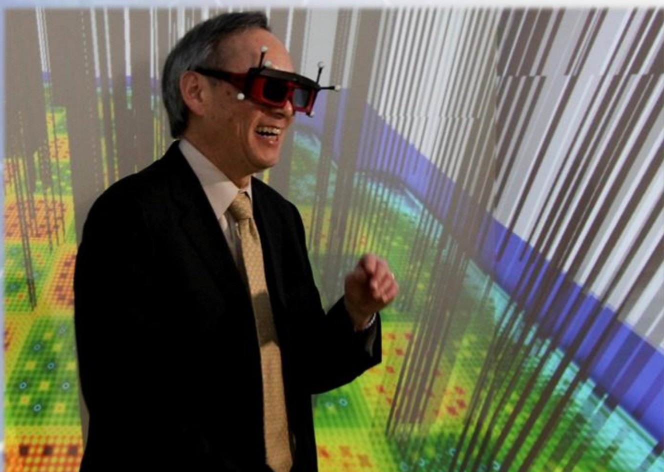
CASL: The Consortium for Advanced Simulation of Light Water Reactors

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

John A. Turner
Oak Ridge National Laboratory
Computer Science & Math Division
Virtual Reactor Integration Lead, CASL



SOS16
Santa Barbara, CA
Mar 15, 2012

CASL
Consortium for Advanced Simulation of LWRs

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

What is a DOE Energy 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
- 03/08/2010: proposals due
- 05/27/2010: CASL selected
- 07/01/2010: first funding arrives

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The Consortium for Advanced Simulation of Light Water Reactors (CASL)

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

Challenges

- High visibility
- Geographically-dispersed
- Diversity of experience
- Wide range of motivation / priorities
- Proprietary codes and data
- Role of commercial codes
- Export control

Individual contributors

ASCOMP GmbH

CD-adapco, Inc.

City University of New York

Florida State University

Imperial College London

Rensselaer Polytechnic Institute

Southern States Energy Board

Texas A&M University

University of Florida

University of Tennessee

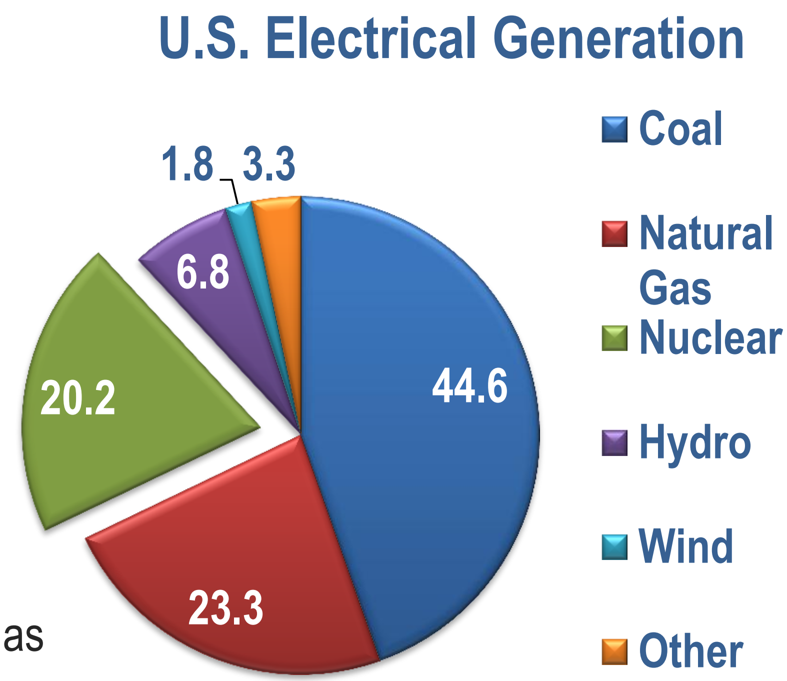
University of Wisconsin

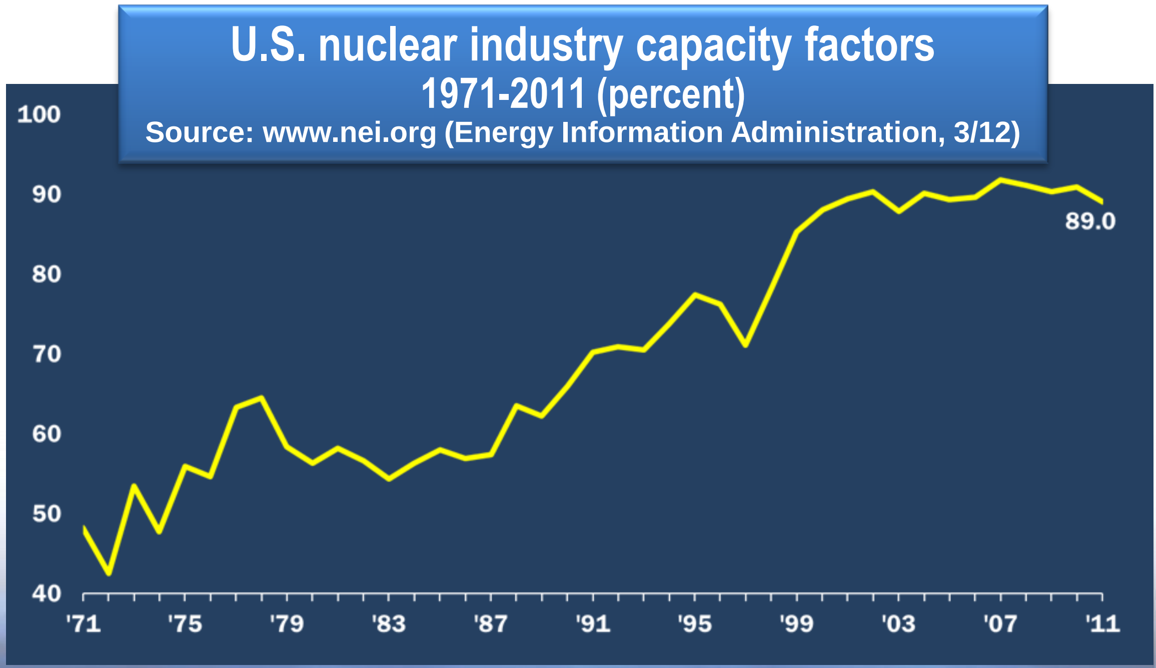
Worcester Polytechnic Institute

Nuclear Energy Overview

Source: Nuclear Energy Institute (NEI)

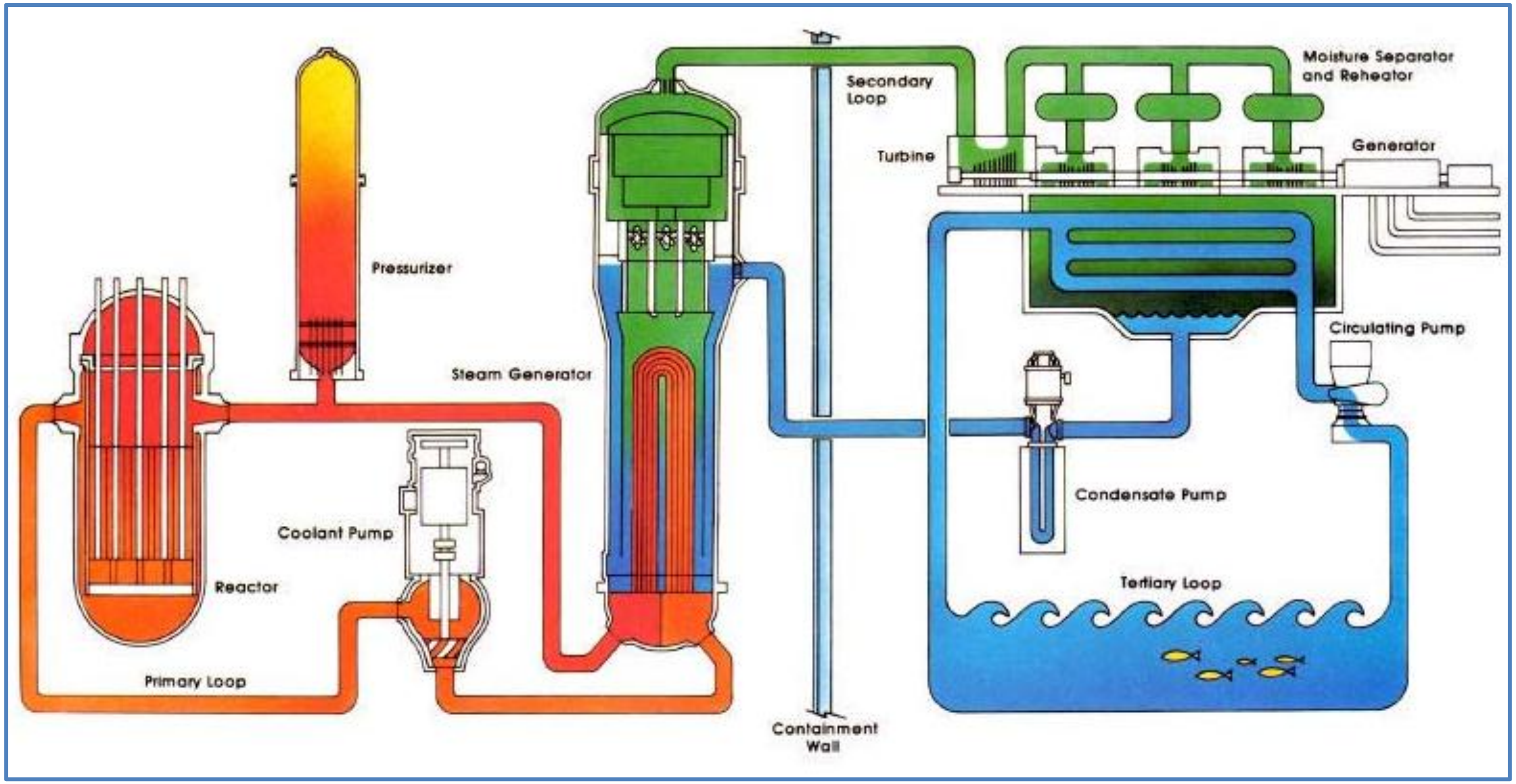
- World nuclear power generating capacity
  - 439 plants (U.S.- 104 plants in 31 states)
  - 373 GWe (U.S.- 100.7 Gwe, 798.7 TWh in 2009)
  - ~90% capacity factor
- U.S. electricity from nuclear: 20.2%
  - One uranium fuel pellet provides as much energy as
    - one ton of coal
    - 149 gallons of oil
    - 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:

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

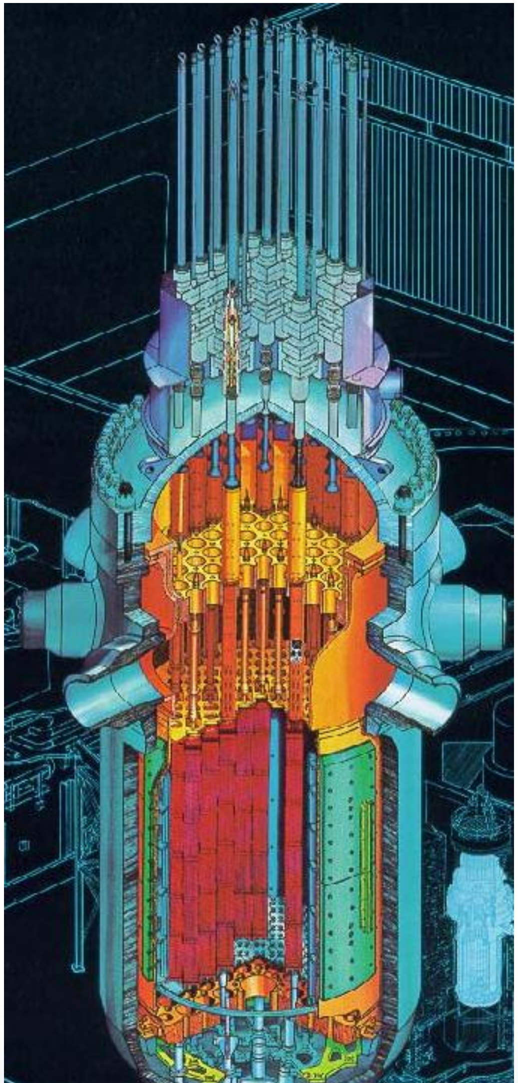
Coolant: pressurized water (2250 psia), T_{in} ~ 545°F, T_{out} ~ 610°F, 134M lb/h (4 pumps)

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

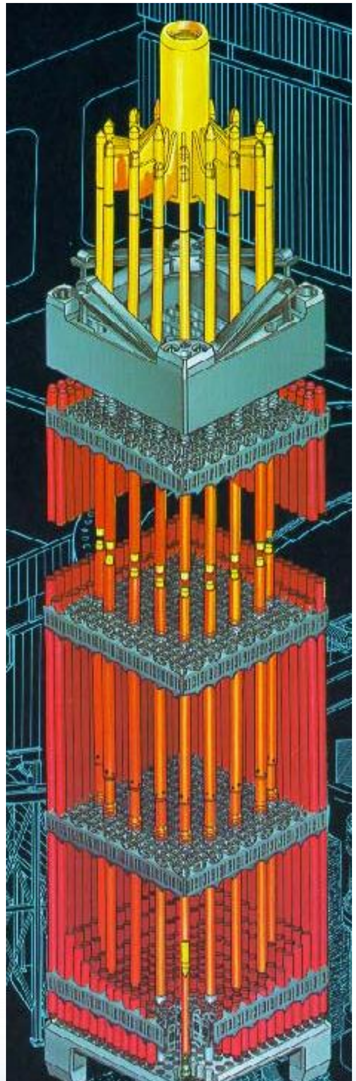
Containment Building: 115’ diameter x 156’ high steel / concrete

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 mission is to improve reactor performance
(initially currently-operating LWRs)

Power uprates

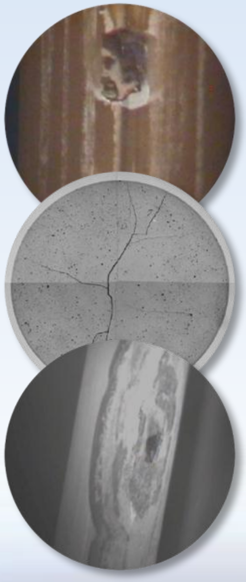
- 5–7 GWe delivered at ~20% of new reactor cost
- Advances in M&S needed to enable further uprates (up to 20 GWe)
- **Key concerns:**
  - Damage to structures, systems, and components (SSC)
  - Fuel and steam generator integrity
  - Violation of safety limits

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



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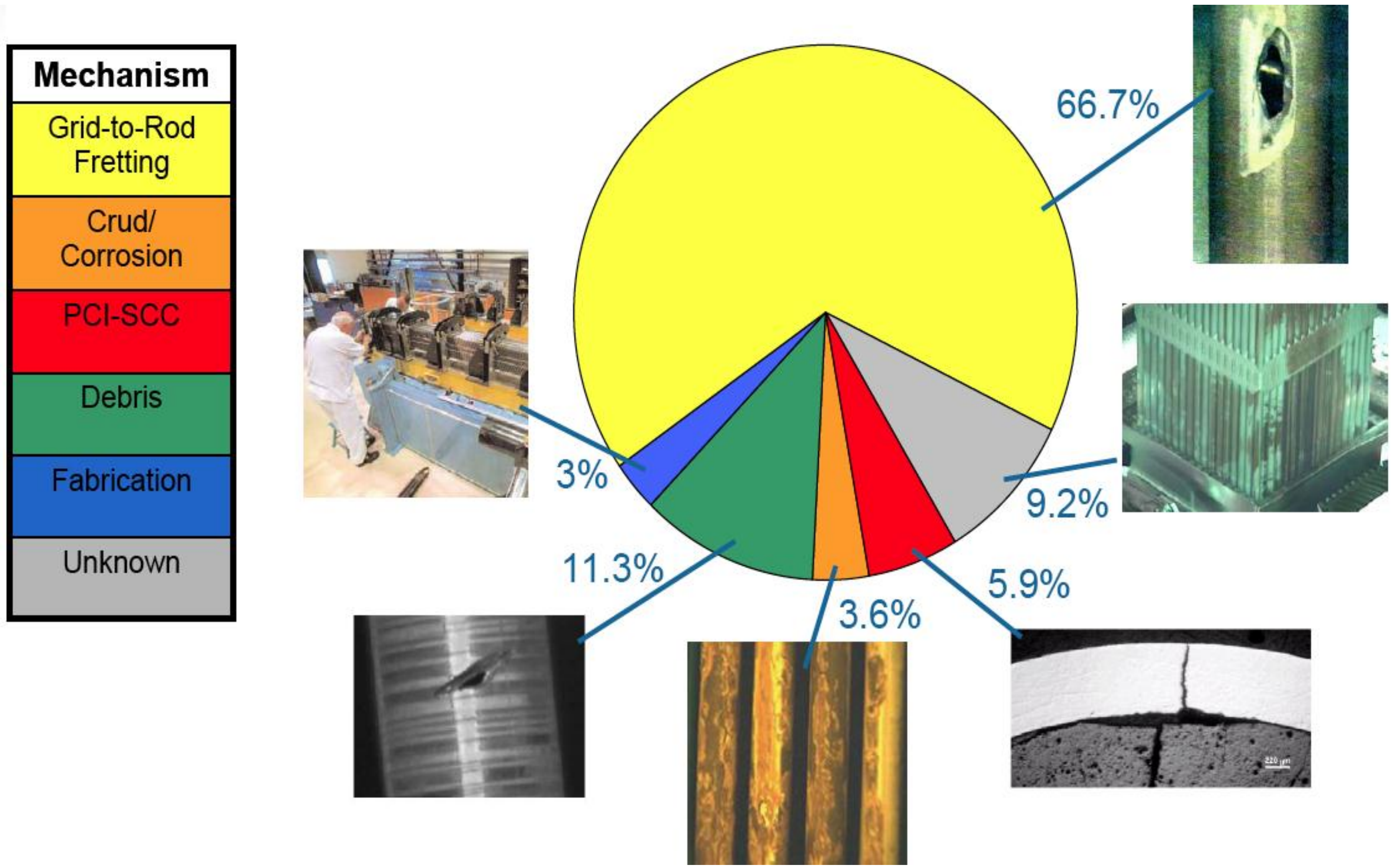
CASL Challenge Problems
Summary of US fuel failure mechanisms (2000-2008)

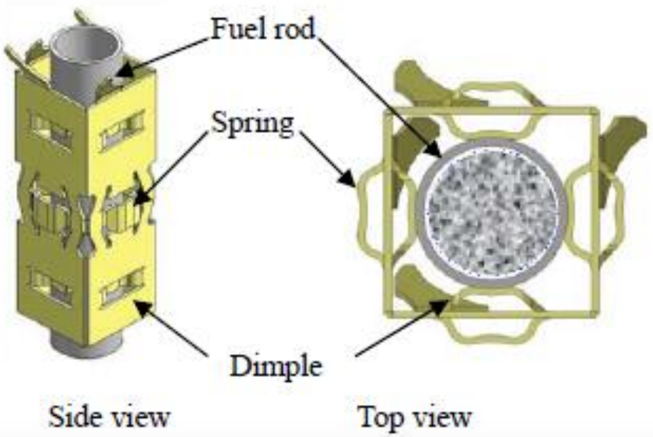


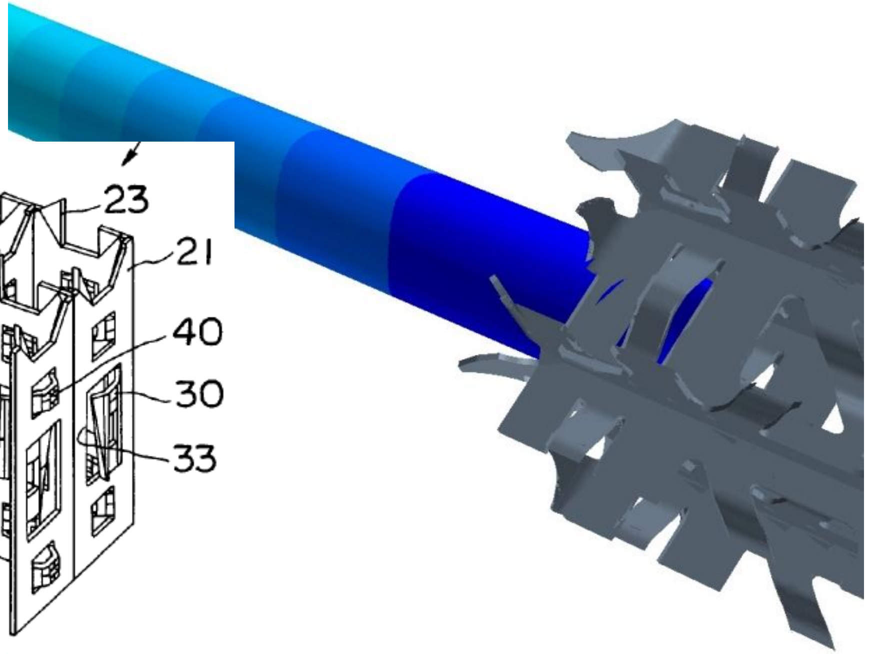
* Edsinger, Stanek, Wirth, JOM **63, no. 8** (2011)

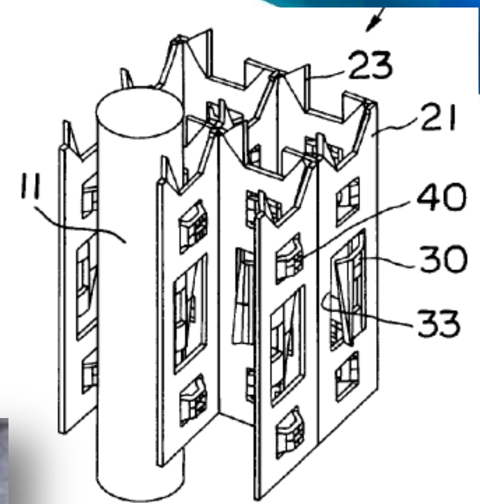
Fuel failure modes provide motivation for CASL activities

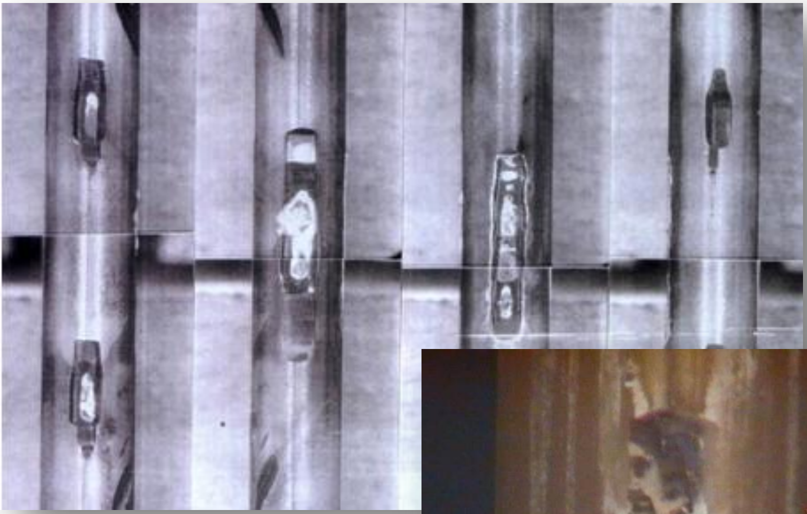
Grid-to-Rod-Fretting (GTRF)

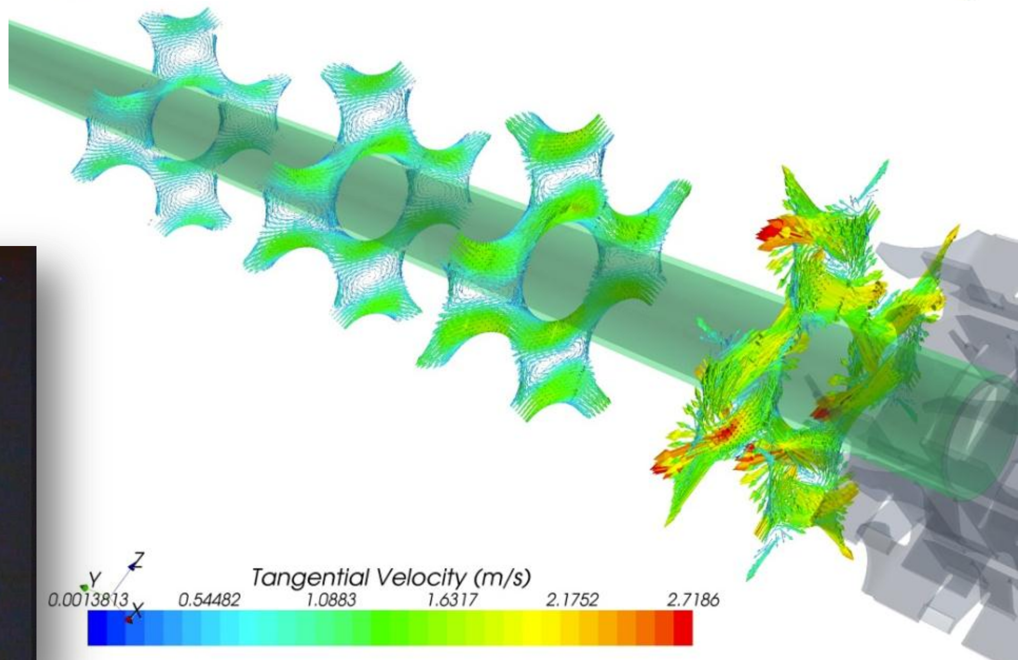
Spacer Grid with Springs/Dimples





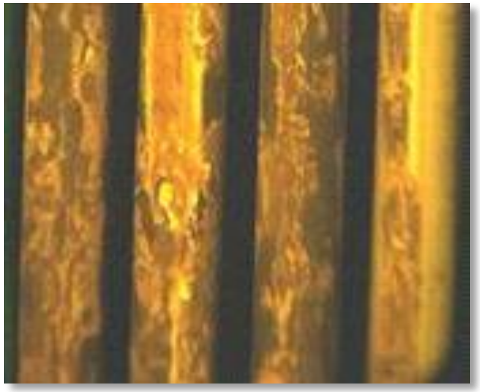




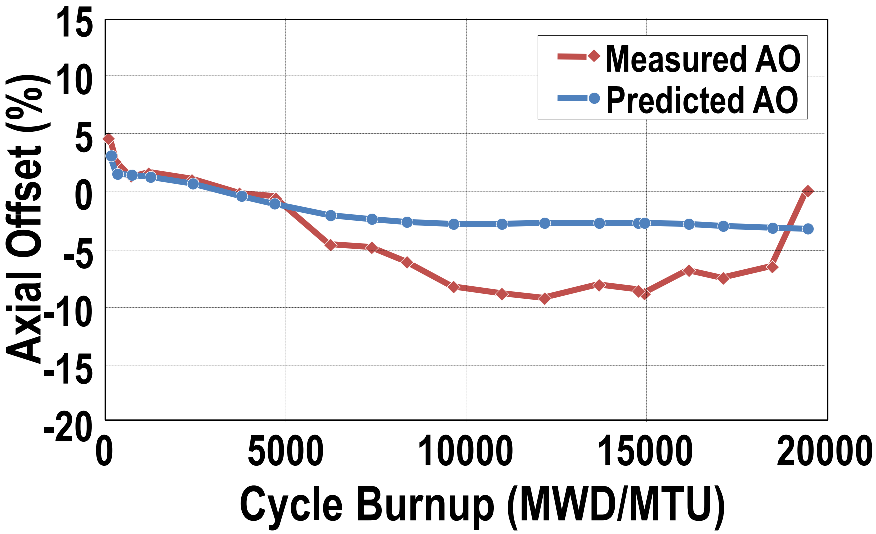


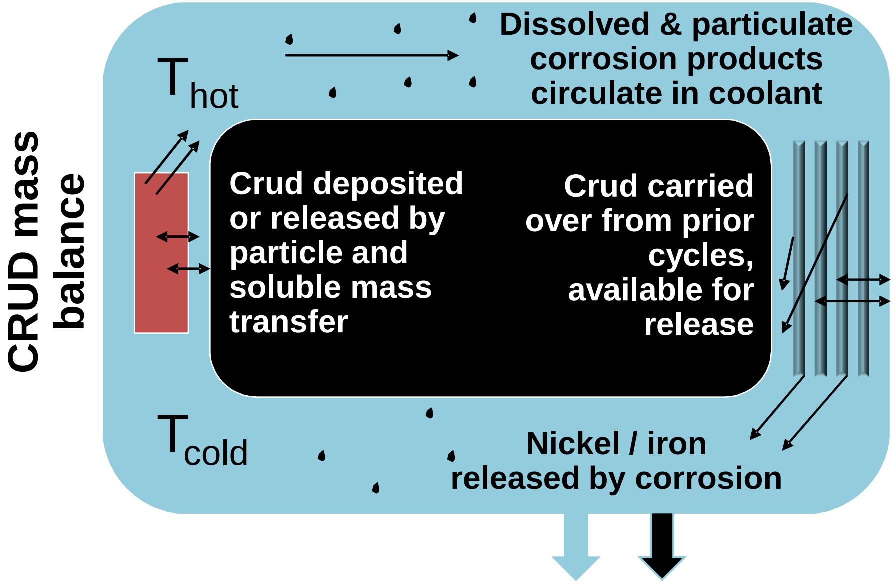
CRUD-induced power shift (CIPS)

- 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



CRUD deposits





Need: Multi-physics chemistry, flow, and neutronics model to predict CRUD growth

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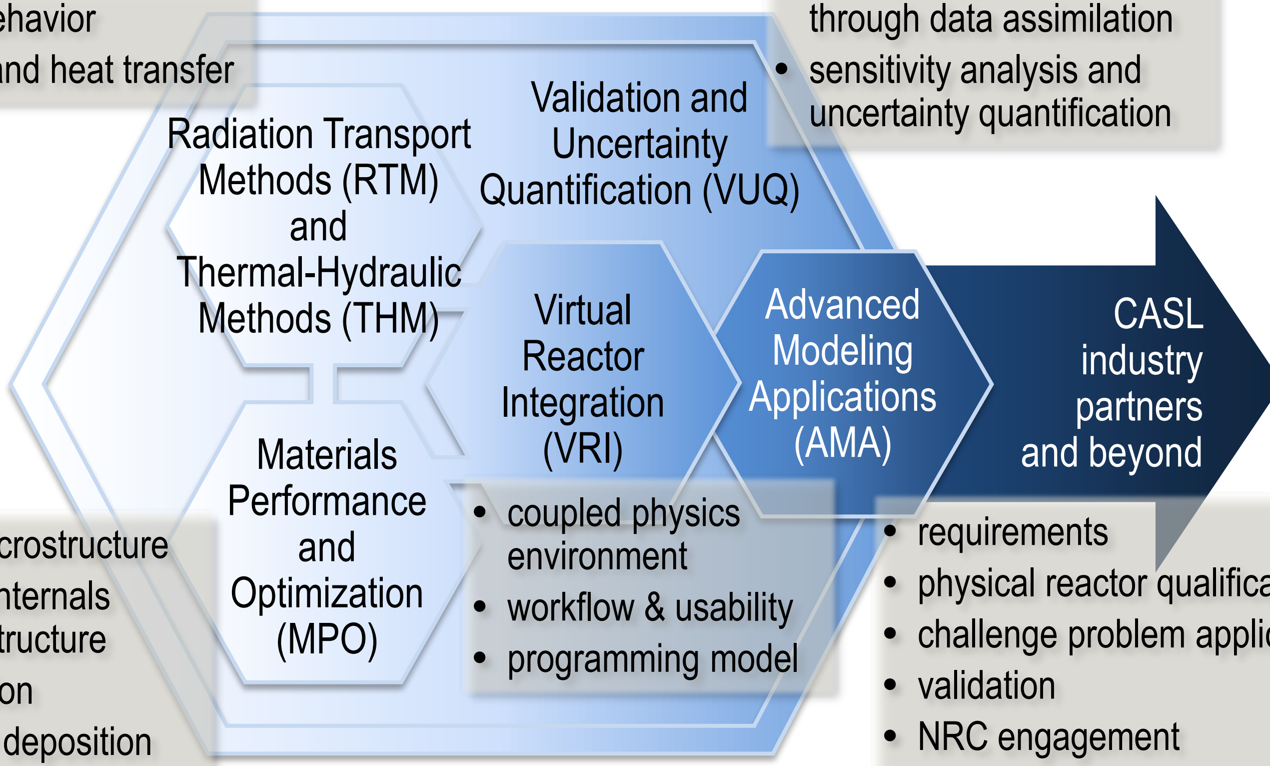
CASL Technical Focus Areas

- neutron behavior
- fluid flow and heat transfer

- V&V and calibration through data assimilation
- sensitivity analysis and uncertainty quantification



- fuel microstructure
- clad / internals microstructure
- corrosion
- CRUD deposition
- failure modes

- coupled physics environment
- workflow & usability
- programming model

- requirements
- physical reactor qualification
- challenge problem application
- validation
- NRC engagement

All Focus Areas span institutions (labs, universities, industry)

Virtual Environment for Reactor Applications (VERA)

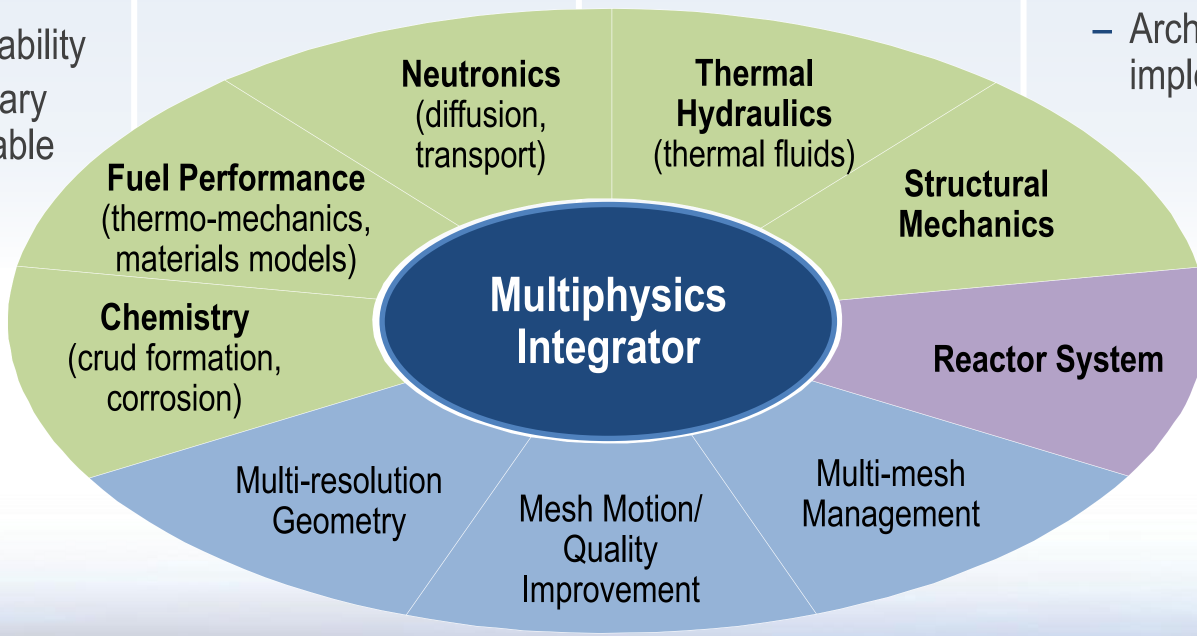
A suite of tools for scalable simulation of nuclear reactor core behavior

- 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



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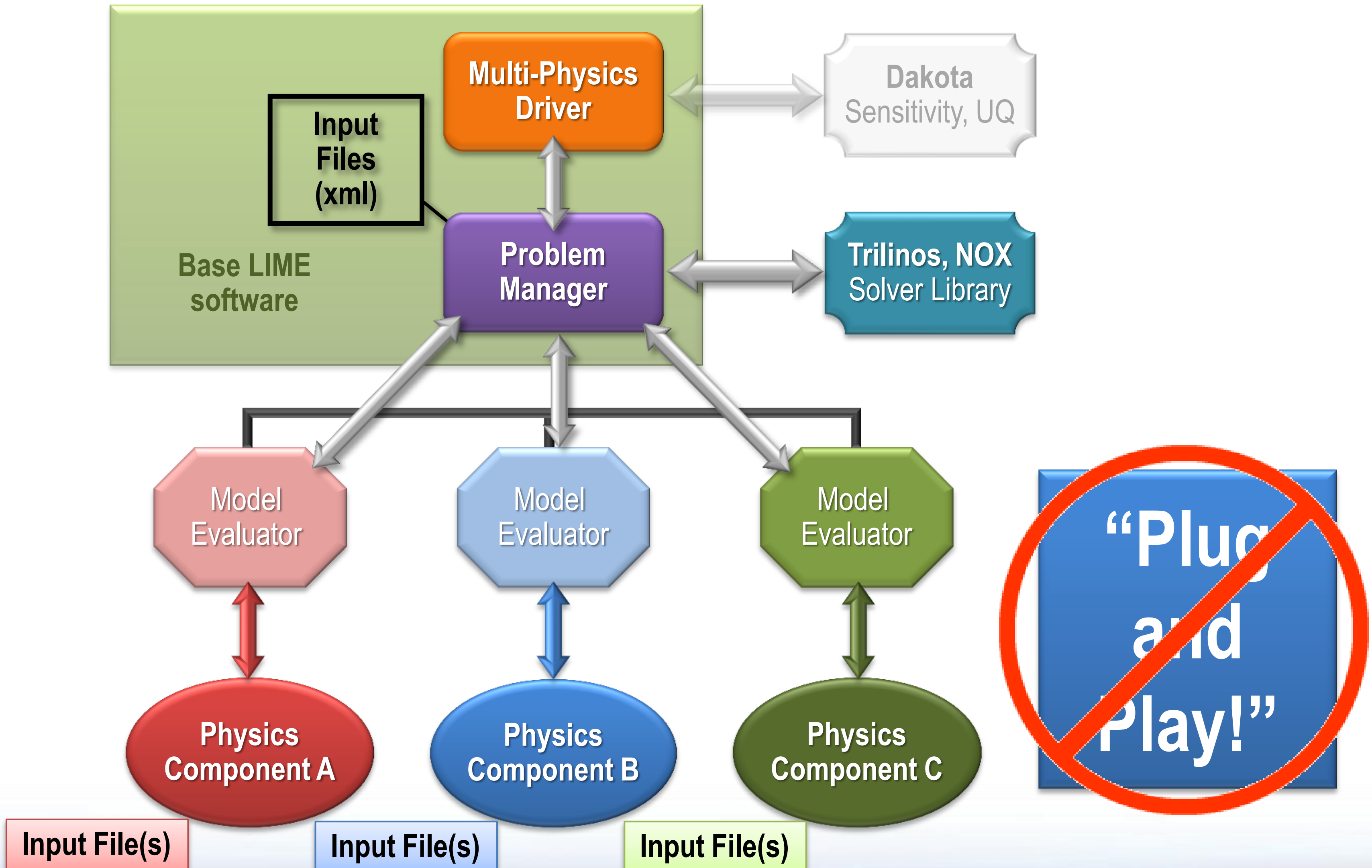
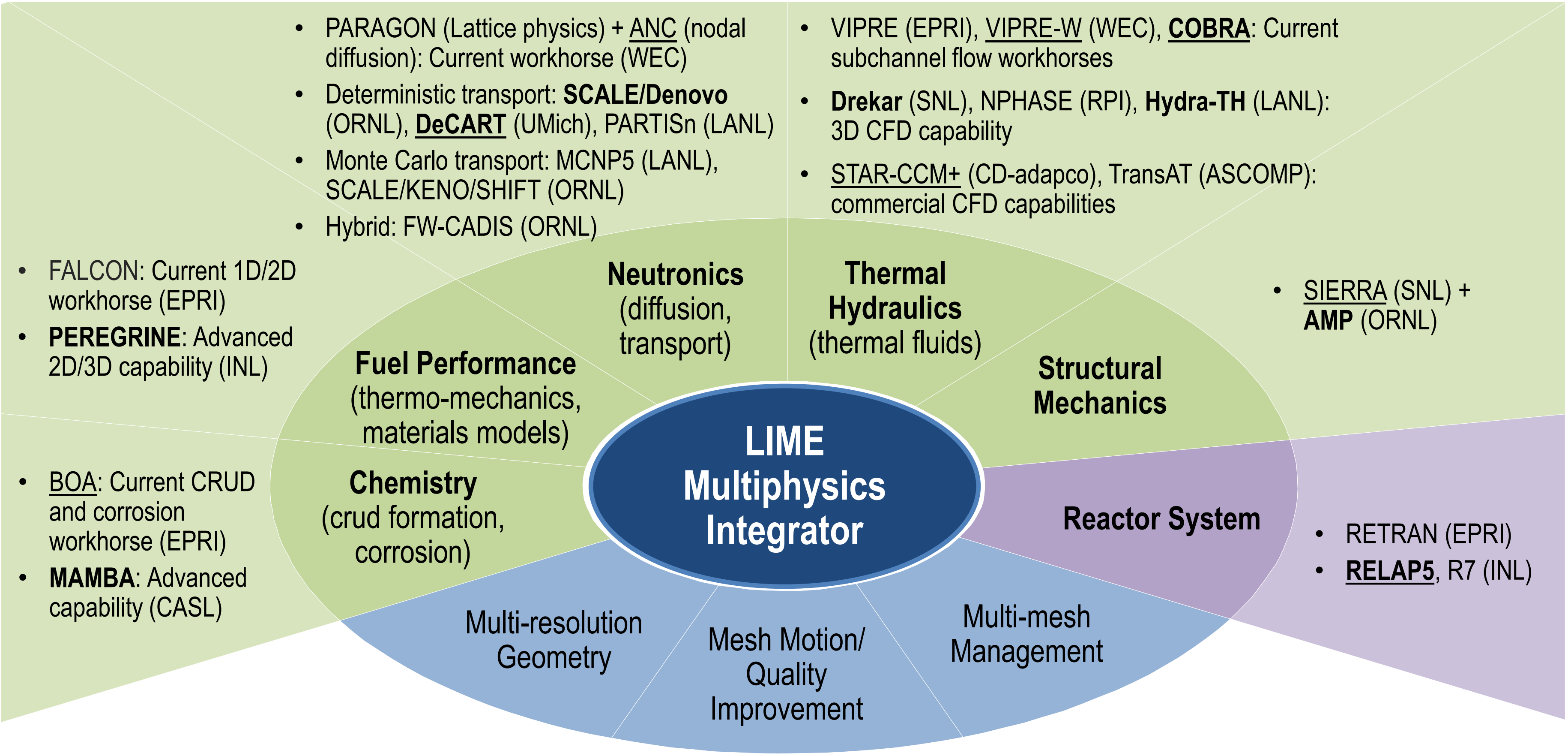
Missing…

- geometry
  - goal is a common geometry database
- material properties
  - again, goal is common libraries
- mesh generation
  - looking at multiple options
- common input / user interface
  - reactor-aware, data-aware
- analysis / design / optimization

Lightweight Integrating Multiphysics Environment (LIME)



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



CASL Challenges

- standing up computational infrastructure
  - institutional access, platforms, development environment
- IP and export control issues
- balancing software quality and research / discovery (NQA-1)
- original plans underestimated requirements for some key elements
  - cross section processing
  - structural mechanics
  - mesh management infrastructure / strategy
- dealing with legacy codes
- priority of analyst workflow and usability
- communication / integration – natural tendency toward “cylinders of excellence”
- terminology confusion
- tension between agility and management by milestones

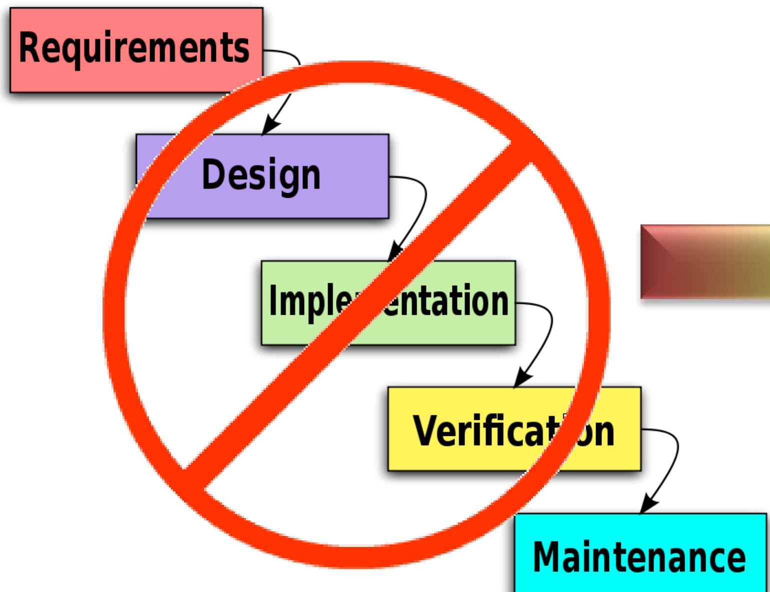
Challenge-problem driven development

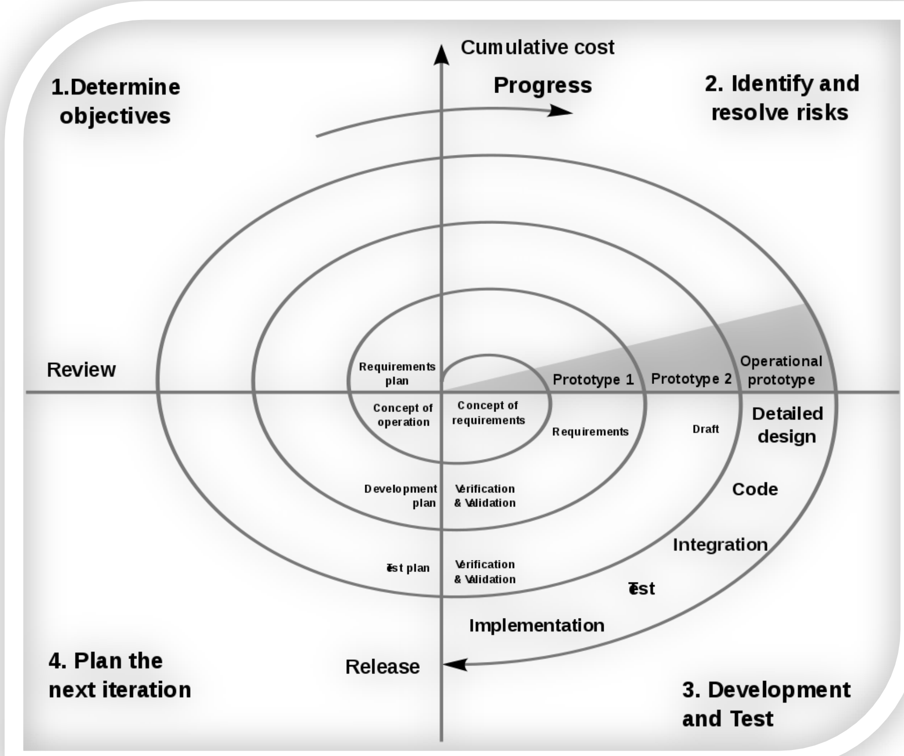
- CASL is following a challenge-problem driven plan
  - use specific relevant problems to drive development of broadly-applicable capability
- could be viewed as large-scale iterative development
- more appropriate for program with significant R&D components
- feedback from customers / users on priorities is critical

Agile software development processes

software development processes:

- processes, practices and activities that drive software development
- customer interactions (e.g. requirements gathering)
- contract models
- planning, day-to-day coordination, releases, etc.



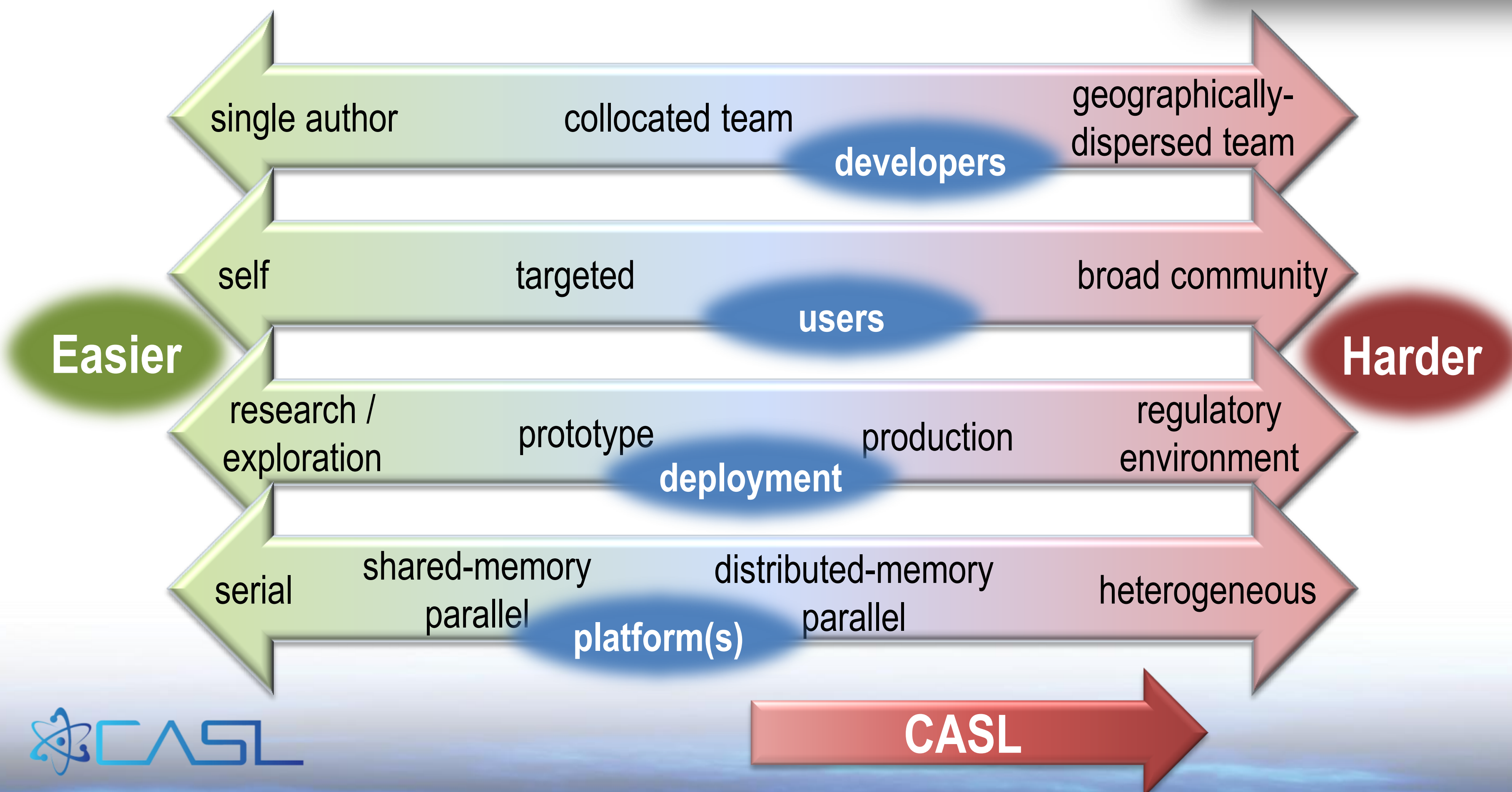


Traditional waterfall approach is unable to accommodate changing requirements and research-driven projects.

Agile methods fix Time (fixed iterations, fixed releases) and Effort (fixed team size) and vary Scope (functionality) based on iterative feedback with customer(s).

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.



CASL is using an Agile software development process

- 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

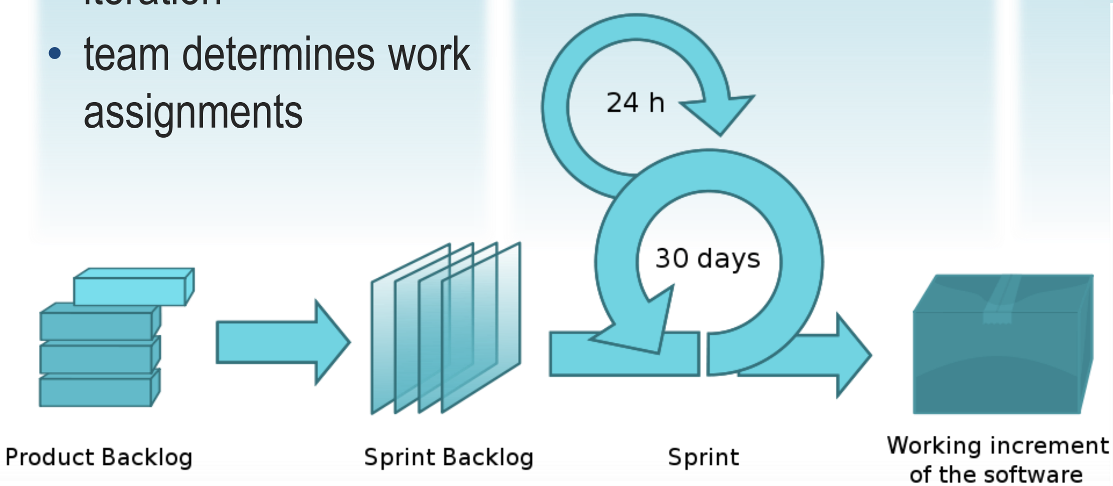
- users prioritize goals for next 4-week iteration
- team determines work assignments

Execute

- two 30-minute standup meetings each week

End

- deliver and demonstrate to users
- review and plan next iteration



Scrum: http://en.wikipedia.org/wiki/Scrum_%28development%29

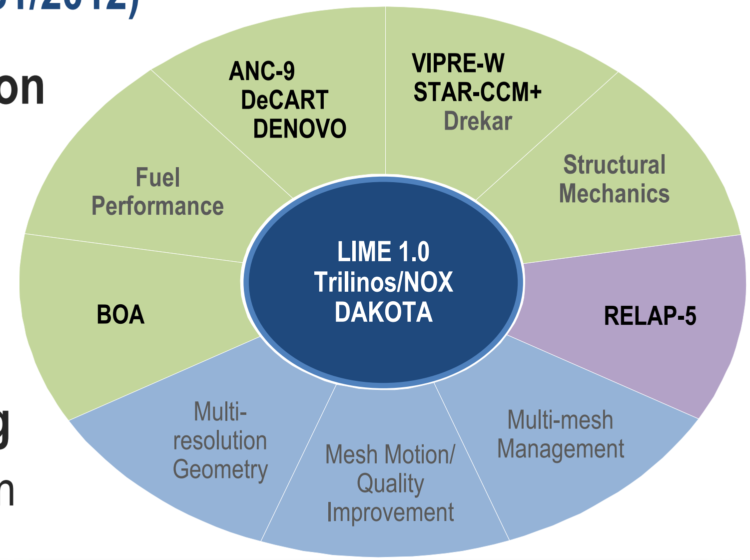
Desirable attributes

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

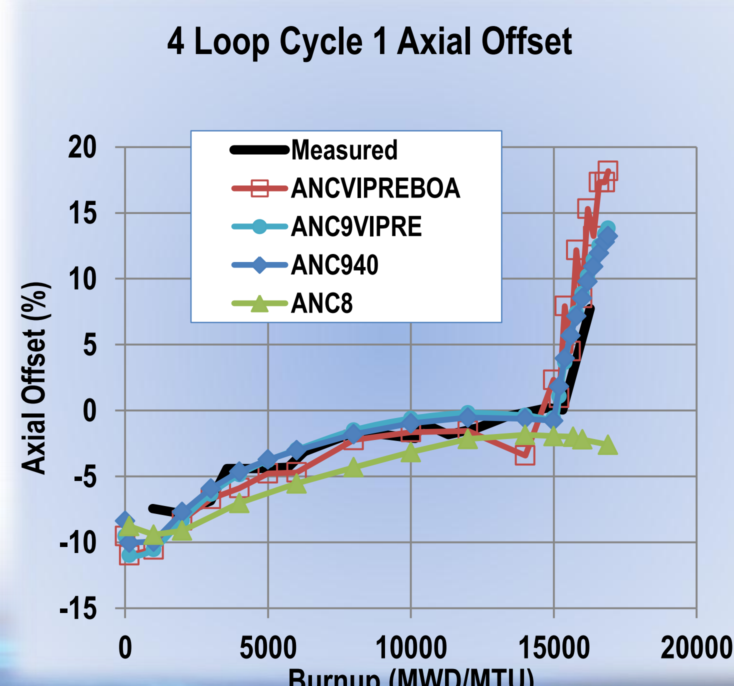
Agility + Formality

Virtual Environment for Reactor Applications (VERA)

v1.0 (3/31/2011), v1.1 (9/30/2011), v1.2 (12/15/2011), v2.0 (3/31/2012)



- **software framework for physics capability integration**
  - based on widely-used advanced open numerical software infrastructure (Trilinos, NOX, LIME, etc.)
  - initial integration with optimization, sensitivity analysis, and uncertainty quantification (DAKOTA)
- **baseline industry capability with improved coupling**
  - based on Westinghouse and EPRI codes as demonstration
    - ANC, VIPRE-W, and BOA standalone
    - Coupled ANC-VIPRE-W and ANC-VIPRE-W-BOA
- **initial advanced capabilities**
  - University of Michigan effort coupling neutronics (DeCART) and commercial CFD (Star-CCM+)
  - developing National Lab capabilities in neutronics (Denovo/SCALE) and CFD (Drekar, HYDRA-TH)
- **initial coupling to reactor system capability**
- **design documents for VERA and infrastructure**



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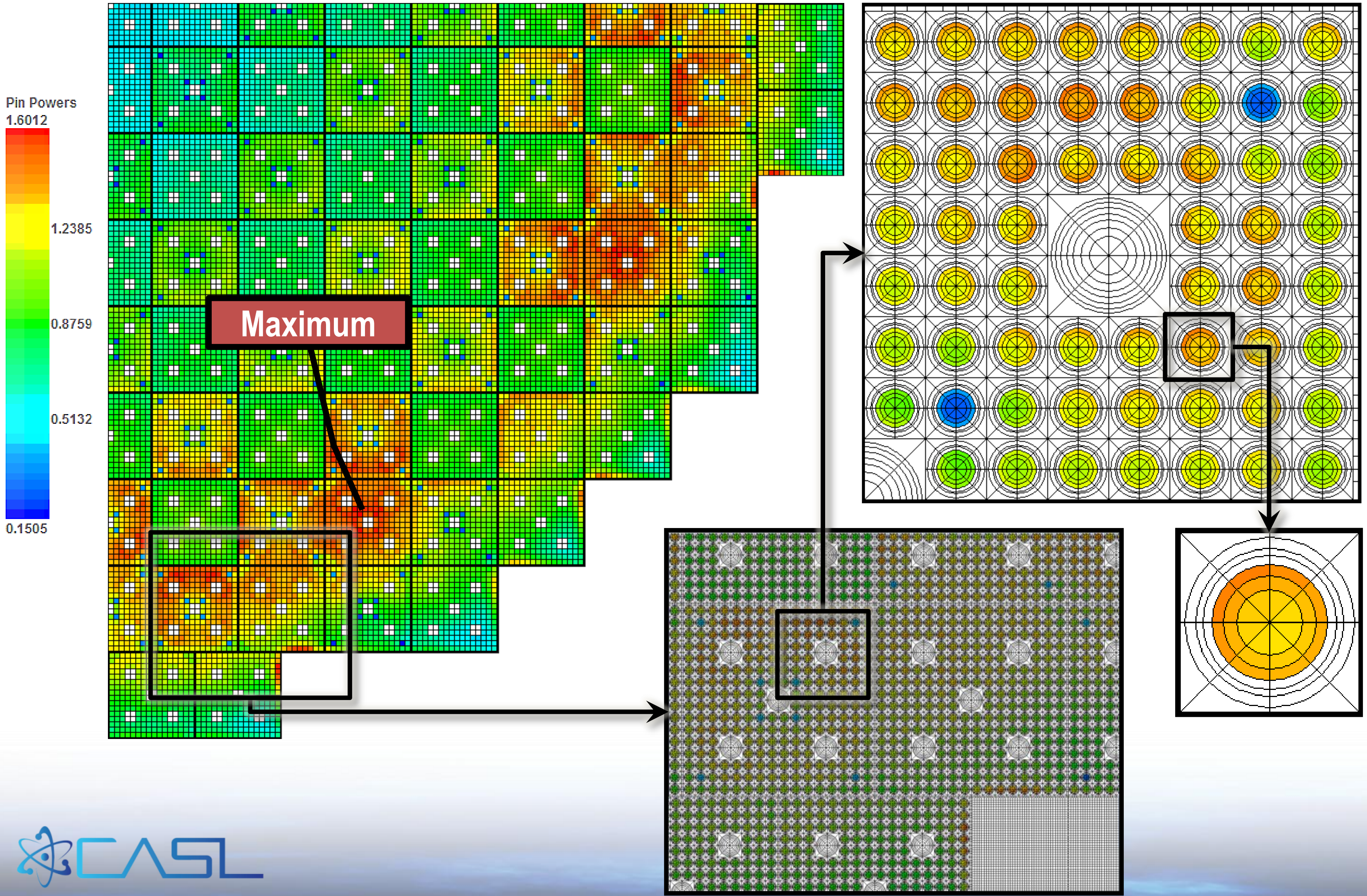
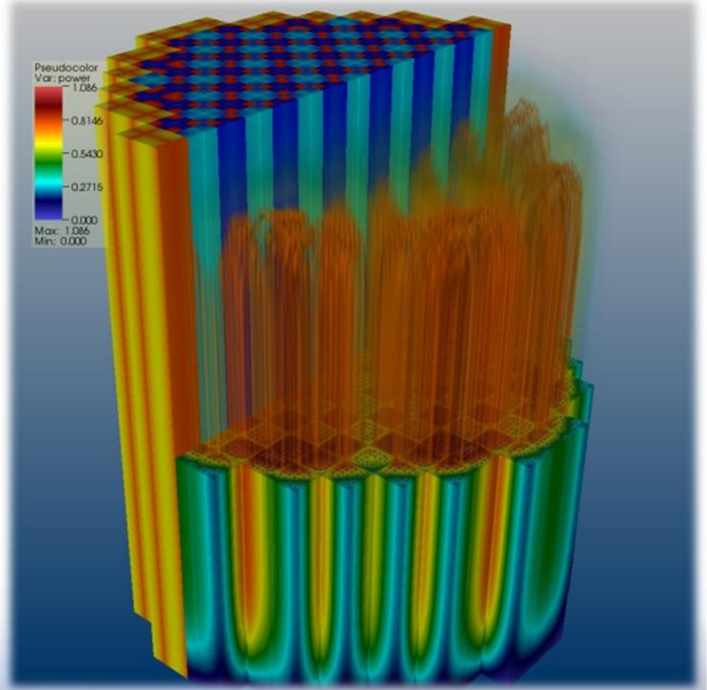
Pin-resolved simulation of neutron behavior

multiscale simulation to obtain axial and azimuthal power distributions



Code Algorithmic Features: Denovo

- 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



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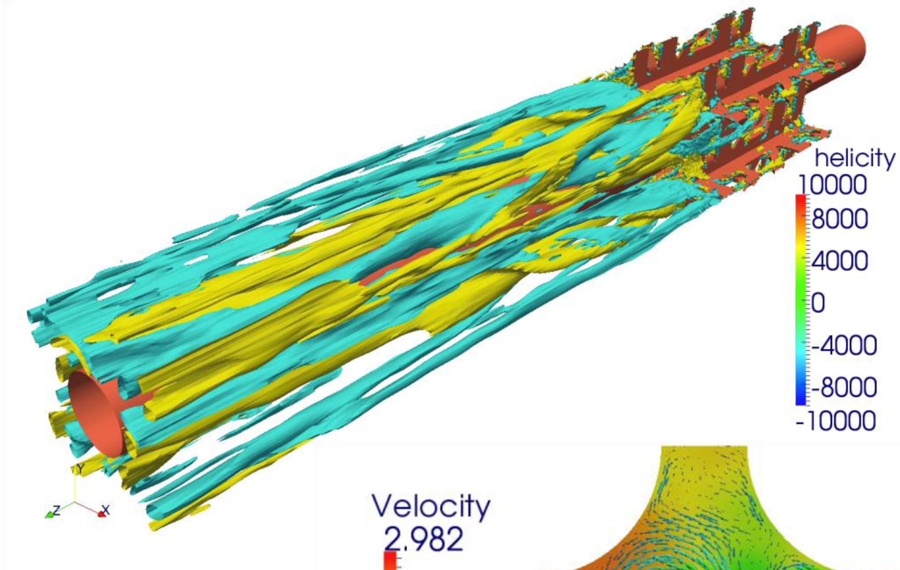
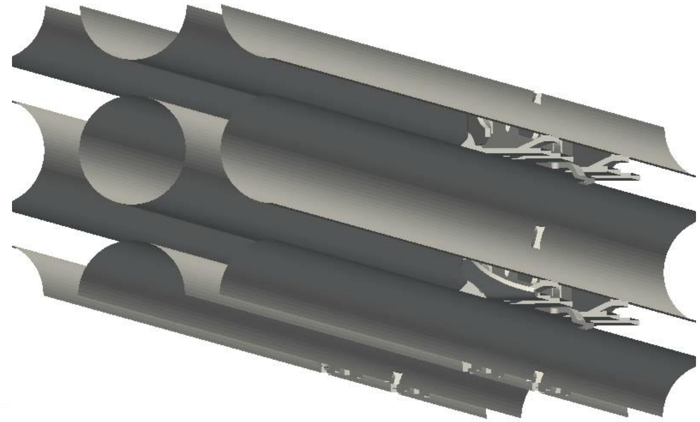
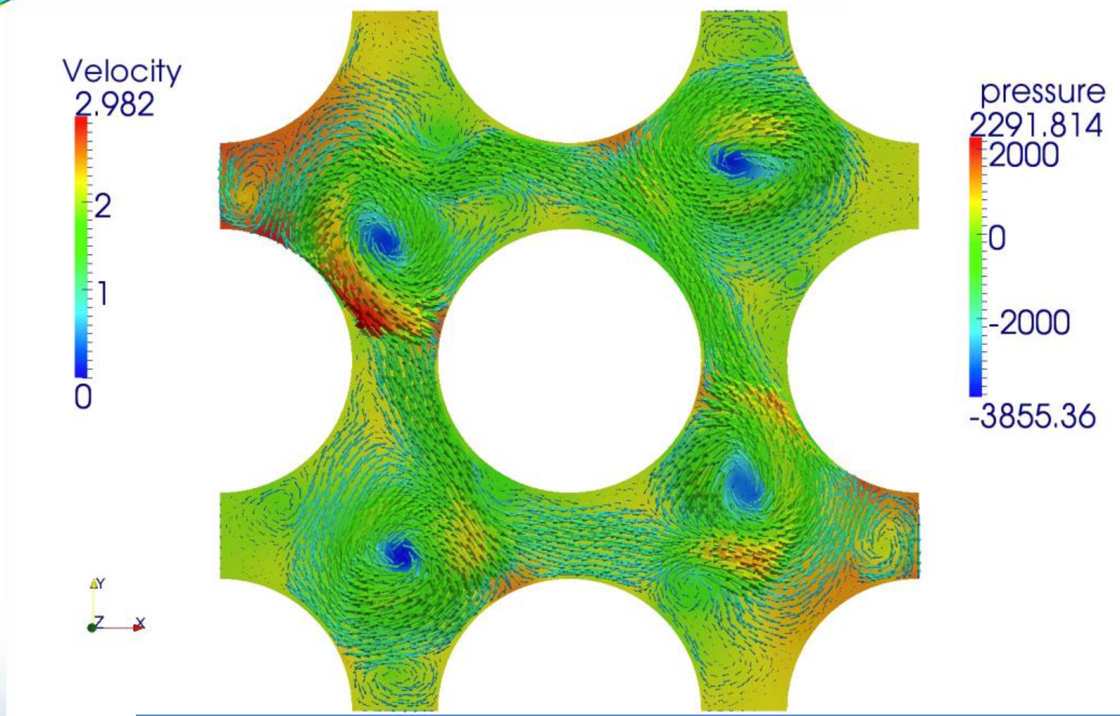
Advanced computational fluid dynamics

Fuel grid-to-rod-fretting analysis with CASL's HYDRA-TH capability





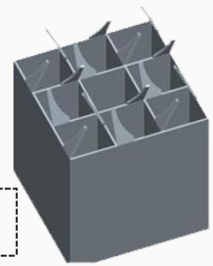


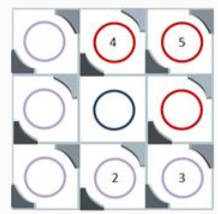
Providing forces for structural analysis

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

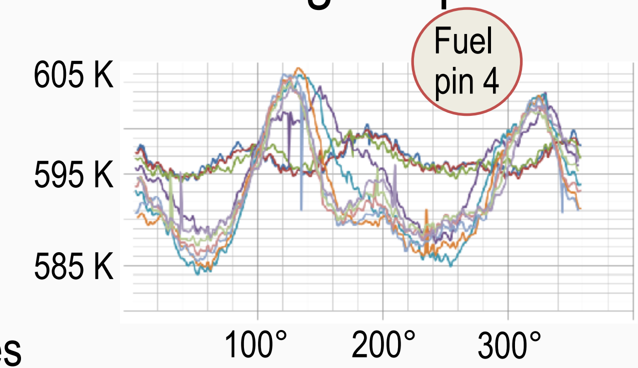
Fuel rod (80 cm section)

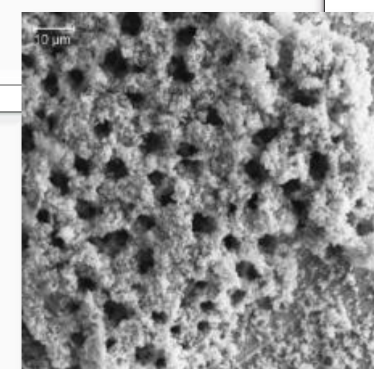




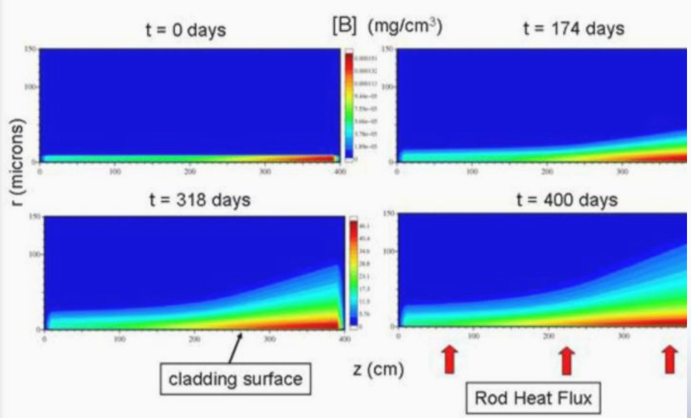
Spacer with mixing vanes

Large azimuthal variation in fluid/cladding temperature

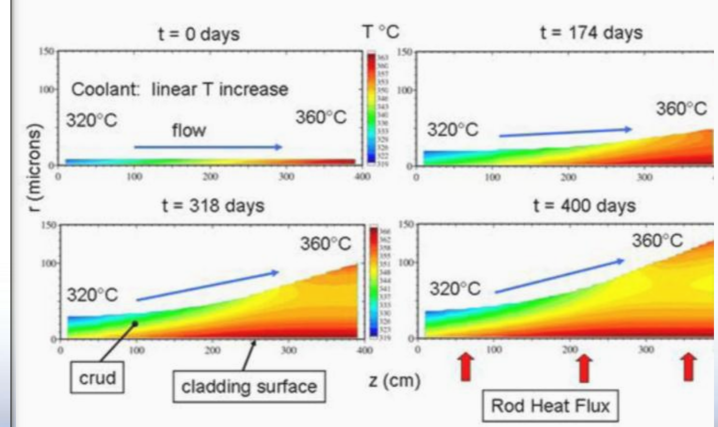




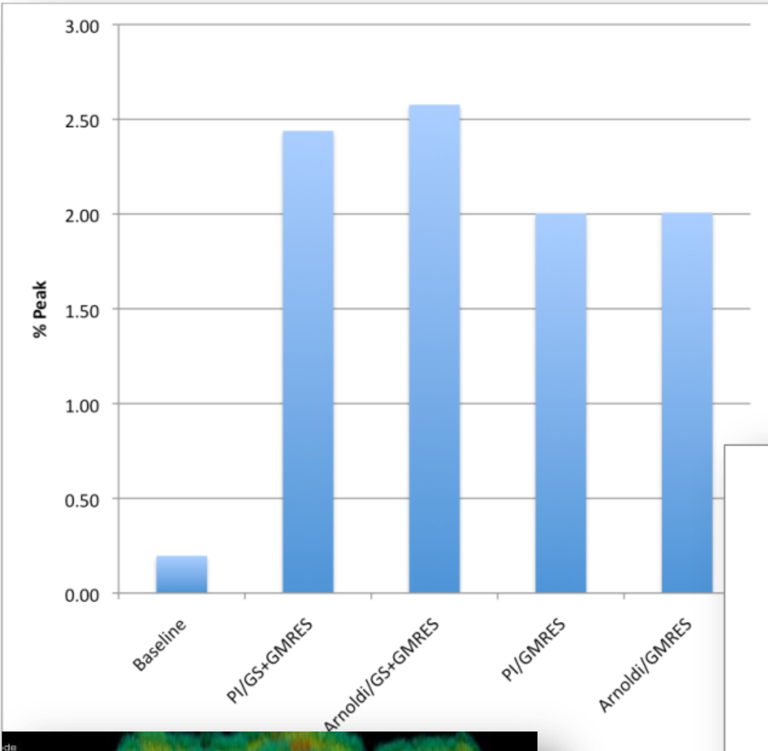
Boron concentration



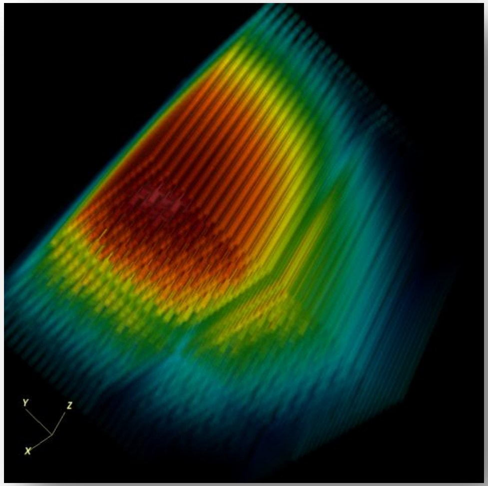
Crud deposition

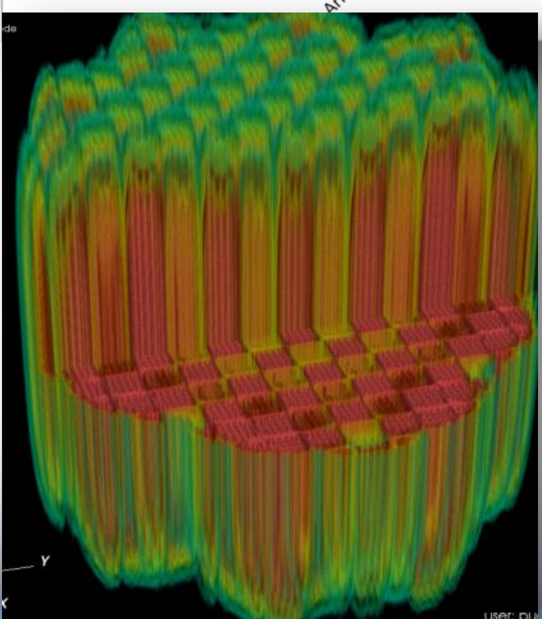


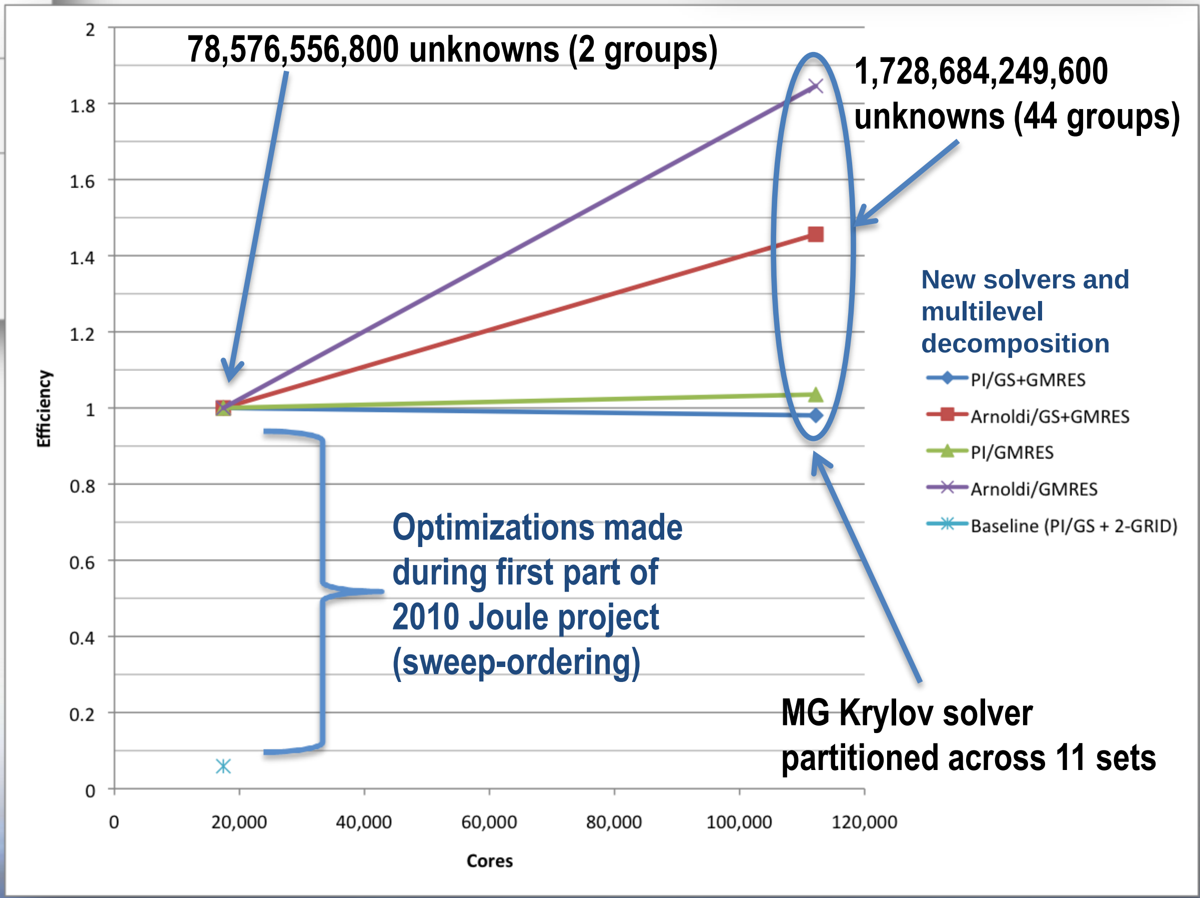
Denovo Parallel Performance



Factor of 10x increase in peak efficiency gained through Joule project + ASCR OLCF-3 project work



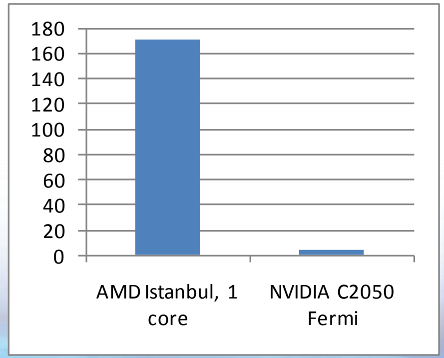




Denovo Transport Sweep GPU performance

- compare performance of sweep on Jaguar Cray XT and on Yona GPU cluster
- single core / single GPU comparison
- test problem: same per-node problem as targeted problem, reduced by half to fit into 3GB C2050 memory

	AMD Istanbul 1 core	NVIDIA C2050 Fermi	Ratio
Kernel compute time	171 sec	3.2 sec	**54X**
PCIe-2 time (faces)	--	1.1 sec	
TOTAL	**171 sec**	**4.2 sec**	**40X**



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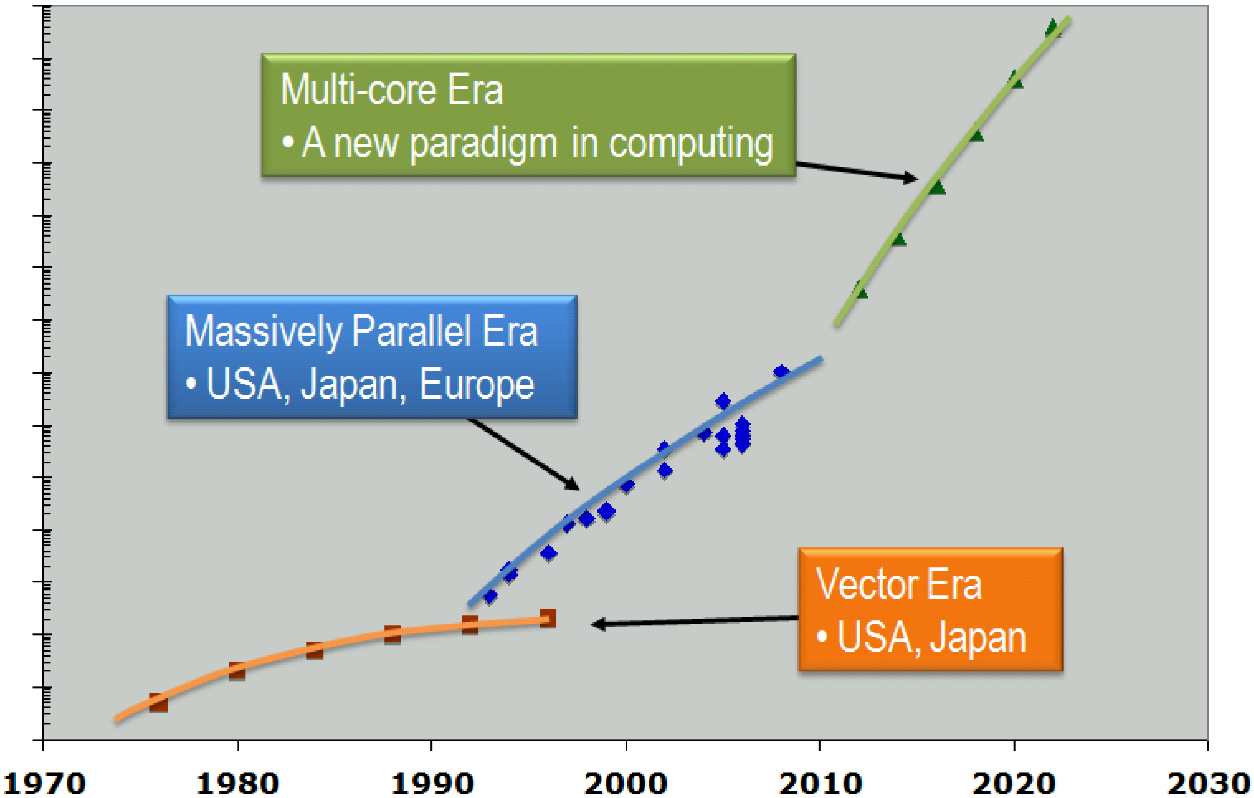
Future large-scale systems present challenges for applications

- 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



Exascale Initiative Steering Committee

Future ~~large-scale~~ desktop systems present challenges for applications

- Dramatic increase in node parallelism increases
  - 10 to 100× by 2015
  - 100 to 1000× by 2018

to

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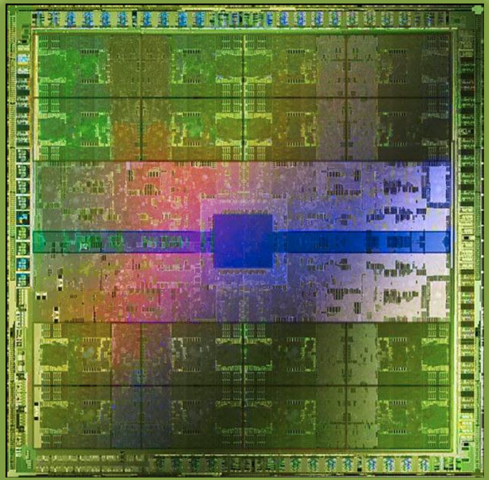
ver

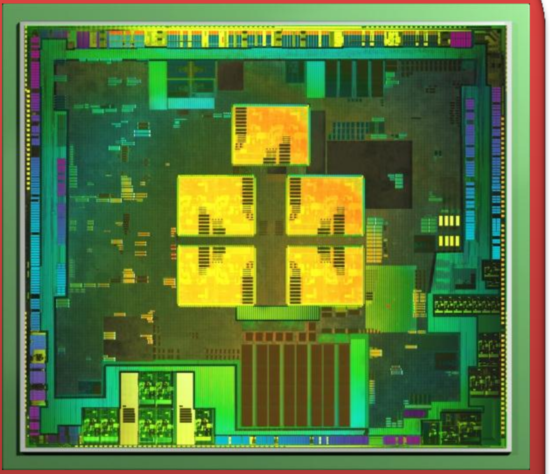
s are

currently immature and in a state of flux

Intel 48-core experimental chip shipped in 2010



NVIDIA 512-"core" Fermi GPU



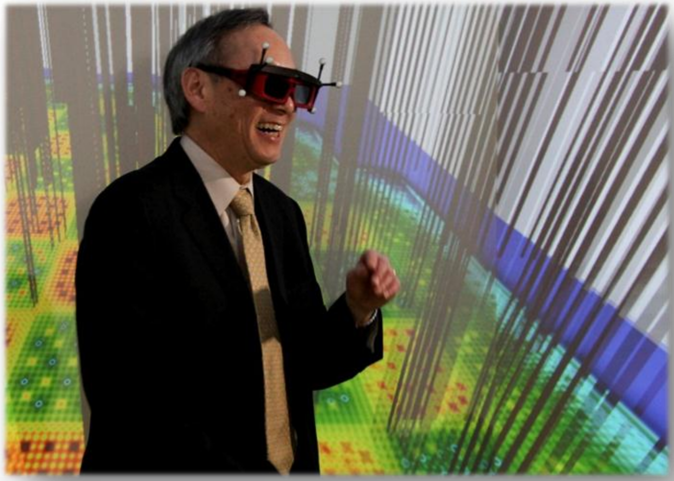
NVIDIA Tegra 3

designed for mobile devices, but will be used in next HPC system at Barcelona Supercomputing Center

Over the life of CASL, these challenges will become increasingly significant at the desktop level

CASL Status

- rapid startup, anchor facility at ORNL
- progression of snapshots of VERA provided to internal customers
  - formal release of infrastructure this summer
  - more formal limited beta release of VERA this fall
- established baseline industry and advanced R&D capability in VERA for neutronics, thermal hydraulics, and corrosion chemistry



- applied selected aspects of VERA to operational PWR core scenarios with conditions relevant to challenge problems
  - corrosion buildup ("CRUD"), pellet-clad interaction (PCI), grid-to-rod-fretting (GTRF)
- integrated within VERA sensitivity and optimization capability to support uncertainty analysis of reactor operational and safety scenarios
- demonstrated that newly established multi-dimensional simulation capabilities exceed industry capabilities

Questions?

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