



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:

Delivering Insight
Not Allowed by Policy
Too Fast, Too Dense

SciDAC REVIEW
Too Small

Integrated Behaviors Too Complex

Too Far Away

Too Long

Too Expensive

Too Hard for Optimization

Traditional Means

- Theory
- Experiments
- Empirical Based Modeling and Simulation





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.



Dr. Gilbert G. Weigand

National Nuclear Security Administration

Dr. Weigand has distinguished himself with his passion for excellence along 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 long-term 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, his 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.

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

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

“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.”





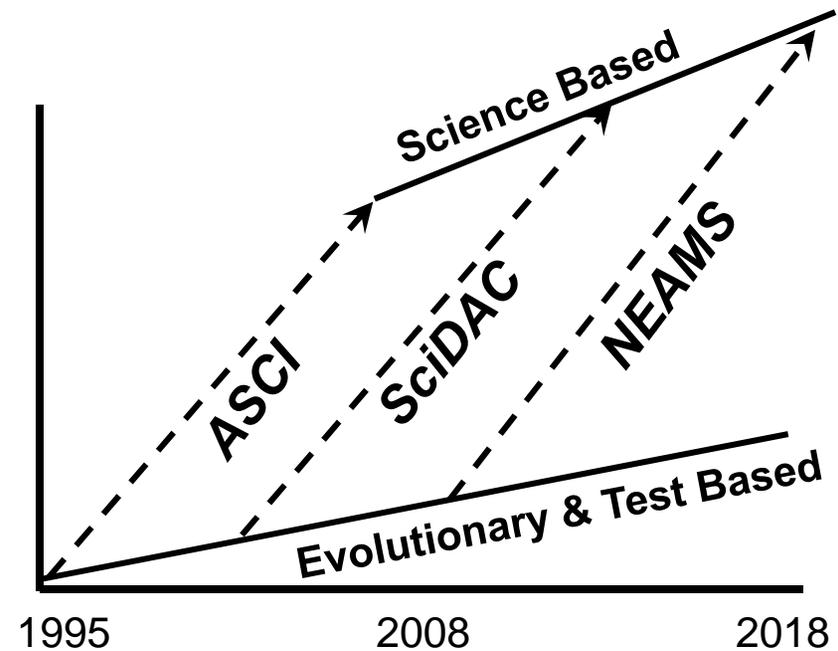
Its Time to Step Up -- Again!

■ 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

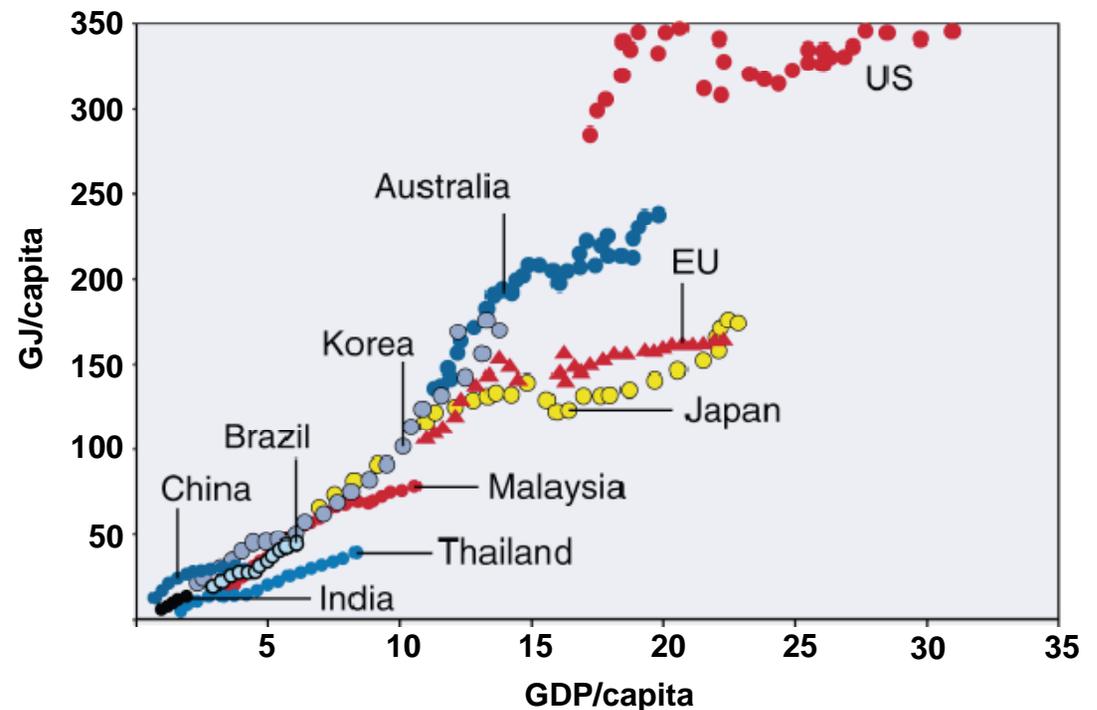




The Worldwide Energy Challenge

- 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





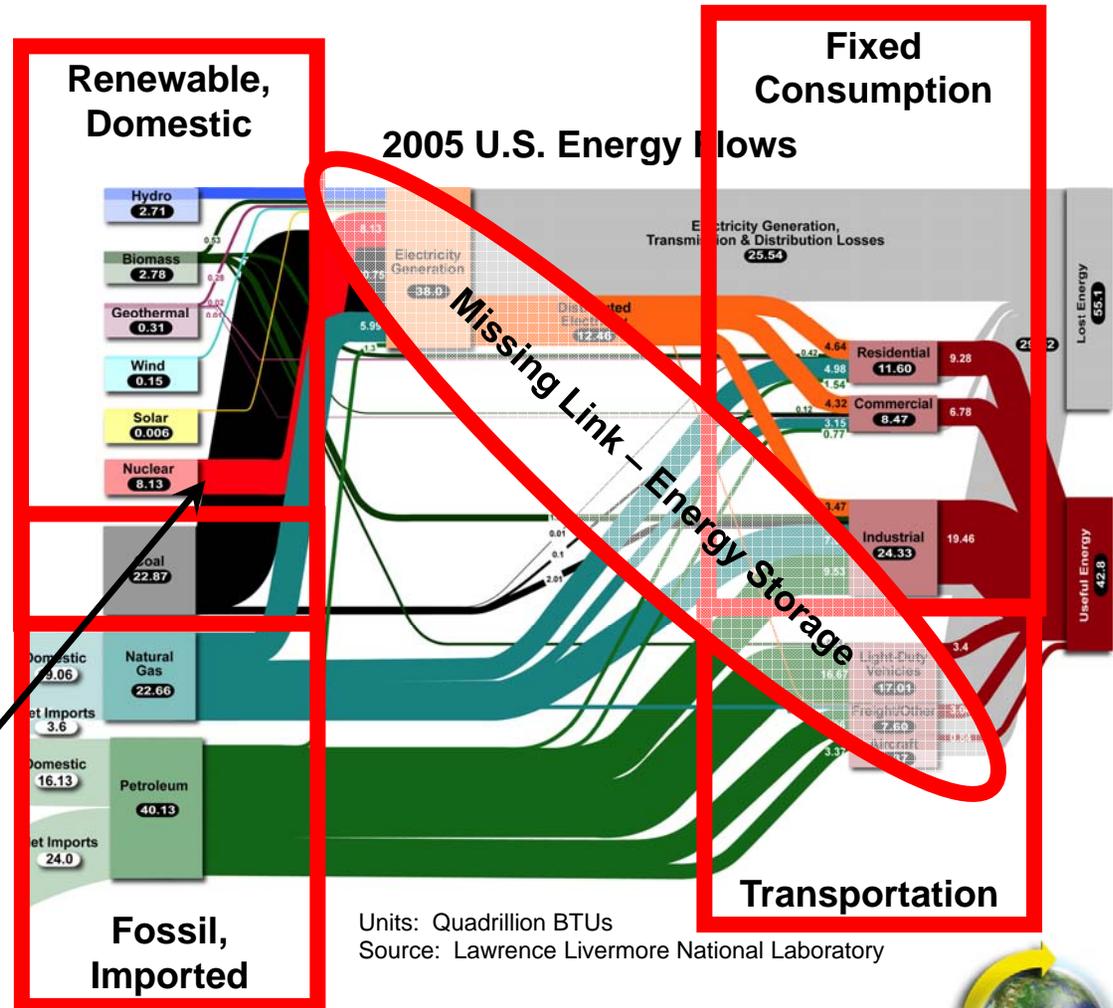
Improving U.S. Energy Security

■ 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

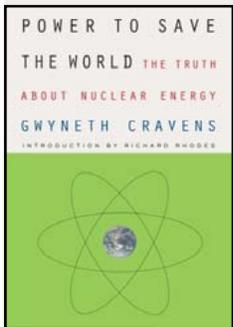
■ Improving Energy Security requires advances in all domestic, clean, and reliable forms of energy

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



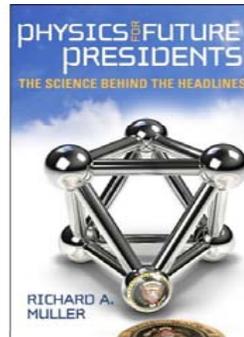


Doing Nuclear Energy & Doing It Better



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

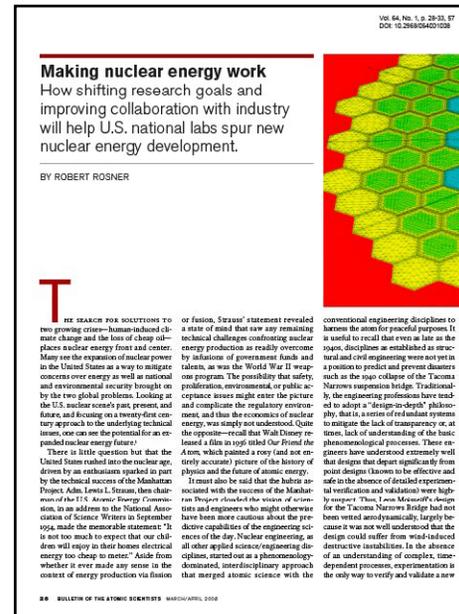
- Meeting these challenges of advancing the use of nuclear energy requires
 - A new generation nuclear energy systems and facilities





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)**

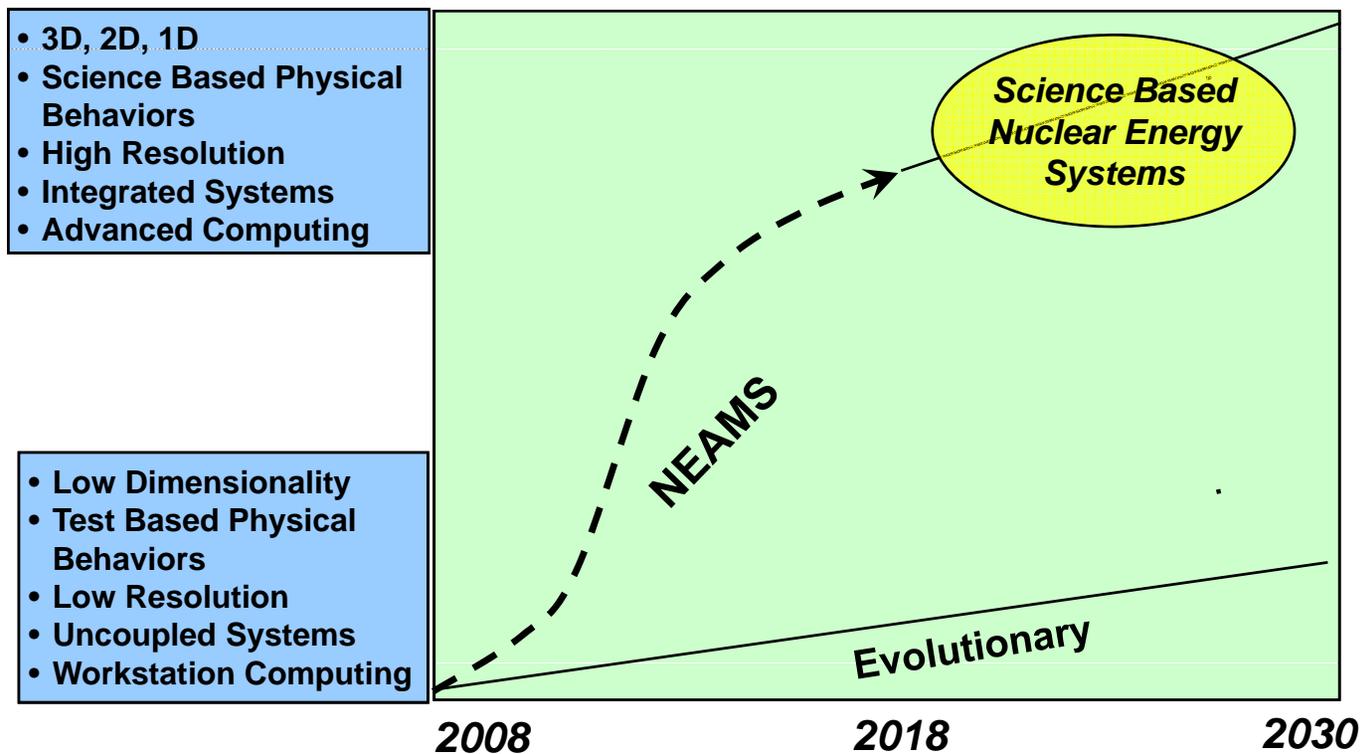




Stepping Up to New Capabilities That Enable Scientific Insight

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.



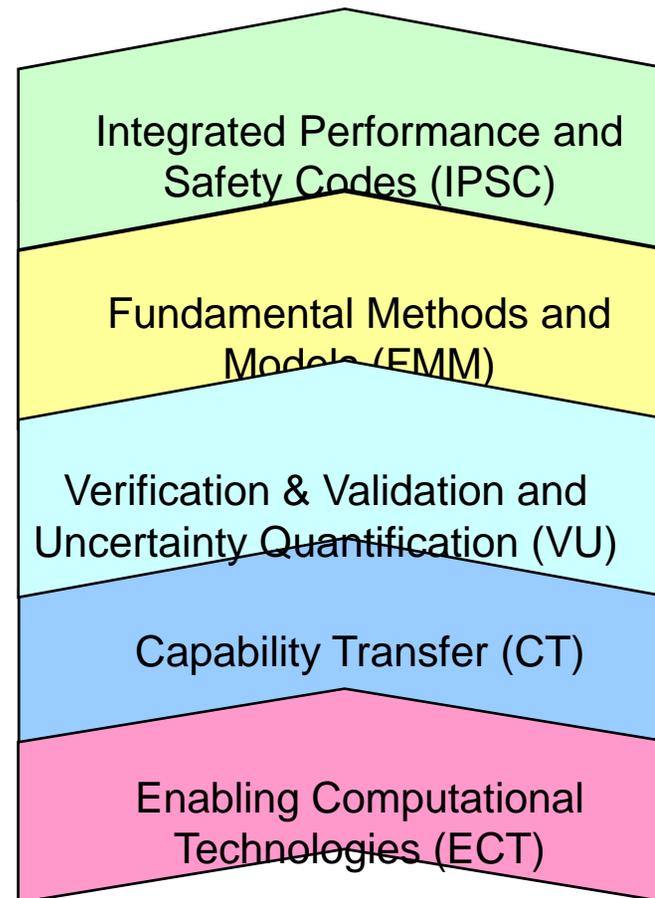


Nuclear Energy Advanced Modeling and Simulation

■ 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:





Details of NEAMS Program Elements

■ Integrated Performance and Safety Codes (IPSC)

- End-to-end codes to understand the detailed integrated performance of new nuclear systems
- Includes:
 - *Nuclear Fuels*
 - *Reactor Core & Safety*
 - *Separations and Safeguards*
 - *Waste Forms and Near Field Repositories*

■ Fundamental Methods and Models (FMM)

- Smaller length scale material modeling work, and Atomistic-to-Continuum (AtC) multi-scale simulation
- Provide understanding and improved properties and models for integrated codes
- This element also identifies and drives small scale experimentation necessary to generate the data needed for physical and engineering models.





Details of NEAMS Program Elements

■ Verification, Validation and Uncertainty Quantification (VU)

- Develops methodologies to be used by IPSC and FMM program elements to create confidence that the simulation results are a reflection of nature and to quantify the uncertainties inherent in modeling and simulation.
- Principal interface with the NRC
- Capture and preserve existing experimental data needed to implement methodologies and interface with experimental program to obtain needed data.

■ Capability Transfer (CT)

- NEAMS success depends on use of capabilities by the nuclear energy industry and licensing bodies.
- Include strategies such as turning scientific codes into engineering tools to be used by industry
- Work to improving the "usability" of HPC codes and systems.

■ Enabling Computational Technologies (ECT)

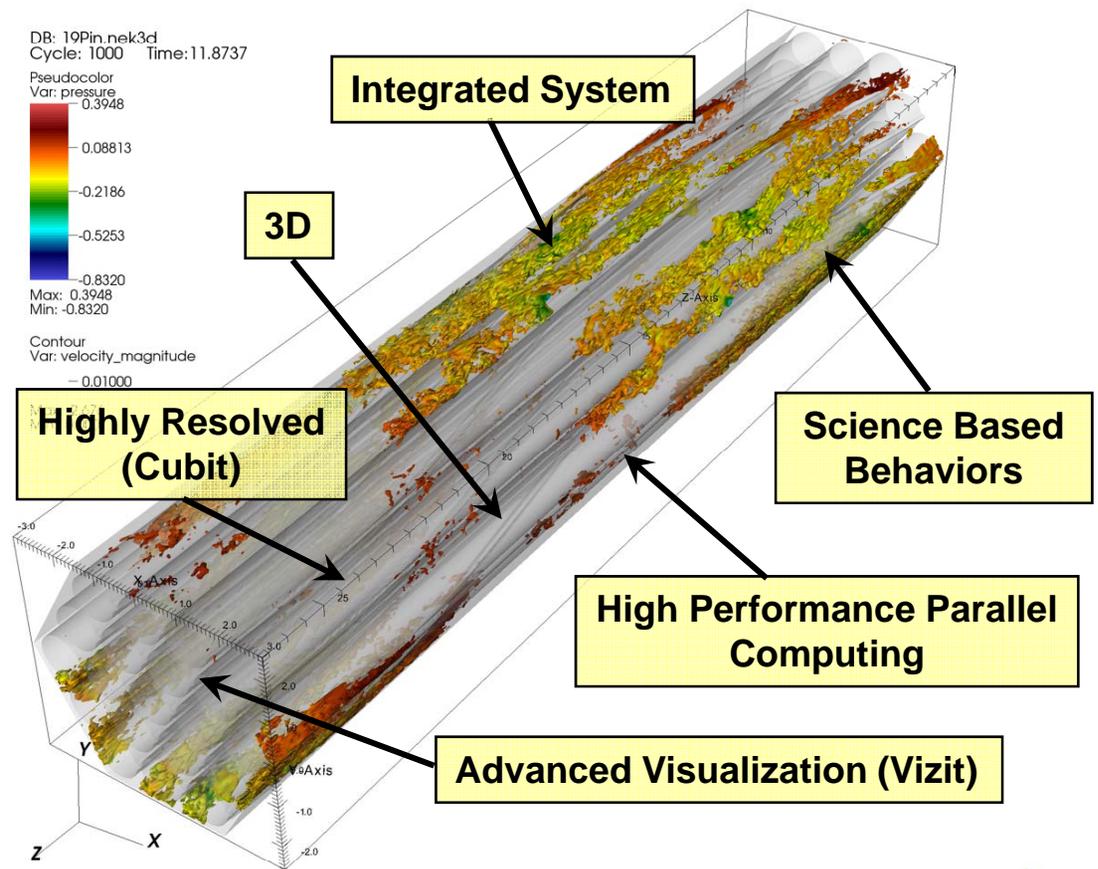
- An essential element of NEAMS is to ensure that the enabling technologies are available to make the first four program elements possible.
- Includes the platforms required to support the code development and the application work





Results of Stepping Up – Improved Science Based Insight

- **Verified and validated capabilities needed to apply a science based approach to understanding complex physical behaviors**
- **For the design, implementation and operation of new nuclear energy systems**
- **Critical to improving U.S. Energy Security and thus:**
 - *National Security*
 - *Economic Security*
 - *Environmental Security*



Early Results from ANL Fast Reactor Simulation of 19 Pin Fuel Assembly

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Fri Jan 4 11:47:32 2008

