Modeling & Simulation Goals and Accomplishments

Paul Turinsky (NCSU), Chief Scientist
On behalf of the CASL Team
(which produced the results to be presented)
S&T Program: Presentation Outline

• Team, Mission & Approach
• S&T Capabilities Needed for Challenge Problems
• Highlighted Accomplishments (to date)

Note addressed is work on supporting experiments, validation data needs, and SQA aspects

Lots to cover, so let’s get on with it!
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

~230 people involved
(most part time)
5 years - $US122M
Prospect for 5 year renewal

Individual contributors
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
Notre Dame University
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 mission: Develop and apply the Virtual Reactor simulator (VERA) to address 3 critical performance goals for nuclear power

1. **Reduce capital and operating costs** per unit energy by:
   - Power uprates
   - Lifetime extension

2. **Reduce nuclear waste** volume generated by enabling higher fuel burnups

3. **Assure nuclear safety** by enabling high-fidelity predictive capability for component and system performance from beginning of life through failure
CASL vision: Create a virtual reactor (VR) for *predictive* simulation of LWRs

**Leverage**
- Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications
- Existing systems and safety analysis simulation tools

**Develop**
- New requirements-driven physical models
- Efficient, tightly-coupled multi-scale/multi-physics algorithms and software with quantifiable accuracy
- Improved systems and safety analysis tools
- UQ framework

**Deliver**
- An unprecedented predictive simulation tool for simulation of physical reactors
- Architected for platform portability ranging from desktops to DOE’s leadership-class and advanced architecture systems (large user base)
- Validation basis against 60% of existing U.S. reactor fleet (PWRs), using data from TVA reactors
- Base M&S LWR capability

**CASL vision: Create a virtual reactor (VR) for predictive simulation of LWRs**
Tackling the Multi-Scale Challenge of Predictively Simulating a Reactor Core

From full core to fuel assembly to fuel subassembly to fuel pin/pellet to meso & micro scales

Time = 2 years
Burnup = 30.3 MWd/kgU
Why think now achievable? Advances in computer hardware, along with comparable advances in numerical solvers, provide computational base.

Current top performance ~ 50 PF
ORNL’s “Titan” Hybrid System: Cray XK7 with AMD Opteron and NVIDIA Tesla processors

**SYSTEM SPECIFICATIONS:**
- Peak performance of 27.1 PF
  - 24.5 GPU + 2.6 CPU
- 18,688 Compute Nodes each with:
  - 16-Core AMD Opteron CPU (141 GFLOPs peak)
  - NVIDIA Tesla “K20x” GPU (1.31 TFLOPs peak)
  - 32 + 6 GB memory
- 512 Service and I/O nodes
- 200 Cabinets
- 710 TB total system memory
- Cray Gemini 3D Torus Interconnect
- 8.9 MW peak power
CASL Challenge Problems (all focused on PWR cores)

Key safety-relevant reactor phenomena that limit performance

Safety Related Challenge Problems

- Departure from Nucleate Boiling
- Cladding Integrity
  - During LOCA
  - During reactivity insertion accidents
  - Use of advanced materials to improve cladding 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

Operational Challenge Problems

- Crud
  - Deposition
  - Axial offset anomaly
  - Hot spots
- Grid-to-Rod Fretting
- Pellet-Clad Interaction
Virtual Environment for Reactor Applications
CASL’s evolving virtual reactor for in-vessel LWR phenomena

Required functional capabilities

VERA
- Thermal-Hydraulics
  - Commercial CFD
  - Research CFD
  - Subchannel Thermal-Hydraulics
- Neutronics
  - Neutron Transport
  - Isotopes
  - Cross Sections
- Geometry / Mesh / Solution Transfer
- Physics Coupling Infrastructure

Baseline
- VABOC
- BOA
- ANC9
- VIPRE-W
- FALCON

Initial / Demo
- DeCART
- Star-CCM+

VERA
- DAKOTA
- MOOSE
- LIME
- Trilinos
- PETSc

Solvers / Coupling / SA / UQ
- DTK
- MOAB
- libMesh
- STK

Common Input
- NiCE
- front-end

Input / Output
- Reactor System

Neutronics
- Insilico
- MPACT

Thermal-Hydraulics
- COBRA-TF
- Hydra-TH
- Drekar

Fuel Performance
- PEREGRINE

Chemistry
- MAMBA2D
- MAMBA3D
- MAMBA-BDM

Version 3.1 (August 2013)
## VERA Usage for Challenge Problems

<table>
<thead>
<tr>
<th>Challenge Problem</th>
<th>Time Scale (Seconds, Minutes, Hours, Days, Years)</th>
<th>Spatial Scale of Phenomena</th>
<th>Code Coupling Required</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crud-CIPS</td>
<td>Y (<em>always implies VERA-CS depletion</em>)</td>
<td>Core-wide</td>
<td>MPACT- COBRA - MAMBA</td>
</tr>
<tr>
<td>Crud-CILC</td>
<td>Y</td>
<td>Few pin-wide</td>
<td>MPACT/Insilico – Hydra – Peregrine – MAMBA</td>
</tr>
<tr>
<td>GTRF</td>
<td>Y + 50 Hz</td>
<td>Few pin-wide</td>
<td>MPACT - Hydra – Peregrine – STK?</td>
</tr>
<tr>
<td>PCI</td>
<td>Y + M to H</td>
<td>Few pin-wide</td>
<td>MPACT/Insilico - Hydra - Peregrine</td>
</tr>
<tr>
<td>DNB</td>
<td>Y + S to M</td>
<td>System to assembly-wide</td>
<td>MPACT – COBRA/Hydra – Peregrine - RELAP</td>
</tr>
<tr>
<td>LOCA</td>
<td>Y + S to M</td>
<td>Pin-wide</td>
<td>Peregrine (B.C. from WEC)</td>
</tr>
<tr>
<td>RIA</td>
<td>Y + S</td>
<td>Few pin-wide</td>
<td>MPACT – Hydra – Peregrine</td>
</tr>
</tbody>
</table>
# VERA-CS vs. Industry Core Simulators

<table>
<thead>
<tr>
<th>Physics Model</th>
<th>Industry Practice</th>
<th>VERA-CS</th>
</tr>
</thead>
</table>
| **Neutron Transport** | 3-D diffusion (core)  
  2 energy groups (core)  
  2-D transport on single assy | 3-D transport  
  23+ energy groups                           |
| **Power Distribution** | nodal average with pin-power reconstruction methods                             | explicit pin-by-pin(*)                      |
| **Thermal-Hydraulics** | 1-D radial node-averaged                                                         | subchannel (w/crossflow)                    |
| **Fuel Temperatures**   | nodal average                                                                  | pin-by-pin(*)  
  2-D or 3-D                                    |
| **Xenon/Samarium**       | nodal average w/correction                                                       | pin-by-pin(*)                                |
| **Depletion**           | infinite-medium cross sections  
  quadratic burnup correction  
  history corrections  
  spectral corrections  
  reconstructed pin exposures | pin-by-pin(*)  
  with actual core conditions                  |
| **Reflector Models**     | 1-D cross section models                                                         | actual 3-D geometry                          |
| **Target Platforms**     | workstation (single-core)                                                       | 1,000 – 300,000 cores                        |

(*) pin-homogenized or pin-resolved depending on application
**Organization to support work scope**

**Advanced Modeling Applications**
- #1 2D HZ 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 BOI Assembly
- #7 HFP Boron Physical Reactor w/ Xenon
- #8 Physical Reactor Startup Flux Maps
- #9 Physical Reactor Depletion
- #10 Physical Reactor Refueling

**Virtual Reactor Integration**
- Baseline
  - VABOC
  - STK
  - DAKOTA
  - VABOC
  - MODFLOW
- Initial / Demo
  - DnCART
  - Star-CCM+
  - MPACT
  - HYDRA
- VERA
  - MOOG
  - LIME
  - Trilinos
  - Hybrid
- Energy
  - MAMBA 2D
  - MAMBA 3D

**Thermal Hydraulic Methods**
- Explicit
- Operator-Splitting
- Segregated (Parallelization)
- Newton-based
  - Fully-Implicit
  - HYDRA-TH
  - HYDRA-TH
- Fractional Steps
- NERLY-IMPLICIT (RELAP5-4.0)
- SEMI-IMPLICIT (RELAP5-4.0)
- SIMPLEx
- GCBA
- MCB
- JFNN
- PHYSICS-Based Preconditioning (Wrigley)
- NK (Anisotropic Jacobi)
- CATYRA-1D

**Radiation Transport Methods**
- MPACT
- SHIFT
- INSILICO
- RELAPS system
- STAR-CCM+
- DnCART
- Initial / Demo
- VERA
- VERA
- VERA
- VERA
- VERA
- VERA
Organization to support work scope

Validation & Uncertainty Quantification

Virtual Office, Computing & Community

Materials Performance and Optimization

**VUQ best practices to select approaches**

**PIRT to identify parameters, FOM**

**VERA User Input**

**VERA Coupling, Mesh Parameters**

**VERA Code 1**

**VERA Code 2**

**VERA Output**

**Figures of Merit**

**How to specify overall study/workflow? NICE?**

---

**MAMBA**

**MAMBA-BDM**

**Peregrine**

**Falcon**

[Graph showing measured vs. calculated temperature with Peregrine and Falcon data]
• Thermal-Hydraulic Methods (THM)
  ➢ Development of robust, parallel solution algorithms for multiphase/multi-field CFD (Hydra-TH)
  ➢ Assessment of subcooled boiling and bubble flow closure relationships using experimental data & DNS (energy partitioning, wall effect lift & drag force, bubble departure characteristics)

Scaled to 36,000 cores on Titan, 192 Million element mesh
Single and Multiphase flow algorithms and the Hydra multiphase flow strategy/roadmap

- Fully-implicit projection algorithms
- “Option 1” with momentum transfer (drag)
- “Option 3” – Fully-implicit with physics-based preconditioning
Fully-Implicit Algorithms based on Projection Methods

- Projection method acts a physically-based preconditioner providing an approximate factorization of the discrete Navier-Stokes Equations

Vortex Shedding Test Problem

Hydra

Open-Foam

• Projection method acts a physically-based preconditioner providing an approximate factorization of the discrete Navier-Stokes Equations

Vortex Shedding Test Problem

Hydra

Open-Foam

Temperature

Kinetic energy

Lagrange multiplier

Godunov Projection

Semi-Implicit Projection

Fully-Implicit Projection

CFL=7

CFL=3.5

CFL=7

CFL=15

CFL=15

CFL=30

CFL=60

CFL=35

CFL=30

CFL=60
Hydra-TH Validation: 5x5 V5H grid strap study shows good agreement with experimental data

- Re = 28,000
- Predicted mean peak velocities within 5% of experiments

- Time-averaged velocity profiles downstream of mixing vanes (96M mesh)
Demonstration and Assessment of Advanced Modeling Capabilities for Multiphase Flow with Sub-cooled Boiling

- A ‘tour de force’ effort used to coordinate/integrate research among the broad and diverse set of researchers in THM
- Primarily supports DNB Challenge Problem, but also positions THM for future applications

**Visuals and Diagrams**

- VERA-CFD (Hydra-TH)
  - Algorithms & Architectures
    - Advanced CFD Algorithms
    - Multiphase Solution Methods
    - Advanced Architectures – NVIDIA nvAMG Library
  - DNS - Interface Tracking
    - Fundamental Understanding
    - Multiphase Closure Models
    - Code Validation
  - 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

**Institutions**

- (LANL, INL)
- (MIT)
- (CCNY)
- (TAMU)
- (NCSU)
- (Notre Dame)
• Radiation Transport Methods (RTM)
  
  ➢ Development of integrated x-section generation/transport solver capability (Insilico), using Sn or newly developed SPn
  
  ➢ Refactored 2D MOC/1D Diffusion code (MPACT) with convergence issue understood & addressed and developed full 3D MOC capability (MPACT-3D)
  
  Below shows analysis (Larsen et. al.) to determine optimum extrapolation parameter value with regard to axial coupling for 2D/1D approach

\[
\theta_{opt} = \begin{cases} 
\frac{2}{2-c} & \text{if } \frac{2}{\sqrt{3c}} < \Sigma_t \Delta z , \\
\frac{2}{2+3(1-c)(\Sigma_t \Delta z)^2} & \text{if } \Sigma_t \Delta z \leq \frac{2}{\sqrt{3c}} , \\
\frac{c}{2-c} & \text{if } \frac{2}{\sqrt{3c}} < \Sigma_t \Delta z , \\
\frac{2}{2+3(1-c)(\Sigma_t \Delta z)^2} & \text{if } \Sigma_t \Delta z \leq \frac{2}{\sqrt{3c}} .
\end{cases}
\]

\[
\rho = \begin{cases} 
\frac{2}{2+3(1-c)(\Sigma_t \Delta z)^2} & \text{if } \Sigma_t \Delta z \leq \frac{2}{\sqrt{3c}} , \\
\frac{2}{\sqrt{3c}} & \text{if } \frac{2}{\sqrt{3c}} < \Sigma_t \Delta z , \\
\frac{c}{2-c} & \text{if } \Sigma_t \Delta z \leq \frac{2}{\sqrt{3c}} .
\end{cases}
\]

Figure 2: Spectral Radius $\rho$ vs Axial Optical Thickness $\Sigma_t \Delta z$ for $c = 0.9$
Insilico (SPn Pin-Homogenized): Need for Low Order Transport

• 3D pin-resolved transport is very computationally expensive
  – A single state point calculation for a full/quarter core model with reasonable fidelity may require most (if not all) of a Titan-class computer for hours

• Multiphysics (T/H, depletion, etc.) simulations require numerous transport calculations
  – Run time of resolved transport makes this intractable
  – Goal for $SP_N$ is to be cheaper than transport, more accurate than diffusion
Environment
Insilico ($S_{n}$) Performance Results – 3D Assembly

- 23 energy groups
- $S_{5}$, $P_{1}$ scattering
- 4x4 mesh per pin, 2 in. axial mesh (143,325 cells)
- 9.9 million total unknowns
- 36 compute cores

<table>
<thead>
<tr>
<th>Eigen solver</th>
<th>Preconditioner</th>
<th>Iterations</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power Iteration</td>
<td>ILUT</td>
<td>861</td>
<td>5126</td>
</tr>
<tr>
<td>Arnoldi</td>
<td>ILUT</td>
<td>21</td>
<td>2608</td>
</tr>
<tr>
<td>Davidson</td>
<td>ILUT</td>
<td>1515</td>
<td>1610</td>
</tr>
<tr>
<td>Davidson</td>
<td>ML</td>
<td>316</td>
<td>745</td>
</tr>
<tr>
<td>Davidson</td>
<td>MGE(ILU)</td>
<td>47</td>
<td><strong>300 [0.08 hrs]</strong></td>
</tr>
</tbody>
</table>

- Denovo $S_{N}$ (LD) runtime on same problem with coarse quadrature is around 1.5 hours
## Watts Bar Cycle 1 2D Core
### INSILICO vs. KENO

#### X100 Delta Assembly Power
(Labels are delta powers)

<table>
<thead>
<tr>
<th></th>
<th>0.4</th>
<th>0.4</th>
<th>0.3</th>
<th>0.3</th>
<th>0.2</th>
<th>-0.0</th>
<th>-0.4</th>
<th>-1.0</th>
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</thead>
<tbody>
<tr>
<td>0.4</td>
<td>0.4</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.2</td>
<td>-0.1</td>
<td>-0.2</td>
<td>-0.9</td>
</tr>
<tr>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
<td>0.4</td>
<td>0.3</td>
<td>0.2</td>
<td>-0.3</td>
<td>-0.8</td>
<td></td>
</tr>
<tr>
<td>0.3</td>
<td>0.3</td>
<td>0.4</td>
<td>0.4</td>
<td>0.5</td>
<td>0.2</td>
<td>-0.0</td>
<td>-0.7</td>
<td></td>
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<tr>
<td>0.2</td>
<td>0.2</td>
<td>0.3</td>
<td>0.5</td>
<td>0.6</td>
<td>0.3</td>
<td>-0.1</td>
<td></td>
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</table>

#### X100 Delta Pin Power
(Labels are assembly powers)

<table>
<thead>
<tr>
<th></th>
<th>1.065</th>
<th>0.990</th>
<th>1.015</th>
<th>0.935</th>
<th>1.125</th>
<th>1.065</th>
<th>1.057</th>
<th>1.069</th>
<th>0.782</th>
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<tbody>
<tr>
<td>1.065</td>
<td>0.997</td>
<td>0.994</td>
<td>1.061</td>
<td>1.057</td>
<td>1.167</td>
<td>1.052</td>
<td>0.631</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.045</td>
<td>0.999</td>
<td>1.055</td>
<td>1.039</td>
<td>1.170</td>
<td>1.044</td>
<td>1.087</td>
<td>0.791</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.046</td>
<td>1.081</td>
<td>1.056</td>
<td>1.163</td>
<td>1.099</td>
<td>1.451</td>
<td>1.041</td>
<td>0.643</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.042</td>
<td>1.056</td>
<td>1.170</td>
<td>1.095</td>
<td>1.314</td>
<td>0.911</td>
<td>0.943</td>
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<tr>
<td>1.055</td>
<td>1.157</td>
<td>1.144</td>
<td>1.151</td>
<td>0.511</td>
<td>0.924</td>
<td>0.626</td>
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<tr>
<td>1.052</td>
<td>1.057</td>
<td>1.041</td>
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<td>0.626</td>
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<tr>
<td>0.785</td>
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</tr>
</tbody>
</table>
Validation Against PWR Zero Power Physics Tests
Watts Bar Unit 1-Cycle 1

KENO = MC  NEXUS = Nodal Diffusion  VERA = Insilico SP\textsubscript{n}
### MPACT (2D {Planar} MOC/1D {Axial} Diffusion) – Pin-Resolved Results: C5G7 3-D Benchmark

- **OECD transport benchmark**
  - Heterogeneous geometry

- **Original Benchmark**
  (Full height assembly without rods)

<table>
<thead>
<tr>
<th></th>
<th>Axially Integrated Powers</th>
<th>Slice Power Errors</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>keff</td>
<td>min</td>
</tr>
<tr>
<td><strong>MPACT</strong></td>
<td>1.18390</td>
<td>0.24</td>
</tr>
<tr>
<td><strong>Error</strong></td>
<td>-9</td>
<td>2.38%</td>
</tr>
<tr>
<td><strong>Axially Integrated Powers</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Rodded A</strong></td>
<td>1.12744</td>
<td>0.26</td>
</tr>
<tr>
<td><strong>Error</strong></td>
<td>62</td>
<td>0.05%</td>
</tr>
<tr>
<td><strong>Rodded B</strong></td>
<td>1.07751</td>
<td>0.35</td>
</tr>
<tr>
<td><strong>Error</strong></td>
<td>26</td>
<td>-0.16%</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>3.7%</td>
</tr>
</tbody>
</table>
MPACT-(3D MOC) - Pin-Resolved Results: PWR Assembly

Axial Description

- Upper Core Plate (4.92 cm)
- Top Nozzle Gap (6.56 cm)
- Upper End Grid (3.28 cm)
- Intermediate Spacer Grid (3.28 cm)
- Fuel (47.56 cm)
- Bottom Nozzle (6.56 cm)
- Lower End Grid (3.28 cm)
- Lower Reflector (9.84 cm)

Radial Description

Problem Size Parameters

<table>
<thead>
<tr>
<th></th>
<th>3-D MOC</th>
<th>2-D/1-D</th>
</tr>
</thead>
<tbody>
<tr>
<td># of Segments</td>
<td>55,952,023,038</td>
<td>28,981,236</td>
</tr>
<tr>
<td># of Rays</td>
<td>2,238,077,088</td>
<td>407,008</td>
</tr>
<tr>
<td># of Regions</td>
<td>3,697,984</td>
<td>157,496</td>
</tr>
<tr>
<td>Directions per octant</td>
<td>36</td>
<td>64</td>
</tr>
</tbody>
</table>

3-D MOC and 2-D/1-D Comparison

<table>
<thead>
<tr>
<th></th>
<th>3-D MOC</th>
<th>2-D/1-D</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{\text{eff}}$</td>
<td>1.17180</td>
<td>1.17323</td>
</tr>
<tr>
<td>No. of Iters.</td>
<td>7</td>
<td>18</td>
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<tr>
<td>Processors</td>
<td>16704</td>
<td>368</td>
</tr>
<tr>
<td>Run Time</td>
<td>2103 s</td>
<td>630 s</td>
</tr>
</tbody>
</table>
Summary of Parallel Decomposition

Spatial decomposition

Angular decomposition

Ray Decomposition

angle 1
angle 2

Thread 1
Thread 2
Deterministic Neutron Transport with Denovo
Part of the CASL/ORNL Exnihilo neutronics system

- Solves 6-D Boltzmann transport equation (space, angle, energy group)
- 3-D, Cartesian orthogonal structured (nonuniform) grids
- Steady-state fixed-source and eigenvalue modes
- Spatial domain decomposition (DD) parallelism using the Koch-Baker-Alcouffe (KBA) sweep algorithm
- Krylov and source-iteration within-group solvers
- Multigroup with optional thermal upscattering
- Multiple spatial differencing schemes, including
  - step characteristics (slice balance) (SC), linear-discontinuous finite element (LD), and trilinear-discontinuous finite element (TLD)
- Reflecting, vacuum, and surface source boundary conditions
Denovo \( (S_n) \) Whole Core Reactor Problem – Pin Homogenized

PWR-900 Whole Core Problem

- 2 and 44-group, homogenized fuel pins
- 2×2 spatial discretization per fuel pin
- 17×17 fuel 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
### Results

<table>
<thead>
<tr>
<th>Solvers</th>
<th>Blocks</th>
<th>Sets</th>
<th>Domains</th>
<th>Solver Time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PI + MG GS (2-grid preconditioning)</td>
<td>17,424</td>
<td>1</td>
<td>17,424</td>
<td>150.15</td>
</tr>
<tr>
<td>PI + MG Krylov</td>
<td>17,424</td>
<td>1</td>
<td>17,424</td>
<td>52.99</td>
</tr>
<tr>
<td>Arnoldi + MG Krylov</td>
<td>17,424</td>
<td>1</td>
<td>17,424</td>
<td>23.62</td>
</tr>
<tr>
<td>Arnoldi + MG Krylov</td>
<td>17,424</td>
<td>2</td>
<td>34,848</td>
<td>12.81</td>
</tr>
</tbody>
</table>

Total unknowns = 59,867,852,800  
Number of groups = 2  
$k_{eff}$ tolerance = 1.0e-5
Denovo ($S_N$) 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
Continuous-Energy Shift Monte Carlo Code Verification

2D Lattice Problem

Power Distribution Relative Error vs CE-KENO VI

<table>
<thead>
<tr>
<th>Problem</th>
<th>Code</th>
<th>Avg Keff</th>
<th>Avg Keff Abs Error (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>t_r = 565 K</td>
<td>KENO VI</td>
<td>1.18619 +/- 0.00007</td>
<td>20.260 +/- 9.586</td>
</tr>
<tr>
<td></td>
<td>Shift</td>
<td>1.18590 +/- 0.00011</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MCNP</td>
<td>1.18528 +/- 0.00007</td>
<td></td>
</tr>
<tr>
<td>t_r = 600 K</td>
<td>KENO VI</td>
<td>1.18294 +/- 0.00007</td>
<td>30.454 +/- 9.703</td>
</tr>
<tr>
<td></td>
<td>Shift</td>
<td>1.18251 +/- 0.00012</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MCNP</td>
<td>1.18187 +/- 0.00007</td>
<td></td>
</tr>
<tr>
<td>t_r = 900 K</td>
<td>KENO VI</td>
<td>1.17239 +/- 0.00008</td>
<td>16.591 +/- 10.007</td>
</tr>
<tr>
<td></td>
<td>Shift</td>
<td>1.17216 +/- 0.00012</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MCNP</td>
<td>1.17146 +/- 0.00007</td>
<td></td>
</tr>
<tr>
<td>t_r = 1200 K</td>
<td>KENO VI</td>
<td>1.16315 +/- 0.00007</td>
<td>11.754 +/- 9.984</td>
</tr>
<tr>
<td></td>
<td>Shift</td>
<td>1.16299 +/- 0.00012</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MCNP</td>
<td>1.16313 +/- 0.00007</td>
<td></td>
</tr>
<tr>
<td>IFBA</td>
<td>KENO VI</td>
<td>0.77237 +/- 0.00008</td>
<td>22.634 +/- 18.183</td>
</tr>
<tr>
<td></td>
<td>Shift</td>
<td>0.77223 +/- 0.00008</td>
<td></td>
</tr>
<tr>
<td></td>
<td>MCNP</td>
<td>0.77125 +/- 0.00006</td>
<td></td>
</tr>
</tbody>
</table>

All benchmarks show excellent comparison with established CE Monte Carlo codes
• Materials Performance & Optimization (MPO)

Microscale activities underway to provide mechanistic/physical insight into complex degradation phenomena
Approach to CRUD

Pragmatic multiscale approach, complementary to BOA, to address the physics/chemistry of CRUD formation and growth, and subsequent impact on CIPS and CILC.

Thermodynamics
Mostly atomistic scale calculations that address CRUD phase stability, nonstoichiometry, solvation and potentially source term.

MAMBA-BDM
Microscale CRUD formation/growth model, which can be used for CILC-risk analysis

1D or 2D MAMBA
Pin-scale CRUD formation/growth model, which can be used for VERA-CS CIPS-risk analysis (assemblies) {Embarishingly parallel}

3D MAMBA
Pin-scale CRUD formation/growth model, which can be used for VERA CIPS-risk analysis (single to few pins)

Benefit to Industry:
1. 3D CRUD pin scale model
2. Improved materials models
3. Coupled CRUD, neutronics and thermal hydraulics model
Crud: Initial high resolution crud simulations of a 4x4 subassembly using STAR-CCM+ / MAMBA (with fixed power)
Peregrine: 2D & 3D Fuel Performance (material, thermal & mechanical coupled behaviors) [Moose/Bison based]
Predictions versus experimental data (Halden & Riso) & Falcon predictions

Embarishingly parallel at rod level
Improved Mechanistic Models of Cladding Deformation

Improved models for clad deformation required for PCI and safety assessments

Atomistic simulation for defect behavior, including mobility and interaction with dislocations

Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal)

Peregrine engineering scale fuel performance

TEAM:
Carlos Tome
Alankar
Gopinath Subramanian
Stas Golubov
Sasha Barashev
Roger Stoller
Jason Hales
Oxidation, Hydrogen Uptake and Hydride Formation and Growth

Gary Was and Peng Wang

Thermodynamics of Zr-O (and H) system

Anton van der Ven and Brian Puchala

H Pickup and Distribution in Zr-4 Experiments

Katsuyo Thornton and Andrea Jokisaari

Zr-O-H Phenomenological Model – Peregrine Interface

Izabela Szlufarska and Dane Morgan

Hyrax Phase Field Model of Hydride Formation and Growth

The University of Wisconsin Madison
• Physics Integration (PHI)
VERA-CS (core simulator) is a subset of VERA capabilities

VERA contains:
- Solvers
- Coupling
- SA / UQ
- Geometry
- Mesh
- Solution Transfer
- Neutronics
- Cross Sections
- Isotopes
- Thermal-Hydraulics
- Subchannel Thermal-Hydraulics
- Research CFD
- Fuel Performance
- 2D r-z
- 3D
- Chemistry
- CRUD
- Deposition
- Corrosion
- Reactor System

Front-end & back-end (workflow / analysis)
VERA input is comfortable for current industry users and extensible.

- ability to create, archive, compare, and modify input similar to current industry workflows
- attributes of real reactors
  - assemblies, poisons, control rods, non-fuel structures, baffle, power, flow, depletion, boron search, detectors, etc.
- eliminate inconsistencies between physics components through use of a common geometry description
- will evolve as needed
- currently using VERA input
  - Insilico ($S_N$, $S_P$, Monte Carlo)
  - COBRA-TF
  - MPACT
  - Peregrine

![Diagram of file types and input processes]

Plain Text (ASCII) ➔ XML ➔ C++ objects ➔ Files/Memory

1. GUI (e.g. NiCE)
2. Script
3. Plain Text
4. XML
5. C++ objects
6. Files
7. Memory
8. Insilico
9. COBRA-TF
10. Peregrine
11. Hydra-TH
12. Mesh
13. COBRA-TF Input
14. Peregrine Input
15. Files
16. Memory
Progression toward VERA-CS multiphysics capability

Using DTK in support of multiphysics integration
Coupled results for 17x17 WEC Assembly

Fission rate (from Insilico) and temperature in Peregrine for a selected rod. The plot on the right is scaled to show clad temps.

Insilico averaged fuel temp. and fission rate
Next: Full Core HFP Model of Watts Bar Unit 1-Cycle 1

Insilico/MPACT - Cobra-TF

Parallel Cobra-TF Performance
• Validation & Uncertainty Quantification (VUQ)

**DAKOTA Input File**
- Commands
- Options
- Parameter definitions
- File names

**DAKOTA Parameters File**
- \{x1 = 123.4\}
- \{x2 = -33.3\}, etc.

**DAKOTA Output Files**
- Raw data (all x- and f-values)
- Sensitivity info
- Statistics on f-values
- Optimality info

**DAKOTA Executable**
- Sensitivity Analysis, Optimization, Uncertainty Quantification, Parameter Estimation

**DAKOTA Results File**
- 999.888 f1
- 777.666 f2, etc.

**DAKOTA executes**
- `sim_code_script`
to launch a simulation job

**User-supplied** automatic post-processing of code output data into f-values

**Use APREPRO/DPREPRO**
to cut-and-paste x-values into code input file

**Code Input**
- CALORE thermal analysis
- ALEGRA shock physics
- SALINAS structural dynam
- Premo high speed flow
  (your code here)

**Code Output**

Loose coupling of DAKOTA to a generic application
Data Assimilation & UQ: Prediction intervals for DREAM versus DRAM MCMC data assimilation algorithms

Test case with 16 parameters

Other area of R&D emphasis has been on reduced order modeling
Verification: Denovo (Sn) Downscatter Problem

• There are significant numbers of outliers. These are “ignored” effectively.

RMR space-angle LD+LS

\[ F = 0.0881292 \pm 0.000107 + A h^{3.840 \pm 0.217} + B/n^{3.100 \pm 0.493} \]

RMR angle for LDFE

\[ F = 0.0883713 \pm 0.0000002 + B/n^{4.985 \pm 2.70} \]

GCI angle for LDFE

\[ F = 0.088322 \pm 0.000148 + B/n^{10.825} \]
CASL projected future computing needs.

- Computing requirements of course vary with physics and geometry
  - Values shown are estimates based on experience to date and professional judgment
  - As VERA capabilities are deployed and applied, we are refining estimates

<table>
<thead>
<tr>
<th></th>
<th>Current Need</th>
<th>Need at End of Phase 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Geometry</td>
<td>Number of Cores</td>
</tr>
<tr>
<td>Input / Meshing</td>
<td>NA</td>
<td>100 – 1,000</td>
</tr>
<tr>
<td>Neutronics</td>
<td>Quarter Core</td>
<td>1,000 – 10,000</td>
</tr>
<tr>
<td>Thermal Hydraulics</td>
<td>Quarter Core</td>
<td>100 – 1,000</td>
</tr>
<tr>
<td>CFD</td>
<td>Assembly</td>
<td>1,000 – 100,000</td>
</tr>
<tr>
<td>Fuel Performance</td>
<td>Single Pin</td>
<td>1,000 – 5,000</td>
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<tr>
<td>Chemistry</td>
<td>Assembly Section</td>
<td>1,000 – 10,000</td>
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<tr>
<td>Structural</td>
<td>Assembly</td>
<td>10,000 – 100,000</td>
</tr>
<tr>
<td>Uncertainty Quantification</td>
<td>Assembly</td>
<td>10,000 – 100,000</td>
</tr>
<tr>
<td>Output / Analysis</td>
<td>NA</td>
<td>1,000 – 10,000</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td><strong>25,200 – 337,000</strong></td>
</tr>
</tbody>
</table>