NEUP Nuclear Energy University Programs
U.S. Department of Energy

July 27-28, 2010

FY2011 NEUP Workshop Modeling and Simulation Breakout Session

Rockville, Maryland

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Nuclear Energy Advanced Modeling and Simulation (NEAMS) Reactor IPSC

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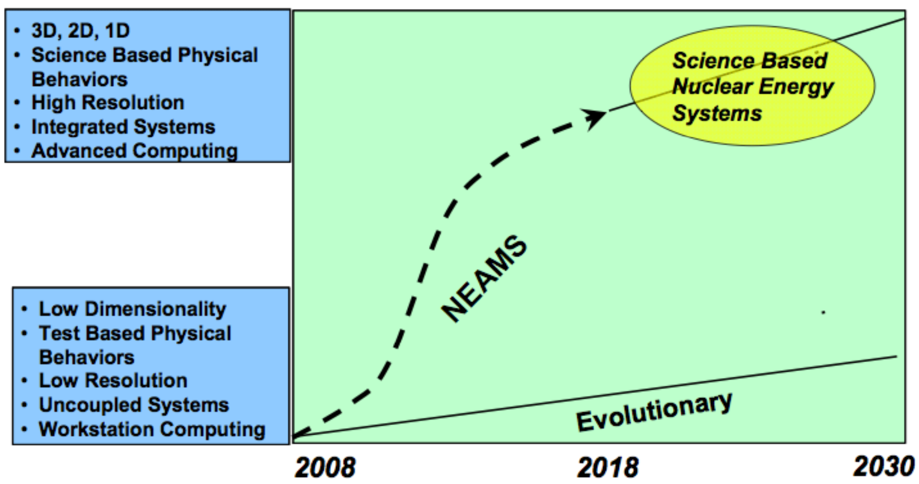
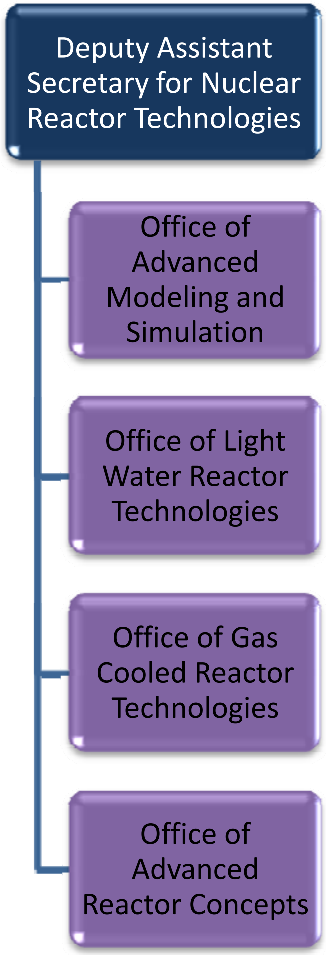
NEAMS

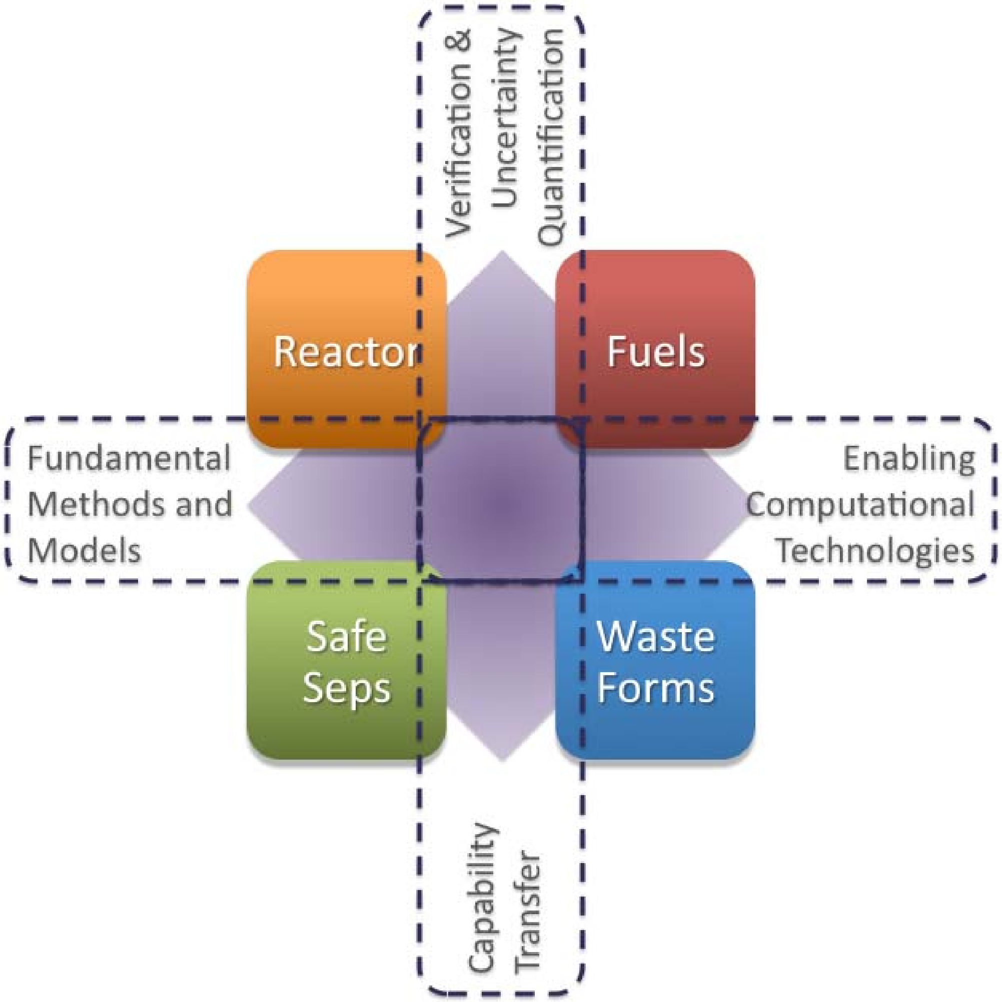
- Vision
  - To rapidly create and deploy "science-based" verified and validated modeling and simulation capabilities essential for the design, implementation, and operation of future nuclear energy systems with the goal of improving U.S. energy security





NEAMS Organization

- Integrated Safety and Performance Code (IPSC) Development Teams
  - Reactors
  - Fuels
  - Waste Forms
  - Safeguards and Separations
- Supporting Cross-cut Elements
  - Fundamental Methods and Models
  - Enabling Computational Technologies
  - Verification and Uncertainty Quantification
  - Capability Transfer



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  - **Reactors**
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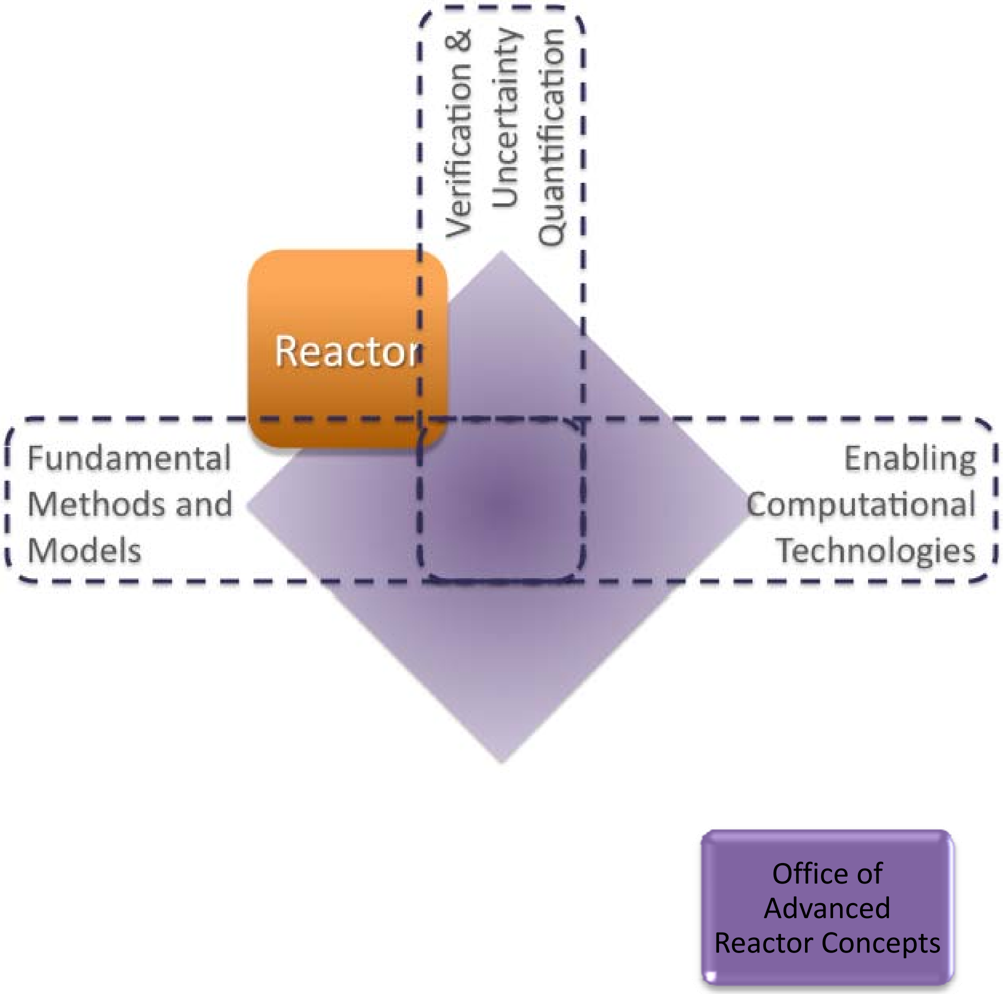
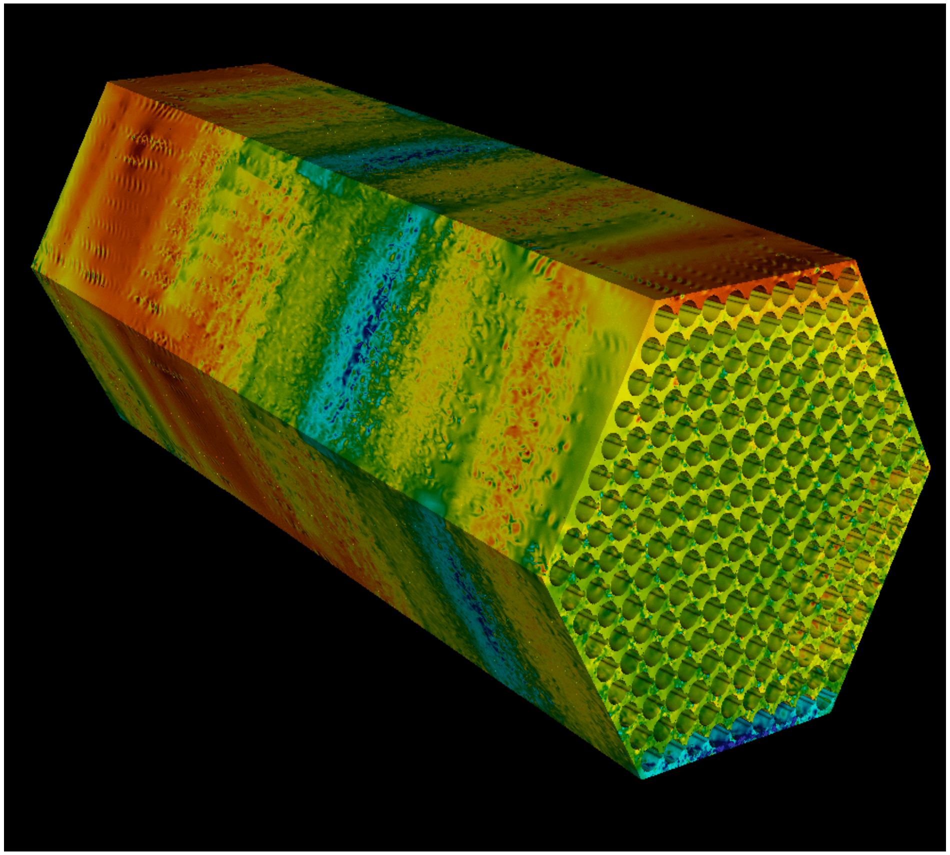


Motivation and Objective

- Apply modern, high-performance techniques to nuclear reactor modeling
  - Improve turn-around time for reactor design iterations
  - Understand and reduce uncertainty of computational models
  - Use advanced simulation tools to improve safety, reduce cost, explore advanced designs
- Maintain a balanced approach
  - Allow for both rapid-turnaround reactor-scale calculations (desktop) and detailed, high-fidelity simulations to augment experiments (petascale)
  - Deliver near-term capability and insight while also developing next-generation tools and integrated capabilities
- Extensive leveraging with other DOE projects
  - INCITE, SciDAC, ASC

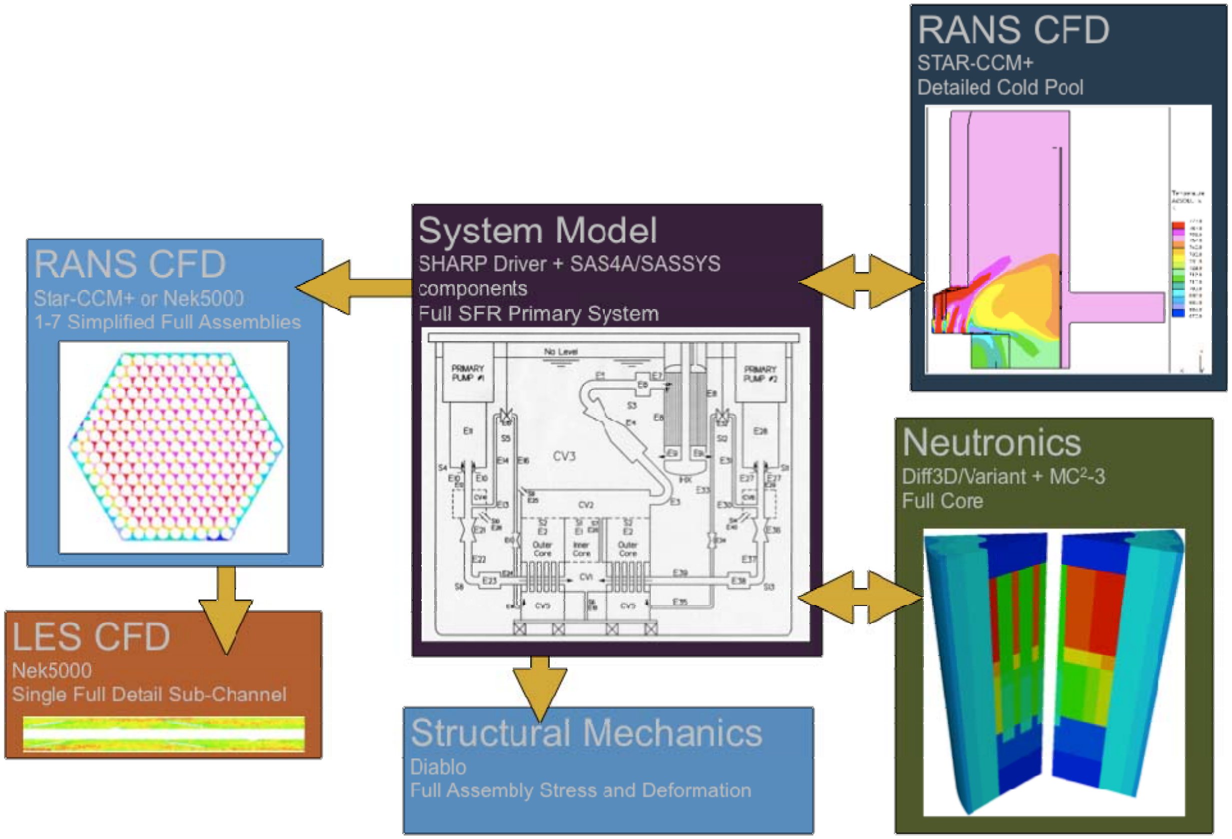
REACTOR IPSC

- Scope
  - Predict performance and safety of reactor over 40-60 year lifetime
  - Initial focus on Sodium-Cooled Fast Reactors (SFR)
  - Primary development efforts in core modeling, extending to full system
  - Many underlying physical processes (e.g. thermodynamics, neutronics) extensible to other reactor types (gas-cooled, light water)



Reactor IPSC

- Develop integrated high fidelity multi-physics simulation capabilities
- Verification, validation and benchmarking of developed tools
- Integrated reactor primary system simulations



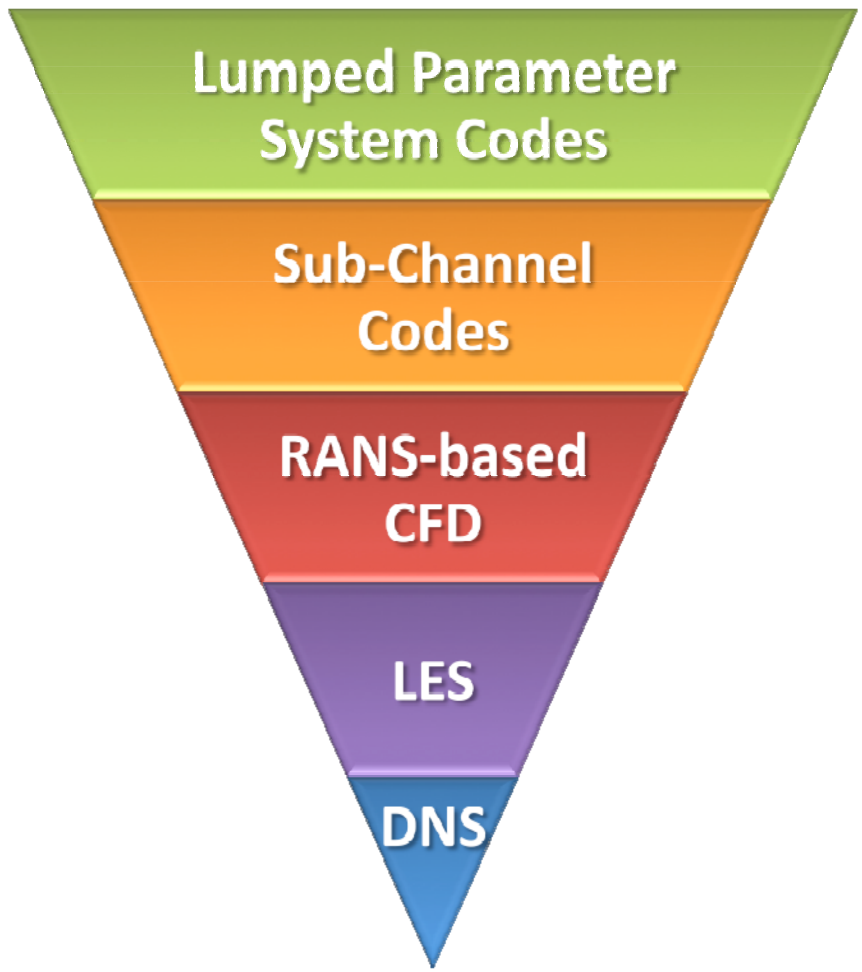
Reactor IPSC Challenge Problems

- Challenge Problem #1: Core Radial Expansion
  - Important for operational, design-basis, and beyond design-basis transients.
  - Critical component of passive safety story. Difficult/impossible to measure.
  - Suspected of playing a role in unexplained PHENIX reactivity transients.
  - Requires coupled neutronics, thermal hydraulics, and structural mechanics.

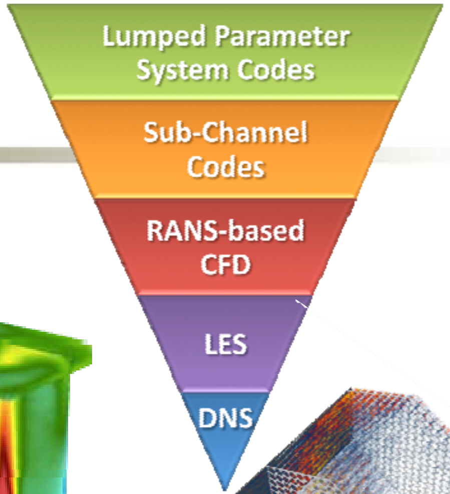
- Challenge Problem #2: Outlet Plenum Mixing
  - Critical to normal operations: thermal striping and fatigue, upper internal structure performance, reactor vessel/head performance, instrumentation and control optimization
  - Critical to transients: thermal (SFR/LFR) or density (VHTR) stratification, natural convection cooling, decay heat removal, control-rod driveline expansion, core restraint system performance
  - Outlet plenum design may either aid or hinder passive safety performance.
  - Requires coupled thermal hydraulics and structural mechanics (with impacts on neutronics)

Hierarchal Thermal Fluid Simulation System

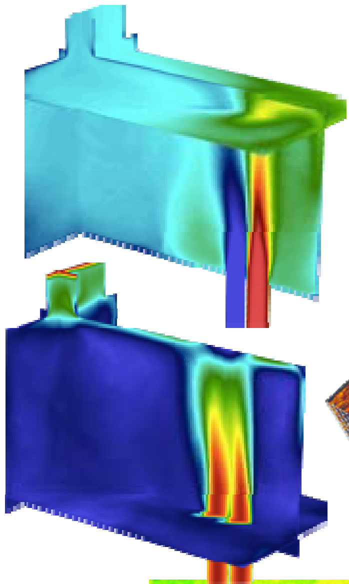
- Apply appropriate scale of resolution to capture relevant local physics and/or fit within available computational capacity.
- Couple through boundary conditions and integral engineering model coefficients
- Codes available to the SHARP virtual reactor
  - SHARP Driver
    - SAS4A Libraries
  - SASSYS1 Subchannel Solver
  - STAR-CD/STAR-CCM+/OpenFOAM RANS
  - Nek5000/STAR-CCM+/OpenFOAM LES
  - Nek5000/OpenFOAM DES

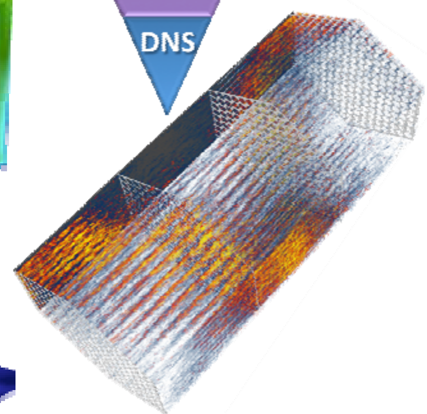


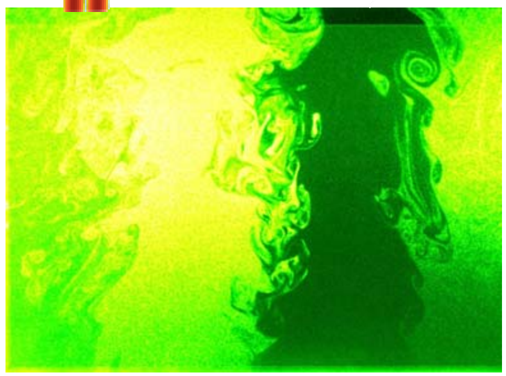
Thermal Hydraulics



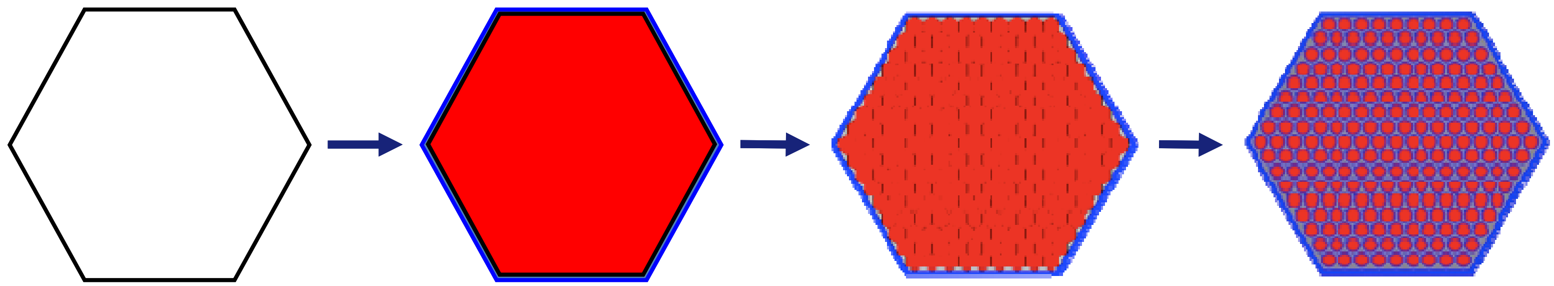
- FY11 Activities
  - Develop multi-resolution simulation hierarchy components
  - Verification, validation and benchmarking
  - Core and system component simulations
- Needs
  - Methods to enable extension to other reactor types
    - High fidelity multi-phase simulation
  - Reduced order modeling methods for acceleration of high-fidelity simulations
    - Modal Analysis Using Proper Orthogonal Decomposition
  - Subgrid models for rod bundle turbulence
  - High spatial and time resolution validation data
  - Thermophysical and thermomechanical property libraries



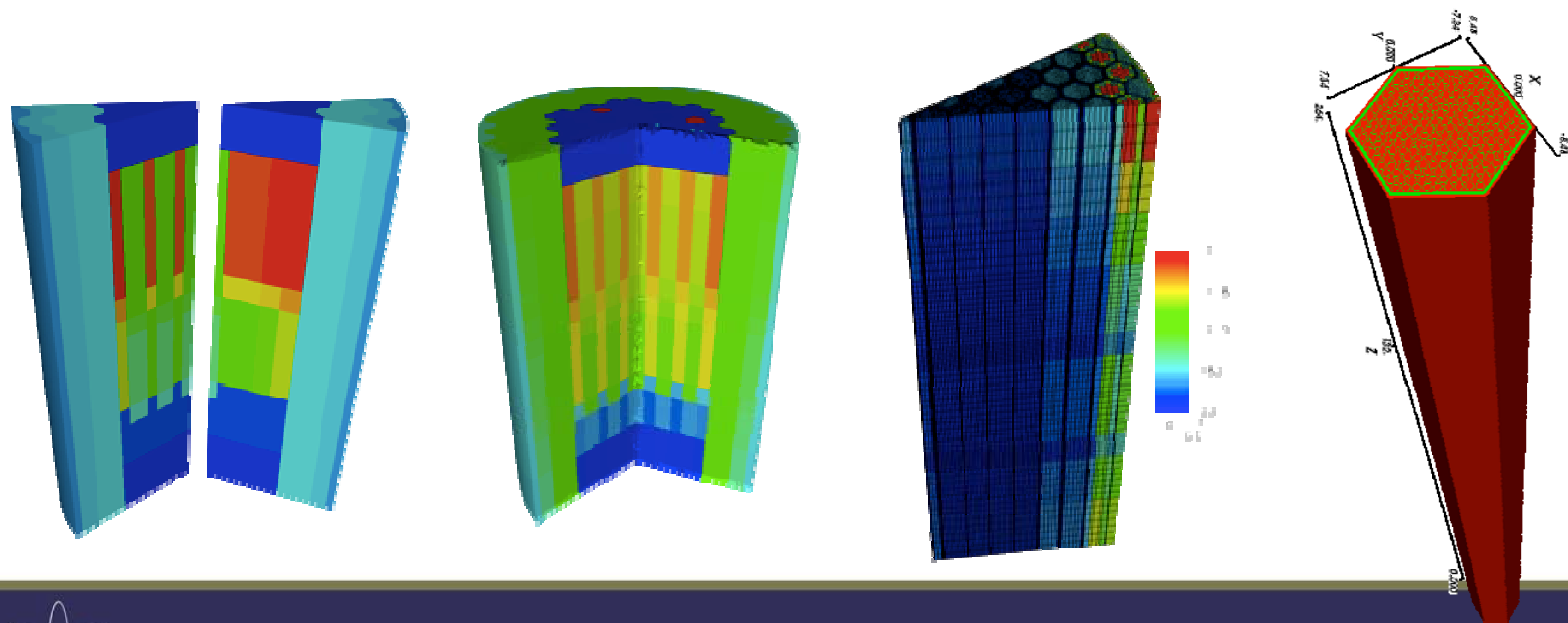




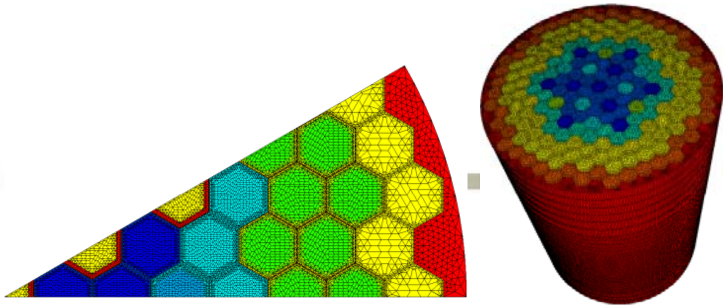
Hierarchal Neutronics Approach



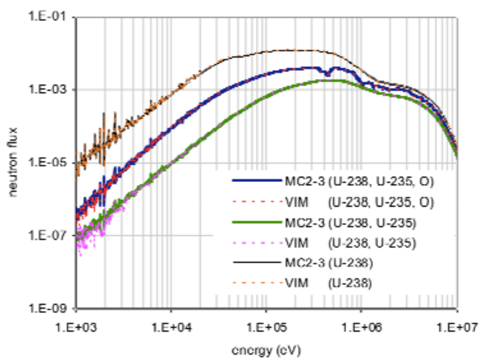
Homogenized assembly | Homogenized assembly internals | Homogenized pin cells | Fully explicit assembly



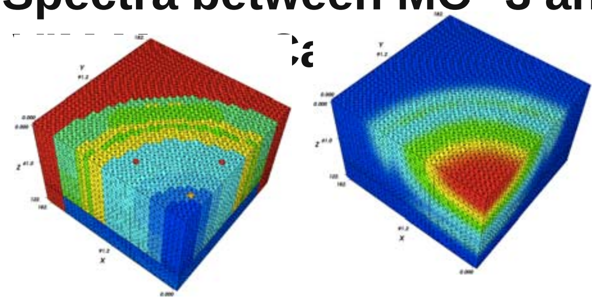
Neutronics



Whole-core



Comparison of Neutron Spectra between MC^2-3 and

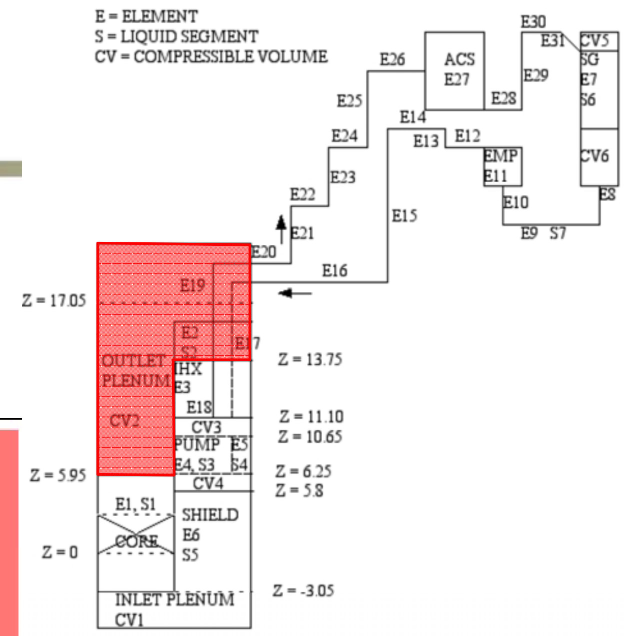


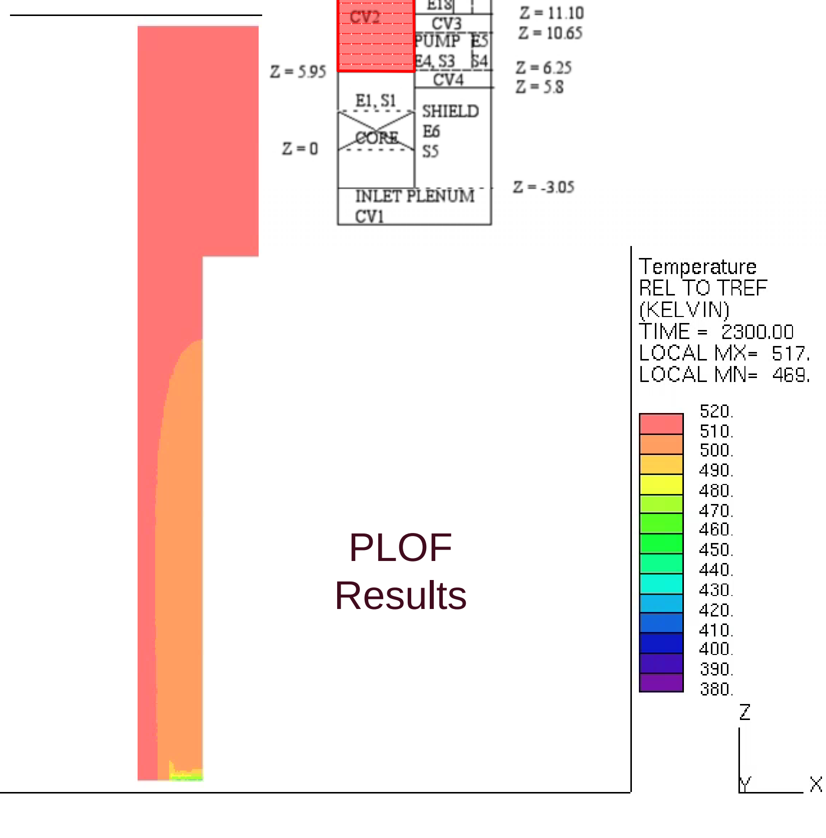
ZPPR-15 Critical Experiment

- FY11 Activities
  - Deliver a production version of the multi-group cross section generation code MC^2-3 by combining the advanced ultrafine group spectrum solver and the 2D method of characteristics (MOC) solver of UNIC
  - Develop an intermediate fidelity flux solver for VHTR analysis which is based on hexagonal pin-cell geometry with structured mesh.
  - Continue to improve the performances of the high-fidelity Sn, Pn and MOC solvers of UNIC on high performance computers
  - Needs
    - Improved x-section data based on nuclear modeling
    - nucleonic structure calculations to complement experimental measurements
      - Minor actinides
      - Fission fragments for high burnup
      - High-fidelity co-variance data for use in transport calculations
      - Fission x-sections

System Simulations

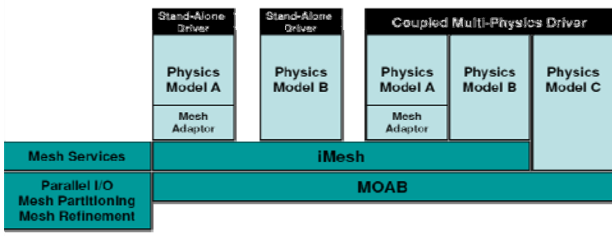
- FY11 Activities
- Develop and demonstrate an initial implementation of the SHARP driver code, providing global system modeling capability and support for a wide range of modeling choices for individual reactor components.
- Develop scalable intermediate fidelity (IF) assembly modeling method to support full-core transient modeling coupled to existing and emerging fuel performance models.
  - Enable parametric analyses like those currently done with subchannel codes, but utilize information from high fidelity simulations in place of experimentally derived correlations
- Needs:
  - Time-stepping strategies for coupled multi-scale simulations of transient system response
  - Models and methods to enable application to other reactor types
  - Multi-scale validation data with adequate resolution to evaluate coupling of high and low resolution methods

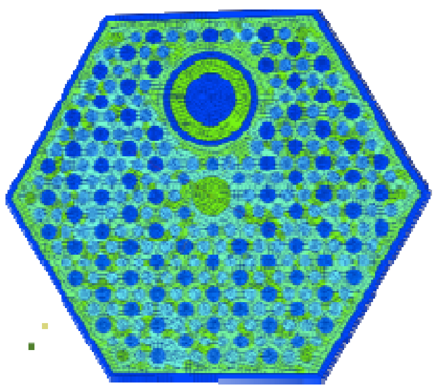


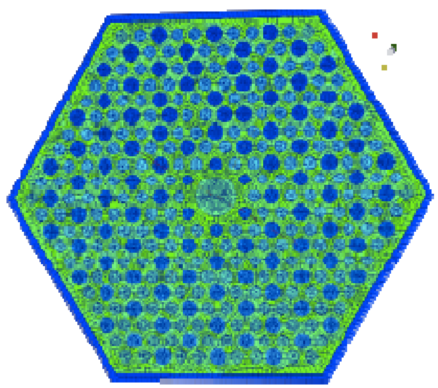


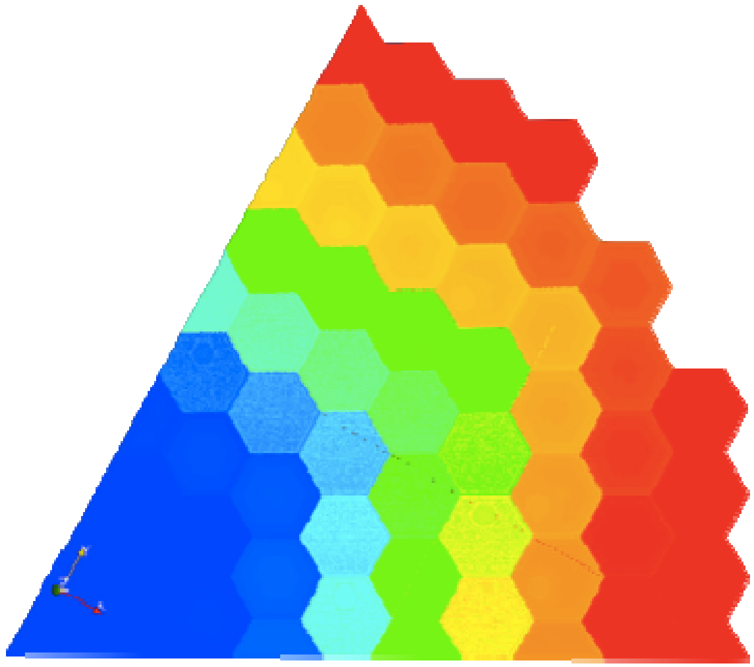
Framework

- FY11 Activities
  - Development of geometry/mesh generation tools built on a foundation including CUBIT, the MeshKit library, and the STAR series of tools.
  - Provide capability for boundary/initial condition coupling from systems models to TH module. Coupling will be performed based on mesh and solution representation in the MOAB mesh library.









The scope for ECT in FY11 spans 4 areas

Software Quality Assurance

- NEAMS SQA Plan
- IPSC risk assessments
- Best practices and tools
- Centralized server of SQA tools and consulting expertise

Cross-cut libraries

- Pre-processing tools such as geometry and meshing
- Post-processing tools such as visualization and data analysis
- Materials interface and library

Common Frameworks

- Assess need for commonality across IPSC teams
  - Release/Distribution
  - Configure/build
  - Workflow and execution
  - Data and information
  - Code coupling
- Propose and develop solutions

Compute Cycles

- Evaluate INL/ORNL capacity computing resources
- Improve accessibility and usability
- Provide guidance on additional options (e.g. INCITE)

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