CASL: The Consortium for Advanced Simulation of Light Water Reactors

A DOE Energy Innovation Hub for Modeling and Simulation of Nuclear Reactors

Douglas B. Kothe
CASL Director

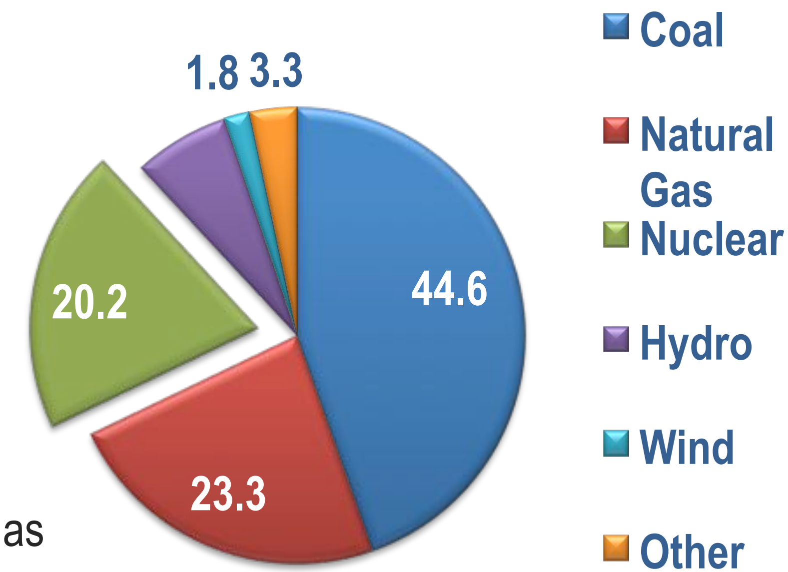
John Turner
CASL Virtual Reactor Integration

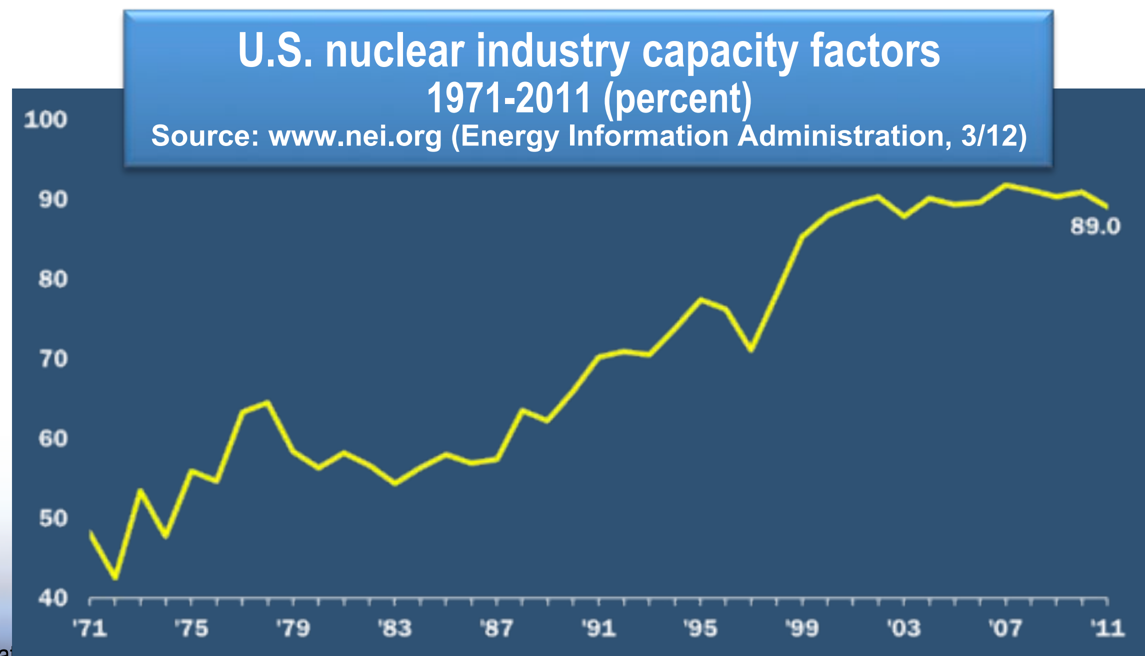
Accelerating Applications
Washington, DC
Mar 30, 2012

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. in 2009: 100.7 GW_e)
  - ~90% capacity factor
- 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

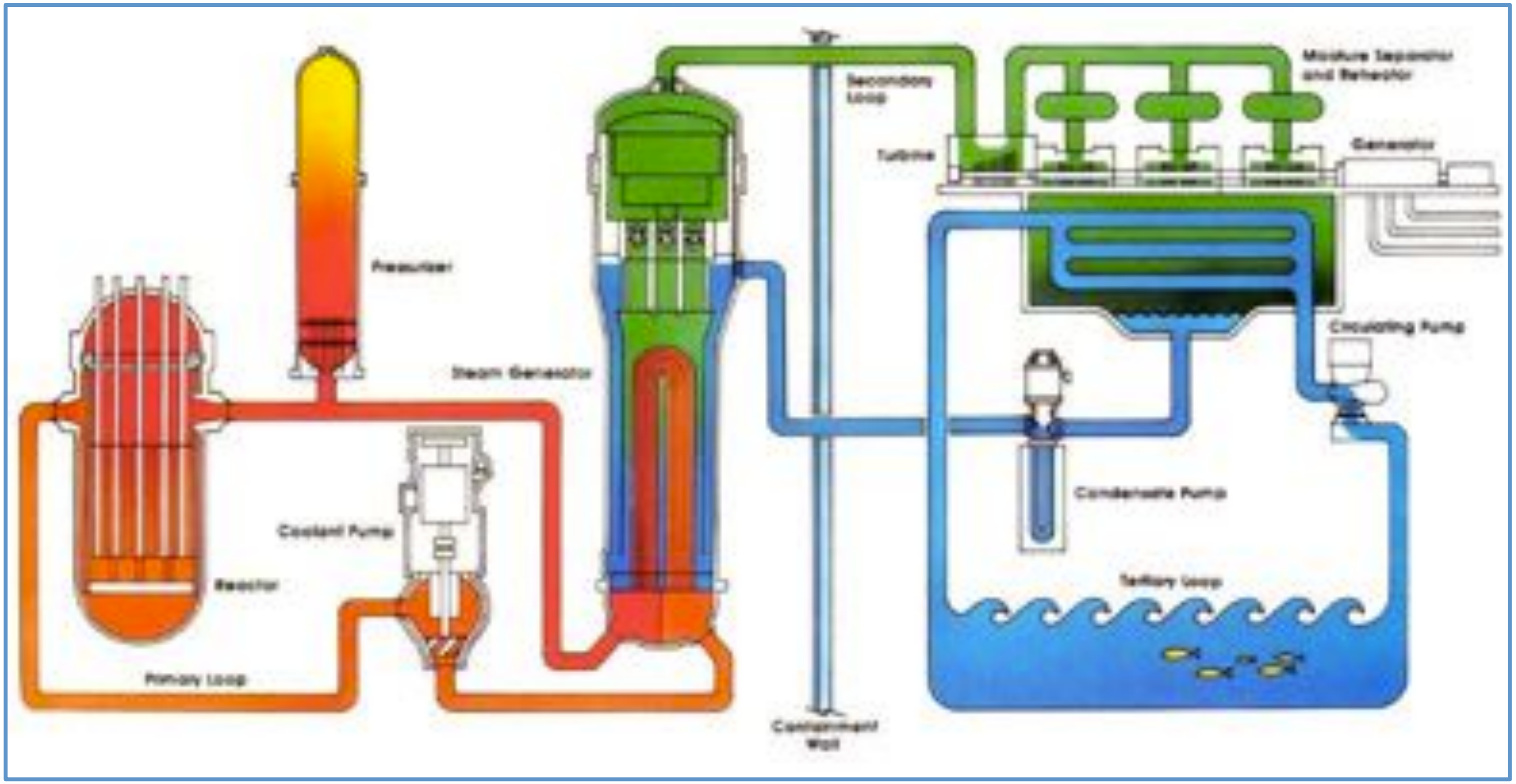
U.S. Electrical Generation





Anatomy of a Nuclear Reactor:

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



Power: ~1170 MWe (~3400 MWth)

Core: 11.1’ diameter x 12’ high, 193 fuel assemblies, 107.7 tons of UO_2

Coolant: pressurized water (2250 psia), T_{in} ~ 545°F, T_{out} ~ 610°F, 134M lb/h (4 pumps)

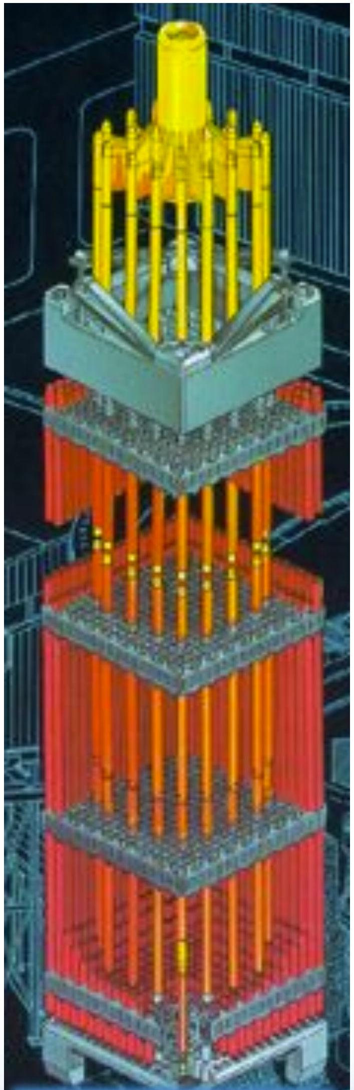
Pressure Vessel: 14.4’ diameter x 41.3’ high x 0.72’ thick alloy steel

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

Anatomy of a Nuclear Reactor

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

reactor vessel and internals



17x17 fuel assembly

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

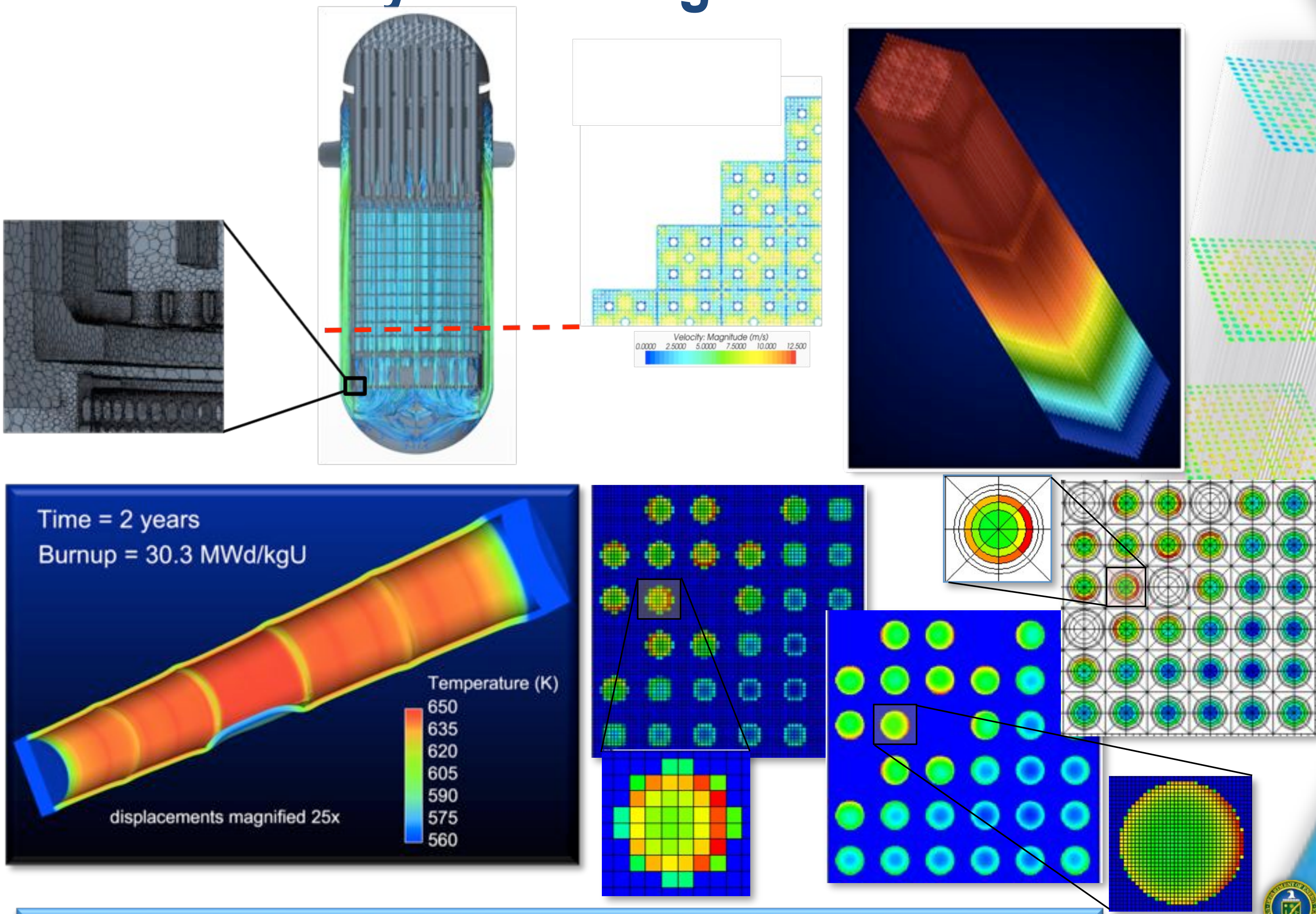
Fuel Pins
- ~300-400 pellets stacked within 12' high x 0.61 mm thick Zr-4 cladding tube

Fuel Pellets
- 9.29 mm diameter x ~10.0 mm high

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

~51,000 fuel pins and over 16M fuel pellets in the core of a PWR!

CASL Tackles the Multi-Scale Challenge of Predictively Simulating a Reactor Core



From full core to fuel assembly to fuel subassembly to fuel pin/pellet

CASL is . . .

- The first DOE Energy Innovation Hub (awarded July 2010)
- Applying existing and developing advanced modeling and simulation capabilities to create a usable “virtual reactor” environment for predictive simulation of light water reactors
- Driven by three key issues for nuclear energy: cost, reduction in amount of used nuclear fuel, and safety. All three can be enabled by power uprates, lifetime extension, and higher fuel burnup, with predictive simulation being an important facilitator
- Focused on the performance of the PWR core, vessel, and in-vessel components to provide greatest impact within 5 years
- Guided by an Industry Council who reviews plans, specs, and products; advise on gaps and critical needs; and advises on incremental technology deployment thru Test Stands & Pilot Projects
- Independently assessed by a Science Council for whether scientific work planned & executed supports attaining overall goals

Clear milestone-driven technical strategy for solving real-world reactor problems
More at www.casl.gov . . .

CASL Charter

Mission

Provide forefront and usable modeling and simulation capabilities needed to address light water reactor operational and safety performance-limiting phenomena

Vision

Confidently predict the safe, reliable, and economically competitive performance of nuclear reactors, through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy enterprise

Goals

1. *Develop and Effectively Apply Modern Virtual Reactor Technology*
2. *Assure Key Design, Operational and Safety Challenges for LWRs*
3. *Engage the Nuclear Enterprise Through Modeling and Simulation*
4. *Deploy New Partnership and Collaboration Paradigms*

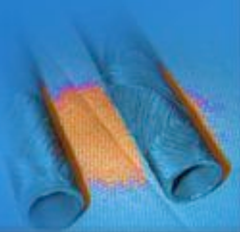
CASL became the first DOE Energy Innovation Hub upon receiving a 5-year, $122M award in July 2010

CASL
Focus on key safety-relevant reactor phenomena that limit performance

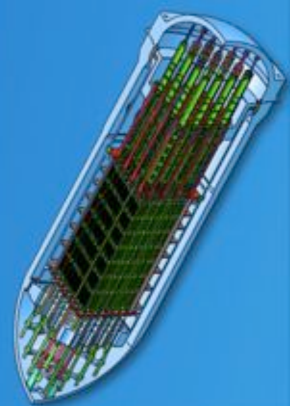
Consortium for Advanced Simulation of LWRs

Departure from Nucleate Boiling

Cladding Integrity
- During LOCA
- During reactivity insertion accidents
- Use of advanced materials to improve cladding performance

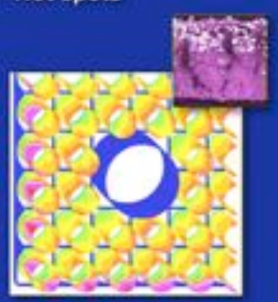


Reactor Vessel and Internals Integrity

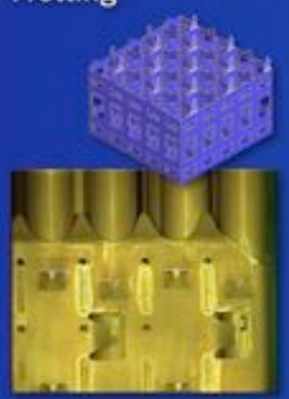


CASL is committed to delivering simulation capabilities for
- Advancing the understanding of key reactor phenomena
- Improving performance in today's commercial power reactors
- Evaluating new fuel designs to further enhance safety margin

Crud
- Deposition
- Axial offset anomaly
- Hot spots

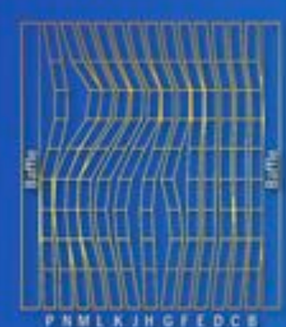


Grid-to-Rod Fretting



Pellet-Clad Interaction

Fuel Assembly Distortion



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

Virtual Environment for Reactor Applications (VERA)

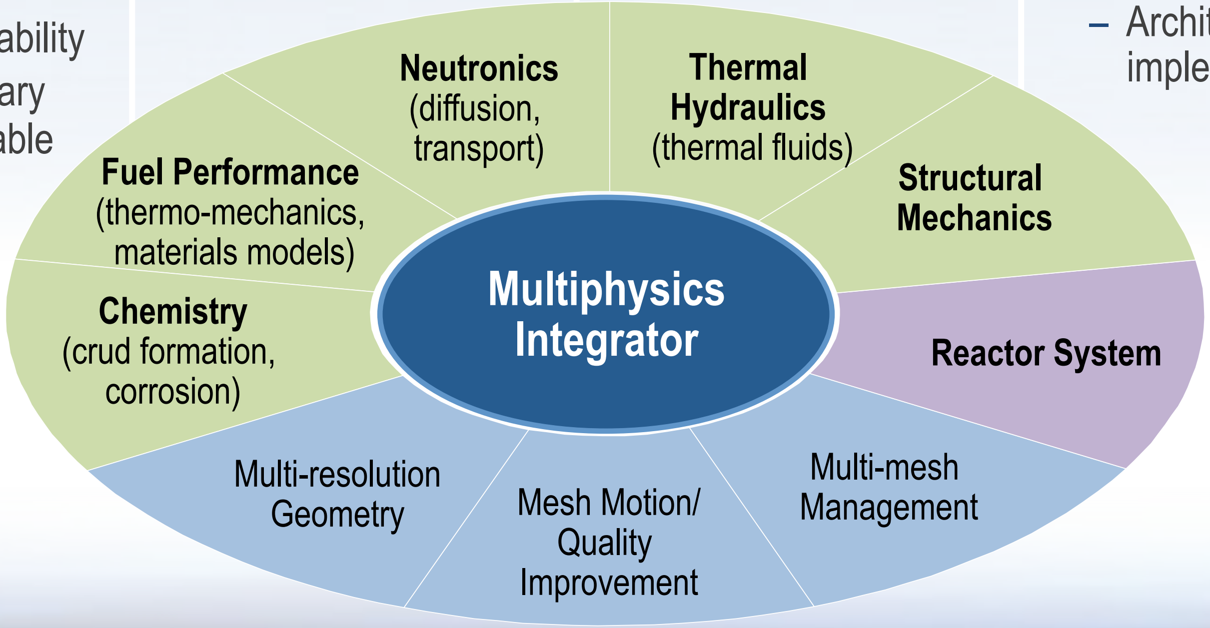
A suite of tools for scalable simulation of nuclear reactor core behavior

- 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

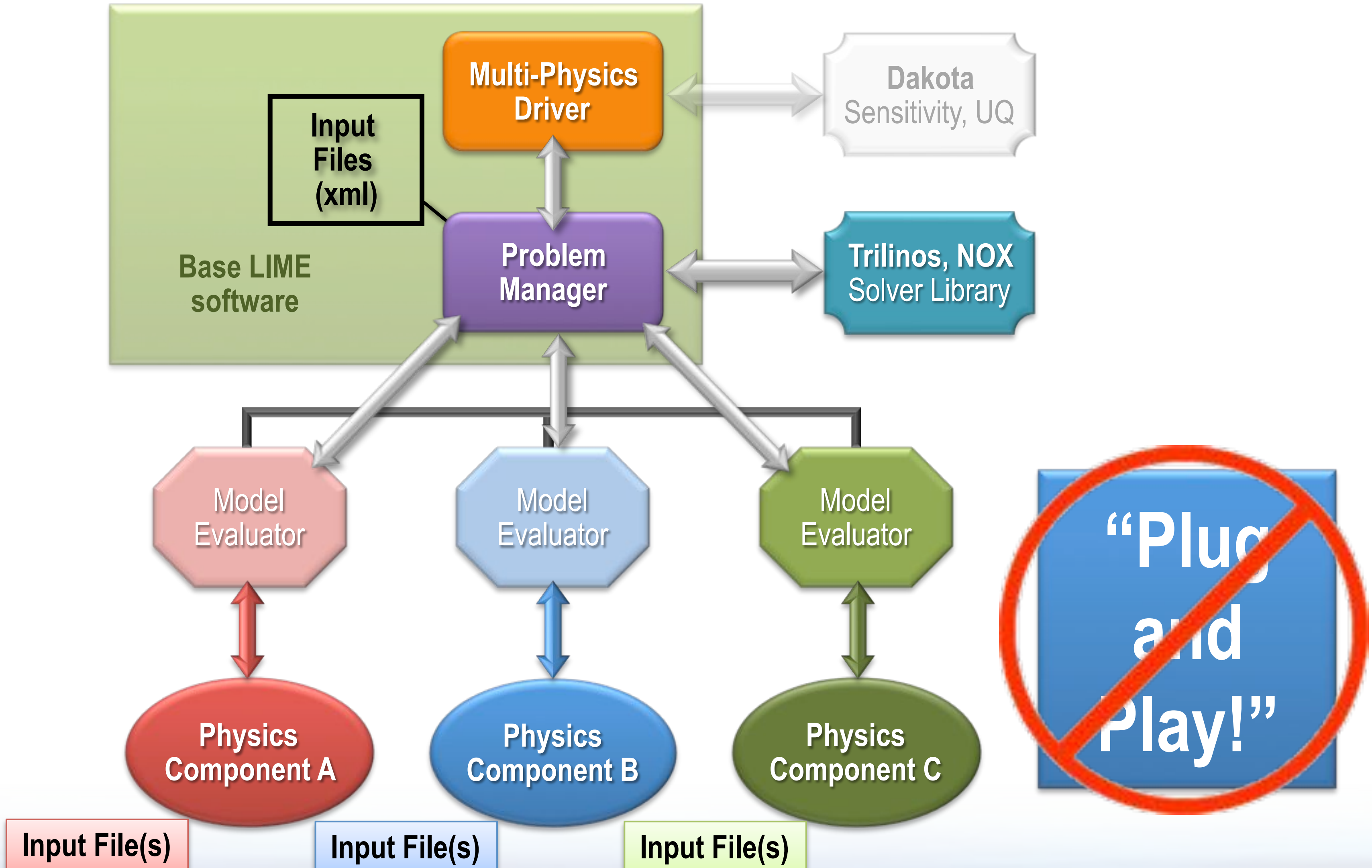
- Development guided by relevant challenge problems
- Broad applicability

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



CASL

Lightweight Integrating Multiphysics Environment (LIME)



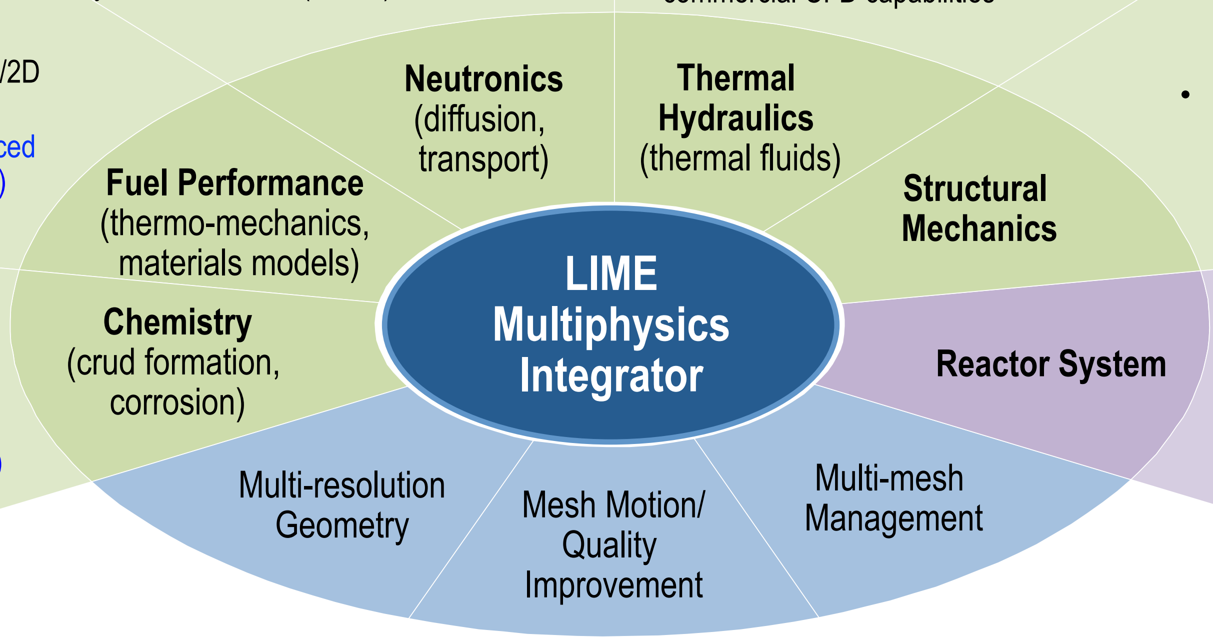
VERA (Virtual Environment for Reactor Applications) combines advanced capabilities with mature, validated, widely-used codes.

- PARAGON (Lattice physics) + ANC (nodal diffusion): Current workhorse (WEC)
- Deterministic transport: **Denovo** (ORNL), **DeCART** (UMich), PARTISn (LANL)
- Monte Carlo transport: SHIFT (ORNL)
- Hybrid: FW-CADIS (ORNL)

- VIPRE (EPRI), VIPRE-W (WEC), **COBRA**: Current subchannel flow workhorses
- **Drekar** (SNL), NPHASE (RPI), **Hydra-TH** (LANL): 3D CFD capability
- STAR-CCM+ (CD-adapco), TransAT (ASCOMP): commercial CFD capabilities

- FALCON: Current 1D/2D workhorse (EPRI)
- **PEREGRINE**: Advanced 2D/3D capability (INL)

- SIERRA (SNL) + **AMP** (ORNL)

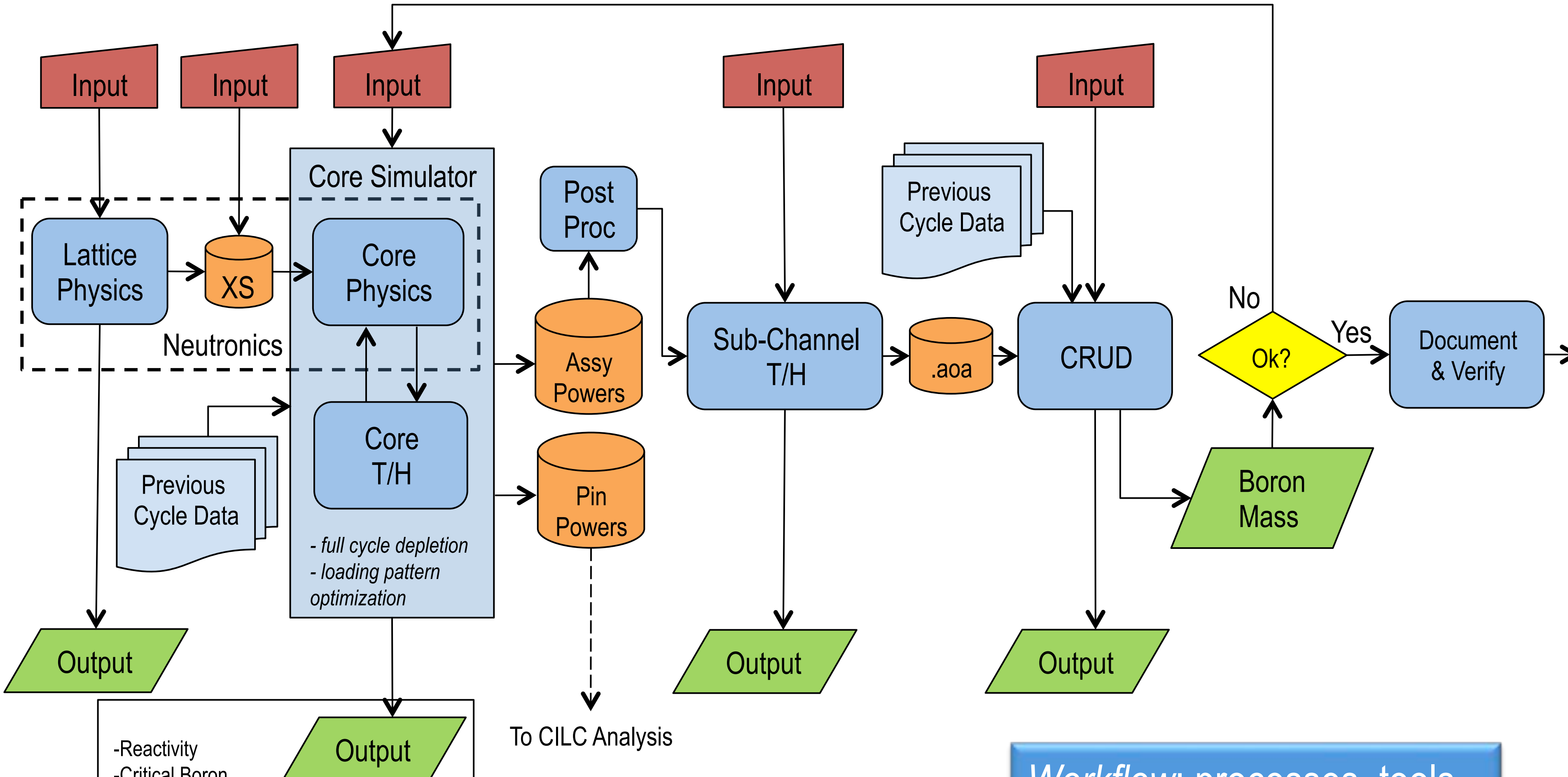


- BOA: Current CRUD and corrosion workhorse (EPRI)
- **MAMBA**: Advanced capability (LANL/MIT)

- RETRAN (EPRI)
- **RELAP5**, RELAP7 (INL)

An Example Nuclear Industry M&S Workflow

Crud Induced Power Shift Risk Evaluation



-Reactivity
-Critical Boron
-Critical Control Rod Positions
-Assembly and Rod Powers
-Assembly and Rod Exposures
-Core Coolant Density Distribution
-Core Axial Offset
-Instrument Response
-Neutron Fluence

Criteria

Compare calculated Boron mass over entire cycle to a 'low risk' threshold = X lbm Boron

Workflow: processes, tools, and technologies used to take a problem to a solution or a concept to a design

CASL Example Applications for PWR Core Analysis

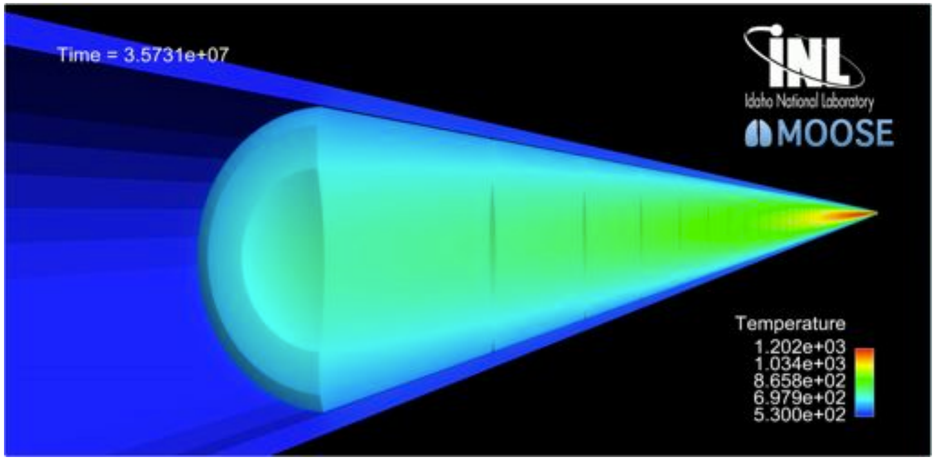
- Nuclear fuel behavior and performance
  - Spatial scale: fuel pellet to fuel pin to fuel sub-assembly (3x3 pins)
  - Application: Peregrine (INL)
- Single-phase thermal hydraulics
  - Spatial scale: fuel sub-assembly (3x3 pins) to fuel assembly (17x17 pins)
  - Application Drekar (SNL)
- Multi-phase thermal hydraulics
  - Spatial scale: fuel assembly (17x17 pins) to full core (193 assemblies or >51K pins)
  - Application: Hydra-TH (LANL)
- Neutron transport
  - Spatial scale: fuel pellet to fuel pin to fuel assembly to full core; also 2D lattice
  - Application: Denovo (ORNL)
- Coolant chemistry and CRUD deposition/buildup
  - Spatial scale: fuel pellet to fuel pin to fuel subassembly(?)
  - Application: MAMBA/MBM (LANL/MIT)

Multiscale Nuclear Fuel Analysis

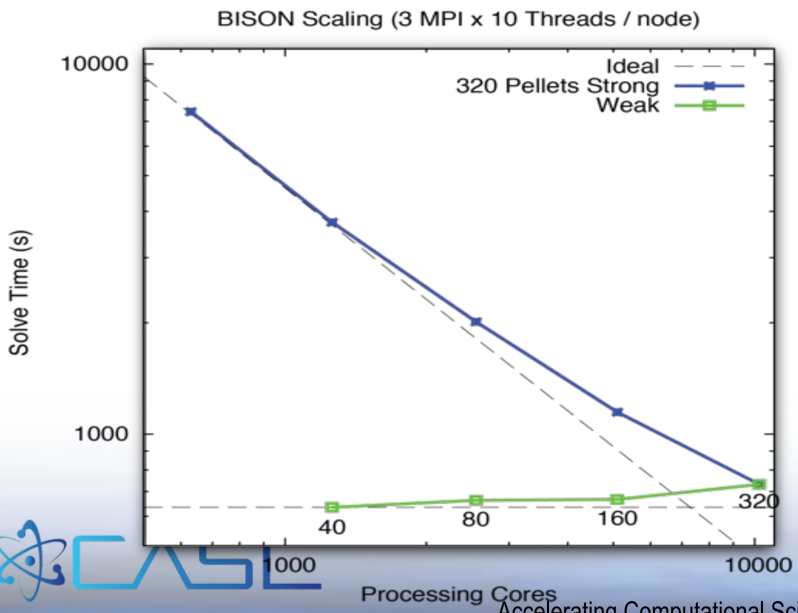
Atomistic to Engineering Scale Linkage For "Science-Based" Predictive Analysis

Science Objectives and Impact

- Strategy: Leverage a massively parallel, multiphysics framework (MOOSE) to deliver predictive simulation
- Driver: Accident tolerant fuel design and fabrication
- Objective: Predict nuclear fuel behavior for "off-normal" conditions and non-existent designs / formulations
- Impact: Mitigating nuclear accident scenarios



Application Performance



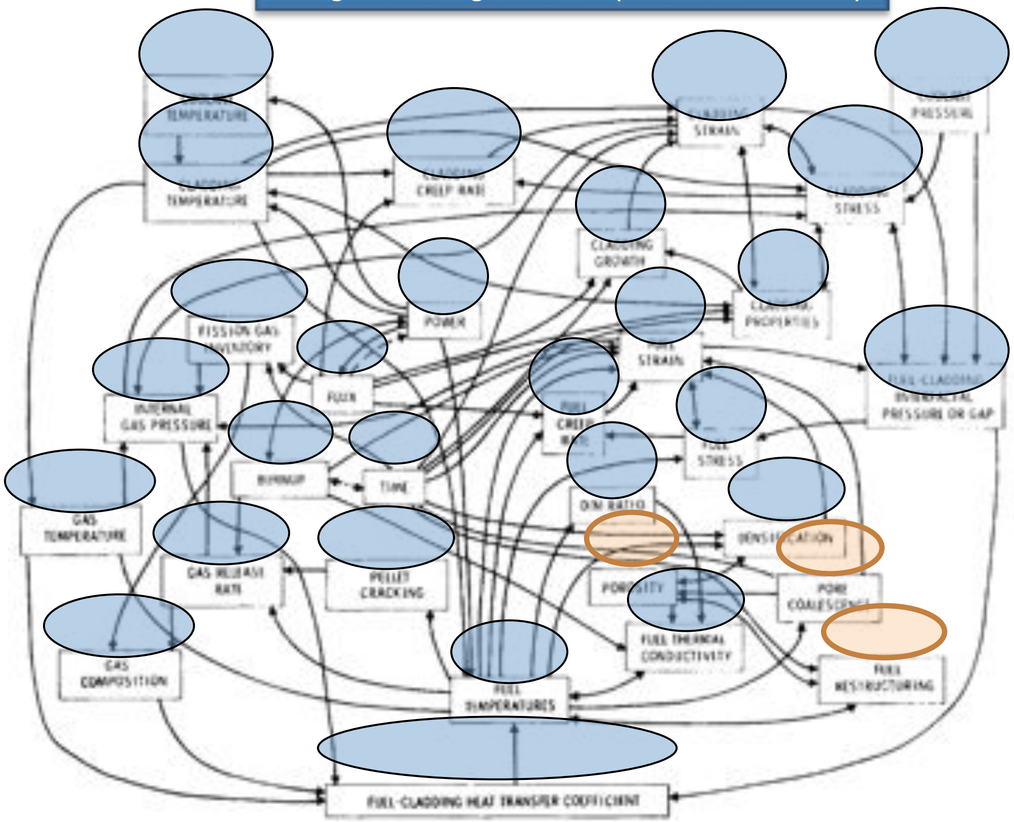
Science/Engineering Results

- First of a kind full, 3D, full-pin (320 Pellets), fully-coupled, fully-implicit, nonlinear fuels performance calculations.
  - Physics: Thermo-mechanics, fission gas release, pellet-clad interaction, gap heat transfer, plenum pressure and more
  - Strong and weak scaling up to ~12,000 cores (plot to left)
- 3D evaluation of fuel manufacturing defects (Missing Pellet Surface).
- Predictive simulation through fully coupled mesoscale and engineering scale simulations
- Engineering design analysis for metal fuel

Multiscale Nuclear Fuel Analysis

Complex Multiscale, Multiphysics Analysis of Nuclear Fuel

Engineering Scale (PEREGRINE)



Meso-Scale (MARMOT)

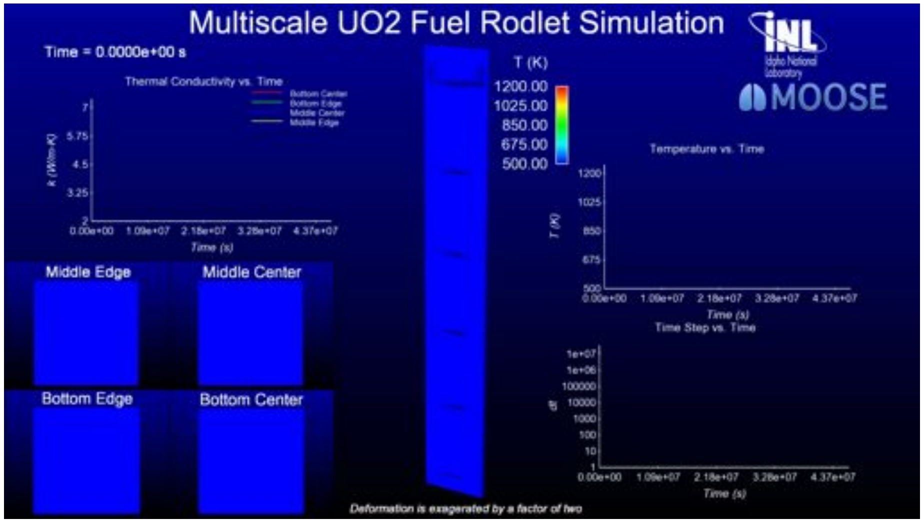
Lassmann, J. Nuc. Mat., **57**, 17 (1980)

- **Multiphysics**
  - ➢ Fully-coupled nonlinear thermomechanics
  - ➢ Multiple species diffusion
  - ➢ Neutronics
  - ➢ Thermalhydraulics
  - ➢ Chemistry
- **Multi-space scale**
  - ➢ Important physics at atomistic and microstructural level
  - ➢ Practical engineering simulations require continuum level
- **Multi-time scale**
  - ➢ Steady operation (Dt > 1 week)
  - ➢ Power ramps/accidents (Dt < 0.1 s)

Nuclear fuel is a complex multiscale, multiphysics problem

Multiscale Nuclear Fuel Analysis

Current Capability



- Small / medium sized, fully-impilicit, fully-coupled multiscale analysis.
- Result to left: Fuel rodlet (5 pellets) coupled to 4 mesoscale simulations.
  - Microstructure evolution impacts engineering scale thermo-mechanics
  - Neutron flux / heat conduction at engineering scale impacts microstructure
- Run using hundreds of processors
- ~1,000,000 Degrees of Freedom

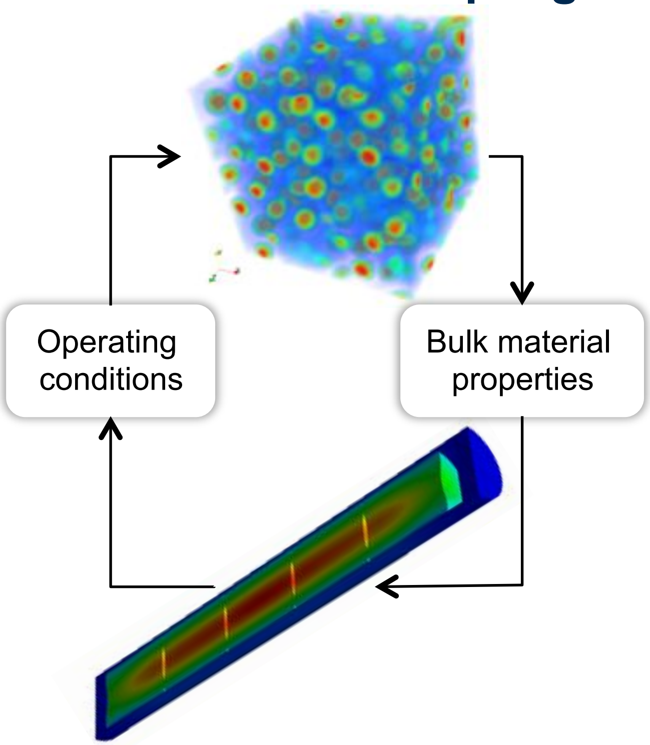
- R.L. Williamson, J.D. Hales, S.R. Novascone, M.R. Tonks, D.R. Gaston, C.J. Permann, D. Andrs, R.C. Martineau, Multidimensional multiphysics simulation of nuclear fuel behavior, Journal of Nuclear Materials, Volume 423, Issues 1–3, April 2012, Pages 149-163
- Michael R. Tonks, Derek Gaston, Paul C. Millett, David Andrs, Paul Talbot, An object-oriented finite element framework for multiphysics phase field simulations, Computational Materials Science, Volume 51, Issue 1, January 2012, Pages 20-29

Current computational capability allows for initial investigation into multi-scale effects

Multiscale Nuclear Fuel Analysis

Future Capability and Needs

Concurrent Coupling



- Tool for predictive simulation
- Captures interaction between scales
- Can locate important coupled behaviors
- Computationally challenging

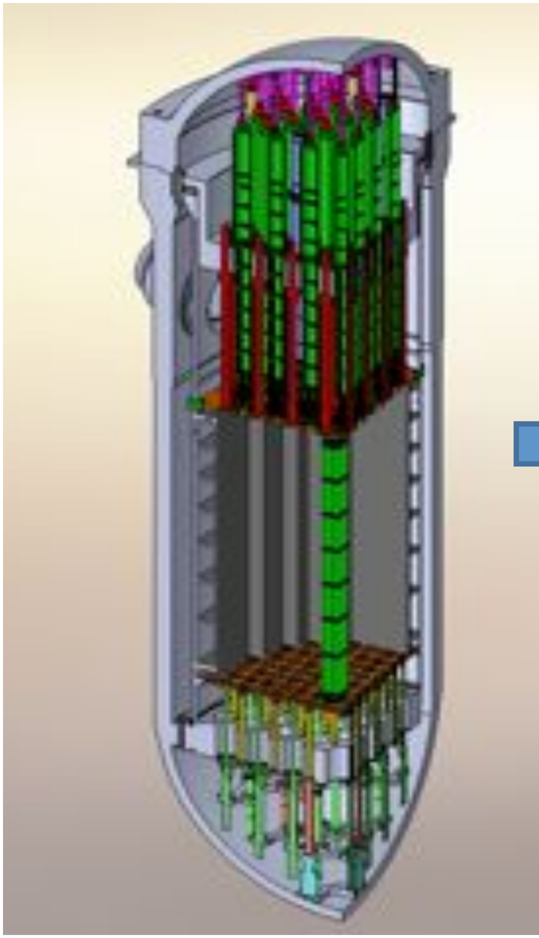
- 3D, full rod, fully-coupled, multiscale analysis
- Track microstructure evolution at multiple points within each pellet for predictive simulation of fuel behavior
- ~300 Million Degrees of Freedom (DoFs) for the engineering scale
- At least ~3,000 lower length scale simulations with 1 Million DoFs each: 3×10^9 DoFs
- Computational resources needed to simulate **one** rod over its lifetime in a reactor: ~330,000 processors for ~30 hours
- 50,000+ rods in a reactor....

Predictive simulation of nuclear reactors requires massive computational resources

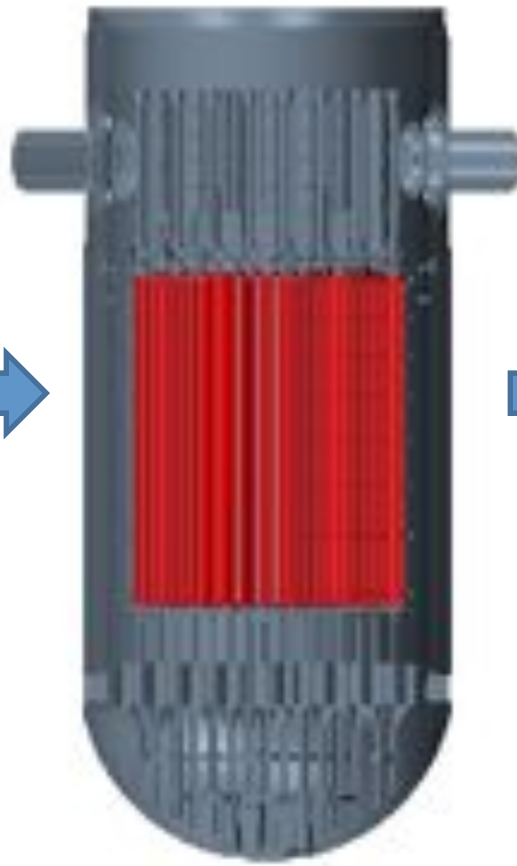
CASL

Full Core Modeling of Reactor Thermal Hydraulics

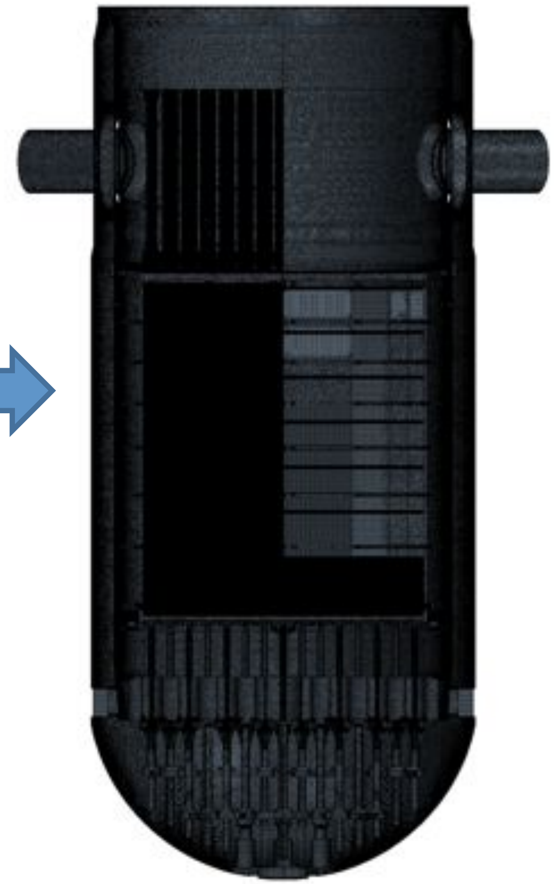
Key geometric features (fuel assembly grid structures) not resolved @ 1B cells



CAD Model



CFD Model

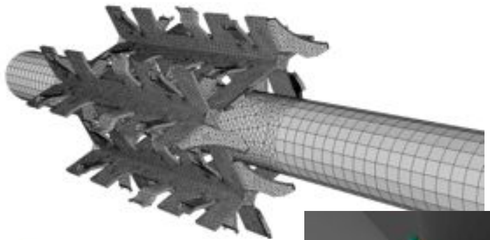


333M cell porous grid model
1 Billion cell detailed grid model

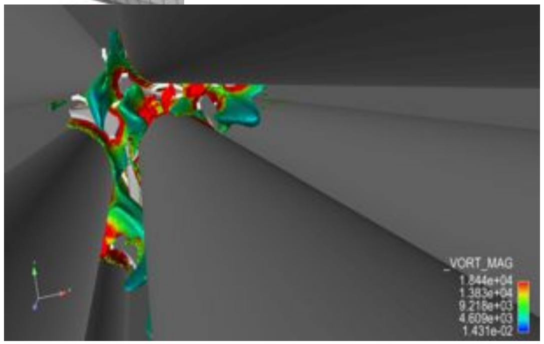
Drekar: Thermal Hydraulics Modeling of Reactor Core Sub-assemblies (Shadid, Pawlowski, Smith, Cyr, Weber – SNL)

Science Objectives and Impact

- Driver: **Modeling for reactor design and evaluation**
- Objective: **Predictive CFD and heat transfer for reducing margins of uncertainty and facilitating power uprates, life extensions and future reactor design**
- Strategy: **Employ next-generation implicit unstructured mesh CFD technology with robust and scalable Newton-Krylov Solvers and embedded UQ technology**
- Impact:
  - **Increase scalability & accuracy over current CFD capabilities.**
  - **Enable studies of critical aspects of flow and heat transfer to help understand failure points due to rod-vibration, localized hot spots and CRUD formation**
  - **Allow validation and uncertainty quantification (UQ).**

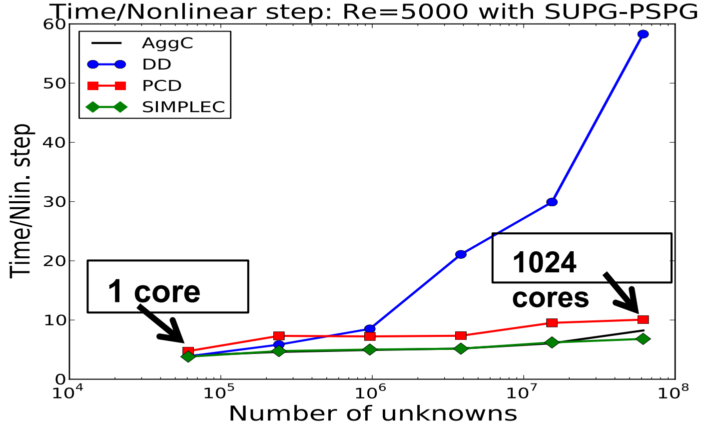


FE Mesh for Fuel Rod and Mixing Vane



Time Avg. LES Flow Iso-Vorticity Surface

Excellent Scaling Performance for Physic-based AMG Preconditioners

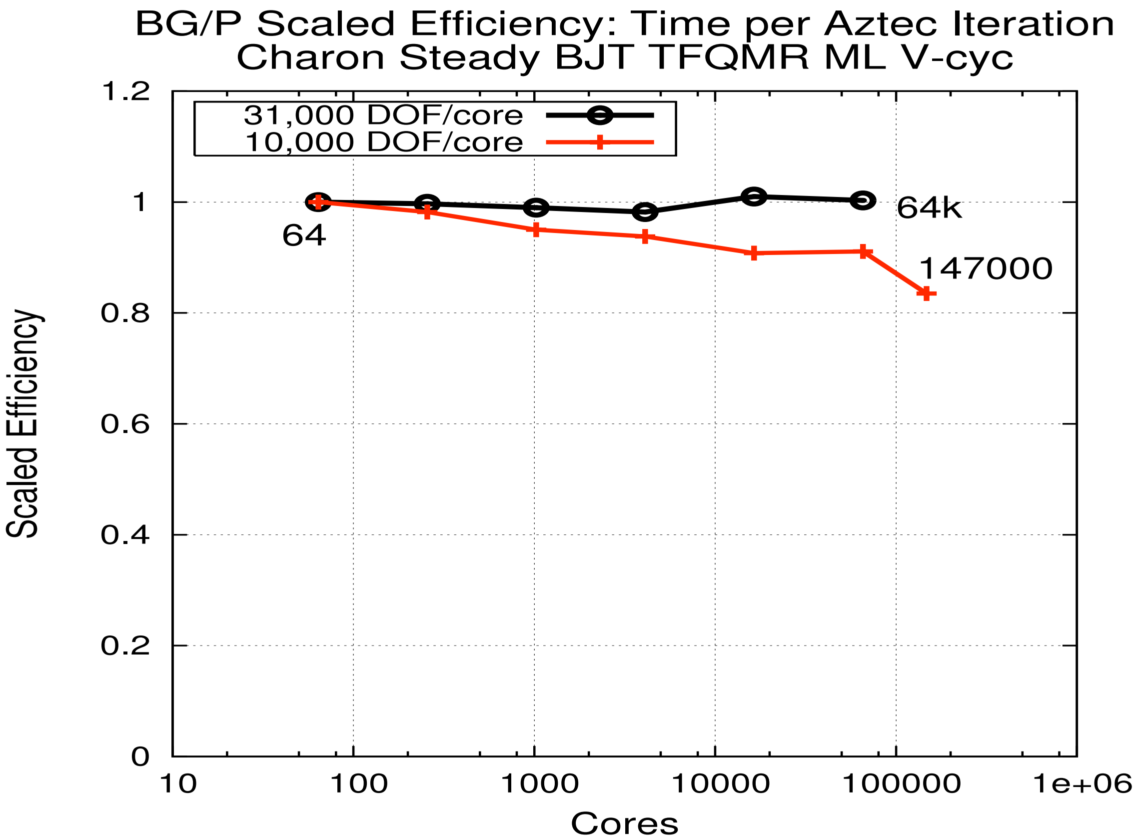


Science/Engineering Results

- LES simulations of 3x3 with mixing vanes;
- LES Pressure forcing and rod vibration simulation w/SIERRA
- Conjugate heat transfer in fluid / rod
- Recent runs of CASL relevant swirling jet flows (LES, RANS). On up to 215M elements, 1.3B unknowns 128K cores of Jaguar

Drekar: Thermal Hydraulics Modeling of Reactor Core Subassemblies
Turbulent fluid flow and heat transfer for rod vibration and localized host spots

Recent Optimization of ML AMG V-cycle Scaling is Critical to Performance*



*P. T. Lin, IJNME, 2012; Performance on a BlueGene/P
This is the fully-coupled AMG solver used in Drekar being run on a semi-conductor drift-diffusion simulation problem

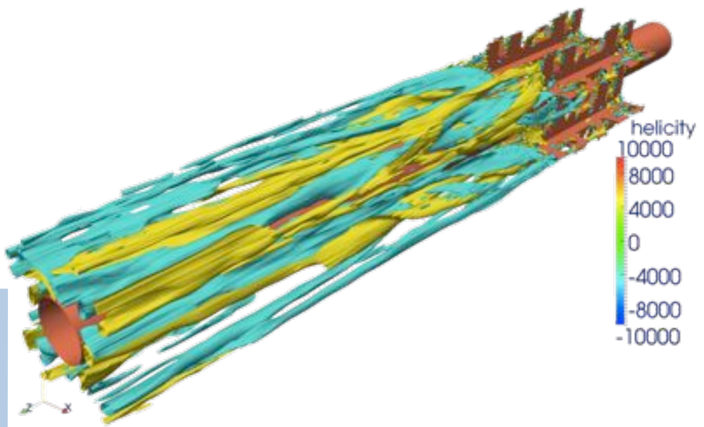
- We believe scaling on Jaguar will also be very good. Hope to have AMG V-cycle scale to ~300K cores for large-problems
- Now doing optimization of AMG setup phase
- Doing scaling studies on Jaguar now
- Working on Joule Metric Effort (Jaguar)

Thermal Hydraulics using Hydra-TH

Turbulent Flow in Grid-to-Rod Fretting

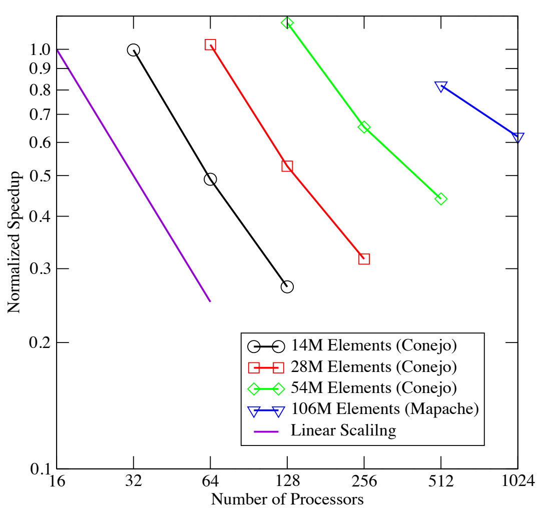
Science Objectives and Impact

- Strategy: Assess the performance of multiple turbulence models for the prediction of time-dependent forces in grid-to-rod fretting
- Driver: Improve in-core rod & spacer design to reduce rod fatigue and cladding
- Objective: Perform high-fidelity simulations of in-core flow around fuel rods and grid-spacer
- Impact: Stakeholders and DOE are focused on extending operating life cycle, reliability and safety while reducing cost



Application Performance

Preliminary Scaling Study



Science/Engineering Results

- Demonstrated the ability of Hydra-TH to predict grid-to-rod fretting forces due to high-Reynolds number flows using implicit large-eddy and detached-eddy simulation
- Showed the feasibility of using Hydra-TH in modeling in-core thermal hydraulics flow processes at reactor scale

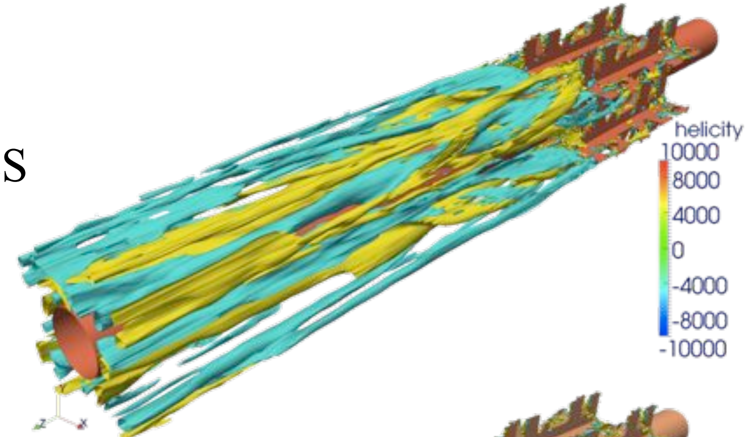
Thermal Hydraulics using Hydra-TH

Turbulent Flow in Grid-to-Rod Fretting

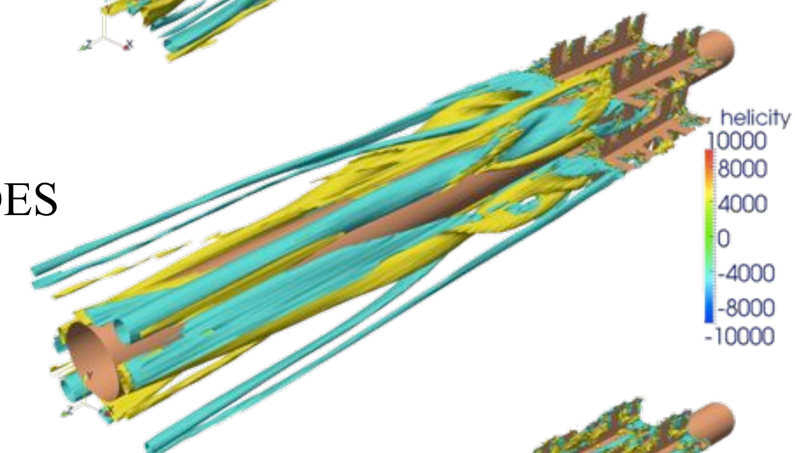
Helicity isosurfaces $(v \bullet \omega)$

- All models capture some level of detail in the longitudinal vortical structures and swirl
- With Spalart-Allmaras, eddies appear more damped, rotation around rod is smeared

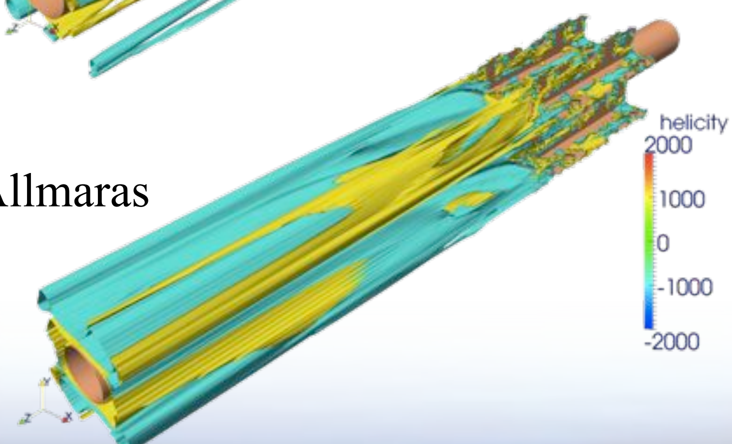
ILES

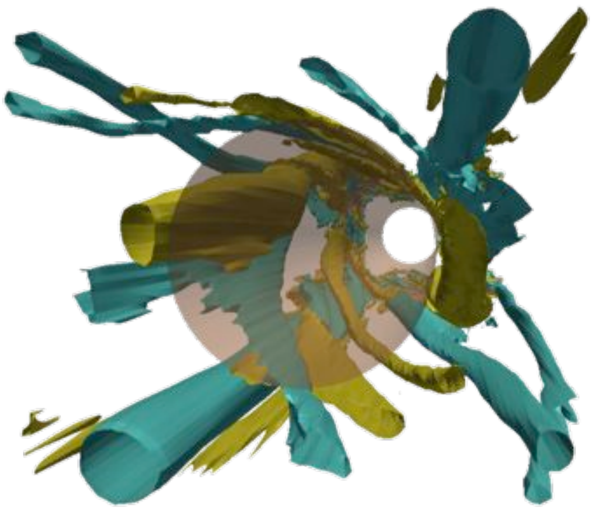


DES



Spalart-Allmaras

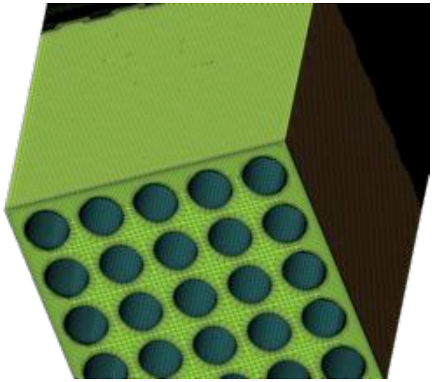




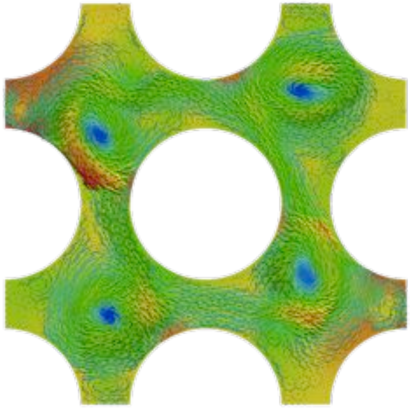
End-view of fuel rod showing swirl in coherent structures

Hydra-TH for Thermal Hydraulic Applications

- Hydra-TH is built on the Hydra toolkit
- The Hydra toolkit provides a collection of lightweight components with flexible data-structures
- Partial list of Hydra-TH capabilities:

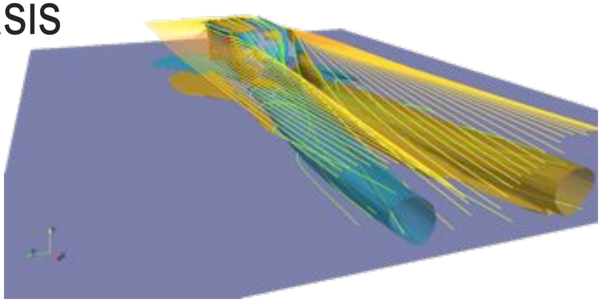


  - Runtime parallel load-balancing with data migration (static and dynamic)
  - I/O interfaces with plug ‘n play multi-reader/multi-writer model
  - Physics centric output delegates for derived output – automatically linked to input
  - State, surface and history output
  - Linear algebra interface w. access to rich suite of Krylov solvers & preconditioners
  - Material models – simple and field-dependent interfaces
  - Keyword input – shared parsing for common input with run-time selectable physics
  - Temperature or enthalpy energy eq.
  - Error handling for both exceptions and cumulative errors
  - Turbulence models
    - ILES, DES, Spalart-Allmaras, RNG k-ε
    - SST k-ω (under constuction)
    - k-sgs (under construction)
  - Porous media flow
  - CHT/FSI interfaces
  - Time-dependent BC’s
  - Passive outflow BC’s
  - Generalized body forces
  - Hybrid meshes (tet, hex, wedge, pyramid)
  - Monotonicity-preserving advection
  - Eulerian or ALE w. deforming mesh
  - Automatic time-step control
  - . . .



Hydra-TH on Jaguar

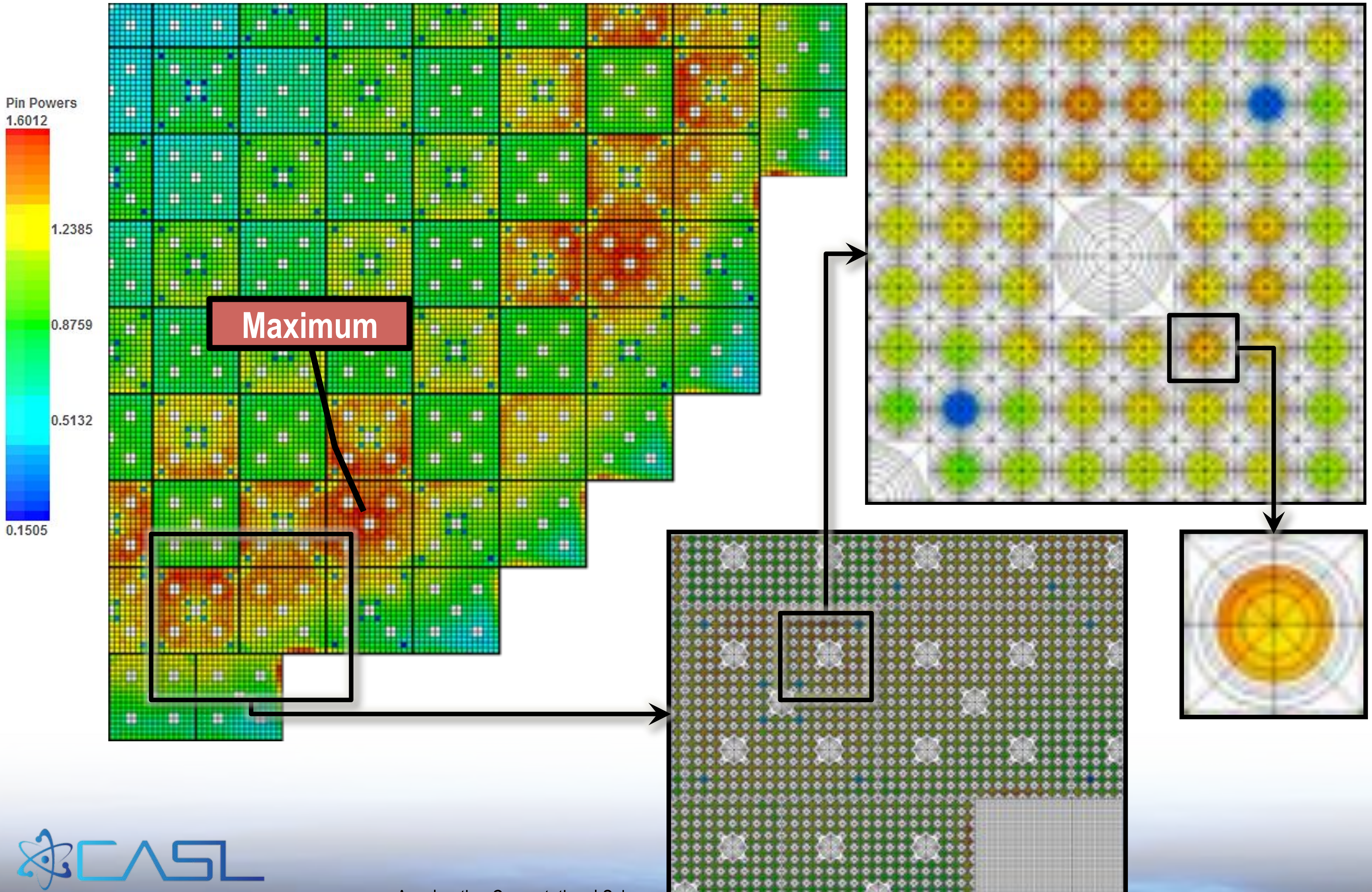
- Hydra-TH was ported to the XT5 system in FY2011
  - Initial scaling studies performed
  - Preliminary channel mesh calculations exercised on ~8000 cores
- Hydra-TH has been ported to the XK6 system
  - Full suite of regression tests exercised on a weekly basis (approx.)
  - Currently working towards scale-up beyond 8000 cores for grid-to-rod fretting problems



- GPU Usage on XK6
  - Sparse linear algebra is the pacing technology for using GPU's with hybrid parallelism in Hydra-TH
  - Hydra-TH already provides interfaces for "native" GPU Krylov solvers, and will make use of advances in PetSC and TRILINOS for GPUs
  - The Hydra toolkit provides threading ready "workset" interfaces for the other portions of the flow physics which will be used for grid-based computations on GPUs

Pin-Resolution of Neutron Behavior is Required

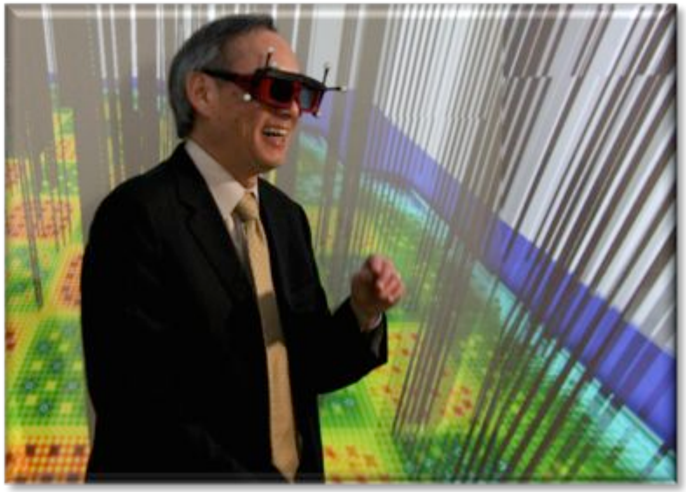
Current practice is to construct 3D power distributions with 1D/2D/nodal

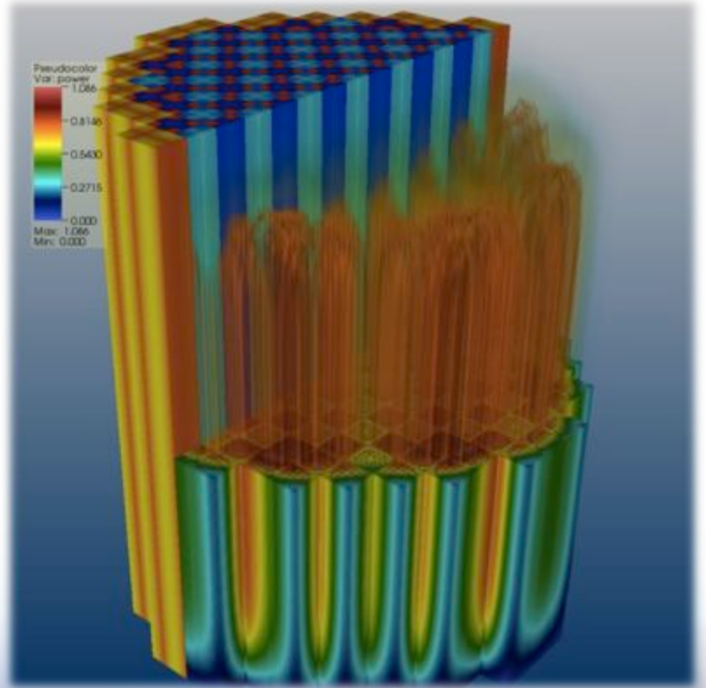


Deterministic Neutron Transport with Denovo

See Tom Evans talk next

- 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)
  - trilinear-discontinuous finite element (TLD)
- Reflecting, vacuum, and surface source boundary conditions



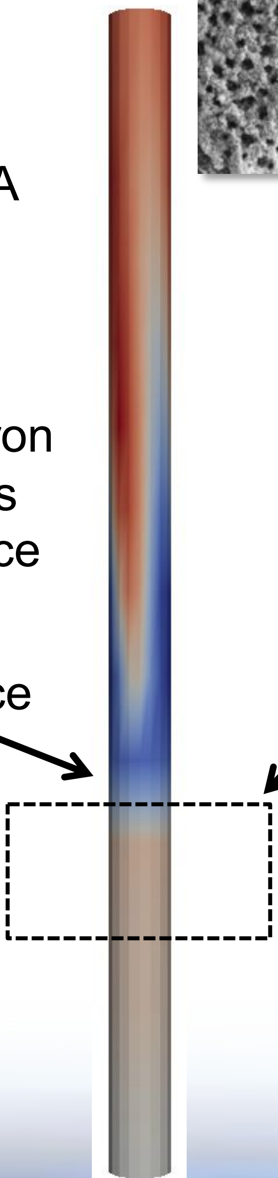


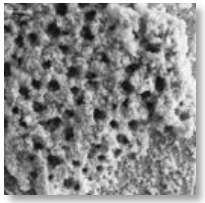
CASL

Coolant Chemistry and CRUD Growth with MAMBA

Thermal hydraulics + transport + fuel performance + chemistry + structural mechanics

Boron concentration within crud layer (colored contours) grown within MAMBA over 60 days of operation





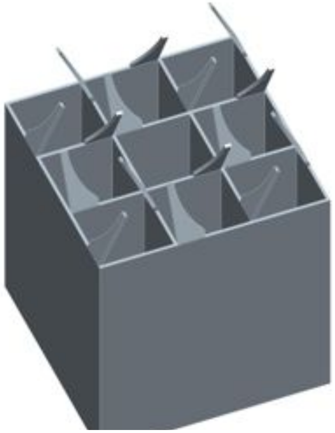
Variations in crud thickness and boron due to T variations on cladding surface

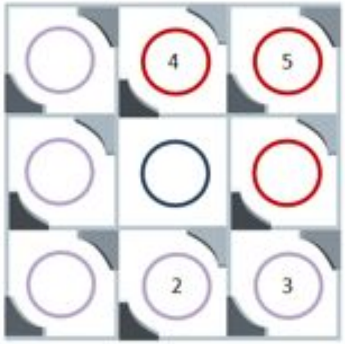
Reduced crud and boron due to turbulence behind mixing vanes

80 cm section of fuel rod

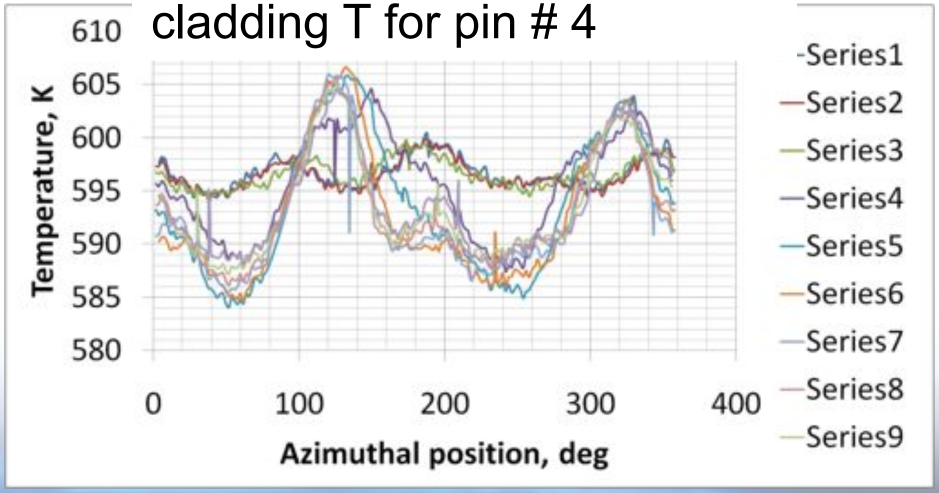
Large azimuthal variation in fluid/cladding temperature computed by STAR-CCM+ (U. Mich. group)

Spacer with mixing vanes



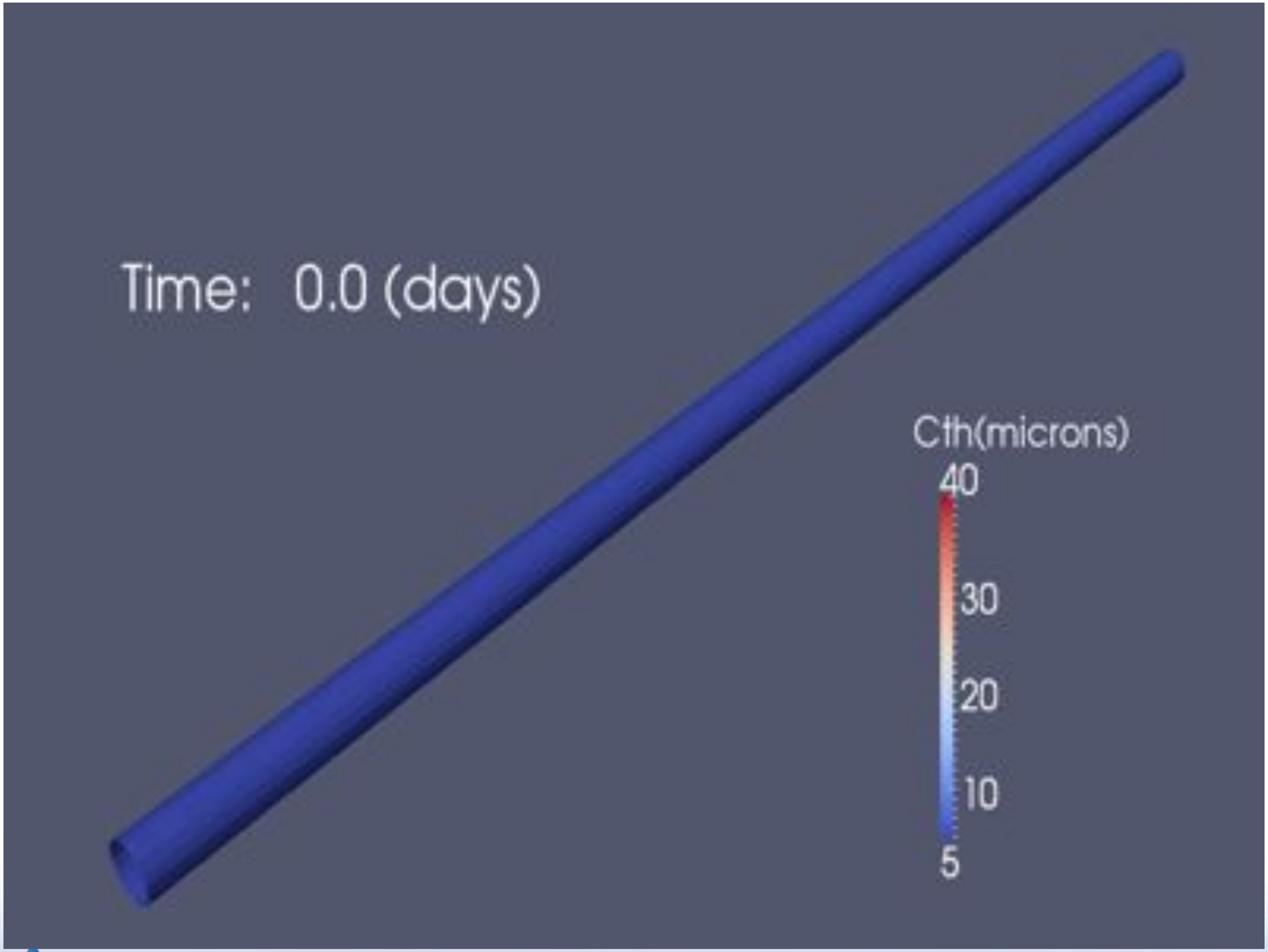


CFD (Star-CCM+) computed cladding T for pin # 4



3D MAMBA + CFD Simulation (movie)

Simulation of full pin with 3-spacer grids – CRUD thickness varies due to T variation and surface erosion



Initial steps of coupling CRUD thickness predictions of B incorporation to DeCart for predicting Axial Offset Anomaly

Questions?

http://www.casl.gov/ -or- info@casl.gov