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Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program Update

Christopher R. Stanek
NEAMS National Technical Director

June 17, 2016

Nuclear Energy Advisory Committee Meeting
Arlington, VA

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Outline

- **Overview**
  - Updated organizational structure
  - Program elements (Fuels, Reactors and Integration Product Lines)
- **NEAMS Support of TREAT**
- **High Impact Problems**
  - Accident Tolerant Fuel
  - Steam Generator – Flow Induced Vibration
- **GAIN, Validation**
- **Interaction with CASL and NRC**
- **NEUP/SciDAC**
- **Science and International highlights**

Themes:
* Proactive engagement with customers of NEAMS tools (both DOE and industry);
* Relationship with CASL;
* Advanced modeling and simulation: predictive multiscale and multiphysics

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NEAMS Organizational Structure

National Technical Director
Chris Stanek (LANL)

Leadership Council

ATF HIP
Jason Hales (INL)

Fuels Product Line
Steve Hayes (INL)

Integration Product Line
Brad Rearden (ORNL)

Reactors Product Line
Tanju Sofu (ANL)

SGFIV HIP
Elia Merzari (ANL)

Dan Funk
Advanced Modeling & Simulation Office (NE-41)

Shane Johnson
Deputy Assistant Secretary, Office of Science and Technology Innovation (NE-4)

Develop, apply, deploy, and support a predictive modeling and simulation toolkit for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities.

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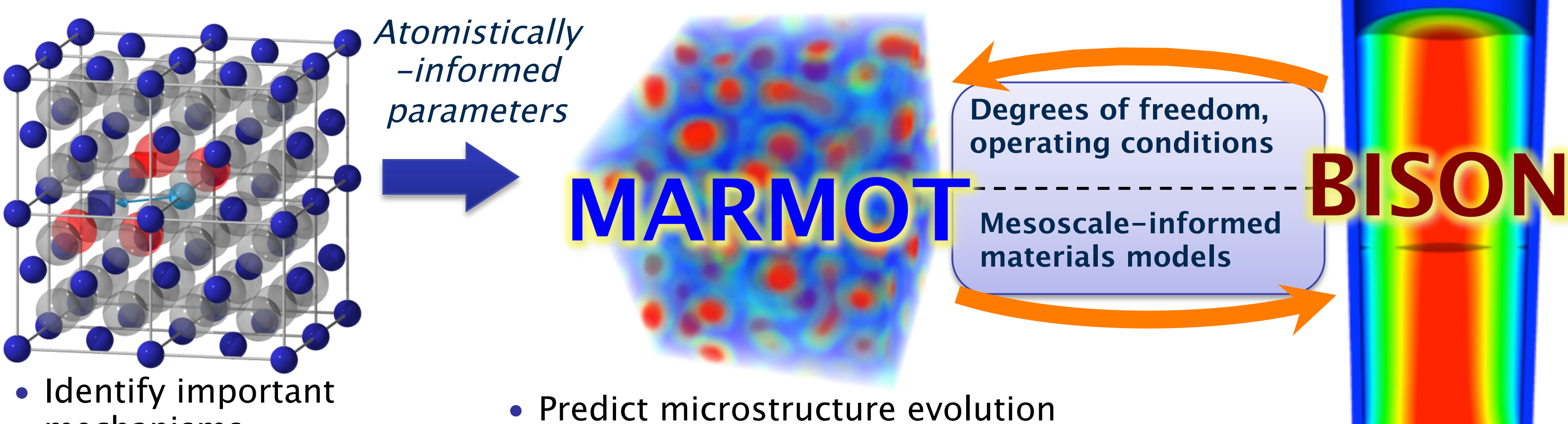
Fuels Product Line (FPL)

- **Empirical models can accurately interpolate between data, but cannot accurately extrapolate outside of test bounds**
- **Goal: Develop improved, mechanistic, and *predictive* models for fuel performance using hierarchical, multiscale modeling – applied to existing, advanced (including accident tolerant) and used fuel.**

Atomistic simulations | **Meso-scale models** | **Engineering scale fuel performance**



- Identify important mechanisms
- Determine material parameter values

- Predict microstructure evolution
- Determine effect of evolution on material properties

- Predict fuel performance and failure probability

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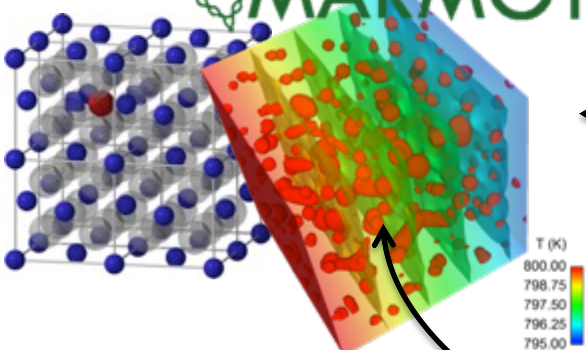
MBM: MOOSE-BISON-MARMOT

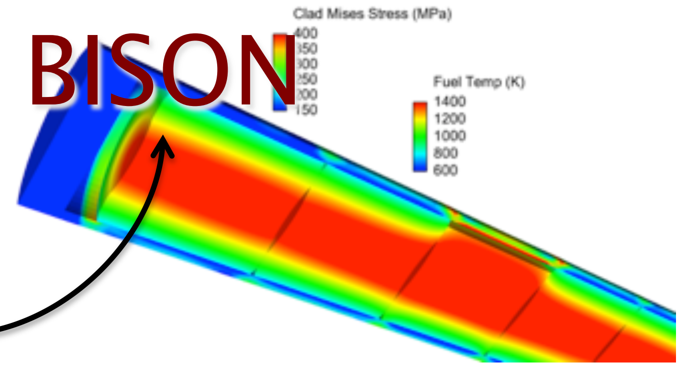
MOOSE-BISON-MARMOT toolset provides an advanced, multiscale fuel performance capability

MARMOT



Mesoscale Material Model Development Tool
- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models

BISON



Engineering-scale Fuel Performance Tool
- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations

MOOSE
Multiphysics Object-Oriented Simulation Environment
- Simulation framework enabling rapid development of FEM-based applications

R&D 100 2014 Winner

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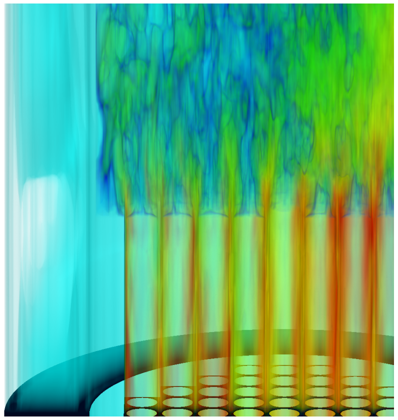
Reactor Product Line: *Sharp*

Develops and deploys high-fidelity, coupled-physics simulation capability for advanced reactors using the *Sharp* code suite, which consists of:

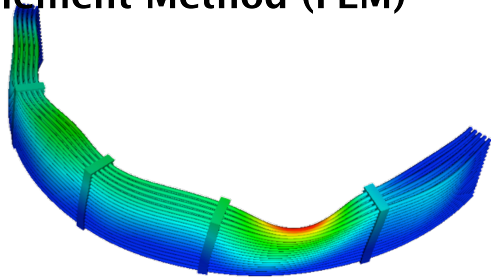
Nek5000 –Thermal-Hydraulics

Highly-scalable solvers for multi-dimensional heat transfer and fluid dynamics



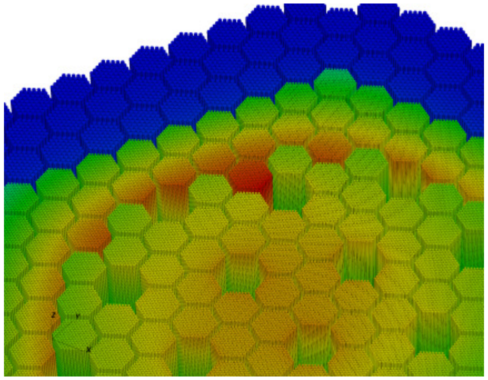
DIABLO – Structural Dynamics

3-D thermal-structural and thermal mechanics analysis using a time implicit Finite Element Method (FEM)



PROTEUS – Neutronics

Can be used to analyze a fast reactor's entire fuel cycle, including cross section generation, radiation transport and fuel cycle modeling



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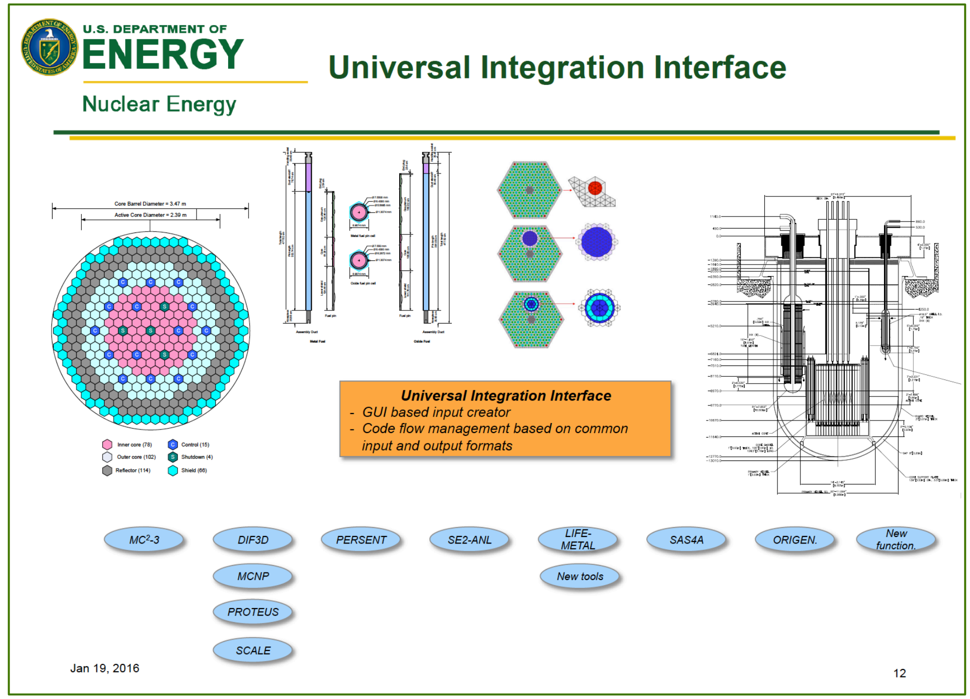
Integration Product Line

NEAMS LC changes (IPL, RPL and NTD) and priority shift have resulted in refactored Integration Product Line.

When defining 5 year goals and path to achieve them, emphasis placed upon: Proactive customer engagement to ensure relevance, *i.e. deployment.*

Specific near-term question:

- *How to provide technology of value to Advanced Reactor Technologies (ART) Program?*



Dialogue with ART = "universal" interface

- Improved use of existing tools
- Gateway to modern tools
- Focus on consistency and ease-of-use

(Slide: T.K. Kim - ANL)

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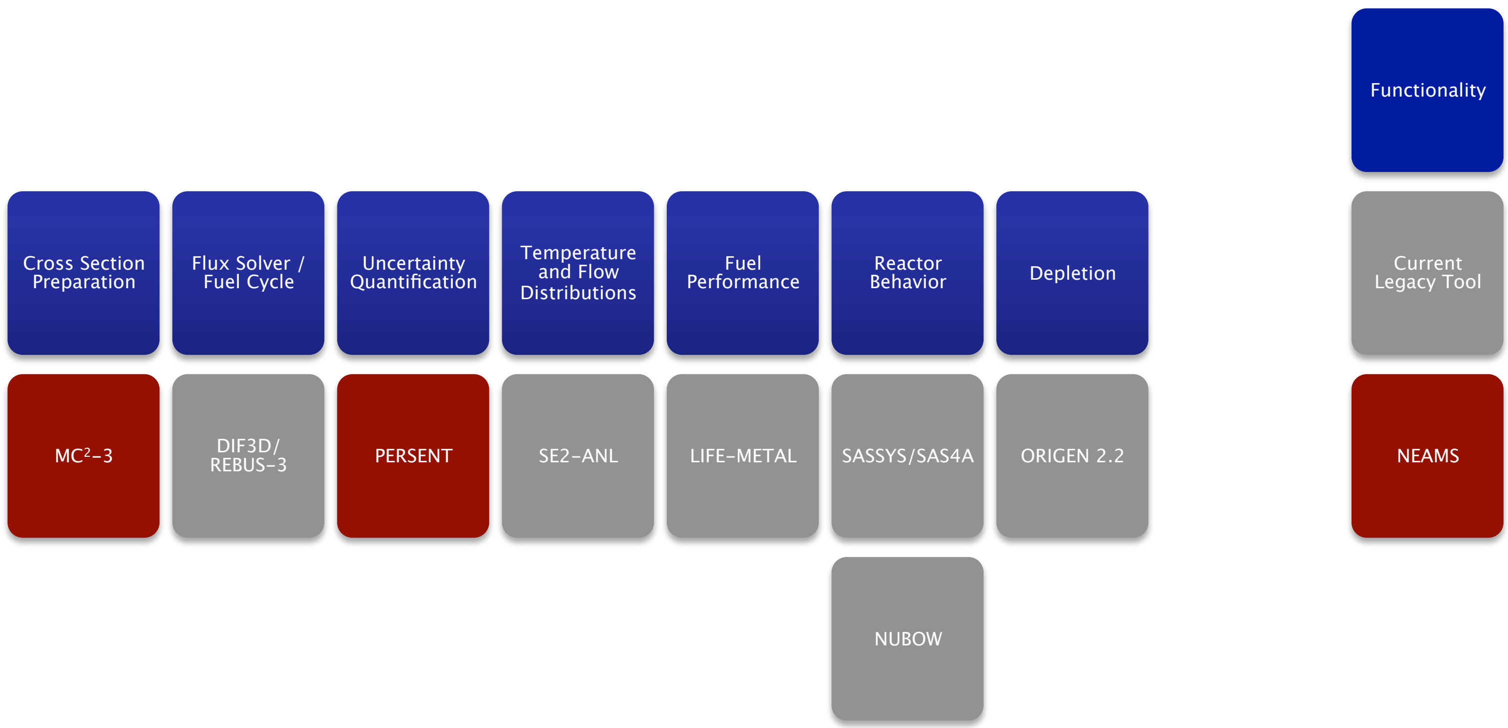
Current ART Code Suite



Limited Choices of Low-Fidelity Physics

Each Code has Unique Input/Output
Data Transfers Require Hand Manipulation with Excel/Python

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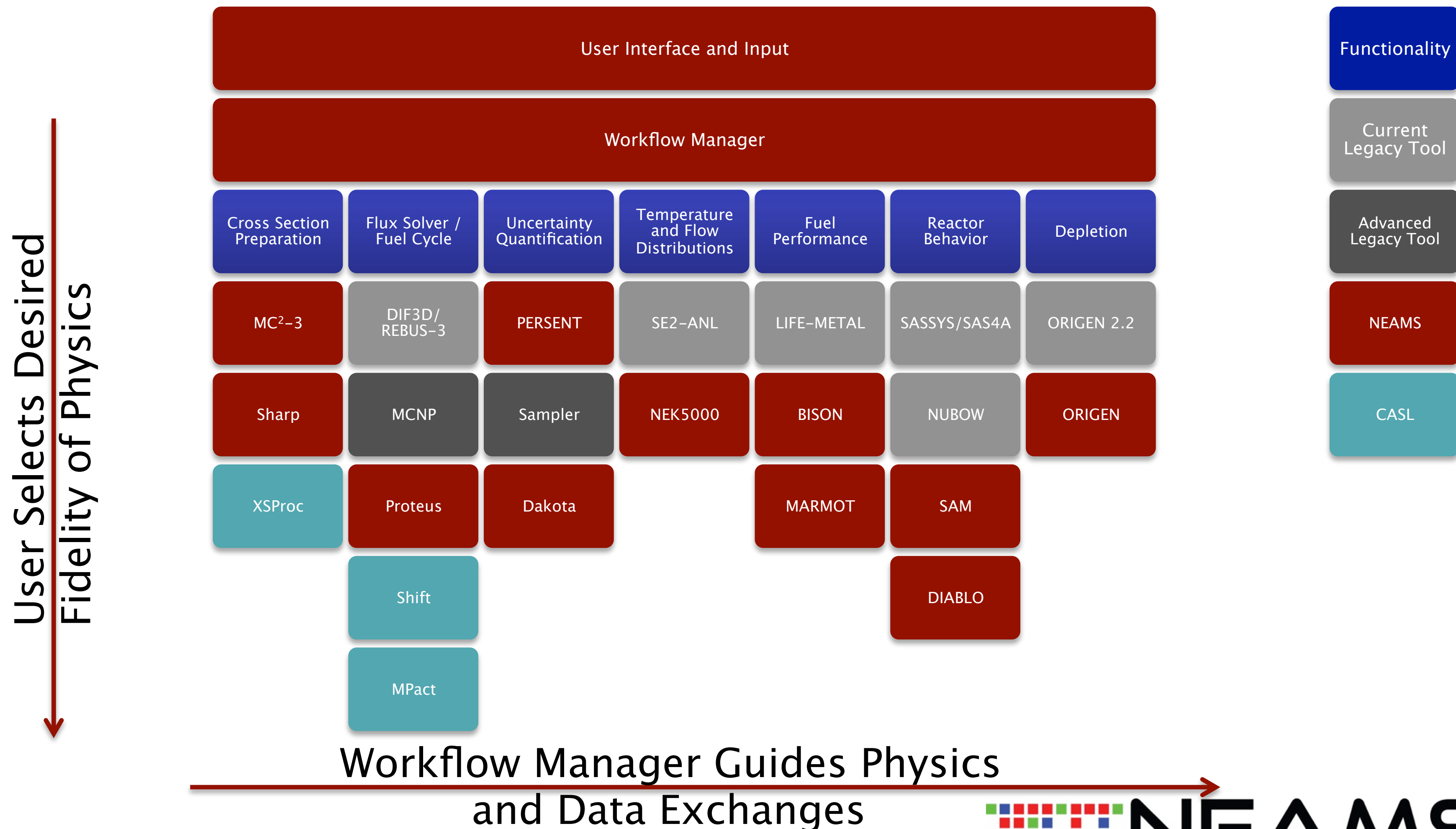
Example NEAMS "Workbench" Implementation for SFR Analysis



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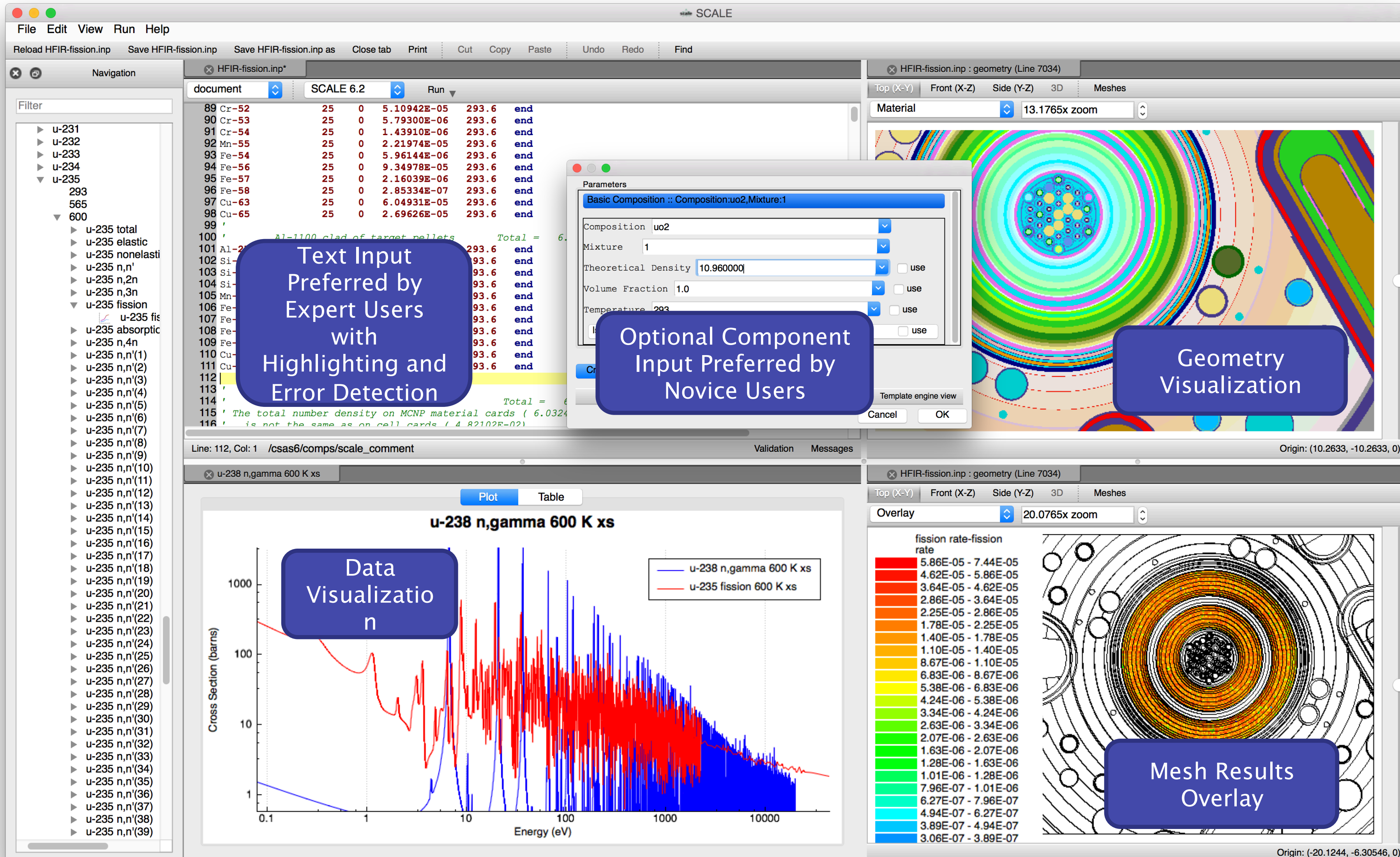
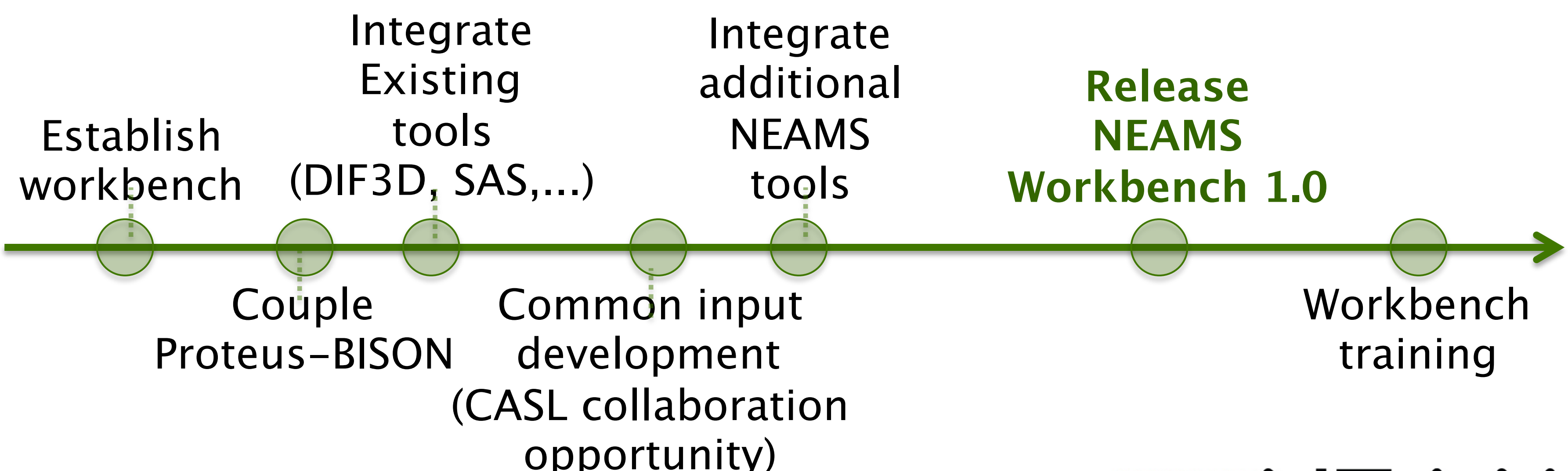
Snapshot of Fulcrum user interface (from SCALE)



NEAMS Workbench

- **Development of a *workbench* has been initiated, which aims to allow users to efficiently manage workflow of existing tools as well as serve as a gateway to advanced *(and integrated)* NEAMS tools.**
- **Initial guidance workbench structure from ART, but intend to leverage modern user interface from SCALE, which is co-sponsored by NRC**
- **Aim is to (1) optimize usage of existing tools, (2) lower barrier to use of advanced NEAMS tools, and (3) seamlessly integrate NEAMS tools.**



NEAMS Support of TREAT

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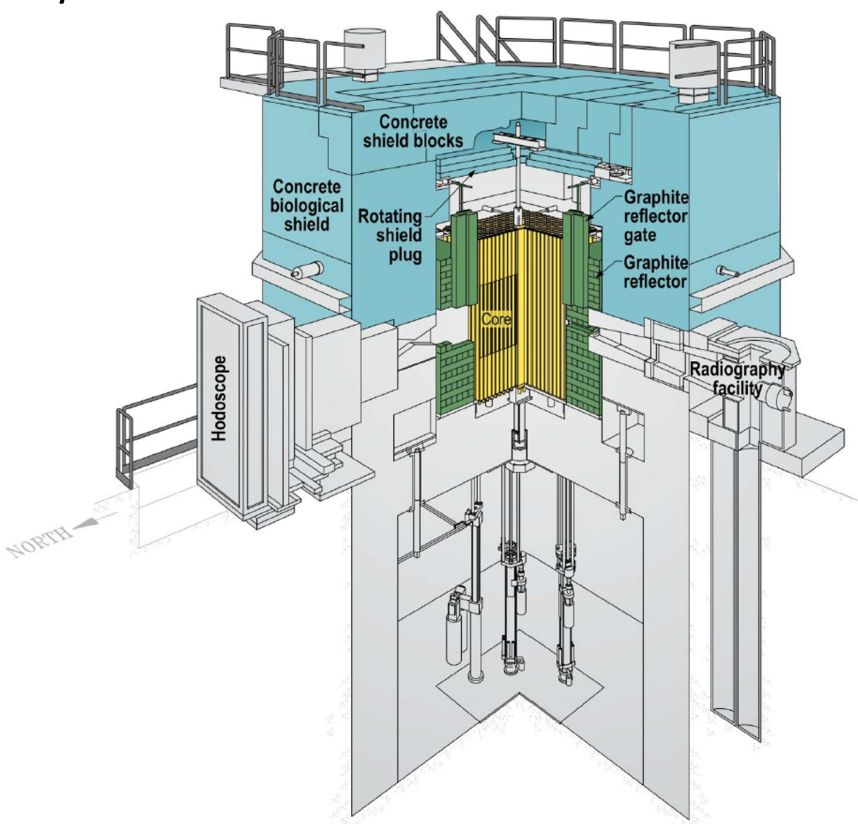
NE Mission Need – *Support resumption of high power/short duration transient testing at the INL TREAT facility with advanced computational tools that will enhance R&D capabilities*



Require high-resolution reactor physics models (eventually coupled to fuel performance for irradiated fuel) to assist operation (e.g. reduce the number of calibration tests) and provide improved predictive capability for analysis of TREAT experiments.

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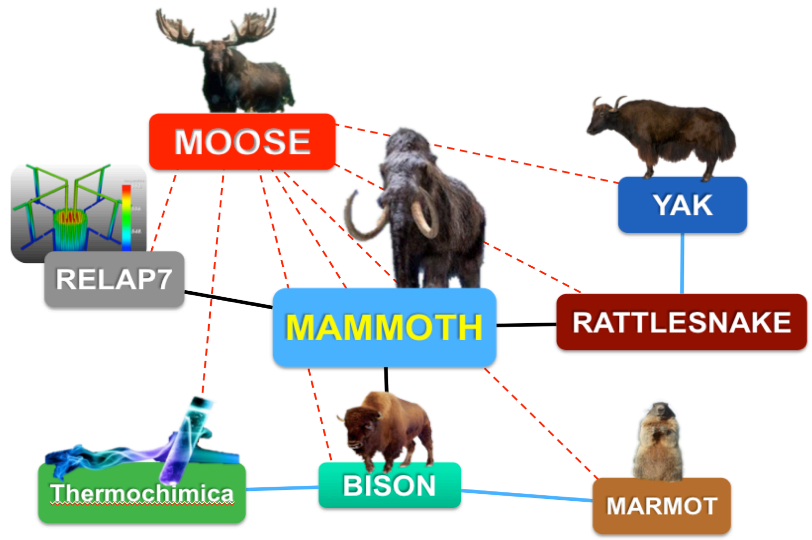
Modeling TREAT Experiments

- **Primary interest is the multi-physics coupling of the core physics and the fuel experiment:**
  - core behavior with low resolution low order operator (diffusion)
    - Preferred as fastest solution
  - and experiment with high resolution high order operator (S_N)
    - Preferred as most detailed solution in smaller experiment.
- **But, in order to have the necessary flexibility for experiment design and analysis, a 3-D M&S capability is necessary to accurately predict:**
  - rapid transient behavior with detailed non-linear temperature feedback effects, and
  - high-resolution flux, fluence, power, temperature distributions and fluid states in the experiment.



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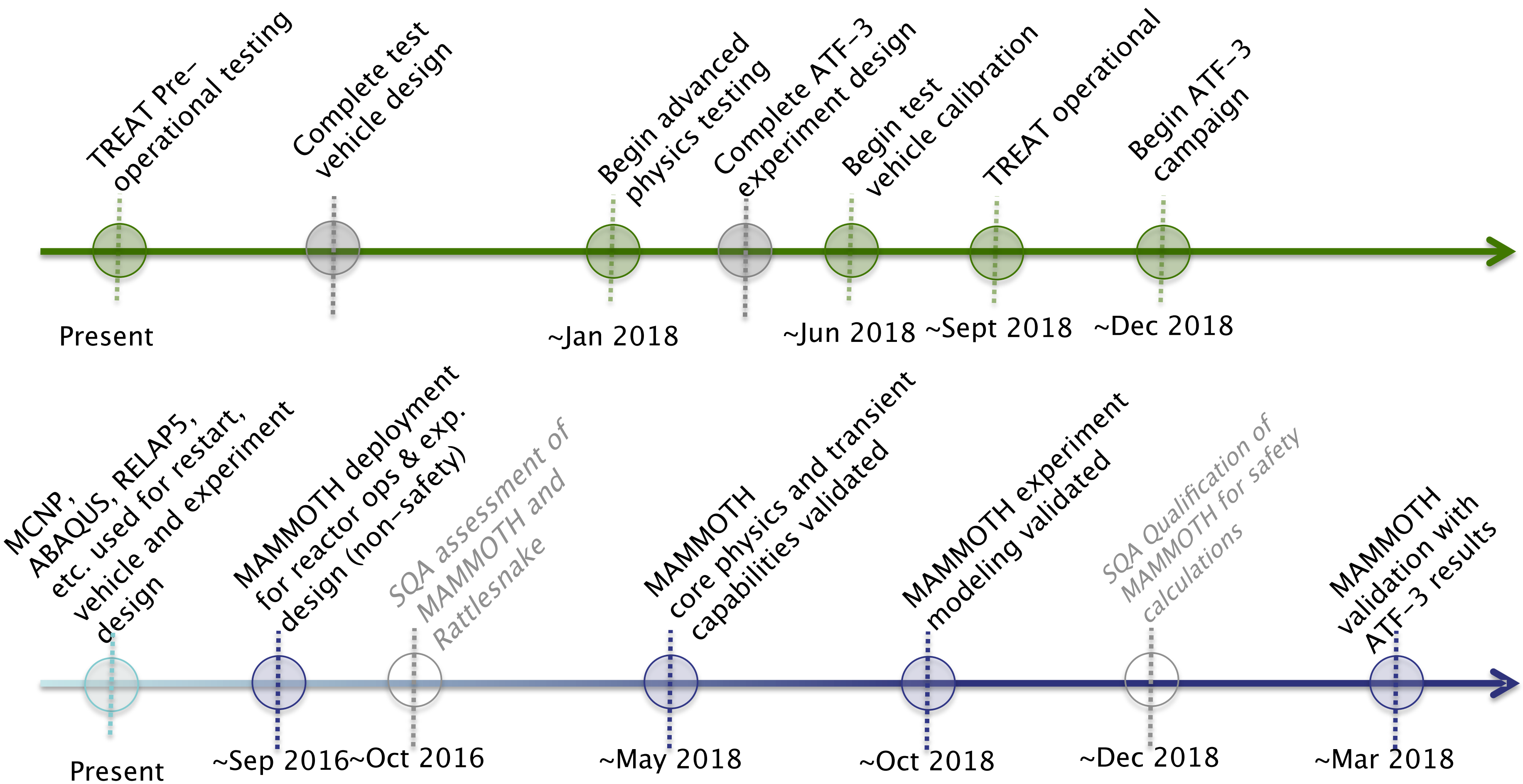
NEAMS Development Plan Tied to TREAT Schedule



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High Impact Problems (HIPs)

- **High impact program concept introduced as a mechanism by which to direct NEAMS tools to address problem of applied relevance.**
  - Core program is the "chassis" upon which HIP is built

- **3-year, ~$3M projects with a defined customer.**

- **Two HIPs initiated in FY15:**
  - *Evaluation of Representative Accident Tolerant Fuel (ATF) Candidates for the Advanced Fuels Campaign*
    - Customer = Advanced Fuels Campaign
  - *Numerical Evaluation of Advanced Steam Generators for SMRs*
    - Customer = NuScale

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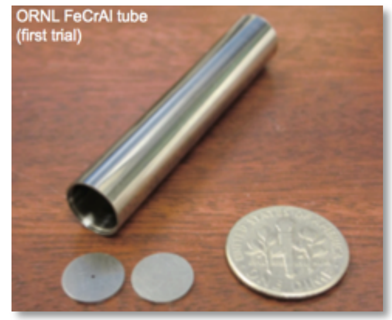
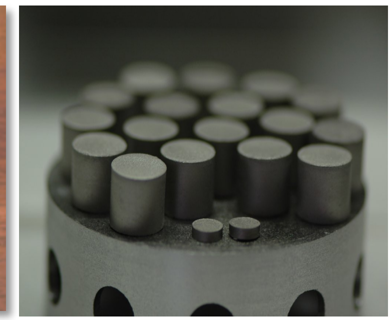
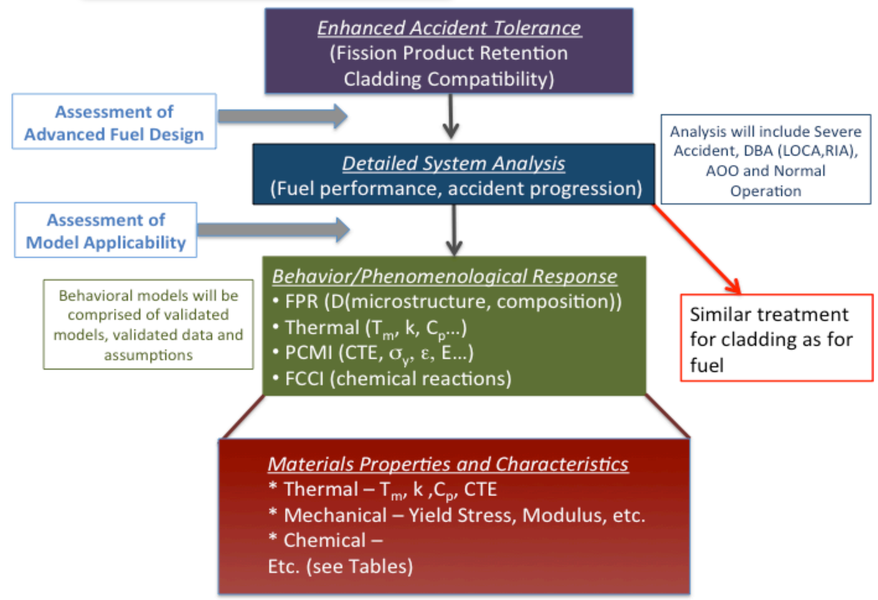
Accident Tolerant Fuel (ATF) HIP

- **ATF HIP supports the Advanced Fuels Campaign (AFC) by developing capabilities to assess ATF designs**
- **Not actively involved in design of ATF concepts, rather providing analysis support**
- **Initial consideration of FeCrAl cladding and U-Si fuel.**
- **Westinghouse Phase 2 ATF proposal to include joint CASL-NEAMS test stand for ATF analysis.**







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Development of fuel performance models for ATF concepts

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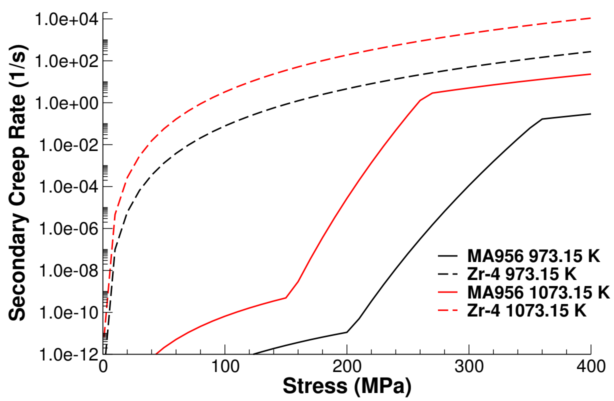
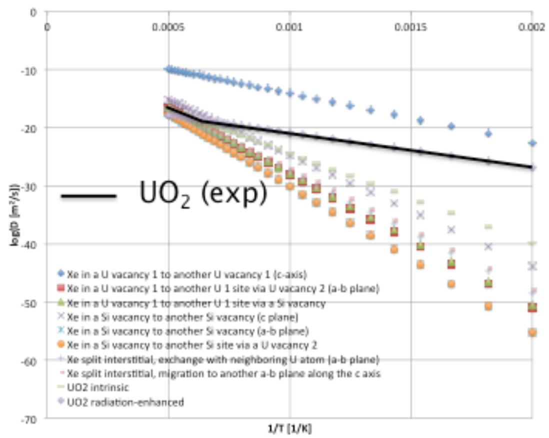
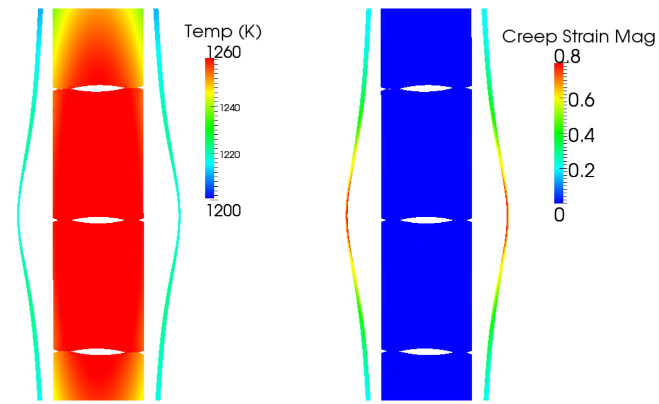
Thermo-mechanical models for FeCrAl alloys are being implemented in BISON



Materials and behavioral models being developed for U-Si fuels



Analyze ATF concepts (including during accidents) using BISON



Capability to analyze advanced fuel designs (e.g. high density, which may also be "accident tolerant") is being developed.

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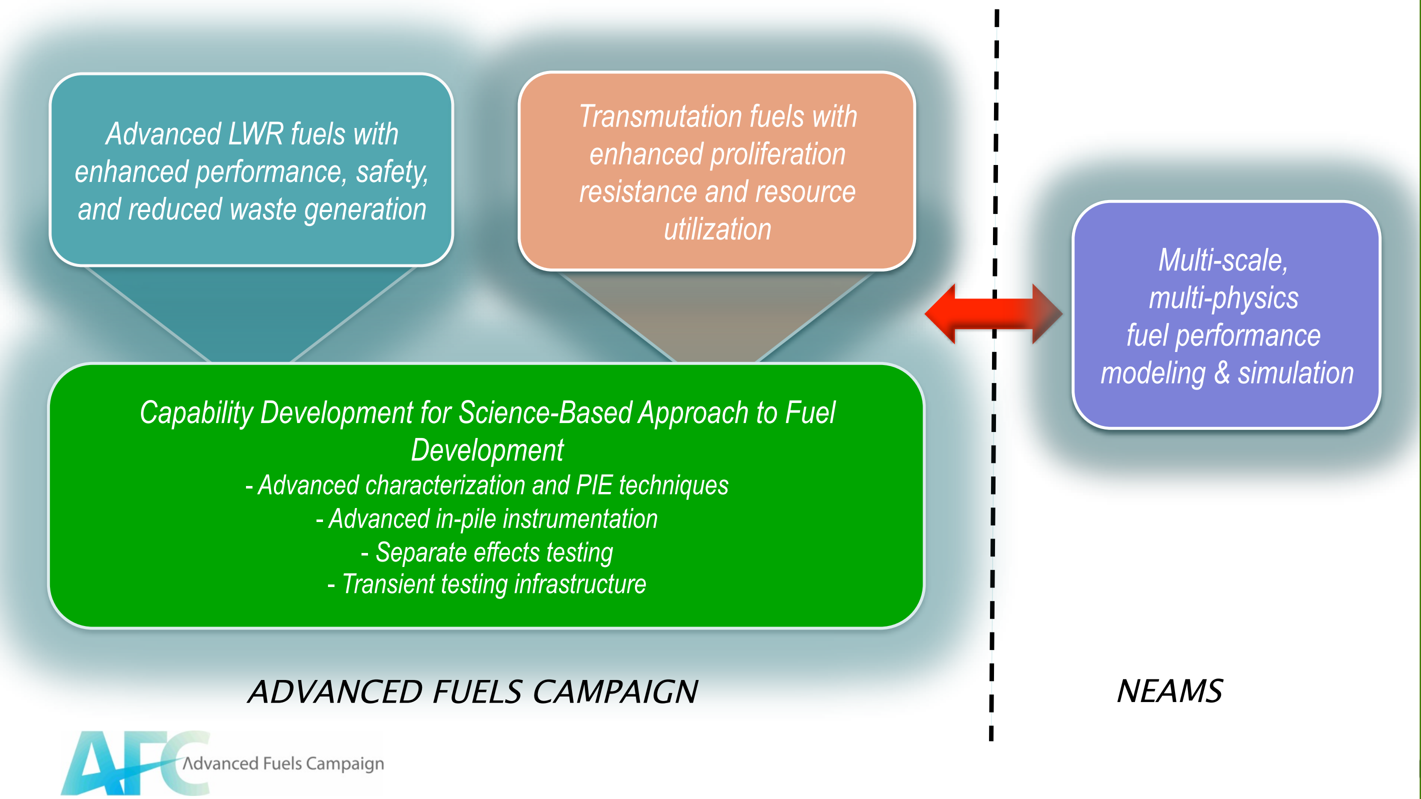
ATF HIP fully integrated in AFC path forward

*The FCRD Advanced Fuel Campaign is tasked with development of near term **accident tolerant LWR** fuel technology and performing research and development of **long term transmutation** options.*



Slide courtesy of Jon Carmack, AFC NTD

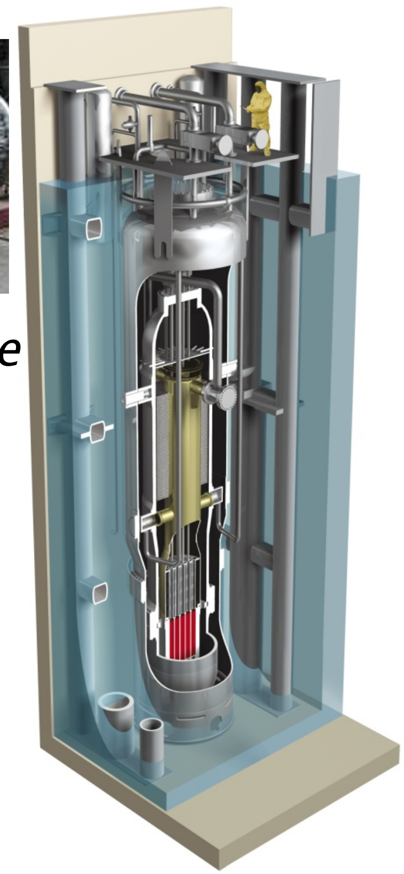
Steam Generator – Flow Induced Vibration (SGFIV) HIP

- **Steam generators may be subject to Flow Induced Vibrations (FIVs).**
- **Designing steam generators that can withstand FIVs is critical (support structures, anti-vibration bars).**
- **Legacy tools/methods, rely on heuristic assumptions or severe simplifications.**
- **Inadequate predictions of flow-induced vibration (FIV) phenomena within SGs can be <u>crippling</u> (SONGS)**
- **Steam generators in integral PWR (SMRs) are <u>internal vessel components</u>.**
- **Recognized limitations of current methods and lack of data for the design of helical SGs (e.g., support structures)**

U-tube

NuScale Power

Helical tube,
this is NOT the NuScale design



NuScale SMR, cartoon

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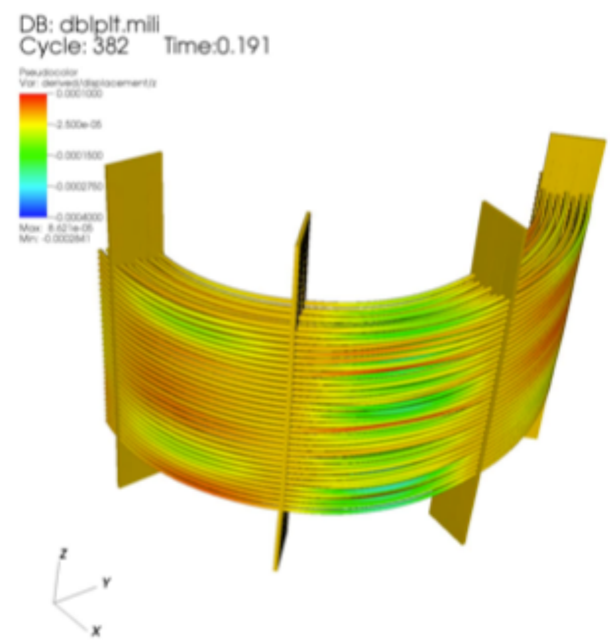
SHARP Applied to NuScale Helical Steam Generator Design

- **Development of validated, predictive capability to simulate Flow Induced Vibrations with SHARP (Nek5000 + Diablo) to assist design of NuScale helical steam generator**

- **Nek data used to drive dynamic simulations in Diablo (~150 Gb data transferred over ~3M points)**
- **Midterm is focused on verification/ validation of FIV capability**
- **Project will culminate with Nek5000+Diablo simulations in support of of full scale test at Areva loop facility (Erlangen)**
- **Exploring potential GTRF simulation and comparisons/evaluation joint with CASL**



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NEAMS Role in GAIN

What is GAIN?

Through GAIN, DOE is making its state-of-the art and continuously improving RD&D infrastructure available to stakeholders to achieve faster and cost-effective development of innovative nuclear energy technologies toward commercial readiness. The capabilities accessible through GAIN include:

- Experimental capabilities with primary emphasis on nuclear and radiological facilities but also including other testing capabilities (e.g. thermal-hydraulic loops, control systems testing, etc.).
- Computational capabilities along with state-of-the art modeling and simulation tools.
- Information and data through knowledge and validation center.
- Land use and site information for demonstration facilities.
- Assistance through the regulatory process. The Nuclear Regulatory Commission (NRC) will provide regulatory expertise and guidance through GAIN.

https://gain.inl.gov/Shared%20Documents/GAIN-FactSheet_rev4.pdf

Emphasis of NEAMS program on proactive customer engagement is consistent with GAIN.

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Validation-based milestones

- Validation cases being added to current suite that correspond to specific capability development.
- Future capability development milestones to be linked to specific targeted validation cases.
- Advanced codes have validation requirements beyond existing datasets.

Overview of the main integral experimental data used for validation of BISON.

Experiment	Rod	Final Burnup (MWd/kgU)	FCT	FGR	Rod Dia
IFA-431	1[a]	≈4	X		
IFA-431	2[a]	≈4	X		
IFA-431	3[a]	≈4	X		
IFA-431 (3D)	4[a]	≈4	X		
IFA-432	1[a]	≈32	X		
IFA-432	2[a]	≈32	X		
IFA-432	3[a]	≈32	X		
IFA-515.10	A1[b]	86.6	X		
IFA-534	18	59.0		X	
IFA-534	19	59.0		X	
IFA-535	809	54.4		X	
IFA-535	810	54.4		X	
IFA-562.2	15	56.7	X	X	
IFA-562.2	16	56.2	X	X	
IFA-562.2	17	56.2	X	X	
IFA-597.3	8	68.1	X	X	
Risø-2	GE-m	15.8		X	X
Risø-3	AN2	40.7		X	X
Risø-3	AN3	42.0	X	X	
Risø-3	AN4	42.0	X	X	
Risø-3	GE7	40.9		X	X
Risø-3	II3	17.6	X	X	X
Risø-3	II5	47.6	X	X	X
OSIRIS	H09	46.1		X	X
OSIRIS	J12	26.7		X	X
REGATE		47.0		X	X
USPWR 16x16	TSQ002	53.2		X	X
USPWR 16x16	TSQ022	58.1		X	X
R.E. Ginna	2	51.2		X	X
R.E. Ginna	4	57.0		X	X
HBEP	BK363	76.0		X	
HBEP	BK365	78.3		X	
Tribulation	BN1/3	50.7		X	X
Tribulation	BN1/4	50.6		X	X
Tribulation	BN3/15	51.1		X	X

[a] Only considered first rise to power.
[b] Included first rise to power in beginning of life comparisons.

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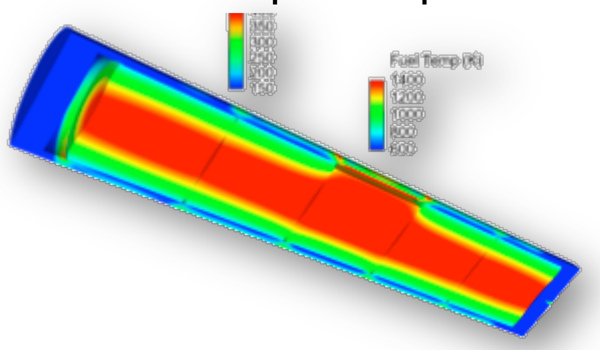
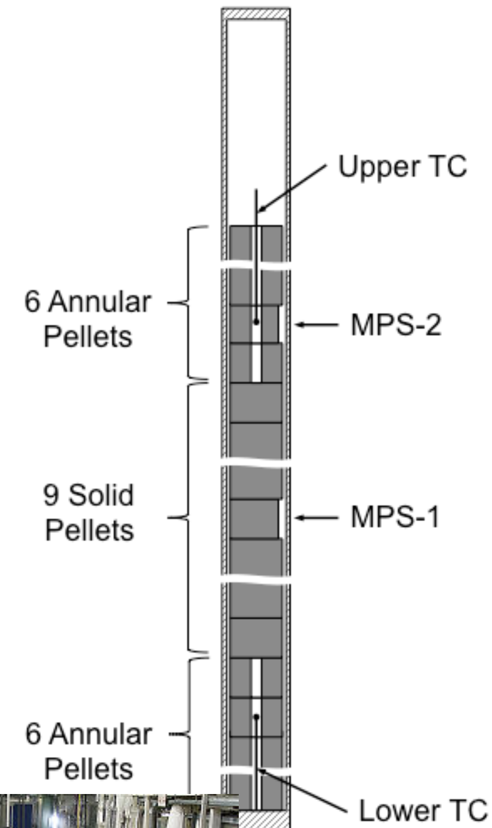
Advanced Validation: *Halden Missing Pellet Surface Experiment*

Manufacturing flaws (“missing pellet surface” defects) in fuel pellets have been root cause of fuel failures. Pellet-cladding interaction (PCI) is a CASL challenge problem.

Validation experiments being planned for the Halden reactor later this year.

Example of a 3D fuel performance code addressing a 3D applied problem – which requires specific validation



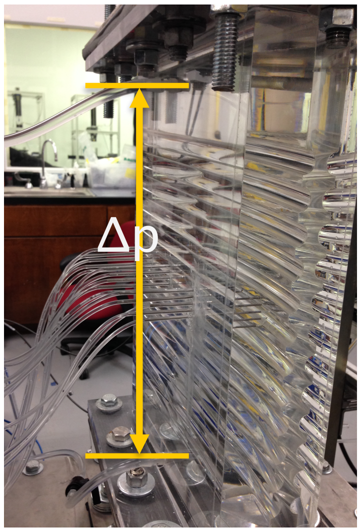


Once validated, further analysis using BISON to define an MPS geometry threshold could used to inform fuel manufacturing tolerances.

The OECD Halden Reactor Project

Texas A&M facility for FIV validation

<Experiment>



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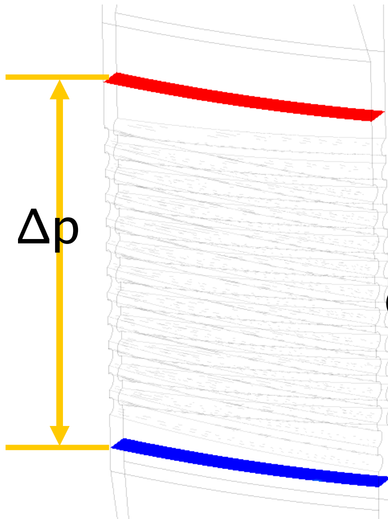
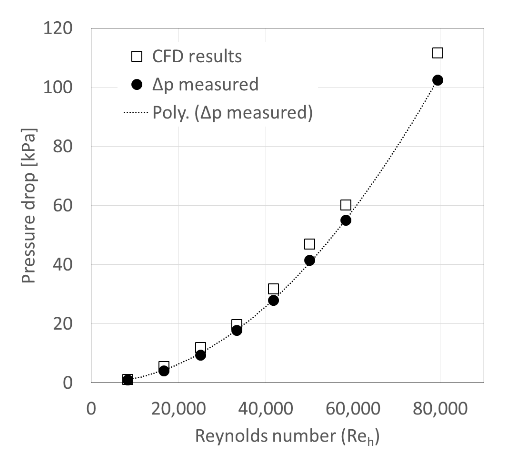
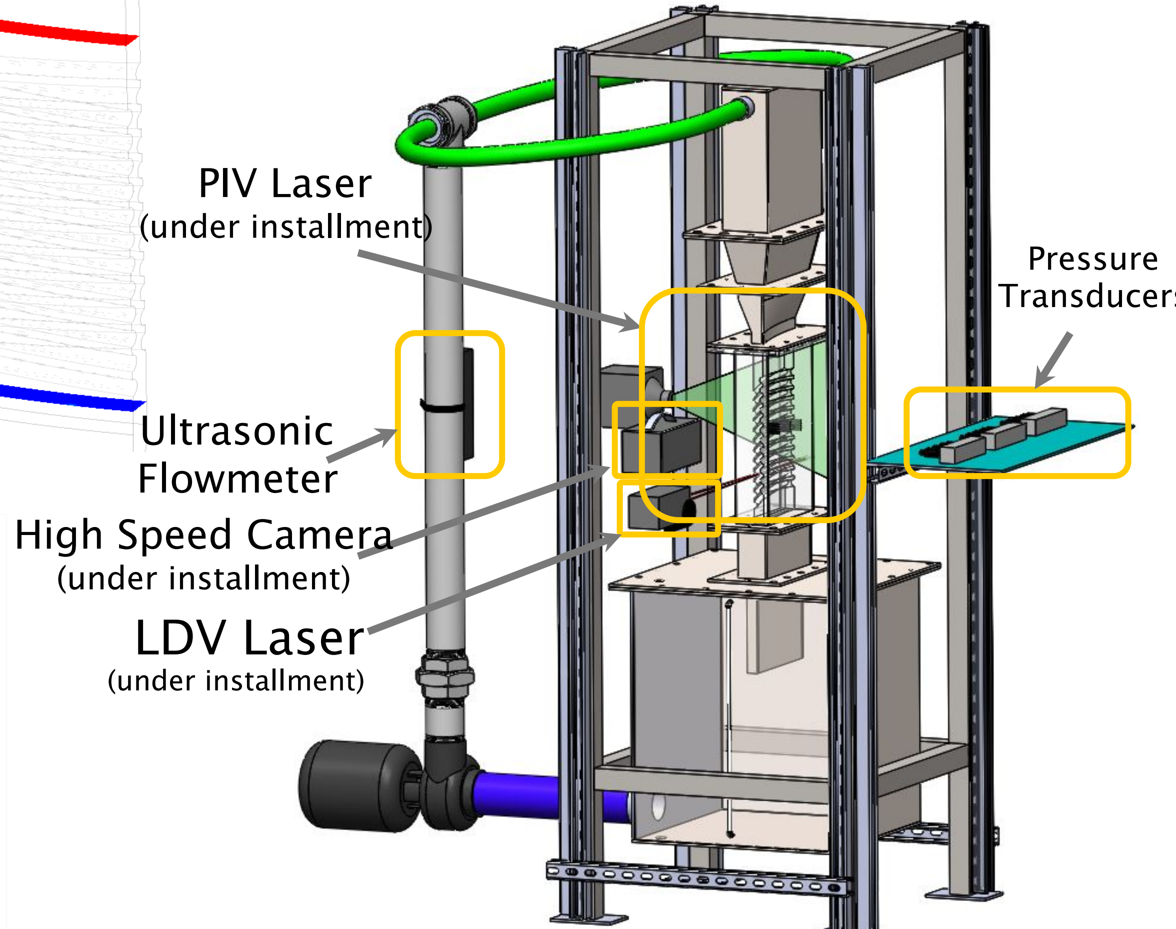






Interaction with NRC

- **Initial technical exchange held (April 2016) between BISON and FRAP teams to identify opportunities where both teams might benefit from each other's completed or ongoing work.**
- **A number of opportunities were identified (some of which NEAMS will continue to pursue), including:**
  - Information exchange on data sources/assessment cases
  - Unified fission gas model, fission gas release during LOCA
  - Extension to spent fuel (low T cladding creep, fission product diffusion)
  - Lower length scale modeling, e.g. O diffusion (in UO_2) for cladding inner diameter oxide growth (relevant to 50.46c)
  - Accident tolerant and advanced reactor fuel.

Regular information exchanges will ensure productive relationship. Potential to emulate for other NEAMS program elements.

CASL coordination

- **NEAMS and CASL leadership teams are currently developing an interaction strategy that addresses near term coordination of effort, but also lays ground work for a comprehensive modeling and simulation suite.**

- **Certain aspects of CASL Phase 2 scope present natural collaboration opportunities with NEAMS (e.g. RIA/LOCA in CASL and ATF-HIP). Those opportunities have been and are being identified for mutual benefit.**

- **Near-term scope coordination also enables strategic planning of comprehensive effort.**

- ***Frequent interaction is critical:* Next meeting between CASL and NEAMS leadership (lab, university and DOE) on Aug. 17.**

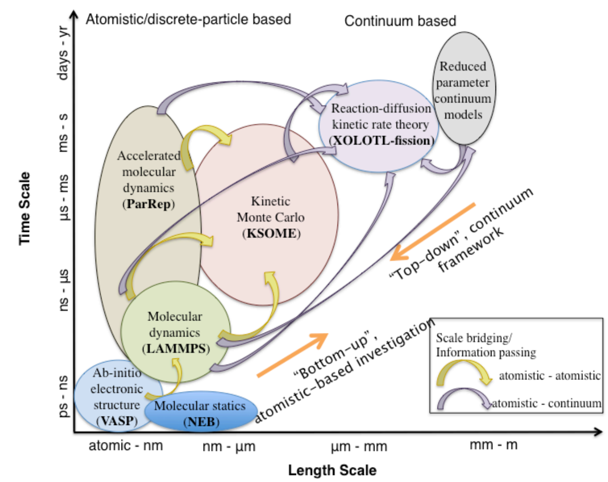
NEUP and Pilot SciDAC

- **NEAMS benefits from NEUP program and will continue to explore how to maximize benefit.**

- **Although still in procurement process, a proposed a pilot SciDAC Partnership between ASCR/Office of Science and Office of Nuclear Energy (NE)**
  - *"Advancing Understanding of Fission Gas Behavior in Nuclear Fuel Through Leadership Class Computing,"* Prof. Brian Wirth (PI)

- Will bring together state-of-the-art computational science and materials science in order to predict fission-gas bubble formation in and its impacts on nuclear fuel.

- Proposed research both extends and complements NEAMS activities.



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Exciting science directed at applied problems

nature COMMUNICATIONS

ARTICLE

Received 9 May 2014 | Accepted 27 Jun 2014 | Published 1 Aug 2014 DOI: 10.1038

Anisotropic thermal conductivity in uranium dioxide

K. Gofryk[1,†], S. Du[2,†], C.R. Stanek[3], J.C. Lashley[1], X.-Y. Liu[3], R.K. Schulze[1], D.D. Byler[3], K.J. McClellan[3], B.P. Uberuaga[3], B.L. Scott[4] & D.A. Andersson

Nuclear Engineering and Design 295 (2015) 48–58

Contents lists available at ScienceDirect

Nuclear Engineering and Design

journal homepage: www.elsevier.com/locate/nucengdes

ELSEVIER

A porous medium model for predicting the duct wall temperature of sodium fast reactor fuel assembly

CrossMark

Yiqi Yu[a,*], Elia Merzari[b], Aleksandr Obabko[b], Justin Thomas[a]

[a] Nuclear Engineering Division, Argonne National Laboratory, Lemont, IL 60439, United States
[b] Mathematics and Computer Science Division, Argonne National Laboratory, Lemont, IL 60439, United States

Journal of Nuclear Materials 469 (2016) 89–9

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

ELSEVIER

Development of a multiscale thermal conductivity model for fission gas in UO_2

CrossMark

Michael R. Tonks[a, b, *], Xiang-Yang Liu[c], David Andersson[c], Danielle Perez[b], Aleksandr Chernatynskiy[d], Giovanni Pastore[b], Christopher R. Stanek[c], Richard Williamson[b]

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Participation in International Activities

- **IAEA Coordinated Research Projects**
  - FUMAC – Fuel Modeling Under Accident Conditions
  - ACTOF – Analysis of Options and Exp. Examination of Fuels for Water-Cooled Reactors
- **OECD/NEA**
  - Pellet-Cladding Mechanical Interaction (PCMI) Benchmark and Reactivity Insertion Accident (RIA) Benchmarks
  - Uncertainty Analysis in Modeling (UAM) Benchmark
  - Halden Reactor Project. NEAMS researcher embedded in Halden team; 3D Bison validation.
  - Nuclear Science Committee – Working Party for Reactor Physics (WPRS): Expert Group on Reactor Physics and Advanced Nuclear Systems (EGRPANS), Expert Group on Radiation Transport and Shielding (EGRTS), Expert Group on Uncertainty Analysis in Modeling (EGUAM), International Reactor Physics Experiment Evaluation (IRPhE), Working Party on International Nuclear Data Evaluation Co-operation (WPEC), Working Party on Nuclear Criticality Safety (WPNCS)
- **I-NERI – U.S.-Euratom Collaboration Framework**
  - Code-to-code benchmarks for CFD simulations of SFR fuel assembly coolant flow
- **Horizon 2020**
  - *Planned- Thermal-Hydraulics Simulations and Experiments for the Safety Assessment of MEtal Cooled Reactors (SESAME)*.
- **US-UK**
  - DOE-DECC Action Plan
  - National Nuclear Laboratory (NNL): Fast Fuel Capability Development, LWR Validation.
- **DOE-CEA Bilateral**
  - Cadarache collaboration on UO_2 fuel physics

NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Summary

- **Success of the NEAMS program looks like:** *customers (both DOE-NE and industry) using NEAMS-developed technology to change the way they do business.*

- **Many of the NEAMS tools are approaching a maturity level that they can be deployed. What more can we do to facilitate deployment?**

- **What research questions (too applied for Office of Science, but too fundamental for industry) must be tackled for the capabilities to reach the next level of maturity?**

- **Pursuing continued interaction with customers (NE programs, e.g. CASL and industry) to identify problems of mutual interest.**