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Nuclear Energy University Programs (NEUP) Fiscal Year (FY) 2013 Annual Planning Webinar

Nuclear Energy Advanced Modeling and Simulation (NEAMS) Program

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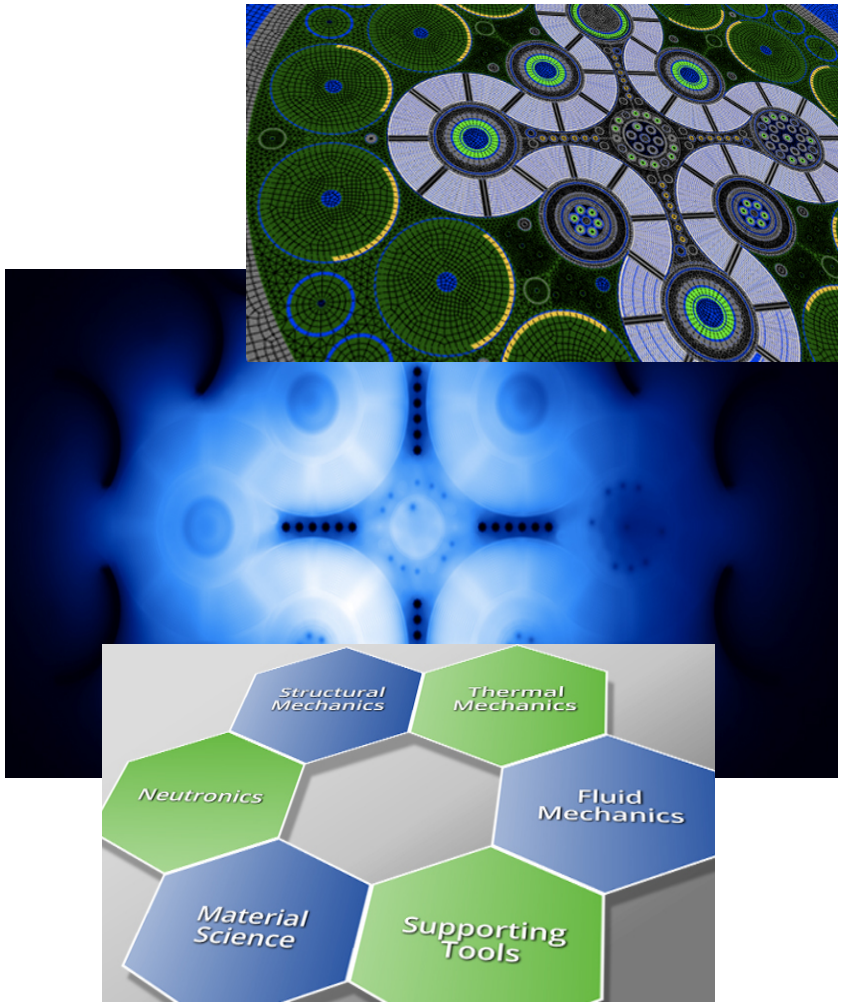
NEAMS Overview –
Benefits of an Advanced Modeling and Simulation Program

- Provides the ability to gain new insights about the performance and safety of nuclear energy technologies
- Works in partnership with theory and experiment to enhance NE R&D
- Develops simulation toolsets for use by R&D community and industry to impact design and analysis of future reactors



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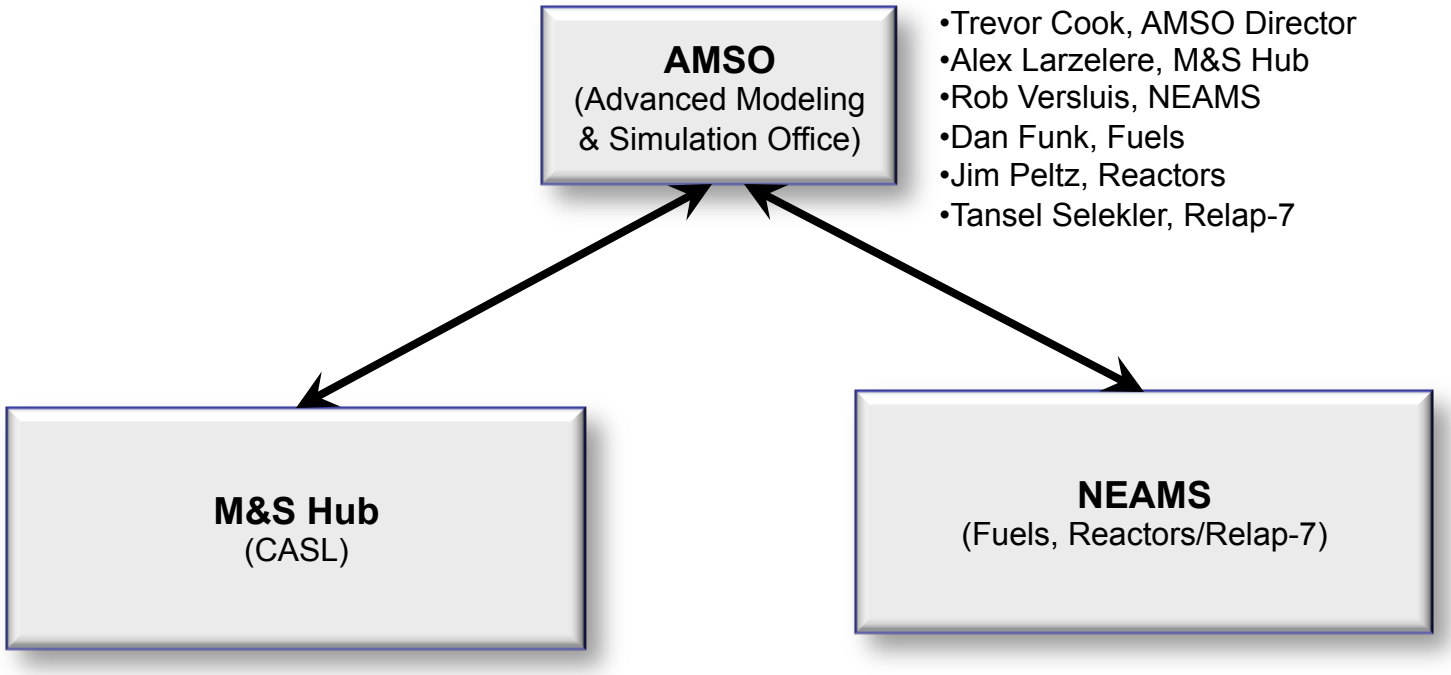
NEAMS Overview –
How Does NEAMS fit into NE, AMSO?

- **AMSO (Trevor Cook, NE-41) is under the Deputy Assistant Secretary for Science & Technology Innovation, (Shane Johnson, NE-4)**
- **NEAMS is a program within AMSO**



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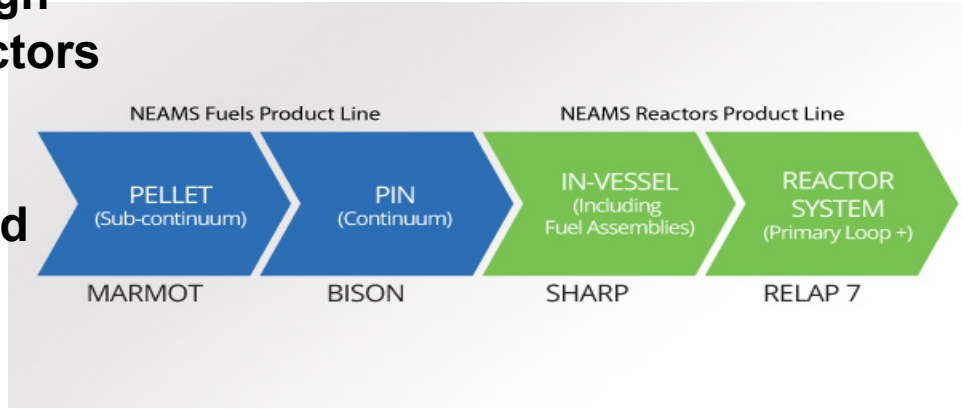
NEAMS Overview –
Management and Technical Structure; "NEAMS Toolkit"

NEAMS
(Two Product Lines: Fuels and Reactors)
- NTD – **Keith Bradley**, ANL
- FUELS – **Steve Hayes**, INL
- REACTORS – **Dave Pointer**, ANL

- **Focused on advanced simulation capabilities for performance of advanced reactors and fuels**
- **Developing a comprehensive "pellet-to-plant" simulation toolkit through two product lines: Fuels and Reactors**
- **Part of the NE approach to implementation of a science-based approach to performing nuclear energy R&D**



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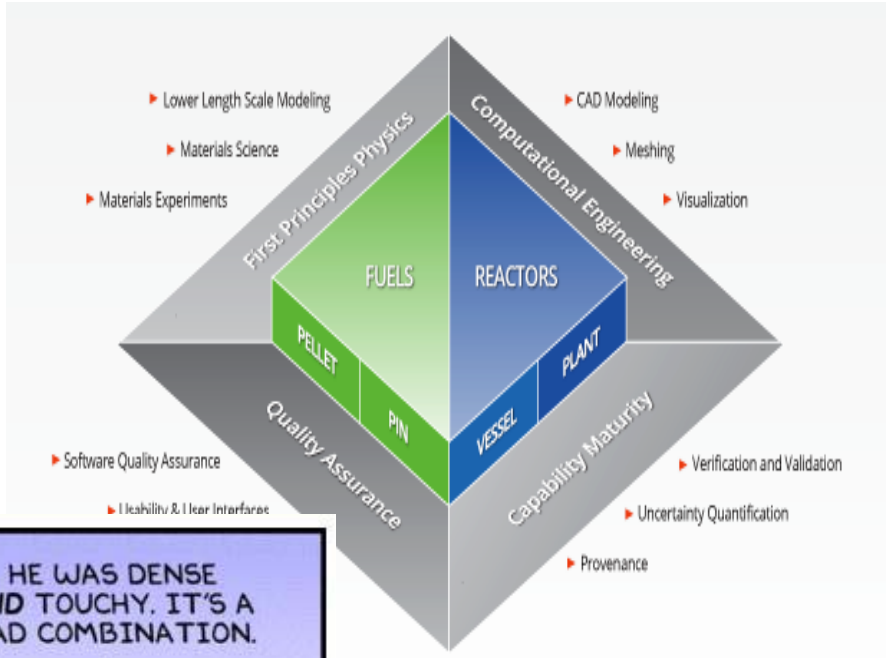
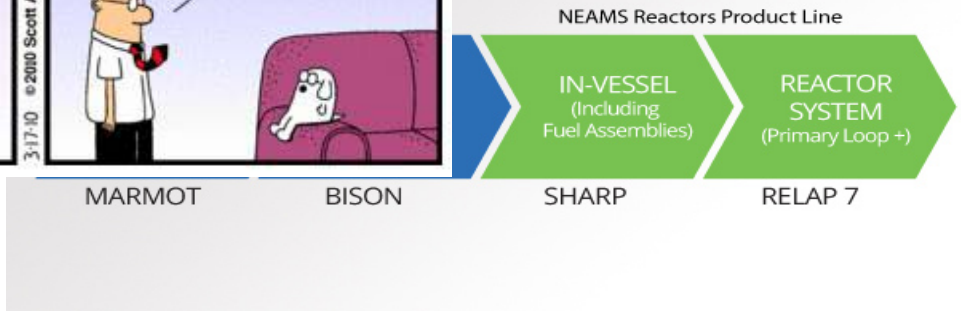


- **Technical vs Program Perspective**
  - **One key challenge: how to integrate them**



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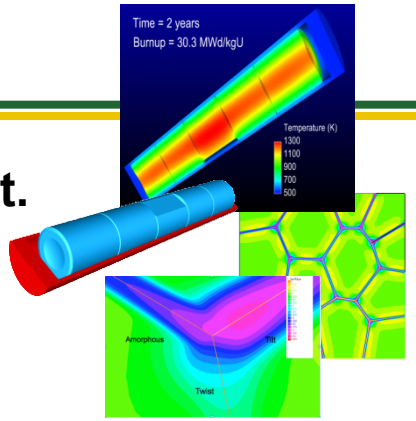
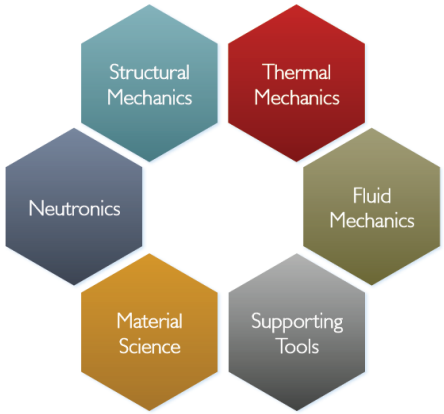
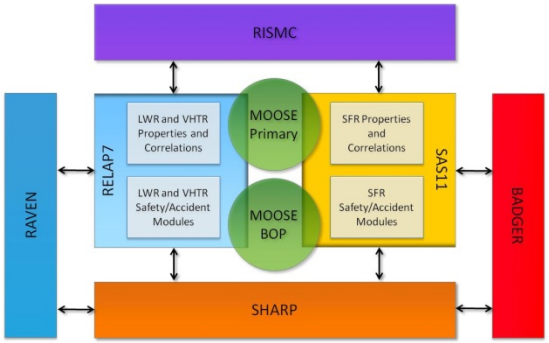
NEAMS Overview –
Product Lines



- **Fuels Product Line**: Support advanced fuels development. Extend functionality of FRAPCON/FRAPTRAN with mechanistic behavior models, modern computational technology and up-to-date computer hardware

- **Reactors Product Line:** Support advanced reactors development. Provide a 3D, high-fidelity, coupled-physics simulation capability for advanced reactors (non-LWRs). Also support Relap-7 development to address plant safety and analysis issues by combining modern computational methods and the latest thermal hydraulic and reactor physics models to extend RELAP 5





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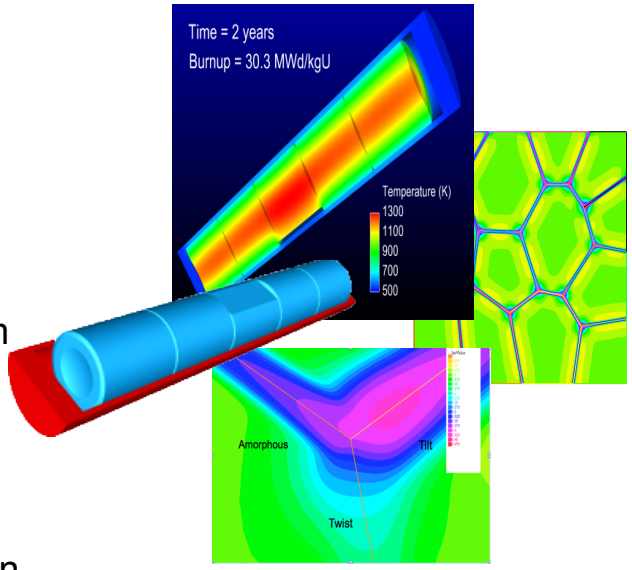
NEAMS Overview–
Fuels Product Line

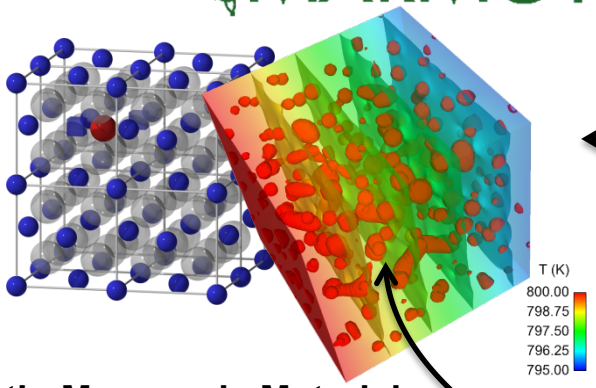


- **Goal is to be able to apply the FPL Toolset (in the NEAMS Toolkit) to several Fuels R&D areas**
  - Advanced fuel designs
  - Accident-tolerant fuels research
  - Could be extended to simulate behavior of used fuel in long term storage
- **Focus is to develop mechanistic (truly predictive) computational capabilities**
  - *Near-term emphasis*: oxide fuels for LWR applications; irradiation performance in quasi-steady state, operational transients, accident scenarios; assessment vs. FRAPCON, FRAPTRAN, FUMEX-III experimental databases; integration at assembly-scale with RPL toolset
  - *Longer-term emphasis*: metallic fuels for SFR applications; irradiation performance in steady-state and transient scenarios; assessment in conjunction with EBR-II & FFTF experimental data; full coupling at assembly-scale with RPL toolset

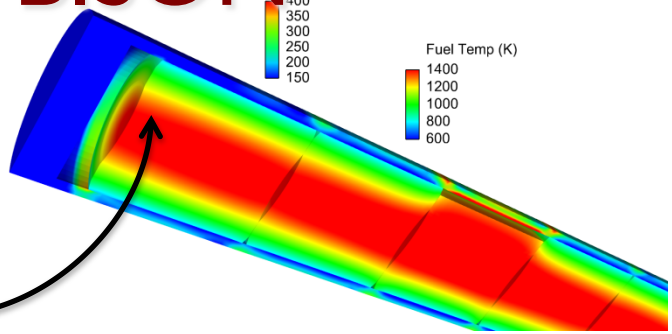
NEAMS Overview–
What is the Fuels Product Line Toolset?

- **FPL Toolset: MOOSE-BISON-MARMOT (advanced, multiscale fuel performance capability)**

MARMOT



BISON



Atomistic-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

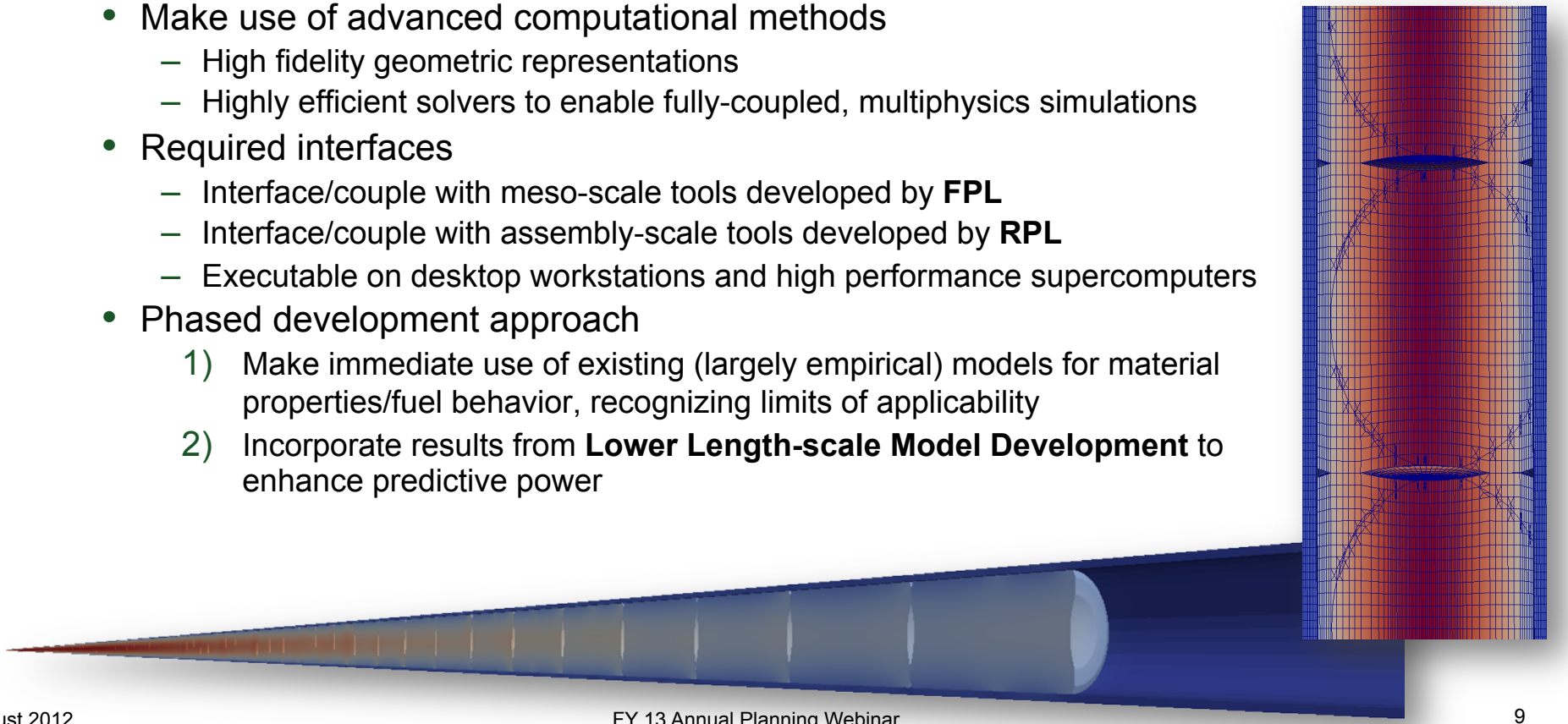
Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

NEAMS Overview–
Fuels Product Line Toolset (BISON)

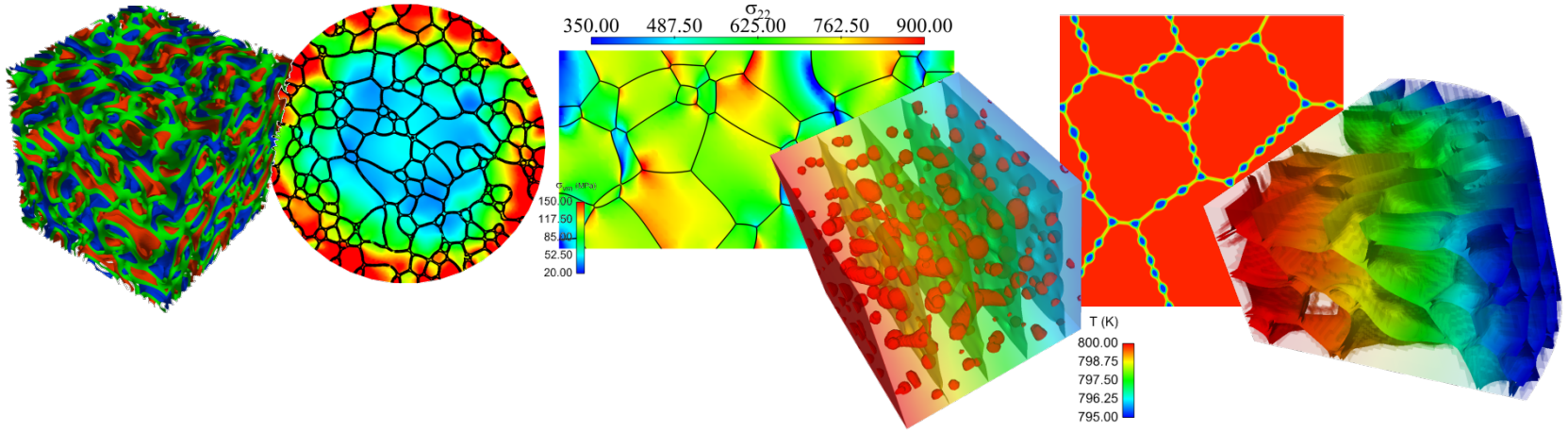
- **BISON - predicting fuel performance at the engineering scale**
  (*e.g.*, pellet-resolved fuel pins)

  - Applicable to normal, off-normal, accident conditions
  - Make use of advanced computational methods
    - High fidelity geometric representations
    - Highly efficient solvers to enable fully-coupled, multiphysics simulations
  - Required interfaces
    - Interface/couple with meso-scale tools developed by **FPL**
    - Interface/couple with assembly-scale tools developed by **RPL**
    - Executable on desktop workstations and high performance supercomputers
  - Phased development approach
    1) Make immediate use of existing (largely empirical) models for material properties/fuel behavior, recognizing limits of applicability
    2) Incorporate results from **Lower Length-scale Model Development** to enhance predictive power



NEAMS Overview–
Fuels Product Line Toolset (MARMOT)

- **MARMOT (Lower Length-scale) - simulating meso-scale, microstructure evolution under irradiation**
  - **Atomic-scale simulations** to enable meso-scale modeling
  - Tools to be used to
    - Develop fundamental material property/fuel behavior models
    - Up-scale to inform fuel performance simulations at engineering-scale
  - Reduce dependence on empirical correlations/models
  - Enable true predictability in compositional or operational regimes where little or no experimental data exists.



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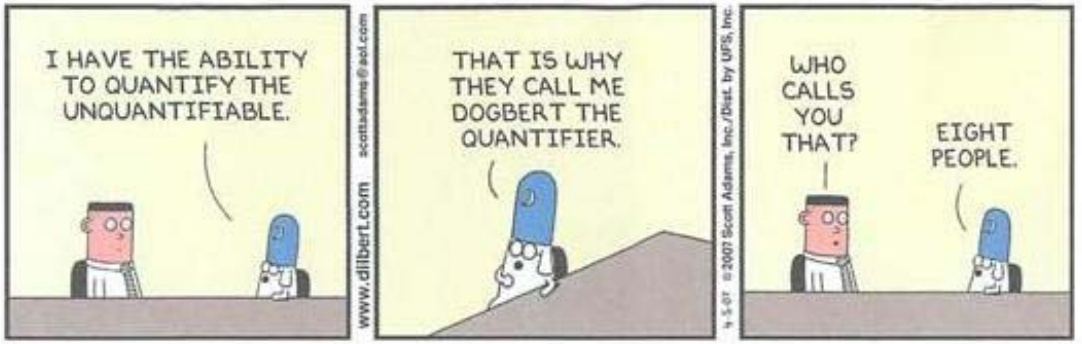
NEAMS Challenges & Needs

- **Validation**
- **Uncertainty Quantification**
- **Early Users**



- **Crucial questions:**
  - How should we design experiments to produce validation data (diagnostics, procedures)?
  - How do we deal with UQ (both models and experiments)?
  - How do we accumulate a portfolio of evidence that allows an objective observer the opportunity to trust (or not trust) a simulation result?
  - What do we mean by high fidelity experimental validation data? How do we obtain it and confirm its usefulness?
    - 3D/Higher spatial and temporal resolution (*e.g.*, fuel microstructure evolution under irradiation)
    - Inclusion of separate effects, to the extent possible
    - Good definition of initial/boundary conditions for input to simulations

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NEAMS Workscope Description

- **NEAMS 1.1-Validation Methodologies**
  - Develop and demonstrate validation methodologies to support the Fuels Product Line at engineering and/or meso-scales (*i.e.*, resolved microstructure)
    - Including but not limited to experiments; ways to design and conduct experiments (*e.g.*, could deliver a project product that is a diagnostic or a procedure, rather than simply data)
    - May include separate effects experiments that explore mechanical, thermal and chemical interactions of relevant fuel microstructures in an unirradiated, ion-irradiated or neutron irradiated environment
- **NEAMS 1.2-Validation Assessment Studies**
  - Assess the engineering scale tool (**BISON**) against experimental data for PWR fuel pins in the existing FRAPCON, FRAPTRAN, and FUMEX-III experimental databases
    - Both deficiencies in irradiation performance models as well as gaps in the experimental databases should be identified in these studies