Where in NE are programs for developing and deploying advanced modeling and simulation tools managed? Who manages them?

NE Federal Manager for Advanced M&S
Dan Funk, dan.funk@hq.doe.gov (until August 31)
Dave Henderson, david.henderson@hq.doe.gov (after August 31)
NE currently executes two complementary advanced M&S programs, each tailored to focus on a particular reactor technology area using computational tools uniquely suited to the particular reactor moderator(s) and fuel(s).

**Energy Innovation Hub for Modeling and Simulation (Hub)**

**Objective:** Develop and apply M&S tools focused on LWR technologies for an improved understanding of important operational and safety issues in existing reactors.

**Nuclear Energy Advanced Modeling & Simulation (NEAMS)**

**Objective:** Develop and deploy predictive analytic computer methods for the analysis and design of advanced reactor and fuel cycle systems focused on non-LWR technologies.
Advanced Modeling & Simulation

ADVANCED M&S CAPABILITY DEVELOPMENT
(Develop and distribute leading-edge, predictive modeling and simulation tools for use by industry, labs, and universities)

INDUSTRY EARLY-STAGE DEVELOPMENT

ACCELERATING ADVANCED REACTOR CONCEPTS

SOLVING HIGH-ImpACT PROBLEMS

LEADING-EDGE RESEARCH

NE ADVANCED REACTOR & FUEL RESEARCH

NRC RESEARCH & ANALYSIS

University Research
Advanced Modeling & Simulation
Underpins NE’s Mission Focus Areas

- Address core performance issues that increase operational costs
- Assure the long-term availability and market competitiveness of nuclear energy

- Accelerate concept development and commercialization
- Meet otherwise cost-prohibitive data needs
- Support NRC confirmatory analyses

- Confirm higher burn-up fuel strategies to slow production of used nuclear fuel (UNF) – VERA
- Support UNF R&D with high-fidelity analysis and prediction of fuel and cladding performance - NEAMS
Advanced Modeling & Simulation
Supporting NE’s Mission Focus Areas

- Critical role in accelerating design and deployment of advanced reactors
  - Design optimization is required to fully realize the economic and technological advantages of advanced concepts
  - Advanced M&S tools will help the NRC expand capabilities as needed to perform confirmatory analysis on advanced reactor concepts

- Only way for vendors to economically address data needs, which otherwise could require cost-prohibitive experimentation
  - Reduce the amount of experimental testing needed
  - Identify, design, execute, and analyze more effective high-value experiments

- The advanced reactor industry is already using our Advanced M&S tools to:
  - Reduce cost and time for license applications to the NRC
  - Enhance potential for successful commercialization - accelerated development crucial to economic viability
Accelerating concept development for timely commercialization is absolutely critical to the future success of advanced reactors

- Without acceleration enabled by Advanced M&S, commercialization of promising advanced reactor concepts may not be possible, which could have a long-range adverse impact on the energy sector; certainly a major opportunity lost

Similarly, application of Advanced M&S tools is critical to the optimized use of advanced test reactors that support advanced reactor and fuels development

- Establishing and executing a modern strategy to simulate experiments and analyze measurement data is central to maximizing the impact of any advanced test reactor experimental program
- Deploying Advanced M&S tools as a tightly coupled research platform enables comprehensive understanding of the multi-scale and multi-physics performance of the advanced reactor experimental capabilities through intelligent feedback between simulations and experiments
## Advanced Modeling & Simulation: Tools to Solve Industry’s Priority Problems

<table>
<thead>
<tr>
<th></th>
<th>LWRs (and water based SMRs)</th>
<th>Advanced Reactors</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Integration</strong></td>
<td>VERA</td>
<td>Workbench</td>
</tr>
<tr>
<td><strong>System Analysis</strong></td>
<td>Plant</td>
<td>RELAP-7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>SAM</td>
</tr>
<tr>
<td><strong>Core Analysis</strong></td>
<td>Neutronics-Pin Resolved</td>
<td>MPACT</td>
</tr>
<tr>
<td></td>
<td>Neutronics-Monte Carlo</td>
<td>Shift/External Codes</td>
</tr>
<tr>
<td></td>
<td>Neutronics-Kinetics/Depletion</td>
<td>MPACT</td>
</tr>
<tr>
<td></td>
<td>Neutronics-Cross Sections</td>
<td>AMPX/SCALE - MC2-3</td>
</tr>
<tr>
<td></td>
<td>T-H Low Res</td>
<td>Cobra-TF (CTF)</td>
</tr>
<tr>
<td></td>
<td>T-H Hi Res (CFD)</td>
<td>External codes/Nek5000</td>
</tr>
<tr>
<td></td>
<td>Structural Mechanics</td>
<td>External codes</td>
</tr>
<tr>
<td><strong>Fuel Analysis</strong></td>
<td>Continuum</td>
<td>BISON</td>
</tr>
<tr>
<td></td>
<td>Microstructure</td>
<td>Marmot</td>
</tr>
<tr>
<td></td>
<td>Component Aging</td>
<td>Grizzly</td>
</tr>
<tr>
<td></td>
<td>Chemistry</td>
<td>MAMBA</td>
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</tbody>
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PROTEUS/MC²-3
Pin Resolved Neutronics

- High-fidelity FEM neutron transport module and matching cross-section generation capabilities
- Unstructured grid for complex geometries
- On-line cross section generation
- Excellent scalability for parallel computing
<table>
<thead>
<tr>
<th>PROTEUS/MC²-3 Papers</th>
</tr>
</thead>
</table>

**MC²-3: Multigroup Cross Section Generation Code for Fast Reactor Analysis (Nuclear Science & Engineering)**

- Improved methods and performance of the MC2-3 code, which is a multigroup cross-section generation code for fast reactor analysis

**NEAMS Neutronics: Development and Validation Status (ICAPP)**

- Status of advanced neutronics capabilities at Argonne National Laboratory (high-fidelity neutron transport code PROTEUS, and advanced multigroup cross section generation code MC²-3); includes validation results and discussion

**High Fidelity Multiphysics Calculations Of Hot Channel Factors For Sodium-Cooled Fast Reactors**

- Reduction or elimination of modeling uncertainties in the calculation of HCFs using high fidelity advanced modeling and simulation tools; high fidelity HCFs calculated with PROTEUS-MOCEX and Nek5000 are compared to legacy HCFs for similar reactor types (SFRs)

**POC – Tanju Sofu (tsofu@anl.gov)**
Nek5000
CFD/Thermal-Hydraulics

- CFD with high-order spectral elements on an unstructured (but conformal) hexahedral grid
- Incompressible and weakly-compressible flow
- DNS, LES, and RANS formulations for turbulence
- Excellent parallel scaling (1M+ ranks)
Comparison Of Experimental and Simulation Results On Interior Subchannel Of A 61-Pin Wire-Wrapped Hexagonal Fuel Bundle

Joint project with AREVA, ANL, TAMU, and Terrapower. Comparisons are made between particle image velocimetry velocity field measurements to ANL’s large-eddy simulation results at an interior subchannel for a Reynolds number of 19,000

POC – Elia Merzari (emerzari@anl.gov)
BISON/MARMOT
Multiscale Mechanistic Modeling of Nuclear Fuels

- **Objective**: Use hierarchical, multiscale modeling for improved, mechanistic, and increasingly predictive models of fuel performance
- Mechanistic fuel behavior models: 1) minimize form errors, 2) provide insight where experimental data is sparse, and 3) may require less (or different) experimental data for validation

- Identify important mechanisms
- Determine material parameter values
- Predict microstructure evolution
- Determine effect of evolution on material properties and fuel behaviors
- Predict fuel performance and failure probability
<table>
<thead>
<tr>
<th>Mechanistic materials modeling for nuclear fuel performance</th>
<th>Mechanistic materials modeling approach based on the current state of the evolving microstructure rather than on burn-up, with experimental data used to inform the development of these models.</th>
</tr>
</thead>
<tbody>
<tr>
<td><a href="https://doi.org/10.1016/j.anucene.2017.03.005">https://doi.org/10.1016/j.anucene.2017.03.005</a></td>
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<tr>
<td><strong>BISON Theory Manual: The Equations Behind Nuclear Fuel Analysis</strong></td>
<td>Theoretical and numerical foundations of BISON for a range of fuel types and physical properties and behavior, with discussion of resulting models</td>
</tr>
<tr>
<td><strong>Assessment of BISON – A Nuclear Fuel Performance Analysis Code (Release 1.4)</strong></td>
<td>Perhaps the most important comprehensive report on Bison. Summary of assessments of Bison’s predictive capability. Primary focus on LWR fuel, with secondary focus on TRISO fuel.</td>
</tr>
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POC – Rich Williamson (Richard.williamson@inl.gov)
Focus is extend the applicability and utility of the NEAMS tools to provide support for advanced fast reactors (e.g., micro-reactors) and for experimental use of fast test reactors

- Expected to support the experimental program (experiment design, analyses, et al) for the Variable Test Reactor project
- Collaboration should include NEAMS and VTR project

IRP is comprised of two primary Tasks

- Task 1 - Accelerate extension of NEAMS computational tools to simulation of relevant metallic fuel behavior and performance, including both high-fidelity and fast-running capabilities as needed.
- Task 2 - Accelerate coupled Neutronics and Thermal-Hydraulic Analysis capabilities to support experimental use of test reactors such as the VTR, and support related advanced fast reactor commercialization (e.g., micro-reactors)
Task 1 – Extension of BISON/MARMOT has two focus areas

- Mechanistic model and transient simulation developments that incorporate or enhance capabilities for key phenomena, including
  - Fuel and cladding temperature distribution (as calculated by the NEAMS neutronics and thermal-hydraulics analysis tools),
  - Fuel-to-cladding and cladding-to-coolant heat transfer,
  - Axial burnup distribution in the fuel,
  - Thermal conductivity of the fuel and cladding for fresh and as-irradiated fuel,
  - Thermal expansion of the fuel and cladding,
  - Fission gas production, transport, and release,
  - Production and transport of lanthanide fission products,
  - Solid and gaseous fission product swelling,
  - Fuel constituent redistribution,
  - Cladding strain due to internal fission gas pressure and fuel-cladding mechanical interactions, and
  - Thinning of the cladding due to fuel-cladding chemical interactions

- Validation of new models by leveraging the available EBR-II and FFTF, and transient fuel testing data, to support both the VTR project as well as relevant industry end-users
Task 2 – Extend Coupled Neutronics and Thermal-Hydraulic Analysis Capabilities

- Review of the hot-pin/channel factors developed for the earlier SFRs (EBR-II, CRBR and FFTF)
- Identification of a subset of these factors as potential candidates for reduction or elimination through high-fidelity simulations
- Application of NEAMS multiphysics analysis capabilities to the calculation of hot-pin and hot-channel factors, where the overall mature capability is expected to subsequently support the test reactor experimental efforts and help meet certain advanced reactor concept commercialization needs
Advanced Modeling & Simulation
Integrated Research Project (IRP)Scope

- Program (IRP-NEAMS-1)
- Federal POC
  - Dave Henderson (david.Henderson@hq.doe.gov)
- TECHNICAL POCs
  - Chris Stanek (stanek@lanl.gov)
  - Tony Hill (hilltony@isu.edu)
- Up to 3 Years and $4,000,000
Questions?