U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

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Why Advanced Modeling and Simulation?

National Goals for Nuclear Energy Technology Development

- Decrease costs
- Improve performance
- Increase pace of deployment
- Enhance innovation
- Responsively deal with nuclear waste
- Promote non-proliferation

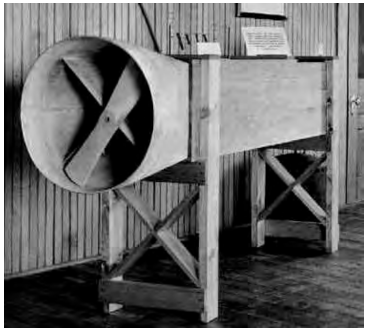
- **We need to go beyond traditional "test-based" approach to understanding nuclear energy**
  - **Very successful for over last 40 years – current fleet is very safe and performs well**
  - **However, test-based approach is:**
    - Very slow
    - Very costly
    - Very hard to optimize

- **Development, deployment and use of advanced modeling and simulation will:**
  - **Provide a new means of obtaining science-based insight that will**
    - Increase the pace of innovation
    - Reduce costs by eliminating unnecessary margins
    - Optimize operations
    - Reduce uncertainty and risk

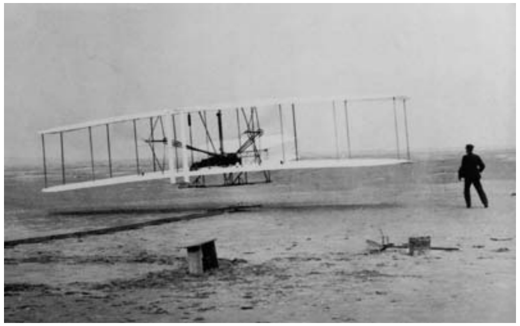
But First Two Questions . . .

Why did these guys fly?

1901 Wind Tunnel



These guys invented this

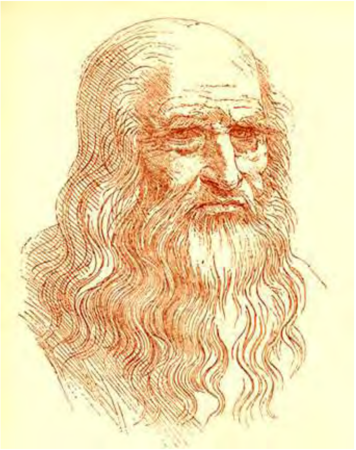


Before they did this in1903

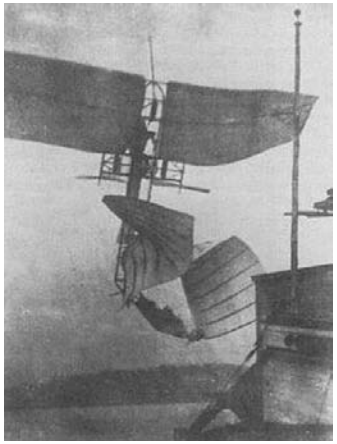
Modeling and Simulation is in the wind tunnel invention business.

When this guy could not?

This guy spent his time studying birds.

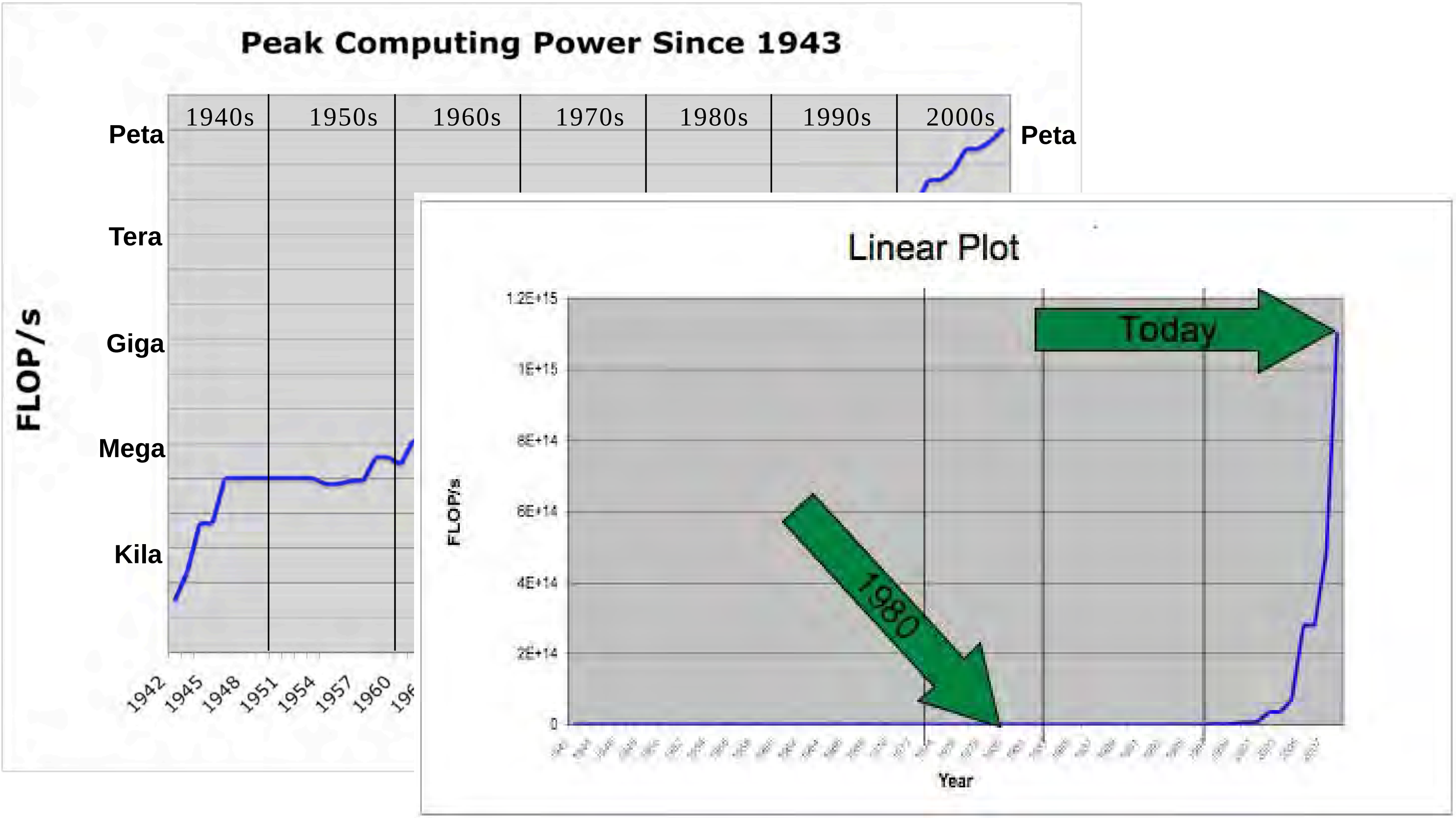


And his airplane looked like this.

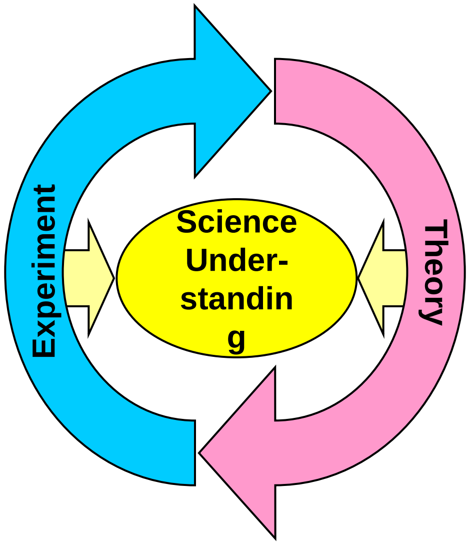


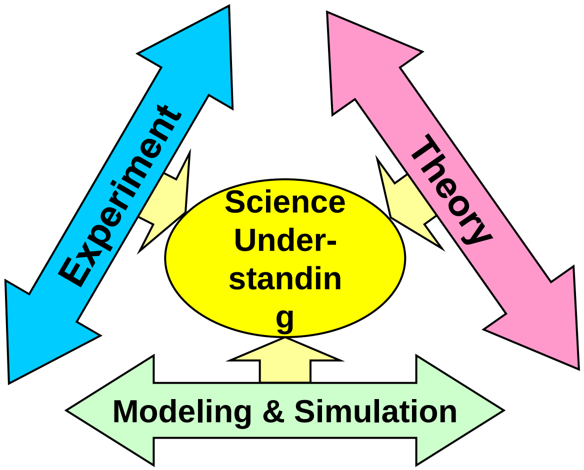
But flew like this.

And It Will Be a Really, Really Good Wind Tunnel



Essential for Enabling the Shift to a Science Based Approach

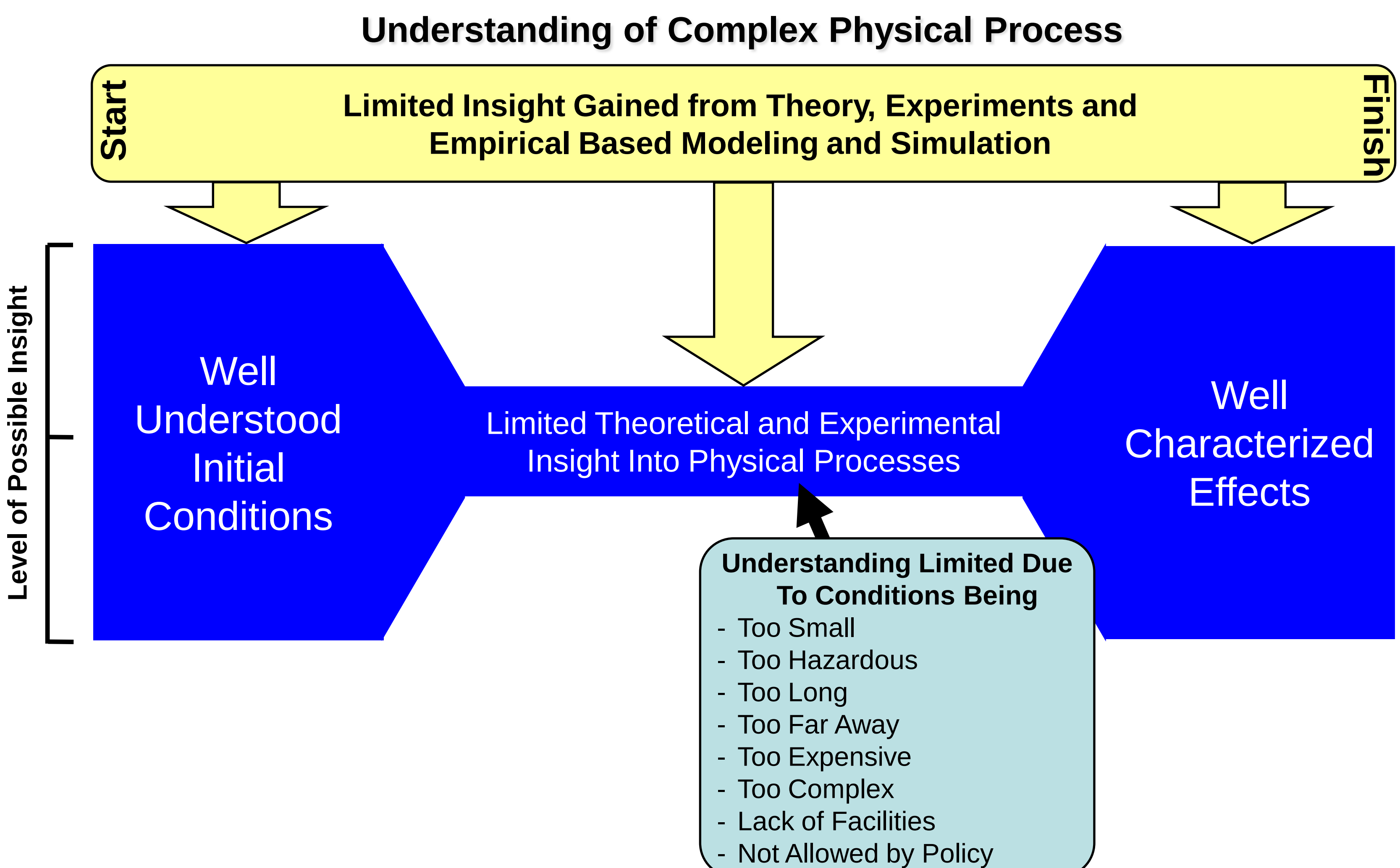




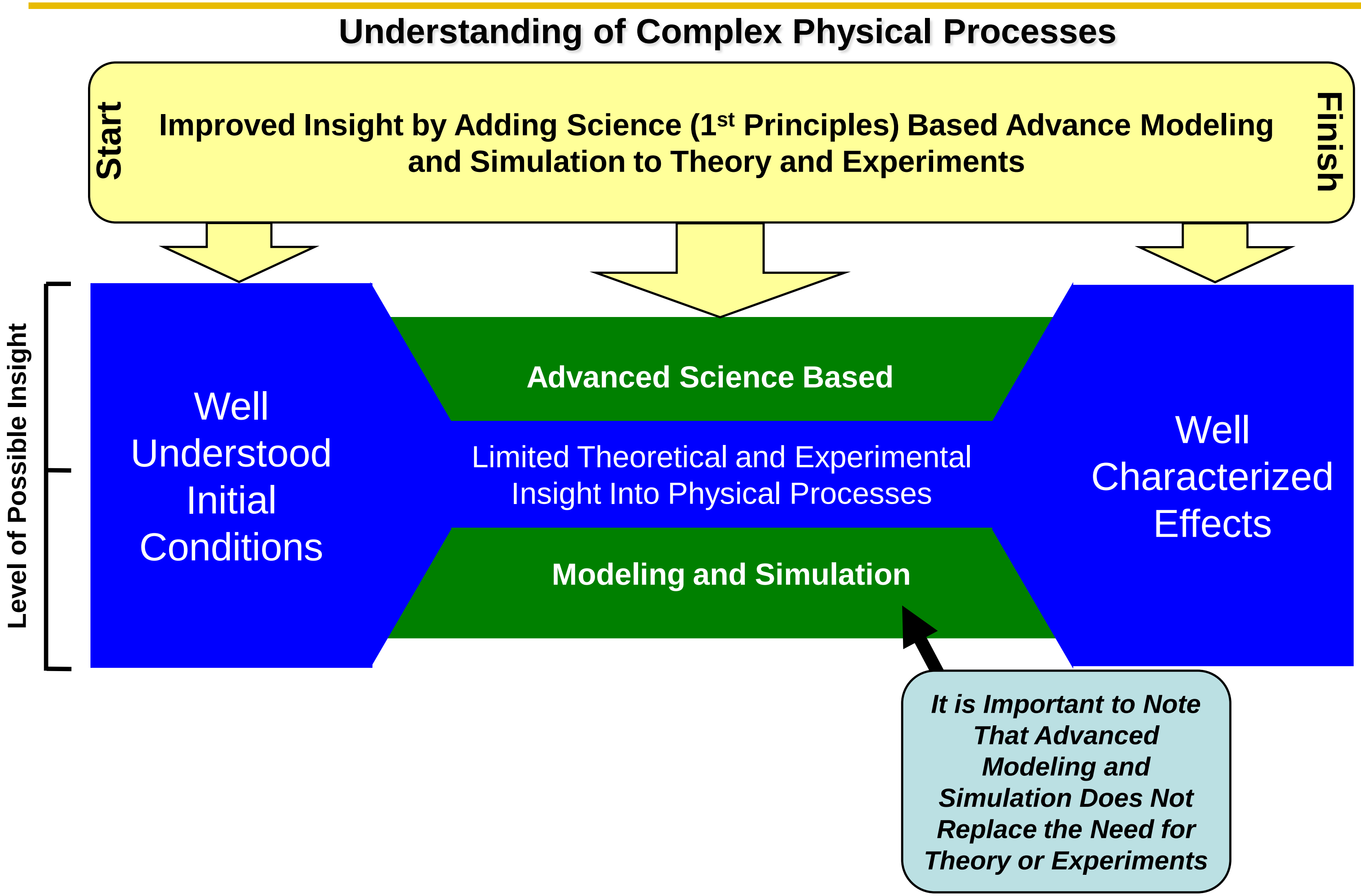
- **Traditional Science Approach**
  - Theory drives design of Experiments
  - Experiments provides discoveries to drive Theory
  - Empirically based modeling and simulation heavily dependent on staying close to experimental basis

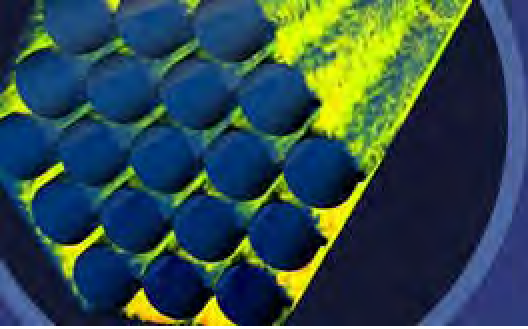
- **Addition of Science Based Modeling and Simulation**
  - Science (1st principles) based modeling and simulation used to extrapolate and predict beyond tested states
  - Can quickly confirm or disprove Theory hypotheses
  - Improve experiments by predicting “areas of interest” and expected results

Why Step Up to New Methods of Gaining Insight?



Supplements Theory and Experiment to Explain "How" Things Happened





Science Based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale

May 11 and May 12, 2009 - Washington DC

Chairs

Ernie Moniz

Bob Rosner

Workshop Charter: This workshop will explore what a "science-based" approach to nuclear energy technology issues involves. We define this approach as the development of technologies needed to advance the safe and environmentally conscious use of nuclear energy as an important source of non-carbon-emitting energy.

This workshop will define the ***actions needed to advance the state-of-the art in the modeling and simulation of nuclear energy and fuel cycle systems.***

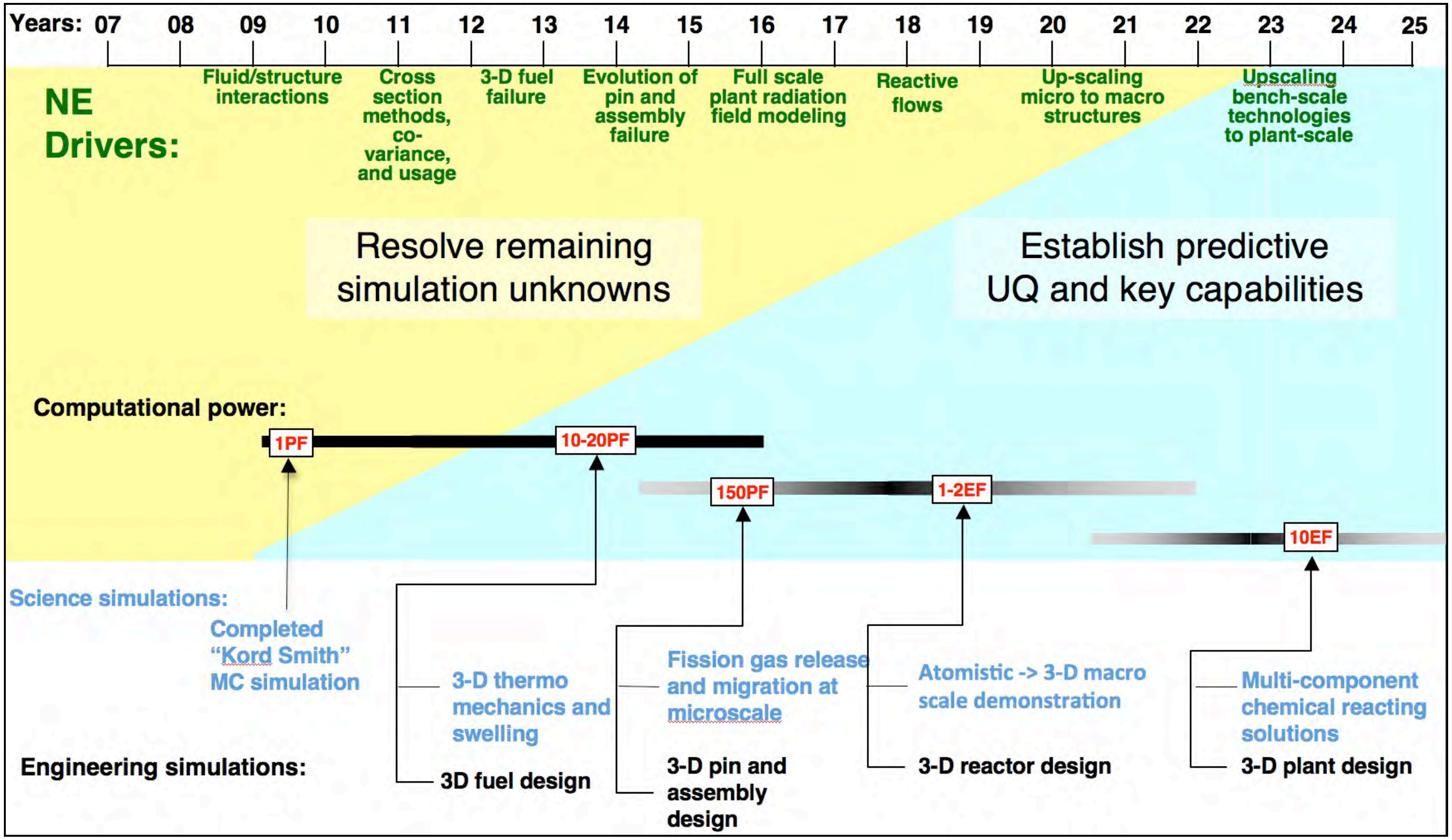
Organized into 4 Panels

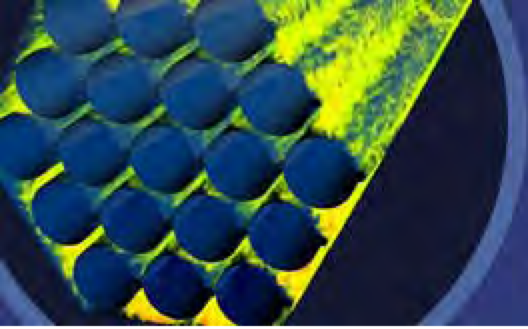
- ***Integrated Performance and Safety Codes***
- ***Advanced Materials***
- ***Verification, Validation and Uncertainty Quantification***
- ***Systems Integration***

Participants Included
(and about 30 additional)

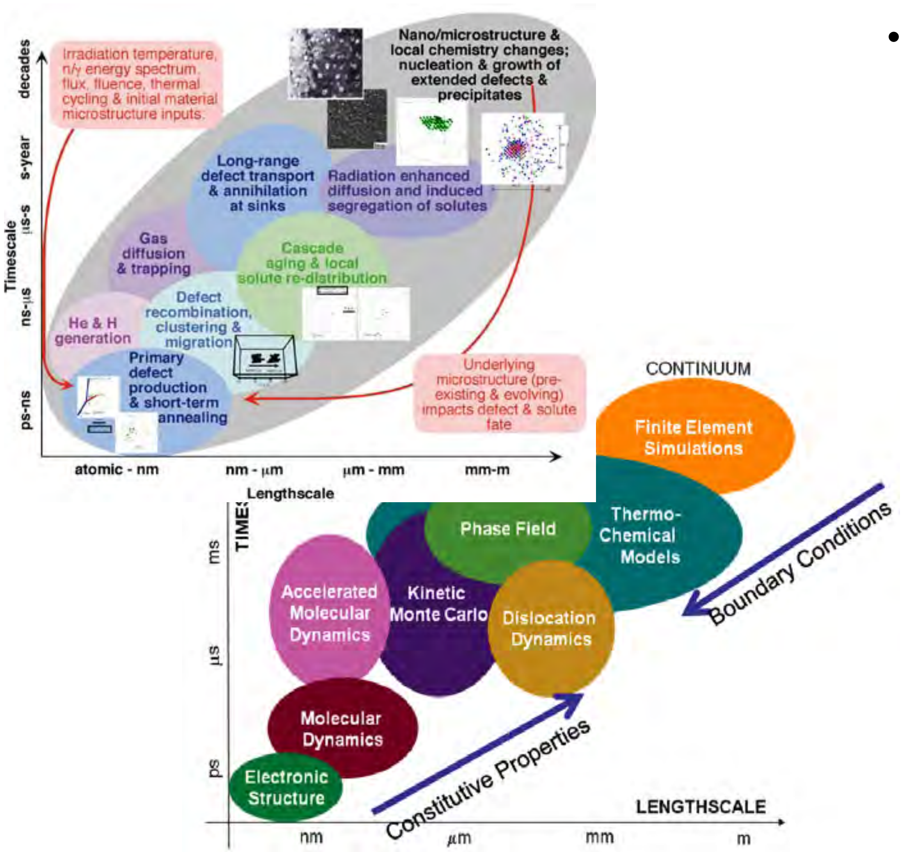
Marv Adams	Texas A&M	Stephen Lee	Los Alamos
Tom Arsenlis	Livermore	Paul Lisowski	U.S. Dept of Energy
Pete Beckman	Argonne	Barney MacCabe	New Mexico
Lali Chatterjee	U.S. Dept of Energy	William Martin	Michigan
Dana Christensen	Oak Ridge	Paul Messina	Argonne
Phil Colella	Berkeley	Parviz Moin	Stanford
Matt Crozat	U.S. Dept of Energy	Jeffery Nichols	Oak Ridge
Julian Cummings	CalTech	David Nowak	Argonne
Tomas Diaz de la Rubia	Livermore	Mark Peters	Argonne
Lori Diachin	Livermore	Vic Reis	U.S. Dept of Energy
Tom Downar	Purdue	Ahmed Sameh	Purdue U
Charles Forsberg	MIT	Buzz Savage	U.S. Dept of Energy
Steven Goldberg	Argonne	Andrew Siegel	Argonne
Anath Grama	PURDUE U	Glen Sjoden	Florida
Sherrell Greene	Oak Ridge	Marius Stan	Los Alamos
Bob Hill	Argonne	Thomas Sterling	LSU
Thuc Hoang	NNSA	Rick Stevens	Argonne
Miachael Holland	OMB	Michael Strayer	U.S. Dept of Energy
Leland Jameson	NSF	Paul Turinsky	North Carolina State
Art Kerman	MIT	John Turner	Oak Ridge
Richard Klein	UC Berkeley	Gil Weigand	Oak Ridge
Ken Koch	Los Alamos	Brian Wirth	UC Berkeley
Doug Kothe	Oak Ridge	Sid Yip	MIT
Alex Larzelere	U.S. Dept of Energy	Thomas Zacharia	Oak Ridge

Nuclear Energy Integrated Performance and Safety Code Panel





Material Behavior in Extreme Environments Panel



Verification, Validation and Uncertainty Quantification

- Our top priority recommendation is that a V&V and UQ program for nuclear systems' simulation take a two-pronged approach.
  - First, focus on research into the critical issues and challenges
  - Second, a concurrent study using the V&V and UQ process to analyze a number of critical, integrated physics applications would provide a problem focus and address the issues of coupled multi-scale physics and UQ.

System Integration Panel

Recommendation for an "Open Source," Flexible, and Extensible, Energy Enterprise Model

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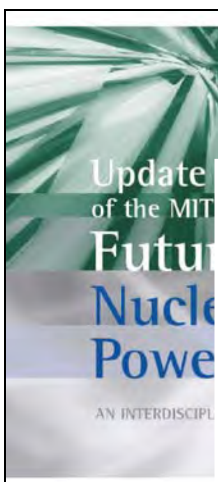
Calls by Experts for NE Advanced Modeling and Simulation

MIT 2003 Report

We call on DOE, perhaps in collaboration with other countries, to establish *a **major project for the modeling, analysis, and simulation** of commercial nuclear energy systems.*

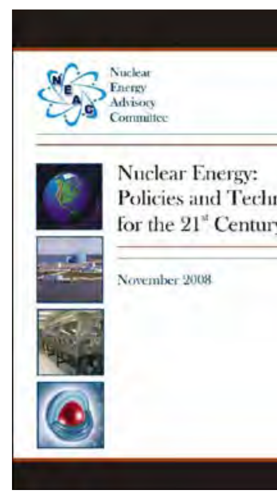
Robert Rosner 2008 Bulletin of Atomic Scientists Article

High-fidelity (science-based) integrated simulations must form the core of design efforts, allowing for rapid prototyping that minimizes the need to experiment.



MIT 2009 Update

Modeling and simulation The 2003 study emphasized the need for greater analytic capability to explore different nuclear fuel cycle scenarios based on realistic cost estimates and engineering data acquired at the process development unit scale. The **DOE program has moved in this direction but much remains to be done.**



2008 NEAC Report

An advanced modeling and simulation effort can lead to better understanding of nuclear energy systems and has the potential to resolve longstanding uncertainties associated with the deployment of these systems.

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

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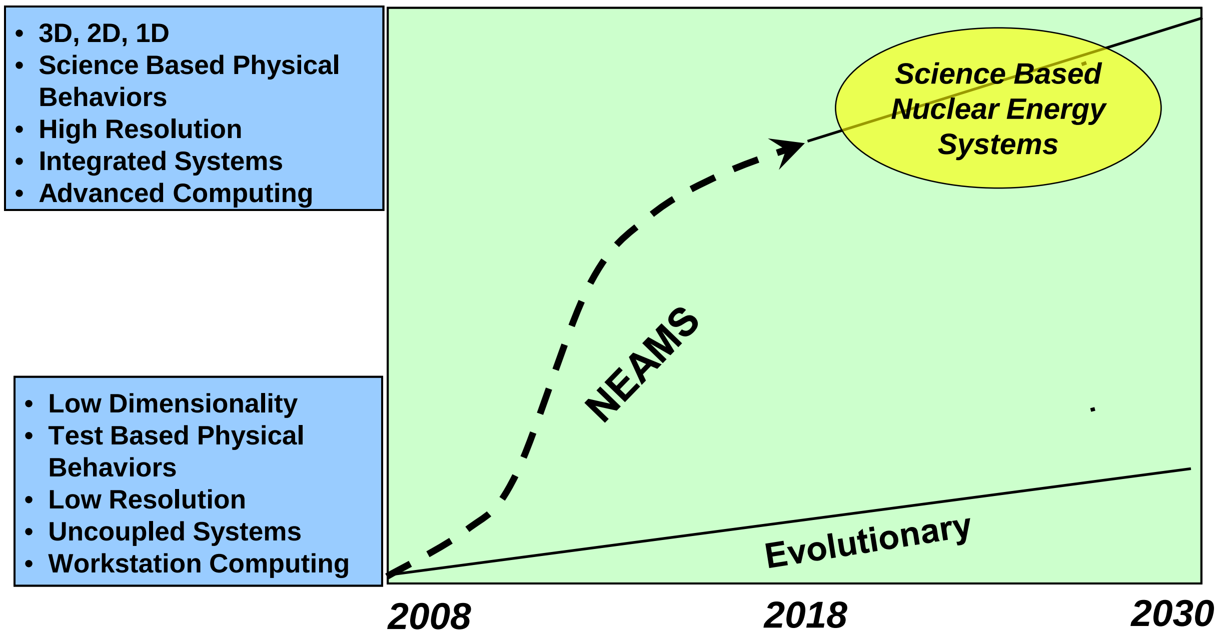
Vision

To rapidly create and deploy "science-based" verified and validated modeling and simulation capabilities essential for the design, implementation, and operation of future nuclear energy systems with the goal of improving U.S. energy security



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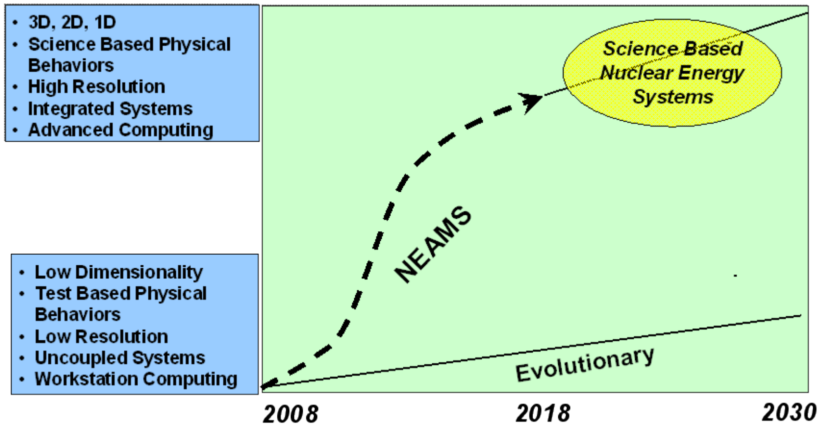
NEAMS Will Deliver . . .

- **Continuously increasing capability for predictive simulation of the performance and safety of:**
  - Nuclear reactors
  - Fuels
  - Safeguarded Separations
  - Waste Forms in a Repository Environment



- **These capabilities will be flexible so they can be applied to differeny types of nuclear energy technologies**

- **NEAMS will implement a comprehensive approach that ensures that new capabilities are fully developed and "born" with appropriate verification, validation and uncertainty quantification.**

- **Modeling and simulation capabilities that can be used to create scientific understanding, design, and license nuclear energy technologies for:**
  - Sustainment of the current LWR fleet
  - Near term deployment of new advanced reactors
  - Innovative uses of nuclear energy
  - Proper disposal of waste
  - Closing the fuel cycle

NEAMS Builds on the Success of ASCI & SciDAC

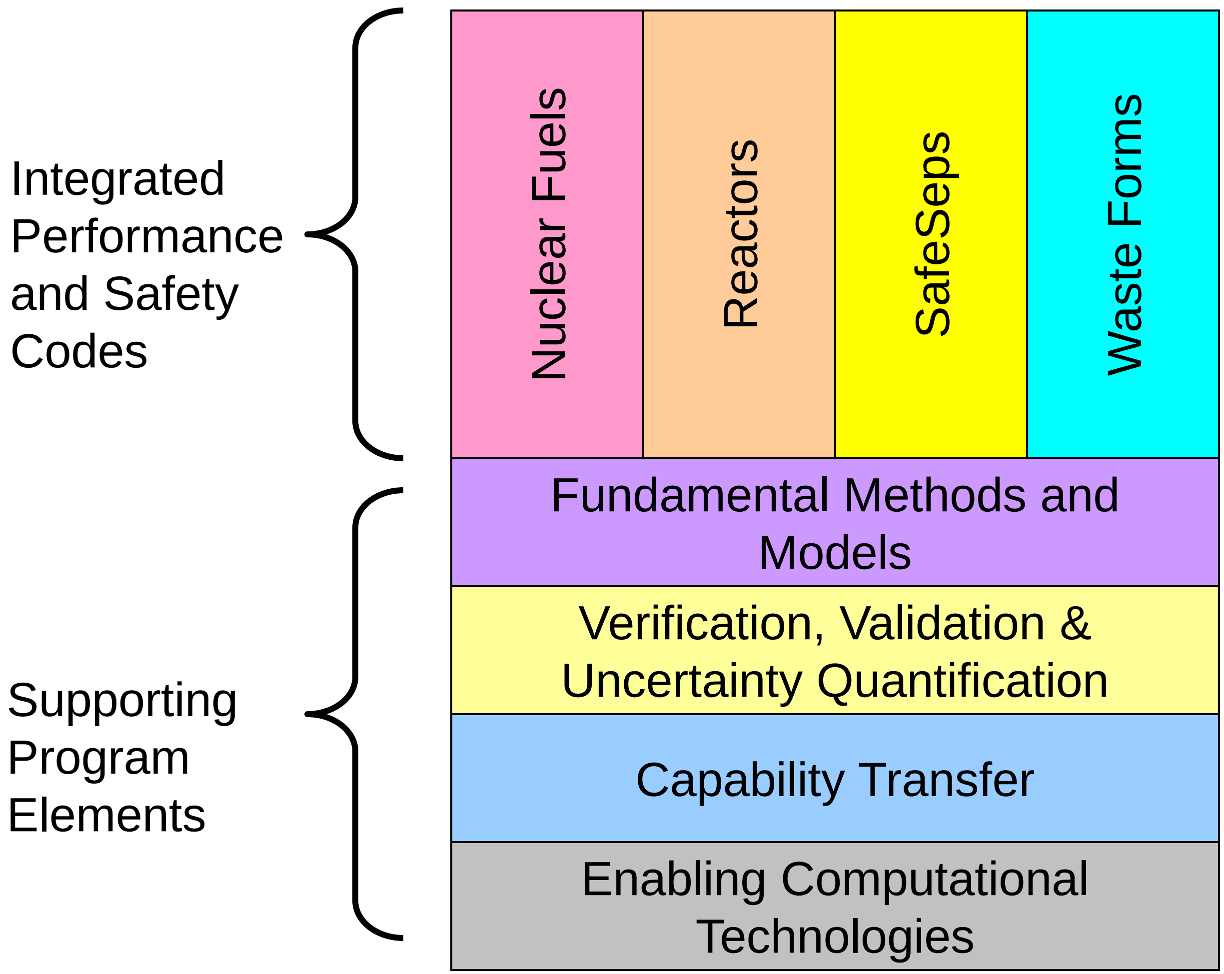
Important Lessons from ASCI

- **Vision** – Have a clear and compelling vision of the mission, and develop a <u>comprehensive program</u> to create new capabilities
- **Leadership** – Headquarters need a “team of rivals” at the national laboratories for leadership of the program
- **Partnership** – Success requires the best from universities, industry and national laboratories
- **Endurance** – Accomplishing the ambitious goals will take time and funding. But it must deliver increasing capabilities “early and often”

NEAMS Users

- **Research and Development**
  - To make discoveries and obtain insight into the physical behavior of nuclear energy technologies (e.g. reactors, fuels, waste)
- **Technology Designers**
  - To conduct design studies for new nuclear energy technologies to understand performance, safety, and cost with the potential of a design of a system submitted for licensing.
- **Regulators**
  - To evaluate submitted designs and supporting analysis to determine if the technologies will meet the requirements to protect human health and the environment
- **Utilities & Operators**
  - To understand and optimize the operations of nuclear energy technologies

NEAMS Organization Provides All Essential Components



NEAMS Program Overview

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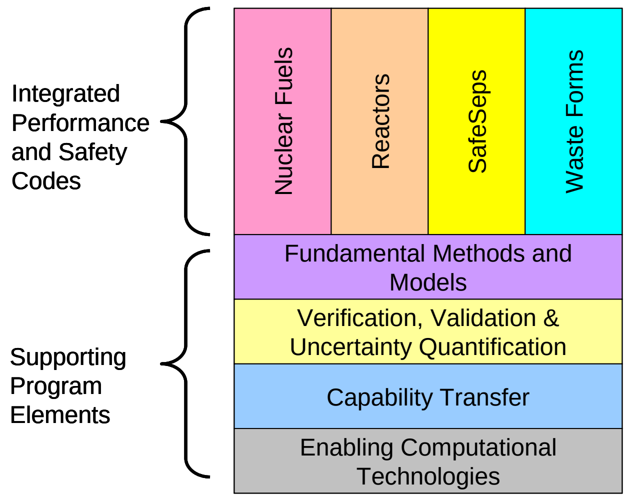
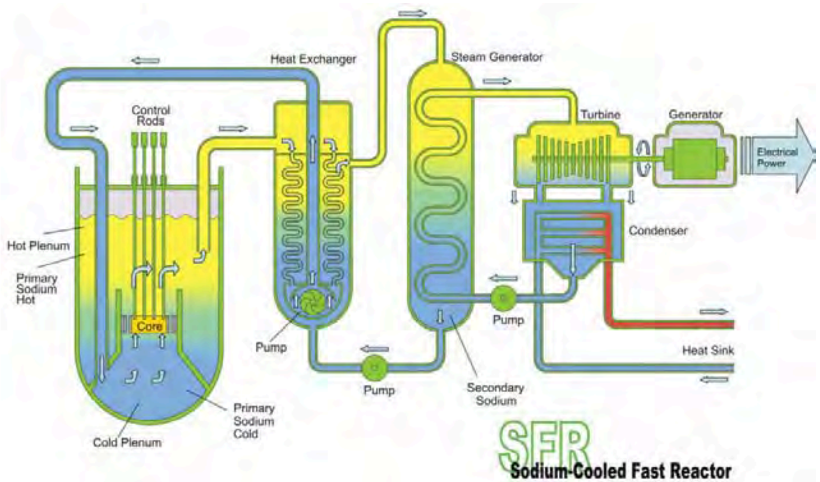
- **Integrated Performance and Safety Codes (IPSC)**
  - Continuum level codes that will predict the performance and safety of nuclear energy systems technologies
  - Attributes include 3D, science based physics, high resolution, integrated systems
  - Large code teams (~25 people)
  - Single “center of gravity”
  - Long-term commitment (~10 years)
  - Codes “born” with verification, validation and uncertainty quantification
  - Using interoperability frameworks and modern software development techniques and tools



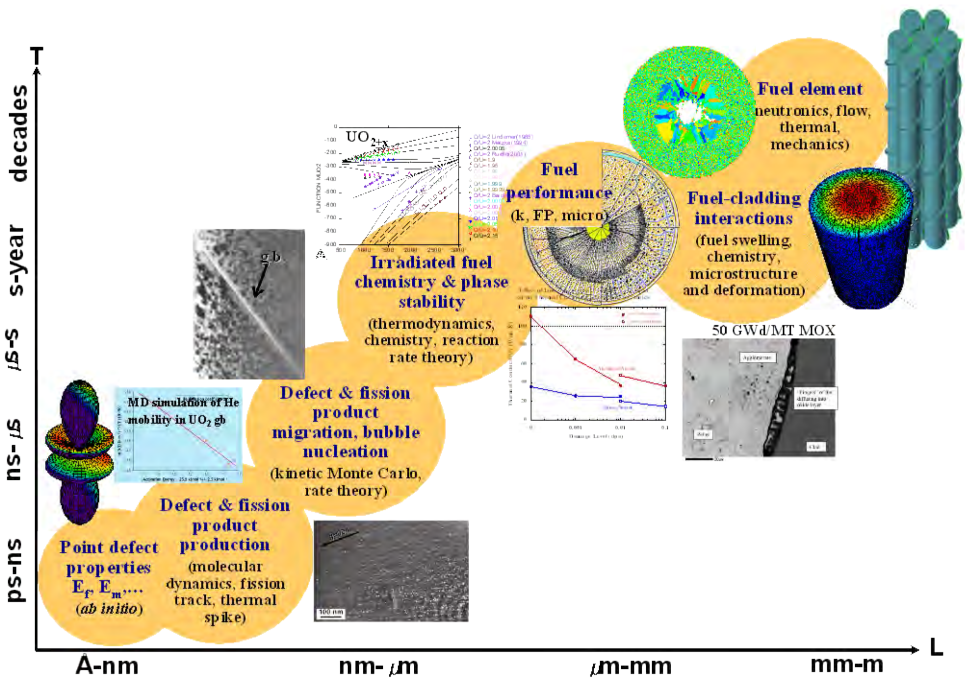
- **Program Support Elements**
  - Develop crosscutting (i.e. more than one IPSC) required capabilities
    - Fundamental Methods and Models
    - Verification, Validation and Uncertainty Quantification
    - Interoperability frameworks
    - Enabling Computational Technologies
  - Provide a single NEAMS point of contact for crosscutting requirements (e.g. experimental data, computer technologies)
  - Smaller, more diverse teams to include laboratories, universities and industries.
  - Shorter timelines

Reactor IPSC



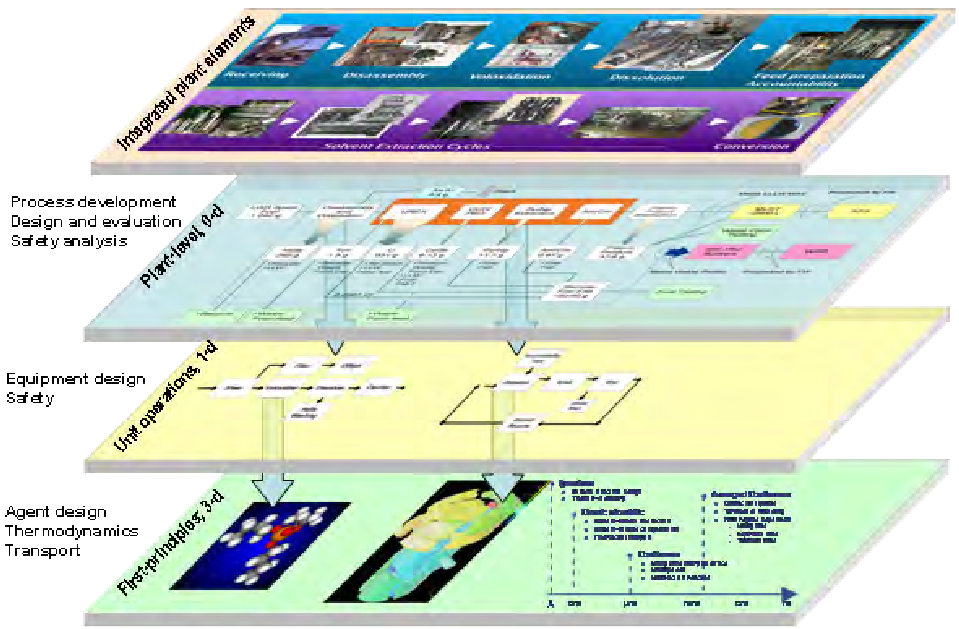
- **Scope**
  - Predict performance and safety of fast reactors over 40 – 60 year lifetime
  - Initial focus on reactor core
  - As code progresses will extend to additional systems
  - Many underlying physical processes (e.g. thermodynamics, neutronics) extensible to other reactor types (gas-cooled,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

Nuclear Fuels IPSC



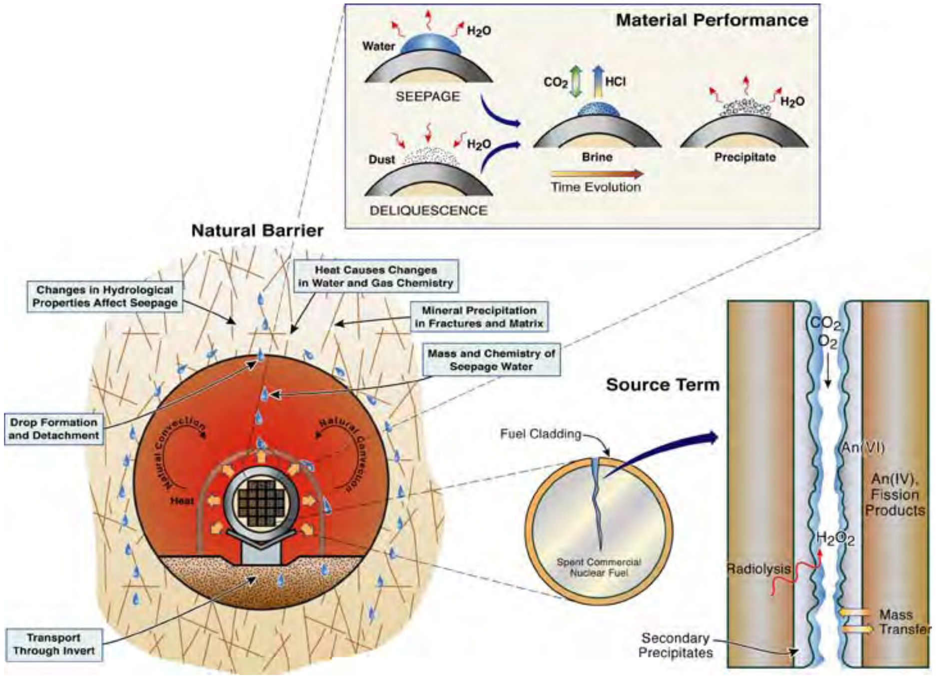
- **Scope**
  - Develop a coupled, predictive three-dimensional, predictive computational tool to predict the performance of nuclear fuel pins and assemblies, applicable to both existing and future advanced nuclear reactor fuel design, fabrication
  - Develop a multi-scale multi-physics framework with 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)

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

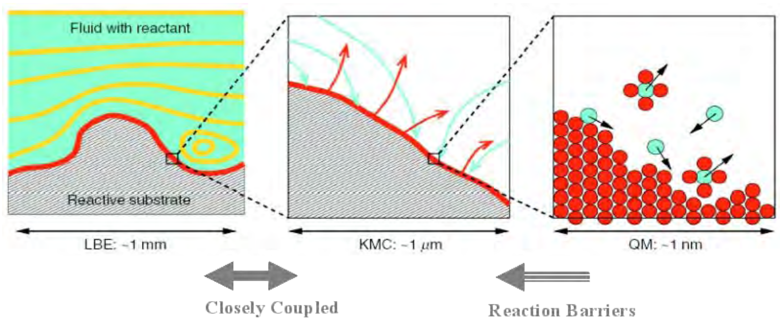
Waste IPSC

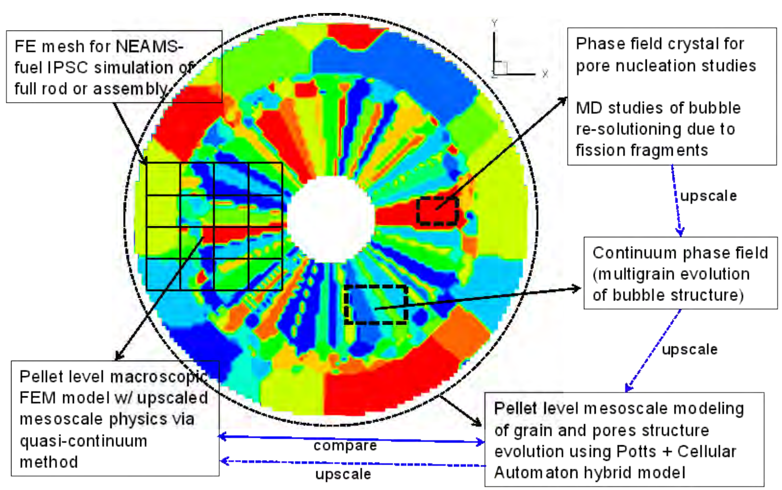


Scope

- 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 mezzo scale to the continuum
- Develop with flexibility to extend to different waste types in different repository environments

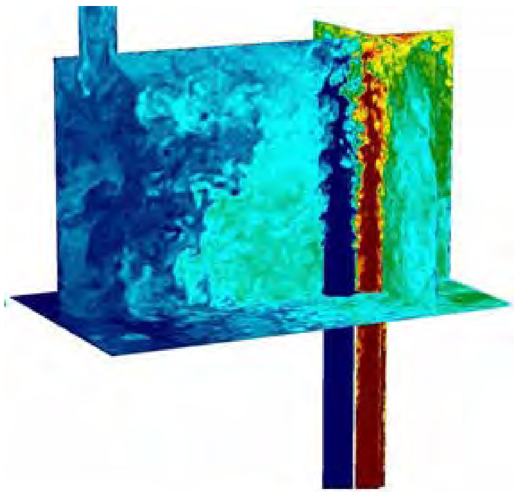
Fundamental Methods and Models (FMM)

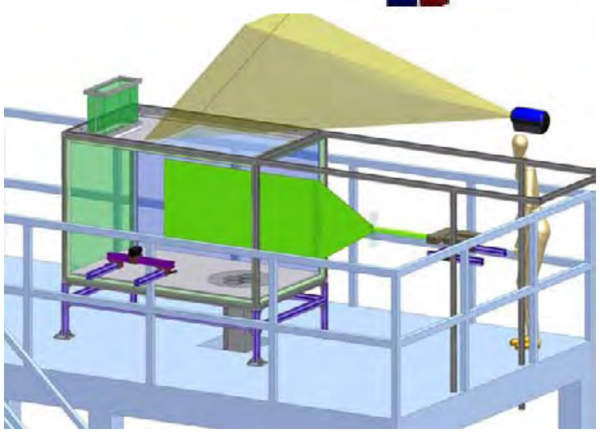




- **Scope**
  - Develop crosscutting models and methods for lower length scale materials performance needed to support IPCSs
  - This includes material modeling at the molecular or quantum scale
  - Also includes methods required for upscaling behaviors to IPSC scale
  - Provide a single NEAMS point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

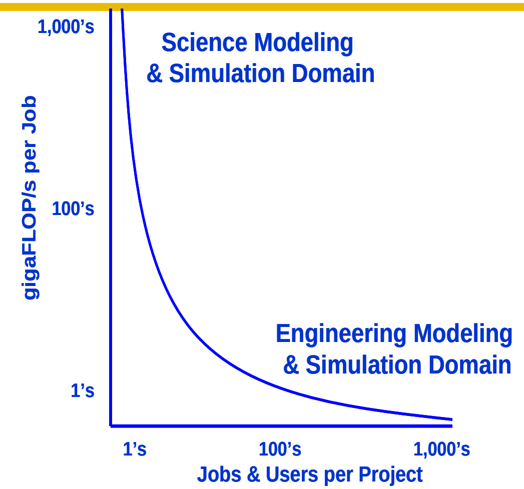
Verification, Validation and Uncertainty Quantification (VU)

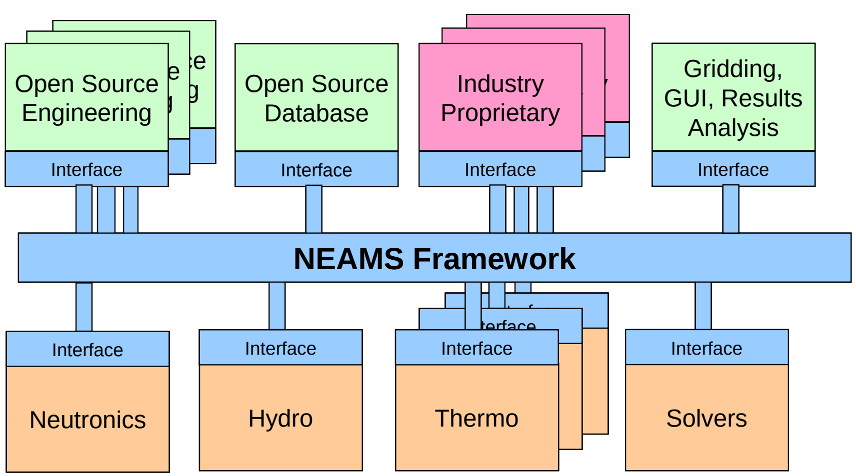




- **Scope**
  - Methodologies
    - Develop NEAMS requirements for verification, validation and uncertainty quantification of IPSCs
    - Conduct analysis of existing methodologies and select “best in class” to serve as basis
    - Extend methodologies as needed
    - Assist IPSCs in executing methodologies
  - Data
    - Serve as NEAMS single point of contact for experimental data
    - Develop NEAMS requirements for experimental data needed to support methodologies
    - Understand availability of existing data
    - Interface with experimental Campaigns for the development of new data
  - Regulatory
    - Serve as primary interface with NRC and other regulatory agencies
    - Understand regulatory requirements for V&V, UQ

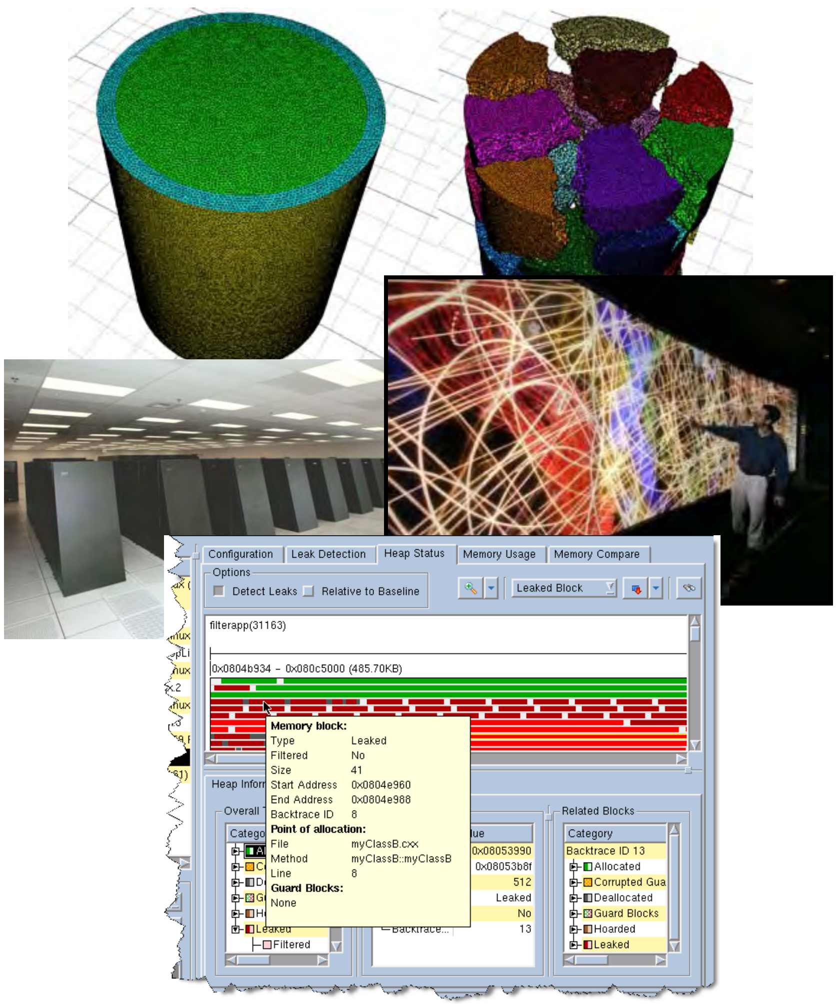
Capability Transfer (CT)





- **Scope**
  - Enable the efficient transfer of advanced modeling and simulation capabilities from the science domain to the industry engineering domain
  - Understand the roadblocks and where possible provide technologies to overcome them
  - One identified roadblock is the interoperability of existing codes, proprietary codes, open source and newly developed advanced codes
  - To overcome this, CT is developing the NEAMS interoperability framework

Enabling Computational Technologies (ECT)



- **Scope**
  - Software quality
  - Application development tools
  - Problem setup tools (e.g. mesh generation)
  - Numerical libraries (e.g. solvers)
  - Results analysis (e.g. visualization)
  - Facilitate compute cycle and data storage availability
  - Leverage other program capabilities and laboratory infrastructure when possible
  - Develop NEAMS funded capabilities when needed
  - Assist and advise IPSC and other supporting elements on the state-of-the-art computational technologies

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

NEAMS Has Assembled the "A" Team of Labs, Universities and Industry

- **Integrated Performance and Safety Codes**
  - Nuclear Fuels
    - LANL – lead
    - ORNL
    - LLNL
    - INL
    - Texas A&M
    - UC Davis
    - Oklahoma State
  - Reactors
    - ANL – lead
  - SafeSeps
    - LANL – lead
    - ORNL
    - ANL
    - SUNY Stonybrook
  - Waste
    - SNL – lead
    - LBNL
    - ANL

- **Supporting Program Elements**
  - Fundamental Methods and Models
    - PNNL – lead
    - SNL
    - ORNL
    - North Carolina State
    - Michigan
    - Nevada, Reno
    - Wisconsin
  - Verification, Validation and Uncertainty Quantification
    - INL – lead
    - SNL
    - LANL
    - University of Idaho
  - Capability Transfer
    - ORNL
    - ANL
    - IBM
  - Enabling Computational Technologies
    - LLNL

DOE Interface Activities

- **Office of Science**
  - Pending MOU
  - Joint SC/NE Workshop
  - Computer Cycles
    - INCITE Awards
    - Director Allocations
- **EM**
  - Assisting with proposal for an EM subsurface modeling and simulation program
  - Assisting with formation of a modeling and simulation program for waste form development
  - Similar to NEAMS efforts in the Waste IPSC
- **NNSA**
  - ASC
    - NSF & NAS Study of Mathematics Foundation for V&V, and UQ
  - NA-20
    - Safeguards and Separations IPSC
    - Proposal review
- **FE**
  - Early discussions about collaboration on subsurface modeling for Carbon Sequestration

International Interfaces

France

- Visit to CEA and EDF in October 2008
- Collaboration on CT Framework
  - Using EDF's Salome to create functional spec
  - Collaborating on the open source Saturn CFD code

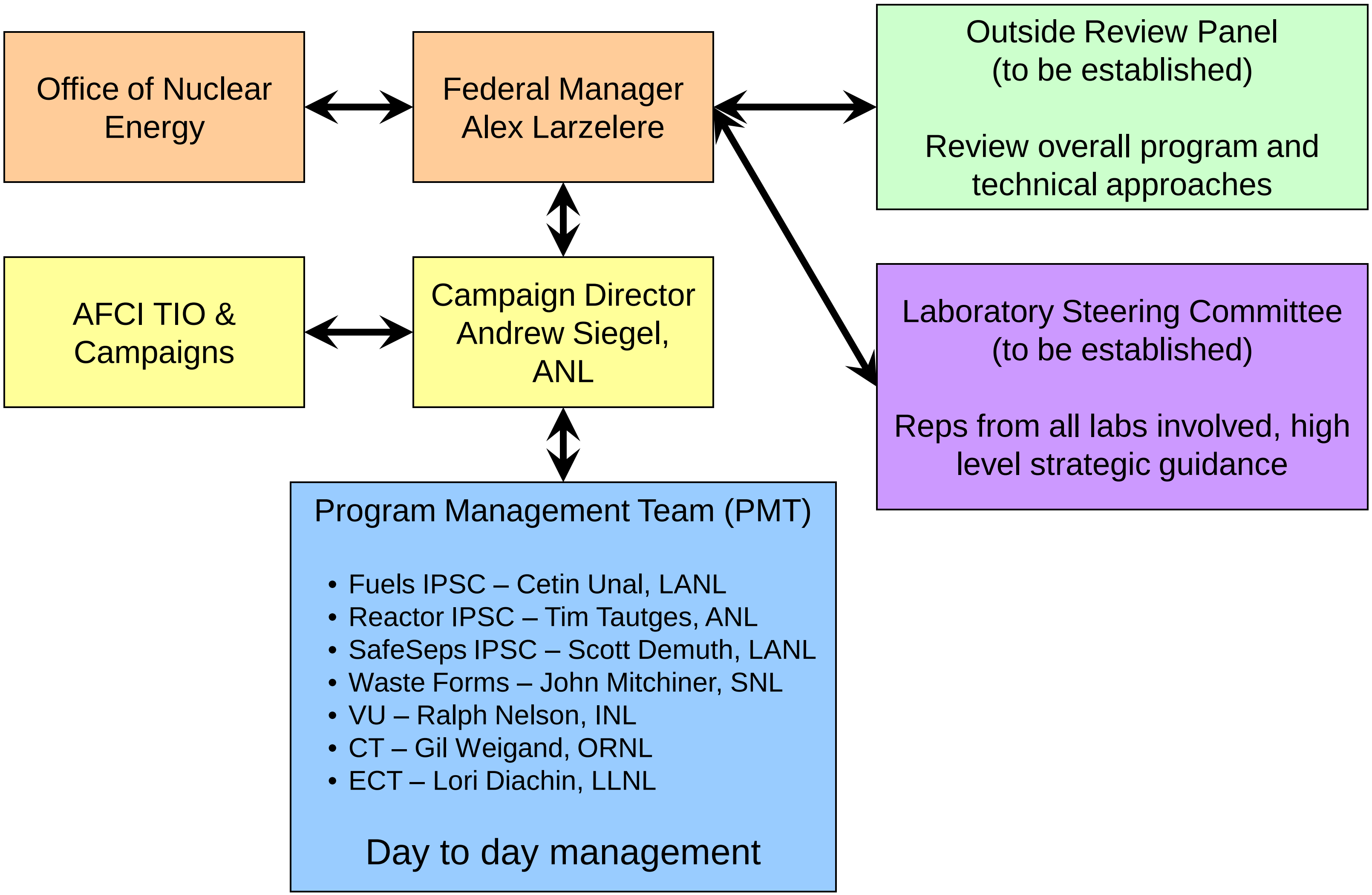
Russia

- Sodium Fast Reactor
  - Early discussions about the role of advanced modeling and simulation in support of SFR collaboration

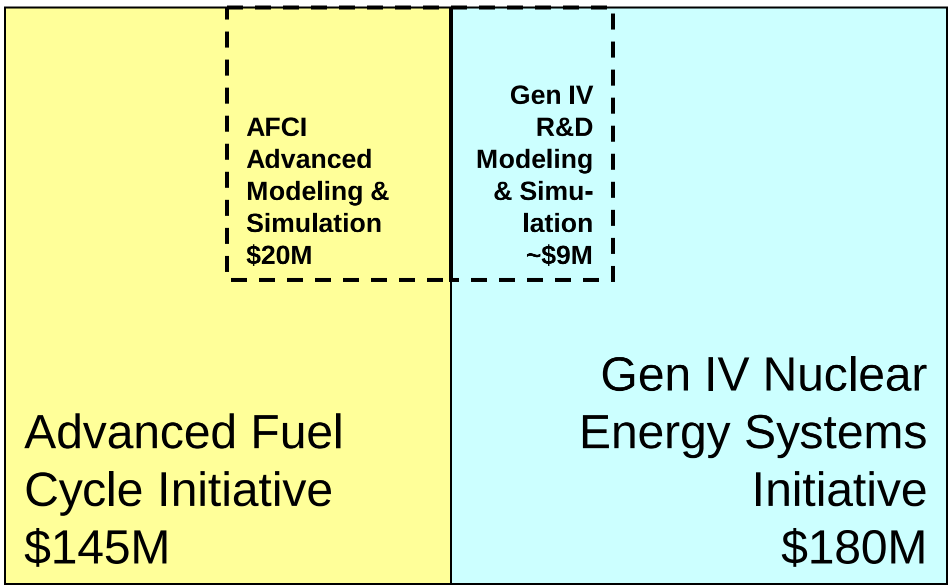
Japan

- Seismic Modeling
  - Whitepaper underway to discuss the seismic modeling problem and recommended actions
  - FY-10, planning to conduct a simulation of a seismic test problem
  - Japan provides – real world geometries and seismic damage observations
  - NEAMS provides – modeling using modern 3D seismic codes on high performance computers
  - Jointly – analysis of simulated vs. real world, assessment of gaps
- Safeguards and Separations Modeling
  - Early discussions

NEAMS Management Structure



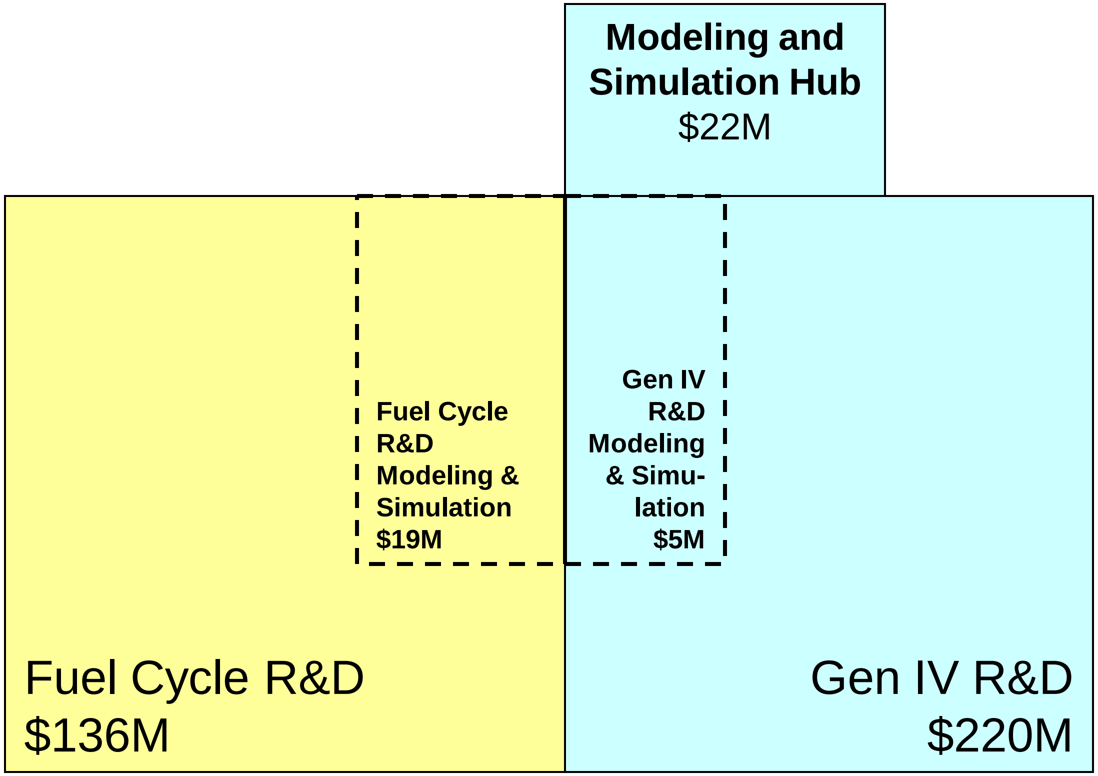
Modeling and Simulation Activities in NE FY-09 Organization



- **NEAMS has been only fully funded since April 2009 (post-CR)**
  - Prior years it was a crosscut at about $7.5M
- **AFCI Budget Overview**
  - $20M in FY-09 Budget
    - Fuels – $6.2M
    - Reactor IPSC – $5.1M
    - Safeguard & Separations IPSC – $1.35M
    - Waste IPSC – $1.5M
    - FMM – $2.1M
    - VU – $2M
    - CT – $0.5M
    - ECT – $0.5M
    - Campaign – $0.6M
  - ~$4M in FY-08 FOA Awards
    - Meso-scale Fuel Modeling – $2M
    - Framework Specification – $2M
  - ~$6M in NE University Program Awards

FY-10 Budget

FY-10 Budget Appropriation



Energy Innovation Hub for Modeling and Simulation

Vision

Nuclear Energy Can Benefit from Modeling and Simulation in the Near, Mid, and Long Terms

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Time (* Dates Approximate)

Nuclear Energy Issues

2010 | 2020 | 2040

Deployment of Gen III+ Reactors

Power Uprates

Higher Burnups

NGNP

Small Modular Reactors

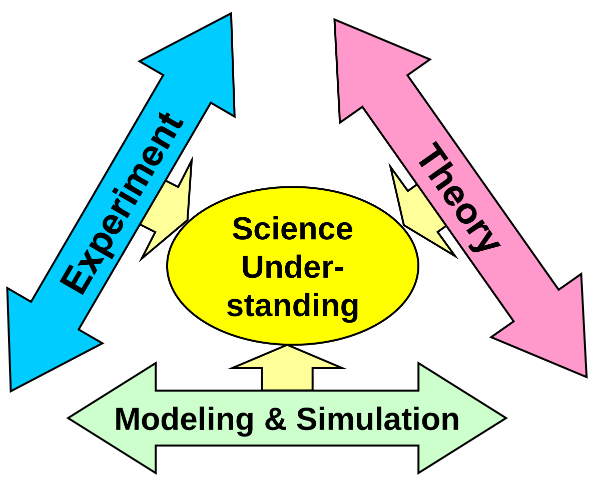
License Extensions

Gen IV Reactors

Waste Repository

Closed Fuel Cycle

Near-Term | Mid-Term | Long-Term



New means of improved understanding nuclear energy Issues

Modeling and simulation has become a peer to theory and experiment to develop science insight

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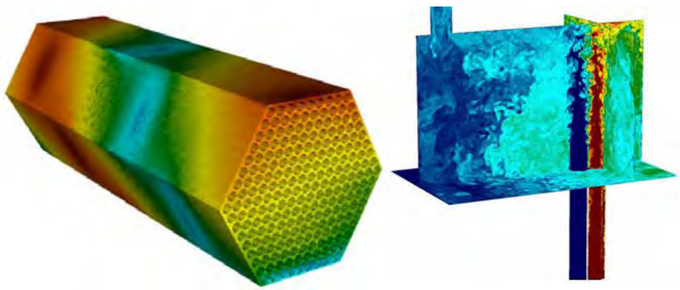
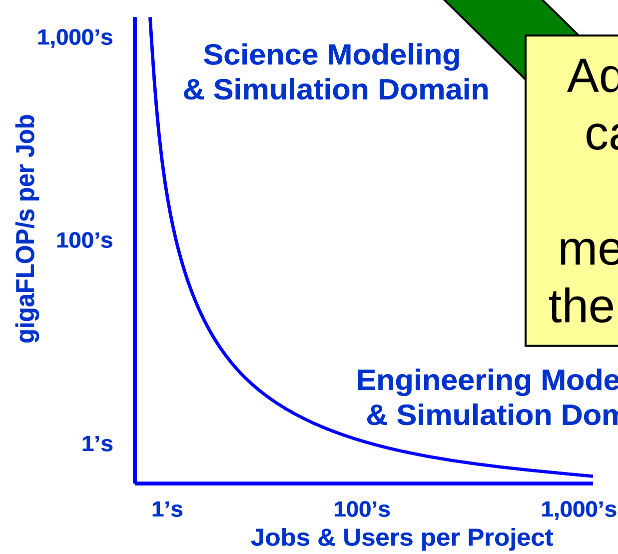
How Can the NE Modeling and Simulation (M&S) Hub Change the Game?

Existing Advanced Modeling and Simulation Capabilities



Currently in the Science Domain

- Few users
- Few jobs
- Very big computers/job
- Long runtime



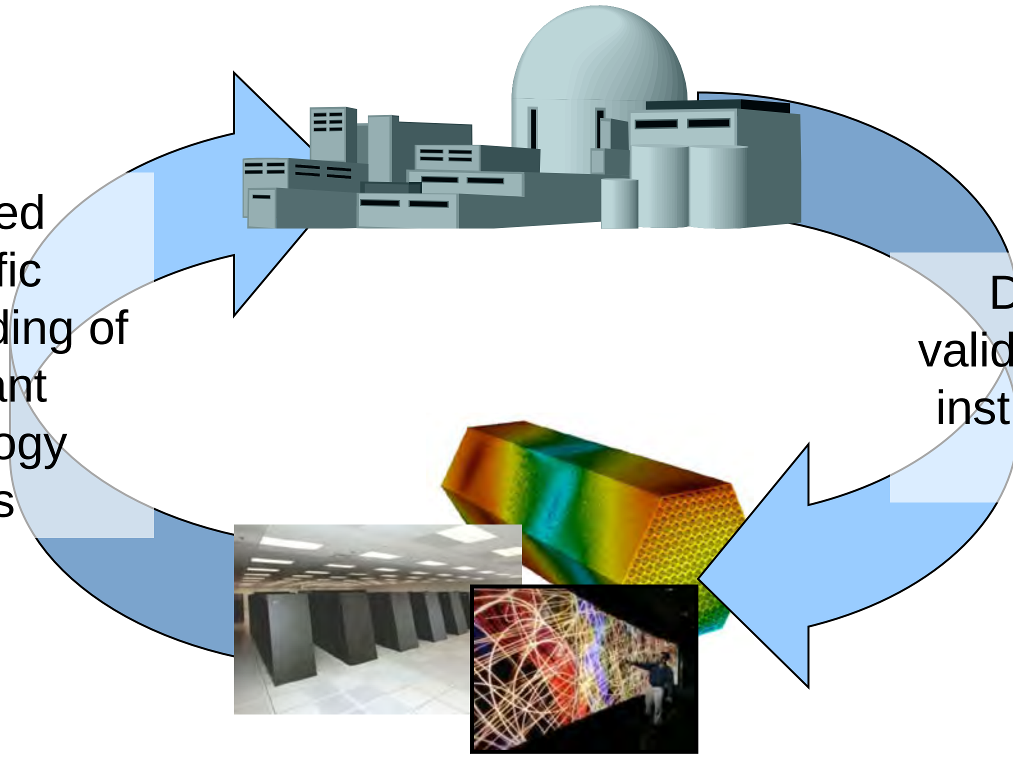
Adapt **Science Domain** capabilities to address issues for the near, medium and long term in the **Engineering Domain**

Change the Game by Accelerating the Use of Advanced Modeling and Simulation to Address Near Term Nuclear Energy Issues

Engineering analysis is different

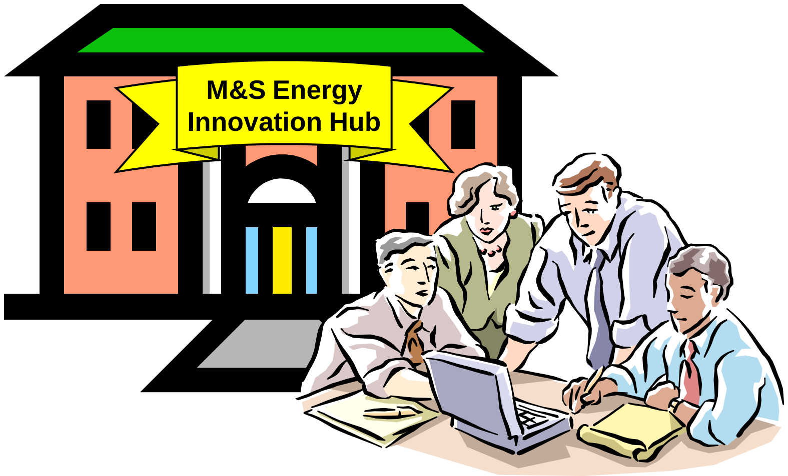
- Short, high pressure timelines
- Requirement for many, short jobs
- Many users
- User environment straightforward

Achieving the Promise of the Hub Requires a Mission Focus



Advanced Modeling and Simulation of the Operating Reactor
(aka "Virtual Reactor")

Modeling and Simulation Hub Activities



- Ideally one physical location
- Competitively awarded to a team of National Laboratories, Universities and/or Industries
- One co-located team of ~75 to ~100 multi-disciplinary researchers
- With access to (but not own) high performance computing resources
- Deliver, in 5 years, an engineering environment using advanced modeling and simulation to address near-term nuclear energy issues

Scope of Work

- Identifying near term nuclear energy technology issues
- Creating requirements for modeling and simulation tools
- Surveying existing capabilities
- Creating interoperability frameworks to link existing capabilities
- Developing additions to capabilities that address nuclear energy technology challenges
- Building architectures to allow code interoperability
- Deploying new user environments to allow the use of advanced modeling and simulation in engineering domains

Competition Considerations

Proposal Factors

- **Proposed "Virtual Reactor" Problem** – Define particular physical reactor to be modeled and problems to be addressed.
- **Approach** - Describe chosen approach to improve modeling and simulation usability
- **Team** - Qualification of team to implement approach and address the proposed nuclear energy problem

Process

1. **Draft FOA** – Issue draft for comments and questions

1. **Workshop** - Refine problem definition and address FOA questions

2. **Final FOA** – Issue FOA with detailed problem definition and proposal requirements

3. **Proposals & Evaluation** - Submission and evaluation of proposals

4. **Site Visits** - Visits to teams deemed to be in the competitive range

5. **Award** - Negotiate contract and make award to winning team

6. **Start Work** - Stand up Hub and start required research and development work

U.S. DEPARTMENT OF ENERGY
Nuclear Energy

NE Modeling and Simulation Hub Fills an Important Gap