NEUP Nuclear Energy University Programs
U.S. Department of Energy

July 27-28, 2010

FY2011
NEUP Workshop
Separations, Waste Forms and Used Fuel Disposition:

NEAMS Perspective

Rockville, Maryland

Overview

- **NEET and NEAMS**
- **Overview of NEAMS**
- **Two IPSCs:**
  - **Waste Form**
  - **Safeguard and Separations**
- **FY11 NEUP Scope from NEAMS**
- **Expectations and Deliverables**

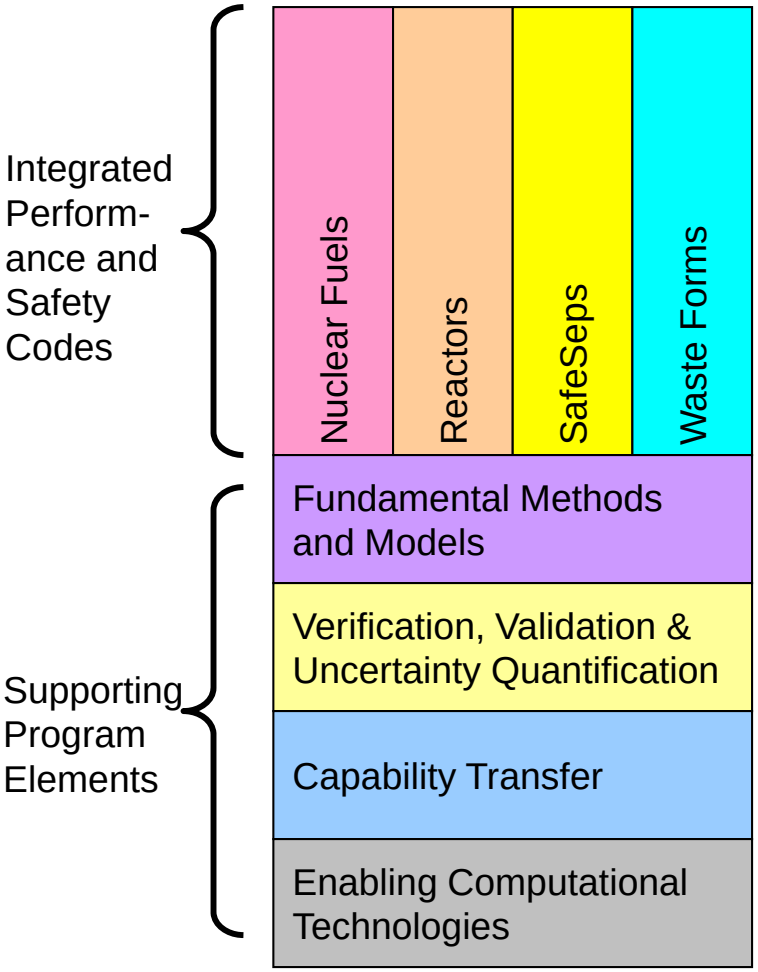
Funding and Programmatic Overview

- **Nuclear Energy Enabling Technologies (NEET)**
  - Crosscutting Technologies
    - Modeling and Simulation
- **Nuclear Energy Advanced Modeling and Simulation (NEAMS)**
  - Waste form
  - Safeguard and Separations

Purpose of NEAMS

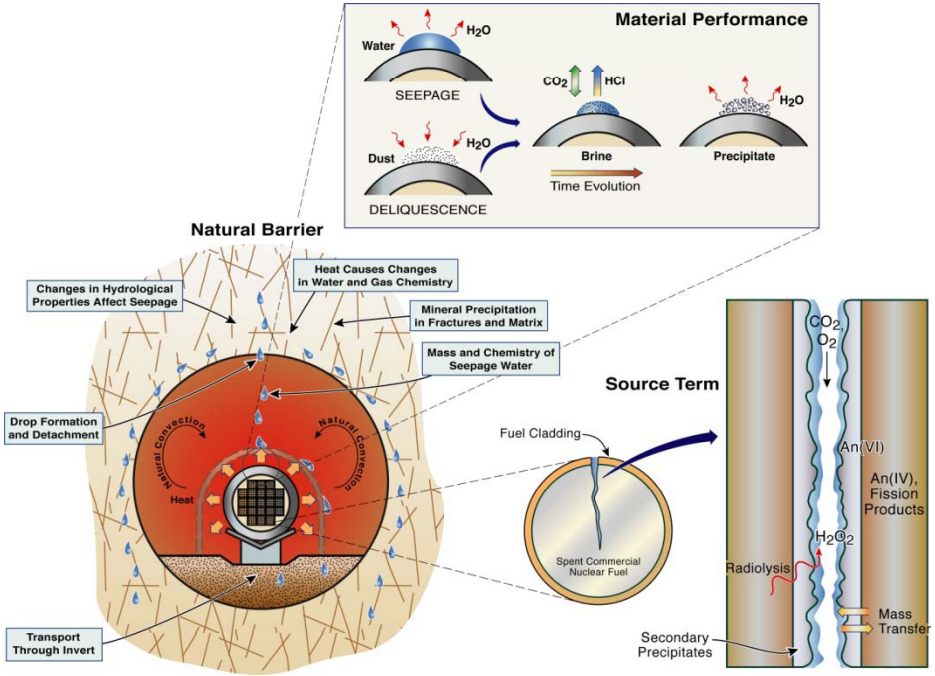
Produce and deliver computational tools to designers & analysts that *predict behavior* in relevant operating regimes, particularly beyond the test base.

NEAMS Program Elements



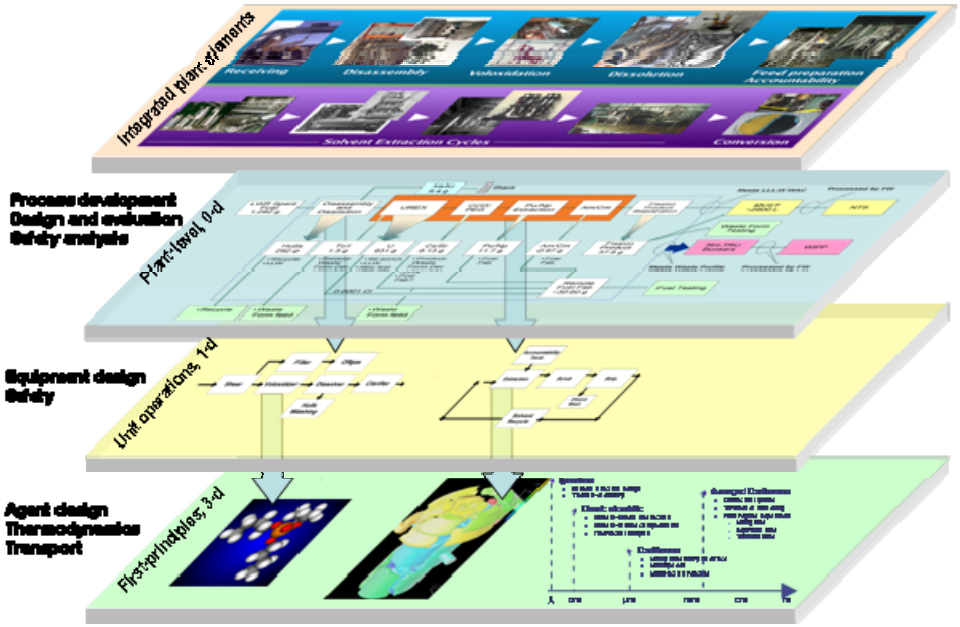
- **Integrated Performance** and **Safety Codes (IPSC)**
  - –Continuum level codes that will **predict** the **performance** and **safety** of nuclear energy systems technologies
  - –Attributes include 3D, science based physics, high resolution, integrated systems
  - –Long-term commitment (~10 years)
  - –Codes with verification, validation and uncertainty quantification
  - –Using interoperability frameworks and modern software development techniques and tools
- Supporting Elements
  - –Develop crosscutting (i.e. more than one IPSC) required capabilities
    - ▪Fundamental Methods and Models
    - ▪Verification, Validation and Uncertainty Quantification
    - ▪Interoperability frameworks
    - ▪Enabling Computational Technologies
  - –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.
  - –Shorter timelines

Waste Form IPSC



- Scope
  - Predict the performance of waste forms under repository conditions for their expected lifetimes (potentially up to a million years)
  - Currently scope is limited to near-field repository conditions, but could be extended if needed
  - Similar to the multi-scale, multi-physics approach used for the Nuclear Fuels IPSC
  - Develop suite of modeling tools to predict microscale behaviors and couple them through the meso scale to the continuum
  - Develop with flexibility to extend to different waste types in different repository environments

Safeguard & Separations IPSC



- Scope
  - Provide coupled performance of safeguards and separation systems
  - Allow the implementation of “safeguards by design” to separation systems
  - Understand performance and safety of separation processes at the molecular and plant scale levels
  - Use plant scale models to provide overall integration of both separations and safeguard processes
  - “Drill-down” to increasing levels of detail where needed to understand performance of critical systems
  - Includes devices used for separations as well as safeguard diagnostics

FY11 NEUP Scope on Waste Form

- **Modeling of radiation and thermal effects on waste forms.**
- **Development of robust, accurate, and validated methods for modeling the chemistry and transport of actinide species at a sub-continuum scale.**
- **Waste form design and assessment.**
- **Waste form corrosion and dissolution.**
- **Waste form corrosion validation experiments.**

FY11 NEUP Scope on Waste Form – cont'd

- **Near-field chemistry.**
- **Aqueous speciation and surface sorption at elevated temperatures and high-ionic strength.**
- **Geochemical transport models.**
- **Upscaling model development methods.**
- **Fidelity of predictions over geologic time scales.**

FY11 NEUP Scope on Safeguard and Separations

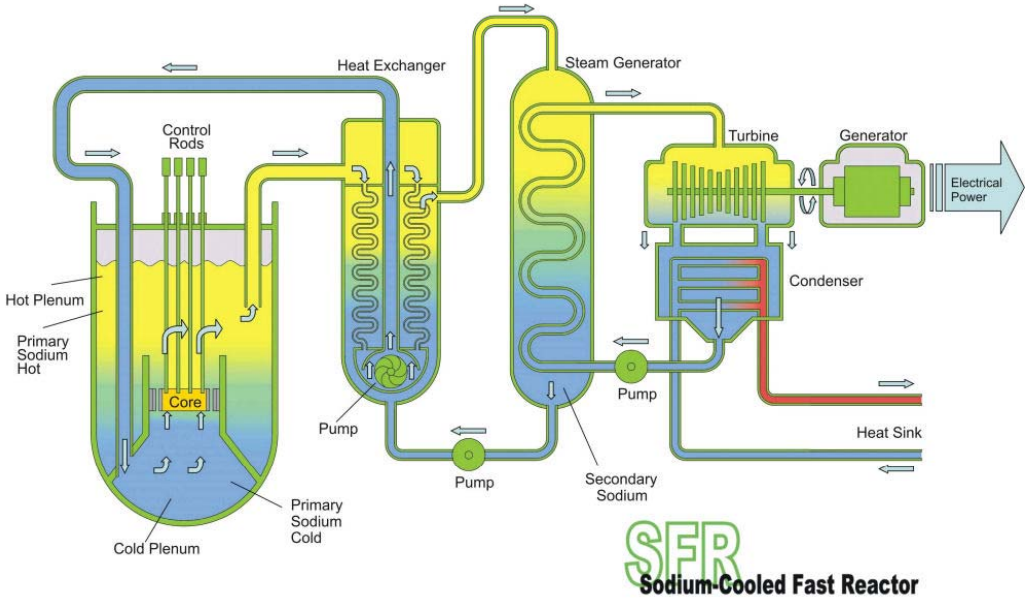
- **Interfacial electrochemistry.**
- **Validation data.**
- **Design of new chemical processes.**
- **Off-gas treatment.**

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**

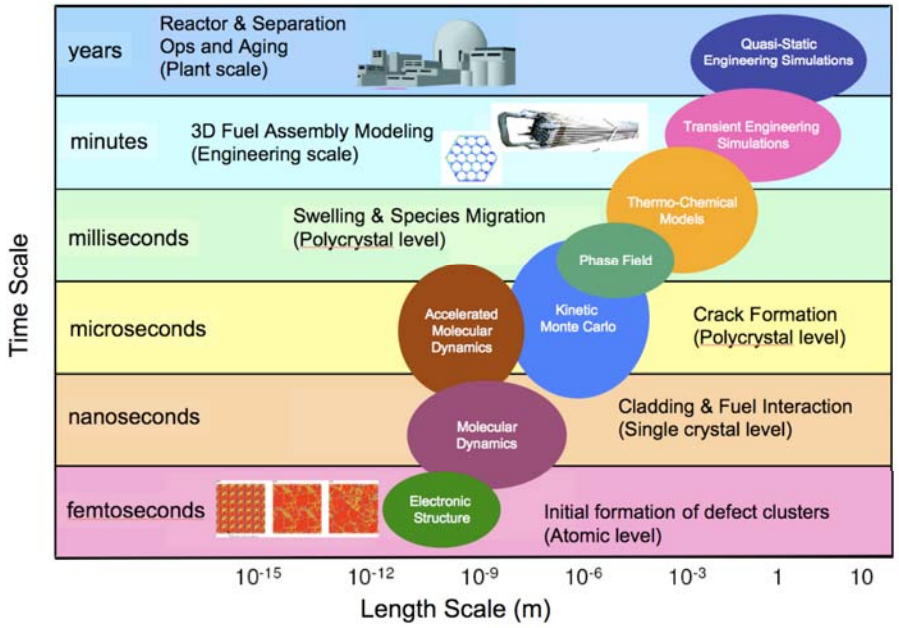
Backup Slides

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)