

U.S. Global Leadership in Energy and Beyond Through Modeling and Simulation

White Paper

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The year 2008 was a defining moment when the confluence of energy and financial crises altered national economies and shifted geopolitical influence. In response, the United States increased financial liquidity and invested in critical infrastructure, including energy, through short-term economic stimulus. Although the United States appears to have weathered the financial crisis, the imperatives of energy security and sustainability present the nation with competitive challenges and economic opportunities that urgently require new long-term energy policies, strategies and investments.

The U.S. Department of Energy (DOE) will lead the transformation, through research, development and deployment of low-carbon energy sources and energy efficient technologies. Capturing the full value of the innovation chain from scientific discovery to manufacturing is essential to maximizing the return on public investment and maintaining U.S. competitive advantage in the global market place. DOE is poised to leverage its intellectual, computational and experimental assets to enable the nation to do this.

Energy Innovation hubs

Energy Innovation Hubs are a key component of DOE's aggressive strategy to solve the most intractable energy technology problems, significantly increasing U.S. energy security and sustainability. The solutions for these problems require long-term, focused scientific and engineering research and development, and critical public-private partnerships to ensure technology deployment. All of these characteristics are part of the Energy Innovation Hubs strategy.

The DOE hubs are designed to develop and deliver transformational energy technologies that will be deployed by the private sector or by public-private partnerships. The hubs are multidisciplinary, multi-investigator, multi-institutional integrated research and technology-deployment centers. They will attract outstanding scientific leadership and the best researchers and scientists from academia, industry and government.

1. Modeling and Simulation for Development and Delivery of Transformational Energy Technologies

High performance computing (HPC) modeling and simulation are essential to addressing the energy problem in areas ranging from climate change, the design of a smart U.S. electric grid, coal gasification and the requirements for successful carbon sequestration to more fuel efficient transportation systems, better performing energy storage systems and safer power plants. HPC modeling and simulation are vital to all phases of the innovation process—from science to applications, manufacturing and commercialization—and are thus crucial components of the DOE hubs. The nuclear energy hub, funded in FY10, is focused on modeling and simulation, and other energy hubs need modeling and simulation as part of their toolkit.

During the last 3 years, the United States has begun to move from descriptive to predictive computing capability. Many—perhaps most—of the problems that must be solved are not amenable to analytic theory or laboratory experiments. In the cases where experiments are possible, they are often expensive, time consuming and provide less data than could simulations. Even when modeling and simulation are incomplete, they provide important insights, save time, save money and prevent mistakes.

HPC modeling and simulation are equally important for manufacturing and commercialization in the energy sector and beyond. The use of HPC has provided a competitive advantage for many of the manufacturing Fortune 50. These companies employ in-house advanced computing as well as having access to HPC hardware, software and technical resources through partnerships with national laboratories and universities. For U.S. leading manufacturers, to out-compete is to out-compute.

However, barriers and obstacles exist that inhibit the full exploitation of HPC modeling and simulation by manufacturing companies and prevent its use by many of the manufacturing Fortune 100 and their suppliers. It is essential that these barriers and obstacles be removed or reduced so that the use of HPC broadens to include many more manufacturing firms and deepens to include many more of their suppliers. This will enable U.S. industry to compete on innovation, not on cost, preventing the movement of jobs overseas and creating quality, high-paying jobs in the United States.

The United States leads in the development and use of HPC for research, technology design and production. Greater exploitation of HPC will enable more creative design to optimize energy technologies, improvement of prototypes, a shorter time-to-market, optimal and sustainable use of natural resources for energy production and many other factors. DOE has tremendous computational assets and intellectual capital that can be leveraged to help solve national energy challenges. These reside in all parts of DOE, including the Office of Science (SC), the applied offices and the National Nuclear Security Administration (NNSA). Greater collaboration among the different parts of DOE can accelerate transfer of new energy discoveries and technologies to U.S. manufacturers.

2. Proposed Solution

DOE should exploit the hubs to launch an initiative that will use the cross-cutting importance of HPC modeling and simulation to increase collaboration among all parts of DOE, and that will advance HPC modeling and simulation in U.S. manufacturing in the energy arena and beyond. The hubs are ideally suited for this because they will:

- Apply HPC modeling and simulation to the entire innovation chain from scientific discovery to application, commercialization and manufacturing;
- Include manufacturers as participants and partners;
- Have the scale and stability needed for major software development;
- Provide computational capacity for verification, validation and certification, which are important to manufacturing technologies; and
- Can serve as anchors for sites in each state that would broaden and deepen the use of HPC modeling and simulation in manufacturing.

To accelerate the ability of the hubs to advance HPC modeling and simulation, DOE Secretary Steven Chu issued “a national call to service” to leading manufacturing companies and invited the company CEOs to serve the nation through participation in a public-private sector HPC Manufacturing Council focused on modeling and simulation as best practice to preserve U.S. global leadership and create quality, high-paying jobs in the United States. The leading manufacturing companies’ contribution to the HPC Manufacturing Council would include:

- Experience with HPC applications for manufacturing leadership;
- Counsel, guidance and collaboration on shaping computational problem definition;
- Knowledgeable company employees to the projects; and
- Financial support for company employee efforts and travel expenses.

The Council on Competitiveness is prepared to assist the DOE by convening the HPC Manufacturing Council, drawing on its long advocacy for HPC modeling and simulation in manufacturing and its strong relationships with leading manufacturers through the Council's HPC Advisory Committee, and to play a leadership role in the HPC Manufacturing Council. The initial proposed scope is to:

- a. Assess the current landscape in preparation for an HPC modeling and simulation initiative to revitalize the U.S. manufacturing base, particularly in the energy arena;
- b. Encourage development of a new generation of industrial strength, science-based software codes informed by proven science and engineering practice, and capable of running efficiently on current and future computer architectures;
- c. Facilitate formation of HPC research consortia involving the DOE hubs, national laboratories and universities to serve as regional points of access for the industrial base;
- d. Enable greater access to the consortia's leadership class HPC for competitive activities—design, data analysis, and other development and production activities. Resource requirements will be substantially larger than past government programs (i.e., the DOE INCITE program);
- e. Advise on design, plan and operation of current and future (including exascale) leadership class super-computer facilities to enable industry to be major users. The companies participating in the “call to service” will provide key resources for application requirements. The goal is for terascale and petascale leadership-class computing systems to quickly become commoditized computing for a higher return on investment;
- f. Inform software development for greater use and access by the U.S. manufacturing base for energy technology deployment;
- g. Address intellectual property (IP) issues for industry collaboration (use of proprietary software, collaborative improvements to proprietary software, availability of ISV software licenses, protection of proprietary results, no publication requirement for proprietary results, etc.); and
- h. Address issues of:

Scalability	Verification and validation
Compatibility	Large parallel, robust, and fault tolerant codes
Interoperability	Software support, stability, and access
Visualization	Hardware support, stability, and access
Data security and compatibility	