U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Idaho National Laboratory

Nuclear Energy Advanced Modeling and Simulation

Fuels IPSC FY-10 Overview

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Outline of Presentation

- Fuels IPSC Objectives
- Fuels MS/MP Framework and the R&D Objectives from NE Roadmap
- FY10 Budgets and Work Packages
- Progress on Program Integration
- Introduction of Technical Talks

Fuels IPSC Objective

- **The Fuels IPSC objective is to deliver a science-based (truly predictive) computational tool for nuclear fuel pin/assembly analysis and design**
  - Near term: oxide & metallic fuels, thermal & fast spectra, irradiation performance of fuel pins in the quasi-steady state
  - Longer term: additional fuel forms, irradiation performance of fuel pins and assemblies during transients, support of fuel fabrication development

- **Potential Applications**
  - Existing LWRs: better informed safety margins, better informed operational constraints, burnup extension, support life extension?
  - Advanced Reactors: design of new fuels

- **Approach:** *Multi-scale, multi-physics based fuel performance simulations in 3D*
  - Make use of theory/first principles, minimal reliance on empirical models
  - Develop atomistically-informed meso-scale models to simulate evolution of microstructure under irradiation
  - (Validate physics models vs. separate effects and integral experiments)
  - Predict fuel properties and performance at engineering scale

Fuels Challenge Problems

- **Lower Length Scale Physics**
  - Understand the thermodynamic and kinetic relationships between multi-dimensional defect structures and predict their evolution under irradiation
  - Up-scale results to inform engineering scale
- **Irradiation Performance at Engineering Scale**
  - Predict properties and integral performance of fuels under irradiation
  - Assess safety margins (including failure probabilities) with quantified uncertainties for both normal operating conditions and transients
  - Develop methodologies to optimize fuel designs/constrain reactor operations in order to minimize fuel degradation and avoid fuel failure
- **Fabrication Process Support**
  - Sintering process simulations of oxide (ceramic) fuels to predict the microstructural characteristics in order to control/optimize as-fabricated properties
  - Casting process simulations of metallic fuels to optimize melt utilization, minimize fabrication loses and waste generation

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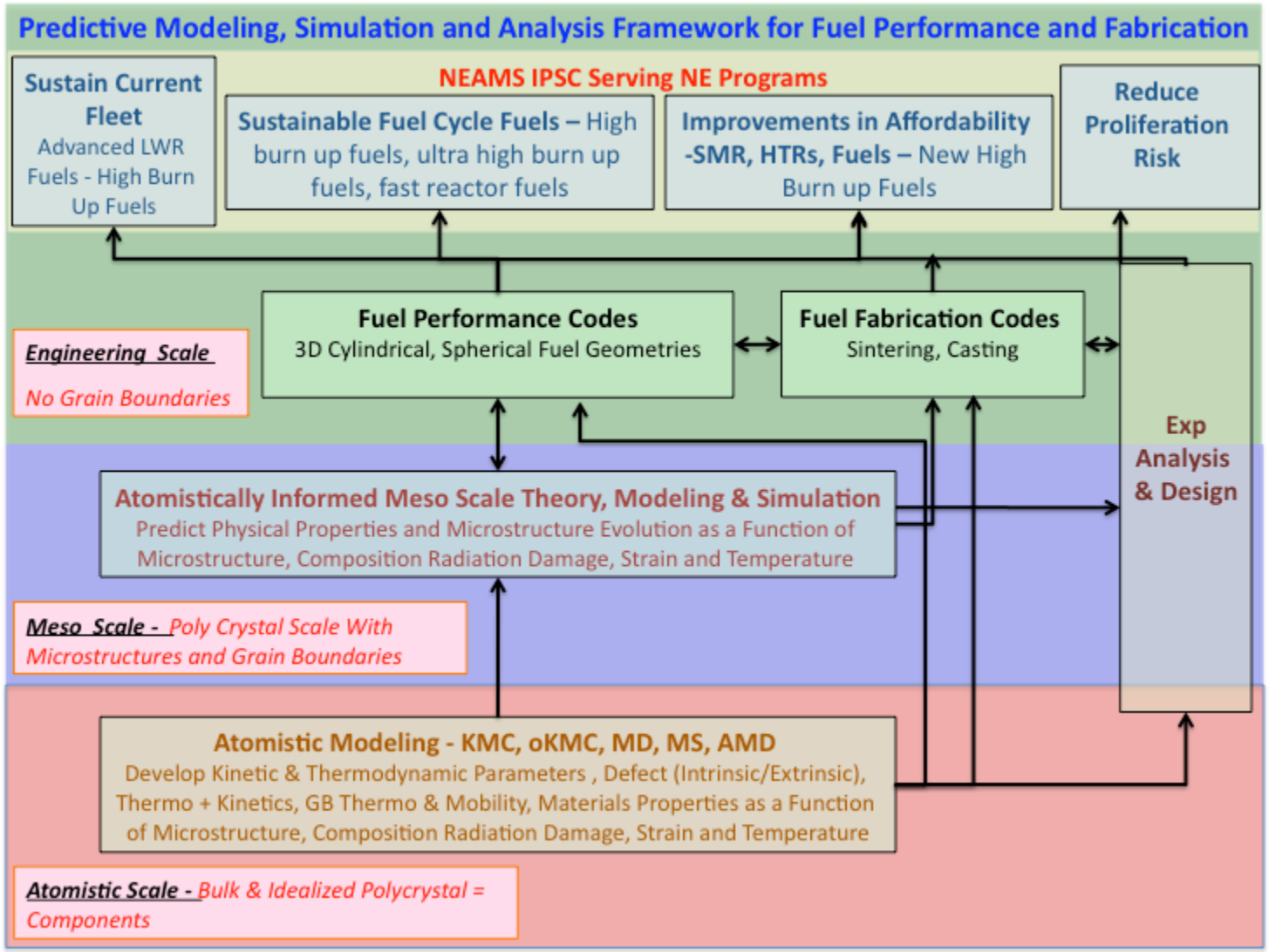
Fuels MS/MP Framework and the R&D Objectives from NE Roadmap



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FY09: $6.05M + $2M (FOA) = $8.05M
FY10: $7.4M
FY11: $5.1M + $0.8M (FMM) = $5.9M

	WP No.	FY10 Allocation	FY09 Carryover	FY10 Total Available
Integrated Performance and Safety Code - Fuels				
Fuels IPSC - ANL	AN1015090601			
Task 1: Sensitivity analysis and validation data support		250,000		250,000
Task 2: A modified gas release model for uranium oxides		150,000		150,000
	Total ANL	**400,000**	**18,927**	**418,927**
Fuels IPSC - INL	IN1015090602			
Task 1: The AMP Nuclear Fuel Performance Code at the Engineering Scale		1,150,000		1,150,000
Task 2: Meso scale modeling		800,000	451,749	1,251,749
	Total INL	**1,950,000**	**451,749**	**2,401,749**
Fuels IPSC - LANL	LA1015090603			
Task 1: The AMP Nuclear Fuel Performance Code at the Engineering Scale		690,000	43,515	733,515
Task 2: Atomistic Scope - Atomistic simulations of mass and thermal transport in oxide fuel for input in to mesoscale models		590,000	149,156	739,156
Task 3: Fuels Meso-scale Scope – Meso-scale simulations of mass transport (fission gas redistribution) in oxide fuels		340,000		340,000
Task 4: Clad Meso Scale - Modeling Creep of Core Reactor Clad and Duct Components Subjected to In-Service Conditions of Irradiation, Stress and Temperature		340,000	94,954	434,954
Task 5: The Integration, Interface, Vision and Requirements Development, Project Management		440,000	34,322	474,322
	Total LANL	**2,400,000**	**321,947**	**2,721,947**
Fuels IPSC LLNL	LL1015090604			-
Task 1: -Atomistic Simulation : Microstructural Evolution and Mechanical Performance of Ferritic-Martensitic Cladding		700,000	139,000	839,000
Task 2: - Atomistic/Mesoscale: CALPHAD thermodynamics database development with ab intio input			117,610	117,610
	Total LLNL	**700,000**	**256,610**	**956,610**
Fuels IPSC ORNL	OR1015090605	-		
Task 1: The AMP Nuclear Fuel Performance Code at the Engineering Scale		1,583,333	423,234	2,006,567
Task 2: Mesoscale Potts Modeling of Fission Gas Release		83,333	50,000	133,333
Task 3: Atomistic Scope – Development of Improved Models for Fission Gas Resolutioning and Thermal Transport in UO2 Based on Atomistic Simulations		283,333	50,000	333,333
	Total ORNL	**1,950,000**	**523,234**	**2,473,234**
	Total All	**7,400,000**	**1,572,467**	**8,972,467**

Fuels Program Integration

- **MS/MP Roadmap was drafted and published**
- **<u>Science-Based Integrated Approach to Advanced Nuclear Fuel Development</u> (LA-UR-10-06182)**
  - Important Sections
    - *Science-based Integrated Approach to Advanced Nuclear Fuel Development – Vision, Approach, and Overview*
    - *AMP: Advanced Modeling and Simulation of Nuclear Fuel Performance*
    - *Science-Based Integrated Approach to Advanced Nuclear Fuel Development – Atomistically Informed Meso Scale Theory and Scale Bridging to Engineering Scale*
    - *Atomistic Simulations and Atomistic-to-Meso Scale Bridging*
    - *Atomistically Informed Mesoscale Modeling of Cladding Materials*
    - *Oxide Fuel Fabrication Modeling and Simulation*
    - *Casting Process Modeling and Simulation*
  - Each section addresses
    - *Background and objective*
    - *Strategy and formulation, modeling targets, approach & current status*
    - *Validation data requirements and suggested experiments*
    - *Scale integration requirements*
    - *Computational requirements*
    - *5 year plan*

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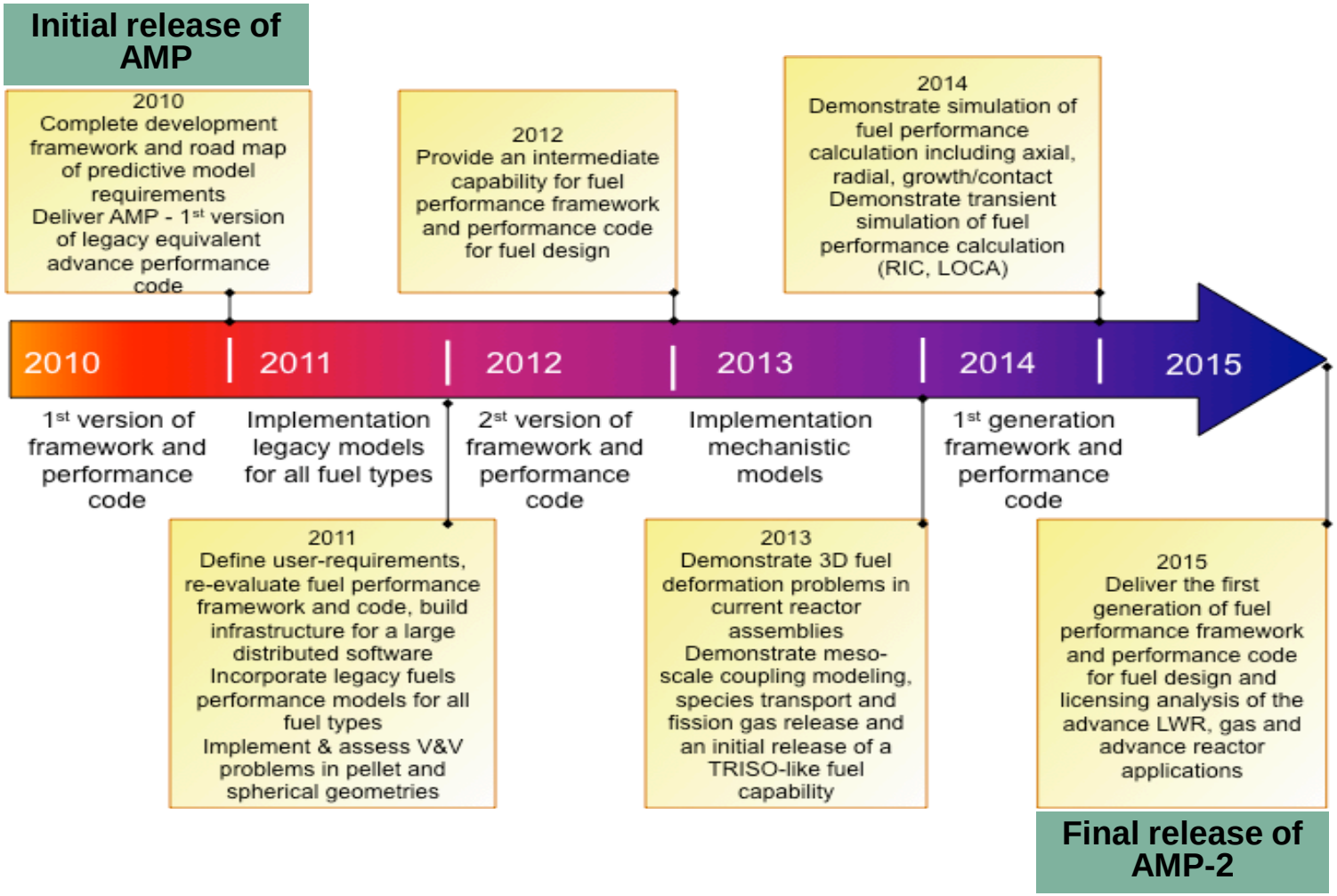
Short-Term Objectives: Consistent with FCRD Advanced Fuels Campaign



Integration with Other Program Elements

- **Validation Methodology & Uncertainty Quantification**
  - R. A. Nelson, C. Unal, J. Stewart, B. J. Williams, “Using Error and Uncertainty Quantification to Verify and Validate Modeling and Simulation Capabilities,” Los Alamos National Laboratory Report, LA-UR-10-06125, September 2010.
- **FMM & ET Elements**
  - Areas where support needed were identified and communicated
- **FCRD Advanced Fuels Campaign**
  - “Advanced Fuels Separate Effects Tests R&D Plan,” Idaho National Laboratory Report, INL/LTD-10-18313 (DRAFT), September 2010.

Synergy with the FCRD Advanced Fuels Campaign

- **Advanced Fuels Campaign Execution Plan (FY10)**
  - **3** Areas of Emphasis in Irradiation Testing (FY11 - FY15)

1. Feasibility testing of emergent, innovative fuel concepts that address the "Grand Challenges".
2. Separate effects testing to broadly advance the theoretical understanding of nuclear fuel behavior and inform/validate the advanced modeling and simulation effort.
3. Assessments to gain an understanding of the differences and/or limitations between testing in neutron-shrouded positions in thermal test reactors vs. prototypic fast-spectrum environments.

Open Scientific Publications

- **High degree of productivity evidenced this year by numerous publications in the open scientific literature**
  - 11 journal articles either published or accepted in FY10
  - 25 conference papers presented during FY10

Introduction of Technical Talks

1. **Chris Stanek (LANL), "Lower Length Scale Simulations of Transport in Oxide Fuel"**

2. **Kevin Clarno (ORNL), "The Initial Release of the AMP Nuclear Fuel Performance Code"**

3. **Bill Cochran (ORNL), "The AMP Backplane: Discreet Management of Numerical Libraries and Multiphysics Data"**