



U.S. DEPARTMENT OF
ENERGY

Nuclear Energy

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

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

NEAMS Organizational Structure



National
Technical
Director
Chris Stanek
(*LANL*)



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*)

Leadership Council

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

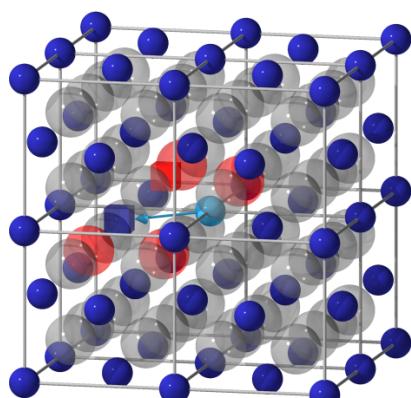
**Shane
Johnson**
Deputy Assistant
Secretary,
Office of Science
and Technology
Innovation
(NE-4)

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.

Fuels Product Line (FPL)

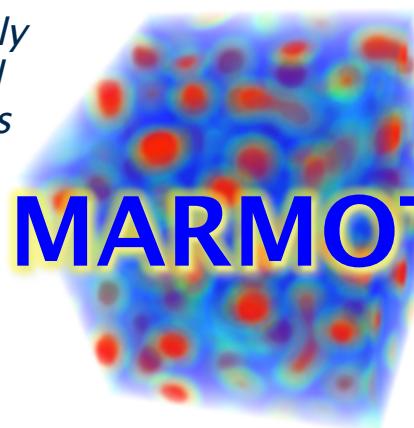
- Empirical models can accurately interpolate between data, but cannot accurately extrapolate outside of test bounds
- **Goal:** Develop improved, mechanistic, and *predictive* models for fuel performance using hierarchical, multiscale modeling – applied to existing, advanced (including accident tolerant)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

Atomistic simulations



- Identify important mechanisms
- Determine material parameter values

Meso-scale models



Atomistically -informed parameters

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

Engineering scale fuel performance

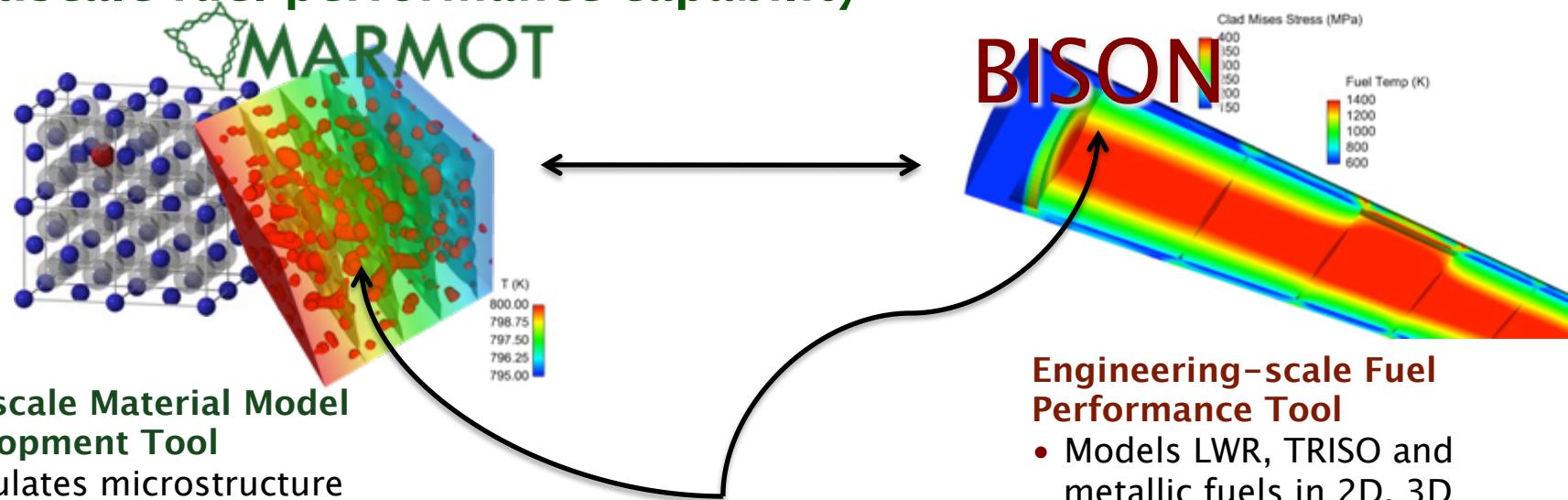


Degrees of freedom, operating conditions
Mesoscale-informed materials models

- Predict fuel performance and failure probability

MBM: MOOSE–BISON–MARMOT

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



Mesoscale Material Model Development Tool

- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models

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

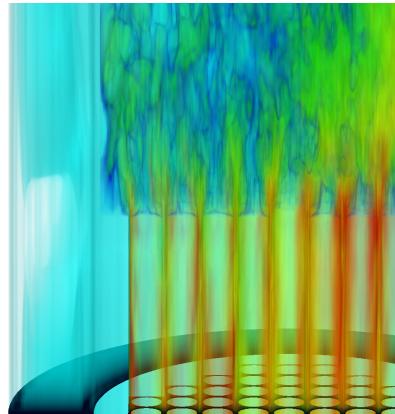
 **NEAMS**
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Reactor Product Line: *Sharp*

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

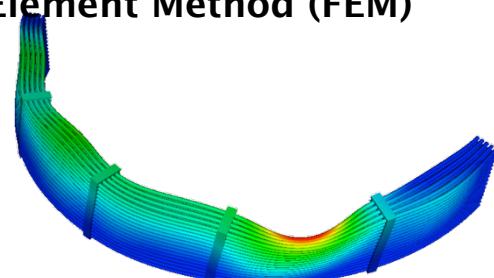
Nek5000 - Thermal-Hydraulics

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



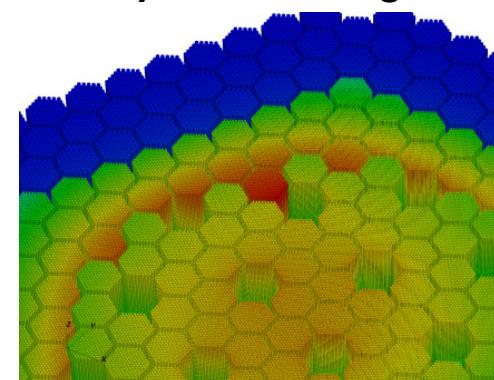
DIABLO - Structural Dynamics

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



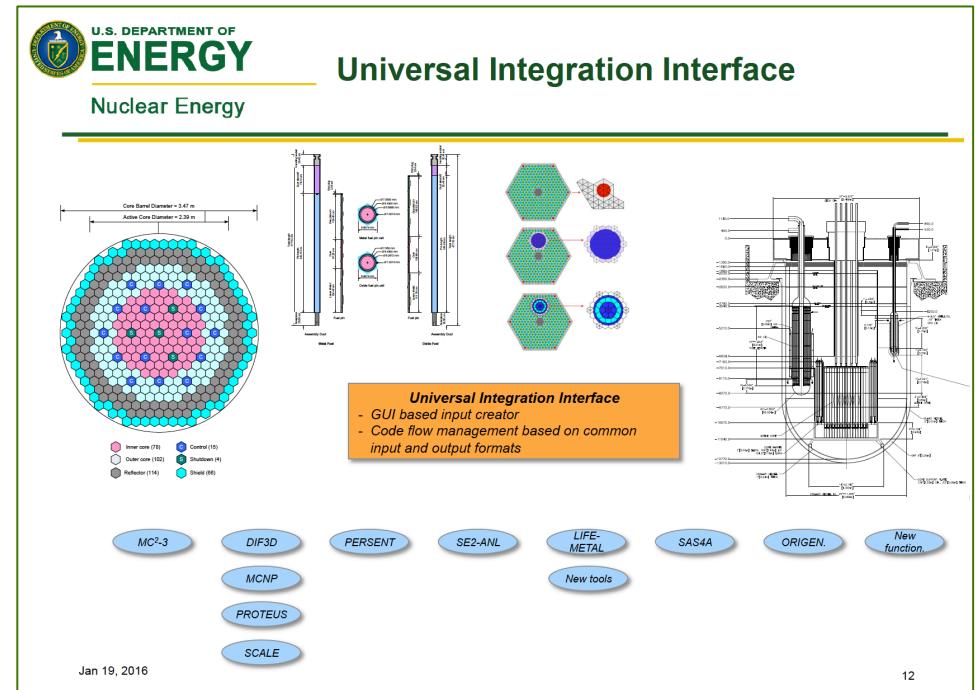
Integration Product Line

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?*



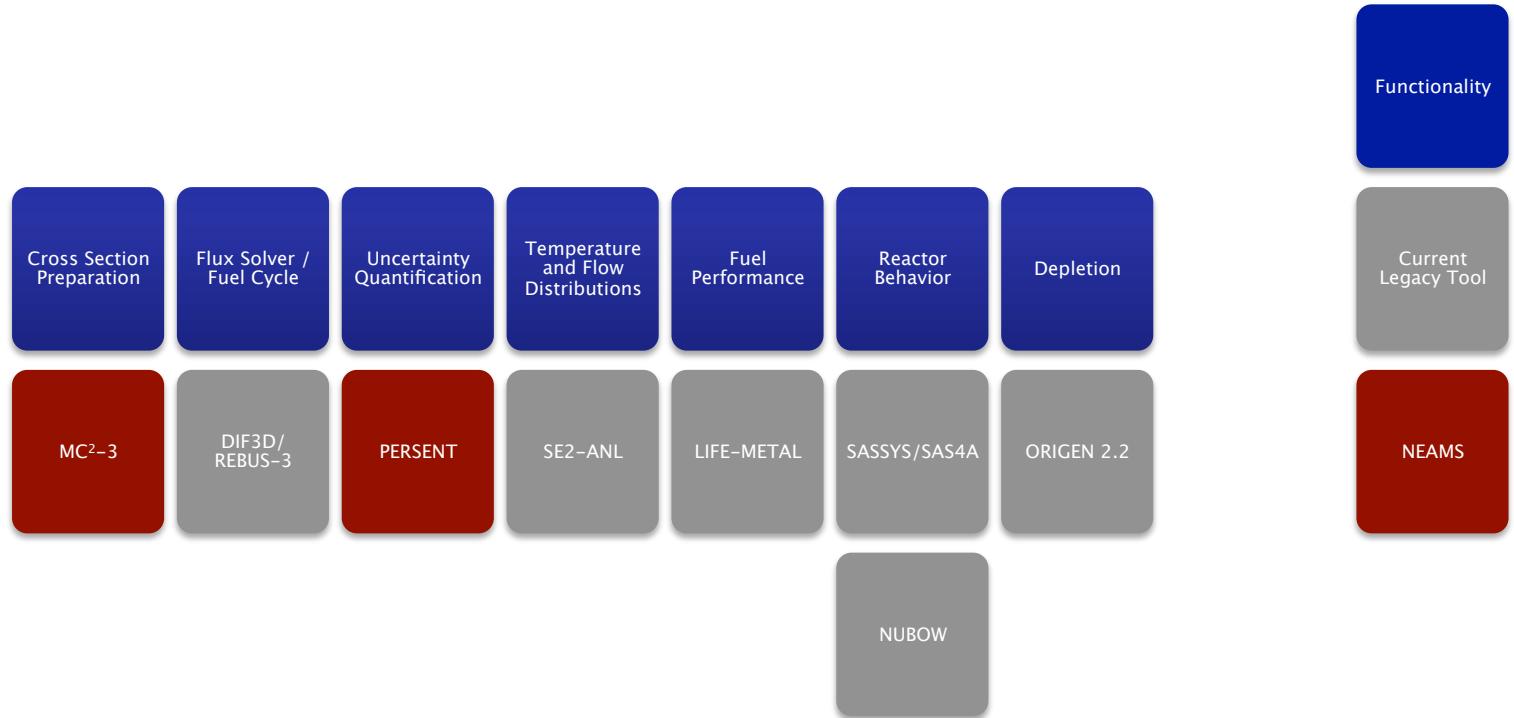
Dialogue with ART = “universal” interface

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

(Slide: T.K. Kim - ANL)

Current ART Code Suite

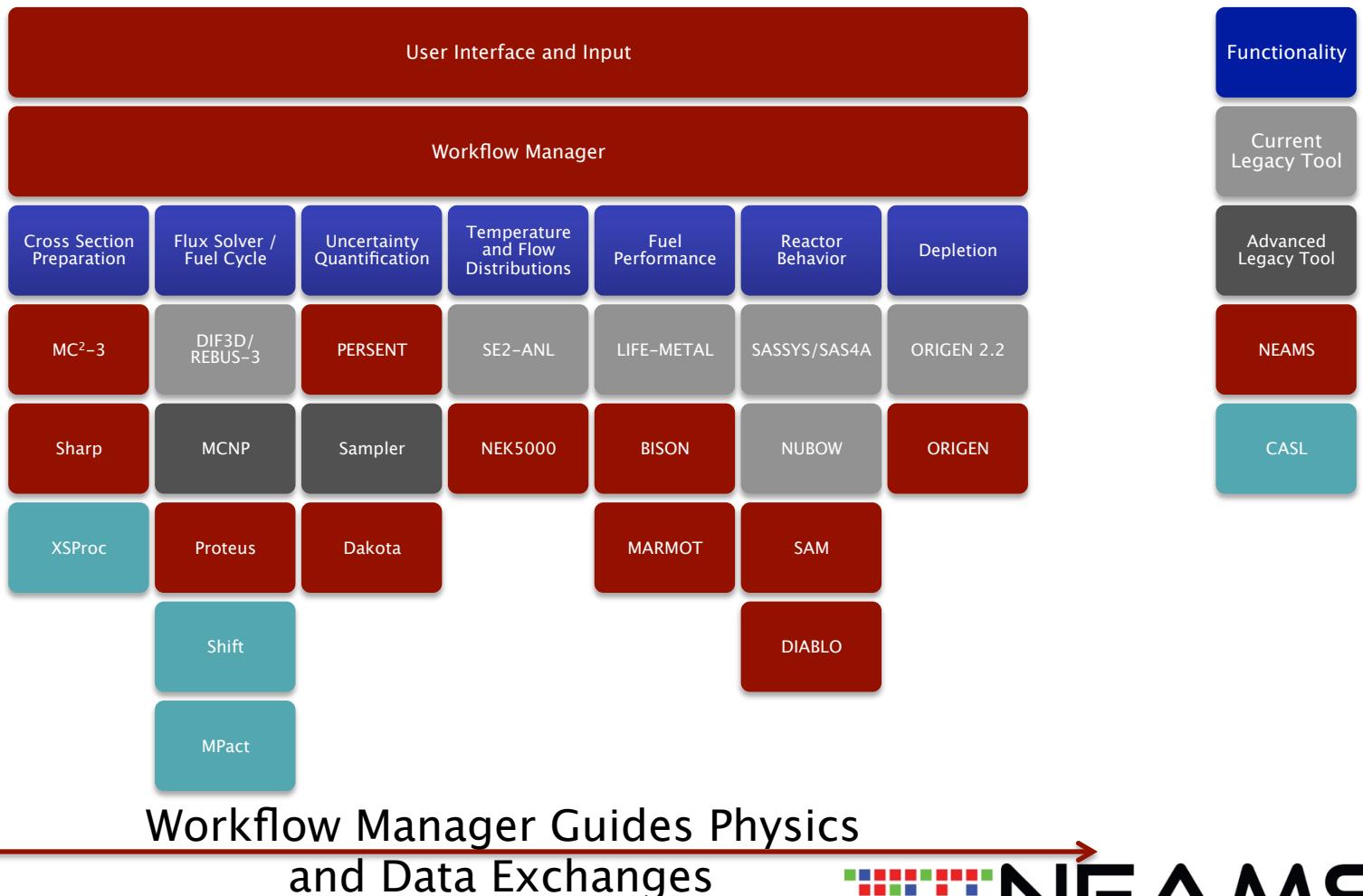
Limited Choices
of Low-Fidelity Physics



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

Example NEAMS “Workbench” Implementation for SFR Analysis

User Selects Desired
Fidelity of Physics



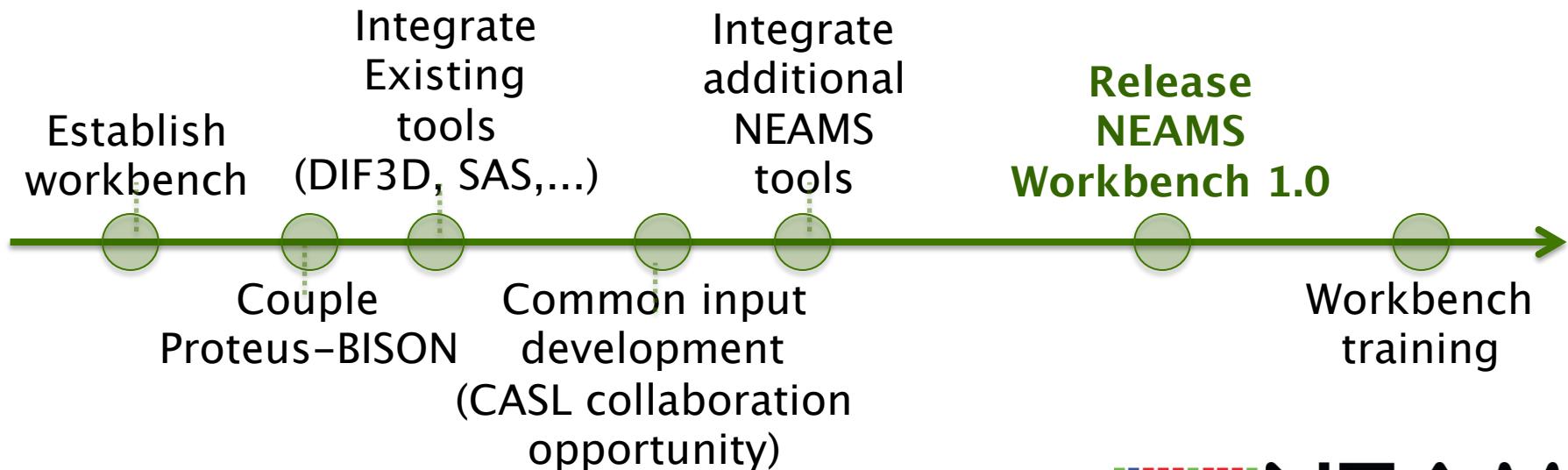
Snapshot of Fulcrum user interface (from SCALE)

The screenshot displays the Fulcrum user interface for the SCALE 6.2 application. The interface is organized into several panes:

- Navigation:** A sidebar on the left containing a tree view of input cards and a text input field for comments.
- Input Files:** The main window shows several input files: "HFIR-fission.inp*", "HFIR-fission.inp : geometry (Line 7034)", and "HFIR-fission.inp : geometry (Line 7034)" (a duplicate tab).
- Parameter Dialogs:** A "Parameters" dialog is open, showing fields for "Composition" (uo2), "Mixture" (1), "Theoretical Density" (10.960000), "Volume Fraction" (1.0), and "Temperature" (293).
- Text Input:** A callout box highlights the text input field in the navigation sidebar with the text: "Text Input Preferred by Expert Users with Highlighting and Error Detection".
- Optional Component Input:** A callout box highlights the "Parameters" dialog with the text: "Optional Component Input Preferred by Novice Users".
- Geometry Visualization:** A 3D visualization of a reactor core structure with various colored regions representing different materials or components.
- Data Visualization:** A plot titled "u-238 n, gamma 600 K xs" showing the cross section (barns) versus Energy (eV) for two components: u-238 n, gamma 600 K xs (blue line) and u-235 fission 600 K xs (red line).
- Mesh Results Overlay:** A 3D visualization of the reactor core with a color-coded overlay representing fission rate or fission rate-fission rate, with values ranging from 5.86E-05 to 3.08E-07.

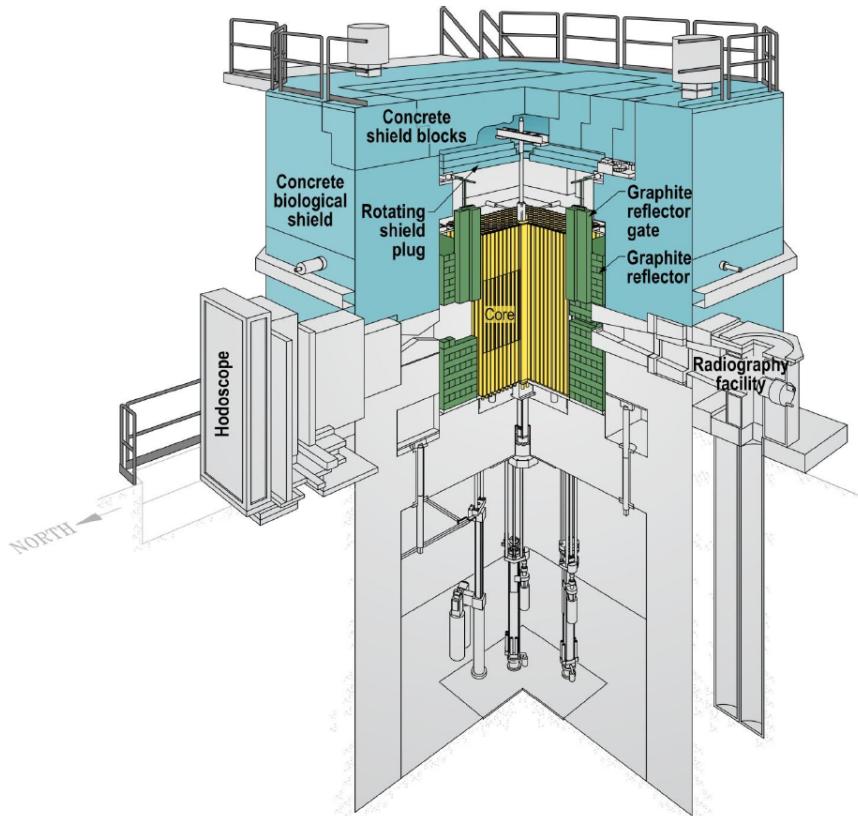
NEAMS Workbench

- 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

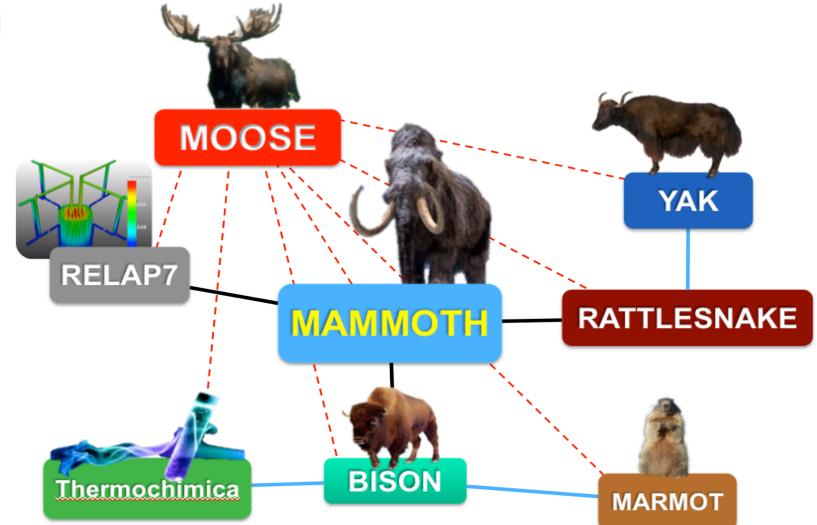
NE Mission Need – *Support resumption of high power/short duration transient testing at the INL TREAT facility with advanced computational tools that will enhance R&D capabilities*



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.

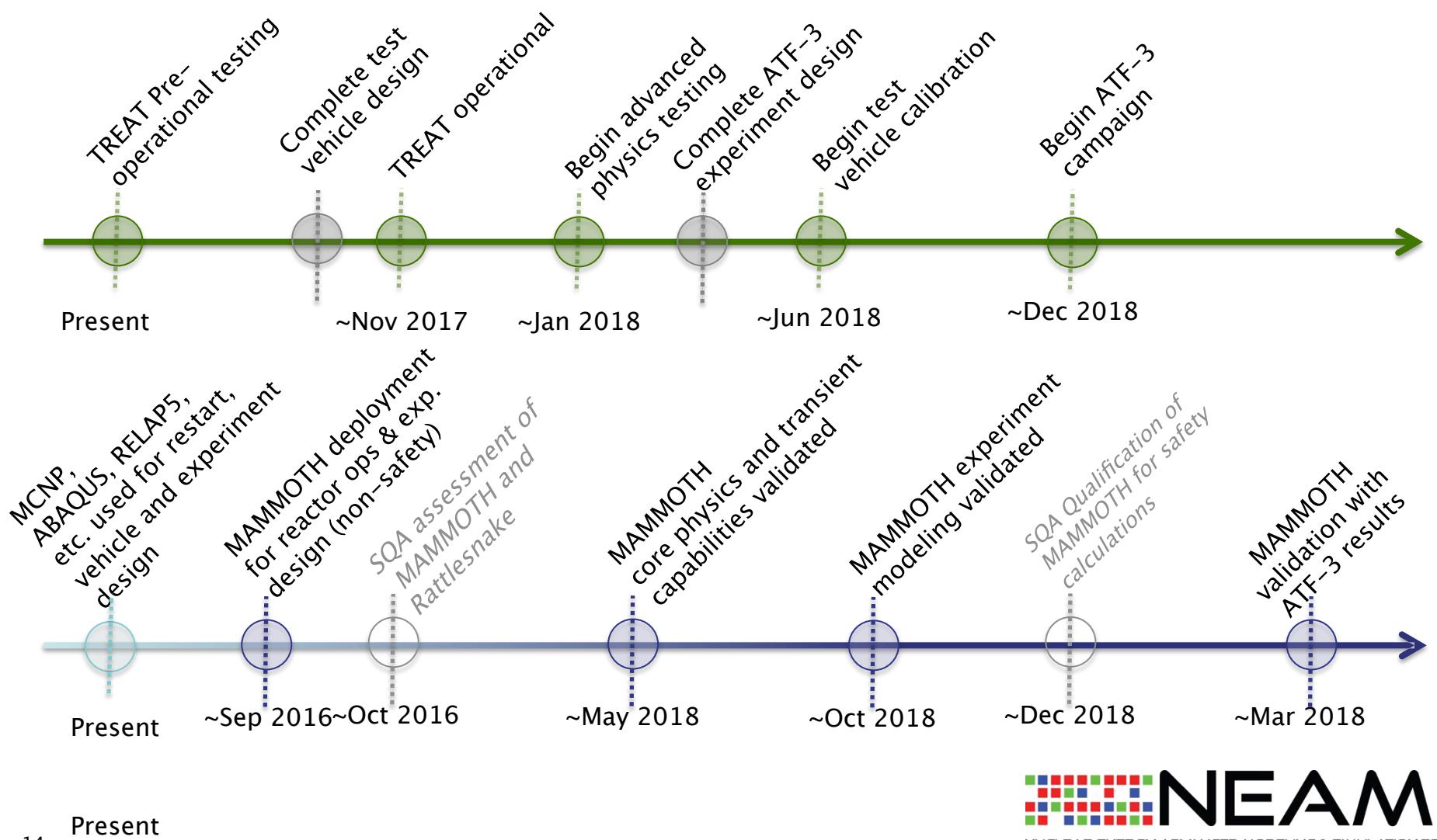
Modeling TREAT Experiments

- n 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.
- n 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.





NEAMS Development Plan Tied to TREAT Schedule

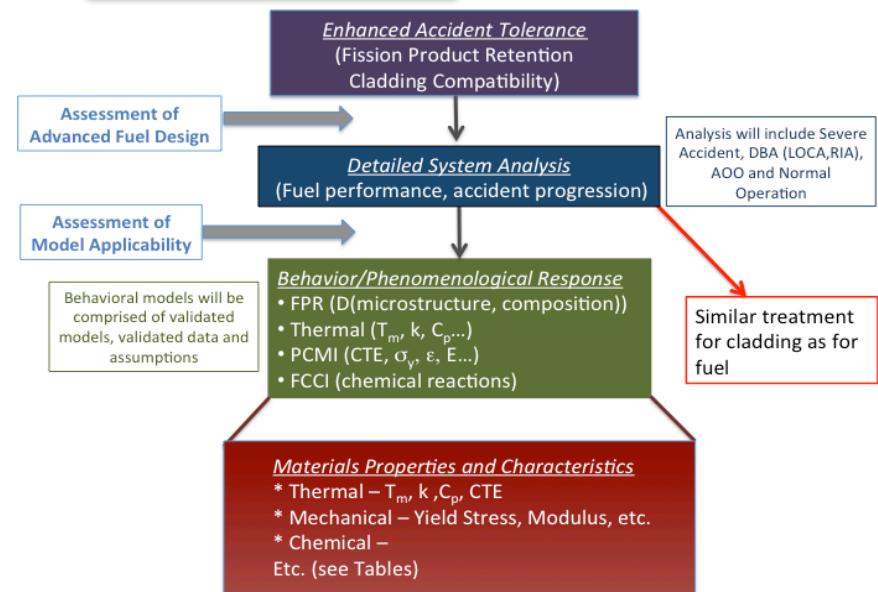
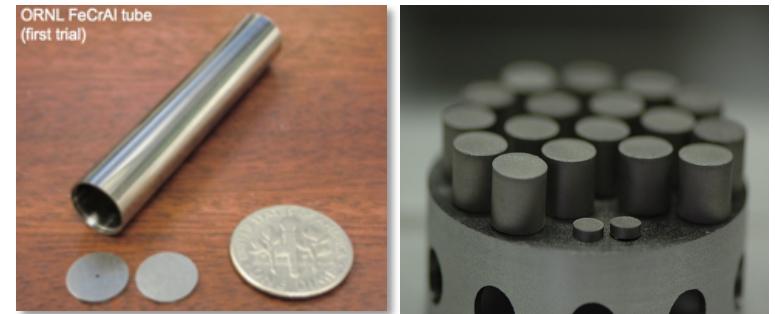


High Impact Problems (HIPs)

- 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

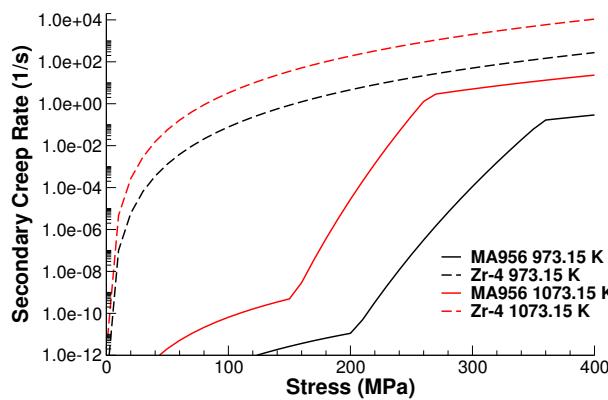
Accident Tolerant Fuel (ATF) HIP

- 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.

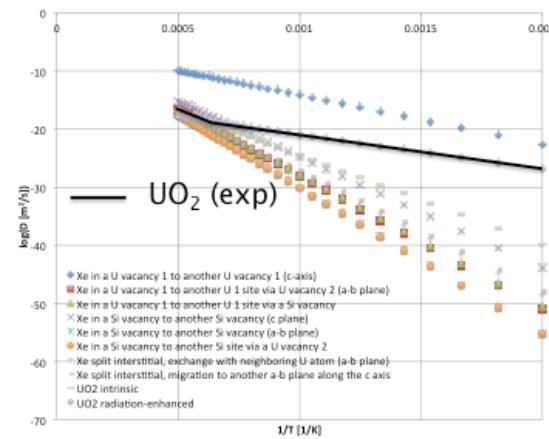


Development of fuel performance models for ATF concepts

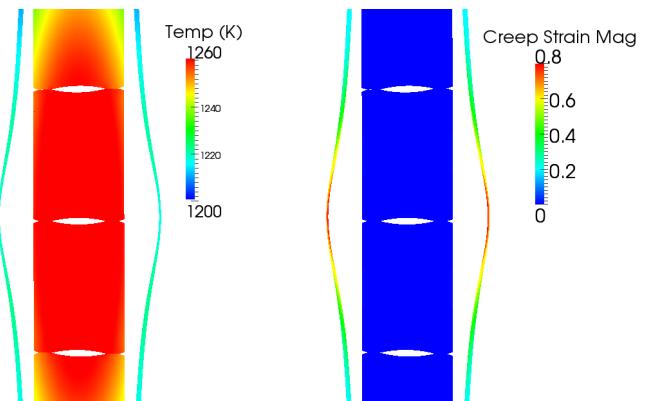
Thermo-mechanical models for FeCrAl alloys are being implemented in BISON



Materials and behavioral models being developed for U-Si fuels

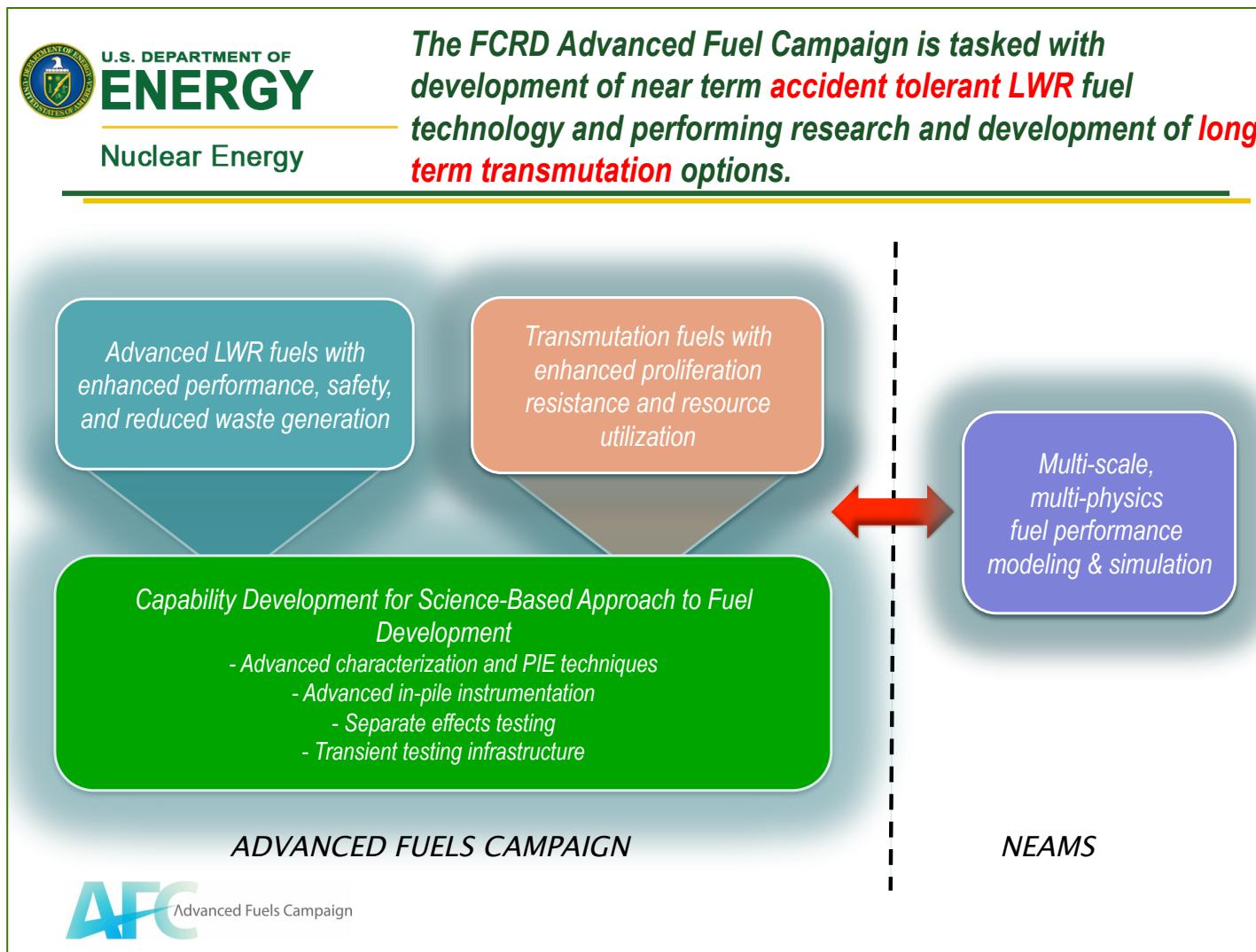


Analyze ATF concepts (including during accidents) using BISON



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

ATF HIP fully integrated in AFC path forward



Steam Generator – Flow Induced Vibration (SGFIV) HIP

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



U-tube



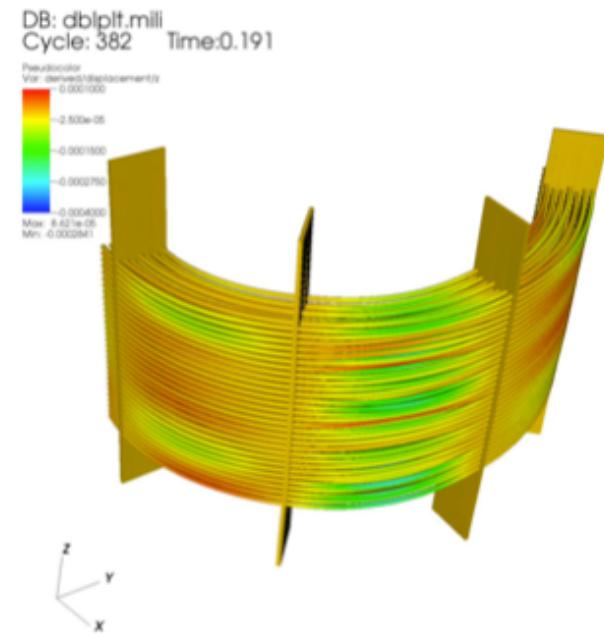
*Helical tube,
this is NOT the NuScale
design*



NuScale SMR, cartoon

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 full scale test at Areva loop facility (Erlangen)
- Exploring potential GTRF simulation and comparisons/evaluation joint with CASL

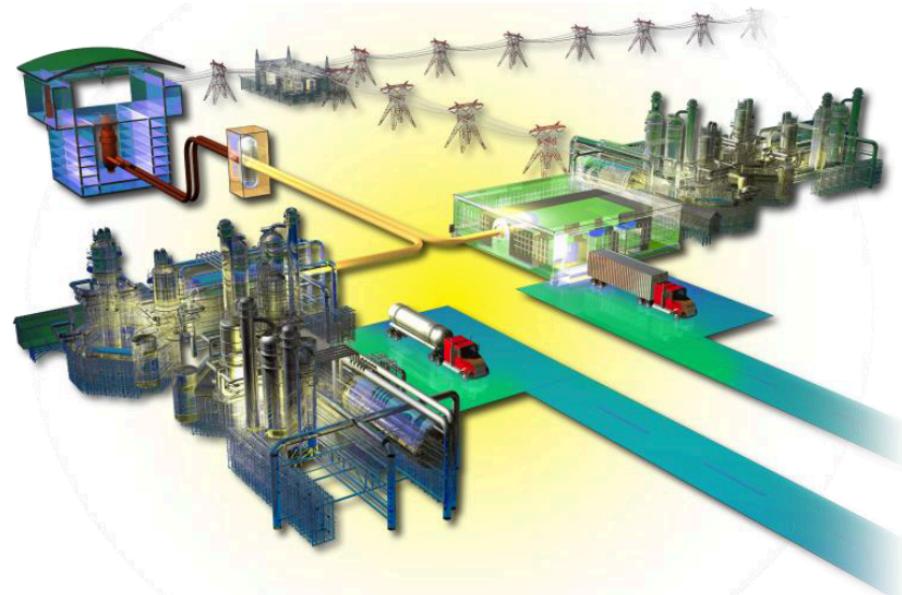


NEAMS Role in GAIN

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.

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.

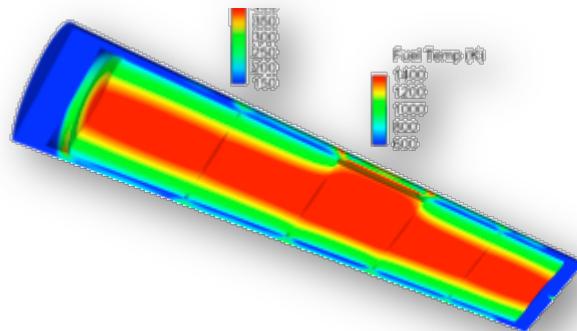
^b Included first rise to power in beginning of life comparisons.

Advanced Validation: *Halden Missing Pellet Surface Experiment*

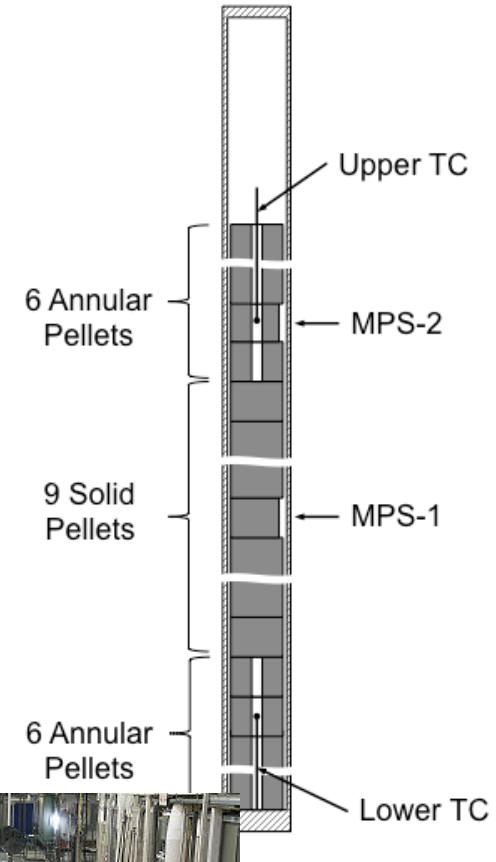
Manufacturing flaws (“missing pellet surface” defects) in fuel pellets have been root cause of fuel failures. Pellet-cladding interaction (PCI) is a CASL challenge problem.

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



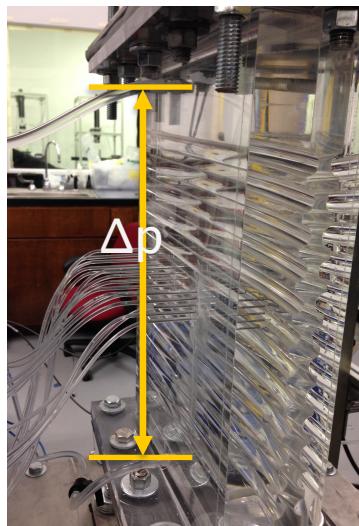
Once validated, further analysis using BISON to define an MPS geometry threshold could be used to inform fuel manufacturing tolerances.



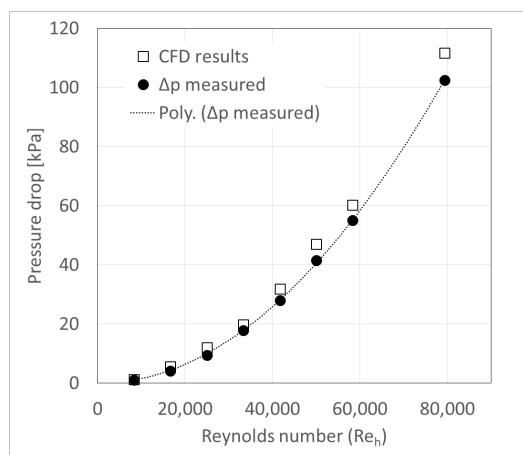
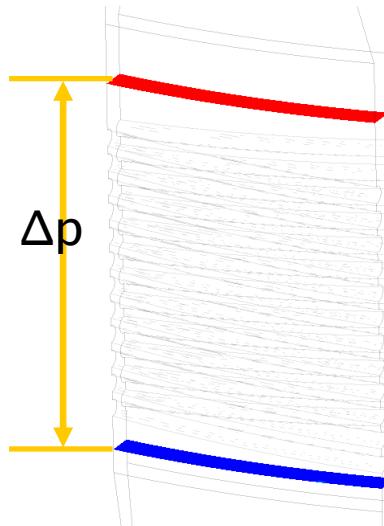
AMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Texas A&M facility for FIV validation

<Experiment>



<CFD>



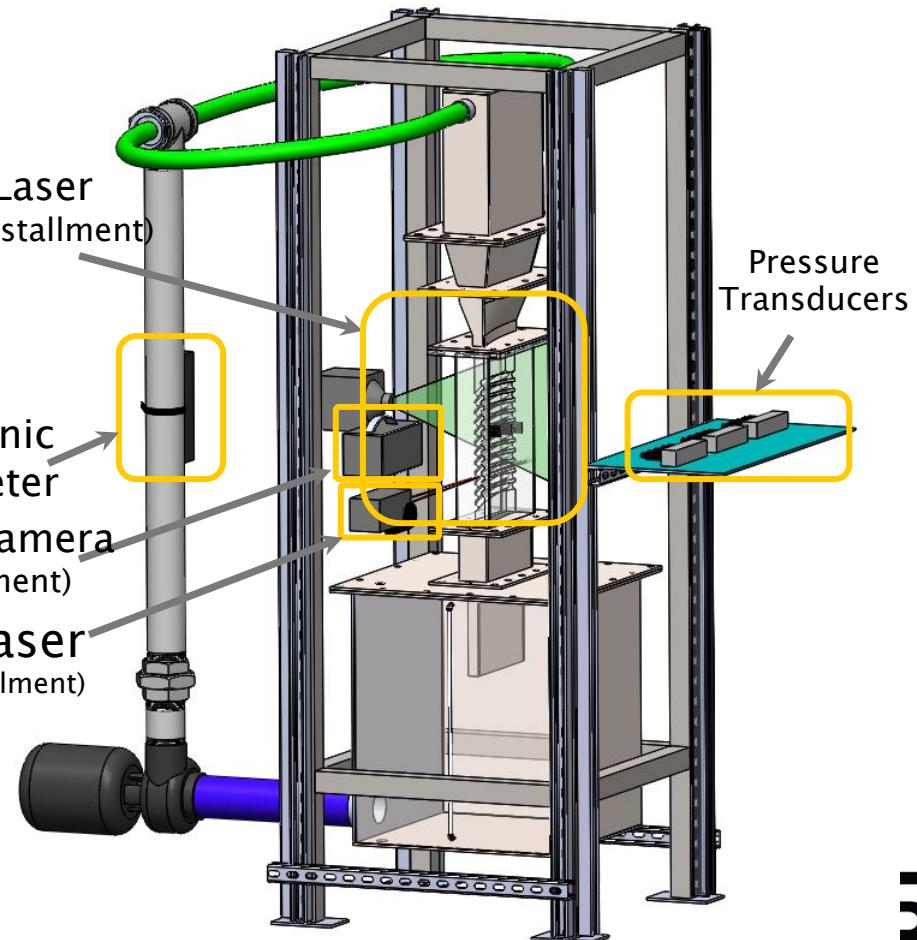
High Speed Camera
(under installment)

LDV Laser
(under installment)

PIV Laser
(under installment)

Ultrasonic
Flowmeter

Pressure
Transducers



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.

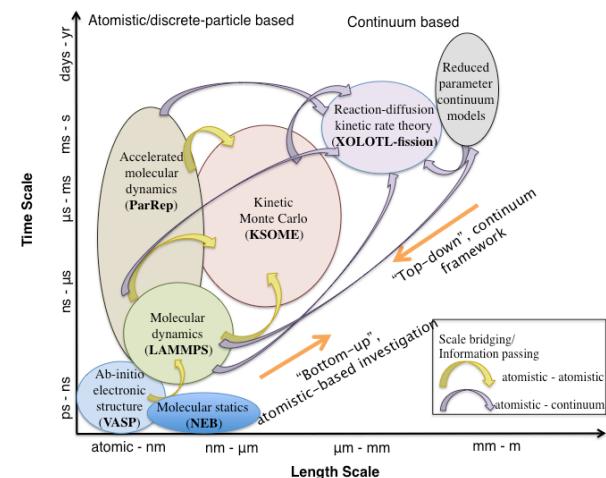
Regular information exchanges will ensure productive relationship.
Potential to emulate for other NEAMS program elements.

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.



Exciting science directed at applied problems

nature COMMUNICATIONS

ARTICLE

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Anisotropic thermal conductivity in uranium dioxide

K. Gofryk^{1,†}, S. Du^{2,†}, C.R. Stanek³, J.C. Lashley¹, X.-Y. Liu³, R.K. Schulze¹, D.D. Byler³, K.J. McClellan³, B.P. Uberuaga³, B.L. Scott⁴ & D.A. Andersson¹

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

Nuclear Engineering and Design
An International Journal devoted to aspects of Nuclear Science Design

CrossMark

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

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

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Journal of Nuclear Materials

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Development of a multiscale thermal conductivity model for fission gas in UO₂

Michael R. Tonks ^{a,b,*}, Xiang-Yang Liu ^c, David Andersson ^c, Danielle Perez ^b, Aleksandr Chernatyntskiy ^d, Giovanni Pastore ^b, Christopher R. Stanek ^c, Richard Williamson ^b

Participation in International Activities

n IAEA Coordinated Research Projects

- FUMAC – Fuel Modeling Under Accident Conditions
- ACTOF – Analysis of Options and Exp. Examination of Fuels for Water-Cooled Reactors

n 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)

n I-NERI – U.S.-Euratom Collaboration Framework

- Code-to-code benchmarks for CFD simulations of SFR fuel assembly coolant flow

n Horizon 2020

- *Planned- Thermal-Hydraulics Simulations and Experiments for the Safety Assessment of MEtal Cooled Reactors (SESAME).*

n US-UK

- DOE-DECC Action Plan
- National Nuclear Laboratory (NNL): Fast Fuel Capability Development, LWR Validation.

n DOE-CEA Bilateral

- Cadarache collaboration on UO₂ fuel physics

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.