U.S. DEPARTMENT OF ENERGY | Nuclear Energy

The State of

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

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NE-71

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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"**

ASCI History Available at https://asc.llnl.gov/asc_history/Delivering_Insight_ASCI.pdf

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Assessing the State of NEAMS

- **Vision**
  - A problem of national significant
  - Having a vision of how to impact it
- **Plan**
  - Understanding "what" is required to implement the vision
  - Understanding of the process required to achieve the "what"
- **Team**
  - Assembling the highly qualified team members to accomplish the "whats"
  - Organizing the team to ensure that everybody knows their role
- **Endurance**
  - Execution – success breeds success
  - Ensuring that adequate resources (e.g. money, compute cycles, technologies) are available to implement the plan

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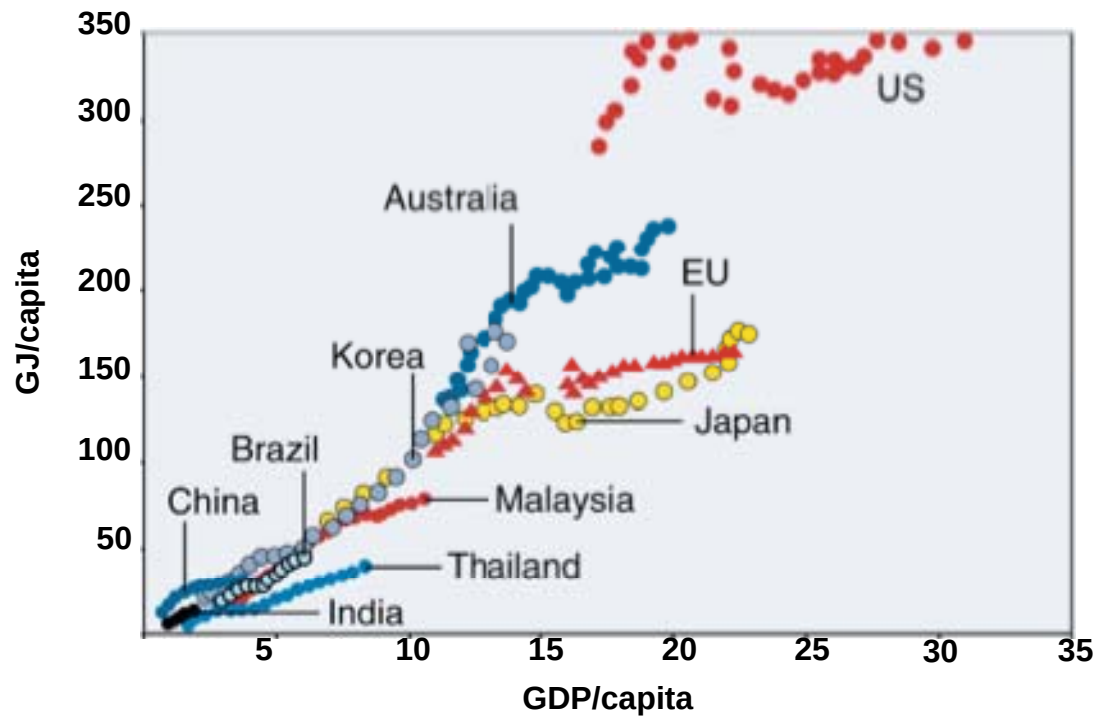
Problem of National Significance

- Energy and economic growth are clearly linked
- As the U.S. and other countries advanced economically, there will be greater competition for energy supplies
- The question is: **How will the U.S. satisfy energy demand in a tightening global energy marketplace?**

Growth in Energy Consumption and GDP per Capita Over Time



Source: Royal Dutch Shell: Exploring Future Energy Needs, Choices and Possibilities

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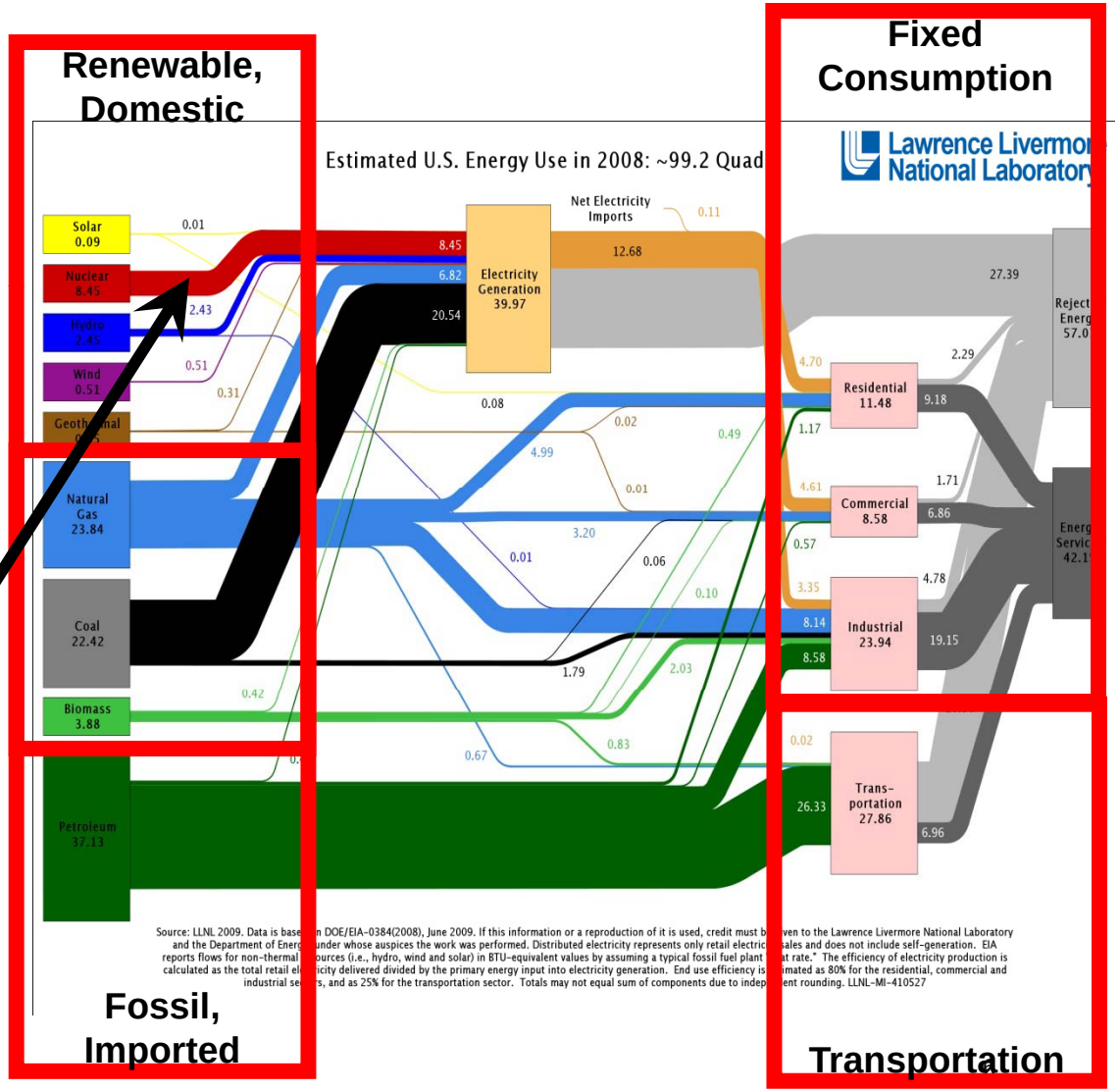
Improving U.S. Energy Security

- **Elements U.S. Energy Security**
  - National Security
    - ***Avoiding dependence on unreliable sources***
  - Economic Security
    - ***Assured supplies at affordable prices***
  - Environmental Security
    - ***Obtaining and using energy in ways that do not harm the environment***
- **Improving Energy Security requires advances in all domestic, clean, and reliable forms of energy**
  - Biomass
  - Geothermal
  - Wind
  - Solar
  - Conservation
  - and . . . **Nuclear**



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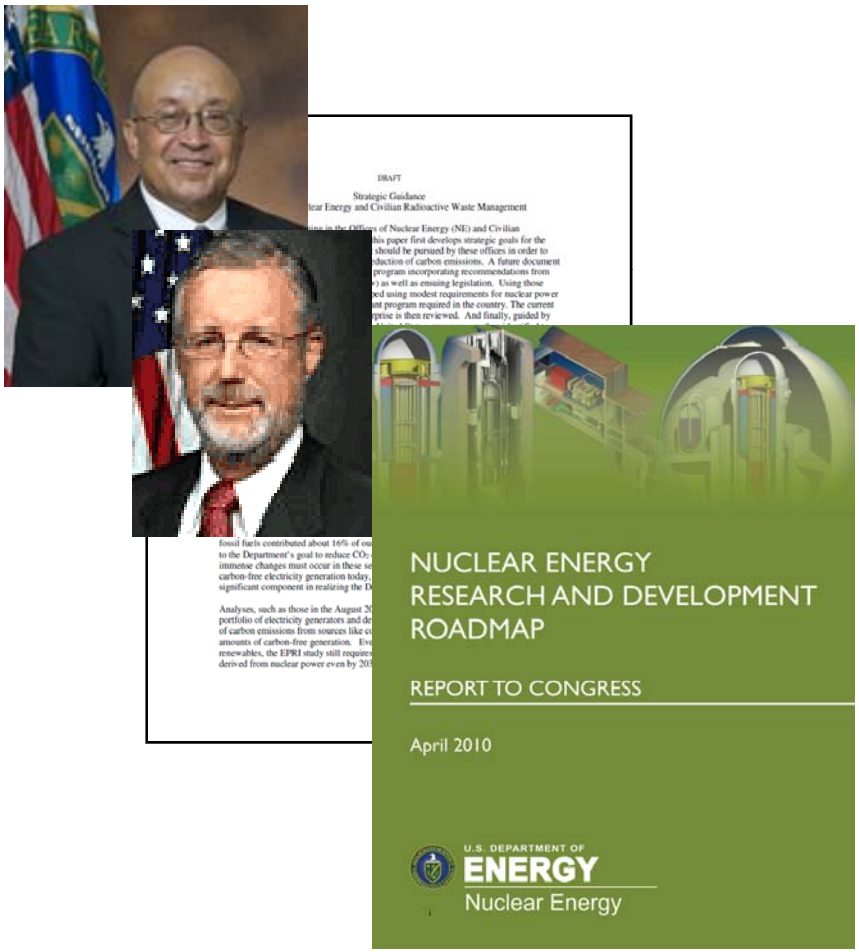
NE R&D Roadmap



- ***R&D Objective 1*** – Develop technologies and other solutions that can improve the reliability, sustain the safety, and extend the life of current reactors.
- ***R&D Objective 2*** – Develop improvements in the affordability of new reactors to enable nuclear energy to help meet the Administration's energy security and climate change goals.
- ***R&D Objective 3*** – Develop sustainable nuclear fuel cycles.
- ***R&D Objective 4*** – Understand and minimize the risks of nuclear proliferation and terrorism.

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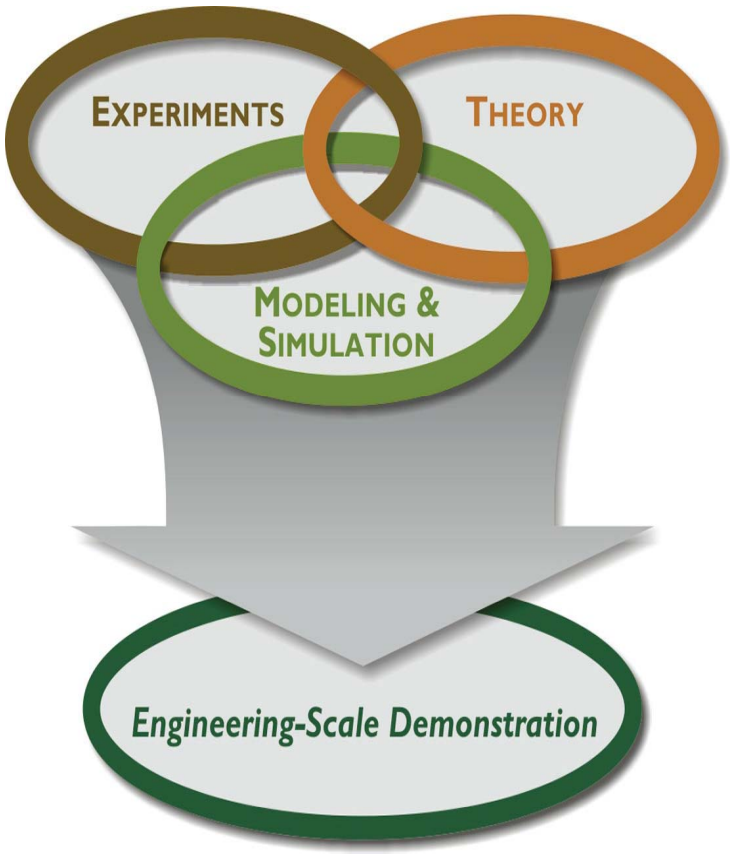
Modeling and Simulation Is An Essential Element



- **Advanced Modeling and Simulation Tools –** Conduct R&D needed to ***create*** a new set of modeling and simulation capabilities that ***will be used*** to better understand the safety performance of the aging reactor fleet. These tools will be fully three-dimensional, high-resolution, modeling integrated systems based on first-principle physics. To accomplish this, the modeling and simulation capabilities will have to be run on modern, highly parallel processing computer architectures.

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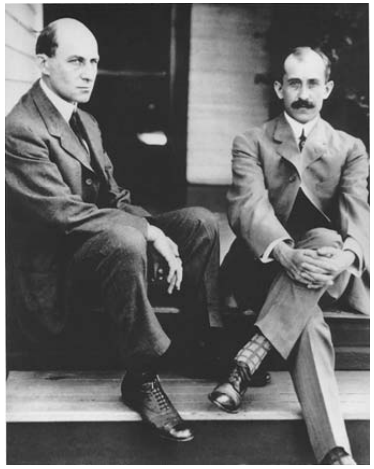
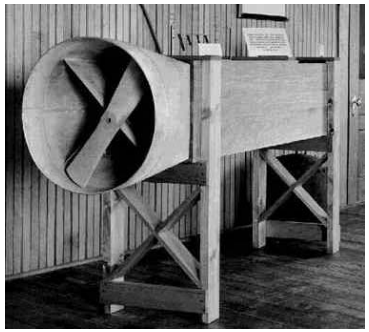
But First A Question . . .

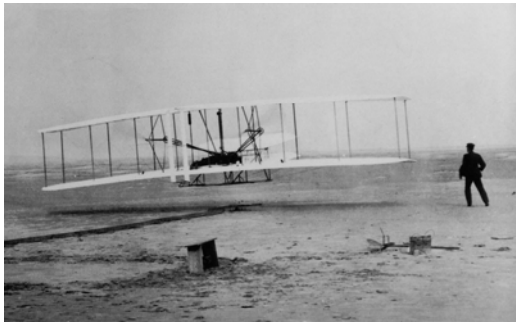
Why did these guys fly?



1901 Wind Tunnel



These guys built and used one of these

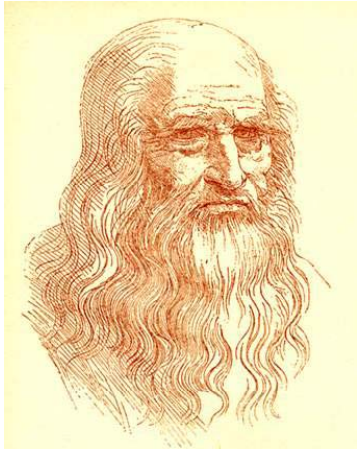


Before they did this in1903

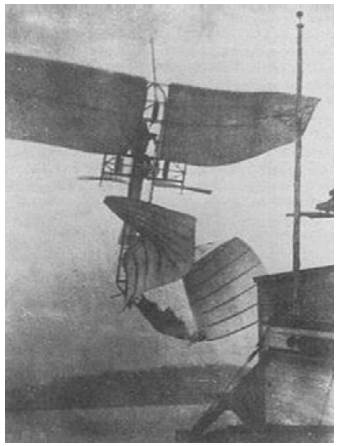
AMSO is in the wind tunnel invention business.

When this guy could not?

This guy spent his time studying birds.



And his airplane looked like this.



But flew like this.

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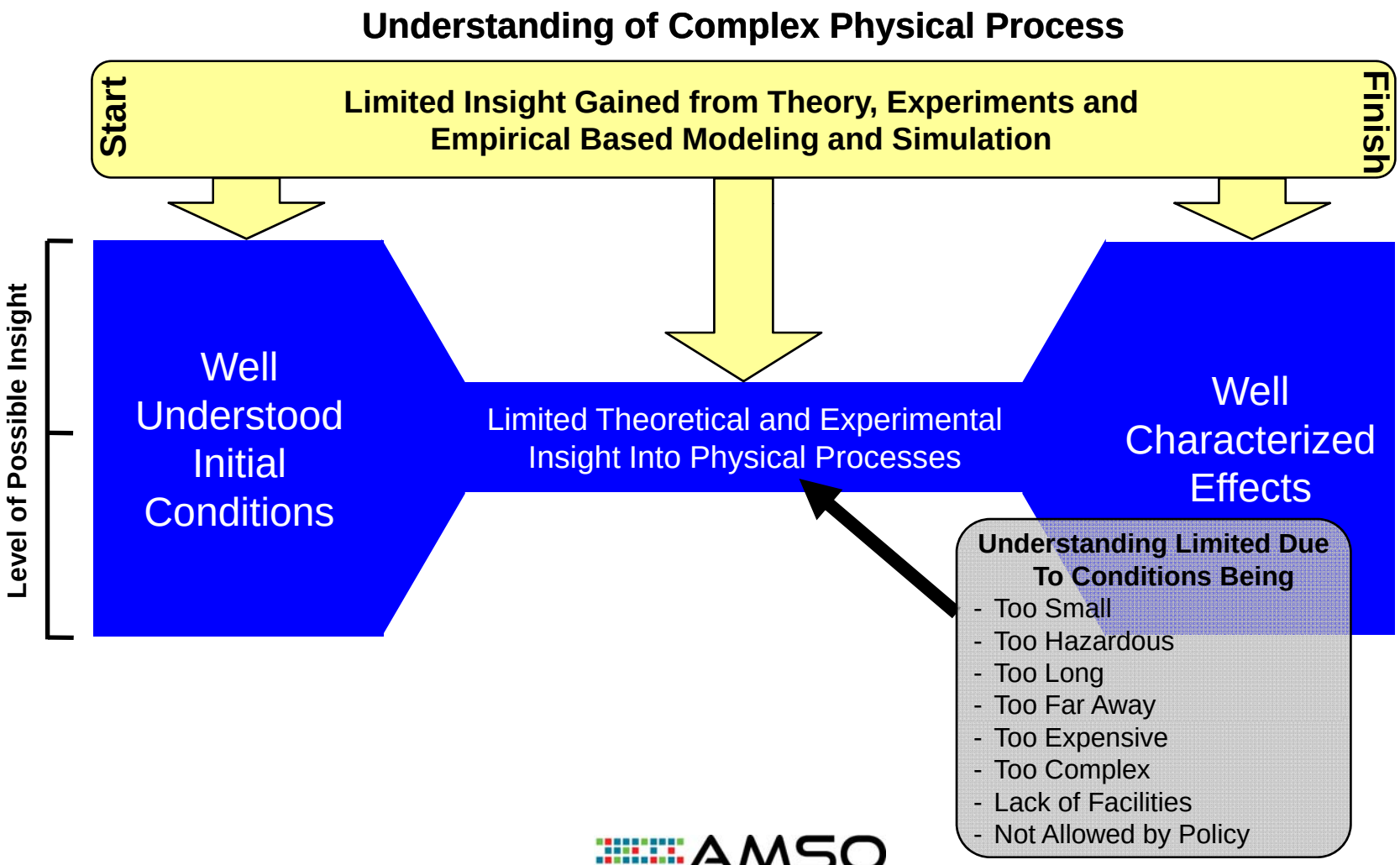
Why Step Up to New Methods of Gaining Insight?



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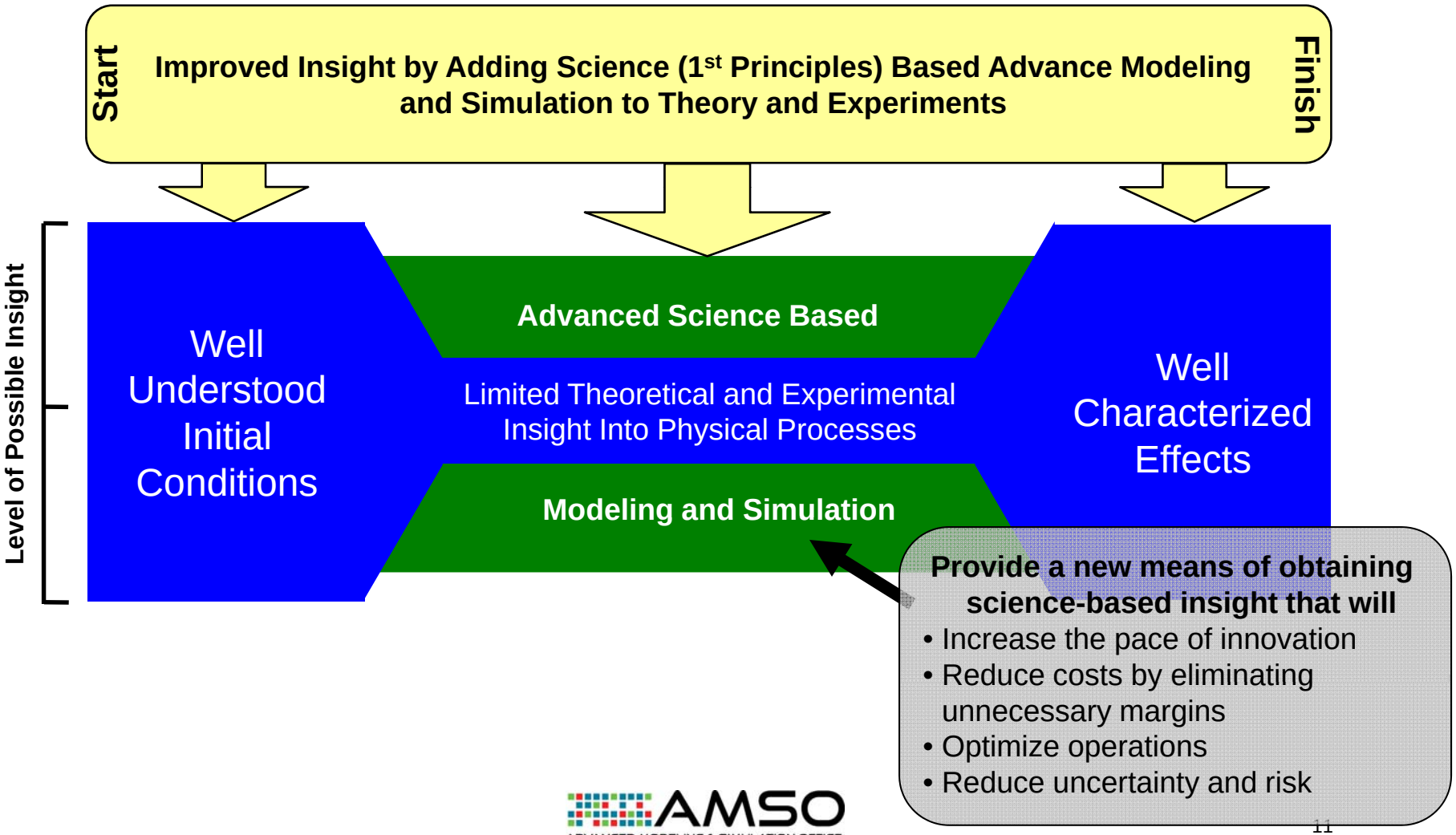
Supplements Theory and Experiment to Explain "How" Things Happened

Understanding of Complex Physical Processes



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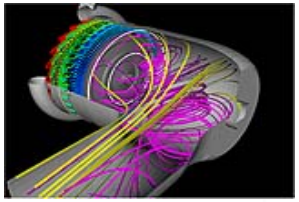
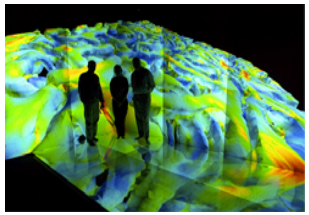
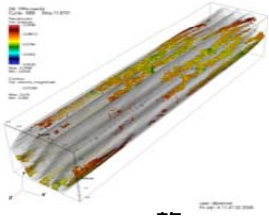
What Industry Has Learned About the Value of Modeling and Simulation Tools

Industry Sector	Problem	20th Century	Today	Value of Change
Aerospace	■ Reduce weight ■ Increase fuel efficiency	■ Physical models ■ Wind tunnels ■ Build and fly prototypes	■ Computational – CFD – Structural Mechanics ■ Build and fly confirmatory test	■ 20% Fuel Savings ■ 50% Composite materials ■ 30% Nox emission reduction
Automobile	■ Reduce weight ■ Increase safety ■ Improve mileage	■ 5-7 year product cycle ■ Wind tunnels ■ Full scale models ■ 7-10 crash tests	■ Extensive use of computational – CFD – Structural mechanics	■ Product cycle reduced to 2 years ■ 85% Reduction in crash testing
Oil & Gas	■ Find new reserves ■ Optimize reservoir output without damaging the field	■ Drill test wells ■ Best-guess reservoir management ■ Limited seismic analysis	■ Computation seismic time pre-stack migration ■ Computational simulations of well planning and reservoir management	■ Improved discovery rates in geologically challenging areas ■ Reduced time for well planning by factor of 100 ■ Improved extraction from secondary and tertiary methods
Nuclear Energy	■ Upgrade reactor power ■ Extend licenses	■ Test & sample-based analysis ■ Empirically based modeling and simulation tools	■ 20 year extensions granted based on samples and analysis ■ Power upgrades allowed	■ Extended availability of profitable energy from nuclear ■ Improved output per reactor







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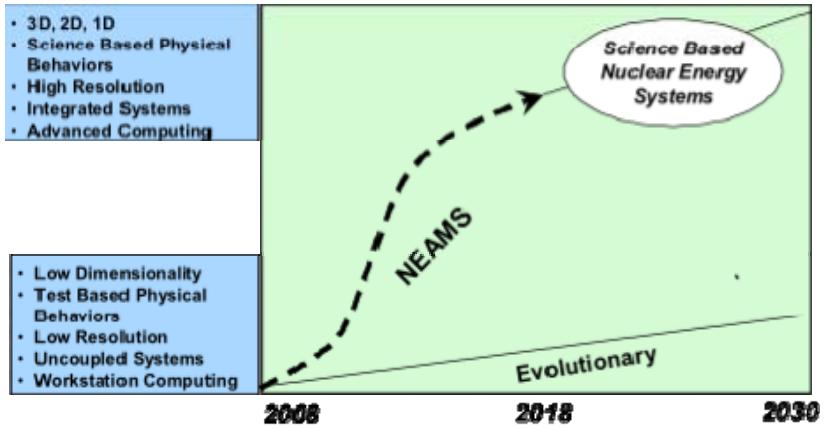
NEAMS Vision (since 2008)

- **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

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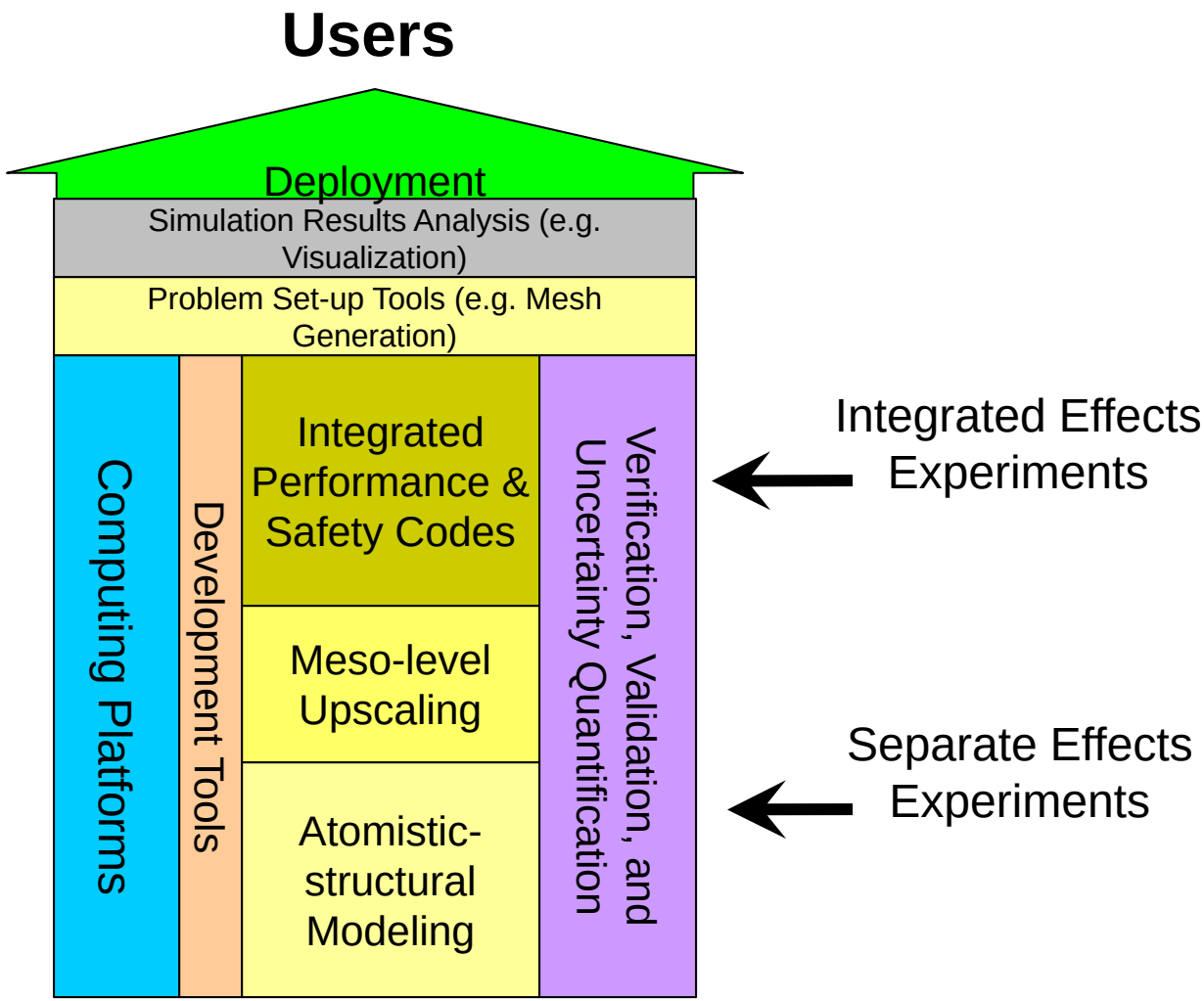
Generic Advanced Modeling and Simulation Capability Architecture

Note: An advanced modeling and simulation program does not have to build all of the elements. However, it must ensure that all of the elements exist and are integrated in order to build advanced capabilities



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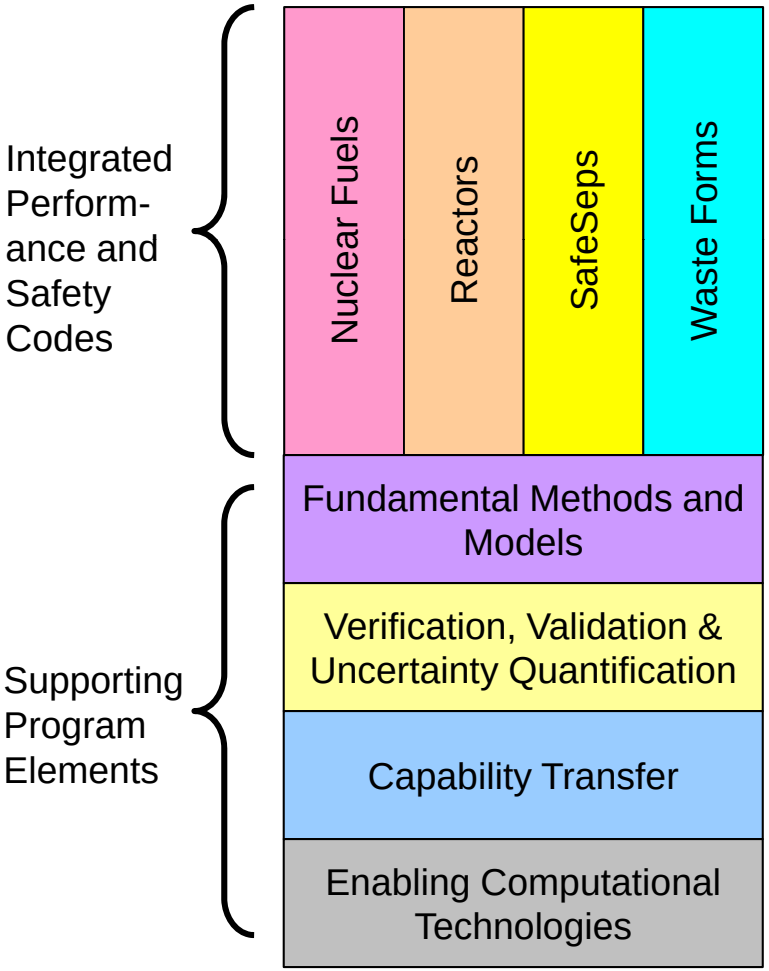
NEAMS Program Elements



- **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**
  - **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**

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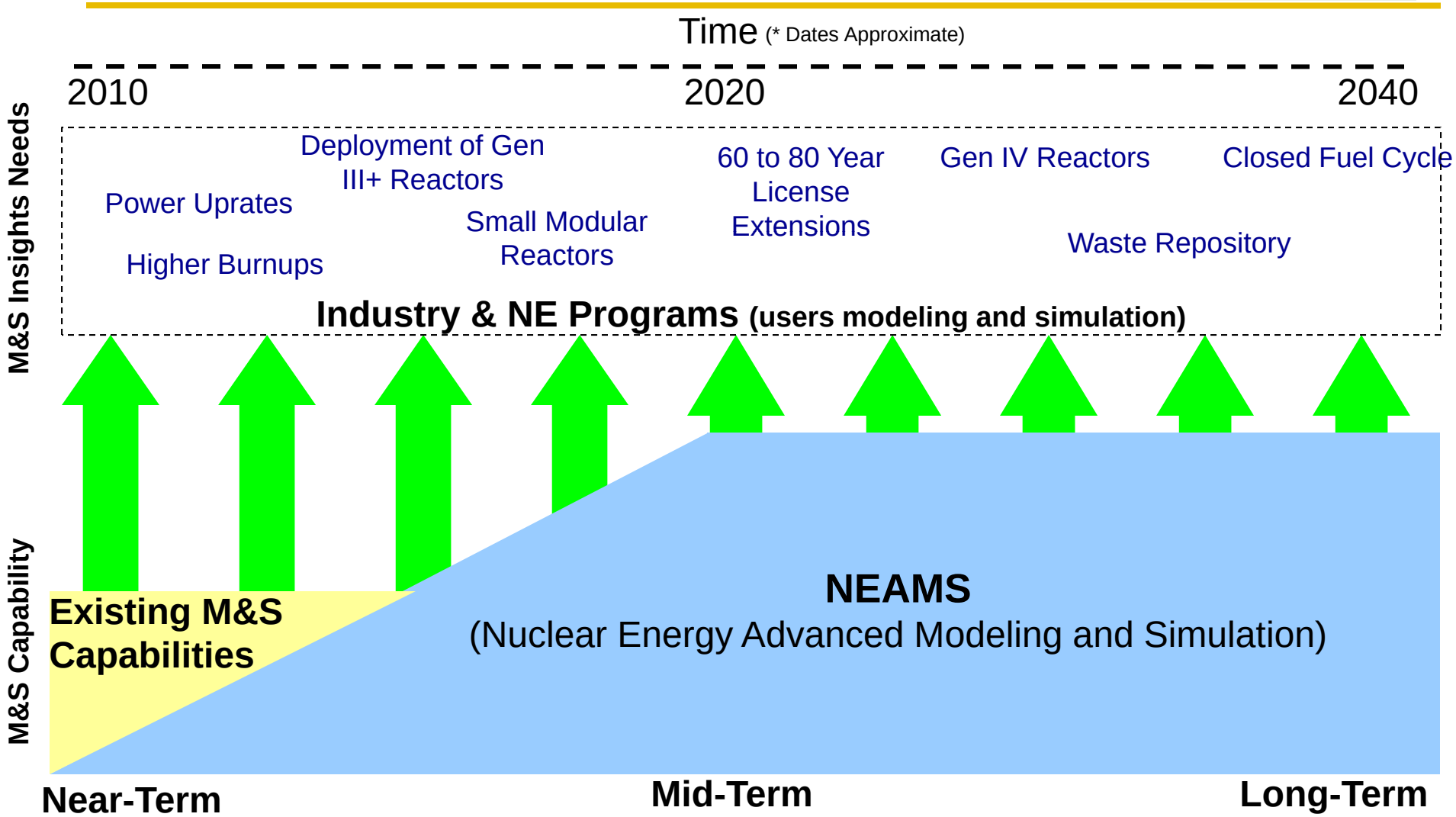
NEAMS Planned Role (circa 2009)



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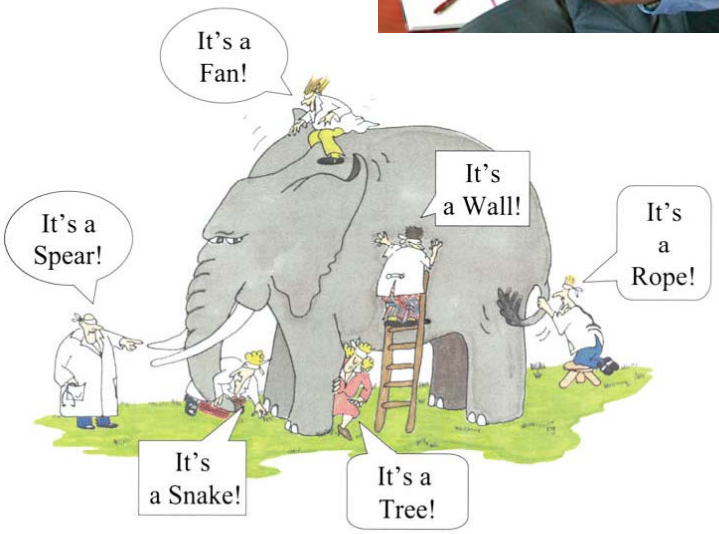
And Then a Surprise Walked the Room



"The proposed Energy Innovation Hubs will take a very different approach – they will be multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges"

- **Leadership**
  - **Outstanding scientist leaders who will have flexibility on a day-to-day basis to guide Hub activities**
- **Connection to NE R&D**
  - **Focused on a small range of important problems to maximize impact**
- **Funding**
  - **Lower ($25M per year for 5 years), but stable**

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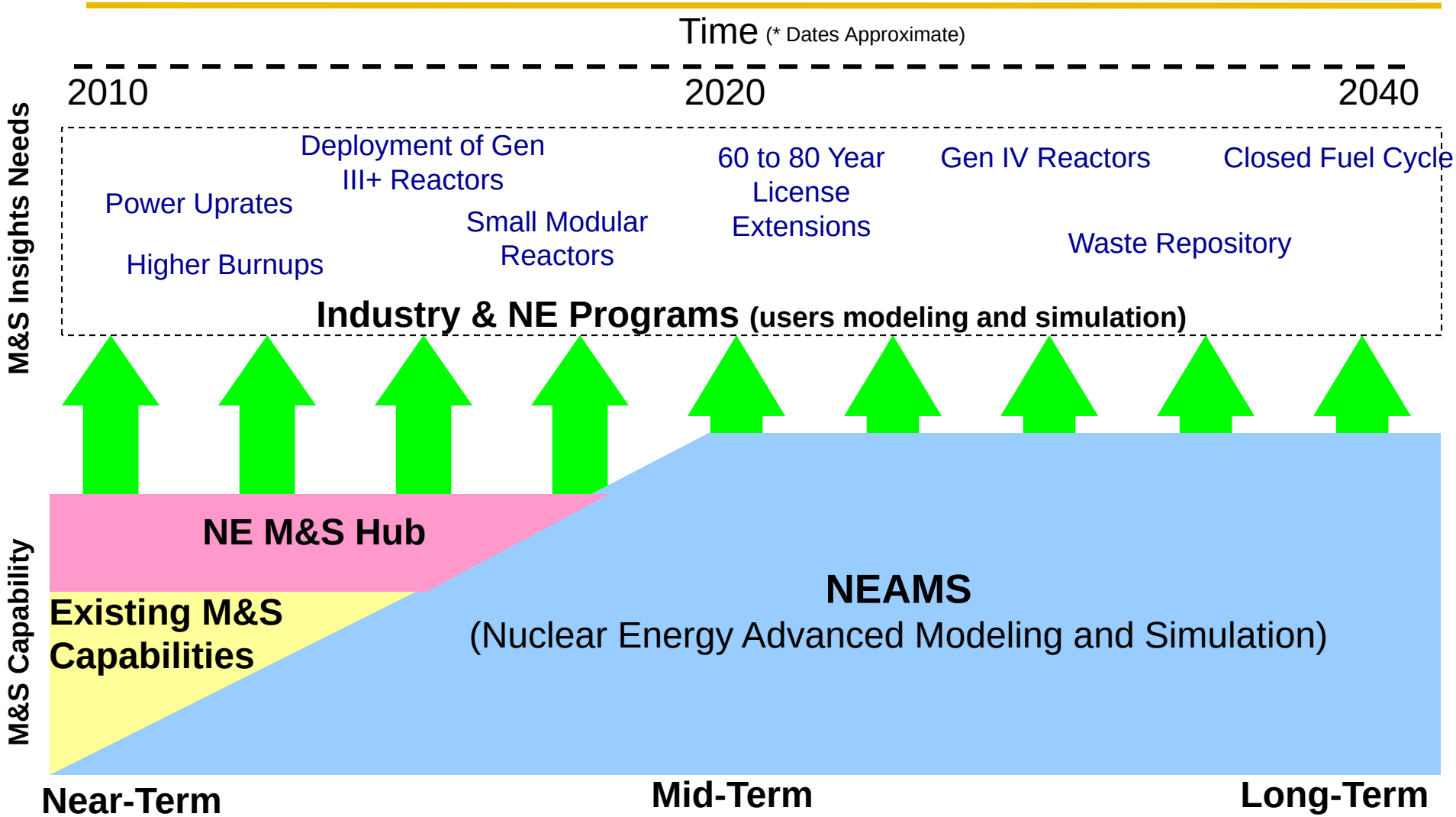
NEAMS and the Hub – Support the Full Range of NE Modeling and Simulation Needs



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Consortium for Advanced Simulation of LWRs

- **Near Term**
  - In 2 to 4 years create advanced modeling and simulation tools to better understand fuel performance in the current generation of nuclear reactors
  - This understanding, quickly deployed to industry, can lead to power uprates, and deeper burn rates
- **Mid Term**
  - These same tools will be used to improve the power output of the next generation (Gen III & III+) reactors
  - The tools will also impact the performance and safety of the near term small modular reactors

CASL

Bottom Line: ***The Hub, if successful, should enable at least 5,000 to 7,000 MW(e)* of additional domestically produced, non-carbon emitting, affordable energy on the grid.***

*Source: Westinghouse, TVA, and EPRI estimates

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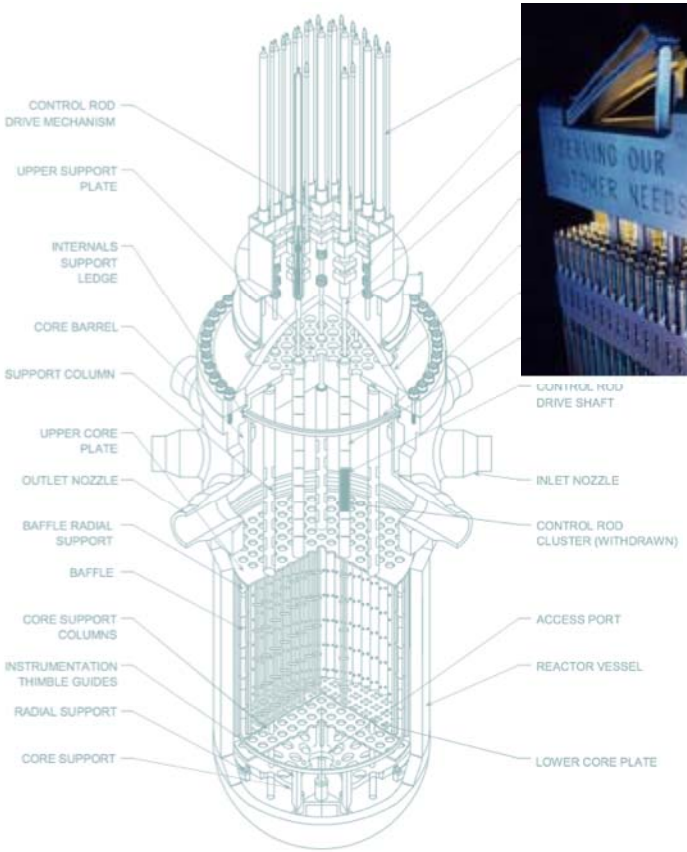
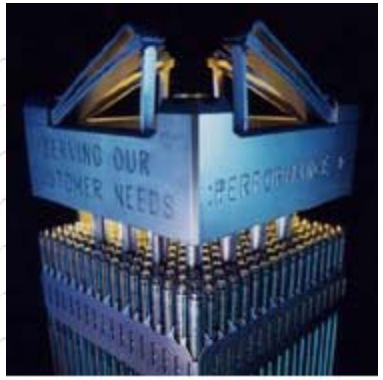
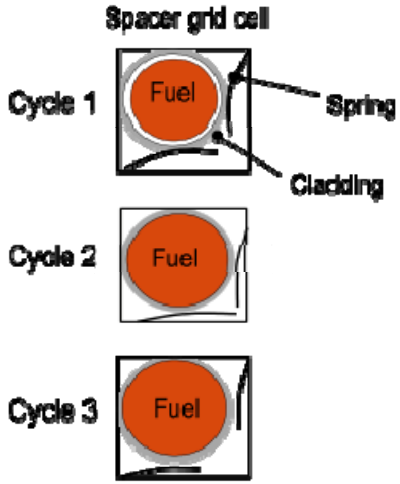
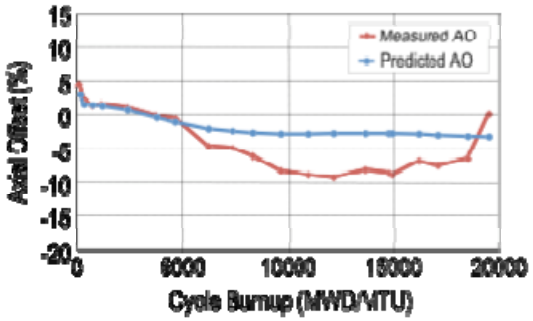
How will the Hub accomplish this?

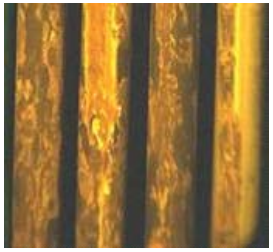
The primary power limiting factor for the current generation of reactors is understanding nuclear fuel performance











CRUD deposits

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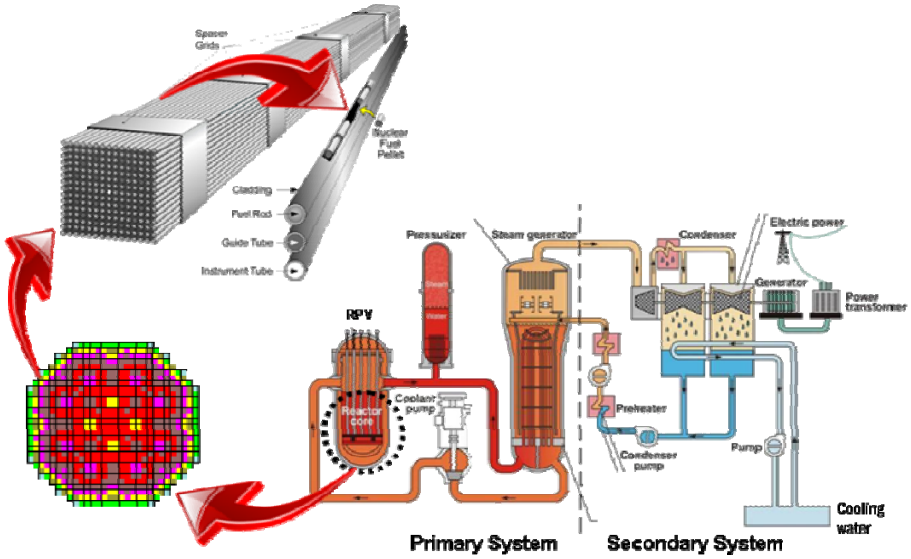
Full Problem Set

TVA Owned

Sequoya 1 & 2

Watts Bar 1 (& 2 Through Startup Testing)



Operational
CRUD-induced power shift (CIPS)
CRUD-induced localized corrosion (CILC)
Grid-to-rod fretting failure (GTRF)
Pellet-clad interaction (PCI)
Fuel assembly distortion (FAD)
Safety
Departure from nucleate boiling (DNB)
Cladding integrity during loss of coolant accidents (LOCA)
Cladding integrity during reactivity insertion accidents (RIA)
Reactor vessel integrity
Reactor internals integrity

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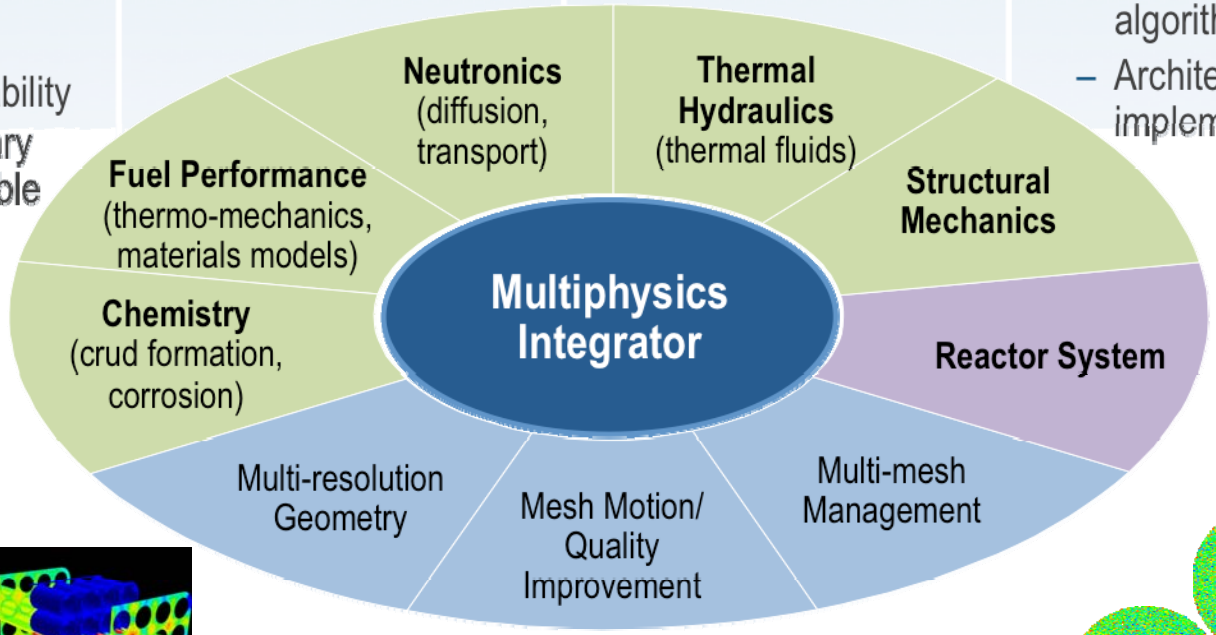
Approach to the Virtual Reactor

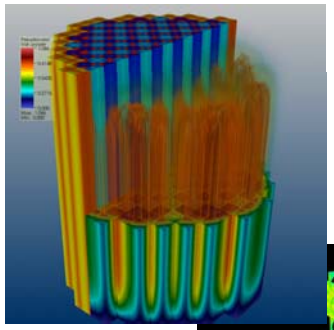
- Flexible coupling of physics components
- Toolkit of components
  - Not a single executable
  - Both legacy and new capability
  - Both proprietary and distributable

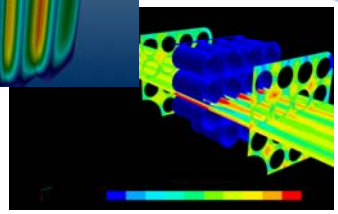
- Attention to usability
- Rigorous software processes
- Fundamental focus on V&V and UQ

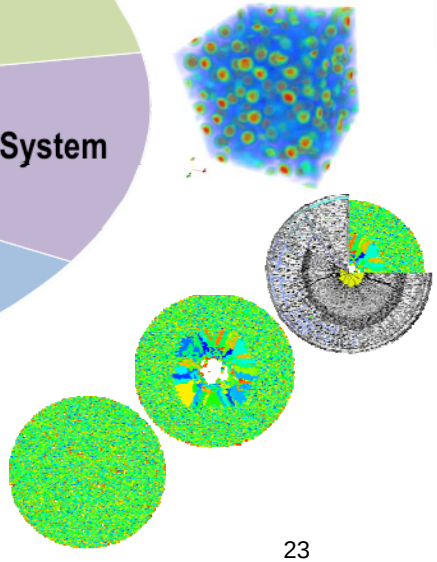
- Development guided by relevant challenge problems
- Broad applicability

- Scalable from high-end workstation to existing and future HPC platforms
  - Diversity of models, approximations, algorithms
  - Architecture-aware implementations









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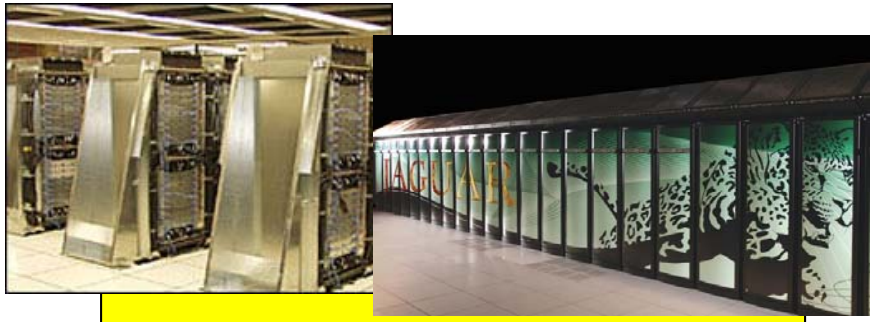
Other Benefits from the Hub

- Due to the hiatus of new nuclear reactor construction in the U.S., designers and engineers did not invested heavily in advanced modeling and simulation (like the aerospace and the automotive industries)
- If the Hub is to be successful, it will have to improve the "usability" of modern high performance computing (HPC) and "lower the bar" for engineers to successful apply these tools to solve problems
- Doing this will have a ripple effect on all users of HPC and will improve U.S. competitiveness in the world markets



HPC Simulation at the Speed of Thought!

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Understanding NEAMS Potential 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

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

- **Integrated Performance and Safety Codes**
  - **Nuclear Fuels**
    - **LANL – lead**
    - **ORNL**
    - **LLNL**
    - **INL**
    - **Florida State**
    - **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
    - INL – lead
    - IL
    - RNL
    - rth Carolina State
    - Michigan
    - Nevada, Reno
    - Wisconsin
  - Verification, Validation and Uncertainty Quantification
    - INL – lead
    - SNL
    - ANL
    - iversity of Idaho
  - apability Transfer
    - RNL - Lead
    - ANL
    - IBM
  - Enabling Computational Technologies
    - LLNL

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NEAMS Management Structure

Office of Nuclear Energy

Federal Manager
Alex Larzelere

Outside Review Panel
(to be established)

Review overall program and technical approaches

Deputy TIO for Adv Modeling and Simulation,
Hussein Khalil, ANL

National Technology Director,
Keith Bradley, ANL

Laboratory Steering Committee
(to be established)

Reps from all labs involved, high level strategic guidance

Program Management Team (PMT)

- Fuels IPSC – Steve Hayes, INL
- Reactor IPSC – Dave Pointer, ANL
- SafeSeps IPSC – Prabhat Sadasivan, LANL
- Waste Forms – Randy Summers, SNL
- VU – Jim Stewart, SNL
- CT – David Bernholdt, ORNL
- ECT – Lori Diachin, LLNL

Day to day management

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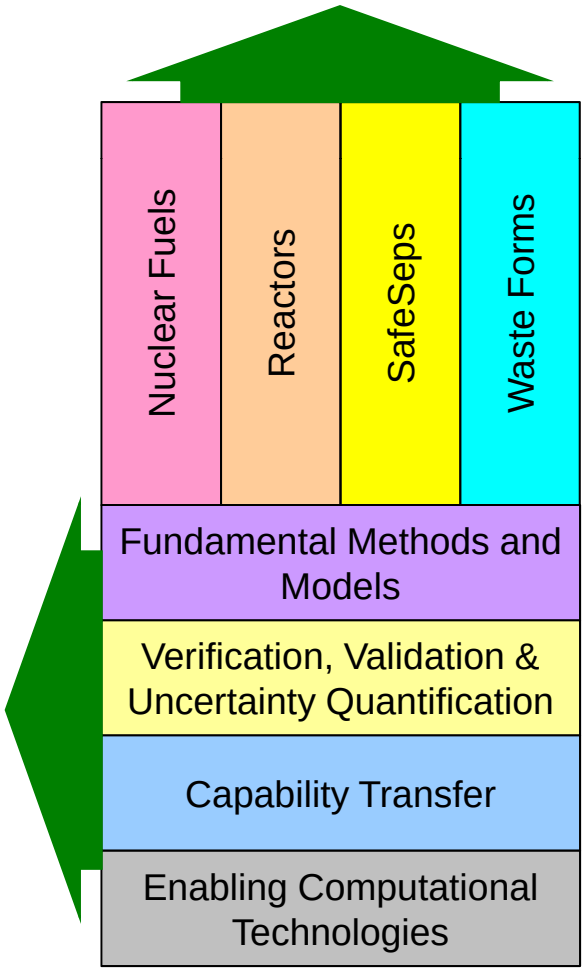
NEAMS Meeting Structure & Interfaces

- **2010 NEAMS Meetings**
  - **January PMT Face-to-Face**
    - **Program coordination**
  - **April PI Meeting**
    - **Kick-off of FY-11 planning**
  - **July PMT Face-to-Face**
    - **Review and coordination of master work packages**
  - **October PI Meeting**
    - **Technical progress review**
- **Fuel Cycle and Reactor Technologies R&D Meetings**
  - **IPSCs attend as necessary**
- **NNSA and Office of Science Interface Meetings**
  - **Supporting elements attend as necessary**

Primary Interface to NE R&D Programs



Primary interface to Office of Science, NNSA, NRC, Industry and Universities

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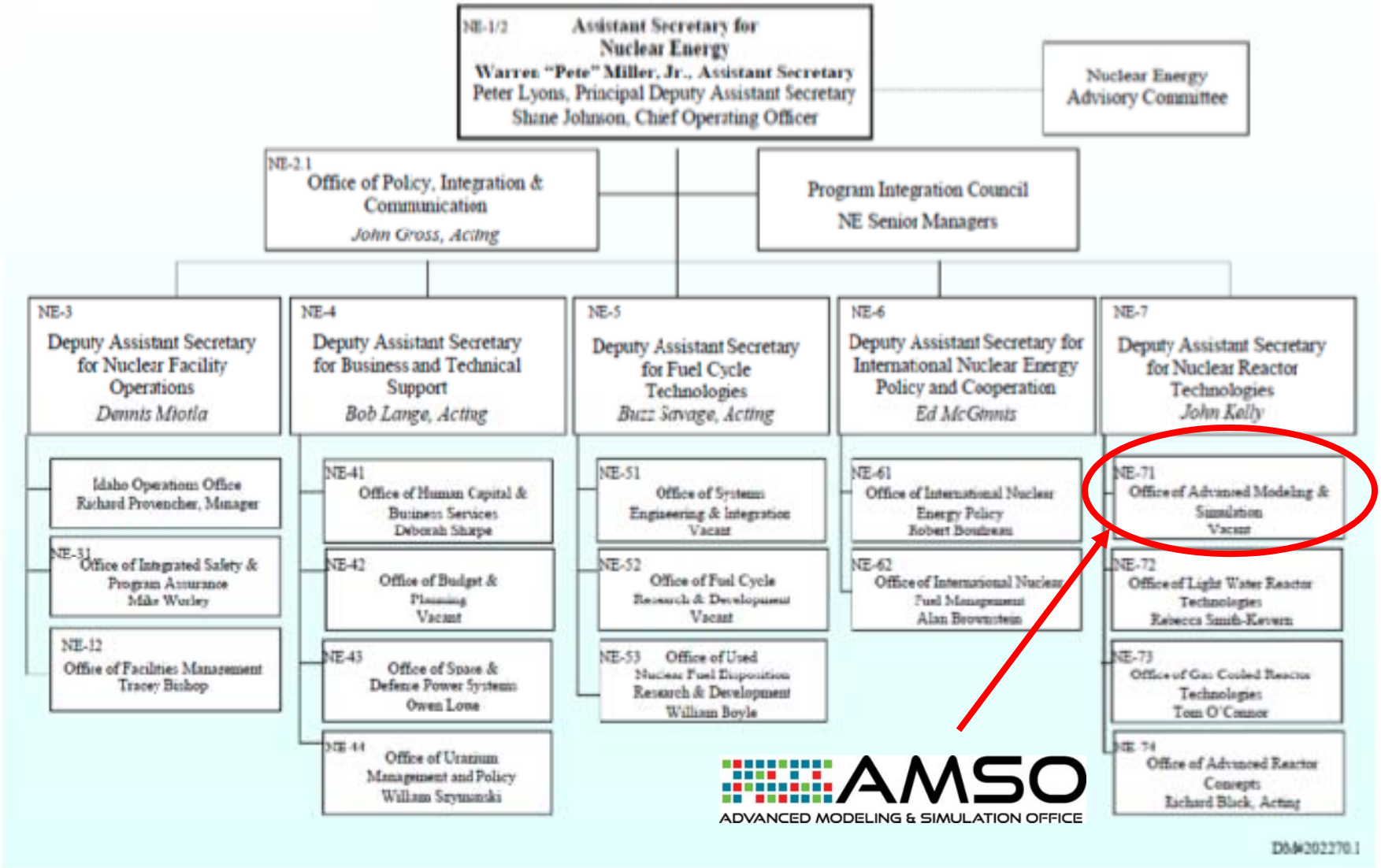
NE-71 Established



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Lots of New Players in FY-2010

DOE Side

- **Pete Miller - Asst Sec for NE**
- **Pete Lyons - Principal DAS**
- **John Kelly - Reactor Technologies DAS**
- **Trevor Cook - Deputy, AMSO**
- **Rob Versluis - Fed Manager, Fuels and Reactors IPSC, AMSO**
- **Dan Funk - Fed Manager, SafeSeps and Waste IPSC, AMSO**
- **Jim Peltz - Fed Manager, Supporting Elements**

Lab Side

- Hussein Khalil (ANL) – TIO Deputy for Adv Modeling and Simulation
- Keith Bradley (ANL) – NEAMS National Technology Director
- Steve Hayes (INL) – Lead, Fuels IPSC
- Dave Pointer (ANL) – Lead, Reactor IPSC
- Randy Summers (SNL) – Lead, Waste IPSC
- Jim Steward (SNL) – Lead, VU

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Assessing the State of NEAMS

- Vision
  - A problem of national significant
  - Having a vision of how to impact it
- Plan
  - Understanding "what" is required to implement the vision
  - Understanding of the process required to achieve the "what"
- Team
  - Assembling the highly qualified team members to accomplish the "whats"
  - Organizing the team to ensure that everybody knows their role
- Endurance
  - Execution – success breeds success
  - Ensuring that adequate resources (e.g. money, compute cycles, technologies) are available to implement the plan

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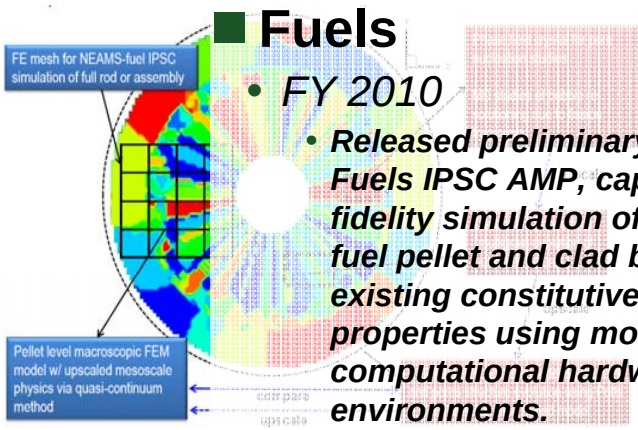
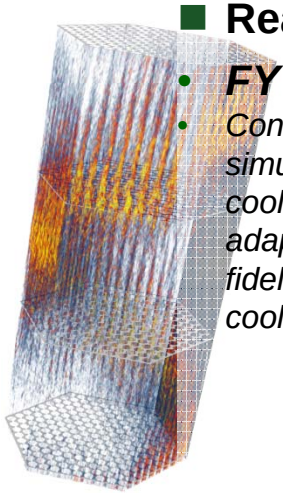
NEAMS IPSC Achievements

Fuels



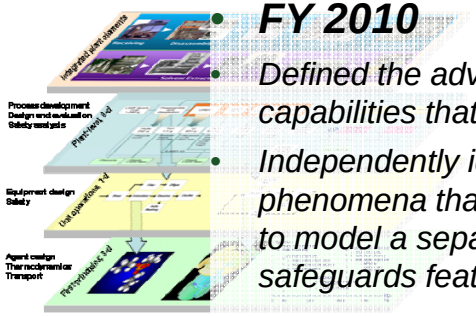
- *FY 2010*
  - ***Released preliminary version 1 of the Fuels IPSC AMP, capable of high-fidelity simulation of uranium-oxide fuel pellet and clad behavior using existing constitutive materials properties using modern computational hardware and software environments.***

Reactors



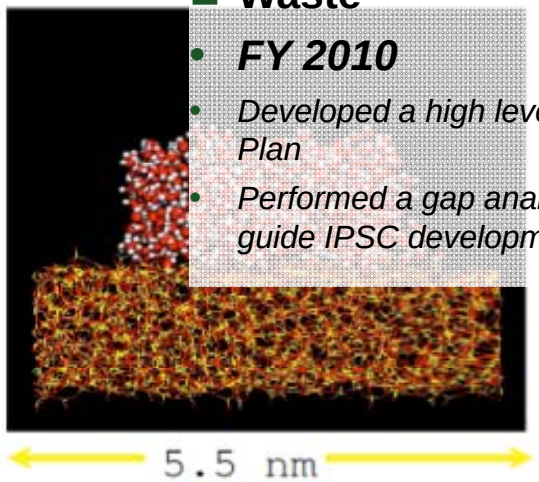
- ***FY 2010***
- *Continued to improve the SHARP modeling and simulation framework for simulating sodium-cooled fast-spectrum reactors and completed adaptations of the SHARP framework for high-fidelity simulation of high-temperature, gas-cooled reactors*

SafeSeps



- ***FY 2010***
- *Defined the advanced modeling and simulation capabilities that comprise the Safe Seps IPSC*
- *Independently identified and ranked the phenomena that must be understood in order to model a separations plant, and its integrated safeguards features*

Waste



- ***FY 2010***
- *Developed a high level Verification & Validation Plan*
- *Performed a gap analysis on key phenomena to guide IPSC development*

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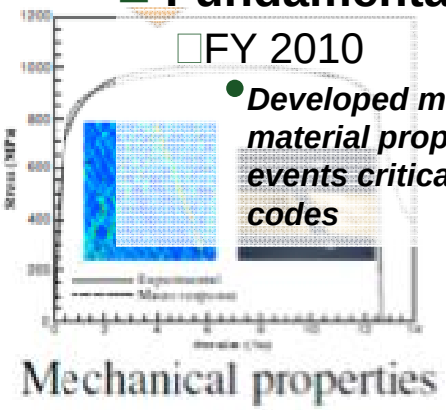
NEAMS Supporting Element Achievements

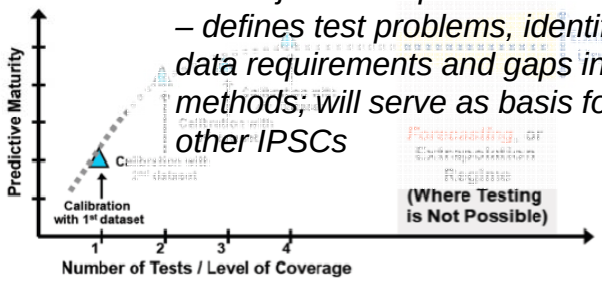
Fundamental Methods & Models



- FY 2010
  - ***Developed models and methods to predict material properties and simulate atomistic events critical to advanced fuels and reactor codes***

V&V, UQ

- ***FY 2010***
- *Issued joint V&V plan for the waste form IPSC – defines test problems, identifies validation data requirements and gaps in error UQ methods; will serve as basis for V&V plans with other IPSCs*

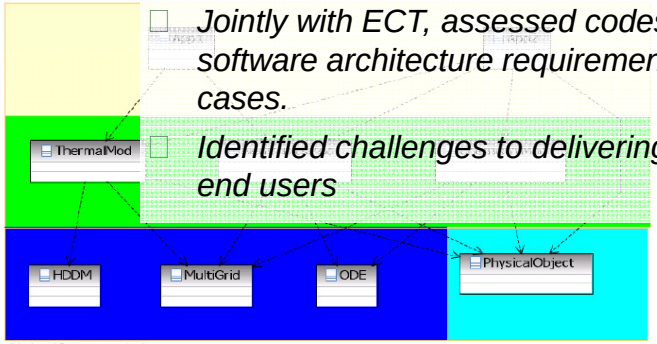


Enabling Computational Technologies

- ***FY 2010***
- *Completed risk assessments as basis for IPSC-specific Software Quality Assurance plans*
- *Demonstrated mesh-to-mesh coupling technology for reactor IPSC*

Capability Transfer

- ***FY 2010***
- *Jointly with ECT, assessed codes to develop software architecture requirements and use cases.*
- *Identified challenges to delivering codes to end users*



(Notional Representation)

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FY 2010-11 Budget Summary

dollars in thousands

	FY 2010 Approp.	FY 2011 Request	FY 2011 House	FY 2011 Senate
Energy Innovation Hub for Modeling and Simulation *	**21,384**	**24,300**	**12,150**	**16,000**
NEAMS		**25,413**		
NEUP	**0**	**2,550**		
SBIR/STTR	**616**	**1,037**		

*Hub was funded in the GEN IV Program in FY 2010

- **Sources of NEAMS funding in FY 2011**
  - **FCR&D = $15,570 (NEUP and SBIR already deducted)**
  - **Advanced Reactor Concept R&D = $2,000**
  - **NEET = $5,000**
  - **SMR = $3,750**
  - **NGNP = $1,500**
  - **LWRS = $500**

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The State of NEAMS is Good

- **Vision**
  - A problem of national significant
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- **Plan**
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But There is Some Bad, & Ugly Along With the Good

- **The Good**
  - **Having Pete Miller, Pete Lyons, and John Kelly join DOE**
  - **Publication of the NE R&D Roadmap and how it defined the role of modeling and simulation**
  - **The addition of the Hub and the fact that the competition ran smoothly and did not disrupt NEAMS (too much)**
  - **All NEAMS Meetings held as planned**
  - **The FY-11 work planning process up to the final preparation of the work packages**
  - **Establishment of NE-71**
  - **The addition of new Federal and Laboratory managers**

- **The Bad (or at least worrisome)**
  - Lots of turnover of people
  - The uncertainty and competition caused by the addition of the Hub
  - Adjustment of the scope and players for some IPSCs
  - Still need to improve interfaces (particularly with NEUP)
  - Need to establish Lab Steering Committee and Outside Review Panel

- **The Ugly**
  - The FY-2011 work planning preparation process and the need for one work package for one NEAMS element for one lab participant for each source of funding (over 70 separate work packages)

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And Continues to Get Better!

- **The future of AMSO, that includes NEAMS and the Hub, looks bright!**
- **NEAMS builds on a solid foundation based on NE programmatic funding**
  - **Established management team and structure (both at HQ and the labs)**
  - **Has a clear technical scope (building advanced modeling and simulation to be used to support NE R&D)**
  - **Solid record of delivery and achievement**
- **While new – the Hub is moving quickly to deliver modeling and simulation products to be used to increase nuclear energy generated electricity**
  - **Quickly stood up and operating – expects to fully cost FY 2010 & 2011 funds by the end of FY 2011**
  - **Delivering "first drop" of the virtual reactor code in December 2010**
  - **Tightly connected to industry and regulatory bodies to ensure deployment as soon as possible**