that prioritize data movement over compute cycles
- Expressing this parallelism and data movement in applications
  - Programming models and tools are currently immature and in a state of flux
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Over the life of CASL, these challenges will become increasingly significant at the desktop level
Questions?  http://www.casl.gov/ -or- info@casl.gov
Supplemental
CASL Technical Focus Areas

- Radiation Transport Methods (RTM) and Thermal-Hydraulic Methods (THM)
- Materials Performance and Optimization (MPO)
- Validation and Uncertainty Quantification (VUQ)
- Advanced Modeling Applications (AMA)
- V&V and calibration through data assimilation
- Sensitivity analysis and uncertainty quantification
- Coupled physics environment
- Workflow & usability
- Programing model
- Requirements
- Physical reactor qualification
- Challenge problem application
- Validation
- NRC engagement

All Focus Areas span institutions (labs, universities, industry)
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Virtual Environment for Reactor Applications (VERA)
A suite of tools for scalable simulation of nuclear reactor core behavior

- Chemistry (crud formation, corrosion)
- Fuel Performance (thermo-mechanics, materials models)
- Neutronics (diffusion, transport)
- Thermal Hydraulics (thermal fluids)
- Reactor System
- Structural Mechanics
- Multi-physics Integrator
- Multi-resolution Geometry
- Mesh Motion/Quality Improvement
- Multi-mesh Management
- Workflow (analysis / design / optimization)
- Geometry
- Mesh generation
- Material properties
- Input / user interface
CASL has embraced Agile software development processes

• based on methodologies being used by partners
  – combine attributes of Scrum and Kanban methodologies
  – customized for CASL and refined as needed (iteratively)
• enabled diverse team to be productive very quickly

Start
• users prioritize goals
• team determines work assignments

Execute
• two 30-minute standup meetings each week

End
• deliver and demonstrate to users
• review and plan next iteration

Desirable attributes
• emphasis on collaboration and adaptability
• constant communication / interaction
  – both within team and with user community
• accommodates changing requirements & unpredictability


Agility + Formality
CASL advanced CRUD modeling predictions

- Colored contours: boron concentration within crud layer
- Findings:
  - Crud thickness and boron vary with $T$ variations on cladding surface
  - Crud and boron reduced by turbulence behind mixing vanes

**Fuel rod (80 cm section)**

**Large azimuthal variation in fluid/cladding temperature**

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>100°</th>
<th>200°</th>
<th>300°</th>
</tr>
</thead>
<tbody>
<tr>
<td>605 K</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>595 K</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>585 K</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Spacer with mixing vanes**

**Boron concentration**

<table>
<thead>
<tr>
<th>Time (days)</th>
<th>$[B]$ (mg/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>t = 0 days</td>
<td>$[B]$</td>
</tr>
<tr>
<td>t = 174 days</td>
<td>$[B]$</td>
</tr>
<tr>
<td>t = 318 days</td>
<td>$[B]$</td>
</tr>
<tr>
<td>t = 400 days</td>
<td>$[B]$</td>
</tr>
</tbody>
</table>

**Crud deposition**

- Coolant: linear $T$ increase
- Coolant: linear $T$ increase
- Rod Heat Flux
- Rod Heat Flux

*Image of boron concentration and crud deposition*