Nuclear Energy University Programs

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Materials: NEAMS Perspective

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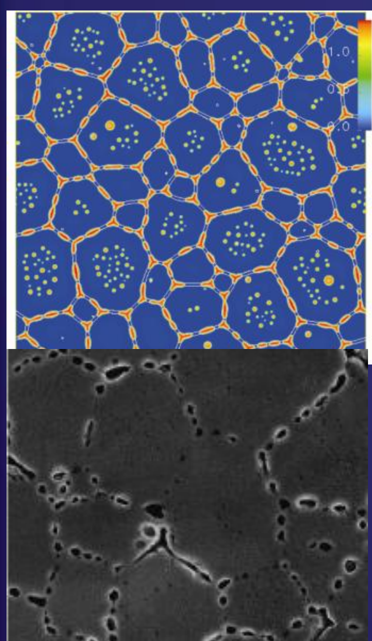

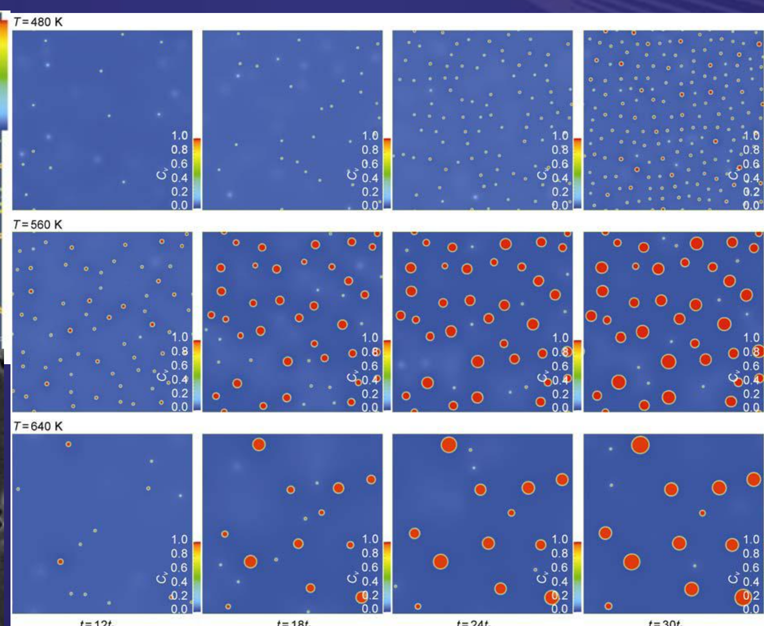

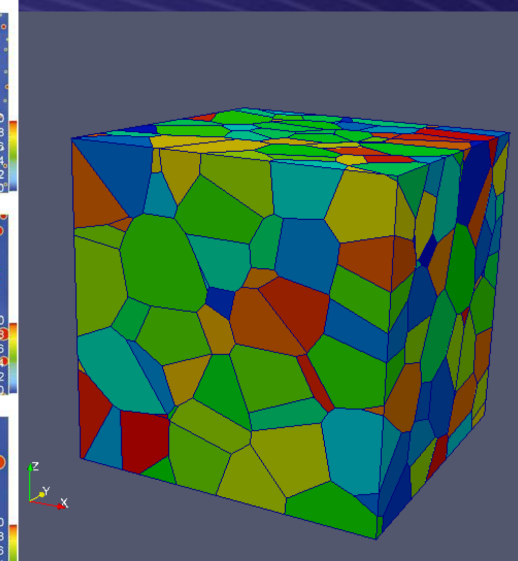

Overview

- NEET and NEAMS
- Overview of NEAMS
- Fundamental methods and models on materials are a supporting element
- FY12 NEUP Scope from NEAMS
- Expectations and Deliverables

Funding and Programmatic Overview

- Nuclear Energy Enabling Technologies (NEET)
  - Crosscutting Technologies
    - Modeling and Simulation
- Nuclear Energy Advanced Modeling and Simulation (NEAMS)
  - Supporting Elements
    - Fundamental Methods and Models (FMM)
- In FY 2012 NEAMS will be supported by NEET

Purpose of NEAMS

Produce and deliver computational tools to designers & analysts that *predict behavior* in relevant operating regimes, particularly beyond the test base.

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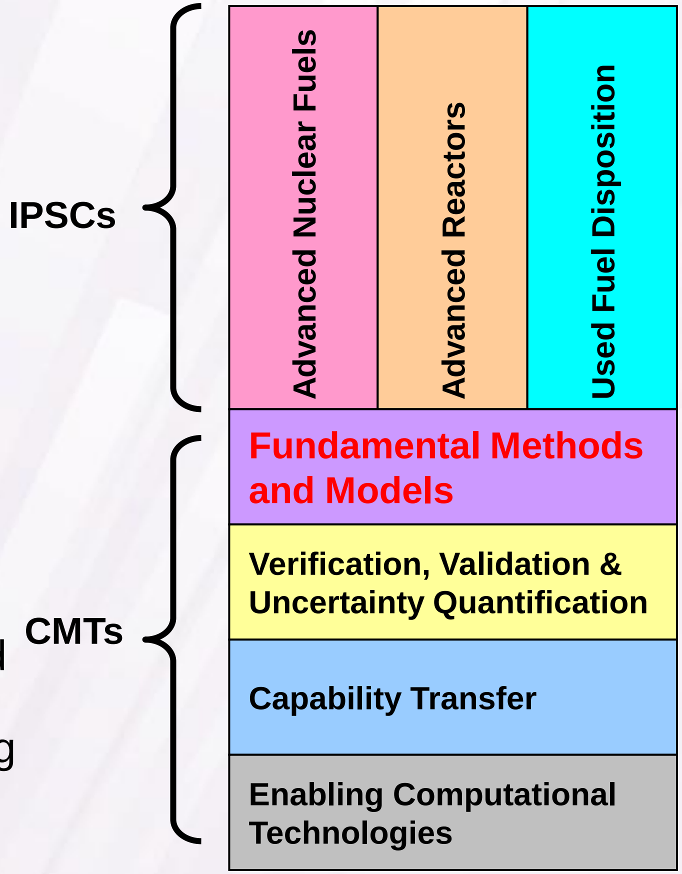
NEAMS Program Elements

- **Integrated Performance and Safety Codes**
  - Continuum level codes that will **predict** the **performance** and **safety** of nuclear energy systems technologies
  - Attributes include 3D, science based physics, high resolution, integrated systems
  - Long-term development horizon (~10 years)
  - Codes with verification, validation and error uncertainty quantification
  - Using interoperability frameworks and modern software development techniques and tools
- **Crosscutting Methods and Tools**
  - Develop crosscutting (i.e. more than one IPSC) required capabilities
  - Provide a single NEAMS point of contact for crosscutting requirements (e.g. experimental data, computer technologies)
  - Smaller, more diverse teams to include laboratories, universities and industries.
  - "Tool Development" with shorter timelines



Roles of Fundamental Methods and Models (FMM)

- Develop crosscutting models and methods for lower length scale materials performance needed to support IPSCs
  - This includes material modeling at the molecular or quantum scale
  - Also includes methods required for upscaling behaviors at the continuum scale
- Provide a single NEAMS point of contact for separate effects experiments needed to validate models
- Collect requirements from IPSCs and develop solicitations for FMM work
  - FMM funded university programs
- Coordinate relevant NE university program work to deliver capabilities to IPSC

FMM Technical Approach

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Scale bridging methodology

Structure scale

Integrated Performance and Safety Codes (IPSC) elements

Effective properties: Stress vs. strain curves, strength, ductility, fracture toughness, thermal conductivity, creep properties, thermal expansion coeff.

macroscale

Crystal plasticity, homogenization, statistical mechanics, microstructure-based finite element…

Microstructure; Microstructure evolution kinetics; Relationship between microstructure and materials property

mesoscale

Phase field, rate theory, kMC, DDD,…

microscale

First principle, MD, DD, kMC…

Thermodynamic and kinetic data, rate of defect generation, defect-defect interaction, inside grain diffusivity and at grain boundary …

Work Plans for FY12

- Hierarchical models and upscaling methodologies for material property prediction under irradiation
  - Statistical model for microstructure reconstruction
  - Accurate and computationally efficient upscaling methodologies
  - Hierarchical multi-scale model development for material property evolution under irradiation
- Development of quantitative phase field framework for mesoscale microstructure evolution prediction
  - Formulation of quantitative phase field models
  - Scalable parallel finite element implementation of the quantitative phase field models
  - Developing methods to link atomistic to continuum diffusion- inputs to the quantitative phase field model
- Development of Potts and KMC based mesoscale models for microstructural evolution
  - Potts model for fission gas migration and sintering
  - Hybrid Potts kMC-phase field model development

FY12 NEUP Scope on Materials

- Predictive Models for Material Degradation at Different Scales:
  - Development of atomistic level chemical kinetics parameters
  - Development of meso-scale methodologies to predict microstructural and chemical evolution kinetics
  - Prediction of continuum level thermal mechanical properties

- Small-Scale Separate Effects Experiments for Model Validation

- Methodology Development for Scale Bridging

Expectations and Deliverables

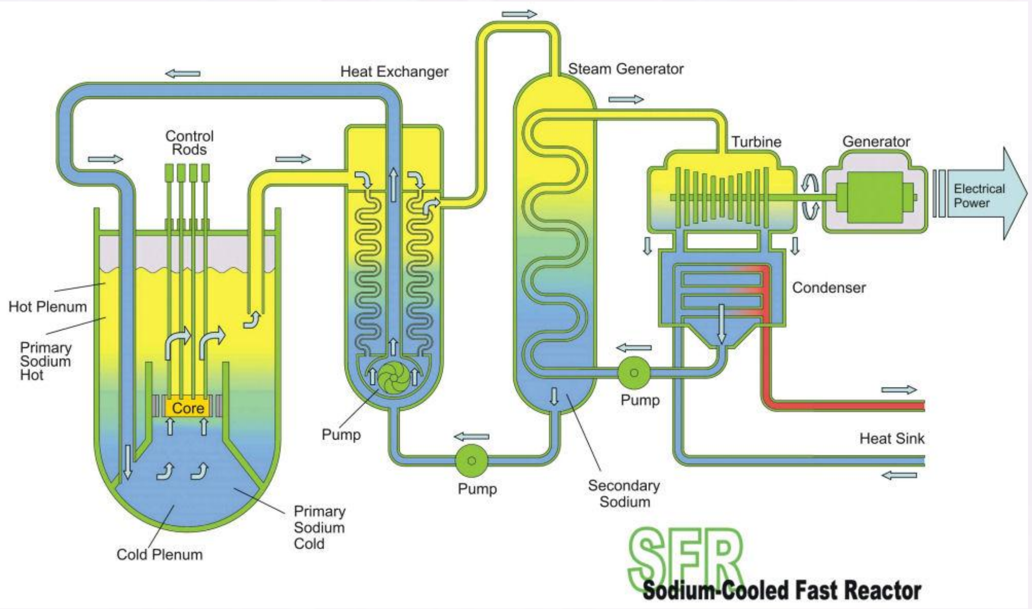
- **Mission-driven expectations**
  - 20% relevance
  - 80% technical

- **Deliverables clearly tied to IPSCs/Campaigns and identified in proposals**
  - Specific
  - Measurable
  - Achievable
  - Realistic
  - Time-bound

- **Performance feedback**

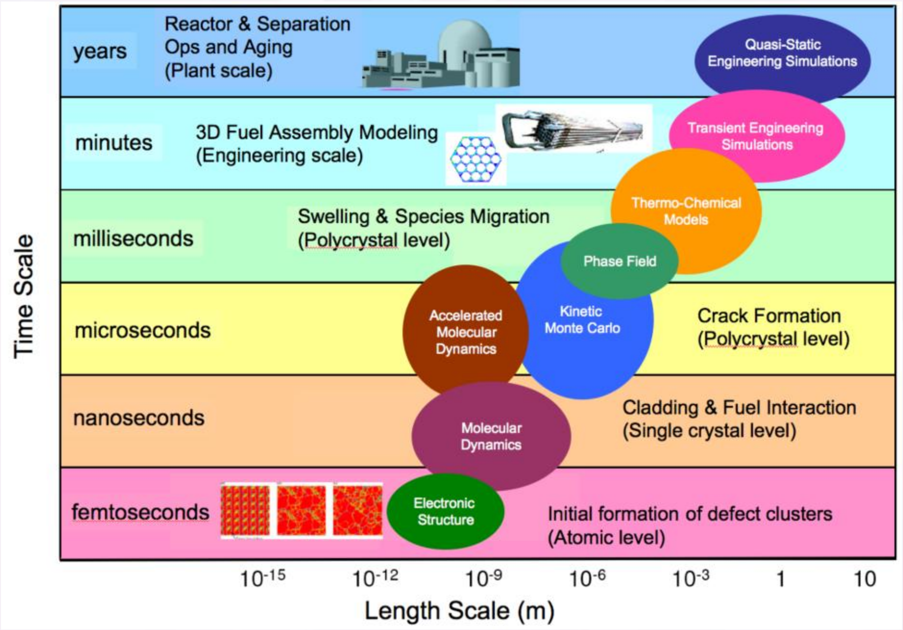
Backup Slides

Reactor IPSC



- **Scope**
  - Predict performance and safety of fast reactors over 40 – 60 year lifetime
  - Initial focus on reactor core
  - As code progresses will extend to additional systems
  - Many underlying physical processes (e.g. thermodynamics, neutronics) extensible to other reactor types (gas-cooled, light water)

Nuclear Fuels IPSC



- **Scope**
  - Develop a coupled, predictive three-dimensional, predictive computational tool to predict the performance of nuclear fuel pins and assemblies, applicable to both existing and future advanced nuclear reactor fuel design, fabrication
  - Develop a multi-scale multi-physics framework with appropriate scale bridging techniques
  - Develop atomistically informed, predictive meso-scale microstructure evolution model that can be bridged to the engineering scale
  - Develop with flexibility to extend to nuclear fuels for other reactor types (gas, light water)