U.S. DEPARTMENT OF ENERGY | Nuclear Energy

An Overview of NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Nuclear Energy University Programs (NEUP)
Consolidated Innovative Nuclear Research (CINR)
Fiscal Year 2017 Annual Planning Webinar

Advanced Modeling & Simulation Office (NE-41)
Office of Science and Technology Innovation (NE-4)
U.S. Department of Energy

August 2016

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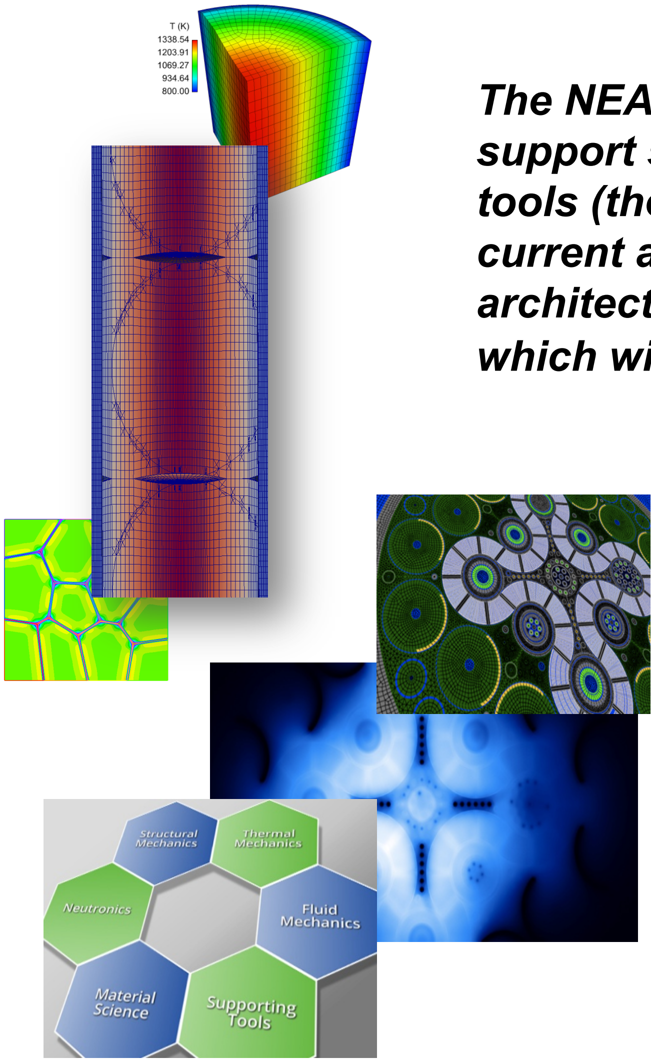
Nuclear Energy Advanced Modeling and Simulation (NEAMS)



The NEAMS Value Proposition: Develop, apply, deploy, and support state-of-the-art predictive modeling and simulation tools (the NEAMS ToolKit) for the design and analysis of current and future nuclear energy systems using computing architectures from laptops to leadership class facilities, which will –

- **Enable transformative scientific discovery and insights otherwise not attainable or affordable**
- **Accelerate both the solutions to existing problems as well as the deployment of new designs, for current and future (advanced) reactors**
- **Solve problems identified as significant by industry, and consequently expand validation, application, and long-term utility of these advanced tools**

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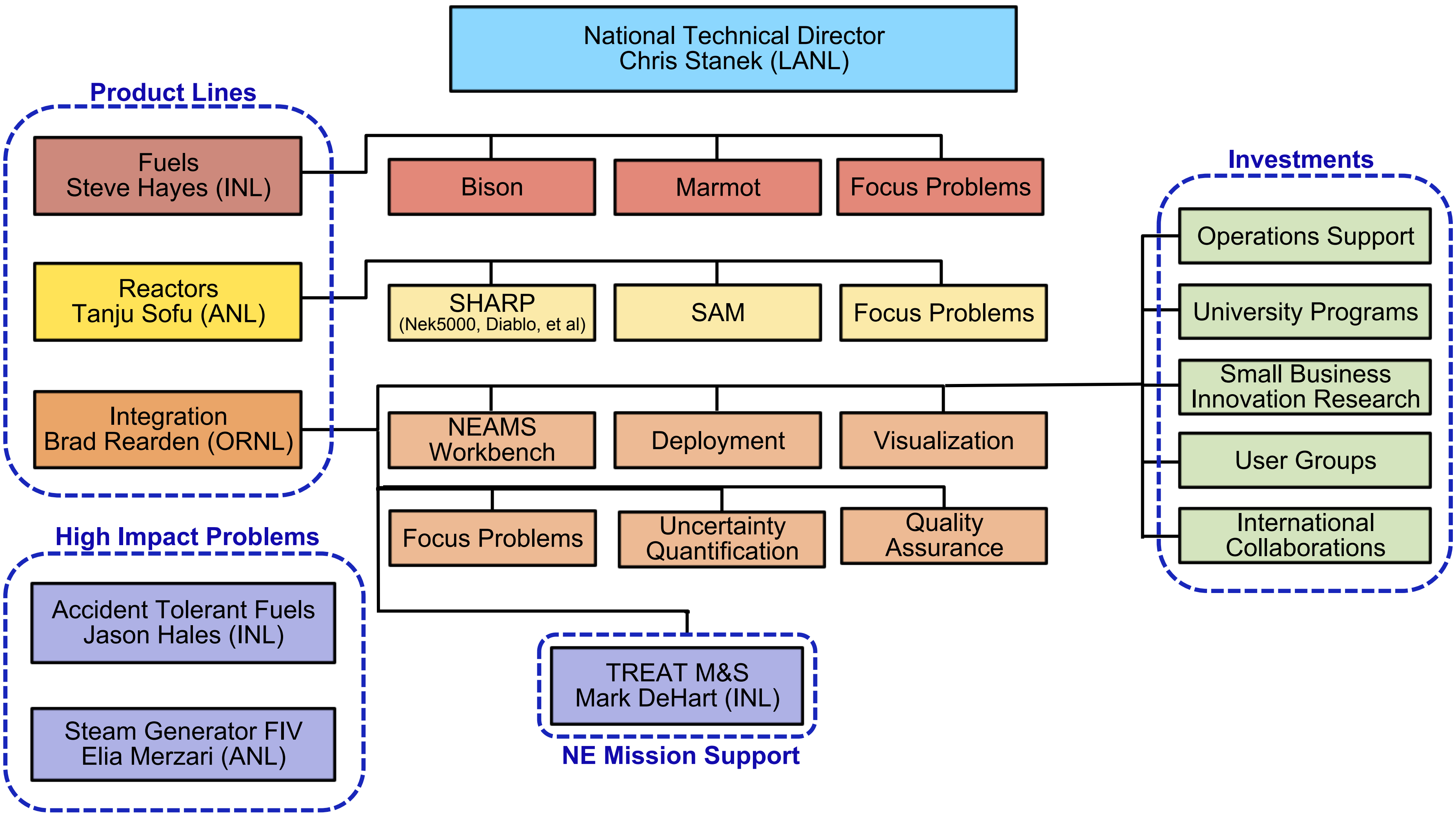
NEAMS Mission Areas



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NEAMS Organizational Structure

Leadership Council

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)

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

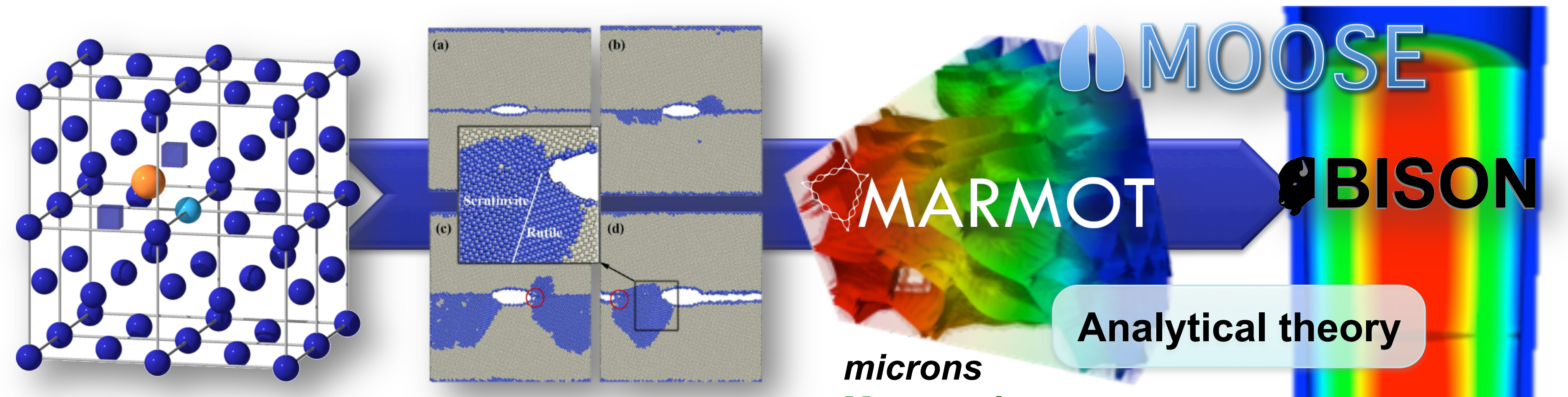
Shane Johnson
Deputy Assistant Secretary, Office of Science and Technology Innovation (NE-4)

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.

FPL

NEAMS - Fuels Product Line (FPL)

- **Atomistic simulations identify critical mechanisms and determine parameters required for mesoscale model development.**
- **Mesoscale modeling and simulation is used to inform the development of analytical theory for fuel material behavior.**



nanometers
First Principles
- Identify critical bulk mechanisms
- Determine bulk properties

100's of nanometers
Molecular Dynamics
- Identify interfacial mechanisms
- Determine interfacial properties

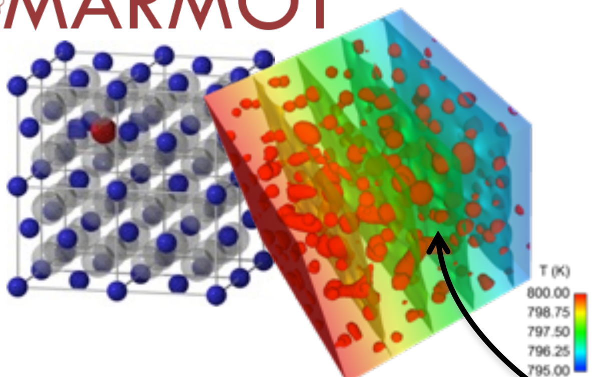
microns
Mesoscale
- Predict microstructure evolution
- Determine impact on properties

millimeters and up
Engineering scale
- Use analytical theory
- Predict fuel performance

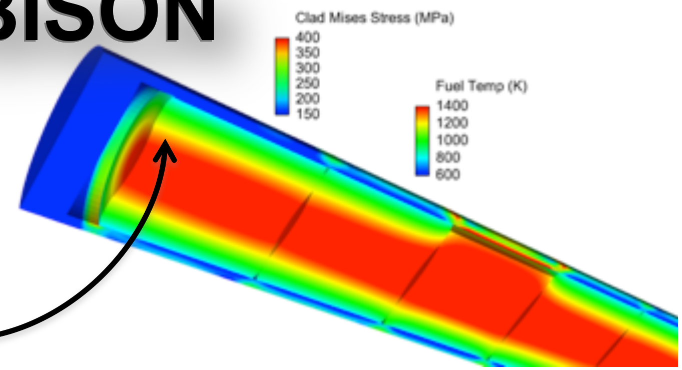
NEAMS - MOOSE-BISON-MARMOT

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

MARMOT



BISON



Mesoscale Material Model Development Tool

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

MOOSE

Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

Engineering-scale Fuel Performance Tool

- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations

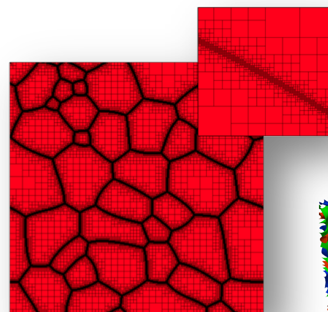
R&D 100 2014 Winner

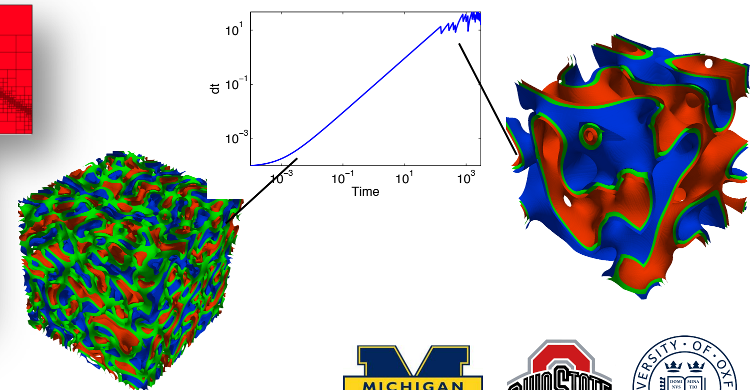
NEAMS – MARMOT

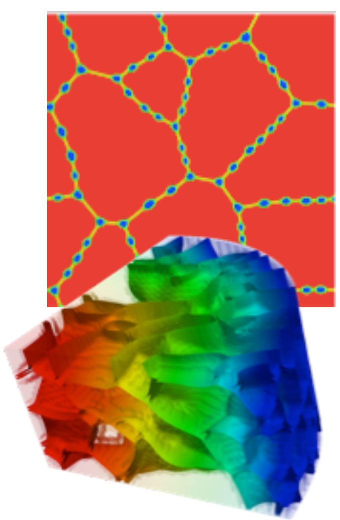
- **MARMOT predicts coevolution of microstructure and physical properties in fuel and cladding materials due to applied load, temperature, and radiation damage**

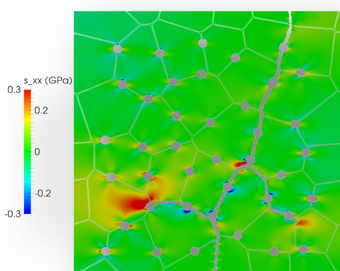
All models implemented in MARMOT are:

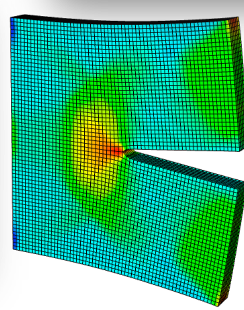
- 1D, 2D or 3D
- Massively parallel, from 1 to 1000's of processors
- Able to employ mesh and time step adaptivity

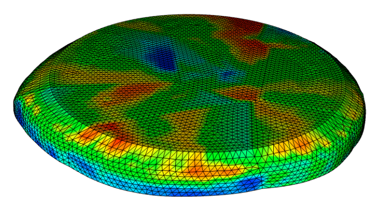












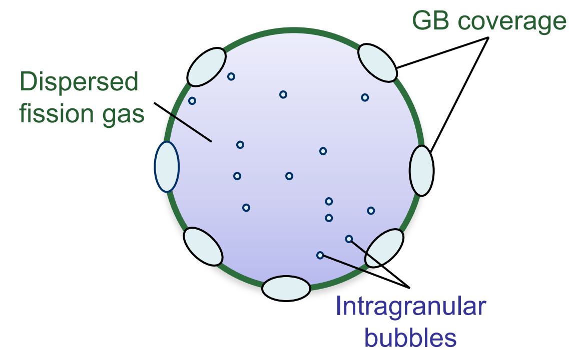
Physical models include:

- UO_2 (grain growth, fission gas release, fracture)
- U-Zr (species transport, phase change, swelling)
- U-Si (fission gas transport and swelling)
- Zircaloy cladding (hydride formation)
- FeCr (microstructure evolution)

MICHIGAN
OHIO STATE
UNIVERSITY OF OXFORD
BYU IDAHO
Massachusetts Institute of Technology
Argonne NATIONAL LABORATORY
Los Alamos NATIONAL LABORATORY EST. 1943
PennState
THE UNIVERSITY of WISCONSIN MADISON
WASHINGTON STATE UNIVERSITY
Pacific Northwest NATIONAL LABORATORY
PURDUE UNIVERSITY

NEAMS – Atomistic to Meso-scale

- **Example: Various methods are employed at different scales to investigate the different stages of Fission Gas (FG) release:**
  - Diffusion of individual FG atoms in bulk UO_2
  - Resolution of intragranular bubbles.
  - Xe segregation, clustering and bubble nucleation
  - Bubble growth and coalescence
  - Percolation in polycrystalline networks

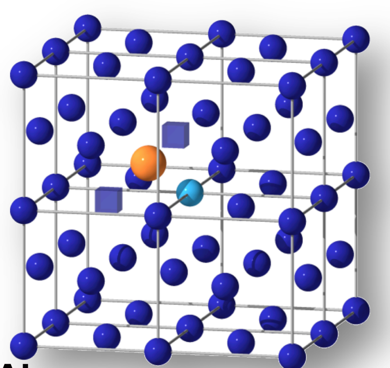


Xe Segregation to GBs

- MD simulations were employed to determine the *segregation energy* of Xe to different GB types.
- These results were used with a mechanistic model of Xe diffusion to predict the impact of GB character on gas transport in MARMOT.

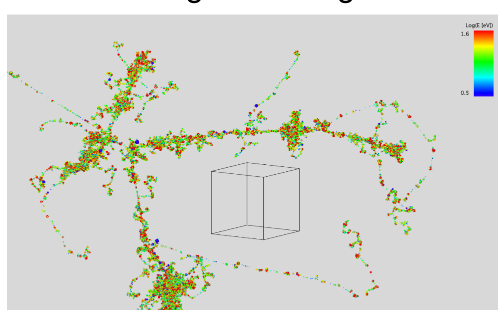
Atomistic simulations of diffusion

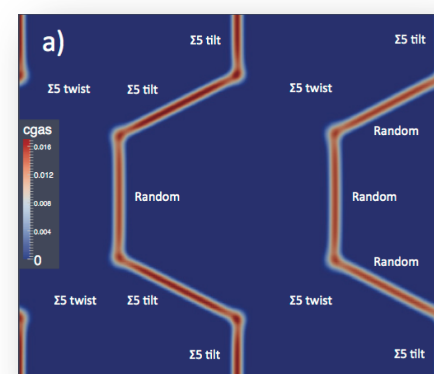
- DFT and MD calculations identified mechanisms and diffusivities for intrinsic and radiation-assisted FG diffusion.



Fission gas re-solution

- Binary collision Monte Carlo simulations were used to investigate homogeneous re-solution.





NEAMS – NEUP/CINR
Work-scope Description

- **Mission Support in NEET/NSUF – NSUF-1.3c; requests are sought for innovative, separate effects irradiation tests of nuclear fuels and/or materials that would provide data important to informing and validating mechanistic, microstructure-based models of fuel behavior under development using MARMOT, the NEAMS tool for simulating microstructure evolution under irradiation**
  - MARMOT models under active development are summarized under NEAMS 1.1 and in the MARMOT Assessment Report
  - Fuel systems of interest for which separate effects experiments are desired are:
    - The LWR fuel system (*i.e.*, both the historic UO2 fuel and Zirconium-based cladding, as well as emerging Accident Tolerant Fuel concepts)
    - The SFR fuel system (*i.e.*, U-Zr and U-Pu-Zr metallic fuel and steel-based cladding)