



Exascale for Energy

The role of exascale computing in energy security

How will the United States satisfy energy demand in a tightening global energy marketplace while, at the same time, reducing greenhouse gas emissions? Exascale computing—expected to be available within the next eight to ten years—may play a crucial role in answering that question by enabling a paradigm shift from *test-based* to *science-based* design and engineering.

Energy security has two key dimensions: reliability and resilience. Reliability means that energy users are able to access the energy they need, when they need it, at affordable prices. Resilience means the ability of the system to cope with shocks and change.

In today's world, energy security, economic security, national security, and environmental security are all closely interrelated. For example, world energy consumption is projected to grow by 44 percent over the 2006 to 2030 period, according to the Energy Information Administration's (EIA) 2009 International Energy Outlook (Figure 1). Competition for energy supplies is certain to increase; but with U.S. oil production declining (Figure 2), economic security and national security may be at risk unless we can obtain assured fuel supplies from reliable sources.

At the same time, environmental security requires that the world transition to carbon-neutral energy sources that do not contribute to global warming. This constraint is hardly altruistic. In the 2007 report *National Security and the Threat of Climate Change*, a blue-ribbon panel of military experts concluded that climate change is a threat multiplier in already fragile regions, exacerbating condi-

tions that lead to failed states—the breeding grounds for extremism and terrorism—while adding to tensions even in stable regions of the world. Climate change, national security, and energy dependence are a related set of global challenges.

Improving America's energy security while stabilizing the earth's climate requires, in the near term, widespread implementation of existing conservation and energy efficiency technologies that reduce carbon dioxide emissions; in the mid-term, substantial improvement of existing energy technologies; and in the long term, development of new technologies and fuel sources.

Modeling and simulation using exascale computers—capable of one million trillion (10^{18}) calculations per second—will make a significant contribution to mid- and long-term advances in energy technologies by enabling a paradigm shift from test-based to science-based design and engineering. Computational modeling of complete power generation systems and engines, based on scientific first principles, will accelerate the improvement of existing energy technologies and the development of new transformational technologies by pre-selecting the designs most likely to be successful for experimental validation, rather than relying on trial and error.

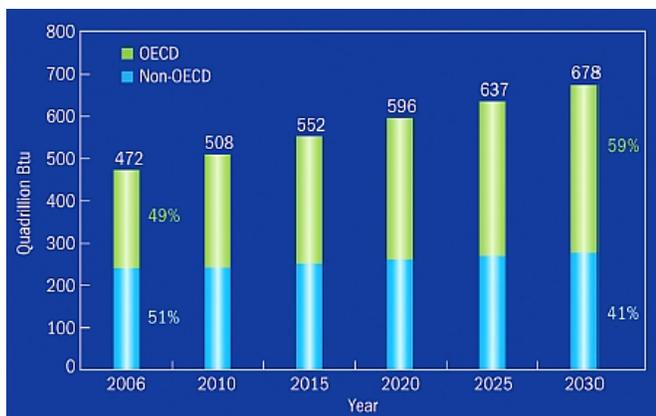


Figure 1. World energy consumption is projected to grow by 44 percent over the 2006 to 2030 period, with non-OECD (Organisation for Economic Co-operation and Development) countries accounting for 82% of the increase. *Source: EIA*

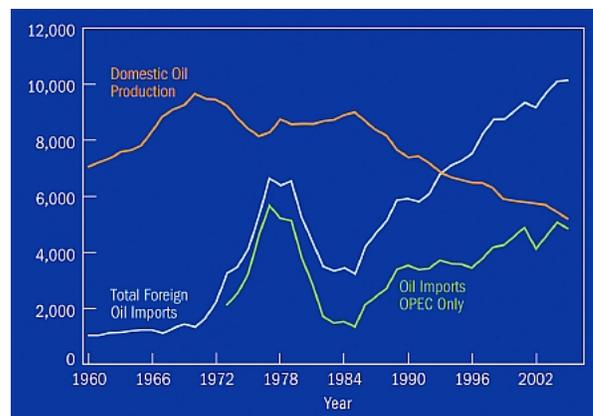


Figure 2. U.S. oil production and foreign oil imports (thousands of barrels per day). *Source: EIA*

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The predictive understanding of complex engineered systems made possible by computational modeling will also reduce the construction and operations costs, optimize performance, and improve safety. Exascale computing will make possible fundamentally new approaches to quantifying the uncertainty of safety and performance engineering.

This report discusses potential contributions of exascale modeling in four areas of energy production and distribution: nuclear power, combustion, the electrical grid, and renewable sources of energy, which include hydrogen fuel, bioenergy conversion, photovoltaic solar energy, and wind turbines. Nuclear, combustion, the grid, photovoltaics, and wind turbines represent existing technologies that can be substantially improved, while hydrogen and biofuels represent long-term R&D projects that will be needed for a carbon-neutral economy. More detailed analyses of these topics can be found in the reports listed at the end of this article. Examples of current research are taken from projects funded by the U.S. Department of Energy (DOE) Office of Science at universities and national laboratories, with a special focus on research conducted at Lawrence Berkeley National Laboratory (Berkeley Lab).

Nuclear Power

Nuclear fission plays a significant and growing role in world energy production. Currently, 436 nuclear power plants in 30 countries produce about 15% of the electrical energy used worldwide. Sixteen countries depend on nuclear power for at least a quarter of their electricity. The USA is the world's largest producer of nuclear power, with more than 30% of worldwide nuclear generation of electricity. America's 104 nuclear reactors produced 809 billion kWh in 2008, almost 20% of total electrical output.

Despite more than 30 years with almost no new construction, U.S. reliance on nuclear power has continued to grow. The U.S. nuclear industry has maximized power plant utilization through improved refueling, operating efficiency, maintenance, and safety systems at existing plants. There is growing interest in operating existing reactors beyond their original design lifetimes.

The Energy Policy Act of 2005 has stimulated investment in a broad range of electricity infrastructure, including nuclear power. Over the last few years more than a dozen utility companies have announced their intentions to build a total of 27 new nuclear reactors. In addition, to meet the rising demand for carbon-free energy, a new generation of advanced nuclear energy systems is under development that would be capable of consuming transuranic elements from recycled spent fuel (see reactor sidebar, page 5). These advanced reactors would extract the full energy value of the fuel, produce waste that does not create long-term hazards, and reduce proliferation of nuclear weapons materials.

Exascale computing is poised to play a major role in the development of next-generation nuclear plants. By enabling the high-fidelity modeling and simulation of

complete nuclear power systems, exascale computing would change nuclear engineering from a *test-based* to a *science-based* discipline. Such modeling can benefit nuclear energy in several ways:

- Accelerate the iteration cycle of technology evaluation, design, engineering, and testing to optimize existing and new nuclear energy applications.
- Shorten the licensing process by providing reliably predictive integrated performance models that reduce uncertainties.
- Reduce construction and operations costs while also reducing uncertainty and risk.

Modeling has always played a key role in nuclear engineering, design, and safety analysis. Computational analyses based on large experimental databases have been used to analyze material properties, fuel performance, reactor design, safety scenarios, and waste storage. But legacy applications do not provide the high fidelity required to understand fundamental processes that affect facility efficiency, safety, and cost, including:

- **Determination of material properties** of fuels and structural materials under both static and dynamic conditions, including nuclear (e.g., neutron and gamma reactions), thermophysical (e.g., thermal conductivity), mechanical (e.g., fracture toughness), and chemical (e.g., corrosion rates). Nuclear fuel assemblies must perform in extreme environments where they are subjected to stress, heat, corrosion, and irradiation, all of which can lead to progressive degradation of the fuel cladding materials and other structural components. Researchers hope that simulations will help them discover new ways of preventing or mitigating material degradation.
- **Spent fuel reprocessing** is an option that was abandoned in the 1970s but is now looked on more favorably. Reprocessing involves dissolving the spent fuel in acid, treating the fuel in a series of solvent extraction processes, and fabricating it into fuel or waste forms. Current models provide only qualitative descriptions of process behavior and are unable to answer many key questions. To support the detailed design and safe operation of reprocessing plants, advanced reprocessing models require improved chemistry, fluid dynamics, interfaces with nuclear criticality calculations, and whole-plant modeling.
- **Fuel development and performance evaluation** is currently an empirical process that takes decades. New fuels must be fabricated, be tested in a test reactor under multiple accident scenarios, undergo post-irradiation examinations, and finally be placed in an operational reactor for several cycles. Fuel performance simulation tools could reduce the current 10- to 15-year qualification time by a factor of three. But these tools must be comprehensive enough to predict the thermal, mechanical, and chemical response of the fuel rod throughout its irradiation lifetime.

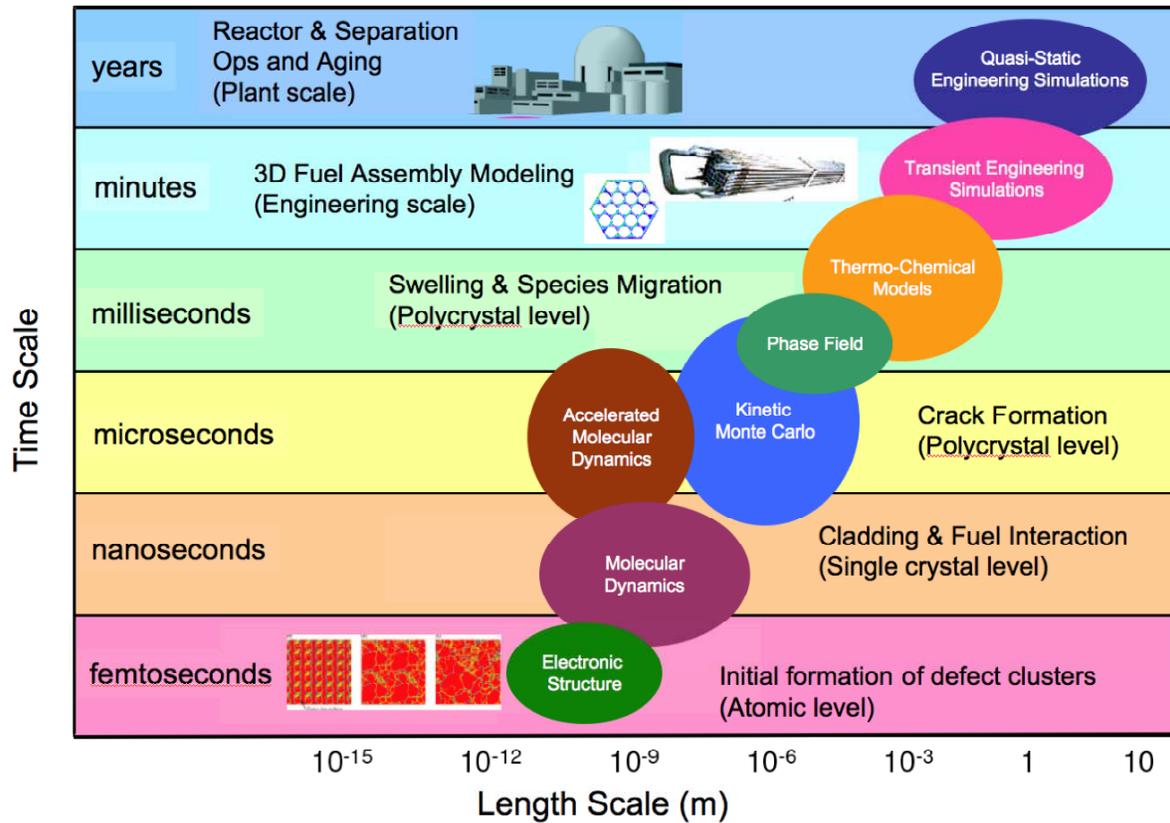


Figure 3. Individual simulation tools and integrated performance and safety codes (IPSCs) involve different physical phenomena at varying scales of interest. Source: Science Based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale workshop

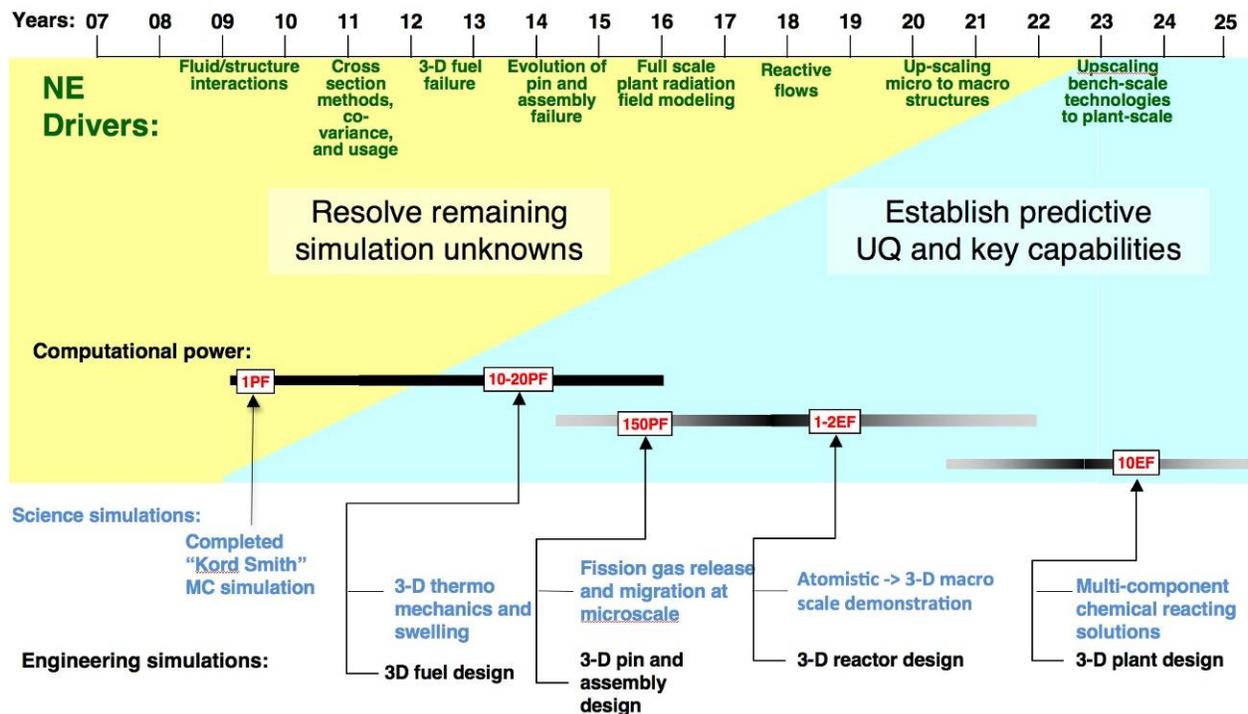


Figure 4. Computational requirements for nuclear energy modeling: PF = petaflops, EF = exaflops. Source: Science Based Nuclear Energy Systems Enabled by Advanced Modeling and Simulation at the Extreme Scale workshop

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- **Reactor design and safety** simulation tools need improved physical, numerical, and geometric fidelity.

There are multiple challenges in modeling the design, performance, and safety of a nuclear reactor. Figure 3 illustrates the multiscale physical challenges that a nuclear reactor faces in size (length) and time.

A May 2009 workshop sponsored by the DOE Office of Science and Office of Nuclear Energy developed a detailed picture of the computational requirements for nuclear energy modeling, culminating in a 10 exaflop requirement by the year 1024. The timeline in Figure 4 includes nuclear energy drivers, science simulations to resolve science unknowns, and engineering simulations that use integrated codes. The workshop participants estimated that it will take nearly 15 years to resolve many of the scientific questions identified in Figure 4 and to establish fully predictive, integrated codes that can quantify uncertainties. But they also estimated that exascale modeling could reduce the construction cost of a large-scale nuclear plant by 20%, saving as much as \$3 billion on a \$15 billion plant.

Exascale resources will improve the geometric, numerical, and physics fidelity in modeling key phenomena such as the evolution of fuel pin microstructure and behavior (Figure 5):

- **Improved geometric fidelity** will extend lower-length-scale fidelity to sub-10 μm resolution of three-dimensional phenomena such as microstructure evolution and material failure, validated with uncertainty quantification methodologies.
- **Improved numerical fidelity** will involve bridging vastly different time and length scales with multi-physics phenomena, such as bubble–fission fragment interactions (including molecular dynamics), and scaling up oxide and metal models into pellet simulations.
- **Improved physics fidelity** will apply to modeling phenomena such as fission gas bubble formation, transport, and release; fuel chemistry and phase stability; fuel–cladding mechanical interactions; and thermal hydraulics, turbulence, and coolant flow in pin assemblies, and their effect on fuel and cladding evolution.

The creation of integrated performance and safety codes faces considerable technical challenges that range from improvements in software engineering and numerical methods to the development of more fully integrated physics models. But if these challenges are met with a sustained and focused effort, exascale computing can revolutionize the modeling and design of nuclear energy systems.

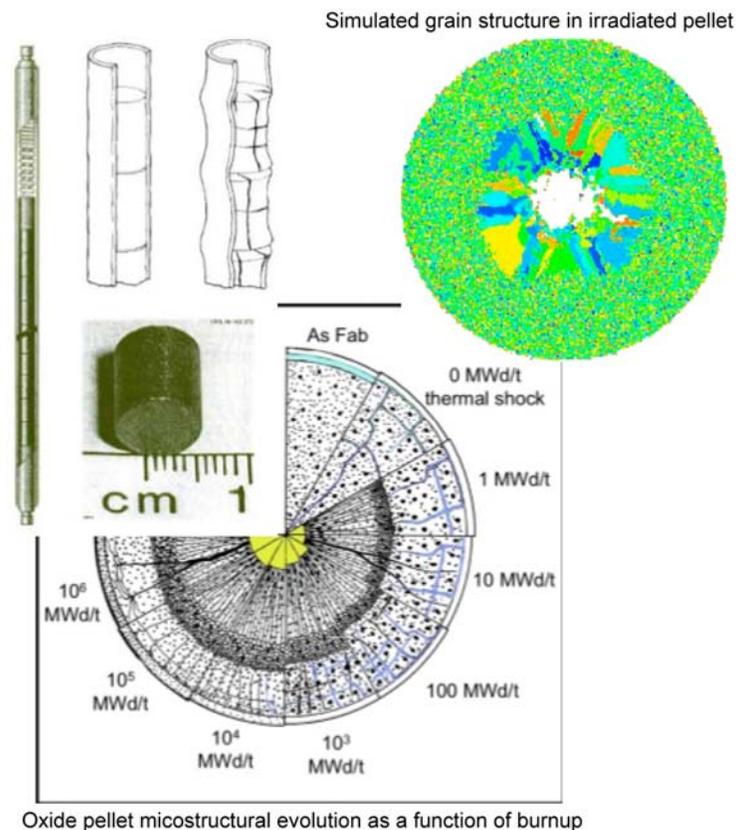


Figure 5. Three-dimensional predictive simulations of fuel pin behavior from microstructure evolution will require exascale resources. *Source: DOE Exascale Initiative*

Simulating Reactor Core Coolant Flow

Liquid-metal-cooled fast reactors are expected to play a key role in the Department of Energy's Global Nuclear Energy Partnership (GNEP). These advanced burner reactors (ABRs) are expected to be safer, to produce more power, and to produce as much as 100 times less waste than today's reactors. Furthermore, ABRs will burn waste recycled from today's nuclear plants as fuel, thus reducing the burden on underground waste repositories. The new generation nuclear plants will operate at temperatures much higher than today's reactors. And instead of water, they will use liquid metals such as sodium or a liquid fluoride salt to cool them. GNEP is thus expected to be an economically viable approach to addressing the issues of energy security, carbon management, and minimal nuclear waste.

With a grant of 30 million processor hours on the Argonne Leadership Computing Facility's IBM Blue Gene/P from the DOE Office of Science's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, Argonne's "Reactor Core Hydrodynamics" project is carrying out large-scale numerical simulations of turbulent thermal transport in sodium-cooled reactor cores to gain an understanding of the fundamental thermal mixing phenomena within ABR cores that can lead to improved safety and economical performance.

Figure 6 shows a recent simulation of turbulent coolant flow in a 217-pin subassembly of the reactor core, conducted with the Nek5000 code. Each pin of nuclear fuel, about a centimeter in diameter and about 1.2 meters long, has a wire twisted around it in a gentle spiral to separate the pins and to promote coolant flow around them. The pins partition the hexagonal canister

into 438 communicating subchannels. (A reactor may include hundreds of these canisters.) This simulation used 2.95 million spectral elements of order $N = 7$ and ~988 million grid points on 32,768 processors of the Blue Gene/P. These fine-scale simulations are providing data and physical insight previously accessible only through experiment.

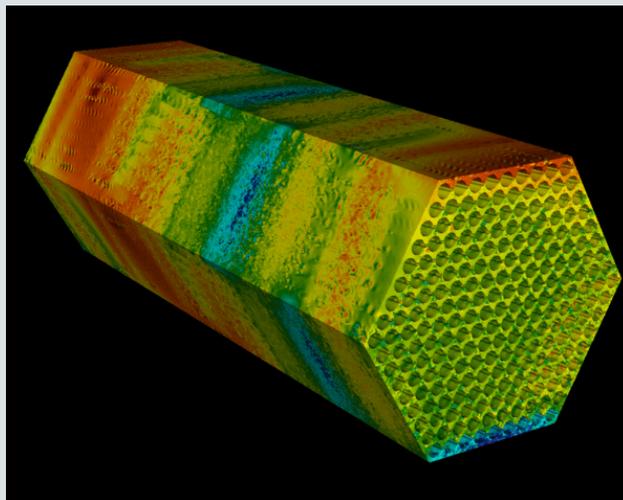


Figure 6. Early-time pressure distribution for simulation of coolant flow in a 217-pin wire-wrapped subassembly, computed on 32,768 processors of the Argonne Leadership Computing Facility's BG/P using Nek5000. The Reynolds number is $Re \sim 10,500$, based on hydraulic diameter. The mesh consists of 2.95 million spectral elements of order $N = 7$ (~988 million grid points). *Source: P. Fischer, ANL*

Combustion

Currently 85% of our nation's energy comes from hydrocarbon combustion, including petroleum, natural gas, and coal (Figure 7). Although there may be long-term alternatives to combustion for some uses, changes in fuels and energy technologies tend to happen gradually (Figure 8). High infrastructure costs suggest that combustion may continue to be the predominant source of energy for the next 30 to 50 years.

Transportation is the second largest energy consumer in the U.S., accounting for two-thirds of petroleum usage. Transportation technologies provide opportunities for 25% to 50% improvement in efficiency through strategic technical investments in both advanced fuels and new low-temperature engine concepts. These improvements would result in potential savings of 3 million barrels of oil per day, from the total current U.S. consumption of 20 million barrels.

A 2006 DOE Office of Basic Energy Sciences workshop on Basic Research Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels identified a single, overarching grand challenge: the development of a validated, predictive, multi-scale, combustion

modeling capability to optimize the design and operation of evolving fuels in advanced engines for transportation applications.

Concern for energy security is driving the development of alternative fuel sources, such as oil shale, oil sands, syngas, and renewable fuels such as ethanol, biodiesel, and hydrogen. These new fuel sources all have physical and chemical properties that are very different from traditional fuels. New combustion systems, for both stationary power plants and transportation, need to be developed to use these fuels efficiently while meeting strict emissions requirements.

Modeling internal combustion engines is a complex, multi-physics, multi-scale problem. Engine combustion processes involve physical and chemical phenomena that span a wide dynamic range ($\sim 10^9$) in spatial and temporal scales, involving hundreds of chemical species and thousands of reactions. The microscopic reaction chemistry affects the development of the macroscopic turbulent flow field in engines, and the change in temperature due to the altered flow dramatically affects the reaction rates. Changes in fuel composition directly affect phenomena at several scales. For example, at microscopic scales, fuel

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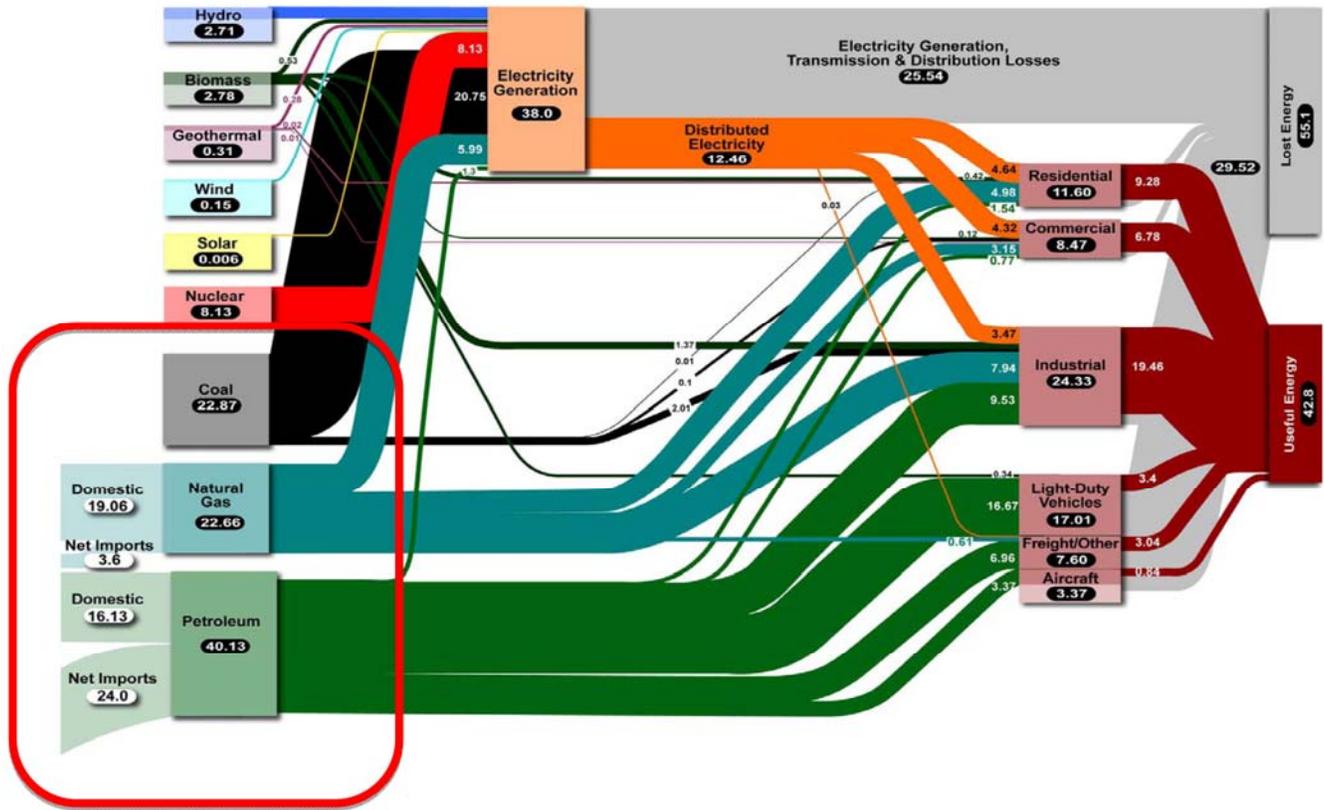


Figure 7. Combustion accounts for 85% of the energy used in the United States. Source: LLNL

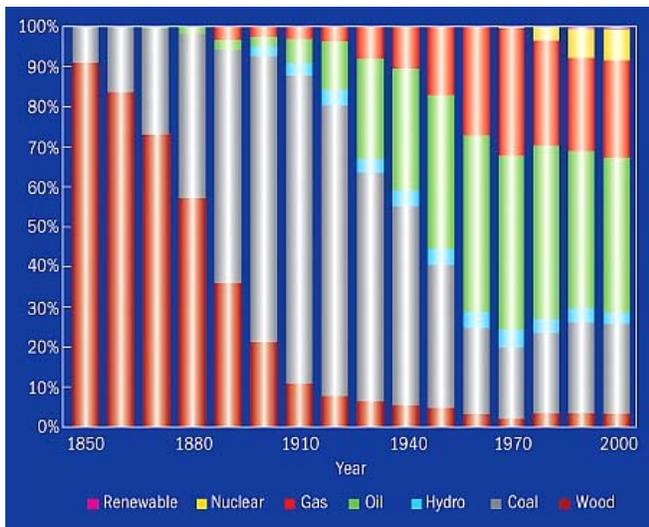


Figure 8. Gradual changes in the U.S. energy supply from 1850 to 2000. Source: EIA

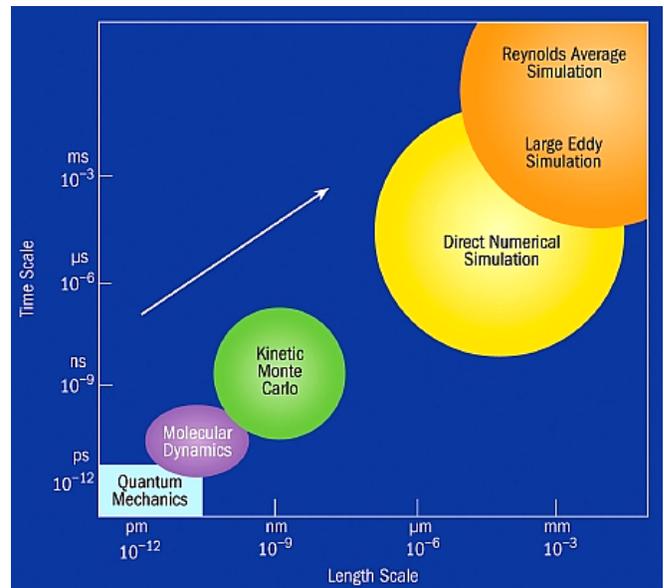


Figure 9. Multi-scale modeling describes internal combustion engine processes from quantum scales up to device-level, continuum scales. Source: DOE Exascale Initiative

changes affect some reaction rates; at larger scales, changes in bulk liquid properties affect fuel injection and evaporation.

Understanding how changes at specific scales affect the overall performance of an engine requires very careful coupling across the scales, as well as a wide variety of computational techniques, such as quantum dynamics,

molecular dynamics, kinetic Monte Carlo, direct numerical simulation, large eddy simulation, and Reynolds-averaged simulation (Figure 9).

Fuel and engine technologies should be developed together if we want to move them as quickly as possible from the laboratory to the marketplace. This co-develop-

ment requires a new approach to engineering research and development: instead of hardware-intensive, experience-based engine design, which is slow and labor intensive, we need a relatively faster, simulation-intensive, science-based design process. High-fidelity multiscale modeling on exascale computers will play a key role in enabling this transition.

Lean premixed burners are one example of a new technology being considered for stationary gas turbines, which provide a significant portion of our electric power generation. Theoretically these burners could operate cleanly and efficiently with a variety of fuels, such as hydrogen, syngas, and ethanol, because of their high thermal efficiency and low emissions of NO_x due to lower post-flame gas temperatures. However, the lean fuel mix makes some burners susceptible to flame instability and extinction, emissions of unburned fuel, and large pressure oscillations that can result in poor combustion efficiency, toxic emissions, or even mechanical damage to turbine machinery. An important exception to this trend is the low-swirl burner, which produces a stable flame (see sidebar, page 8).

Researchers are only beginning to acquire a fundamental understanding of the dynamics of premixed flame propagation and structure for the variety of different fuels that is required to meet the engineering design goals for lean premixed burners. Exascale computing will play a deciding role in whether we are able to design these types of systems.

Effective design of both power generation and transportation systems will require new computational tools that provide unprecedented levels of chemical and fluid

dynamical fidelity. Current engineering practice is based on relatively simple models for turbulence combined with phenomenological models for the interaction of flames with the underlying turbulent flow. Design computations are often restricted to two-dimensional or relatively coarse three-dimensional models with low-fidelity approximations of the chemical kinetics.

A dramatic improvement in fidelity will be required to model the next generation of combustion devices (Figure 10). Theory cannot yet provide detailed flame structures or the progression of ignition in complex fuels, while experimental diagnostics provide only a limited picture of flame dynamics and ignition limits. Numerical simulation, working in concert with theory and experiment, has the potential to address the interplay of fluid mechanics, chemistry, and heat transfer needed to address key combustion design issues.

The grand challenge is to develop a validated, predictive, multiscale, combustion modeling capability that can optimize the design and operation of evolving fuels in advanced engines and power plants. Using exascale computing systems, thousands of design iterations—each corresponding to a high-fidelity multiscale simulation—could accelerate the optimization and implementation of new technologies.

Other scientific challenges related to combustion include capturing and using the energy currently dissipated as waste heat, and capturing and storing the carbon dioxide released by combustion to help stop global warming. Computational simulations are already playing a key role in both efforts, as described in the sidebars on pages 9 and 10.

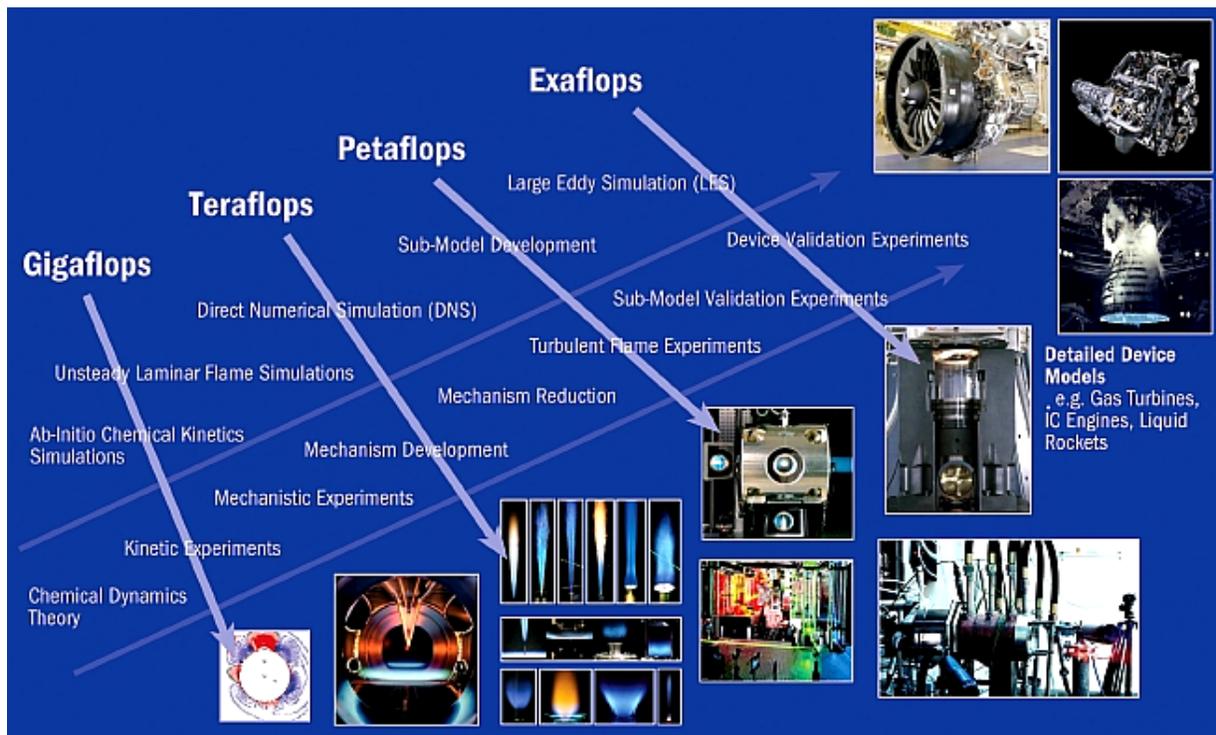


Figure 10. Combustion science breakthroughs enabled by algorithms, applications, and HPC capability.
Source: J. Oefelein and R. Barlow, SNL

Low-swirl combustion: Experiments and simulations working together

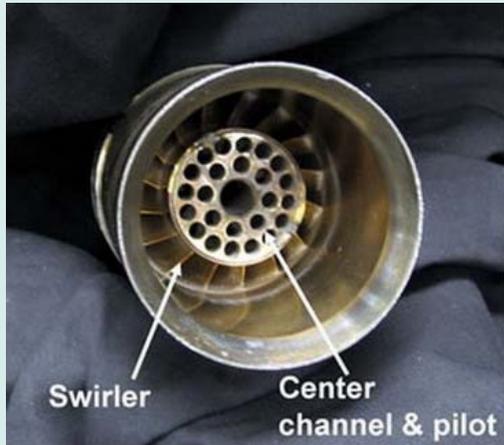


Figure 11. The heart of the low-swirl burner is a vane-swirler that has two flow passages. The fuel/air mixture flows through the openings of the center channel and the gaps between the surrounding swirl vanes. This design creates the low-swirl flow which supports a stable lifted or floating flame. *Source: R. Cheng, Berkeley Lab*

Researchers at Lawrence Berkeley National Laboratory (Berkeley Lab) have invented a unique, clean-burning combustion technology known as the low-swirl burner (LSB), which was honored with a 2007 R&D100 Award (Figures 11 and 12). The basic LSB principle is fundamentally different than the conventional high-swirl combustion method and defies many established notions of turbulent flame properties and burner engineering concepts. The new technology not only burns efficiently and cleanly, producing a very low level of nitrogen oxides, it is also more economical to manufacture and operate than many conventional burners. The LSB has been scaled for devices ranging in size from home furnaces to industrial boilers and power plants.

For much larger turbines capable of generating 250 MW of electricity, the Department of Energy is supporting research to evaluate the low-swirl combustion technology as a candidate for the hydrogen turbines in DOE Office of Fossil Energy's FutureGen Clean Coal Project. FutureGen is a public-private partnership to design, build, and operate the world's first zero-emissions fossil fuel power plant, using the Integrated Gasification Combined Cycle (IGCC) approach to produce hydrogen, which is separated from a concentrated CO₂ stream. The CO₂ is then sequestered in the earth, preventing emissions to the atmosphere that contribute to climate change.

Continued development of low-swirl burners and other advanced combustion technologies for large-scale generation of electricity depends on improving our understanding of basic flame structure, stabilization mechanisms, emissions, and response to changes in fuel. Numerical simulation has the potential to address some of these issues, but simulation of advanced burners has proven to be difficult because of the large range of spatial and temporal scales in these systems. The bulk of the analysis to date has been based on laboratory experiments.

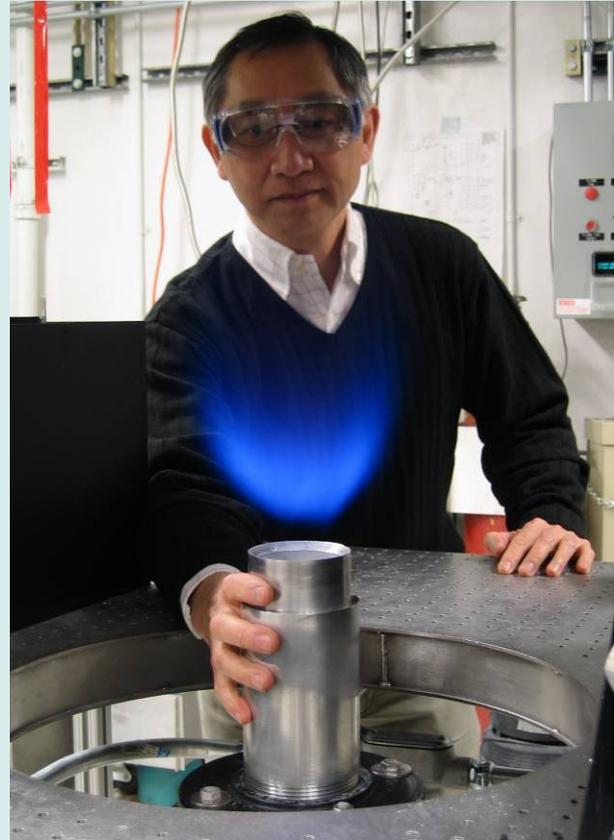


Figure 12. The low-swirl burner remains cool to the touch because the lifted flame does not heat up its body. The lifted flame originally was thought to be highly undesirable because in other burners it leads to unstable flame behaviors. But the unique divergent flow field of the LSB allows the lifted flame to self-adjust and remain robust even with a very lean fuel mixture. *Source: R. Cheng, Berkeley Lab*

The detailed structure of lean premixed flames becomes particularly important and difficult to simulate when the fuel is hydrogen. Burning hydrogen in a gas turbine presents significant technical and engineering challenges because of the high reactivity of hydrogen, its fast flame speed, and the propensity of the hydrogen/air mixture to auto-ignite and explode.

Lean hydrogen-air flames burn in cellular structures—localized regions of intense burning, separated by regions of local extinction. In this regime, the flame surface is broken into discontinuous segments. This type of structure introduces severe difficulties in applying standard turbulence/chemistry interaction models, which are based on the presence of a highly wrinkled but continuous flame surface. The cellular burning patterns also make the analysis of experimental data problematic, and can lead to significant inaccuracies or misinterpretations.

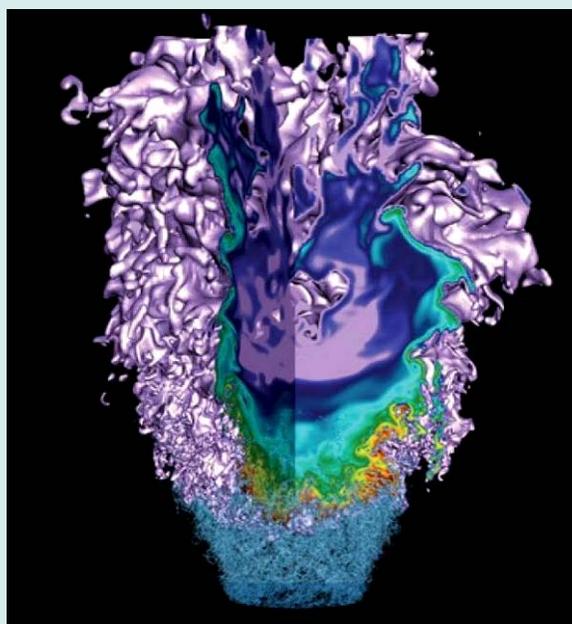
Despite these difficulties, Berkeley Lab's Center for Computational Sciences and Engineering (CCSE), supported by two successive INCITE grants totaling 5.6 million processor hours, has succeeded in producing a series of direct numerical simulations of lean, premixed

hydrogen flames on laboratory-scale low-swirl burners (Figure 13).

Using a low Mach number formulation and adaptive mesh refinement, the simulations incorporate detailed chemistry and transport without relying on explicit models for turbulence or turbulence/chemistry interaction. The simulations capture the cellular structure of hydrogen flames and provide a quantitative characterization of enhanced local burning structure.

This work lays the foundation for a program of closely collaborative investigations between computational and experimental combustion scientists. Since the simulations of a laboratory-scale burner required millions of hours on a tera-scale system, future simulations of power plant burners will clearly require exascale capabilities.

Figure 13. Simulations that ran on as many as 4000 cores of the Franklin Cray XT4 supercomputer at the National Energy Research Scientific Computing Center (NERSC) captured the detailed structure of a lean hydrogen flame on a laboratory-scale low-swirl burner. This image shows concentration of the flame radical hydroxyl and the turbulent vorticity field (gray). *Source: M. Day, Berkeley Lab*



Thermoelectrics: Turning waste heat into electricity

Automobiles, industrial facilities, and power plants all produce waste heat, and a lot of it. In a coal-fired power plant, for example, as much as 60 percent of the coal's energy disappears into thin air. One estimate places the worldwide waste heat recovery market at one trillion dollars, with the potential to offset as much as 500 million metric tons of carbon per year.

One solution to waste heat has been an expensive boiler-turbine system; but for many companies and utilities, it does not recover enough waste heat to make economic sense. Bismuth telluride, a semiconductor material, has shown promise by employing a thermoelectric principle called the Seebeck effect to convert heat into an electric current, but it's also problematic: toxic, scarce, and expensive, with limited efficiency.

What's the solution? Junqiao Wu, a materials scientist at the University of California, Berkeley and Lawrence Berkeley National Laboratory, believes the answer lies in finding a new material with spectacular thermoelectric properties that can efficiently and economically convert heat into electricity. (Thermoelectrics is the conversion of temperature differences, that is, differences in the amplitude of atomic vibration in a solid, into an electric current.)

Wu knew from earlier research that a good thermoelectric material needed to have a certain type of density of states, which is a mathematical description of distribution of energy levels within a semiconductor. "If the density of states is flat or gradual, the material won't have very good thermoelectric properties," Wu says. "You need it to be spiky or peaky."

Wu also knew that a specialized type of semiconductor called highly mismatched alloys (HMAs) could be very peaky because of their hybridization, the result of forcing together two materials that don't want to mix atomically, akin to mixing water and oil. He hypothesized that mixing two semiconductors, zinc selenide and zinc oxide, into an HMA, would produce a peaky density of states.

Beginning in late 2008, Wu collaborated with other researchers to run computations on the Franklin supercomputer at NERSC. After months of number crunching, Wu's idea held up (Figure 14). Theoretically, at least, mixing the two materials enhanced their thermoelectric performance considerably, producing a new, highly efficient, potentially low-cost thermoelectric material.

Wu is now working on synthesizing this material in the lab, a process that could take three to five years. If Wu's experiments are successful, it might be another five years before his material is adapted into a thermoelectric device and sent out to recover waste heat.

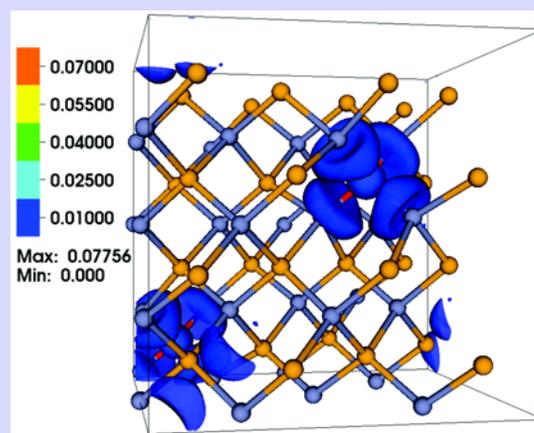


Figure 14. Contour plots of charge density in a zinc selenide/zinc oxide alloy. *Source: J. Wu*

Adapted from "Thermoelectrics: A matter of material" by Rachel Shafer, in *Innovations: Research & News from Berkeley Engineering*, Vol. 4, No. 5, June 2010.

Carbon capture and sequestration: Putting the brakes on CO₂ emissions

Carbon capture and sequestration—injecting carbon dioxide (CO₂) into the Earth’s subsurface instead of releasing it into the atmosphere—is one of the most promising ways for reducing the buildup of greenhouse gases in the atmosphere. In fact, even under the most optimistic scenarios for energy efficiency gains and the greater use of low- or no-carbon fuels, sequestration will likely be essential if the world is to stabilize atmospheric concentrations of greenhouse gases at acceptable levels.

CO₂ sequestration in geologic formations includes oil and gas reservoirs, unmineable coal seams, and deep saline reservoirs. These are structures that have stored crude oil, natural gas, brine, and CO₂ over millions of years. Many power plants and other large emitters of CO₂ are located near geologic formations that are amenable to CO₂ storage. In many cases, injection of CO₂ into a geologic formation can enhance the recovery of hydrocarbons, providing value-added byproducts that can offset the cost of CO₂ capture and sequestration.

While pilot projects have demonstrated the feasibility of carbon sequestration, there are unanswered questions about the behavior of CO₂ in geologic formations and the most economical ways to capture CO₂ at its sources. Three research projects in Berkeley Lab’s Computational Research Division (CRD) are helping to find the answers to those questions. All of the projects involve collaborations with one or more of DOE’s Energy Frontier Research Centers (EFRCs).

When CO₂ is pumped into geologic reservoirs for long-term storage, acidic fluids resulting from CO₂ reacting with groundwater and brine may dissolve some of the minerals in the reservoirs and deposit them downstream as carbonates, changing the pore geometry and flow patterns of the geologic formation. Modeling this process mathematically is the goal of a project called “Advanced Simulation of Subsurface Flow and Transport at the Pore Scale,” led by Phillip Colella of CRD.

This project, a collaboration between the SciDAC Applied Partial Differential Equations Center for Enabling Technology (APDEC) and the Energy Frontier Research Center for Nanoscale Control of Geologic CO₂ (NCGC), will develop the algorithmic and software infrastructure tools to enable NCGC’s goal of modeling molecular- to pore-scale processes in geologic systems. Specifically, the team will develop algorithms and software to model multiphase, reacting flow of CO₂ and water in a complex heterogeneous medium, with modification of microscale pore structures by mineral dissolution and precipitation. The Chombo numerical algorithm software package supported by APDEC will be extended so it can be applied to this class of problems.

Another collaboration, between NCGC and the SciDAC Visualization and Analytics Center for Enabling Technology (VACET), led by E. Wes Bethel of CRD, will give NCGC researchers the necessary tools to visualize and analyze their data effectively and improve their understanding of processes governing carbon sequestration. The project “Visualization and Analysis for Nanoscale Control of Geologic CO₂” intends to bridge the gap between experimental data and numerical simulations by developing image processing and analysis tools to automate measurements in both experimental and simulated data, and by developing geometric analysis techniques to extract relevant features from numerical simulation data that can be compared to experimental data. The tools

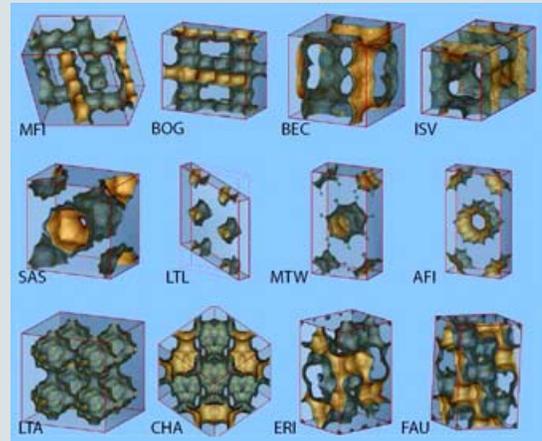


Figure 15. A sampling of pore structures in zeolites, a type of microporous mineral. A research project at Berkeley Lab will automate the computational screening of 2.5 million theoretically possible zeolite structures to search for materials that can economically capture CO₂ at its sources.

developed in this project will accelerate data processing and provide new capabilities for analysis of simulations, thus allowing NCGC researchers to run more experiments and effectively target new experiments.

The cost of capture is one of the main bottlenecks for large-scale carbon capture and sequestration. For example, the conventional technology for capturing CO₂ from the effluent stream of a power plant may require as much as 25% of the electricity being produced. The EFRC for Gas Separations Relevant to Clean Energy Technologies aims to tackle this problem by developing novel porous materials, such as zeolites or metal organic frameworks, that can capture CO₂ economically. But finding the ideal pore topologies from the 2.5 million theoretically possible zeolite structures (Figure 15) requires new computational tools for automated structural analysis.

In the project “Accelerating Discovery of New Materials for Energy-Related Gas Separations through PDE-Based Mathematical and Geometrical Algorithms and Advanced Visualization Tools,” also led by Bethel, the SciDAC VACET center will collaborate with this ERFC to develop state-of-the-art algorithms for analyzing and screening chemical systems, using a combination of advanced partial differential equation (PDE) algorithms to detect and probe geometric structures, and visualization techniques to track the motion of chemical probes through complex structures. Moving these algorithms to high performance computing platforms and deploying advanced data analysis tools will allow the researchers to automatically screen millions of pore structures without human intervention. The most promising structures can then be synthesized and tested.

The Electric Power Grid

The current U.S. power grid is a huge, interconnected network composed of power-generation stations, high-voltage transmission lines, lower voltage distribution systems, and other support components (Figure 16). Supporting the grid operation is an extensive communications and control infrastructure; decision making requires sophisticated computational tools.

The current system is under tremendous stress. Transmission system expansion has been unable to keep pace with the growth in energy demand. Consequently, transmission congestion is creating large electricity price differentials between geographic regions. For the New York Independent System Operator (NYISO) alone, these price differentials account for nearly 25% of the region's electricity costs. Furthermore, the existing grid structure and centralized control philosophy were not designed to handle the proliferation of small power sources resulting from deregulation, the intermittent supply from alternative sources such as wind and solar power, or the demand that could be created by widespread use of electric vehicles.

The power grid is also in the midst of a transformation from the analog to the digital age, exemplified by the term “smart grid.” The smart grid will manage and deliver electrical energy through a combined centralized and distributed system, in which many nodes are capable of producing, consuming, and storing electrical energy; sensors at each node will automatically provide continuous data

about energy use, flow, and system status. Managing transactions on this network will involve extensive communications networks, real-time data monitoring and analysis, and distributed, hierarchical control schemes. Designing and simulating such a network represents a grand computational challenge on an unprecedented scale.

Smart grid technologies, tools, and techniques include hardware, software, and business practices that will generate massive amounts of new data. Near real-time data and visibility of wide-area grid conditions will enhance electric system planning and operations; improve the integration of renewable and energy efficient technologies; increase demand response, electric reliability, and electric asset utilization; and provide better situational awareness and faster response to prevent local disturbances from cascading into regional outages (Figure 17).

On March 30–31, 2009 the U.S. Department of Energy's Office of Advanced Scientific Computing Research (ASCR) and Office of Electricity Delivery and Energy Reliability (OE) conducted a joint technical workshop to discuss data management, modeling and analysis, and visualization and decision tools for the 21st century electric power system. The purpose was to “get ahead of the curve” and anticipate major computational and engineering challenges associated with the extensive amount of new and more detailed data on the status of grid conditions that are expected over the next decade as part of national grid modernization efforts.

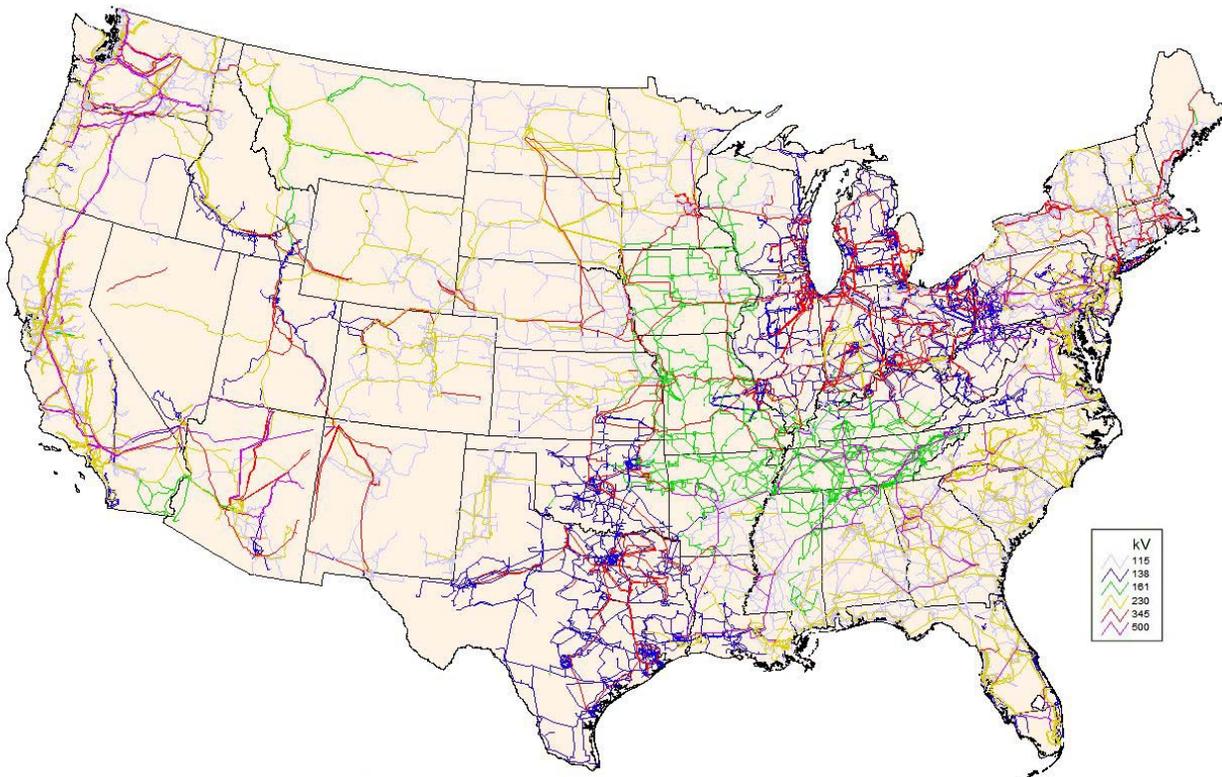


Figure 16. The contiguous U.S. electric power transmission grid. New computational modeling and analysis tools are needed that integrate real-time information to optimize power flow and prevent outages. *Source: FEMA*

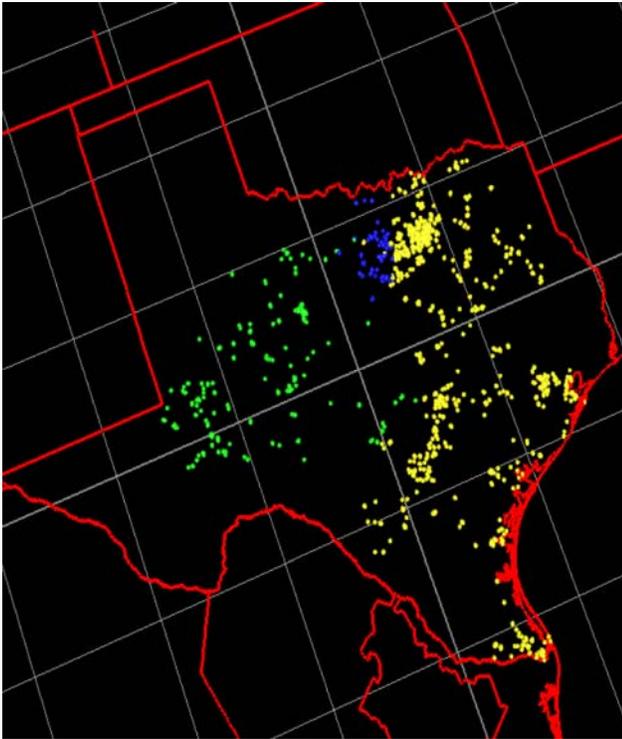


Figure 17. Simulation results show how cascading failures would break the Electric Reliability Council of Texas system into three independent islands (each shown in a different color), leading to blackouts. *Source: "Computational Research Needs for Alternative and Renewable Energy"*

The electric power system has undergone extensive change over the past several decades and has become substantially more complex, dynamic, and uncertain as new market rules, business practices, regulatory policies, and electric generation, transmission, distribution, storage, and end-use technologies have been tried and adopted. There are now hundreds of times more transactions at the bulk power level and emerging requirements for the two-way flow of power and information at the electric distribution level.

The availability of more detailed data about system conditions and advanced metering infrastructure for dynamic pricing and demand response can be a great benefit for improving grid planning and operations; but ways must be found to aggregate, organize, and keep the data secure so that it can be used to upgrade, extend, and replace existing modeling, analysis, and decision making tools.

There are a number of computational challenges that must be addressed to achieve this result. For example, the large volume of more detailed data creates information management challenges, but opens opportunities for grid operators to base decisions on actual measurements rather than estimates. Wide-area visibility that covers a much larger footprint of the power system than is currently possible will create data analysis and visualization challenges, but opens opportunities for interconnection-wide network and state estimation models. Access to information on grid conditions in near real time creates data analysis and

error checking challenges, but opens opportunities to detect operating anomalies and disturbances so that actions can be taken to prevent them from becoming local problems or cascading into regional outages.

A major barrier to addressing the computational challenges is the insufficiency of today's electric system models, and analysis and visualization tools. They cannot be counted on to provide accurate representations and information about the status of the grid, are not able to handle system dynamics properly, and cannot evaluate multiple major contingencies simultaneously. Advanced models are needed for anticipating multiple contingencies that could have severe consequences, for evaluating large-scale cascading outage scenarios, and for developing accurate measures of a system's brittleness or susceptibility to outages from a variety of potential causes.

The ASCR-OE workshop focused on three broad areas: data management, modeling and analysis, and visualization and decision tools.

Effective power system planning, operations, and communications (intra- and inter-entity) requires power system operators to analyze vast amounts of data, such as automated and computer-assisted control data, grid telemetry, market information, environmental information, and others. With the advent of smart grid technologies, data will become richer and denser. More data can yield more precise forecasts and enable more robust active control. However, if not properly managed, data can cause the opposite effect if it has been compromised or if it inundates the system with unnecessary information. Having better data management environments is one of the keys for enabling decision makers to make correct inferences and judgments as they apply this information to making the grid more efficient, reliable, affordable, and secure.

Improving data management for the 21st century grid involves addressing a number of technical challenges. For example, massive amounts of data can introduce unacceptable latency (slow down communications) into energy systems if processed, stored, or utilized on today's architectures. Furthermore, as redundant, missing, and poor quality data substantially increases, so will the likelihood of faulty readings, which could cause energy systems to crash. Concerns about system stability have kept most utilities with access to grid telemetry data from taking advantage of it, because the capabilities to extract good data do not exist today. In addition, achieving an adequate level of cybersecurity and protection of ownership and access rights will be increasingly difficult, because underlying protocols will need to constantly change as they respond and adapt to an increasingly complex energy infrastructure and a highly dynamic risk environment.

Significant effort will be needed in research, development, and demonstration to address these challenges. For example, multidisciplinary teams will need to develop a transition plan from legacy systems to future systems, including building and testing prototype architecture designs for planning, operations, and communications. Cybersecurity technologies and tools also must be developed to appropriately manage trust, security, and risk, and to

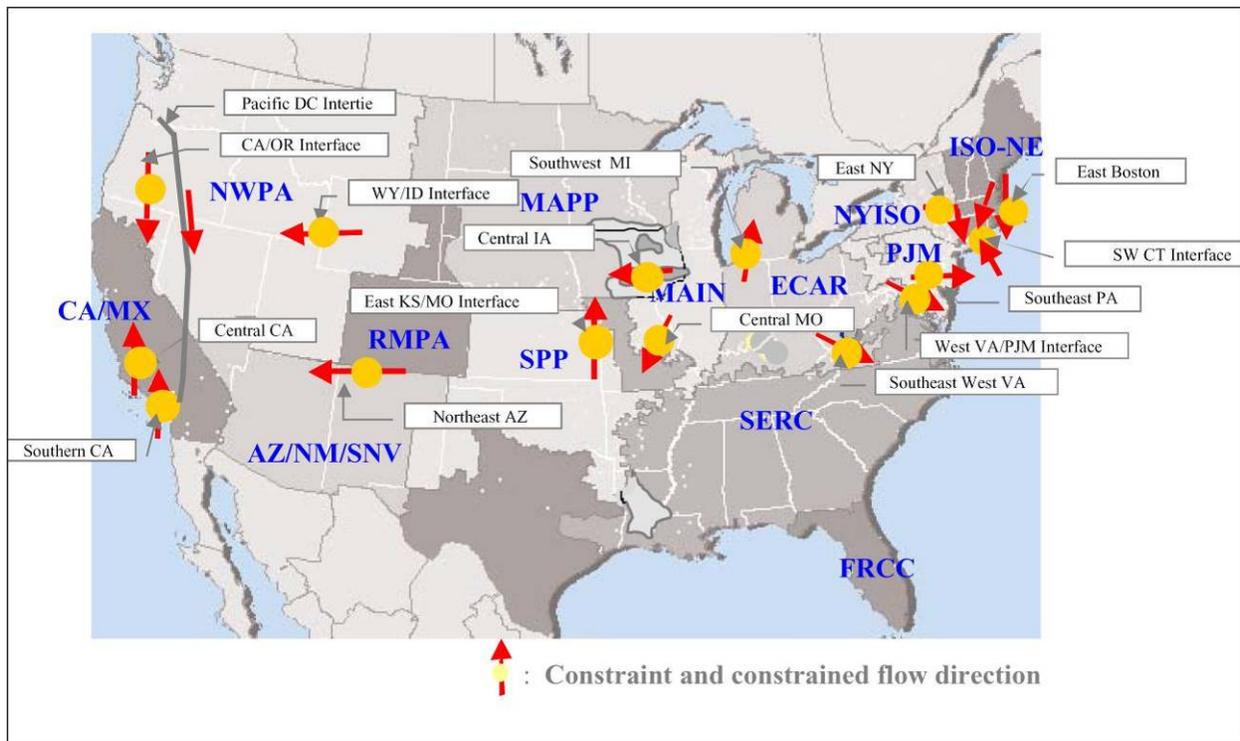


Figure 18. Transmission constraints in the contiguous U.S. from June through August 2000 and 2001. *Source: FERC*

aid compliance management and dynamic data sharing policies.

The transition to a smarter grid means that an enormous amount of data will be collected that will require analysis and verification so that it can be transformed into usable information. Computerized data modeling and analysis can provide a representation of the behavior of the grid system that will contribute to understanding the interaction of the parts of the electric grid and of the system as a whole.

Data modeling and analysis are already used by a number of stakeholders for a diverse set of applications, including operations, planning, training, and policymaking. But the existing algorithms and capabilities that have been used for data modeling and analysis are becoming dated and are not robust enough to handle all of the changes in the electricity and ancillary sectors.

There is a need for algorithms, not just computers, to transform the grid modeling paradigm from static, slow, and deterministic to dynamic, real time, wide area, and stochastic. This new paradigm will enable proactive decision making, not just contingency response.

Transmission congestion is one area that could benefit from proactive modeling and decision making. The Federal Energy Regulatory Commission (FERC) estimated that the economic costs of transmission congestion in the summers of 2000 and 2001 (Figure 18) ranged from less than \$5 million to more than \$50 million per incident. However, for one particular set of conditions in the eastern portion of New York during the summer of 2000, FERC estimated a cost of more than \$700 million. Real-time modeling and proactive decision making may pre-

vent or mitigate these costly transmission constraints in the future.

There are a number of technical challenges associated with data modeling and analysis for the future power system. For instance, one challenge is to conduct streaming data analysis for real-time detection of anomalies and improved forecasting. It is critical that the right kind of data is acquired and that uncertainties are handled properly so that there is confidence that the data is accurate. Another challenge is to develop new algorithms that are robust and scalable as the complexity of the problem increases.

Planning and operating the nation's electric grid is far more complicated today than it was in the past because of institutional, regulatory, market, and technological changes over the past several decades. For example, the level of transactions in bulk power markets is higher; the number of market participants is higher; the level of peak demand is higher; the costs of outages are higher; and public awareness about the environmental consequences of electricity production, delivery, and use is higher.

The market introduction of smart grid technologies, tools, and technologies will provide grid operators, consumers, and policy makers with significantly more information for managing the grid and addressing national energy and environmental priorities such as global climate change, economic recovery, oil import dependence, and critical infrastructure dependence. Having better visualization and decision tools is one of the keys for taking this data, turning it into useful information, and applying it to make the grid more efficient, reliable, affordable, and secure.

Exascale for Energy

Improving visualization and decision tools for the 21st century grid involves addressing a number of technical challenges. For example, the system itself is becoming more complex, uncertain, and dynamic. Grid operators—the primary users of visualization and decision tools—face daily decisions which require near-real-time responses to prevent local disturbances from cascading into regional outages. The grid of the future will also involve real-time decision making by consumers about consumption and their demand response to dynamic pricing. And state, regional, and national policy makers and regulatory officials are becoming more heavily involved with electric resource planners and engineers in assessing needs for new power plants and transmission and distribution facilities. All of these participants—grid operators, planners and engineers, consumers, and policy makers—will need better visualization and decision tools to plan and operate the grid of the future properly.

The planning and operation of the electric power grid involves the deployment of diverse resources under uncertain conditions with imperfect information. From a mathematical viewpoint, many of these problems can be posed as nonlinear stochastic optimization problems containing both discrete and continuous variables. However, in practice, a lack of advanced algorithms and software has necessitated the use of simplified models and heuristics. Decision-making is divided into a series of simpler steps, each of which considers only a subsystem, or focuses exclusively on a particular time-scale or geographic area. The operational and planning decisions that emerge are inevitably inferior to those possible in a more global, multi-scale optimization of the entire system.

Optimal power flow (OPF) modeling is an important tool for determining the most efficient and economical operation of existing power systems as well as for planning future expansion. However, full-scale nonlinear OPF has not been widely adopted in real-time operation of large-scale power systems. Instead, system operators often use simplified OPF tools that are based on linear pro-

gramming and decoupled system models. Historically, this is due both to the lack of powerful computing hardware in the industry and to the lack of efficient and robust OPF algorithms. With the advent of fast, low-cost computers, speed has now become a secondary concern, while algorithm robustness and scalability are the primary issues.

A transmission system operator comparable to the NYISO might contain 10,000 buses, 12,500 transmission lines, 2,000 generators, and 2,000 equipment contingencies, yielding an optimization problem with on the order of 6×10^7 variables, 4×10^7 nonlinear equality constraints, 5×10^7 nonlinear inequality constraints, 2×10^7 linear inequality constraints, for a total of about 1×10^8 constraints of various types. This complex and large-scale problem would adequately represent the situation the NYISO faces every day in its planning and operations. A larger problem would surface when accurately modeling the eastern National Interest Electric Transmission Corridor. Yet the largest OPF problem reliably solved to date is a 2,935-bus reduced-order model of New York without contingencies.

This example illustrates that the most immediate issue for power grid modeling is algorithm and software development, not more computing power. Berkeley Lab researchers are currently collaborating with mathematicians and power engineers from Cornell University and the University of Wisconsin to develop optimization algorithms that detect vulnerabilities in the power grid, analyze cascading outages, and perform resource allocation across multiple locations and times; they will then combine these algorithms into an integrated optimization framework (see sidebar below).

When real-time, wide-area grid modeling, optimization and control software is eventually developed to monitor and manage as many as 100 million distinct nodes, it could easily require continuous access to hundreds of thousands of processors.

Optimization and control of electric power systems

Mathematicians from Berkeley Lab's Computational Research Division (CRD) are working to increase the reliability of the electrical grid and improve the nation's ability to respond to energy disruptions. By advancing the technologies needed to implement a smart grid, Berkeley researchers will play an important role in avoiding costly, cascading blackouts like the August 2003 blackout that affected eight northeastern U.S. states and Canada.

Although improvements to the nation's power grid have since been put in place, further research is needed to expand the grid's ability to simultaneously respond to multiple power outages and automatically re-route electricity to avoid broader blackouts. The three-year project, in which Berkeley Lab researchers are collaborating with mathematicians and power engineers from Cornell University and the University of Wisconsin, will develop optimization algorithms that detect vulnerabili-

ties in the power grid, analyze cascading outages, and perform resource allocation across multiple locations and times. They will then combine these algorithms into an integrated optimization framework.

"The North American power grids combine to make one of the largest interconnected systems on earth," says Juan Meza, head of the High Performance Computing Research Department and Lead Principal Investigator for the project. "It has a complex transmission network, containing more than 9,200 electric generating units connected to over 200,000 miles of transmission lines."

Electricity is distributed across North America on multifaceted grids, which are controlled by a variety of players. These large interconnects are divided among a number of regional utility companies which are responsible for maintaining their portion of the grid and delivering power to consumers.

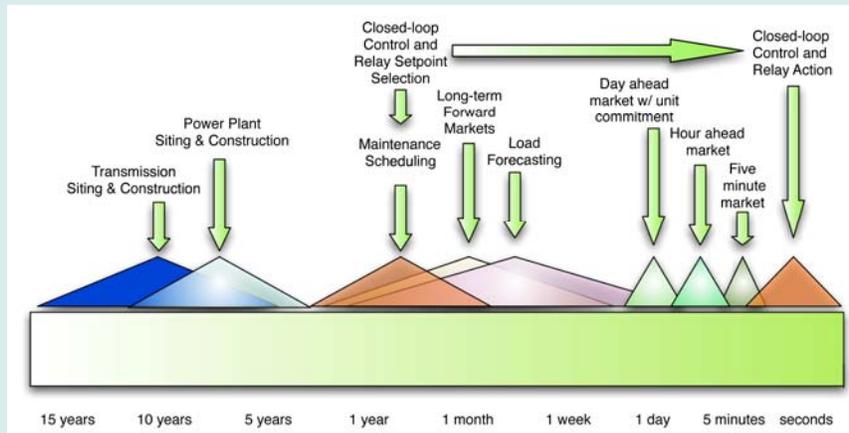


Figure 19. Representative decision-making timescales in electric power systems. Behaviors at very fast time scales (e.g., requirements for grid resilience against cascading failures) impose constraints on longer time scale decisions, such as maintenance scheduling and grid expansion. *Source: J. Meza, LBNL*

Because electricity cannot be stored, the electric power system must constantly be adjusted to ensure that the generation of power matches the demand. This task falls on hundreds of Control Area Operators across the continent using computerized control centers. The regional utility companies are responsible for coordinating the area operators working on their portion of the grid.

“Although interconnectedness ensures that the system is reliable most of the time, it also means that a few critical line failures could potentially cause a massive blackout,” says Meza.

The grid delivers electricity from power plants to consumers via two primary systems, the transmission system and the distribution system. First, the transmission system transports electricity from power plants to substations near populated areas; then the distribution system delivers electricity from substations to consumers’ homes and businesses. If each power plant, substation, and consumer is represented as a point on the electric power grid, then multiple redundant lines connect each point to ensure that power can travel a variety of routes, from any power plant to any substation and consumer. This means that a line failure between any of these points will not cause a power outage for consumers because power can be rerouted.

The problem becomes even more complex because not all transmission lines on the grid are created equal. Some lines and routes are created to carry more power than others, and options for how to reroute power could affect the severity of an outage—will it affect a neighborhood or an entire city?

Meza notes that one current approach for determining the optimal detour routes in the event of a transmission line failure is to build a large-scale model of the grid and test different scenarios to determine which will cause a blackout. Although this approach has worked

so far, experts warn that it will soon be impractical as the demand for power grows and the grid becomes ever more complex.

Instead of building a model of the entire electric power grid, Meza and his collaborators will use combinatorial techniques and graph algorithms to identify all the critical line failure scenarios that could lead to a blackout. He notes that by taking advantage of these mathematical methods, the computational cost is drastically reduced, and the methods can easily be modified to detect vulnerabilities in the grid as it becomes more complex.

Their mathematical methods will also identify optimal detours for rerouting power in the event of multiple line failures, and will rank the solutions from those that will cause minor outages to those leading to severe blackouts. This will help facilitate decision making between the many players involved in both the short- and long-term process of delivering electricity.

“Our combinatorial techniques can analyze vulnerabilities of large complex systems in a fraction of the time needed by previous methods,” says Meza. “This vulnerability analysis will be an important component in decision support and policy making, thereby providing a more reliable and efficient power grid.”

With electricity demand expected to increase by 35% in the next 20 years, maintaining and planning for system reliability is a recognized problem in the national interest. Long-term planning needs to account for actions that take place over a wide range of time scales, from fractions of a second to the 15 years it takes to site and construct transmission lines (Figure 19). Advanced computational tools can take much of the guesswork out of this planning by providing algorithms and software to support optimum power flow across multiple temporal and spatial scales.

Alternative and Renewable Energy Sources

According to the Energy Information Administration’s *Annual Energy Outlook 2006*, renewable energy contributes only 6.8% to the present U.S. energy supply, as shown in Figure 20. Despite the modest percentage of energy currently supplied by renewables, ambitious state and national goals have been set for the future renewable energy supply. These goals include having hydrogen be a major contributor to future transportation fuel, producing sufficient biofuels to reduce gasoline usage by 20% in ten years, deploying market-competitive photovoltaic systems by 2015, and generating 20% of total U.S. electrical supply from wind energy by 2030.

Meeting these ambitious goals will require major technological advances. In response to these challenges,

the DOE Office of Science (SC) and the DOE Office of Energy Efficiency and Renewable Energy (EE) convened a workshop on Computational Research Needs for Alternative and Renewable Energy on September 19–20, 2007, in Rockville, Maryland. Discussions at the workshop made clear that realizing the potential for alternative and renewable energy will require robust computational capabilities—including ultrascale computing systems, scalable modeling and simulation codes, capacious data storage and informatics, and high-speed communication networks.

Four renewable energy technologies which can greatly benefit from computational research are discussed briefly below: hydrogen fuel, bioenergy conversion, photovoltaic solar energy conversion, and wind energy.

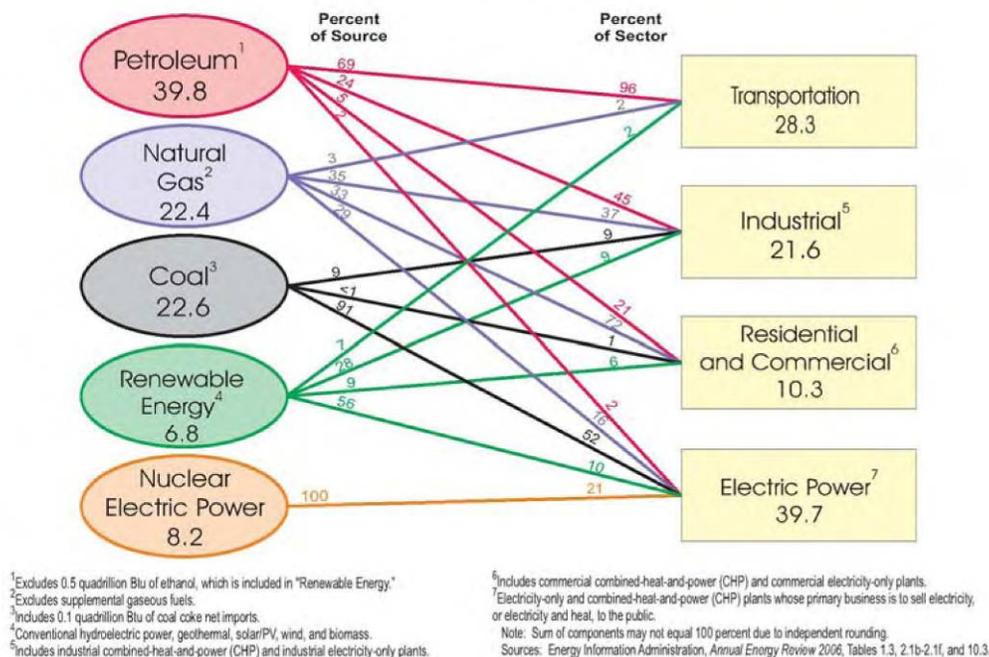


Figure 20. U.S. primary energy consumption by source and sector, 2006 (quadrillion Btu). Source: EIA

Renewable Fuels: Hydrogen

Molecular hydrogen (H₂) is an energy carrier, not an energy source, but it can store energy for later use in both stationary and transportation applications. Hydrogen can be produced using a variety of domestically available sources including renewable solar, wind, and biomass resources, fossil fuels (such as natural gas and coal), and nuclear energy. In a fuel cell, the free energy associated with the formation reaction of water from hydrogen and oxygen is harnessed as electrical energy. Hydrogen can also be combusted in an internal combustion engine.

Advances in computational science are needed to accelerate the rate of discovery and implementation in all aspects of the future hydrogen energy economy. For example, fuel cell technologies require breakthroughs in catalysis, materials design and integration, and a deeper

understanding of ion, electron, and molecular transport mechanisms. Computational models can accelerate experimental research and point the way to more efficient and less costly fuel cells.

For hydrogen fuel to displace our reliance on petroleum, we need to develop methods to store hydrogen inexpensively in vehicles in a safe, convenient, compact, and lightweight package. The DOE has been supporting basic research (DOE Office of Science) and applied research (DOE Office of Energy Efficiency and Renewable Energy) to develop hydrogen storage systems that can be incorporated into vehicles that will be desirable to consumers, but the challenge of producing such systems has not yet been met.

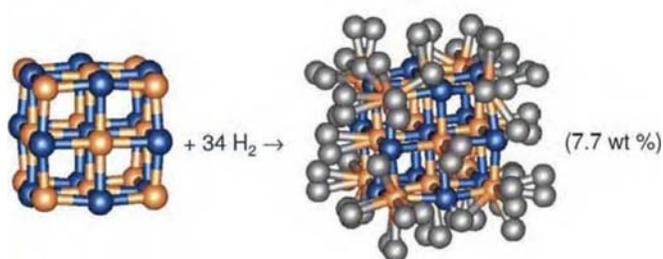


Figure 21. Developing systems for high-density storage of hydrogen is crucial to successful hydrogen technology deployment. The depicted $Ti_{14}C_{13}$ titanium carbide nanoparticle displays aspects of both hydrogen spillover and dihydrogen bonding, and can adsorb 68 hydrogen atoms for nearly 8% weight hydrogen storage. *Source: Y. Zhao et al., NREL*

Computation and theory have already played an important role in advancing next-generation, solid-state hydrogen storage options. For example, first-principles calculations have identified titanium carbide nanoparticles as a candidate hydrogen storage medium (Figure 21). However, much more needs to be done, as no storage method tested to date satisfies all of the requirements for efficiency, size, weight, cost, and safety for transportation vehicles. Computational science will play a critical role in advancing options such as metal hydrides, chemical hydrogen carriers, and sorption materials; but even physical storage methods would benefit from improved computational resources and techniques. For example, a better understanding of the mechanical properties of materials could lead to new, less expensive fibers or composites for containers that could store hydrogen via compression or liquefaction.

The hydrogen panel in the SC/EE workshop identified the following five priority research directions that cut across all hydrogen-related technologies. It is important to note that these priority research directions address core needs associated with specific underlying fundamental processes:

- Rate processes in hydrogen production, storage, and use
- Inverse materials and system design
- Synthesis of targeted materials
- Long-term behavior and lifetime simulation
- Linking models and scales—from atoms to systems.

Renewable Fuels: Bioenergy Conversion

Alternative and renewable fuels derived from biomass offer the potential to reduce our dependence on imported oil, support national economic growth, and mitigate global climate change. However, technological breakthroughs are needed to overcome key barriers to the development and commercialization of these fuels. These barriers include the high cost of pretreatment processes, enzymes, and microbial biocatalysts for biochemical conversion processes.

The lignocellulose in biomass is highly recalcitrant to most of the physical, chemical, and biochemical treatments currently used to liberate sugars. The cell walls of lignocellulose contain highly ordered, water-excluding microfibrils of crystalline cellulose that pose a significant barrier to enzymatic hydrolysis. The cellulose microfibrils themselves are laminated with hemicellulose, pectin, and lignin polymers. This complex matrix of heteropolymers is the main reason why plant biomass has resisted low-cost chemical and enzymatic treatments.

Cellulases can be used to hydrolyze the polysaccharides in the plant cell wall to fermentable monosaccharides, but the large quantities of expensive cellulases that are currently needed make the process cost-prohibitive. Despite Herculean attempts, the specific activity of cellulases has not been improved after more than three decades of research. A better understanding of the structure, function, and relationships governing the activity of soluble enzymes on insoluble polymeric substrates is essential to break this bottleneck. Computation uniquely provides a multiscale framework of understanding to guide and interpret experimentation on complex biological systems.

The priority research directions for biomass conversion identified in the SC/EE workshop include understanding lignocellulosic biomass depolymerization and hydrolysis, and chemical energy extraction from heterogeneous biomass. At Oak Ridge National Laboratory's BioEnergy Science Center (BESC), a new method for molecular dynamics simulation of lignocellulosic biomass is currently being tested.

BESC researchers have developed a strategy for a fast all-atom molecular dynamics simulation of multimillion-atom biological systems on massively parallel supercomputers, using models of cellulose and lignocellulosic biomass in an aqueous solution. Their approach involves using the reaction field (RF) method for the computation of long-range electrostatic interactions, which permits efficient scaling on many thousands of cores. Although the range of applicability of the RF method for biomolecular systems remains to be demonstrated, for the benchmark systems the use of the RF produces molecular dipole moments, Kirkwood G factors, other structural properties, and mean-square fluctuations in excellent agreement with those obtained with the commonly used Particle Mesh Ewald (PME) method.

Due to its complexity, lignocellulose poses significant challenges to molecular dynamics simulation. Among these are the characteristic length scales (\AA – μm) and time scales (ns– μs and beyond) of events pertinent to the recalcitrance of biomass to hydrolysis into sugars. To access these length and time scales, standard molecular dynamics protocols must be modified to scale up to massively parallel machines.

The BESC researchers simulated a system of lignocellulosic biomass containing 52 lignin molecules each with 61 monomers, a cellulose fibril of 36 chains with 80 monomers per chain (Figure 22), and 1,037,585 water molecules, totaling 3,316,463 atoms.

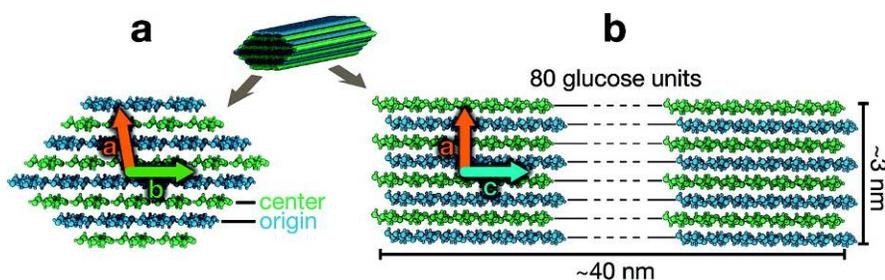


Figure 22. A simulated cellulose fibril showing (a) the cross-section and (b) a side perspective. The fibril consists of 18 origin chains (blue) and 18 center chains (green). The axes of the unit cell are also indicated. *Source: T. Splettstoesser, ORNL*

Their studies showed that the properties derived using the PME method are well reproduced using the computationally less demanding reaction field method. Scaling benchmarks showed that the use of RF drastically improves the parallel efficiency of the algorithm relative to PME, yielding ~30 nanoseconds of simulated reaction time per computing day, running at 16.9 teraflops on 12,288 cores of ORNL's "Jaguar" Cray XT5 system. Consequently, microsecond time scale molecular dynamics simulations of multimillion-atom biomolecular systems now appear to be within reach.

Despite this important advance, some critical biological phenomena, such as ligand binding, require the simulation of relatively long time scales (up to 1000 seconds). For this type of application, exascale computing will be required.

Renewable Electricity: Photovoltaic Solar Energy Conversion

Electrical generation by solar energy capture with photovoltaic systems has virtually no environmental impact beyond device manufacturing, is ideal for individual home or other distributed generation, and taps a virtually unlimited resource. Currently, however, it is two to four times more expensive than most residential or commercial rate electricity. So, although photovoltaic has a number of excellent small markets, it currently supplies only a small fraction of total electricity use and requires further cost reductions and efficiency improvements to be able to make a major contribution to meeting electrical demand.

More than 30 years of experimentation was needed for the relatively simple thin-film silicon solar cell to reach its current efficiency of 24%. In order to develop next-generation solar cells based on new materials and nanoscience fast enough to reduce the global warming crisis, a different paradigm of research is essential. Exascale computing can change the way the research is done—both through a direct numerical material-by-design search and by enabling a better understanding of the fundamental processes in nanosystems that are critical for solar energy applications.

Unlike bulk systems, nanostructures cannot be represented by just a few atoms in computational simulations. They are coordinated systems, and any attempt to understand the materials' properties must simulate the system

as a whole. Density functional theory (DFT) allows physicists to simulate the electronic properties of materials, but DFT calculations are time-consuming; and any system with more than 1,000 atoms quickly overwhelms computing resources, because the computational cost of the conventional DFT method scales as the third power of the size of the system. Thus, when the size of a nanostructure increases 10 times, computing power must increase 1,000 times.

Photovoltaic nanosystems often contain tens of thousands of atoms. So one of the keys to unleashing the energy harvesting power of nanotechnology is to find a way of retaining DFT's accuracy while performing calculations with tens of thousands of atoms.

Researchers at Lawrence Berkeley National Laboratory have demonstrated a way to accomplish this using a divide-and-conquer algorithm implemented in the new Linear Scaling Three-Dimensional Fragment (LS3DF) method. In November 2008, this research was honored with the Association for Computing Machinery (ACM) Gordon Bell Prize for Algorithm Innovation.

In a solar cell, there are a few key steps that determine overall efficiency in the conversion of sunlight to electricity: light absorption, exciton generation, exciton dissociation into separated electron and hole, carrier transport, and charge transfer across nanocontacts. A few aspects of nano solar cells often limit their overall efficiency: weak absorption of light, electron-hole recombination, nanocontact barriers, or large overpotentials. Unfortunately, many of these processes are not well understood. This is one instance where computational simulations can play a critical role.

For example, materials that have separate electron states within the energy band gap, such as zinc tellurite oxide (ZnTeO), have been proposed as next-generation solar cells. Such systems could theoretically increase solar cell efficiencies from 30% to 63%. To test this hypothesis, the Berkeley Lab researchers used LS3DF to calculate the electron wave function of a 13,824-atom ZnTeO supercell on 17,280 cores of NERSC's Cray XT4 system, Franklin (Figure 23). The LS3DF calculation took just a few hours, compared with the four to six weeks it would have taken using a direct DFT method. The results showed that ZnTeO is a good candidate for photovoltaic applications, with a theoretical power efficiency estimated to be around 60%.

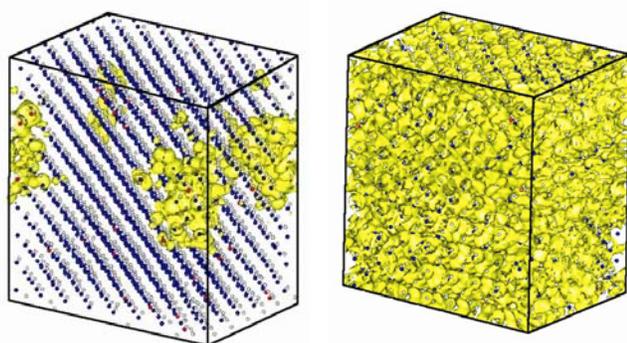


Figure 23. The electron wave functions for an oxygen-induced state (left) and ZnTe conduction band edge state (right) in a ZnTeO alloy with 3% O. The grey, blue, and red dots correspond to Zn, Te, and O atoms respectively. *Source: L.-W. Wang, Berkeley Lab*

In subsequent tests, LS3DF ran on more than 100,000 supercomputer cores, making it the first variationally accurate linearly scaling *ab initio* electronic structure code that has been efficiently parallelized to such a large number of processors.

To go beyond nanoscale simulations, algorithmic breakthroughs like LS3DF, combined with multiscale methods and exascale computers, could be used for the integrated simulation and design of entire photovoltaic systems, shortening the cycle for device development and optimization, and improving the efficiency and cost of photovoltaics.

Improved computational methods, such as those described in the sidebar below, will play a crucial role in this effort.

Scaling-up computational methods for solar energy research

Multicore and heterogeneous computer architectures are setting new records for computing speed and are demonstrating possible paths toward exascale computing. But taking full advantage of faster hardware for solar energy and other fields of research requires new and improved mathematical methods and computational tools.

Researchers in Berkeley Lab's Computational Research Division (CRD) are collaborating on three projects that are working to improve algorithms and codes specifically for solar energy research; but the methods and tools they develop will also have applications in combustion efficiency, materials science, and many other scientific domains.

Computational chemistry codes such as GAMESS, NWChem, and MPQC are among the most widely used in the DOE research community and beyond, with applications in solar energy cell design, combustion efficiency, materials science, nanoscience, nanoelectronics, and related fields. Tuning these codes by hand to make them run efficiently on a particular computer usually requires a high level of expertise and lots of time, especially as computers grow in size and complexity.

One promising way to speed up the process is autotuning—the development of tools and techniques that can automatically generate and test variations of a scientific code, resulting in a tuned code that achieves very high performance on a given system.

The “Autotuning Large Computational Chemistry Codes” project is implementing state-of-the-art performance analysis and autotuning techniques to accelerate some key computational chemistry applications, notably a linear scaling multi-reference configuration interaction (MRCI) module in the GAMESS code. One particular application targeted is a set of large-scale simulations of large hydrocarbons and sulfur-containing hydrocarbons that are components of diesel fuel.

Collaborators include two DOE Energy Frontier Research Centers (EFRCs)—the Combustion EFRC (CEFRC) and the Argonne-Northwestern Solar Energy Research Center (ANSER)—as well as researchers from Lawrence Berkeley, Ames, and Sandia national laboratories and the universities of Tennessee and Oregon.

The “Large-Scale Eigenvalue Calculations in the Study of Electron Excitation for Photovoltaic Materials” project is a collaboration between the SciDAC TOPS (Towards Optimal Petascale Simulations) center and two EFRCs: the Center for Inverse Design at the National Renewable Energy Laboratory (NREL), and the Molecularly Assembled Material Architectures for Solar Energy Production, Storage, and Carbon Capture EFRC at the University of California, Los Angeles (UCLA).

This project is focusing on developing and deploying state-of-the-art solvers for specific large-scale eigenvalue problems. The improved algorithms will help researchers search for nanostructure-based effects for the design of new photovoltaic materials with much higher efficiency, as well as improve the efficiency of organic solar cells and design new solar cell types. The project aims to improve code scalability and performance on modern multicore supercomputers.

Production of solar energy can take many forms, from the direct production of fuels from sunlight through artificial photosynthesis, to the production of electricity through photovoltaics. Using computation to identify promising classes of chemicals that can catalyze such reactions involves multiscale QM/MM (quantum mechanics/molecular mechanics) simulations coupled with higher-level models, all under the coordination of an optimization framework to search for candidate molecules.

The project “Enhancing Productivity of Materials Discovery Computations for Solar Fuels and Next Generation Photovoltaics” brings together a group of computer scientists and applied mathematicians from the SciDAC Performance Engineering Research Institute (PERI) and the Solar Fuels and Next Generation Photovoltaics EFRC at the University of North Carolina. The three major thrusts of this effort are: (1) integrating performance engineering tools and methods with the ongoing development of the chemistry codes; (2) developing advanced simulation-driven optimization methods to apply to this problem; and (3) structuring the computations under a workflow and data management framework to ensure performance portability and productivity across a range of computing systems.

Renewable Electricity: Wind Energy

When it comes to generating electricity, wind power is the technology closest to being cost competitive with fossil-fuel-driven power generating plants. Although its use by utilities is limited by its intermittent nature, there are sufficient wind energy resources in the continental United States to meet a substantial portion of national energy needs at a competitive cost. The goal of generating 20% of the total U.S. electrical supply from wind energy by 2030, while feasible, is highly challenging. Turbine installations are growing dramatically, but they still provide less than 1% of U.S. electricity.

Current wind plants often under-perform predicted performance by more than 10 percent, and wind turbines often suffer premature failures and reduced lifetimes from those predicted during design. Turbine downtimes and failures lead to a reduced return on investment, which lowers the confidence of investors and increases the cost of raising capital necessary to develop a wind plant. A key reason for these early failures is a lack of detailed knowledge about unsteady wind flows and how they interact with turbines.

Standard meteorological data sets and weather forecasting models do not provide the detailed information on the variability of wind speeds, horizontal and vertical shears, and turbulent velocity fields that are needed for the optimal design and operation of wind turbines and the exact siting of wind plants. For example, wind turbines are frequently deployed in regions of undulating topography to take advantage of the expected speed-up of wind as the atmosphere is forced up over the hill. But recent evidence suggests that the drag imposed by trees can create turbulence that can damage wind turbines on subsequent ridges. More research is needed on the planetary boundary layer (PBL, the lowest part of the atmosphere) and how it interacts with the shape and ground cover of the land in specific locations in order to understand unsteady wind flows.

Researchers at the National Center for Atmospheric Research (NCAR) have developed a new large-eddy simulation (LES) code for modeling turbulent flows in boundary layers. Running on as many as 16,384 processors of the Franklin Cray XT4 at NERSC, the NCAR-LES code enables fine mesh simulations that allow a wide range of large- and small-scale structures to co-exist and thus interact in a turbulent flow.

High-resolution flow visualizations in Figures 24 and 25 illustrate the formation of both large and small structures. In Figure 24, we observe the classic formation of plumes in a convective PBL. Vigorous thermal plumes near the top of the PBL can trace their roots through the middle of the PBL down to the surface layer. Closer inspection of the large-scale flow patterns in Figure 24 also reveals coherent smaller scale structures. This is demonstrated in Figure 25, which tracks the evolution of 10^5 particles over about 1000 seconds and shows how dust devil vortices form in convective boundary layers. Coarse-mesh LES hints at these coherent vortices, but fine-resolution simulations allow a detailed examination of their dynamics within a larger-scale flow.

Petascale computing will permit simulation of turbulent flows over a wide range of scales in realistic outdoor environments, such as flow over tree-covered hills. This will allow researchers to resolve 1–10 meter surface features while still capturing 1–100 km energy scales of motion in the boundary layer. Exascale computing will allow simulation of mesoscale systems with resolved clouds and a host of important small-scale processes that are now parameterized.

Improved PBL and turbine inflow modeling capabilities will enable the design of wind turbines that optimize performance by getting more power out of lighter designs, but will also be more cost effective due to longer lifetimes and reduced operations cost.

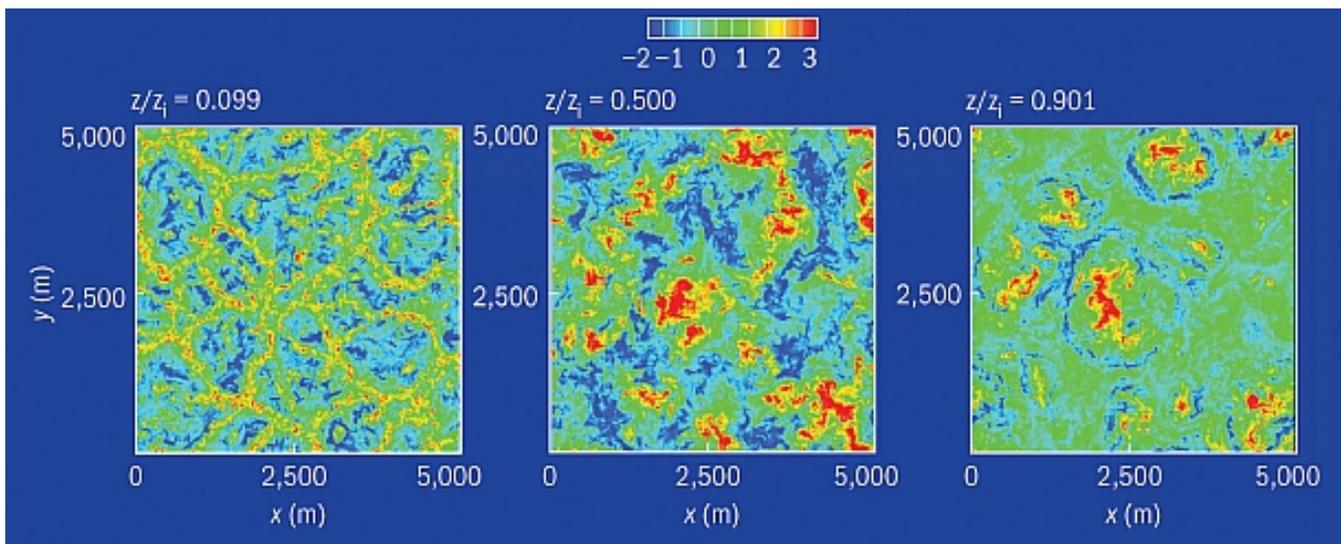


Figure 24. Visualization of the vertical velocity field in a convective PBL at heights of 100 m, 500 m, and 900 m, from a 512^3 simulation. Plumes near the inversion can trace their origin to the hexagon patterns in the surface layer. *Source: P. Sullivan and E. Patton, NCAR*

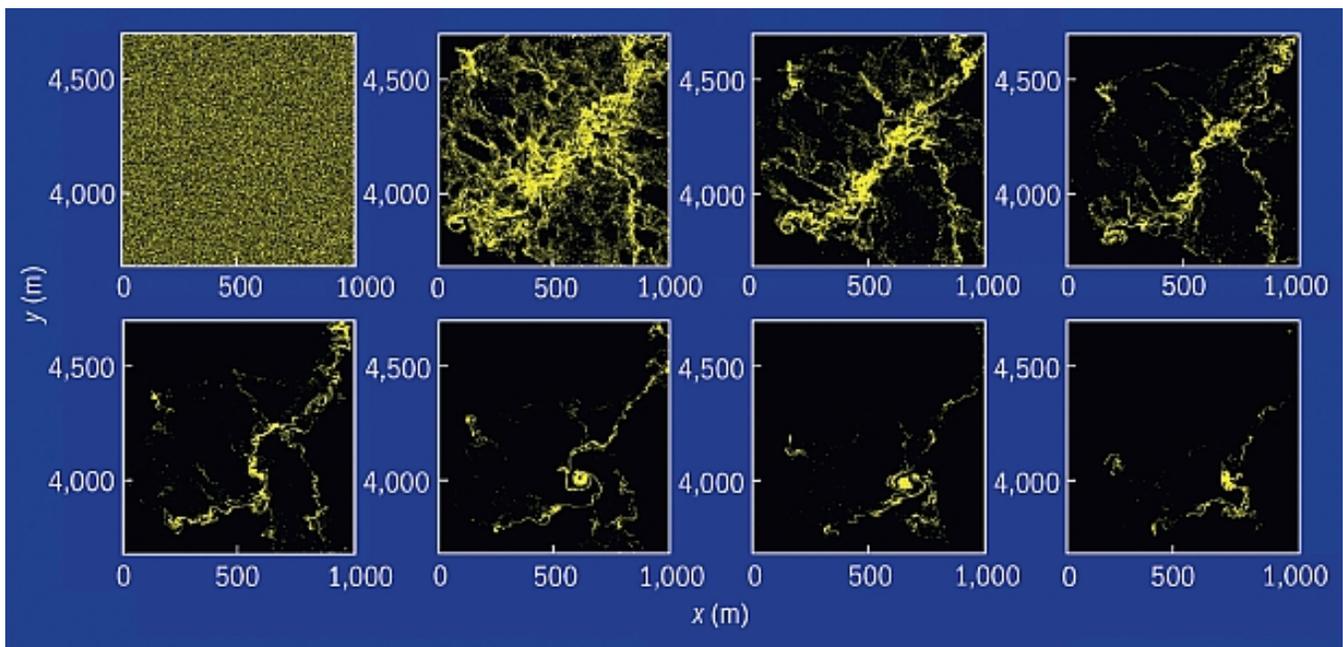


Figure 25. Visualization of particles released in a convective PBL from a 1024^3 simulation of convection. The viewed area is $\sim 3.8\%$ of the total horizontal domain. Time advances from left to right beginning along the top row of images. Notice the evolution of the larger-scale line of convection into small-scale vortical dust devils. *Source: P. Sullivan and E. Patton, NCAR*

Further Reading

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