Report on

A NATIONAL SUMMIT ON ADVANCING CLEAN ENERGY TECHNOLOGIES

Entrepreneurship and Innovation through High Performance Computing

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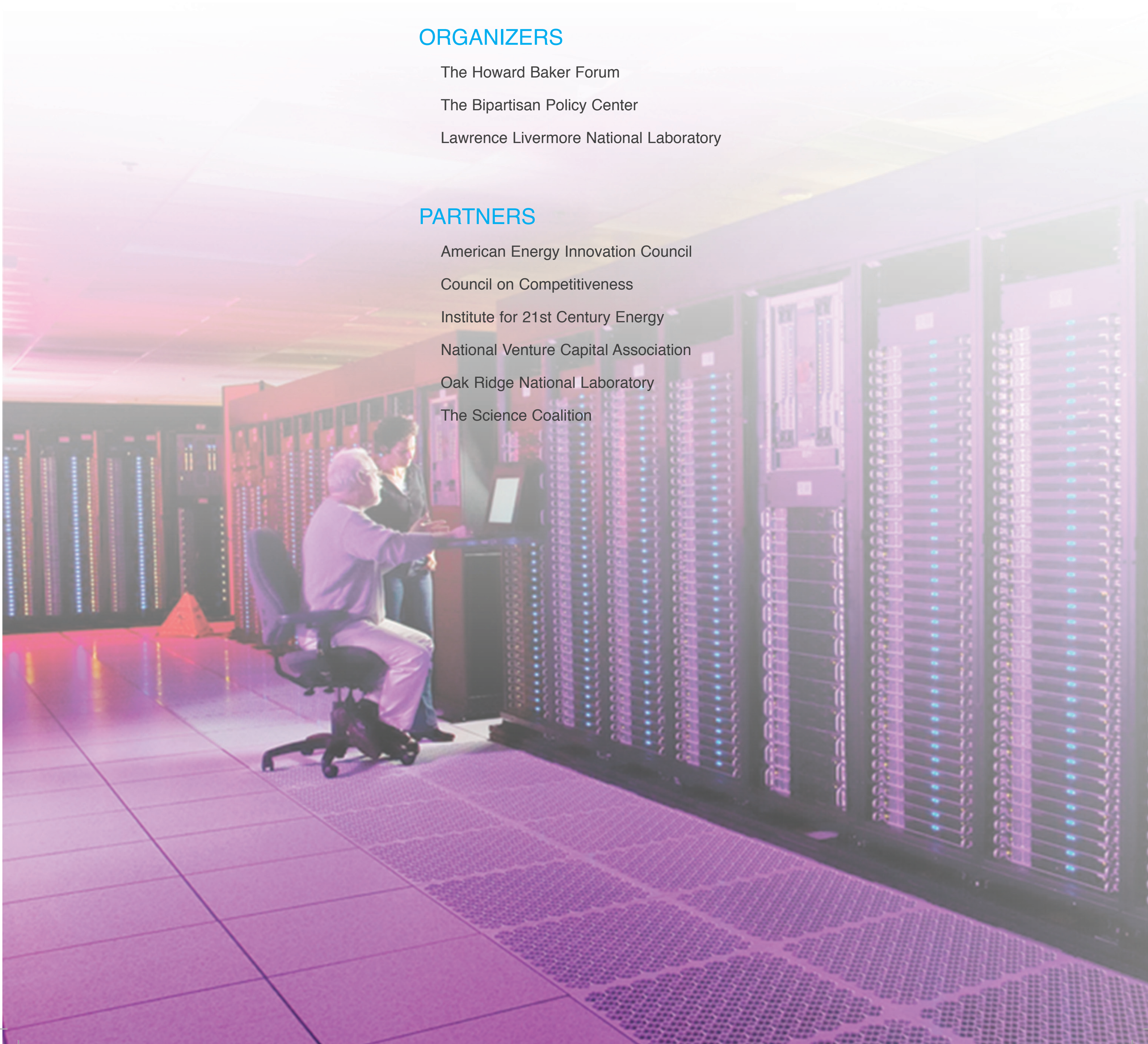


Executive Summary

The demand for energy in the United States is anticipated to grow from 96 quadrillion BTUs in 2009 to 123 quadrillion BTUs by 2035, while adding 1.4 billion metric tons of CO_2 to the atmosphere. In response, the United States has established aggressive goals toward achieving a clean energy society: putting 1 million electric vehicles on the road by 2015, generating 80% of electricity from a diverse set of clean energy sources, making non-residential buildings 20% more energy efficient by 2020, and cutting greenhouse gas emissions by about 17% below 2005 levels by 2020 and 83% by 2050. Meeting these clean energy goals requires huge investments, long lead times, and above all, breakthrough innovations in clean energy technology to lower risks.

In light of demonstrated advances in the defense, aerospace, and pharmaceutical industries, experts agree that tapping America's world-renowned high performance computing (HPC) and simulation capability could help transform the clean-energy industry, creating thousands of new jobs and energizing America's lagging high-tech manufacturing capabilities. HPC is used increasingly by industry because it substantially reduces the time and cost to design, develop, prototype, and deploy new products. HPC enables innovation, lessens uncertainty, and improves options.

Because of HPC's tremendous potential to advance clean energy, 300 experts and practitioners from business, finance, industry, government, academia, and the nation's leading science and computing laboratories met for two days in May, 2011 at a National Summit in Washington, D.C. to discuss how to effectively utilize HPC to advance clean energy solutions.

As a result of the Summit, the meeting's organizers are taking action to better understand how HPC can help advance U.S. innovation in the global energy marketplace and to launch several pilot projects: They will convene science and technology conferences focused on key energy challenges to determine how best to apply HPC in the clean energy sector. In conjunction with these conferences, a Call for Proposals will be issued for sponsored public-private partnerships between companies of all sizes and Department of Energy national laboratories (such as Lawrence Livermore National Laboratory), the acknowledged world leaders in applying HPC to science, defense, and industry. These partnerships will be aimed at demonstrating the effectiveness of HPC to efficiently solve problems. Organizers are also creating a dynamic, innovative, and interactive website for clean energy computing, a portal to provide information, advice, and computing access to clean-energy enterprises and researchers.

National Summit Summary

On May 16–17, 2011, the Howard Baker Forum, Lawrence Livermore National Laboratory, the Bipartisan Policy Center, and other partners with the common goal of accelerating U.S. development of clean energy technology, held a National Summit on Advancing Clean Energy Technologies in Washington, D.C., subtitled Entrepreneurship and Innovation through High Performance Computing. The meeting featured energetic discussions on promising clean energy technologies, with a particular focus on exploring how high-performance computing (HPC) can catalyze rapid advancement of U.S. clean-energy technologies in an increasingly competitive global marketplace.

Senators Howard Baker, Tom Daschle, and Bob Dole co-hosted the summit. Other key speakers included Senator John Hoeven and Senator Byron Dorgan; Marine Corps Gen. Jim Jones (ret.); Department of Energy (DOE) Under Secretary Dr. Steve Koonin; Siemens Corp. President and CEO Eric Spiegel; Rensselaer Polytechnic Institute President Dr. Shirley Ann Jackson; Oak Ridge National Laboratory Director Dr. Thom Mason; Argonne National Laboratory Director Dr. Eric Isaacs; IBM Vice-President of Deep Computing Dr. David Turek; Lawrence Livermore National Laboratory Deputy Director for Science and Technology Dr. Tomás Díaz de la Rubia; and White House Science Advisor Dr. John Holdren.

Many Summit speakers argued that tapping America's world-renowned HPC and simulation capability could transform the clean-energy industry.

Principal speakers were joined by federal elected officials; senior administration officials; banking, venture capital, and industry leaders; and clean energy experts for a two-day examination of the roles of government, industry, national laboratories, and universities in transforming the U.S. energy industry. Summit speakers discussed spurring American competitiveness and job creation through clean energy development and deployment, and the role of private financing in commercializing advanced energy technologies. Participants also described the challenges facing the vast landscape of fossil fuel alternatives, including nuclear, fusion, solar, wind, and geothermal, among others, and ways to speed their commercial development and deployment.

At the Summit, it became evident that the U.S. is not faced with running out of energy; rather, the U.S. is increasingly faced with the economic, political, and environmental risks of fossil-fuel dependence. In his keynote address, White House Science Adviser John Holdren said that although renewable energy is expanding significantly in the United States, fossil fuels still dominate. In particular, Holdren and other Summit speakers pointed to the growing accumulation of greenhouse gases that require dramatic changes to the nation's—and the world's—energy systems. The growing atmospheric concentrations of greenhouse gases add to risks, costs to future generations, and the potential for irreparable harm to ecosystems. As a result, speed is of the essence. Holdren concluded, "Advancement in energy technologies is required to address economic, political, and environmental risks of fossil fuel dependence."

According to Steven Koonin, DOE Under Secretary for Science, the Obama Administration's ambitious energy goals include reducing oil imports by one-third by 2025, putting 1 million electric vehicles on the road by 2015, generating 80% of electricity from a diverse set of clean energy sources, making non-residential buildings 20% more energy efficient by 2020, and cutting greenhouse gas emissions by about 17% below 2005 levels by 2020, and 83% by 2050.

Meeting these clean energy goals by 2050 requires accelerated development, prototyping, and deployment of new low-carbon energy technologies, which in turn requires enormous investments in new power plants, revitalized energy networks, and transformed transportation systems. Part of the challenge we face in meeting the Administration's goals is lowering the risk and cost of transition to a clean energy world while moving as quickly as possible to minimize climate change.

Many Summit speakers argued that tapping America's world-renowned HPC and simulation capability could transform the clean-energy industry, creating thousands of new jobs and energizing America's lagging high-tech manufacturing capabilities. With the promise of HPC in mind, the Summit mobilized the talents and insights of energy technologists and computational experts with the knowledge and experience of energy industry executives and public officials.

Summit speakers noted that HPC, once the specialty of a small group of computational experts, is used increasingly by industry as a tool for commercial survival to design and virtually test a vast range of industrial and commercial products, including jetliners, truck engines, golf clubs, and disposable diapers. HPC has been shown to substantially reduce the time and cost to design, develop, prototype, and deploy new energy materials, components, and systems. As already seen in other sectors like defense, aerospace, and pharmaceuticals, HPC enables innovation, lessens uncertainty, and improves options, thereby allowing companies to become more facile, responsive, and technologically advanced. Through virtual prototyping, hundreds of clean energy-related designs and new materials can be tested and optimized before manufacturing begins.

A NEW APPROACH NEEDED

Participants discussed how a new model for public-private partnerships combining clean energy technology (the grand challenge of our generation) and HPC (the underpinning technology accelerator) could break down barriers to help the nation pioneer innovative solutions. The clean energy challenge is so large and so urgent that we cannot afford to ignore the extraordinary potential of HPC to help make possible abundant clean, green—and reasonably priced—energy to American homes and businesses. At stake is assured clean energy supplies, enhanced national security, the prospect of thousands of new manufacturing jobs, and America's global competitiveness in the all-important energy sector.

FIVE CRITICAL CLEAN ENERGY AREAS

Panels of Summit participants discussed each of these five critical clean energy areas and how HPC could accelerate their development and deployment:

(1) Building Energy Efficiency. Buildings account for 40% of energy use in the U.S. Most stakeholders—builders, owners, occupants—understand the importance of energy savings, as well as the corresponding financial savings. Using HPC to improve building design, modification, and operations would result in significant savings in energy use and corresponding reductions in carbon emissions. HPC can contribute to creating new standards for verifying, validating, and calibrating energy modeling and simulation, used in design and operation of new buildings. Using HPC tools would also permit financially viable retrofits to enable current buildings to exceed 50% reduction in energy use and ultimately enable standards for networks of buildings.

(2) Carbon Capture and Sequestration (CCS). Climate change urgently requires deep cuts in greenhouse gas emissions and carbon capture from fossil-based fuels has great potential in reducing those emissions. Large-scale deployment of CCS is challenged by large technical uncertainties and significant costs associated with research, development, and deployment, including quantification of risks regarding the long-term effectiveness of geological storage. The use of HPC would accelerate permitting and safe operation of geological storage sites as well as finding the best CO_2 capture technology. Simulations would range from interactions of carbon molecules to commercial integration of capture devices in power plants.

(3) Liquid Fuels Combustion. Greater fuel efficiency, reduced greenhouse gas emission standards, and demand for unconventional vehicle architectures are all driving vehicle design. Meeting these challenges requires predictive modeling of in-cylinder processes (combustion, turbulence, sprays, air-fuel mixing), controls, heat transfer, and wear. The use of HPC would shorten time-to-market significantly, reduce development costs, and make products with enhanced long-term performance possible. Simulations could systematically examine countless candidate combinations of engine modifications and advanced fuels, with more rigor and less time, than physically building and testing engines with slight modifications. This approach offers insight into both the most likely and most robust designs possible.

(4) Nuclear Energy. Expansion of nuclear energy inevitably raises concerns about safety, reliability, and the potential for proliferation of nuclear weapons-usable materials. HPC could aid understanding of the safety of the aging reactor fleet and spent fuel storage facilities, speed design and optimize construction of new classes of reactors and new types of nuclear fuels, and perform analyses to determine whether reactor operation is optimized for power or for special nuclear materials production.

(5) Smart Grid and Storage. The current grid system urgently needs higher quality power, improved asset utilization, ability to anticipate and respond to disturbances, and greater resiliency to natural disasters or attacks. In addition, incorporation of renewable energy sources as well as widespread adoption of plug-in electric vehicles will complicate grid management. Studies show that large-scale models would lead to at least a 10% improvement in capital utilization and at least a 10% decrease in operating costs, with improved reliability and market transparency. Compared to conventional methods, HPC simulations would also permit easily running tens of thousands of different energy-use scenarios.

Tapping HPC's Full Potential

IMPROVING TRUCK FUEL ECONOMY BY REDUCING AERODYNAMIC DRAG

The basic configuration of the Class 8 tractor-trailer has not changed in decades. Statistics from 2006 show that, on average, each of the 2.2 million semi-trucks on U.S. highways consumes 12,800 gallons of fuel annually—roughly 12% of America's total petroleum usage.

In partnership with BMI Corp. and other companies, Lawrence Livermore National Laboratory (LLNL) is coupling HPC with physical experimental validation to accelerate the design, prototyping, and deployment of energy-saving technology, rapidly transforming the 30-year-old tractor-trailer design. This effort has already resulted in the design of several devices for Class 8 heavy vehicles, including the SmartTruck UnderTray, that reduce aerodynamic drag by more than 20% and boost fuel economy by more than 10%. This translates into 2.8 billion gallons of diesel fuel saved per year, roughly 2.5 million tons of CO_2 not released into the atmosphere, and $8 billion in cost savings.

Critical drag-producing regions, such as the trailer base, underbody, and tractor–trailer gap, were assessed using HPC.

The U.S. government has made significant investments in HPC, particularly at the Department of Energy (DOE) national laboratories, where HPC has become the "third leg" of science, joining theory and experiment. HPC powers innovation through the astonishing realistic simulations it makes possible. In HPC, thousands of microprocessors work together to mimic physical reality capable of focusing on a single water molecule or an entire ocean and over time periods ranging from billionths of a second to billions of years. Whether it's the folding of a protein, the reactions inside a gasoline engine, or the fusion of hydrogen isotopes, simulations can reveal complex details with stunning clarity. Because of HPC's astonishing power, it's been named one of the most important American inventions of the past 60 years.

DOE national laboratories lead the world in HPC for both scientific and defense applications. Lawrence Livermore, Sandia, and Los Alamos national laboratories use HPC to annually certify the health of the nation's nuclear weapons stockpile without the need for nuclear testing and have broken new ground in simulating the chemistry and physics of reactions, ranging from the birth of stars to the flue gas capture of CO_2 by promising new compounds. These labs are also pioneering new HPC architectures, algorithms, networks, visualization techniques, and storage systems.

A growing number of DOE-sponsored partnerships are already helping U.S. energy businesses use the full potential of HPC to obtain a significant competitive edge over foreign competitors through faster development, deployment, and commercialization of clean-energy technologies. DOE has launched advanced simulation programs through Energy Innovation Hubs for nuclear energy, energy-efficient buildings, and carbon capture and sequestration. These hubs link researchers at national labs, universities, and industry. Also, Advanced Research Projects Agency—Energy (or ARPA-E) initiatives focus on creative, high-risk energy research; projects are modeled after the Department of Defense's successful DARPA Program that developed technologies like the Internet, GPS, and Stealth aircraft. In addition, the DOE Office of Science's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program offers researchers in both the public and private sectors opportunities to explore HPC. General Electric, Boeing, Pratt & Whitney, and General Motors have all used INCITE for product design improvements. General Electric Research, for example, has used INCITE for combustion modeling, wind turbine designs, and improving jet engine performance.

Technical conservatism is the norm in the energy industry and must be overcome. One example of the industry's conservatism is the lack of widespread use of HPC. American energy companies, particularly start-ups, small, and medium-sized businesses, have not taken full advantage of HPC because of the cost of entry, lack of available application software, and insufficient access to trained manpower.

Public-private partnerships and collaborations are key to success and commercialization in using HPC. Numerous reports from the Council on Competitiveness indicate industry's willingness to explore or enhance HPC partnerships with government because of the complexity of HPC technology. The Council's report on the DOE/NNSA/ASC Academic Strategic Alliance Program (ASAP) showed that all 12 commercial firms interviewed (from aerospace, automotive, energy, and software industries) indicated that access to HPC resources was indispensable, the collaborations were overwhelmingly successful, and, given another opportunity to partner, they would do so. Furthermore, the report stated that one-third of the firms

Critical drag-producing regions, such as the trailer base, underbody, and tractor–trailer gap, were assessed using HPC.

PRESIDENT OBAMA'S ADVANCED MANUFACTURING PARTNERSHIP

While launching his administration's Advanced Manufacturing Partnership, President Obama in June 2011 spoke to the benefits of public-private partnerships in computer-based modeling and simulation. The President noted how Procter & Gamble (P&G), in collaboration with Los Alamos National Laboratory, used HPC software, originally designed to study nuclear particles, to improve the performance of diapers. The results saved P&G half a billion dollars over 10 years.

In the same address, President Obama spoke of the administration's efforts to help smaller and medium-sized manufacturers take advantage of the same technology that gave P&G a boost. "To help smaller manufacturers compete, federal agencies are working with private companies to make powerful, often unaffordable modeling and simulation software easier to access."

achieved an important breakthrough or discovered something new; learning new approaches to problem-solving was transformational. Half of the companies reported solving a specific problem—bringing a product to market faster, achieving a cost reduction, or increasing profitability—as a direct result of the partnerships. The report states:

"Although it was never a program goal, ASAP demonstrates that strategic public-private sector partnerships can provide significant value by lifting the country to a higher level of competitiveness. In particular, ASAP provides an opportunity for NNSA to demonstrate in quantifiable terms that it can successfully leverage its HPC resources to both meet national security mission needs and accelerate the nation's economic security and global competitive position—providing an enhanced return on the government's investment in HPC assets." (http://www.compete.org/publications/detail/132/partnering-for-prosperity-nnsa/)

For many large corporations, HPC is essential to business survival because it provides a virtual test bed for new products, materials, and manufacturing processes. For example, Boeing optimized airfoil design, resulting in a seven-fold decrease in testing. Cummins brought a new engine to market solely with modeling and analysis tools, reducing development time and cost, and improved engine performance. Goodyear developed predictive modeling capabilities for a new tire design that enabled a three-fold reduction in product development time, and Ford accomplished virtual aluminum casting, producing a 7:1 return on investment and $100 million in savings.

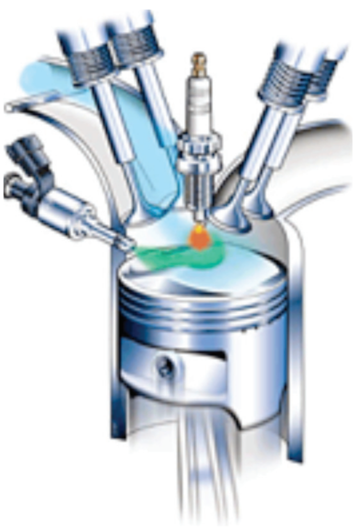
FROM SAFETY TO ECOBOOST: HPC ENABLES INNOVATION AND PRODUCTIVITY AT FORD

(Excerpted with permission from a DARPA-funded Council on Competitiveness case study, available at: http://www.compete.org/publications/detail/1664/case-study-hpc-enables-innovation-and-productivity-at-ford-motor-company/)

After an intense 30-year working relationship with supercomputers—ranging from early water-cooled Crays to today's commodity clusters—engineers at the Ford Motor Company view modeling and simulation with high performance computing (HPC) not as some high-tech miracle, but as an integral part of the business.

Says Nand K. Kochhar, Ford's executive technical leader for global CAE (computer-aided engineering) and chief engineer for global materials and standards engineering, "The combination of HPC and CAE simulation technology is a key enabler of our product development process. We provide advanced computational capabilities for Ford not just as a service, but as an integrated enabler of company business strategy. HPC is key to delivering on our overall business plan, optimizing product development, creating high quality products, and improving time-to-market. With advances in computing technologies, it is possible to accomplish this in a cost effective manner."

HPC and CAE played a pivotal role in the development of Ford's EcoBoost engine technology, which will be available in more than 80 percent of Ford vehicles by 2013.

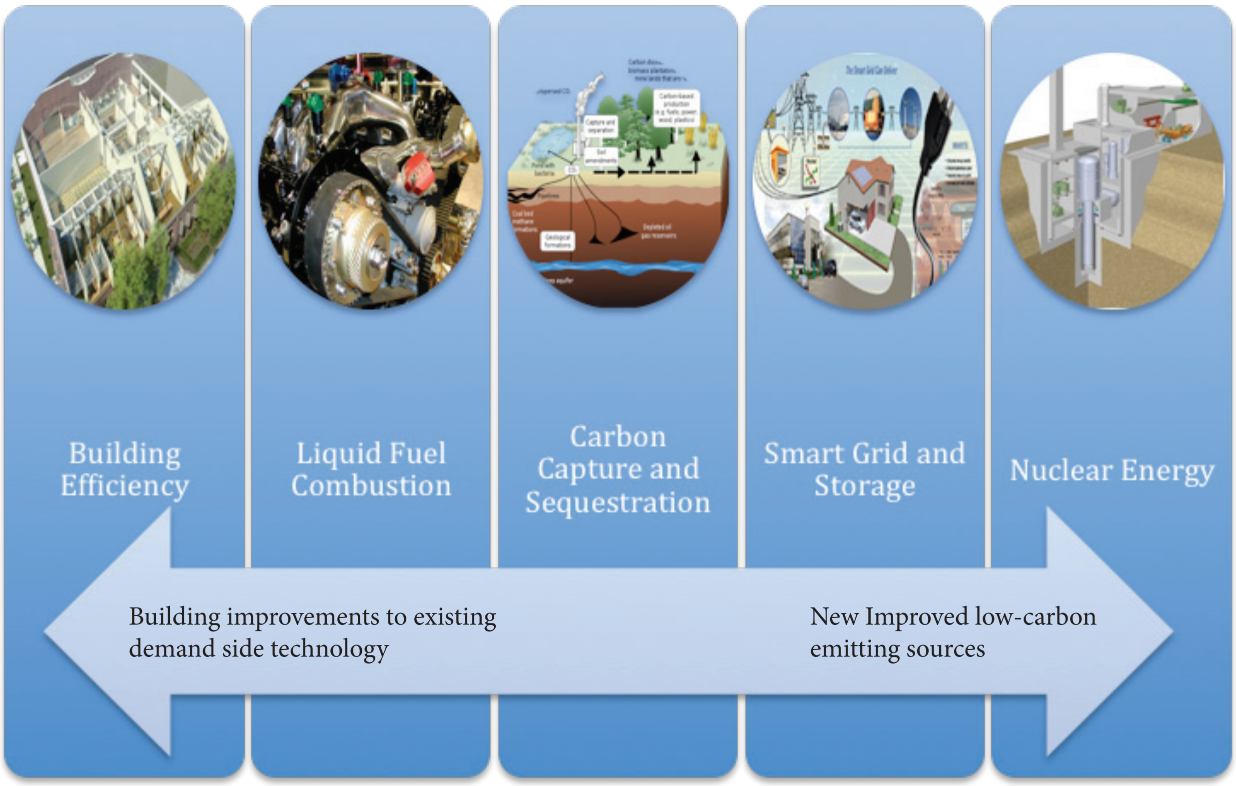


Promising Clean Energy Technologies

The current U.S. energy mix is highly dependent upon classic hydrocarbon-based fuels, and there is a tremendous amount of wasted, or rejected, energy. At the same time, vast amounts of CO_2 continue to pour into the atmosphere. Energy policy experts emphasize that a clean energy future is not solely about deploying zero-carbon and renewable energy sources. Rather, it is also about improving efficiencies of existing technologies in an effort to accommodate the transition to a low-carbon-emitting future while utilizing the enormous infrastructures now in place.

America's energy challenges include creating more efficient combustion systems, advancing nuclear energy systems, developing new approaches to capture and sequester carbon, creating a smarter electrical grid, and enhancing building energy efficiency. Many of these initiatives are already planning to use HPC resources for modeling and simulation, and more could benefit if a resource were readily available. In every case, technical challenges could be met more rapidly and cost-effectively by using HPC to enable breakthrough solutions. During the Summit, industry experts, national laboratory directors, and DOE staff discussed their particular energy sector and the need for HPC, and they offered some Big Audacious Goals (i.e., ambitious goals to be achieved by 2020). Summit participants also discussed the economic benefits of having a coordinated and comprehensive application of HPC to America's clean energy industry:

1. **Building Energy Efficiency**. Buildings in the U.S. (commercial, industrial, and residential) are responsible for 40% of U.S. overall energy use and greenhouse gas emissions. Improving building design and operations could result in massive savings in energy use, reductions in carbon emissions, and cost reductions for building owners and operators. Additionally, new buildings and building retrofits are subject to incrementally "miserly" building and municipal codes. Improved building energy efficiency is achieved by increasingly efficient equipment, better design and optimized building management. While all three of these components are improved by HPC, only appliance and building equipment developed has benefitted from advanced simulation and modeling. It is important for energy efficient designs and



Summit participants discussed integrating HPC into five energy fields spanning the spectrum of clean energy technology and efficiency sectors.

retrofits to be validated for their savings, in some cases to justify costs. Current building operations can be optimized for better, more efficient performance if the building is tuned correctly, and the staff managing the building is properly trained in running a high performing building. Energy efficiency in buildings is accelerated by validated, verified models of buildings, appliance and equipment use, as well as improved workflow design and building control tools, calibrated to real building performance. These models must be easy-to-use for end-users, policymakers, and manufactures alike, and must clearly demonstrate the costs savings of improved energy efficiency to builders, operators, and tenants.

Today there is a diverse array of building models, tools, and operational procedures; however there is no single unifying authority. DOE has funded work in this area, with DOE-2, EnergyPlus, and Energy-10 being the most popular models. These tools enable buildings to be modeled and analyzed for energy use at different timescales and incorporating different technologies. Likewise, the National Institute of Standards and Technology (NIST) has funded tools focusing on building airflow and heat. CAD and design firms have their own approaches to modeling building energy. Many of these tools, however, are expensive, difficult to use, do not account for the inherent variability in building operations (weather, human behavior, equipment performance, etc.) and cannot identify the resulting energy or financial savings from energy efficiency improvements. Also, not all simulation tools have been rigorously verified, validated, and calibrated. Finally, most buildings are not operated by staff capable of interpreting multifaceted data streams (when available) or in running simulations of their buildings, should those simulations be easy to create.

Big Audacious Goals: (1) Deploy ubiquitous, cost-effective measuring, modeling, and control tools to enable financially viable retrofits that make possible the current building stock to exceed 50% reduction in energy use (relative to ASHRAE and California's Title 24 code). (2) Enable future building stock to be zero-net energy. (3) Create a platform and standard for verifying, validating, and calibrating building energy models for both design-phase and operational purposes.

Economic Benefits: HPC would reduce costs to the private sector from energy costs, improved equipment performance and longevity, increase energy security to the federal government and military, lower greenhouse gas risk to building owners and operators, enhance valuation of real estate through more reliable energy services to tenants, and demonstrate the value of already-deployed advanced sensors, specifically Smart Energy Meters.

Moderator: Michael McQuade, United Technologies Corporation Panelists: Charlie Catlett, Argonne National Laboratory; Jim Sexton, IBM T.J. Watson Research Center; James Braun, Purdue University; John Burns, Virginia Polytechnic Institute and State University

2. **Liquid Fuel Combustion**. Vehicles in the United States account for 27% of U.S. energy use. Despite advancements in hybrid and all-electric vehicles, petroleum-based engines will remain a staple of our transportation system (particularly in heavy-duty trucks and jet aircraft) for the foreseeable future. The escalating requirements for greater fuel efficiency and environmental performance drive vehicle manufacturers to adopt increasingly complex systems and components. Engine performance improvements have been achieved by the adoption of new technologies (e.g., direct injection, variable valve actuation, in-cylinder turbulence, etc.) that demand an increasingly sophisticated understanding of sprays, air-fuel mixing, turbulence, and combustion chemistry. These and other advances offer increased thermal efficiency to as high as 50% from current state-of-the-art 35–40%.

To realize the additional latent potential of next-generation technologies, it is necessary to refine, or in some cases to discover, the fundamental processes that underlie performance improvements. Advanced components like direct injectors cannot be fully developed without systematic, quantitative representations. Many of these underlying processes—particularly in-cylinder phenomena—are physically coupled, such that evaluating one element requires a simultaneous understanding of all the other features. Consequently designing advanced engines as complete systems, with detailed physical representations of all components, is virtually impossible today due to the computational complexity involved.

These challenges present a unique opportunity to develop predictive computational design tools for enhancing combustion engine performance. Robust application of HPC could sharply reduce engine development cycles, accelerating time to market, and reducing development costs, while achieving emissions targets and enhancing the competitiveness of U.S. engine manufacturers, even in the face of intense international competition. Concurrently, new fuels will add another layer of complexity, further highlighting the need for rapid, agile product-development with HPC.

Big Audacious Goals: (1) Deploy HPC to achieve 50% brake thermal efficiency for engines compatible across light-duty vehicle classes that meet emission standards. (2) Likewise, deploy HPC to achieve 60% brake thermal efficiency in engines suitable for Class 7-8 heavy-trucks that meet emission standards.

Economic Benefits: A more robust analytical modeling and simulation capability would make firms that currently rely on iterative designs more competitive and responsive, benefitting industry and the nation. For example, every 10% reduction in gasoline translates to about 125 M tonnes of CO_2 saved annually, or \$60B per year @\$4 per gallon. Every 10% reduction in diesel translates to approximately 65M tonnes of CO_2 annually, or about \$30B annually @\$4 gallon.

Moderator: Bob Carling, Sandia National Laboratories; Panelists: Andy McIlroy, Sandia National Laboratories; Wayne Eckerle, Cummins, Inc.; Gary Smyth, General Motors; Charlie Westbrook, Retired from LLNL

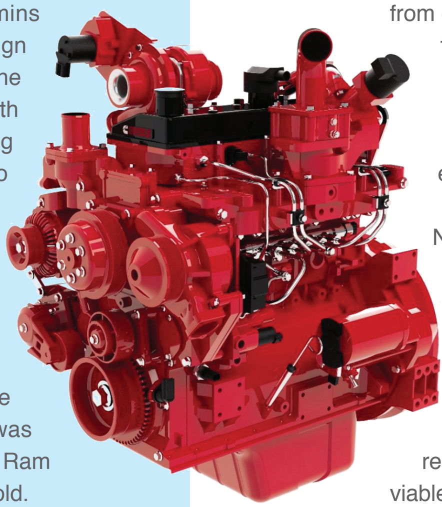
3. **Carbon Capture and Sequestration**. Carbon Capture and Sequestration (CCS) is a key technology toward achieving timely and steep reductions in greenhouse gas emissions while maintaining the benefits of fossil energy. Because 33% of U.S. emissions and 95% of U.S. power emissions come from coal and gas, CCS has the potential to rapidly and economically achieve the steep abatement targets laid out by the President and many states while using assured, domestic energy supplies.

Near-term progress in CCS is challenged by uncertainties in both the regulatory and industrial sectors and the significant costs associated with research, development, and deployment. At present, technological costs remain much higher than economically viable, and more detailed quantification of risks regarding the long-term effectiveness of geological storage are needed. Two primary technical challenges remain: lowering the cost of CO_2 capture, and demonstrating the safety and effectiveness of geological storage. Roughly 90% of the costs associated with CCS are in carbon capture, which requires concentration of CO_2 to very high purities (> 95%). HPC capabilities can greatly assist in all stages of development, from screening of new capture materials (much like the pharmaceutical industry)

DIESEL ENGINE DESIGNED SOLELY WITH COMPUTATIONAL TOOLS

Computational tools for improving combustion engine performance shorten engine development cycles, accelerating time to market and reducing development costs while also achieving energy security and emission-reduction goals. This effort is poised to achieve a great leap in American combustion engine technology that will position the nation as the world leader in next-generation engines.

In 2007, manufacturer Cummins achieved a milestone in engine design by marketing a diesel engine—the ISB 6.7 liter—designed solely with computational tools. Physical testing was conducted only after the fact to confirm performance. In this first effort, Cummins not only reduced development time and cost by about 10%, but also achieved a more robust design, improved mileage, and met all environmental and customer constraints. The ISB 6.7 liter Cummins diesel was first marketed in the 2007 Dodge Ram pickup truck; more than 200,000 sold.



Companies such as Chrysler, Ford, GM, Cummins, and Caterpillar have identified two simulation targets that are achievable in the next 5 years, that could improve efficiency by more than 20%: (1) simulating stochastic in-cylinder combustion processes and (2) simulating the constantly evolving fuel sprays.

to integrated plant simulation and design. Perhaps most importantly, new simulation methodologies and tools can remove costly steps from testing and scale-up, dramatically reducing demonstration costs to government and industry and cutting the time to market by as much as 50%.

HPC can support design and troubleshooting of carbon capture and storage devices, finding the optimal balance of performance, reliability, and cost. Simulations can range from small-scale interactions of carbon molecules to large-scale changes in stability of underground reservoirs, providing governmental and industrial decision makers with the insights needed to enable nationwide deployment.

Big Audacious Goals: (1) Use HPC to reduce the energy penalty of carbon capture from 30–40% (today) down to <15%. (2) Develop long-term, large-scale sequestration projects and related modeling and simulations to better understand the sequestration process in various geological areas to enable commercial deployment of hundreds of large-scale CCS projects injecting well over 1 million tons of CO_2 per year.

Economic Benefits: Without CCS, the goals of the U.S. administration with regard to ameliorating climate change cannot be met. Advanced computer modeling could both accelerate the development and deployment of CCS and reduce the technical and financial uncertainties to success. The CCS field will be led by the country that develops the technology first and then exports to other countries.

Moderator: Carl Bauer, National Energy Technology Laboratory; Panelists: Madhava Syamlal, National Energy Technology Laboratory; David Sholl, Georgia Institute of Technology; Julio Friedmann, Lawrence Livermore National Laboratory; John Tombari, Schlumberger, Carbon Services

CARBON CAPTURE SIMULATION INITIATIVE

The Carbon Capture Simulation Initiative (CCSI) is a partnership among national laboratories, industry, and academic institutions. The partnership is aimed at developing advanced computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to development, demonstration, and ultimately widespread deployment.

Using HPC simulations researchers can watch the molecular-level dynamics of carbon-capturing materials, then scale up to explore how these materials function at the device-level and in a production power plant. This approach reduces costly intermediate-scale testing such as building prototypes. The CCSI Toolset is an integrated suite of validated computational models designed to reduce the risk associated with incorporating innovative technologies into new carbon capture solutions. The CCSI Toolset is speeding the development and deployment of CCS in these ways:

- Promising concepts will be more quickly identified.
- The time to design and troubleshoot new devices and processes will be reduced.
- The technical risk in taking technology from laboratory-scale to commercial-scale will be more accurately quantified.
- Deployment costs will be stabilized more quickly.

The initiative brings together five DOE national laboratories—Los Alamos, National Energy Technology, Pacific Northwest, Lawrence Berkeley, and Lawrence Livermore—as well as partners in academia and industry.

4. **Smart Grid and Storage**. The U.S. electric grid was identified by the National Academy of Engineering as the greatest engineering achievement of the 20th century. Yet, its infrastructure is based on decades-old technologies unable to support the needs of the 21st century. The increasing complexity of electric power demand and supply will require the modernization of electricity generation, transmission, distribution, and individual customer appliances. The smart grid uses new sensor and actuator technologies, new control methods that support two-way power flow, and new human interfaces to provide improvements in products and services, higher-quality power, asset utilization, ability to anticipate and respond to disturbances (self-healing), resilience to natural disasters or attacks, customer choice, and transaction support.

Modernizing the grid will require changes on both the supply and demand side that will significantly increase complexity as well as services that grid operators can provide to generators and end-users. Changes in supply include increased penetration and cost competitiveness of renewable resources, distributed generation, bulk power storage, and market rules that shape the net-metered open access energy market. On the demand side, widespread adoption of plug-in electric vehicles (PEVs) and participation in demand response programs will complicate grid management.

HPC provides a powerful tool to accelerate progress in creating the smart grid by allowing quick analysis and imaging of data. This results in improved performance and by providing better predictive tools for the integration and asset utilization for expanded and efficient deployment of renewable energy. Today, measurements of the grid's physical and electrical parameters are capable of being collected every 4 to 6 seconds, yet models of system stability perform at resolutions of 3 to 5 minutes (when possible), limiting operators' ability to control the system in real time. By employing HPC techniques to grid simulation, grid managers could explore new approaches to system optimization and real-time control of a very complex system; the electric grid spans thousands of miles, contains over 30,000 major physical devices, and communicates with millions of end-use devices. Higher-resolution models could more closely replicate actual systems and develop analytic tools to manage imminent problems and contingencies. In providing real-time error and system security analyses, HPC-powered cyber security tools can improve the robustness and resilience of the electric grid, from end-users to system managers. Also, high-resolution predictive modeling, coupled with grid modernization, could reduce the need to build new transmission capacity.

Big Audacious Goals: (1) Integrate planning and operation of all three U.S. and Canadian interconnections, leading to at least a 10% improvement in capital utilization and at least a 10% decrease in operating costs with improved reliability and market transparency. (2) Manage loads at the distribution level to support complex, individual contracts for energy services (e.g., allow each PEV owner to specify required charge level by a chosen time for the morning commute).

Economic Benefits: Vigorous application of HPC would result in a more efficient use of capital, decreased losses in the system, and lower fuel costs. Because annual U.S. electricity revenues top $350B and total U.S. capital investments exceed $800B, even a small improvement in efficiency provided by a smart grid would generate large savings to individual customers and the U.S. economy. DOE estimates U.S. economic losses of $119B–$188B per year due to power outages and low quality. These inefficiencies and reliability problems pose a threat to U.S. economic competiveness and could be overcome with the help of HPC.

Moderator: Kevin Dasso, Pacific Gas and Electric Co. Panelists: Craig Adams, Exelon Corporation; Daniel Kammen, University of California-Berkeley; Steve Pullins, Horizon Energy Group; Carl Imhoff, Pacific Northwest National Laboratory

5. **Nuclear Energy**. Every MWh of electricity produced with nuclear energy avoids the emission of approximately 1.0 MT of CO_2 if the same amount of energy had been generated with conventional coal-fired technologies (0.6 MT of CO_2 for natural gas). In addition, nuclear power is dependable. It is available day or night, when the wind is blowing and when it is not.

However, continued and increased use of nuclear energy faces several key challenges: First, the capital cost of a large new plant is high and can challenge the ability of electric utilities to build new reactors. The introduction of smaller reactors may reduce capital costs by taking advantage of series fabrication in centralized plants. HPC could provide a virtual test bed for new reactors and their manufacturing processes.

Second, no permanent solution to high-level commercial nuclear waste management has been deployed in the United States. Innovative solutions, as tested first by HPC, will be required to assure that used fuel from nuclear power plants is properly stored. Third, global expansion of nuclear energy raises concerns stemming from access to enrichment and reprocessing activities that might produce weapons-usable materials. A robust simulation capability to evaluate proliferation and terrorism risks is needed here as well.

Finally, the reactors in the current operating fleet have been continuously increasing their power densities to meet rising electricity demand, and the operating fleet will be pursuing license extensions that will push the operating life of current reactors to 80 years. Modeling and simulation is a core part of every license application as it is a measure of the applicant's quantitative understanding of the reactor system and materials performance and limits. These simulations are typically run on single workstations and desktops, and current analysis tools used during severe accident scenarios are unable to provide a real-time snapshot of reactor core reconfiguration (i.e. during an accident which results in a loss of coolant). Given the political and societal concerns in the wake of the Japanese Fukushima event, HPC could simulate severe disaster scenarios as well as help develop intrinsically safer designs.

Big Audacious Goals: Use HPC to better understand the safety performance of the aging reactor fleet and design and optimize construction of new classes of reactors. HPC will (1) Provide real-time analysis of reactors in severe accident conditions (beyond design basis). (2) Perform non-proliferation analyses to determine whether reactor operation is being optimized for weapons material production. (3) Aid license applications for new classes of reactors whose operation and safety cases require a significant departure from reactors in current operation. (4) Simulate, predict, and refine the future safety and performance of reactors and integrated plant systems as they age.

Economic Benefits: 64 GW of new nuclear capacity is equivalent to building about 46 new nuclear plants at an average size of 1,400 MW each. Together, these nuclear plants would produce $1.7 trillion in economic value to local communities near the plants, $365B in tax revenue, 90,000 jobs, and power to 47 million households. In addition, the nuclear plants would save trillions of tonnes of CO_2 from being emitted.

Moderator: Alex Larzelere, U.S. Department of Energy; Panelists: Terry Wallace, Los Alamos National Laboratory; Doug Kothe, Oak Ridge National Laboratory; Eric Loewen, GE-Hitachi Nuclear Energy; Don Langley, The Babcock & Wilcox Company; Kord Smith, Studsvik-Scandpower, Inc.

CONSORTIUM FOR ADVANCED SIMULATION OF LIGHT WATER REACTORS

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is a DOE Innovation Hub that is developing advanced capabilities for predictive simulation of light water reactors. CASL researchers are developing highly sophisticated models that will help accelerate upgrades at existing U.S. nuclear plants. These upgrades could improve the energy output of our existing reactor fleet at a fraction of the cost of building new reactors, while providing continued improvements in reliability and safety. The facility, headquartered at Oak Ridge National Laboratory, brings together four national labs, three industry partners, and three universities in a highly collaborative effort.

CASL's environment for predictive simulation, the Virtual Reactor (VR), is being used to address essential issues in nuclear power plant and design. CASL is validating the VR models against experiments and then against operating reactor data from the existing Tennessee Valley Authority pressurized water reactors fleet. The resulting VR couples state-of-the-art neutronics, thermal hydraulics, structural, and fuel performance models, linked with existing systems and safety analysis tools, to model nuclear power plant performance.

CASL is addressing three key areas of performance: (1) Reducing capital and operating costs per unit energy; (2) reducing the nuclear waste volume generated by enabling higher fuel burnups; and (3) enhancing nuclear safety by enabling high-fidelity predictive capability for component performance through failure.

Action Items for Harnessing HPC

The Summit engaged participants from both the public and private sectors in thinking about a national roadmap that would harness HPC to advance American clean energy technologies. Participants raised a broad range of questions in efficiently harnessing HPC. These include: How can HPC work best in industry? How should technology transfer and intellectual property be assigned in HPC partnerships? How do we obtain sustainable and stable funding for using HPC to advance clean energy technology? What is the role of venture capitalists? How do we make HPC more available to middle and small-size businesses? What are the barriers to accessing HPC, including cost, access, availability, and user-friendly software? What would an accessible HPC user facility provide? What HPC user facility types are presently available nationally and internationally? However, these obstacles present opportunities.

In response, Summit organizers have decided upon three initial action items that will facilitate HPC adoption by U.S. energy companies:

1. Co-sponsor meetings on clean energy technology advancement to determine the HPC state-of-the-art and to identify areas of need for companies at different stages. For example, an energy symposium will be held in North Dakota in partnership with local schools, clean energy companies, and local business. Also, a conference in Washington, D.C. in partnership with related universities and businesses in the field, will examine shale gas and its effects on the energy sector. Organizers will develop a comprehensive report detailing issues of safety, reserve estimates, track record, new capabilities, outlook, and impact on U.S. energy policy.

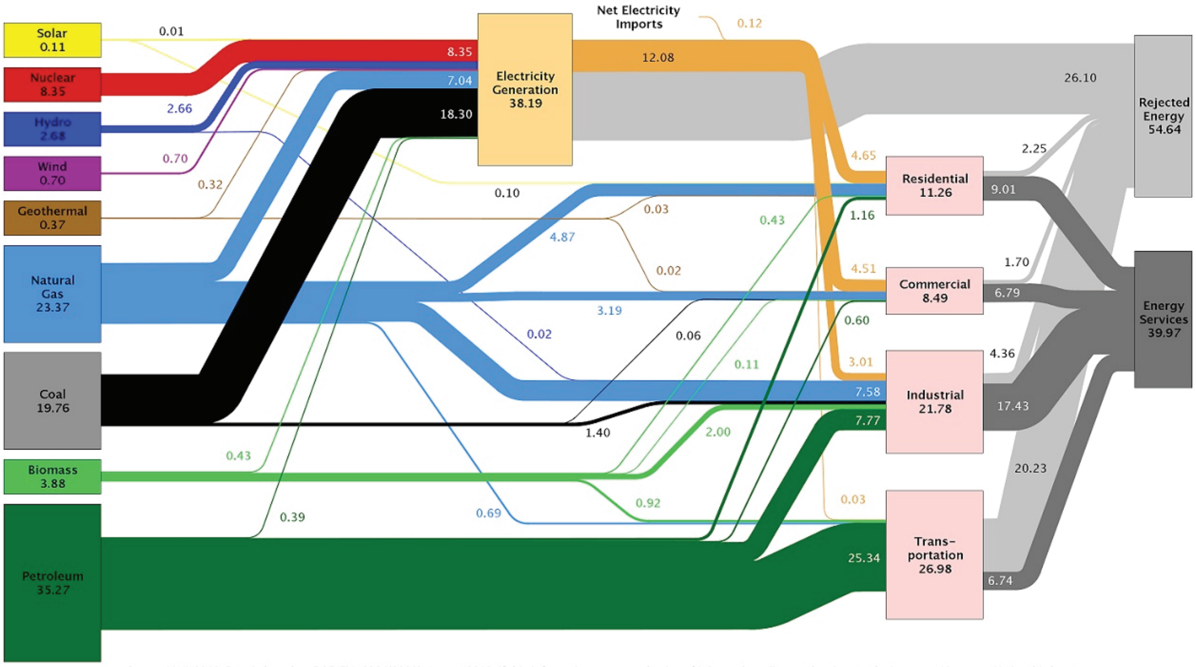
2. Release a Call for Proposals for clean energy businesses of all sizes. Winning proposals will be provided with Lawrence Livermore National Laboratory's (LLNL's) HPC capabilities and expertise for pilot projects aimed at solving specific problems.

3. Generate a dynamic, innovative, and interactive website for clean energy computing. This electronic portal will outline the state-of-the-art for selected energy sectors. It will provide information and advice and track follow-on actions to enterprises, entrepreneurs, and researchers—a one-stop shop for what stakeholders need to know in order to leverage America's HPC assets. The roadmap will also provide concrete next steps and solicit inquiries for use of LLNL HPC capabilities.

We are confident that these three initial actions—workshops and conferences; strong public-private partnerships, and a living website—will spur other, far-reaching actions that together will accelerate the deployment of advanced clean energy technology with HPC. Within a few years, companies large and small will be routinely turning to HPC tools to rapidly design, develop, and deploy new energy products and materials. HPC will be the catalyst that lowers the risk and cost to transition to a clean energy society. The resulting transformation of America's energy future will help ensure U.S. competitiveness in the global energy market, invigorate our high-tech manufacturing industry, and strengthen national security.

Energy use in the U.S., 2009.

Estimated U.S. Energy Use in 2009: ~94.6 Quads



Source: LLNL 2010. Data is based on DOE/EIA-0384(2009), August 2010. If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports flows for non-thermal resources (i.e., hydro, wind and solar) in BTU-equivalent values by assuming a typical fossil fuel plant "heat rate." The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 80% for the residential, commercial and industrial sectors, and as 25% for the transportation sector. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

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