



Building New Means of Scientific Insight for Nuclear Energy

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Advanced Modeling and Simulation Provides New Science Based Ways of Understanding the World

Why Do This? – Traditional Means of Insight Are Not Good Enough:

Traditional Means

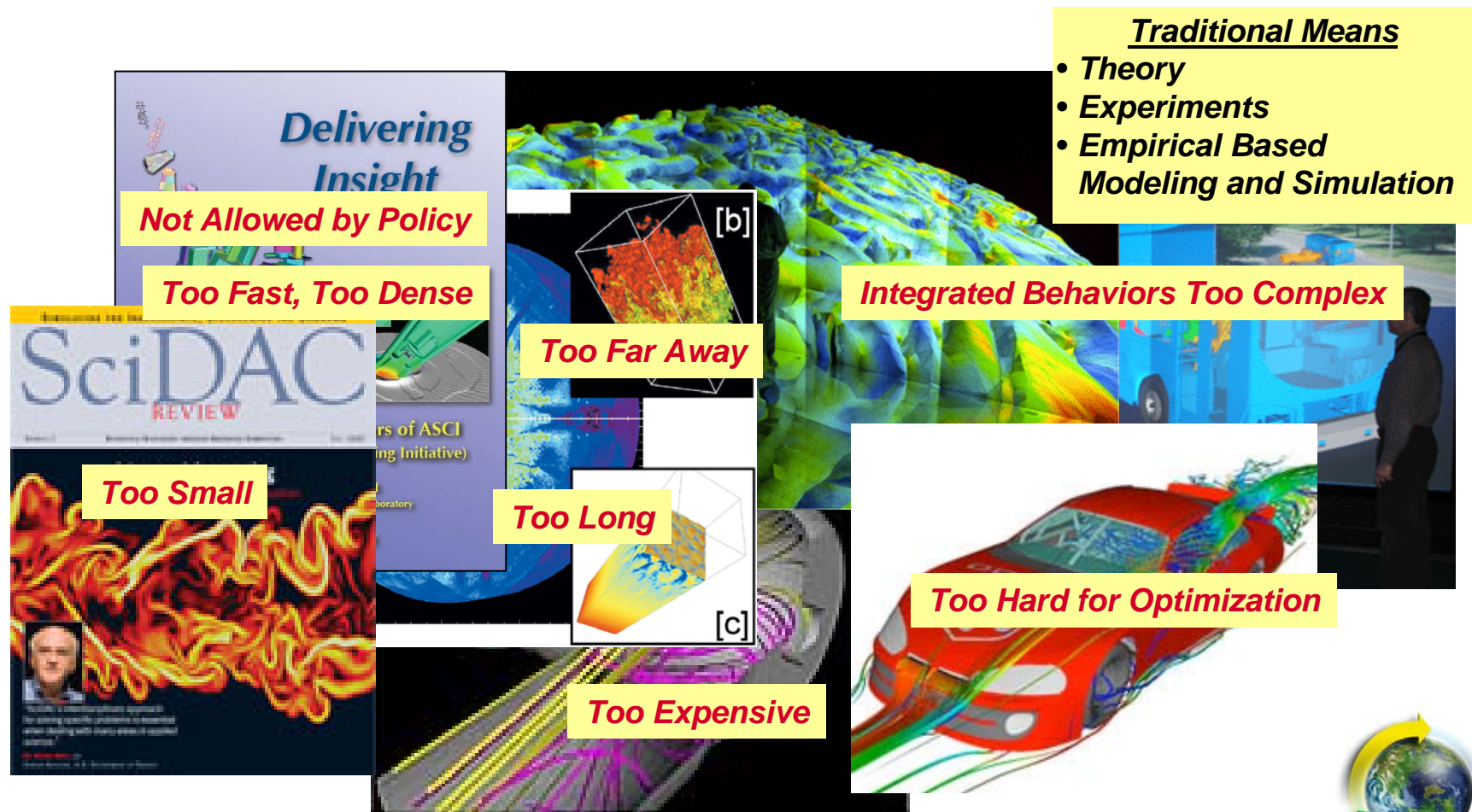
- Theory
- Experiments
- Empirical Based Modeling and Simulation

Delivering Insight
Not Allowed by Policy
Too Fast, Too Dense

SciDAC REVIEW
Too Small

Too Far Away
Too Long
Too Expensive

Integrated Behaviors Too Complex
Too Hard for Optimization





April 8, 2008 - DOE Secretary Bodman Presents the 1st-ever James R. Schlesinger Award.

James R. Schlesinger Award

This award represents the highest non-monetary level of recognition an employee or contractor can receive in the Department. It is named in honor of the first Secretary of Energy and is bestowed upon one individual each year whose outstanding performance is responsible for contributions of national importance or for affecting significant improvement to the successful implementation of the Department's mission.

Award recipient, in the tradition of Dr. Schlesinger, should have a record of consistently demonstrating outstanding leadership in public service and should exhibit the highest levels of integrity, professionalism, and dedication throughout their service to DOE. All DOE employees and contractors who meet the criteria are eligible to receive this award.



"This award represents the highest non-monetary level of recognition an employee or contractor can receive in the Department."

Dr. Gilbert G. Weigand

National Nuclear Security Administration

Dr. Weigand has distinguished himself with his passion for excellence and with his ability to foster and implement the practices and values that are necessary for the protection of our nation. It is because of his vision and determination that the United States is the world leader in high performance computing, that the Department of Energy leads the country with the best scientific and computing tools and scientists, and that we are able today to certify our nuclear weapons stockpile without underground nuclear testing.

Throughout his tenure at the Department of Energy, he has led the development and use of next-generation scientific and technical tools that provide the foundation of today's Stockpile Stewardship program. From this leadership position, he conceived and implemented the Department's most successful technical program to date, the Accelerated Strategic Computing Initiative (ASCI). Dr. Weigand successfully united the needs of the government programs and national laboratories with the knowledge of the U.S. computing industry, and the support of the U.S. Congress, to put together a ten year plan to build the world's best high performance supercomputers. His vision and ability to engage and organize the technical community were the driving forces behind the successes of ASCI and his implementation strategy assured rapid development and effective alignment in computer industry for the goals and computing investments. More importantly, Dr. Weigand's contributions have impacted more than stockpile stewardship. High-performance computing and simulation, at the ASCI level, pervade all areas of science and technology. In addition to the scientific accomplishments of the ASCI program, Dr. Weigand's efforts have provided reassurance in the safety and security of the stockpile and protection of this Nation.

For his intellectual aptitude, drive, determination and unwavering commitment to supercomputing benefiting both the Department of Energy and the Nation, Dr. Weigand is presented the James R. Schlesinger Award.

"Dr. Weigand successfully united the needs of the government programs and national laboratories with the knowledge of the U.S. computing industry, and the support of the U.S. Congress, to put together a ten year plan to build the world's best high performance supercomputers."

"From this leadership position, he conceived and implemented the Department's most successful technical program to date, the Accelerated Strategic Computing Initiative (ASCI)."





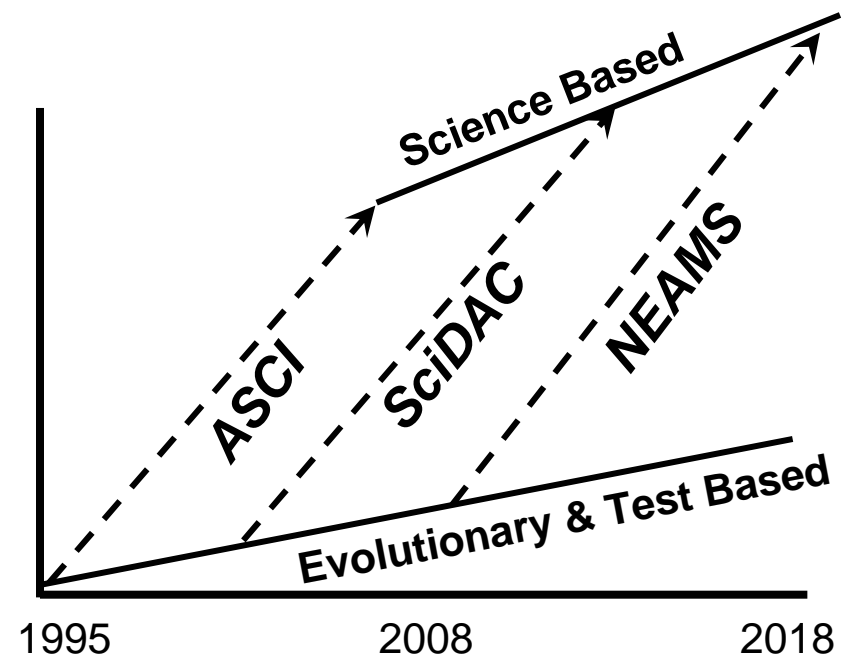
Its Time to Step Up -- Again!

■ Modeling and simulation capabilities that are:

- Science (1st principles) based
- High dimensionality
- High resolution
- Integrated systems
- Adequate modeling of space and time
- Appropriate verification, validation and uncertainty quantification
- Running on the world's most powerful computing platforms using the best programming and results analysis tools

■ ASCI did it for nuclear weapons and the Stockpile Stewardship Program

■ SciDAC did it is for scientific discovery in high energy physics and materials



It is now time to step up again to the next great challenge for the U.S. and the world – Energy Security

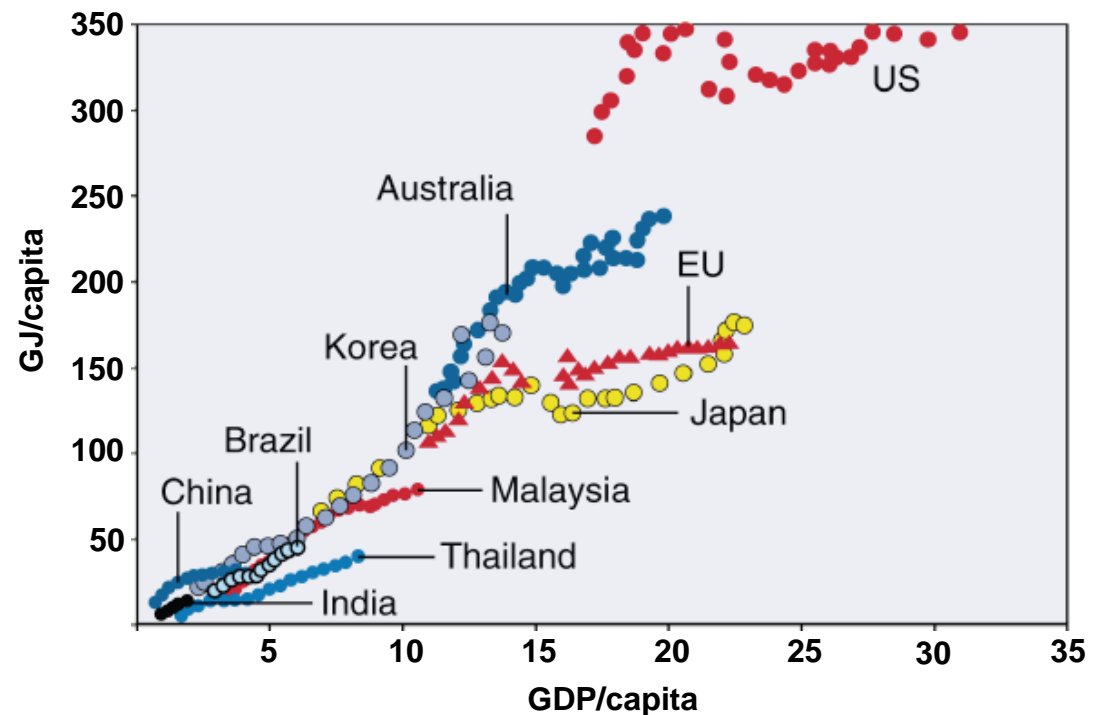




The Worldwide Energy Challenge

- 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





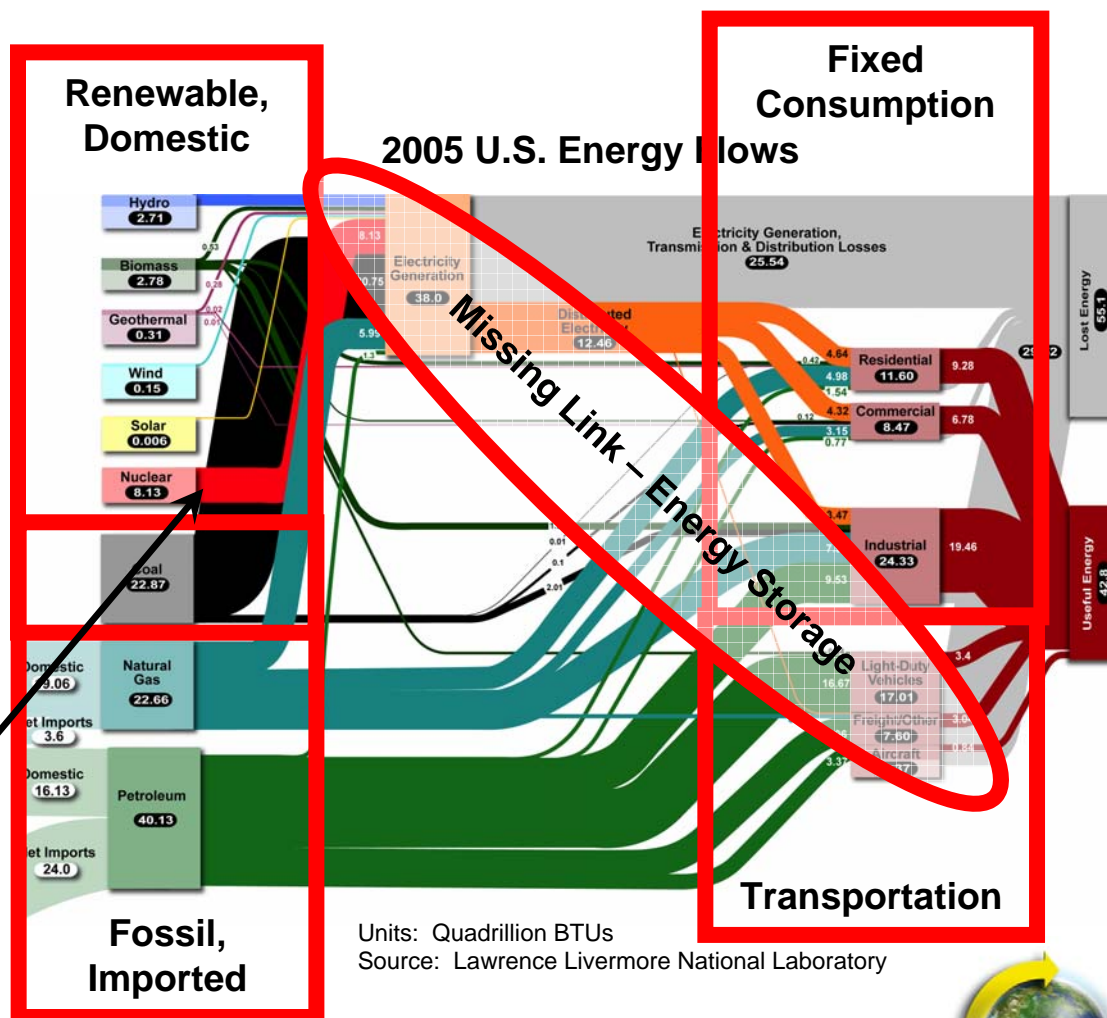
Improving U.S. Energy Security

■ Elements U.S. Energy Security

- **National Security**
 - dependence on unreliable sources
- **Economic Security**
 - need for assured supplies at affordable prices
- **Environmental Security**
 - obtaining energy in ways that does not harm the environment

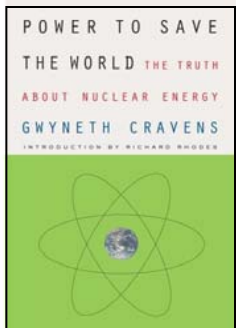
■ Improving Energy Security requires advances in all domestic, clean, and reliable forms of energy

- Biomass
- Geothermal
- Wind
- Solar
- Conservation
- and . . . **Nuclear**



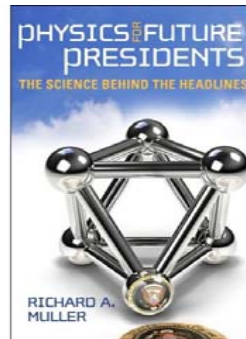


Doing Nuclear Energy & Doing It Better



Power to Save the World by **Gwyneth Cravens**

Physics for Future Presidents by **Richard Muller**



- Proven to be safe, reliable, and environmentally friendly
- Builds on an existing energy distribution network
- Already supplies about 20% of U.S. electrical power
- Already 23 applications expected (and more to come) to be submitted to the NRC for new nuclear electricity generation plants
- Provides 70-80% of the electricity used by France and Japan

■ Long term challenges of nuclear energy:

- Extracting the full energy value of the nuclear fuel through recycling
- The sustainability of the resources needed for nuclear energy
- Creating new waste forms for the un-reusable materials from fuel recycling that do not present long term hazards
- Non proliferation of nuclear materials and technologies

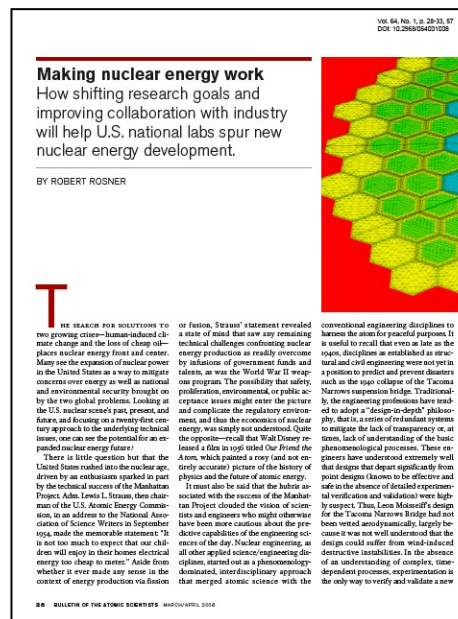
- Meeting these challenges of advancing the use of nuclear energy requires
 - A new generation nuclear energy systems and facilities





Needed – Improved Scientific Insight

- **Nuclear Energy System include:**
 - Fuel recycling reactors
 - Separation plants with appropriate Safeguards
 - New waste forms and optimal use of repositories
 - Policies that encourage countries not to separate used fuel and to depend on assured nuclear fuel sources
- **Previous nuclear systems were developed using a “test-based” approach**
- **A new “science based” approach is necessary**
- **Advanced modeling and simulation is essential to apply science based understanding to new systems**
 - Requires
 - *Higher dimensionality (3D)*
 - *Science (1st principles) based physical behaviors*
 - *High resolution*
 - *Integrated system models*
 - *High performance computers*



Making Nuclear Energy Work

by

Robert Rosner

Bulletin of Atomic Scientists
Mar-Apr '08

- **Done rapidly to impact the design and development of future nuclear energy systems.**
- **Validated by the scientists and engineers with “hands on” experience with similar nuclear systems.**
- **Built on previously successful DOE Advanced Modeling and simulation programs (SciDAC, ASC)**

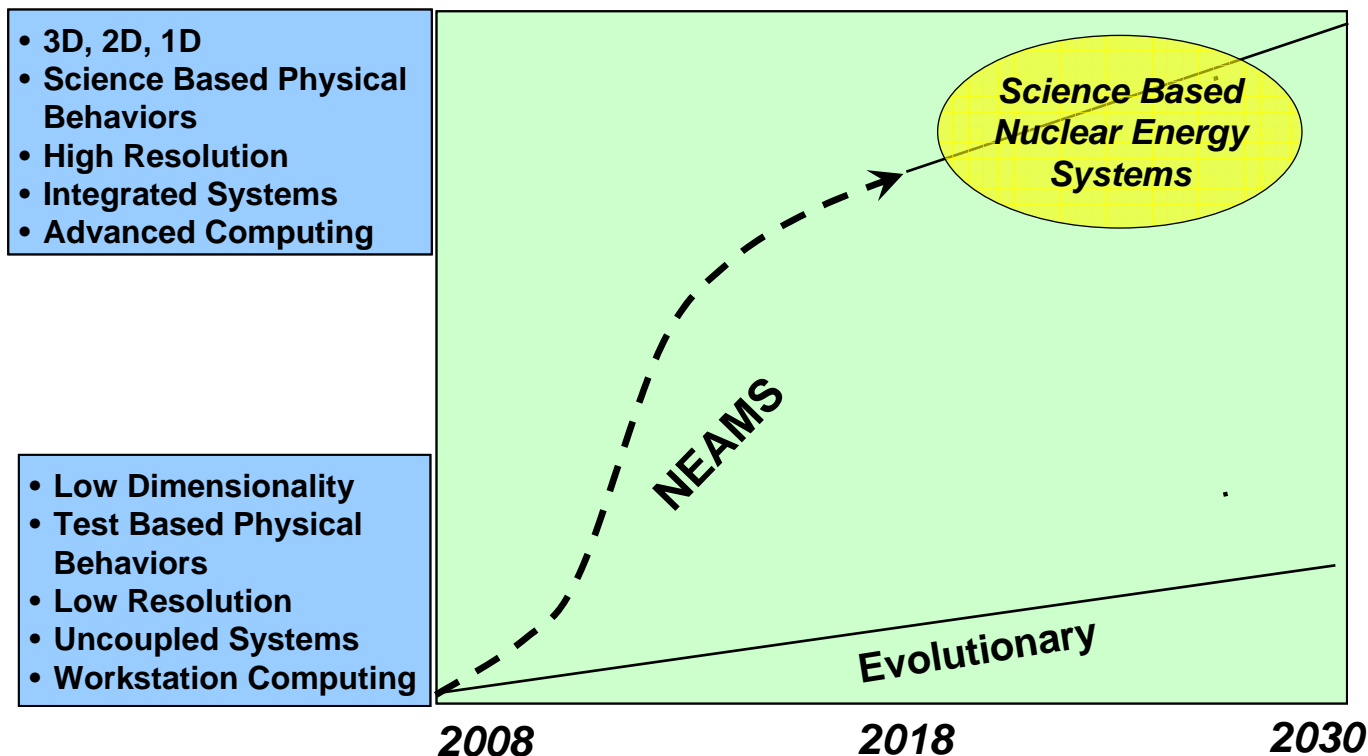




Stepping Up to New Capabilities That Enable Scientific Insight

NEAMS Vision

To rapidly create, and deploy next generation, verified and validated nuclear energy modeling and simulation capabilities for the design, implementation, and operation future nuclear energy systems to improve the U.S. energy security future.



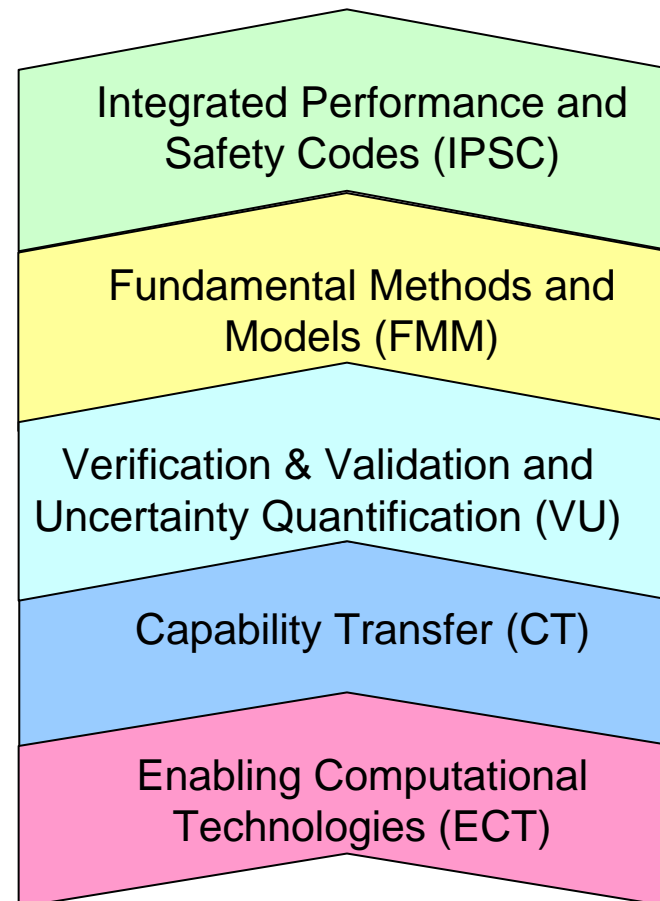


Nuclear Energy Advanced Modeling and Simulation

■ NEAMS Approach

- Built on a **robust experimental** program for model development and V&V
- Appropriate **flexibility** so that the simulation tools are applicable to a **variety of nuclear energy system options and fuel cycles**
- **Continuously deliver** improved modeling and simulation capabilities relevant to existing and future nuclear systems (in the near, mid, and long term)
- Apply the **best ideas** through **open competitive processes** to address the challenges of achieving the vision

■ NEAMS Program Elements:





NEAMS Program Strategy – Integrated Performance and Safety Codes

Integrated Performance and Safety Codes (IPSC)

Strategy Goal

End-to-end codes to understand the detailed integrated performance of new nuclear systems

Strategy Deliverables

- Create overall architecture and development plan for IPSC
- Focus on current leading edge platforms with plans to port to advanced platforms as they become available
- Create requirements for Fundamental Methods and Models solicitations and integrate FMM project results in IPSC
- Utilize V&V and UQ methodologies developed by VU Team
- Create requirements for integrated effects testing needed for V&V for the VU Team
- Create specifications for, and use NEAMS Framework created by Capability Transfer

Approach

- Create large code teams (50 to 75 people) with a centrally located “critical mass”
- Use additional individual or small teams to focus on particular code aspects
- Rough Composition
 - 1/3 Application specific expertise
 - 1/3 Advanced computing expertise
 - 1/3 Team support (V&V, SE and SQA, Support)
- Interface with application users and if not available create teams of “ghost users” to assess usability of applications

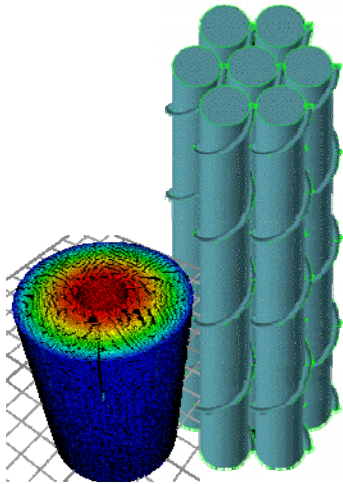
Risks & Issues

- Challenging and very aggressive milestones.
- Need to quickly create integrated code teams at laboratories that may not have experience with large code development.
- Finding the right talent to populate teams.
- Dependence on other NEAMS strategies (FMM, VU, CT, ECT) for success.
- Dependability of funding.





NEAMS Program Strategy – Nuclear Fuels IPSC



NEAMS-Fuels Deliverable

- Coupled, three-dimensional, predictive tool for pins and assemblies, applicable to both existing and future reactor fuel design, fabrication and for both normal and abnormal operating conditions. The validated tool can be used for lifetime extension, development

Milestones

- **Year 2**
 - Develop code to evaluate performance margins under normal and abnormal operations with predetermined burn-up
- **Year 4**
 - Predict evolution of fuel burn-up within an assembly
- **Year 6**
 - Predict transient fuel behavior for DBA and severe accidents
- **Year 8**
 - Predict fuel-clad-coolant chemical interactions

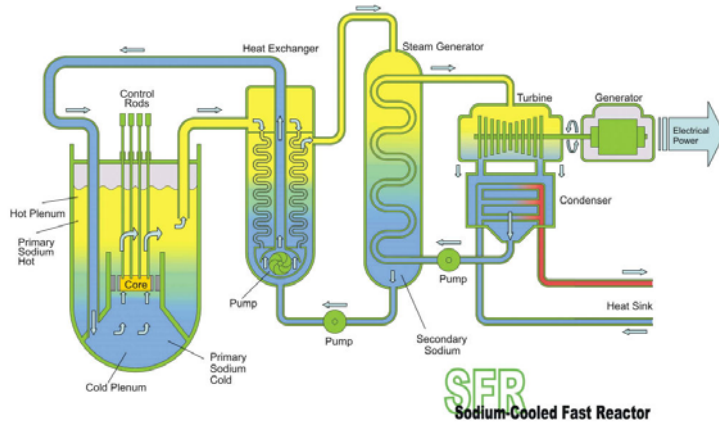
Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$15M	\$20M	\$25M	\$25M	\$30M	\$30M





NEAMS Program Strategy – Reactor Core and Safety IPSC



NEAMS-Reactor Deliverable

- A revolutionary next generation IPSC that integrates and couples high-fidelity models of all relevant physics
 - To enable dramatic shift in the way modeling and simulation is used in design and licensing
 - Science based predictive simulation capabilities

Milestones

- **Year 2**
 - Deliver fully coupled 3D modeling capability of single fuel assembly in core
 - Deliver first generation of advanced science based reactor safety analysis code
- **Year 4**
 - Deliver 3D coupled physics simulation application for full core
 - Deliver next generation of science based safety analysis code
- **Year 6**
 - Deliver verified and validation 3D, science based application for single reactor type.
- **Year 8**
 - Delivery reactor analysis code utilizing NEAMS framework

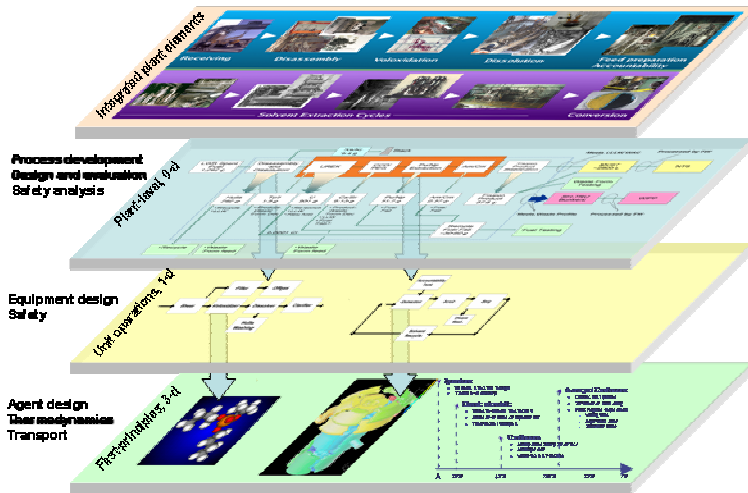
Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$15M	\$20M	\$25M	\$25M	\$30M	\$30M





NEAMS Program Strategy – Separations and Safeguards IPSC



NEAMS-SafeSep Deliverable

- Produce the M & S toolkit.
- Toolkit will enable
 - Design of commercially viable reprocessing options and facilities.
 - A priori integration of separations and safeguards (where appropriate) for detailed analysis and optimization.
 - Scalability of the technology (lab-commercial)
 - Meeting regulatory requirements (validation)
 - Explore advanced separations techniques.
 - Predict with high confidence the quantities and locations of the materials.
 - Fully integrated safeguards simulation from signature creation to interpretation
 - Plant-level model for diversion path analysis and safeguards by design.
 - Real time continuous information management and analysis.

Milestones

- Year 1
 - initial framework spec
- Year 2
 - beta framework populated with legacy codes
- Year 5
 - Integration of priority 1-D unit operations modules
 - Very large scale Bayesian computing for analyses
 - Dynamical analysis.
- Year 10
 - PDE device models
 - Subscale (PMM) models for chemical properties and processes
 - Design Optimization methods

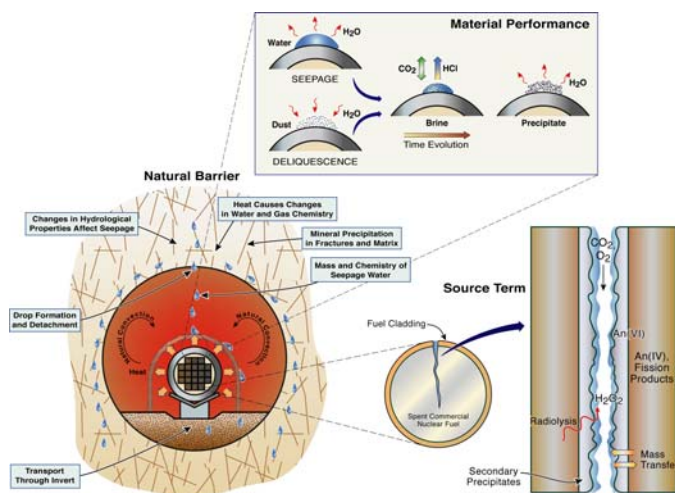
Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$5M	\$15M	\$20M	\$25M	\$30M	\$30M





NEAMS Program Strategy – Waste Forms & Systems IPSC



NEAMS-Waste Deliverable

- An integrated, science-based waste form/repository simulation package that is able to model various waste form and repository environments and captures the full range of multi-scale effects for licensing a repository for waste from a closed fuel cycle

Milestones

- **Years 3-10**
 - coupling waste form models and geochemical models, interface w/ separations, compare to experiments, rigorous uncertainty quantification
- **+5 year**
 - geochemical transport model that captures the chemical and physical processes which govern repository performance
 - waste form modeling package that predicts waste form stability from first principles (radiation damage, FP solubility, chemical evolution, leaching, etc)
- **Years 3-10:**
 - Development of next generation parallel codes
- **Years 0-3:**
 - Modernization of existing models

Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$5M	\$15M	\$20M	\$25M	\$30M	\$30M





NEAMS Program Strategy – Fundamental Methods and Models

Fundamental Methods and Models (FMM)

Strategy Goal

Smaller length scale material modeling work, and
Atomistic-to-Continuum (AtC) multi-scale simulation

Scope

- Provide understanding and improved properties and models for use in integrated codes
- This element also identifies and drives small scale experimentation necessary to generate the data needed for physical and engineering models.

Approach

- Create many small (~\$1-2M/year) projects to create the lower length scale understanding of behaviors
- Select a number of projects (~5) every year that last 2-3 years
- Annual solicitation for projects based on requirements from IPSC projects
- Utilize a FMM Integrator to collect IPSC requirements and deliver FMM results.

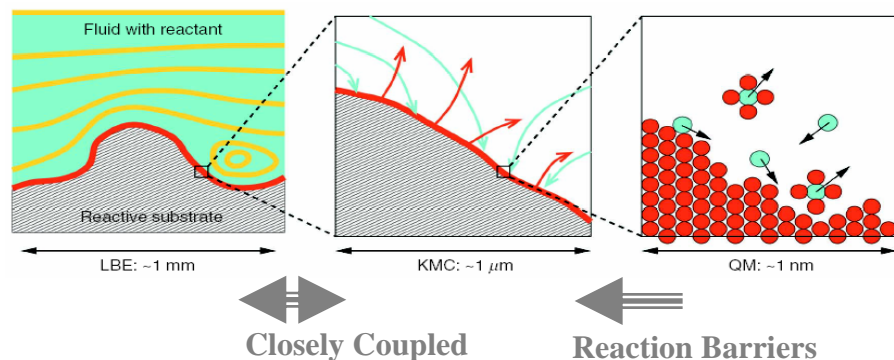
Risks & Issues

- Ability to capture appropriate IPSC requirements for FMM projects
- Management of many (~20 - 25) active FMM projects and deliver results to IPSC projects
- Quality of FMM result physical models and underlying data
- Ability to fund required experiments to support FMM work





NEAMS Program Strategy – Fundamental Methods and Models



Strategy Deliverables

- Deliver methods and models of fundamental physical behavior of material relevant to the integrated performance and safety codes.
- Identify and support separate effects experiments needed for delivering methods and models.

Milestones

- **Year 1**
 - Develop requirements from IPSC teams for FMM work
 - Complete solicitation and compete 5 FMM projects
- **Year 2**
 - Receive results from 1st FMM projects
 - Update IPSC requirements and compete 2nd round of FMM projects
- **Year 3**
 - Receive results from 1st FMM projects
 - Update IPSC requirements and compete 3rd round of FMM projects
- **Year 4 to 10**
 - Continue to refresh FMM projects through competitive process

Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$8M	\$10M	\$15M	\$20M	\$25M	\$25M





NEAMS Program Strategy – Verification, Validation & Uncertainty Quantification

Verification & Validation and
Uncertainty Quantification (VU)

Strategy Goal

Delivery of IPSC codes that are “borne” verified,
validated as assessed for uncertainty quantification.

Scope

- Deliver methodologies to be used by IPSC projects to V&V and UQ their codes.
- Capture existing experimental data and work with integrated effects experiments to create necessary data for V&V and UQ.
- Serve as principle interface with NRC to ensure methodologies are acceptable for licensing purposes.

Approach

- Work with NRC to understand requirements for V&V and UQ methodologies.
- Survey existing methodologies to understand ability and gaps to meet requirements.
- Develop and refine methodologies as necessary.
- Work closely with IPSC teams to understand experimental data requirements.
- Identify sources of existing data and quality of that data.
- Work with other AFCI Campaigns to help set requirements for new integrated effects experiments.

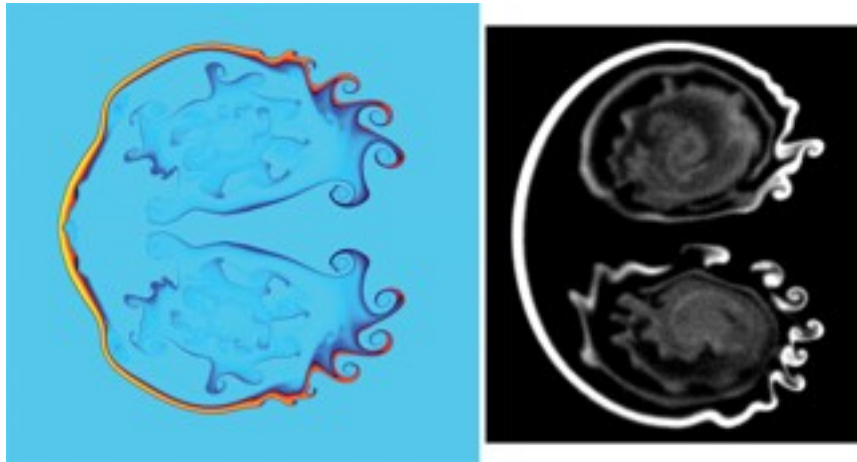
Risks & Issues

- Ability/willingness of the NRC to comment on exactly what are V&V and UQ requirements.
- Developing V&V and UQ methodologies in a vacuum that cannot be implemented in actual IPSC projects.
- Lack and quality of existing experimental that is appropriate for use in IPSC projects.
- Inability to influence new experiments to generate integrated effects experiments needed to implement V&V and UQ methodologies.





NEAMS Program Strategy – Verification, Validation & Uncertainty Quantification



Strategy Deliverables

- System for Quantitative Assessment (and improvement) of Predictive Capability that:
- Tools that enable optimization of benefit/cost from experiments and improved models
- Assessed errors and uncertainties in key measured data
- Structured licensing process built upon this methodology

Milestones

- **2 yrs:**
 - Assessment/inference using these estimates of numerical errors
 - Apply prototype system to at least one integrated code (with selected experimental data)
 - Initial R&D results on effects of assumptions that are “buried” in assessment/inference methodology
 - Establish relationship with licensing organization
 - Help establish relationship between experiments and modeling
- **5 yrs:**
 - Exercise Quantitative Assessment of Predictive Capability on integrated codes, fundamental models, fuel performance simulations, ...
 - Use some data for assessment, then do “prediction” of something else, then compare
 - Quantitative understanding of effects of statistics assumptions
 - Mature relationship with licensing organization
 - Mature relationship between experimentation and modeling

Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$5M	\$10M	\$15M	\$25M	\$30M	\$30M





NEAMS Program Strategy – Capability Transfer

Capability Transfer (CT)

Strategy Goal

Use of NEAMS developed codes for designing, building and operating of new nuclear energy systems.

Scope

- Creation of a modeling and simulation interoperability frame work to facilitate capability transfer.
- Identification and elimination of unnecessary barriers that inhibit capability transfer.

Approach

- Create a team to work with IPSC efforts to identify framework requirements
- Develop high level UML model for framework architecture
- Examine existing frameworks to determine how well they meet specification
- Provide additional development to best existing framework
- Work with technology transfer offices to understand requirements and to remove unnecessary barriers.

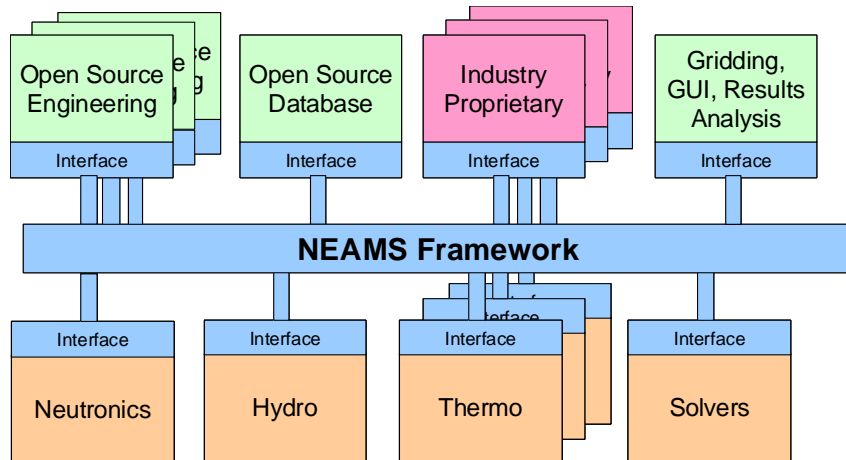
Risks & Issues

- Existing CT is
 - Ad Hoc
 - Slow
 - Realizes on Serendipity
 - Underfunded for years
- Legal Issues
 - Intellectual Property
 - Export Control
 - Licensing
- Limited (in many cases “no”) abilities that allow easy integration of existing and newly developed modeling and simulation capabilities





NEAMS Program Strategy – Capability Transfer



Strategy Deliverables

- NEAMS Framework is the industry standard for nuclear energy modeling and simulation
- Framework attributes
 - Standardized input and output
 - Integration of
 - Research and development modules
 - Existing modules
 - Proprietary modules
 - Modules under export control
 - Support for developers and users
 - Framework documentation
 - Technical support commercially available

Milestones

- **Year One**
 - Initial framework spec
 - Establish industry group
 - Establish NEAMS use cases
 - Deliver prototype (beta) framework
- **Year Three**
 - One IPSC code team using alpha NEAMS framework
 - One industry code using alpha NEAMS framework
 - Exercised legal processes to enable tech transfer
- **Year Five**
 - v1 NEAMS Framework release
- **Year Seven**
 - NEAMS Framework fully integrated into all NEAMS code team

Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$1M	\$5M	\$10M	\$12M	\$15M	\$15M





NEAMS Program Strategy – Enabling Computational Technologies

Enabling Computational Technologies (ECT)

Strategy Goal

Deliver and use a comprehensive set of technologies required to achieve the NEAMS vision of creating new, advanced capabilities

Scope

- Computational capabilities include:
 - Computing platforms
 - Development environments
 - Tools to build, test and run simulation models
 - Capabilities to interpret simulation results and support design decisions for new nuclear energy systems

Approach

- Centrally planned capabilities to support NEAMS requirements for technologies.
- Geographically and institutionally distributed capabilities for efficient operations
- Centrally managed system of technologies to optimally meet NEAMS needs

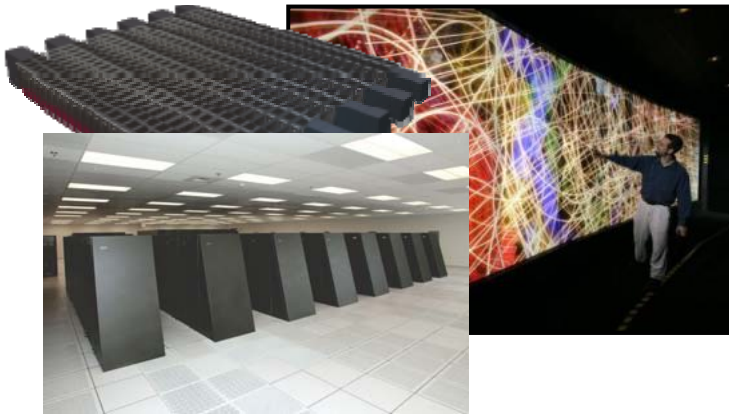
Risks & Issues

- Shifts in computer platform architectures
- Evolving programming models for use of new architectures
- Cross-institutional challenges of capability “ownership”
- Ability of other HPC programs (e.g. ASC and SciDAC) to maintain NEAMS required pace of technology development





NEAMS Program Strategy – Enabling Computational Technologies



Strategy Deliverables

- A centrally planned and operated, but distributed implemented computational capabilities to build and use NEAMS modeling and simulation capabilities.
- Includes:
 - Computer platforms
 - Code development tools
 - Model setup
 - Results analysis and visualization

Milestones

- **Year One**
 - Create NEAMS ECT specification
 - Create NEAMS ECT operational plans
- **Year Two**
 - Start procurement process for ECT computing platforms, visualization system and software tools
- **Year Three**
 - Receive and install ECT software and hardware
- **Year Five**
 - Technology refresh
- **Year Seven**
 - Technology refresh

Budget Requirements

FY09	FY10	FY11	FY12	FY13	FY14
\$1M	\$5M	\$40M	\$50M	\$60M	\$60M

