U.S. Department of Energy Workshop

Computational Research Needs in Alternative and Renewable Energy

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Office of Science
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Energy Efficiency and Renewable Energy
Bringing you a prosperous future where energy is clean, abundant, reliable, and affordable

Cover graphics, clockwise from left:

- Developing systems for high-density storage of hydrogen is crucial to successful hydrogen technology deployment. Numerous promising possibilities are being pursued, and high-performance computer modeling can play a key role. 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.
- Exoglucanases, also known as cellobiohydrolases, are key catalysts in the enzymatic breakdown of cellulose to sugars, perhaps the most critical step in developing the capability to economically produce fuels and chemicals from fibrous biomass as well as sugar or starch.
- Quantum dots are nanoscale photovoltaic crystals that can be "tuned" to particular wavelengths by varying their size, leading to potentially far greater efficiency than bulk materials.
- A two-dimensional section extract of a wind turbine flow field developed with computational fluid dynamics modeling; the intricate structure of the flow field is responsible for powerful aerodynamic loads and complex aeroacoustic emissions. Graphic courtesy of P. Morris, L. Long, and K. Brentner, Pennsylvania State University.
- Many transmission lines of the future electrical grid may look similar to those of today, but they will likely carry information as well as energy, allowing the control of electrical appliances and electrical generators, to better match the real-time needs of the system.

All of these next-generation energy technologies require a vastly increased understanding and manipulation of fundamental processes—capabilities that can be greatly enhanced by high-performance, computing-based models and simulations.

COMPUTATIONAL RESEARCH NEEDS FOR ALTERNATIVE AND RENEWABLE ENERGY

U.S. Department of Energy Workshop Report

Co-Chairs

Greg Bothun, University of Oregon
Steve Hammond, National Renewable Energy Laboratory
Stephen Picataggio, Synthetic Genomic Solutions, Inc.

Organizing Committee

Ross Guttromson, Pacific Northwest National Laboratory
Mike Heben, National Renewable Energy Laboratory
Mike Himmel, National Renewable Energy Laboratory
Kai-Ming Ho, Iowa State University and Ames Laboratory
Moe Khaleel, Pacific Northwest National Laboratory
Shawn-Yu Lin, Rensselaer Polytechnic Institute
Costas Maranas, Pennsylvania State University
Phani Nukala, Oak Ridge National Laboratory
Scott Schreck, National Renewable Energy Laboratory

DOE Office of Science Contact

Gary Johnson, Office of Advanced Scientific Computing Research

DOE Office of Energy Efficiency and Renewable Energy Contact

Sam Baldwin, Chief Technology Officer

Administration

Joree O'Neal, Oak Ridge Institute for Science and Education

Publication

National Renewable Energy Laboratory

EXECUTIVE SUMMARY

America and the world face significant and urgent challenges rooted in the way we power and fuel our economies. The scale of the challenge requires an unprecedented response. Global energy demand is projected to grow dramatically in the coming decades, driven by rising standards of living and by continued worldwide population increases. Developing cost-effective renewable energy sources to meet future energy demand in an environmentally responsible manner is critical to achieving both energy security and overall sustainability.

According to the Energy Information Administration (EIA) report, *Annual Energy Outlook 2006,* renewable energy sources represent only 6.8% of the U.S. energy supply. In spite of this very modest level, 28 states and the District of Columbia have established renewable portfolio standards (RPSs), which mandate that electric utilities generate a certain percentage of electricity from renewable sources within the next one to two decades. The percentages vary by state, from 11% to 30%. In addition to the state mandates, ambitious national goals have been set as well. For example, the President's 2007 State of the Union Address set a goal to produce sufficient biofuels to reduce domestic gasoline usage by 20% in 10 years. The current state of our energy portfolio, coupled with concerns about climate change and projections that world energy demand will double by 2050, make meeting future energy needs in an affordable, reliable, and environmentally sensitive manner a true grand challenge.

Realizing the full potential of alternative and renewable energy will require advances in the underlying technologies as well as adaptations in the existing energy infrastructure. High-performance computing capabilities and state-of-the-art numerical simulation models will play a key role in accelerating the scientific and engineering progress necessary to fulfill this potential and is critical to advancing our understanding of the fundamental phenomena involved, from the smallest spatial and temporal scales to the integration and design of full systems. Advances in high-performance computing, numerical methods, algorithms, and software design now enable scientists and engineers to solve large-scale problems that were once thought intractable.

In response to these challenges, the U.S. Department of Energy (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. The workshop was held September 19–20, 2007, in Rockville, Maryland. It brought together leading renewable energy researchers and computational scientists to identify computational research needs and opportunities in alternative and renewable energy, with a focus on EE mission objectives and SC capabilities.

The workshop was divided into five parallel breakout panels: Renewable Fuels—Hydrogen; Renewable Fuels—Bioenergy Conversion; Renewable Electricity—Photovoltaic Solar Energy Conversion; Renewable Electricity—Wind Energy; and Energy Distribution—Grid Futures and Reliability. Each panel developed a set of priority research directions for a program of computational research in alternative and renewable energy.

- The Hydrogen panel identified five challenges requiring high-performance computing and associated computational research needs, including the simulation of rate processes, new materials, long-term performance of materials, and multicellular devices.
- The Bioenergy Conversion panel focused on challenges and computational research needs for cost-effective enzymatic and thermochemical deconstruction of biomass. In both approaches, numerical simulation is vital to understanding and improving the processes.
- The Photovoltaic Solar Energy panel's priorities correlated to a number of different photovoltaic device technologies. Whether developing novel materials with specific optical and electrical properties or optimizing processes for different solar energy conversion technologies, computer simulation is a key part of planned research efforts.
- The Wind Energy panel's priorities center on research needs based on using large-scale computer simulations to reliably predict complex parameters of wind turbine performance over the turbines' lifetimes—a key need for reducing the cost of energy and risks associated with investment in multimillion-dollar machines.
- The Grid Futures and Reliability panel envisioned the future electrical grid—one that operates more efficiently and better accommodates the intermittent nature of renewable energy electrical generation. The challenge of efficiently and reliably operating a vast network composed of traditional centralized power generation, as well as perhaps millions of distributed renewable energy sources, requires high-performance computing in and of itself. The panel's priorities addressed the impact of policy on such a grid, as well as the transition to it and the related systems needed for it.

The challenge is daunting—to enable alternative and renewable energy technologies to achieve their potential in meeting future energy needs. However, high-performance computing and modeling can play a significant and dramatic role in accelerating the required research. Fortunately, we are seeing continued rapid growth in computational capability and favorable reductions in the cost of large-scale simulation. Together, these two trends are enabling substantial simulation-based research and development breakthroughs in numerous fields of science, technology, and engineering.

Addressing the computational research needs identified in this workshop report will reap tremendous benefits in terms of advancing the basic science underlying alternative and renewable energy technologies. This will lay the groundwork for, and greatly accelerate, the scientific and technological advances that will play a major role in meeting global energy needs—sustainably and cost effectively.

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INTRODUCTION AND BACKGROUND

Renewable energy resources and clean energy alternatives are playing a larger role in diversifying the world's energy future. Using renewable energy sources for electrical generation and transportation fuels can improve energy security, reduce both toxic and greenhouse-gas emissions, and promote the growth of new industries.

In signing the Energy Policy Act of 2005 and promoting his 2006 *Advanced Energy Initiative*, President Bush laid out an agenda for transforming the way we produce and use energy. The *Advanced Energy Initiative* identifies certain technologies that have been in development over several decades. In some cases, these technologies still require significant advances to realize their potential. Predictive modeling and simulation capability used to study the full scientific and technical spectrum—from fundamental properties of materials to full systems—is needed to guide us toward a future alternative energy economy. The Workshop on Computational Research Needs for Alternative and Renewable Energy was held in the spirit of defining the most important objectives.

The workshop sought to obtain input from the research community regarding computational research needs and opportunities in alternative and renewable energy, particularly as they apply to developing new sources of electricity generation and transportation fuels. These needs and opportunities had a specific focus: aligning with U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy mission objectives and DOE Office of Science capabilities. The workshop was convened by those two offices.

The primary goal of the workshop was to identify a set of priority research directions for a program of computational research in alternative and renewable energy. This program, if followed, will significantly contribute to the development of cost-competitive renewable electricity and fuels that will profoundly change the energy production, distribution, and end-use portfolio of the United States.

The successful Scientific Discovery through Advanced Computing (SciDAC) program, with its centers, institutes, and multidisciplinary collaborations, could serve as a model for a new program in computational research in alternative and renewable energy. Fulfilling many of the priority research directions identified by the workshop panel sessions depends on petascale computational capability. Thus, a substantial effort will be needed to ensure that the existing code base using terascale computational resources will also be able to efficiently and effectively use petascale computational capabilities. In addition, the workshop made clear that increased collaboration among computational scientists, mathematicians, and discipline scientists—as well as collaboration between theorists and experimentalists—is an essential part of a successful research program.

THE ENERGY CHALLENGE—URGENT AND FORMIDABLE

The United States and the world face serious economic, environmental, and national security challenges based on our dependence on fossil fuels. The United States has just 2% of the world's oil reserves, but consumes about 25% of current world use. U.S. oil production has been generally declining since 1970, yet our demand has grown. Today, the United States depends on imports for roughly 60% of our oil, even as prices pass $100/barrel. With about 12 million barrels of oil imported per day, this costs the United States nearly $1 million per minute—a tremendous cost to our economy. At the same time, high prices for oil may help prop up political regimes unfriendly to the United States and our allies.

Moreover, the countries of the developing world have also adopted fossil fuels as their initial energy pathway, thus increasing competition for oil resources. This competition is increasingly intense because current global demand is significantly higher than our refinery-limited global output. As the roughly five billion people in today's developing countries strive for the economic lifestyle taken for granted by people in today's industrial countries, competition for oil is growing, not just in price, but also in terms of geopolitical strategies. Finally, high oil costs can constrain economic growth, even for the world powers, and may contribute to political instability in developing countries.

U.S. imports of natural gas are also increasing, with a number of new liquefied natural gas facilities approved and more under consideration. Increasing imports of natural gas will add to our national economic burden. It will also raise further concerns about our dependence on foreign sources of energy.

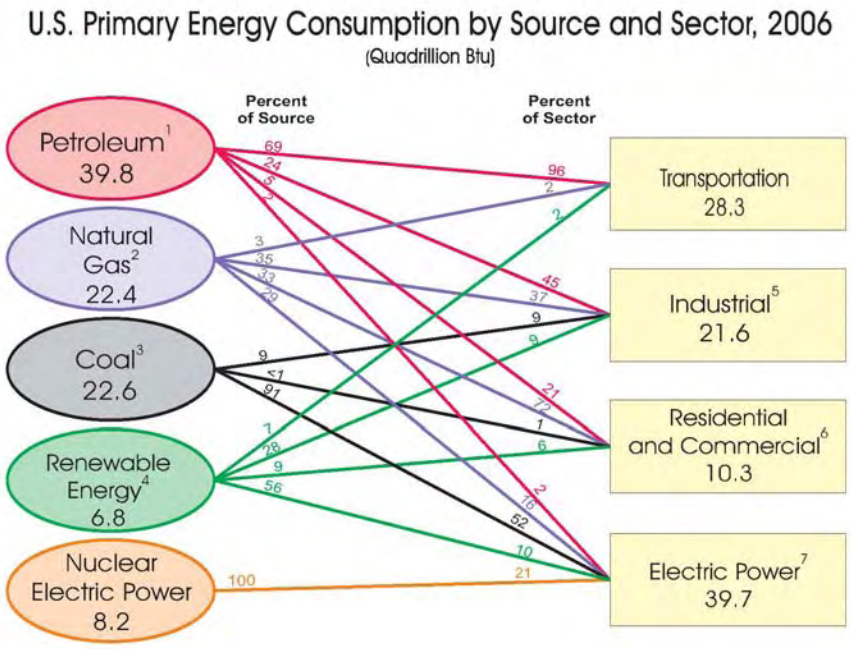
In addition to security and economic concerns, our dependence on fossil fuels also imposes a severe burden on the environment and human health resulting from emissions of particulates, acids (e.g., sulfur oxides and nitrogen oxides), toxins (e.g., mercury), and greenhouse gases (e.g., carbon dioxide). In 2005, the National Academies of Science of Brazil, Canada, China, France, Germany, India, Italy, Japan, Russia, the United Kingdom, and the United States signed a joint statement stating that "The scientific understanding of climate change is now sufficiently clear to justify nations taking prompt action" and "Long-term global efforts to create a more healthy, prosperous, and sustainable world may be severely hindered by changes in climate." They urged all nations to take "prompt action to reduce the causes of climate change."[1] Understanding of the potential consequences of climate change continues to grow, as evidenced by the Intergovernmental Panel on Climate Change Fourth Assessment Report[2] and a steady stream of scientific literature on every aspect of climate change, from observed and projected temperature and rainfall changes, to forest fires, to acidification of the world's oceans.[3]

This global context amplifies the sense of urgency and the magnitude of the energy challenge that we, as a nation and as a world, face collectively. Much can be done to address these energy

[1] "Joint Academies' Statement: Global Response to Climate Change", 2005
[2] http://www.ipcc.ch/ipccreports/index.htm
[3] See, for example: O. Hoegh-Guldberg, et al., "Coral Reefs Under Rapid Climate Change and Ocean Acidification", Science V. 318, 1737-1742 (2007)

challenges with existing technologies: improving the efficiency of buildings, industry, and our transportation system, making use of combined heat and power systems, and deploying renewable energy systems. Many of these are cost competitive, or nearly so, today. But by themselves, these are not sufficient to meet the challenges we face. Substantial improvements in energy efficiency, renewable energy, electrical grid management, and energy storage technologies are essential; their successful development will accelerate the transition to a sustainable energy economy. But developing cost-effective renewable energy and other technologies to meet future energy demand in an environmentally responsible manner is a formidable challenge.

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 the figure below. 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, generating 20% of total U.S. electrical supply from wind energy by 2030, and having a smart electrical grid able to reliably deliver the power needed to meet future demand using the new sources.



[1]Excludes 0.5 quadrillion Btu of ethanol, which is included in "Renewable Energy."
[2]Excludes supplemental gaseous fuels.
[3]Includes 0.1 quadrillion Btu of coal coke net imports.
[4]Conventional hydroelectric power, geothermal, solar/PV, wind, and biomass.
[5]Includes industrial combined-heat-and-power (CHP) and industrial electricity-only plants.
[6]Includes commercial combined-heat-and-power (CHP) and commercial electricity-only plants.
[7]Electricity-only and combined-heat-and-power (CHP) plants whose primary business is to sell electricity, or electricity and heat, to the public.
Note: Sum of components may not equal 100 percent due to independent rounding.
Sources: Energy Information Administration, *Annual Energy Review 2006*, Tables 1.3, 2.1b-2.1f, and 10.3.

Meeting these ambitious goals will require major technological advances. Discussions at the workshop made clear that realizing the potential for alternative and renewable energy will require robust computational capabilities—including petascale computing systems, scalable modeling and simulation codes, capacious data storage and informatics, and high-speed communication networks.

The need to undertake these efforts is urgent on a number of levels. In the context of this workshop, many of the advances in the underlying alternative and renewable energy technologies necessary for renewables to realize their potential to supply a much greater share of U.S. energy demand will be assisted by the research opportunities presented here. The workshop focused on five main areas that could form the backbone of a computational research program in alternative and renewable energy. Background on these five areas is described below.

Hydrogen. Hydrogen is an energy carrier, rather than an energy resource, but it has significant potential to contribute to fueling future transportation systems. It generates only water vapor at point of use and can be generated and transported in a variety of ways. Many people envision that hydrogen production and use will change our whole energy structure, but at this point, hydrogen is an experimental transportation fuel. Key challenges include renewable energy-based hydrogen production technologies, on-vehicle storage systems, and fuel-cell operation. Fuel cells and some of the potential storage systems, in turn, present crucial materials challenges, and all aspects present process optimization challenges. Workshop discussions found that many promising research efforts for developing hydrogen technology have common needs, including the following: to be capable of modeling rate processes; to develop new materials to meet specific needs (as opposed to developing new materials and then finding uses for them); to realize physical manifestations of theoretically proposed materials and processes; to simulate the long-term performance of materials and devices; and to understand relations between processes at different levels (e.g., atomic and operating device). These all present tremendous modeling challenges that could probably not be undertaken without high-performance computing capability.

Bioenergy Conversion. Biomass offers the greatest resource for producing renewable-source liquid transportation fuel. We currently produce about 5 billion gallons of fuel ethanol per year in the United States, mostly as an additive to gasoline. But this is still less than 2% of total gasoline use, and there is a limit to how much corn and other food crops can be allocated to fuel production. A study by DOE and the U.S. Department of Agriculture, however, projected that by 2030 it would be possible to harvest enough biomass to replace 30% of current U.S. petroleum consumption. That replacement would require a fundamental technology change. We would need to use cellulosic biomass—the bulk of plant matter—rather than just starch or sugar from food crops currently used for making ethanol. A key step for biologically converting cellulosic biomass to fuel is breaking the complex polymers down to component sugars (depolymerization and hydrolysis). Alternatively, biomass can be converted to fuels and chemicals through various thermochemical reactions. However, none of these processes are well understood at this time. Planned modeling of chemical and biological catalysts and reaction processes offers promising optimizing processes to be economically and industrially viable. However, this will be highly complex and requires high-performance computing capabilities.

Photovoltaic Solar Energy Conversion. Electrical generation by solar energy capture with photovoltaic (PV) 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 at the location of the end-user. So, although PV 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. Potential avenues for achieving such a cost reduction include the following: developing "thin-film" technologies that can be produced or applied inexpensively; developing concentrator systems that can capture large amounts of solar radiation with small, high-efficiency devices; and both increasing efficiency and decreasing cost for more traditional devices. For each of these approaches, a number of potential technologies are being actively researched. All, however, require understanding and manipulating highly complex atomic-level physics and chemistry. Intricate modeling is essential, and high-performance computing dramatically enhances research capabilities.

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. On a more real-world level, the goal of generating 20% of the total U.S. electrical supply from wind energy by 2030 is feasible, but highly challenging. Turbine installations are growing dramatically, but they still provide less than 1% of U.S. electricity. Because energy capture by turbines increases as the square of rotor diameter, cost effectiveness and energy production per acre both increase with turbine size. Increasingly larger turbines, however, also increase both the need for improved designs and the risk of using new designs. Therefore, a major need for expanding the contribution of wind energy is to be able to reduce the risk associated with installing very large, very expensive turbines by being able to predict their performance more reliably. Sophisticated modeling of aerodynamics, acoustics, design performance, reliability, and longevity are all needed. All are highly complex and depend on high-performance computing capability.

Grid Futures and Reliability. Electrical generation from solar and wind energy is intermittent and much of it is better suited to distributed, rather than central, generation. Electric and plug-in hybrid-electric vehicles, stationary and vehicular fuel cells, and efficient appliances all present opportunities for distributed electrical storage and demand manipulation. Taking advantage of these new technologies, as well as coping with the overall increase in electricity use, requires a new kind of electrical transmission and distribution system—a "smart grid." This smart grid will have to be able to receive feedback interactively from, and control, millions of separate electric devices and distributed electrical generators. To do so effectively while avoiding the risk of system failures requires immensely complex operating models that would not be possible without a high-performance computing capability.

Renewable energy resources and technologies have the potential to greatly reduce our dependence on fossil fuel use. This will greatly enhance energy security, improve air quality, lessen climate impacts, and provide other benefits. Dramatic advances in technologies are

required, however, to fully realize those benefits. Detailed numerical modeling, such as that made possible by high-performance computing, is a central part of the research needed to advance various renewable energy technologies. This workshop brought together leading researchers in key technology areas with computational research experts to identify computational research areas that would most effectively enhance research in alternative and renewable energy technologies. This report describes the priority research directions identified in that collaboration

WORKSHOP LOGISTICS

The workshop sought to help identify specific opportunities for high-performance computer modeling and simulation to enhance renewable energy technologies. The approach was to divide the workshop into research regimes most relevant to developing significant new sources of electricity generation and transportation fuel production over the next one to two decades.

To that end, technical panel discussions focused on five significant areas in which the simulation, modeling, and characterization of advanced materials will play a critical role in advancing research in renewable energy technologies: (1) Renewable Fuels—Hydrogen, (2) Renewable Fuels—Bioenergy Conversion, (3) Renewable Electricity Generation—Solar Energy Conversion, (4) Renewable Electricity Generation—Wind, and (5) Energy Distribution—Grid Futures and Reliability. A common goal of these five panel discussions was to define research needs and opportunities in alternative and renewable energy that would benefit from high-performance computing-based collaborations involving discipline scientists, applied mathematicians, and computational scientists.

More than 150 people participated in this invitation-only workshop. Participants included a broad representation of discipline and computational scientists working in various aspects of renewable energy and representing academia, industry, and national laboratories. These participants were organized via areas of technical competence and personal preferences into one of the five breakout panels.

The first day (Wednesday, September 19) began with welcoming remarks by workshop organizers and representatives of the collaborating DOE offices. The workshop agenda was pursued through the five parallel breakout panels, each consisting of between 20 and 45 panel members. Panel assignments were based on the first and second panel choices that attendees selected when they registered for the workshop. The workshop schedule also included three excellent plenary talks by leaders in the field of renewable energy and computational science. Details of the workshop program, the overall workshop charge, charges to the panels, and plenary presentations are on the conference Web site at http://www.nrel.gov/crnare_workshop/

Discipline scientists led the breakout panel discussions on Wednesday. The intent was to articulate discipline-related research directions in terms of what is needed to help meet or accelerate progress toward ambitious administration, congressional, and department goals. The day concluded with a plenary session in which each panel reported on what they considered to be preliminary priority research directions.

On the second full day of the workshop (Thursday, September 20), discipline and computational science panel leaders together directed the panel discussions to (1) revisit the prior day's priority research directions, (2) suggest priority research directions overlooked in the first day of panel discussions, and (3) identify panel members to serve as lead authors in producing priority research direction documents that will provide comprehensive, easily understood descriptions of each priority research direction.

The second day again concluded with a plenary session in which each panel presented the latest versions of its panel's priority research directions.

On the following morning (Friday, September 21), the Organizing Committee pulled together the various pieces of each of the priority research direction to produce a first draft summarizing the main points raised and discussed during the two previous days. That draft formed the basis for the initial letter report that was sent one week after the workshop concluded, as a prelude to this final workshop report.

SUMMARY OF KEY PRIORITY RESEARCH DIRECTIONS

What emerged from this process was that workshop participants identified a set of key priority research directions pertaining to each of the five selected areas of research. The bulk of this report constitutes the panel reports that elaborate on these priority research directions as they impact our nation's ability to increase our level of energy production from renewable sources. Our future energy independence and sustainability depend critically on the nation's scientific, engineering, and technical ability to develop scalable devices able to capture an appreciable amount of the indigenous energy (e.g., wind, solar, biomass) that surrounds us every day. The investment that will move these important priority research directions forward from merely good ideas to actual devices is crucial if we are to make significant headway in solving our future demand in the areas of electricity generation and transportation fuel. In addition, there is also widespread agreement on the absolute requirement for an intelligent electricity distribution grid to better manage and incorporate new sources of generation on a variety of spatial scales, from our backyards to potentially very large alternative-energy farms. All of the identified research priorities rely heavily on modeling and simulation that is possible only with high-performance computing. Developing that modeling capability should be the highest priority.

Renewable Fuels—Hydrogen. The hydrogen panel determined that the ability to use hydrogen as a future energy carrier critically requires advanced computational resources. These resources are needed especially to advance research in molecules and materials that can potentially store large amounts of hydrogen on both per-volume and per-weight bases. In addition, metascale analysis is required to identify new molecules or materials that will improve the energy efficiency of hydrogen storage, as well as various photochemical methods of producing hydrogen. Priority research directions that particularly need advanced computing capability include:

- Assessing and characterizing rate processes in the production, storage, and end use of hydrogen
- Developing new computation approaches in the area of inverse materials and system design—identifying needs and then determining the materials and system designs to meet

those needs using advanced computation
- Developing new approaches in the area of the synthesis of targeted materials
- Improving the computational tools needed to better assess the long-term behavior and overall lifetime of various advanced materials
- Developing multiscale analysis tools that can scale from individual atoms to entire systems.

Renewable Fuels—Bioenergy Conversion. The biomass conversion panel found a clear need for advanced computational modeling to better understand plant and microbial processes essentially at the individual cell level. The goal here is to improve the efficiency of fermentable sugar recovery and thus increase the potential biofuel yield per unit plant mass or per unit crop acre. Specific priority research directions identified included the need for computational research capabilities to better understand the following:

- Developing lignocellulosic biomass depolymerization and hydrolysis
- Understanding and engineering of biological systems
- Extracting chemical energy from heterogeneous biomass
- Conducting systems analyses of sustainability, life cycle, and land use.

Renewable Electricity—Photovoltaic Solar Energy Conversion. As in the hydrogen area, advanced computational resources are needed for better materials characterization and simulation to advance photovoltaic solar energy technologies. Device-level integration and overall system design are crucial to improving basic PV cell efficiency, and this requires significant modeling of the electronic properties of candidate new materials. Priority research directions, then, include:

- Optimizing materials in inorganic PV devices
- Understanding and modeling organic polymerics and small molecules and inorganic nanostructure PV devices
- Designing and optimizing complex, biomimetic, and hybrid materials for solar electric energy conversion
- Better integrating and designing PV systems
- Simulating processes for PV materials manufacturing.

Renewable Electricity—Wind Energy. To further enhance the attractiveness of wind energy in the commercial market, technological advancement must continue to drive down the cost of wind energy. This can be accomplished by increasing energy capture while decreasing initial capital cost as well as operating and replacement costs. Maximizing wind energy production per unit surface footprint depends on optimizing the fluid-dynamic efficiency of the wind turbine. Cost reduction relies on narrowing design margins due to model uncertainties and on attenuating fatigue loading that prematurely exhausts component structural life. Specifically, once wind turbines achieve diameters on the order of 100 meters, differential flow between the top and bottom can lead to turbulent instabilities that compromise performance and overall system lifetime. Advanced fluid-dynamical modeling and calculations are needed to help achieve good system design at these scales. Priority research directions for key specific capabilities necessitating advanced computing capabilities include reliably predicting wind turbine:

- Aerodynamics and acoustics
- Design and performance
- Reliability and longevity over long lifetimes.

Energy Distribution—Grid Futures and Reliability. The future grid will likely evolve from 10^4 individual power-plant generating sources to a distributed grid in which end-users can store or generate electricity and interact with the grid. Furthermore, the state of the system needs to be known in near real time. Designing and simulating a network so that it works in real time represents a grand computational challenge on an unprecedented scale. The important priority research directions identified will enable the development of capabilities for transforming to and managing the future electrical grid. These include:

- Evaluating the evolution of grid infrastructure and impacts on grid response under various technology development, market, and policy influences
- Evaluating and integrating automation and sustainable operation strategies for the future grid
- Maintaining continuity and interoperability as the grid transforms
- Exploring and evaluating a wide range of attributes and emergent behavior in possible grid futures
- Developing and integrating innovative components and processes for the evolving grid.

COMMON THEMES

During the workshop, nearly all of the breakout groups discussed the following crosscutting needs and challenges that were associated with their particular domain expertise.

Rational Materials and System Design. Traditional design of "materials" has followed the path where a material is synthesized, its properties are characterized, and then we decide how it is best used. A more rational approach is to determine the desired characteristics (e.g., optical and electrical, structural, chemical or thermal properties) and then undertake to determine what material best exhibits those desired properties. We need to develop effective methodologies and computational tools for designing materials starting with the desired properties. This inverse process will require developing techniques to predict the properties of a complex material from its chemistry and structure, as well as developing efficient searching approaches for finding optimum chemistry and configurations. These will include global optimization of N-dimensional parameter spaces, novel general methodologies for correlation of materials and their properties, linked multiscale modeling protocol and software development and hardware capabilities, and mixed integer programming using surrogate models for the objective function. This has huge potential for identifying new materials for hydrogen technology, solar energy conversion, and beyond.

Multiscale Models, from Atoms to Systems. A common theme running through much of this workshop was to develop the ability to link approaches that use different physical laws and different spatial and temporal scales. This is generally termed "metascale" computing or modeling. The challenges include developing computational strategies to bridge scales of length and time from the quantum to continuum. An understanding of the propagation of uncertainly between scales and models needs to be developed, as well as scalable and efficient methods for coupling atomistic models of different fidelity. Strategies for incorporating atomistic computations into continuum models will also be developed, as well as techniques for quantification of integrated uncertainty and improved algorithms for stochastic simulations. This

work will be critical to enabling the design and optimization of realistic systems for solar energy conversion as well as hydrogen production, storage, and utilization in the 5–10 year timescale.

Multidisciplinary Collaboration. Increased collaboration among computational scientists, mathematicians, and discipline scientists, as well as collaboration between theorists and experimentalists, is essential as the effort goes forward. Especially important is the continued collaborative development of new high-performance computing enabling technologies and new algorithmic approaches designed to meet the specific needs of renewable energy research as it applies to electricity generation, distribution, and storage. While many of the large-scale simulation codes being used in this field today can scale to use teraflop computational capabilities, significant effort will be needed to ensure that they can readily use the petascale computational capabilities being planned.

CONCLUSION

America and the world face tremendous challenges in the way we power and fuel our economies. The scale of the challenge requires an unprecedented response as global energy demand is projected to grow dramatically in the coming decades. Developing cost-effective alternative and renewable energy sources to meet future energy demand in an environmentally responsible manner is critical to achieving both energy security and overall sustainability.

At the workshop, many lively and substantive discussions clearly illustrated the urgent need for a program of computational research in alternative and renewable energy to support application areas of interest to DOE's Office of Energy Efficiency and Renewable Energy. DOE as a whole, and EE and SC in particular, have formidable simulation capabilities, scientific software tools, computing platforms, and interdisciplinary researchers without equal in the world. These DOE assets, together with academic- and industry-based researchers, represent an extraordinary resource for advancing research in alternative and renewable energy. In the past decade, renewable technologies have been boosted by a number of progressive national and international energy and environmental policies. However, the necessary scale of implementation, given our current consumption rates, is very large, requiring our very best research and development efforts to produce scalable forms of renewable energy, making use of what nature has provided us in abundance.

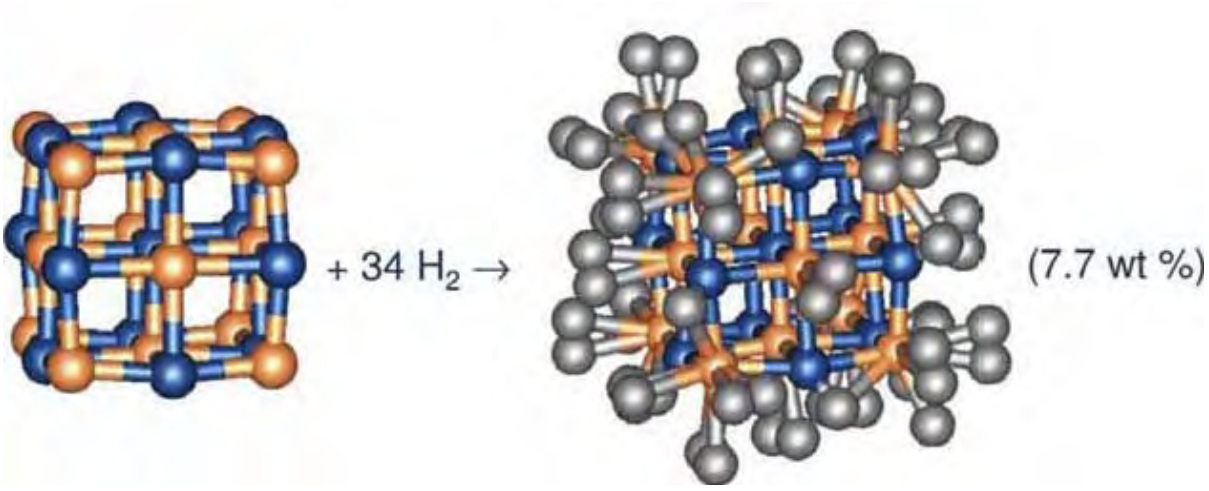
In addition to high-performance computing capabilities, increased collaboration among computational scientists, mathematicians, and discipline scientists—as well as collaboration between theorists and experimentalists—is essential as the effort goes forward. Especially important is the continued collaborative development of new high-performance computing enabling technologies and new algorithmic approaches designed to meet the specific needs of renewable energy research as it applies to electricity generation, distribution, and storage. Although many of the large-scale simulation codes being used in this field today can scale to use teraflop computational capabilities, significant effort will be needed to ensure that they can readily use the petascale computational capabilities being planned.

These collaborations will need to address daunting challenges related to a dramatic increase in the proportion of our nation's energy needs supplied through renewable sources. Indeed, the

total scale of the need is often forgotten amid the technical details of research and development. Thus, new efforts must fully address a multitude of scalability issues as they pertain to real deployment of these new technologies. Fortunately, favorable trends in capability and cost of large-scale simulations are making it possible to conduct simulation-enhanced research in a number of science and engineering areas. This suggests that common facilities and resources will be made available to the research community. The successful SciDAC program and its associated centers and institutes serve as a viable working model toward establishing a similar research program that focuses on the research and development of more efficient alternative energy devices, but also on their deployment and integration with the electrical grid. As the effort for energy independence is a national need, we must develop a similar-scale R&D program and associated facilities.

The reports of the five panels that follow constitute the main body of this workshop report. They provide full details of the research priorities of the five renewable energy technology areas and the ways that a new program of computational research in alternative and renewable energy can help meet the challenges of those research areas—and thereby enable renewable energy to make a substantial contribution to future energy needs.

RENEWABLE FUELS—HYDROGEN



Developing systems for high-density storage of hydrogen is crucial to successful hydrogen technology deployment. Numerous promising possibilities are being pursued, and high-performance computer modeling can play a key role. 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.

CHARGE TO PANEL

As an energy carrier, hydrogen has much promise for reducing our need for fossil-fuel-based energy. To fully realize this potential, we must develop a hydrogen economy based on a network of production, distribution, and storage technologies. Key among these components is the ability to store hydrogen in a cost-effective manner. Advanced methods of hydrogen production must also be developed, as must more distributed end uses of this energy carrier.

The charge to the members of the Hydrogen breakout session is to identify priority research directions in this area related to:

1. Nanostructured and other advanced materials and methods for hydrogen storage
2. Advanced fuel cells
3. Photochemical production of hydrogen
4. Thermochemical production of hydrogen
5. Algae and photobiological production of hydrogen.

SESSION BREAKOUT LEADERS

Dave Dixon, University of Alabama
Bruce Clemens, Stanford University
Mike Heben, National Renewable Energy Laboratory

OVERVIEW AND BACKGROUND

Molecular hydrogen (H_2) is an energy carrier, not an energy source, but it can store energy for later use. Interest in developing a new energy economy with hydrogen as a central focus stems from the fact that hydrogen can be produced from abundant and diverse domestic energy resources; then, it can be stored, and finally, used in highly efficient fuel cells. 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 Gibbs 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, but this process is usually not as efficient as the reaction of hydrogen with oxygen in a fuel cell. The development of efficient, inexpensive hydrogen technologies has the potential to provide a seamless pathway from our current dependence on oil, which increasingly is imported, to the use of domestically available resources. The move to pure hydrogen as a fuel, for both stationary and transportation applications, will decrease the carbon dioxide (CO_2) intensity associated with our energy consumption patterns. Thus, hydrogen is a key piece in our nation's energy puzzle and has great potential for producing a large change in our overall energy economy.

Realizing Hydrogen's Potential

The potential benefits of hydrogen as a fuel cannot be realized without innovative and scalable solutions to several different problems. Among these is the ability to efficiently store and recover hydrogen. The development of advanced storage materials should enable the United States to replace gasoline as the main transportation fuel. Breakthroughs in production and fuel cell technologies are also required. Advances in computational science will clearly accelerate the rate of discovery and implementation.

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. Ideally, computational models would be developed that permit accelerated exploration of possible directions for experimental research and point the way to more efficient and/or less costly implementations. These models need to contain all relevant details to permit control of both physical and chemical aspects, and they span concerns from atomistic to bulk issues. Computational science could also guide research related to cost and manufacturing issues and permit the exploration of new topological configurations.

The potential for hydrogen fuel to displace our reliance on petroleum is contingent on developing methods to store hydrogen inexpensively on-board vehicles in a safe, convenient, compact, and lightweight package. The U.S. Department of Energy (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 [Satyapal, 2007], but the challenge of producing such systems has not yet been met.

As much recent scientific literature has shown, computation and theory have already played an important role in advancing the next-generation, solid-state storage options currently being explored. However, much more needs to be done as no storage method satisfies all of the requirements for efficiency, size, weight, cost, and safety for transportation vehicles. Computational science will clearly 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.

Computational science advances will also have a tremendous impact on hydrogen production technologies. Hydrogen can be produced from renewable resources via a variety of methods that are currently the subject of intense research efforts worldwide. These methods include photoelectrochemical water-splitting using semiconductors; photobiological approaches using algae and cyanobacteria; fermentation, pyrolysis, and gasification of biomass; solar thermochemical processes; and direct electrolysis using electricity derived from photovoltaics or wind energy. The DOE Office of Energy Efficiency and Renewable Energy has an active program that supports development in each of these areas.

The Hydrogen panel 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.

Note also that the specific example research activities discussed in the following pages within the context of the priority research directions are intended to be illustrative rather than complete.

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RATE PROCESSES IN HYDROGEN PRODUCTION, STORAGE, AND USE

ABSTRACT

Rate processes are extremely important in virtually all scientific and technical aspects related to generating, transporting, and transforming hydrogen and hydrogen-containing molecules and materials. Critical rate processes span many orders of magnitude in time and occur on a multitude of physical scales, ranging from the atomic, to the molecular, to the macromolecular, to the solid-state levels. Advances in computational science are required to improve the accuracy and speed at which simulations can be performed.

EXECUTIVE SUMMARY

New computational capabilities in *Rate Processes in Hydrogen Storage, Production, and Use* will provide a more detailed understanding of chemical and physical transformations from the molecular to the system level. Understanding the processes that control molecular transformations will enable experimentalists and engineers to design new catalysts, materials, and strategies to maximize the rates of key processes. These critical rate processes span many orders of magnitude in time and occur on a multitude of physical scales, ranging from molecular (electron transfer) to macromolecular (phase transformations) levels. Key outcomes to benefit hydrogen energy include approaches that enhance charge separation to increase efficiencies of hydrogen production, and approaches that enhance rates of hydrogen sorption and desorption in condensed-phase and molecular materials.

For hydrogen generation, key needs evolve around an understanding of interfacial charge-transport and mass-transfer processes and quantum-mechanical hydrogen tunneling. These issues also tie into hydrogen storage, but it is clear that phase nucleation and ultimate microstructural evolution are also important in adequately describing the storage and release processes. Because hydrogen production, storage, and use involve interfacial processes, associated reaction chemistry may be affected significantly by imperfections in solid materials. Computational approaches that enable a detailed understanding of both thermally and photochemically driven processes will permit the rational design of catalysts to control the processes.

The associated scientific and computational challenges can be grouped into four broad areas:

- Redox reactions and proton-coupled electron transfer
- Temporal and spatial behavior of complex reactions
- Condensed-state, phase-change reaction kinetics of metastable configurations
- Homogeneous and heterogeneous reactions in real-world conditions.

Kinetics—that is, the rates at which chemical or physical processes occur—is critical to the use of hydrogen in future energy economies and is often the critical factor limiting performance in hydrogen technologies. A broad set of computational science needs include:

- Realistic models for interfacial charge-transfer dynamics
- Quantum-mechanical tunneling methods for treating the dynamics of light atoms
- Atomistic modeling of phase nucleation, microstructural evolution, and metastability
- Comprehensive modeling of the role of imperfections in reactions
- Tools for predicting chemical reactions in solution and on surfaces.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

The rates of chemical and physical processes control our ability to generate hydrogen from water by thermal, electrical, or photolytic methods; release hydrogen from a storage system and regenerate the spent fuel or recharge the medium; and generate energy in the form of electricity in fuel cells. Specific examples include the separation of charge in photocatalytic splitting of water to produce hydrogen, controlling rates of hydrogen desorption and resorption in hydrogen storage materials, and the behavior of redox reactions and proton-coupled electron transfer in fuel cells. The main computational challenges in predicting kinetic behavior are: that time is linear and does not necessarily parallelize, with the behavior of the next time-step usually requiring knowledge of the previous time-step; the need to take small time-steps to reliably predict temporal behavior; and the need to cover very large scales in time from the sub-femtosecond ($<10^{-15}$ s) to multiple years. The long timescales are important in terms of predicting how materials change in use—for example, in a hydrogen storage system in a car or a photocell used to split water using sunlight as an energy source. In addition, there is need for an accurate description of the underlying potential energy surface, as well as the need to couple chemical processes with physical transport processes such as diffusion and complicated flows.

The practical generation of hydrogen using either conventional or photon-assisted electrolysis requires surfaces that can efficiently transfer charge with minimum overpotential and no degradation of performance. In hydrogen-generation systems, processes must involve proton-coupled electron transfer, and this is an active area of experimental, theoretical, and computational research [Costentin 2006]. Work on understanding charge-transport processes is very active, and recent efforts have focused on electron transfer at semiconductor/solution interfaces and charge transfer in sensitized solar cells [Durrant 2006]. Excited electronic states and charge transfer are important in either electrical or photochemical generation of hydrogen. The treatment of such states is much more challenging computationally in terms of both the electronic structure and the dynamics and kinetics. Coupled electron transfer and proton transfer leads to very different timescales, and the Born-Oppenheimer approximation currently used for so much of the predictive kinetics can break down. Methods to treat these issues are being developed, but no computationally efficient and general methods are yet available. Photoexcitation in solids can lead to separated electrons and holes, or to electron-hole pairs that are associated as excitons. The dynamics of electrons, holes, and excitons in solids and their coupling to phonon modes is not well understood and requires new theoretical and computational approaches. Realistic methods are needed for modeling both outer-sphere charge transport and transfer processes of chemisorbed species.

Efficient chemical reactions are necessary for hydrogen storage in terms of hydrogen release and regeneration of spent fuel. If the storage system is a solid such as a metal hydride, then an additional complication is the need to predict nucleation and growth in a solid-state phase transformation. In a chemical storage system, the solid-state issues can be present, but researchers might also need to predict the rates of reactions in solution, as well as at the solution-solid interface. In addition, for chemical hydrogen storage, they might also need to be able to predict the effect of catalysts on chemical processes. A catalyst changes the rates at which chemical bonds are formed and broken and can be used to control the yields of desired products versus undesired ones. Catalysts do not change the overall thermodynamics of the process and are usually present in small-percentage quantities. An example from chemical hydrogen storage is the need for catalysts to release H_2 from ammonia borane [Stephens 2007a; Stephens 2007b] and the need for catalysts in the regeneration steps to rehydrogenate spent fuel. An example from solid-state systems is the improved performance of Ti-doped sodium alanates.

Calculations of rate constants for hydrogen generation, storage, and use pose a significant computational challenge because of the size and complexity of active sites and reactant molecules. Transition-state theory (TST) is the simplest approach [Glasstone 1941, Johnston 1966, Kreevoy 1986, Steinfeld 1989, Truhlar 1996, Truhlar 1999, Fernandez-Ramos 2007]—considering that it uses a minimal amount of the potential energy surface to predict rate constants for chemical reactions—and it has recently been used to predict rate constants for chemical hydrogen storage systems [Nguyen 2007, Nguyen 2007, Nguyen 2007]. The simplest form of TST only requires information about reactant and transition-state structures, frequencies, and energetics. However, in a complex system or on a surface, it is often difficult to find the transition state. And in complex systems, the concept of a single transition state may not be meaningful. The number of reaction pathways will increase with system complexity. There may be many transition states with similar energies, leading to many competitive reaction paths that contribute to the actual rates. For reactions in condensed phases, the effects of the environment (such as the solvent, interface, or solid) will significantly influence the rate constants—in general, affecting the pre-exponential factor, A. Reliable predictions of the A factor in a rate expression require accurate predictions of the entropy of the system. Currently, this requires appropriate reliable sampling of multiple configurations, which, at this time, is not computationally tractable. Molecular dynamics (MD) simulations provide an approach for calculating transport properties that are important in hydrogen generation, storage, and use systems. However, MD simulations of complex, multiphase systems cannot currently be readily extended to the sufficiently long timescales necessary to simulate the slow processes of interest.

The efficient conversion of chemical potential to electrical energy in a fuel cell faces similar issues of interfacial charge transfer and proton transport.

Addressing these issues will require the development of:

- New methods to implement quantum chemistry and direct dynamics on advanced computer architectures
- Multiscale approaches to electronic-structure-based dynamics
- Tools to provide accurate information transfer between models of different fidelity
- Improved rare-event sampling methods.

Progress will require developing new methods to implement quantum chemistry and direct dynamics on advanced computer architectures. A critical need is for more robust potential and faster electronic-structure methods to couple with improved potential-energy, surface-sampling techniques to enable faster identification of reaction pathways and rate-limiting steps. New generations of the tight-binding method (self-consistent charge) and reactive force fields (such as ReaxFF) need to be advanced.

Quantum dynamical effects need to be incorporated into accelerated molecular dynamics to deal with light elements such as hydrogen. And there is a need to extend long-timescale methods with the capability to use forces and energies directly from electronic structure methods. This will require multiscale approaches to electronic-structure-based dynamics and procedures to accurately transfer information between models of different fidelity and techniques for handling rare-event sampling. This research will impact kinetics issues for hydrogen production, storage, and use technologies, in which a better understanding will enable the design of materials with improved kinetics. A critical issue with the dynamics of hydrogen is to be able to treat quantum-dynamical effects. Current approaches based on path-integral techniques involving multiple replicas are very inefficient computationally.

There is also a need for improved methods that can use the results from atomic-scale calculations as input to larger-scale models. For example, rates of nucleation and growth processes in hydrogen storage solid-state reactions depend on the surface and interface energies and interface structure and atom-transport processes.

Of critical importance in hydrogen storage is an understanding of the dynamics of hydrogen adsorption/desorption processes and the phase changes that will necessarily occur in the storage host during the process. In addition, the role of imperfections on the kinetics of storage processes is also an issue. Theoretical and computational work on phase changes focuses on extrapolating the behavior of bulk materials from that of small clusters [Proykova 2006], and there is a growing need for computational studies of phase changes accompanying chemical processes.

COMPUTATIONAL SCIENCE NEEDS

The scientific issues and challenges just described require significant advances in computational approaches, coupled with advances in applied mathematics and computer science. New methods for treating kinetics and reactions, as well as molecular-dynamics methods, need to be implemented in algorithms that are appropriate for advanced computing architectures. New methods that scale on large parallel architectures with relatively low memory and storage requirements are especially needed. Efficient algorithms and new methods for determining reaction surfaces and for predicting reaction pathways are also needed, as well as how they can be coupled to kinetics simulations. New phase-space sampling techniques for reactions in complex systems are needed as well.

Success in these areas will enable:

- Tools to enable a fundamental, atomistic understanding of complex phase-change and reaction behaviors
- Multiscale approaches to electronic-structure-based dynamics
- Atomistic approaches to large systems (e.g., phase transitions, chemical reactions).

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

The potential impacts of success in the areas listed above for alternative and renewable energy include:

- Design of new materials for solar hydrogen production with improved kinetic control, including understanding the role of dopants for photochemical water-splitting
- Design of high-hydrogen-capacity storage materials with efficient H_2 release and regeneration
- Design of fuel cells with cost-effective metal catalysts and membranes
- Development of methods to assess stability, leading to synthetic routes to needed materials.

TIME FRAME

Advances in computational science are already impacting the design of metal hydride, chemical hydride, and sorption material systems. Further investments will have a large impact in the 3- to 10-year time frame. For example, faster identification of reaction pathways and rate-limiting steps would aid in the development of more efficient regeneration processes for chemical hydrogen storage materials. Models able to explain the nucleation and growth of the hydride or hydrogenated phases in metal hydride or spillover materials, respectively, would lead to improvements in system efficiency and reversibility. Similar beneficial impacts can also be anticipated for hydrogen production and use technologies.

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INVERSE MATERIALS AND SYSTEM DESIGN

ABSTRACT

The design of unique materials with new and improved physical properties is a consistent theme in many of the research areas associated with alternative and renewable energy. Inverse materials design for specific application in hydrogen production, storage, and use aims at developing a computational protocol for discovering novel materials not yet found or explored experimentally. One approach to address this computational grand challenge requires developing capabilities to take either experimental or computational structural and property data for known or existing materials and to use this information in novel algorithms to elucidate structures of new materials, molecules, or systems from a predetermined set of desired properties. This effort will require developing rapid screening and computational methods for quick-validation protocols. Progress in these areas will lead to the development of novel methodologies and hardware capabilities for computational materials design.

EXECUTIVE SUMMARY

Prediction databases and the tools to efficiently mine these databases need to be developed. An efficient framework is required to discover high-performance materials, molecules, and complex functional assemblies. This effort will require novel mathematical and computational approaches for optimizing the inverse design of materials. Novel high-performance materials are necessary in all areas of a hydrogen economy, including hydrogen generation, storage, and use.

SUMMARY OF RESEARCH DIRECTION

To develop a materials-prediction database and discovery framework, we need to identify and calculate chemical/physical (e.g., electronic, thermodynamic, structural, stability) descriptors that can be used in combination with data-mining tools to predict the property of a given material or suggest the chemical domain of interest of a new material or complex. To calculate molecular descriptors and build a database for compound/chemical classes, we need rapid computational tools based on quantum mechanical, atomistic, and larger united atom/molecule levels. These tools, followed by the development of rapid-screening tools for the database, can be used for design and selection. This process could draw ideas/parallels from experimental high-throughput screening techniques [Potyrailo 2006]. Correlating materials performance in devices to fundamental materials properties by approaches such as structure-activity relationships methods (e.g., QSAR, QSPR), based on multivariate statistical analysis (e.g., cluster analysis, genetic function approximations), is a focus for developing models having predictive capabilities. Some of these techniques have been developed and applied successfully in other research areas such as the pharmaceutical industry [Rogers 1994], chemical sensors (materials selection and sensor response) [Shevade 2006; Ryan 2007], and catalyst design.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

A computational grand challenge is to develop computational methods for materials design based on a fundamental molecular understanding using first principles. The problem of inverse materials design generally involves evaluating the properties of a known material using chemical knowledge and computational tools to find a material that will have a desired property. The challenges are to develop rapid quantum-mechanical/atomistic-based screening tools and use them to derive knowledge, and then to integrate these components to predict materials and system performance. There is a great need to permit rapid surveying of potential materials/molecules/systems to find those that may be most readily synthesized or manufactured.

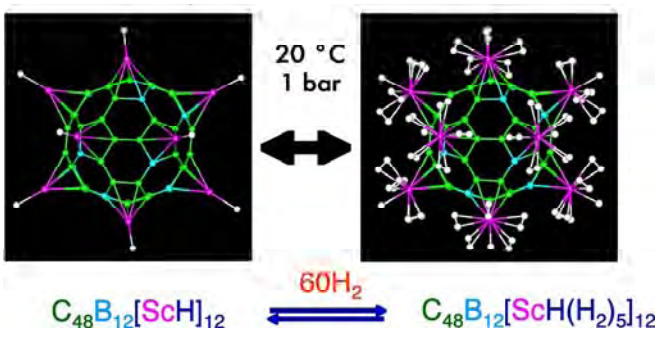

Figure 1: "Synthesis in the computer" has resulted recently in the prediction of many new approaches to hydrogen storage materials. Here, scandium atoms complexed to B-doped "buckyballs" ($C_{48}B_{12}$) present unoccupied d-orbitals with suitable energies to complex 12 dihydrogen species reversibly [Zhao 2005].

Although there is considerable emphasis currently on new concepts for converting sunlight into electricity in photovoltaic devices, hydrogen may be generated by direct water-splitting at the surfaces of illuminated semiconductor surfaces. However, new materials must be identified to realize this potential. Today, the typical approach is a brute-force process involving a long, arduous materials search, coupled with scientific intuition, which often involves multistage synthesis and extensive experimental characterization. The same may be said for biological or biomimetic approaches to hydrogen production. The rate of advancement could be greatly accelerated by developing a computational pathway that would take the desired performance properties and calculate possible structures or approaches (i.e., synthesis in the computer) to meet specific criteria. The motivation for these efforts is based on the recognition that a major energy source in the future will be solar energy. This source fluctuates in time (e.g., day and night, or seasonally); thus, efficient energy storage is required for a future that uses this energy.

Of the possible energy storage systems, energy storage in chemical bonds has the widest applicability. This includes hydrogen storage materials as well as batteries. Significant limitations exist for both these systems, so considerable improvement in material properties is necessary in both areas for future energy-storage needs. Despite significant efforts, ongoing challenges exist in finding the best materials to meet the desired goals. Electrocatalysis, particularly oxygen catalysis (both O_2 reduction and water oxidation), represents a major barrier to the widespread implementation of fuel cells and electrolyzers. Both systems currently require platinum or platinum-group metals (PGMs) to operate efficiently and are limited by the lack of abundance of these noble metals as well as their cost. More than 50 years of research, which

involved looking for more abundant materials with properties even approaching those of the PGMs, has met with limited success. An equally pressing need is the development of an electrolyte for the fuel cell that is mechanically and thermally robust and chemically stable (for at least 5000 hours of operation) and exhibits high proton conductivity at temperatures between 110°C and 130°C at low relative humidity. Materials meeting this need would revolutionize energy systems and, in fact, may be the single greatest materials challenge for the hydrogen economy.

POTENTIAL COMPUTATIONAL SCIENCE NEEDS AND IMPACT

In recent years, materials science has witnessed the emergence of a grand challenge that has implicitly defined this multidisciplinary field—namely, the ability to identify and process specific materials and structures that are predicted to meet or exceed multiple properties/performance criteria stipulated by the designer. Olsen [1997, 2000] labeled this new paradigm as the "goals-means" approach. This approach contrasts sharply with the traditional "cause and effect" approach driven mainly by innovations in processing, which typically focuses on only a limited number of readily manufacturable configurations.

This inverted paradigm of materials design is especially critical for highly constrained design applications, where the designer faces increasingly complex requirements with multiple property objectives/constraints and materials anisotropy affecting system performance. For example, new materials are needed to make solar hydrogen production cost competitive with fossil fuels. Designing solar materials for producing hydrogen requires the design and assembly of two- and three-dimensional photosystems, in which only the optimal spatial arrangement of components can achieve efficient light-harvesting, charge-carrier separation, and catalyzed generation and separation of hydrogen and oxygen.

Although existing simulation tools can model the properties of a prototypical design, developing new designs remains a significant challenge. Optimization techniques can be used to search for new designs, but wrapping a general-purpose (black-box) optimizer around large-scale materials simulation is very expensive because each objective function evaluation (i.e., the computational simulation) is very costly. New optimization techniques are needed that leverage simplified materials models (surrogates) to manage the cost of a design-optimization process.

A particular challenge is that these material-design simulations involve both continuous and discrete choices. Such mixed-integer optimization problems can be quite difficult to solve. Efficient large-scale parallel algorithms for mixed-integer nonlinear programming, or MINLP, need to be developed. In addition, we need general techniques for creating efficient surrogate modeling techniques with controllable accuracy for complex material models.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

This research would identify promising materials/chemicals/complexes and systems for (1) solar water-splitting, (2) hydrogen and electrical energy storage, and (3) fuel cell membranes and catalysts.

TIME FRAME

Advances are having an impact in related research directions. A focused program would have much greater impacts in the 3- to 10-year time frame with applications to real-world systems.

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SYNTHESIS OF TARGETED MATERIALS

ABSTRACT

Many new materials, catalysts, molecular species, and complex systems are being devised by theoretical physics and chemistry methods to overcome critical hurdles associated with deploying the hydrogen economy. This trend is likely to continue as theoretical methods become more ubiquitous in the scientific community. Unfortunately, many of the most promising predictions have not yet been realized because of the difficulty of experimentally synthesizing the highly specialized functional entities/materials, even in small quantities. In many cases, the desired species exist in local metastable minima, and a variety of variables and kinetic and thermodynamic factors are expected to be at play while navigating a complex reaction surface during synthesis. In short, the reaction coordinate and methods by which these needed materials may be synthesized are often completely unknown. Computational science can play an essential role in exploring the synthetic reaction space to winnow possibilities and direct experimental emphases. This mission is daunting and mandates that the phrase "synthesis in the computer" be extended from providing an accurate representation of the endpoint of the reaction (i.e., the product) to the entire reaction coordinate. In time, this effort will result in complete, accurate simulations of large-scale manufacturing processes.

EXECUTIVE SUMMARY

A variety of different hydrogen-related science and technology advances are being promoted to develop an environmentally friendly, efficient, hydrogen energy economy. Hydrogen as a fuel promises load leveling for intermittent renewable energy sources, and permits the development of a carbon dioxide-free energy supply for the transportation sector. A critical need for using hydrogen as a fuel is efficient storage systems with the appropriate equilibrium thermodynamics in terms of the enthalpy and free energy and release/uptake rates of hydrogen. Such systems have very specific engineering constraints in terms of the energetics, overall weight and volume, and life-cycle cost. This places stringent requirements on the materials to be used, whether the hydrogen is stored in a chemical or metal hydride, or via an advanced sorbent technology. There is also the complex issue of how to generate hydrogen economically without impacting the environment, and many important issues related to hydrogen fuel cells also need to be addressed. Computational science can help experimentalists design and build new materials, molecules, complexes, and systems for hydrogen production, storage, and use.

For computational science to have a greater impact on the fabrication of new materials, substantial advances are required in the domain areas, computer science, and applied mathematics. Substantial improvements are required in electronic structure methods for molecules and materials, and in solving scaling issues for new architectures. The ability to make accurate predictions reliably and inexpensively is also required. This will involve developing new density functional theory exchange-correlation functionals, as well as improving other methods for predicting electronic structure, including quantum Monte Carlo approaches. New methods are needed for efficient sampling of phase space to deal with complex potential-energy surfaces, entropic effects, long-time dynamics, multiple phases, and rare events on length scales of 1 to 100 nm. Techniques are needed to incorporate environmental synthetic variables such as

pressure, density, temperature, pH, and ionic strength for materials synthesis. New methods for quantum-dynamical simulations that couple electronic structure and nuclear motion in realistic environments may be needed when light elements such as hydrogen are a component in the synthesis. New approaches need to be developed based on modern computer science methods to deal with and contribute to the knowledge base of complex materials. The organization of knowledge about the relevant materials properties into databases that can communicate with each other—and tools to manipulate the databases and mine them for new knowledge—are expected to have a substantial impact on developing materials, molecules, and systems for hydrogen technologies.

SUMMARY OF RESEARCH DIRECTION

A broad set of computational science needs in terms of the domain areas, computer science, applied mathematics, and computational science are presented. Highlights include the need to develop:

- Tools to calculate pathways for the fabrication of targeted materials, molecules, and systems, including metastable intermediates, as a function of environmental variables (e.g., pressure, temperature, pH)
- Tools for quantum simulations (electronic structure and nuclear motion) in realistic environments for thermodynamics, kinetics, and excited states
- Efficient algorithms/methods to efficiently search phase space for local (reactive intermediates) and global minima, and transition states to model equilibria and transformation between these along the reaction path
- An improved ability to model accurately finite temperature material properties, rare events, and long-time dynamics on length scales of 1 to 100 nm
- New database structures and data-mining tools for materials properties and reaction pathways.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

There is increasing interest in developing hydrogen-based fuel cells as an environmentally friendly power source for the transportation sector. A current critical issue with hydrogen as a fuel for use in on-board transportation systems is the need for efficient hydrogen storage systems with appropriate management of the release/uptake of hydrogen. Hydrogen can be stored physically with high-pressure tanks or in cryogenic systems as liquid hydrogen. These approaches have weight, volume, cost, and safety issues that limit their practical viability. As a result, there is substantial interest in developing hydrogen storage materials that can store hydrogen in sorption, metal hydride, or chemical hydride systems. All of these approaches involve the design of materials or molecules that possess the appropriate hydrogen energetics and release rates and appropriate regeneration schemes. Also, concerns associated with safety, efficiency, and toxicity must be addressed.

Developing computational methods to assist in synthesis will require the ability to calculate competitive pathways involving multiple constituents as a function of environmental variables (e.g., pressure, temperature, composition). The ability to predict reactions in solution will require including pH, ionic strength, and viscosity. Currently, tools for such simulations do not exist.

Understanding synthesis to enable the prediction and optimization of experimentally employed methods will require the ability to model behaviors and reactions across a range of scales of length and time, in a wide variety of gaseous, liquid, and solid-state environments. A significant computational issue is the need to sample enough of the phase to be able to predict the entropy of the reaction and its effect on the reaction rates and thermodynamics, in the case of liquids, or to be able to sample the different sites and the effect of crystallinity and surface roughness on the reaction, in the case of heterogeneous reactions. The case of the solid-liquid interface is even more complex and has currently not been treated with any reliability.

To relate to engineering constraints for synthesis, high accuracy simulations will be required. For example, for a 50:50 starting mixture of two components, a change in the reaction free energy, ΔG, of less than 1.5 kcal/mol leads to a change in the equilibrium constant by a factor of 10, leading to a 90:10 mixture at 25°C. Similarly, a change in the activation energy of 1.4 kcal/mol changes the rate constant by a factor of ten at room temperature (25°C). A factor of 2 to 4 in the rates could determine whether or not a hydrogen storage or production system is economically feasible. Thus, the computational methods for simulation of materials design for hydrogen-related technologies must have an appropriately high accuracy.

To bring computational science to bear on synthetic reactions, high-accuracy descriptions of complex interactions at the electronic structure level in extended systems must be possible. This will require the development of new density functional theory (DFT) functionals with guaranteed accuracy and the ability to treat transition states and weak non-bonded interactions. In addition, the current computational efficiency must be substantially improved, and not just enhanced by going to a larger system. The scaling of the algorithms in terms of single-processor efficiency and parallel performance must be improved. There must be continuing development of reduced scaling methods in electronic structure theory.

One promising area is that the quantum Monte Carlo (QMC) approach, which has some potential computational advantages, but also has many limitations and requires substantial work [Hammond 1994]. In QMC, there are real issues in terms of the starting-guess wavefunctions and the number of nodes that are needed. Substantial work is needed in the area of derivatives for QMC for geometry optimization and frequency calculations, some of the information needed for characterizing the potential-energy surfaces. If the issues with QMC can be addressed, it holds the promise of being a very scalable, accurate method with very different memory requirements. All of the methods dealing with predicting transition states require improved computational treatments of anharmonicity to improve predictions of reaction rates. Accurate methods are needed for treating quantum electronic effects in larger systems from 1 to 100 nm with high accuracy. Currently available electronic structure methods [Frauenheim 2000; Frauenheim 2002] do not offer the accuracy that could be needed for treating quantum effects at the larger nanoscale. This is an unknown area in terms of exactly what properties will exhibit quantum behavior. There is a need to develop improved empirical potentials for all molecules in the Periodic Table, including the ability to include chemical reactions for classical and quantum-dynamical molecular dynamics simulations. Such potentials would enable faster searching of phase space in complex systems and provide substantially improved guesses of starting structures for more accurate simulations. In addition, this would permit improved kinetic and

thermodynamic predictions by enabling the inclusion of more of the environment in the simulation—for example, through combined quantum-mechanical electronic structure theory (QM) with empirical or molecular mechanics (MM) simulations (so called QM/MM methods).

There are also substantial needs to improve our ability to characterize the critical regions of potential-energy surfaces in complex systems, including searching for global minima and transition states. New methods for exploring phase space are required, leading to new materials discovery, the ability to predict finite-temperature material properties, rare events for reaction kinetics, and phase stability. This is an issue because such simulations are linear in time and often require small time-steps for accuracy and, for example, energy conservation. New methods are needed to reduce the time for finding and calculating reaction paths for synthesis, degradation, and systems perturbation in complex materials and molecules. Such simulations will enable the accurate prediction of the entropy and stability of complex materials.

COMPUTATIONAL SCIENCE NEEDS

The above scientific issues and challenges require significant advances in computational approaches, coupled with advances in applied mathematics and computer science. New electronic-structure methods and methods for treating molecular-dynamics methods need to be implemented in algorithms appropriate for advanced computing architectures. New methods that scale on large parallel architectures with relatively low memory and storage requirements are especially needed. Efficient algorithms and new methods for determining reaction surfaces and methods for predicting reaction pathways are needed. New phase-space sampling techniques for reactions in complex systems (e.g., adaptive hybrid methods) would enable substantial progress in designing materials for hydrogen storage, production, and use. Another issue is the need to analyze long-term dynamic simulations when it might not be possible to store all of the intermediate data. How can the researcher perform on-the-fly analysis and abstract critical information—for example, data relevant to the prediction of a reaction rate? New multiscale multiphysics methods will be needed to deal with the size of the temporal and spatial scales, as well as the complex physical and chemical phenomena that may be encountered during synthesis.

As these efforts proceed, new approaches based on modern computer science methods will be needed to deal with a complex and ever-growing materials knowledge base. The organization of knowledge about the relevant reactions into databases that can communicate with each other—and tools to manipulate the databases and mine them for new knowledge—are expected to substantially impact the development of hydrogen production, storage, and use systems.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

The potential impacts of success in the above areas for alternative and renewable energy include:

- Design of new materials for solar hydrogen production
- Design of high-hydrogen-capacity storage materials with efficient hydrogen release and regeneration
- Design of fuel cells with cost-effective metal catalysts and membranes

- Development of methods to assess stability leading to synthetic routes to needed materials.

TIME FRAME

Large impacts can be expected in the 3- to 5-year time frame, with impacts to applications in real-world systems in 10 years.

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LONG-TERM BEHAVIOR AND LIFETIME SIMULATION

ABSTRACT

Materials durability is one of the key issues in hydrogen fuel applications. A better understanding of the mechanisms leading to the failures of the materials and devices for hydrogen production, storage, and fuel cells is essential for a better selection and design of materials and systems. This is a computational challenge that requires broad advances in computational materials science, applied mathematics, and computation. This priority research direction discusses possible mechanisms that affect the long-term performance of the materials and devices for hydrogen production, storage, and fuel cells; it also identifies the computational research needs for making progress in predicting the long-term behavior and lifetime of the materials and devices.

EXECUTIVE SUMMARY

In the search for alternative clean fuels, hydrogen is an excellent candidate as an energy source/carrier for both transportation and stationary applications. However, materials performance degradation is a serious challenge that must be overcome if, for example, hydrogen fuel cell technology is to realize its market potential. Durability problems in materials used for hydrogen storage, hydrogen production, and fuel cells are typically studied by simply measuring degradation after the devices have been run for long periods of time. Experimental data are then analyzed to assess the failure modes. Conclusions are based on limited data sets obtained under controlled, narrowly defined conditions, so real-world degradation mechanisms are often poorly understood. There is an urgent need for a rational, validated, computational accelerated testing method that can predict the long-term performance and lifetime of the materials and fuel cells used for hydrogen technology.

Experiments indicate that there are common phenomena and processes involving the phase transformations during hydrogen (or proton) transport, hydrogenation/dehydrogenation reactions, and the damage accumulations leading up to materials failure in these systems. Elucidating the mechanisms responsible for failure in materials for hydrogen storage and fuel cells is essential for predicting new ways to dramatically improve the stability and life span of hydrogen fuel cells.

Four computational research directions have been identified by the panel to address the long-term behavior and durability issue in hydrogen fuel cell technologies:

1. Hydrogen transport in fuel cells, defective lattices, and related interfaces and topologies
2. Interfacial mobility under the influence of hydrogen and the evolving lattice defects
3. Phase transformation and microstructure evolution in materials involving hydrogen cycling over long times
4. Explicit incorporation of real-world environmental effects.

Computer simulations of failure mechanisms in these systems require a fundamental understanding of hydrogen interactions within a given host system that operates at timescales

ranging from picoseconds (10^{-12} s) to years, and over length scales ranging from atomistic to the continuum. To date, methods to simulate the interactions of hydrogen (or oxygen) with the crystal defects at the appropriate scales of length and time have not been developed and validated by experiments. The development of such multiscale computational approaches will not only aid in understanding the mechanisms of hydrogenation/dehydrogenation, but will also provide the necessary tools for predicting hydrogen fuel cell lifetime.

SUMMARY OF RESEARCH DIRECTION

The ultimate goal of this priority research direction is the quantitative prediction of the long-term behavior of the materials used for hydrogen production, storage, and fuel cells. Computational research will focus on elucidating the underlying physical mechanisms of material damage and degradation and on how to improve the lifetime of materials for energy technologies involving hydrogen. We need to develop event-driven simulation tools for handling specific materials and processes of import to hydrogen.

Hydrogen transport in fuel cells and in defective lattices

Hydrogen and proton transport is an essential process in hydrogen fuel cells. The poor long-term stability of interfacial connections between components, including issues of electrical connectivity and adhesion, often leads to operational difficulties. It is well established that a major source of failure in interconnects of electronic circuits is electromigration. Instabilities develop and grow to break circuits. The baneful effects of defects are also accentuated. The proton electromigration analogy applies to systems in which the hydrogen nuclei can move relatively freely through the material, rather than tunneling from cell to cell. Like electrons, the protons are driven by the electric field, albeit in the opposite direction. The field acting on the atoms will essentially be the same as in the conventional case. For metals, this force is dwarfed by the "wind" force due to ballistic collisions between the carriers and the atom [Ishida 1994; Rous 1994; Bly 1996; Rous 1999]. If there are also positive carriers that are moving in the opposite direction, the wind force will be diminished in comparison to the pure electron-carrier case. Because a proton is about 2000 times as massive as an electron, the proton will move much slower than the electron but will carry comparable momentum. To the extent that there are band effects, these will be drastically different for electrons. A hierarchy of questions of interest arises from this viewpoint. First, one must characterize the motion of the protons. Next, the wind force needs to be modeled, which is usually framed in terms of a large effective charge of the carrier. It has been established that this effective charge increases dramatically in magnitude near defects such as steps on surfaces [Rous 1999] for electrons; it is reasonable to anticipate (but necessary to verify) that similar behavior occurs for proton carriers. After such fundamentals are established, the role of this new force and how it affects the evolution of atoms at narrow junctions in the material or near defects needs to be studied. This will help to determine what the impact on the aging process is, especially as to how it affects the evolution and distortion of defects [Hausser 2007].

In hydrogen-storage systems in which the molecule is dissociated into atoms that reside interstitially in metals, the resulting proton carriers could have similar effects on the aging and eventual failure of materials. For example, the charging of hydrogen can lead to considerable changes in the host metallic lattice parameters or even to the formation of new (hydride) phases,

which, in turn, causes large internal stresses in the materials used for hydrogen production, storage, and fuel cells [Fultz 2002]. Moreover, defects in the host lattice will be acting as hydrogen traps, which will greatly affect the dynamics of the hydrogen or proton transport during the hydrogen cycling [Yamamoto 2002; Sakaki 2006]. It is important to understand hydrogen transport in defective lattices and how defects accumulate, eventually leading to the failure of the materials over long-term hydrogen cycling. Computational research is also needed for accurately determining the energetics of H-cluster formation, H-vacancy and H-dislocation interactions, and migration barriers for H diffusion in the vicinity of lattice defects**,** as well as the dynamics of the hydrogen or proton transport on high-surface-area materials and in defected lattices under nonequilibrium conditions. Similar computational studies are needed for oxygen transport in solid-oxide fuel cells.

Interfacial mobility under the influence of hydrogen and the evolving lattice defects

The appearance of the hydride phase in the some hydrogen storage materials necessarily leads to interface formation. These interfaces and their migration lead to the formation of additional defects in the host lattice. A defect network is created as the result of the large internal stresses between the host and hydrogenated phases. This interface must migrate during the cycling, resulting in a high density of vacancies and dislocations. Therefore, it is important to understand and predict the interfacial mobility under the influence of hydrogen and the evolving lattice defects. Similar concerns can be associated with hydrogen transport on surfaces during so-called "spillover." Computational research is needed for understanding:

- How do the hydrogen and evolving lattice and surface defects (e.g., vacancies, self-interstitials, dangling bonds, and dislocations) affect the interfacial mobility of evolving phases?
- What is the role of fast diffusion paths (e.g., grain boundaries, dislocations, strained surfaces) on these processes and how do they affect the ultimate charge/discharge rates?

Phase transformation and microstructure evolution in materials involving hydrogen cycling over long times

Materials for hydrogen production, storage, and use can undergo phase transformations that consist of nucleation, growth, and coalescence of the parent phase and dissolution of the hydrogen subsystem [Goltsova 1999; Goltssova 2002; Pitt 2002]. With the evolution of large and nonuniform stress fields associated with phase transformations and lattice defects, a damage mechanism may develop that includes formation of microvoids/microcracks that can lead to failure (pulverization) of the hydrogen storage device and/or fuel cell [Joubert 2002]. Therefore, computational studies are needed that simulate and predict phase transformation and microstructure evolution in materials involving hydrogen cycling over long times. Computational research is needed for addressing these questions:

- How does the dislocation network in storage materials reach steady state during hydrogenation/dehydrogenation cycles?
- Where and how do new phases form during hydrogenation and dehydrogenation cycles?
- What is the origin of material damage and degradation, and how does it accumulate and impact performance behaviors?

- What determines whether microvoid nucleation and growth or cleavage-crack nucleation and final unstable crack growth lead to the final failure of the materials?

Durability of systems is also an issue. The poor long-term stability of interfacial connections between components, including issues of electrical connectivity and adhesion, often lead to operational difficulties. The structure of the interfaces between the various cell components can have a huge impact on performance. Therefore, it is important to understand the evolution of interface structures between components involving hydrogen cycling over long times.

Explicit incorporation of real-world environmental effects

Hydrogen storage devices and fuel cells may work in harsh conditions such as high-temperature and corrosive environments; for transportation usage, however, the temperature must be substantially lower, in the range of 80° to 125°C. In most fuel cells, the main issue is "poisoning" or fouling by impurities (e.g., sulfur, hydrocarbons, ammonia, and carbon monoxide) in the hydrogen feed stream. Degradation of the materials will be accelerated by harsh environments and impurities. It is clear that technical advances in high-temperature, corrosion-resistant materials will require a more detailed fundamental understanding of the thermodynamics and kinetics governing the reaction pathways between multicomponent gases and the materials for hydrogen storage and fuel cells. This highly complex problem must be addressed to extend the lifetime of the materials. Computational research is needed for simulating the long-term behavior and lifetime of materials for hydrogen technology that explicitly incorporate these real-world environmental effects. First-principles methods are needed for accurate calculation of the thermodynamics and kinetics governing the reaction pathways between multicomponent gases and the materials for hydrogen storage and fuel cells; they will foster the rational design of materials and devices that are durable and safe from catastrophic materials failures. A critical issue will be the need to develop simulation techniques to deal with low levels of impurities, which, in general, implies large computational system sizes.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

The mechanism of hydrogen transport, phase transformation, and microstructure evolution in these systems is cooperative and collective in nature, leading to complex behavior. Elucidation of the degradation mechanisms in these systems requires a fundamental understanding of hydrogen interactions within a given host system that operates at timescales ranging from picoseconds to years, and in length scales ranging from the atomistic to the continuum. To date, methods to simulate the wide range of degradation interactions of hydrogen with the materials used for storage, fuel cells, hydrogen generation or transport, at the appropriate scales of length and time, have not been developed or validated by experiments. To cover the wide range of behaviors in these processes and their mutual interactions, computational components at different scales need to be developed and linked together seamlessly. Indeed, many of the key phenomena are controlled at the atomistic scale—for example, uphill diffusion, dislocation and vacancy generation, hydrogen trapping and subsequent migration of these lattice defects, subsystem structure evolution, and finally, fracture—but they are demonstrated at the micro, meso, and continuum scales. An understanding of these fundamental individual processes is necessary to describe their mutual interactions and behavior. However, because of the current limitations in the spatial and temporal scales that may be accessed in atomistic simulations with sufficient

accuracy, new techniques will be required to solve these complex problems. Also, new techniques are sought that may permit a more detailed understanding of processes where cooperative and collective phenomena play a major role. Atomistic simulations need to be coupled seamlessly to mesoscale or continuum simulations to model the development of microstructures resulting from the interactions of the host lattice/hydride interfaces with the lattice defects. At the mesoscale, the collective behavior of a very large number of lattice defects (e.g., dislocation junctions, pile-ups, entanglements, and grain-boundary migrations) modifies the internal stress states and creates nonequilibrium conditions for diffusion, structure, and phase transformations. The mesoscale and continuum simulations will use input obtained from atomistic simulations, such as hydrogen-cluster formation energies, hydrogen-vacancy, hydrogen-dislocation, hydrogen-interface interaction energies, and migration barriers for hydrogen diffusion, as well as fundamental kinetic properties. The ultimate scheme for such an approach would be the seamless integration of all length and time scales in a unified computational algorithm. Initially, however, it is probably best to develop methods that accept data as input from the different scales to predict the behavior at a higher or lower scale. Developing such computational approaches will aid in understanding how materials used in hydrogen production, storage, and fuel cells degrade so that such degradation may be avoided.

POTENTIAL COMPUTATIONAL SCIENCE IMPACT

The scientific advancements and computational algorithms and tools for multiscale simulation of hydrogen transport, phase transformation, and structure evolution developed from this research effort will benefit the broader research community as many problems in materials research involve multiscale, multiphysics behavior.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

Achievements from this computational research will lead to better materials and system design, which will extend the lifetime of relevant materials and devices.

TIME FRAME

Large impact can be expected in 3 to 10 years.

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LINKING MODELS AND SCALES—FROM ATOMS TO SYSTEMS

ABSTRACT

Developing the infrastructure to enable hydrogen to become an effective energy carrier will require a detailed, quantitative understanding of the underlying chemical and physical processes in each stage of the hydrogen fuel cycle (i.e., production, storage, and use). To optimize performance and stability, to minimize rare-earth material usage and cost, and to discover more facile manufacturing techniques, system-level (or device-level) design will require research advances in science and engineering at multiple scales, from the atomistic to the continuum. Predictive simulation will require accurate and efficient computational strategies that bridge these scales, as well as a detailed understanding of the uncertainty in single-scale simulations and the propagation of uncertainty and numerical error between scales and between the disparate physical models.

EXECUTIVE SUMMARY

The development of technologies for hydrogen production, storage, and use depends critically on science and engineering from the atomistic to the continuum scale. Efficient and stable long-timescale performance of these devices requires a detailed understanding of fundamental chemical and physical processes; an understanding of catalytic reaction mechanisms; and the ability to design new materials, chemicals, and systems [Dresselhaus 2004]. Meeting these challenges requires the development of advanced mathematical and computational techniques that bridge the scales from quantum to atomistic and molecular physics. Further, to analyze, design, and optimize actual systems requires accurate and scalable computational modeling of complex coupled continuum multiphysics phenomena. This includes fluid flow, thermal energy and chemical species transport, nonequilibrium bulk and surface phase chemical reactions, solid mechanics, and electrical systems modeling, and perhaps photoexcited states.

Predictive computational simulations will require new developments in mathematics and computational algorithms to accurately and robustly link component simulations at individual physics scales. New methods will be required to determine active scales in the space-time domain that need to be included; the strength of the interscale coupling; the required interscale transfer operators; and the appropriate model for each scale that accurately captures the relevant physical behavior. Appropriate interscale coupling algorithms must be developed that allow error, stability control, and uncertainty quantification (UQ) of data at the interface between component-scale models. Advanced multiscale methods must necessarily integrate these component-scale models and the interscale coupling algorithms, to allow continued uncertainty quantification and sensitivity analysis, and to allow for error estimation and control for the entire multiscale simulation. To enable system-scale simulations, there is a critical need to develop new partial differential equation (PDE) solution methods that are accurate, scalable, and robust for integrating the multiple-timescale behavior of these nonlinear, coupled systems for long-time-transient-behavior and steady-state operation. Finally, with the development of new optimization algorithms, system-scale simulations can be carried out to enable the design and optimization of reliable and efficient low-environmental-impact systems for H_2 production, storage, and use.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

Developing hydrogen production, storage, and use technologies depends critically on science and engineering at scales ranging from the quantum level to the continuum. Performance of these devices requires a detailed understanding of fundamental chemical and physical processes; an understanding of catalytic reaction mechanisms; and the ability to design new materials [Dresselhaus 2004]. Critical examples include developing a fundamental theoretical understanding of the following: how hydrogen reacts with a material surface; ionic transport in membranes and various electrolyte materials; electron conductivity mechanisms in electrode materials; an accurate understanding of electron-transfer processes at interfaces; and the susceptibility of catalytic material to impurities that cause poisoning and fouling [Dresselhaus 2004]. Furthermore, this fundamental atomic-level physics must be represented at the continuum level to provide engineering tools for system design.

One challenge of modeling systems for hydrogen production, storage, and use requires the accurate quantitative treatment of hydrogen chemistry in the condensed phase. Quantum chemistry methods are able to obtain this level of accuracy; however, they are currently limited to a relatively small number of atoms. There are two potential approaches to address this problem. The first is to develop new quantum chemistry methods that have dramatically improved algorithmic scaling. The second is to hybridize high-fidelity quantum chemistry methods with other lower-fidelity quantum models such as density functional theory that use a local-density approximation, to compute locally accurate solutions at significantly reduced cost. Even with these types of approaches, the obtainable scales fall well short of the need to describe the dynamical, finite-temperature response of bulk material. A critical challenge in multiscale modeling is to abstract the crucial chemical phenomena from the electron-based quantum chemistry calculations to inform classical (Newtonian) atomistic simulations through empirical force-field models that accurately capture the quantitative chemistry of the electronic structure simulations. Currently, high-fidelity force-field models, and extensions that are capable of modeling chemical reactivity for hydrogen, are very difficult to construct and often have very limited applicability.

Coupling atomic and continuum scales introduces several additional challenges. First, the concepts of scale separation and interscale communication become intertwined. Expressions are needed that quantitatively pass information between the different types of scales. A significant issue is that fluctuations at the atomic scale can introduce stochastic forcing at the continuum scale, which introduces significant discretization issues. Second, accurate modeling and simulation of physical systems requires multiscale multiphysics capabilities. For example, combining advanced models for thermo-electro-mechanical systems is sufficiently challenging within continuum mechanics. Combining such models with atomic-scale simulations, and developing an interaction framework capable of passing information between scales for multiple types of fields, is very difficult. Third, “smart” algorithms need to be developed for efficient and automated adaptive refinement that not only can control the accuracy of the simulation at a given scale, but also can control the appropriate scale for a given region.

At the system scale, effective and scalable steady-state and long-timescale-transient computational modeling tools for multiphysics continuum mechanics are needed to analyze, design, and optimize hydrogen technology devices. This may include fluid flow, thermal energy

and chemical species transport, nonequilibrium bulk and surface-phase chemical reactions, solid mechanics, electrical systems modeling, and perhaps photoexcited states. These systems are strongly coupled, highly nonlinear, and characterized by multiple physical phenomena that span a very large range of scales of length and time. Some of these problems allow application of the same continuum model at all scales; the primary barrier to simulation is computing resources and appropriate scalable computational simulations methods. In other cases, detailed physics at the atomistic/molecular level must be simulated to resolve the small scales, and the mathematical theory required to couple the effects to the continuum level is not fully developed.

Meeting these multiscale challenges will require the development of advanced mathematical and computational multiscale techniques. In this effort, significant research needs to be undertaken to develop mathematical methods to accurately and efficiently model the propagation of uncertainty in—and estimate the sensitivity of—the solution to data, model, and integration error in these complex multiscale solution methods. In addition, multiscale methods at the system level will require new, accurate, and efficient time-integration methods for coupled deterministic and stochastic component mechanisms with error control and UQ capabilities.

SUMMARY OF RESEARCH DIRECTIONS

The development of technologies for hydrogen production, storage, and use begins at the quantum level. Direct simulation of the Schrödinger equation is computationally intractable. Within the chemistry, solid-state physics, and material communities, there are a number of different approximations to the Schrödinger equation that trade fidelity for computational efficiency. New approaches that hybridize approximations of different fidelity to obtain locally high-fidelity approximations at a reasonable computational cost are needed to compute the fundamental hydrogen chemistry for systems. To bridge quantum to continuum simulations, there is a critical need to abstract detailed chemical phenomena from the electron-based quantum chemistry calculations to be useful in classical (Newtonian) atomistic simulations through empirical force-field models that accurately capture the quantitative chemistry of the electronic structure simulations. Systematic approaches for deriving force-field models are needed, along with analysis tools that can characterize the impact of these types of approximations on the accuracy of classical atomistic simulations.

Combining atomistic computations into continuum models has proceeded along two parallel paths. Some approaches couple atomistic and continuum models within a single simulation, with the goal of using the atomistic simulation in regions where complex physical phenomena are expected, and using the coarse-scale continuum methods to emulate realistic component dimensions and produce high-fidelity boundary conditions for the atomistic regions. Other approaches abstract information gleaned at the atomic scale to construct continuum-scale models of the atomistic behavior. The use of spatial and temporal averaging schemes, and of frequency-dependent expressions, to estimate these models is vital. And validating the robustness of such schemes and expressions is necessary, albeit formidable.

Predictive systems-level simulations of multiphysics systems will need to combine accurate integration methods with adaptive spatial discretizations, and provide uncertainty quantification capabilities, while allowing efficient and reliable estimation and control of spatial and long-time integration error. In addition, techniques that efficiently explore the structure and stability of complex nonlinear solution spaces (e.g., see sidebar on fuel cell simulations) and allow determination of optimal designs must be developed. These modeling requirements are complicated by the need to couple information from the atomistic level into continuum-level simulations. Fluctuations at the atomistic level appear as stochastic forcing terms at the continuum level. New approaches are needed that can provide high-fidelity simulations of stochastic PDEs, as is the development of effective UQ-type methods for combined deterministic and probabilistic approaches for multiscale coupling.

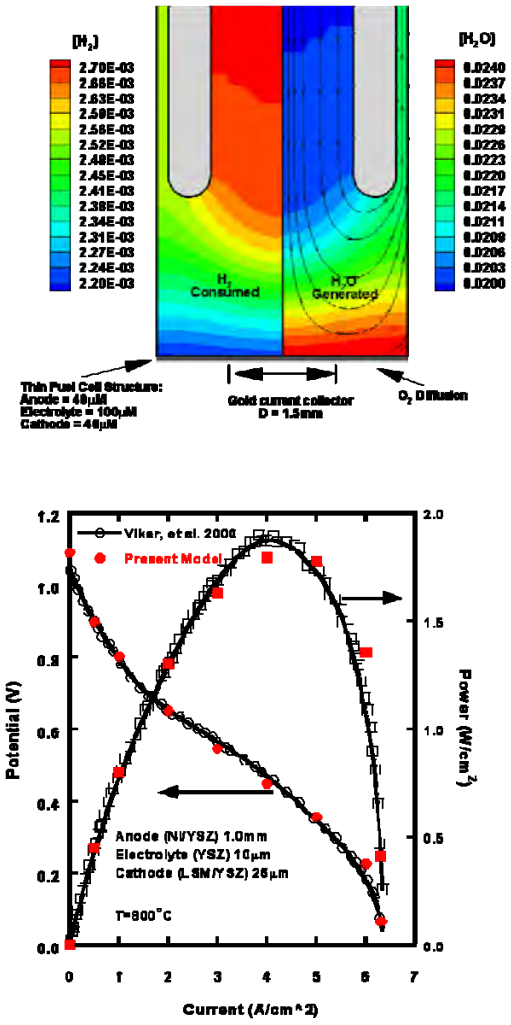

Figure 2: (Top): Hydrogen and water contours for cylindrical concentric tubular solid-oxide fuel cell (SOFC). (Bottom): Comparison of a similar SOFC found in the literature with large-scale parallel simulation code (MPSalsa [Shadid 2006]). (Courtesy of J. Shadid, SNL, and K. Ellwood, Ford Resc.)

COMPUTATIONAL RESEARCH NEEDS

To achieve accurate, stable, efficient, and scalable predictive simulations for the multiple length-scale and timescale physics critical for developing hydrogen technology systems, many advances in numerical methods and computational science are required.

Key areas of research include the need to develop:

- New hybrid approaches for quantum simulation that combine approximations of different fidelity to compute quantum-level chemical information.

- New methods for computing force fields from quantum simulations using mathematical optimization techniques to optimize the empirical parameters that populate the degrees of freedom in defining a force field. Functional forms of the interacting atomic potential functional forms need to be generalized to provide sufficient flexibility to reproduce the desired chemistry/materials science/physics with fidelity.

- New multiscale approaches for transferring information between scales. This information must include specific functional forms for specific physical quantities (e.g., stress, temperature, heat flux, charge, porosity); spatial and temporal averaging schemes; and frequency dependence for dynamic phenomena. These methods must be applicable for analyzing systems in which multiple physical mechanisms are operable.

- Accurate and efficient numerical methods for stochastic partial differential equations that arise from incorporating source terms representing the coupling of atomistic models into continuum systems. Numerical methods for stochastic PDEs have lagged behind developments in deterministic PDEs.

- Stable, accurate, efficient, and scalable temporal integration methods coupled with UQ techniques (deterministic and stochastic) with estimation and control of spatial discretization and long-time integration error for large-scale complex multiple-timescale applications.

- Deterministic UQ tools based on sensitivity and adjoint-based techniques for data, integration, and model error estimation and control. Adjoint methods have been shown to be very promising for estimating and controlling data, model, and long-time integration error. To develop efficient transient adjoint-based techniques, work is required to limit solution storage requirements, memory usage, parallel communication, and cost of the adjoint solve.

- UQ algorithms for probabilistic approaches based on sampling methods (e.g., Monte Carlo), direct methods (e.g., polynomial chaos), and hybrid deterministic/probabilistic approaches.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

The ability to computationally design and optimize the performance of specific materials and entire systems would provide a crucial tool in developing the hydrogen economy. Facilitated by predictive multiscale simulation technologies, the optimal design of high-performance materials and components with stable long-time operating characteristics is possible. These new advanced materials and components, combined with a systems-level computational optimal design capability, can be used to develop highly efficient, stable, and economic hydrogen systems.

TIME FRAME

Time frames are given for developing various algorithms and techniques:

- Multiscale solution algorithms: 5–10 years
- UQ method for combined deterministic and probabilistic methods: 3–5 years
- System-level computational modeling and optimization techniques: 3–5 years
- Improved algorithms for stochastic simulations: 3–6 years.

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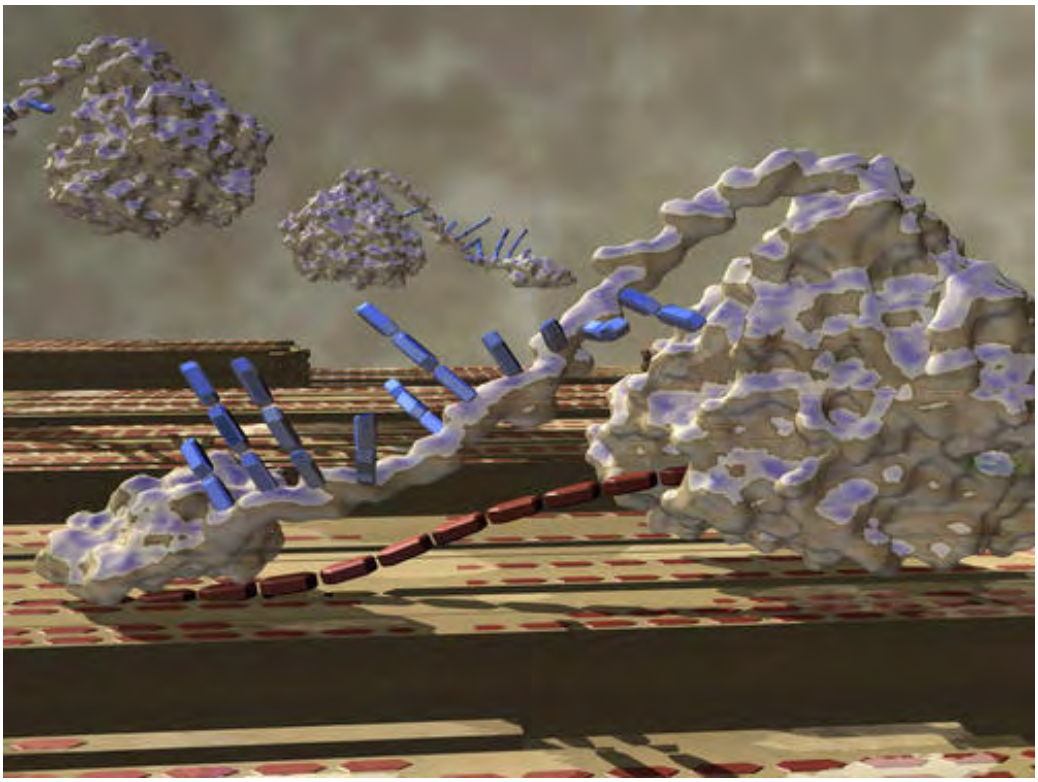
RENEWABLE FUELS — BIOENERGY CONVERSION



Exoglucanases, also known as cellobiohydrolases, are key catalysts in the enzymatic breakdown of cellulose to sugars, perhaps the most critical step in developing the capability to economically produce fuels and chemicals from fibrous biomass as well as sugar or starch.

CHARGE TO PANEL

Alternative and renewable fuels derived from cellulosic biomass offer the potential to reduce our dependence on imported oil, support national economic growth, and mitigate global climate change. However, breakthrough technologies are still needed to overcome the barriers to developing and commercializing these fuels.

Key barriers are the high cost of the cellulose enzymes that convert crystalline cellulose to fermentable sugars and the development of microbial biocatalysts for rapid, efficient fermentation of the mixed sugars in cellulosic hydrolysate streams. Realizing the potential of cellulosic biofuels can be expedited by applying a new generation of biological research and genomic tools. This breakout session will focus on computational research needs that can accelerate the development of cost-effective processes for converting cellulose to fuels.

The charge to the members of the Bioenergy breakout session was to identify priority research directions in this area related to:

1. Dynamic simulation of cellulose depolymerization and hydrolysis
2. Accelerated annotation of microbial genomes and metagenomic libraries
3. In-silico modeling and simulation of complex metabolic networks.

SESSION BREAKOUT LEADERS

Michael Crowley, National Renewable Energy Laboratory
Brian Davison, Oak Ridge National Laboratory
Mike Himmel, National Renewable Energy Laboratory
Costas Maranas, Pennsylvania State University
Leonardo Marino-Ramirez, National Institute of Health
Mark Nimlos, National Renewable Energy Laboratory
Steve Picataggio, Synthetic Genomics, Inc.
Jennie Reed, University of Wisconsin

BACKGROUND AND MOTIVATION

Alternative and renewable fuels derived from lignocellulosic 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 [Foust et al. 2007]. These barriers include the high cost of pretreatment processes, enzymes, and microbial biocatalysts for biochemical conversion processes and selectivity, and the formation of undesirable products from thermochemical processes.

Grow Your Fuel

Significant increases in the efficiency of extracting chemical energy from biomass creates the potential for 20%–40% of domestic fuel use to come from 10% of available crop land devoted to growing high-yield crops such as switchgrass. Realizing this potential will require significant advances in deconstructing complex biomass feedstocks to improve the cost of production of ethanol and other biofuels.

Lignocellulosic biomass is highly recalcitrant to most of the physical, chemical, and biochemical treatments currently used to liberate sugars. Plants naturally possess many structures that resist these treatments [Himmel et al. 2007]. For example, the outer layer of the epidermis in grasses contains dense collections of thick-walled cells protected by waxy or oily materials. In trees, the bark poses a formidable physical and chemical barrier to all but the harshest treatments. The cell wall contains highly ordered, water-excluding microfibrils of crystalline cellulose that pose a significant barrier to enzymatic hydrolysis. The cellulose microfibrils themselves are surrounded by layers of hemicellulose that are covalently linked to heterogeneous aromatic lignins [Ding and Himmel 2006]. This complex matrix of heteropolmers is the main reason why plant biomass has resisted low-cost chemical and enzymatic treatments. Cellulases are now used to hydrolyze the polysaccharides in the plant cell wall to fermentable monosaccharides. However, the high loadings of expensive cellulases that are currently needed to achieve the necessary hydrolysis yields are 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/relationships governing the activity of soluble enzymes on insoluble polymeric substrates is essential to break this bottleneck [Himmel et al. 2007].

BIOCHEMICAL TECHNOLOGIES

Economical biochemical conversion of lignocellulosic biomass to fuels requires harsh pretreatment steps to liberate the hexose and pentose sugars from the complex polysaccharide matrix before they can be fermented by microbial biocatalysts. Furthermore, these pretreatment steps also generate substantial amounts of acetate and other compounds that inhibit the subsequent fermentation process. The feedstock represents the largest component of the operational cost for producing biomass-derived liquid fuels; so, maximizing the yield of

fermentable sugars from these feedstocks is essential for a commercially feasible process [Perlack et al. 2005].

Cellulosic Ethanol

Cellulosic ethanol can be produced using biochemical and thermochemical technologies. With biochemical approaches, the polysaccharides in plants are deconstructed into constituent sugars, which are then fermented into ethanol. The thermochemical approach involves gasification of biomass into synthesis gas and thermocatalytic conversion of the gas to ethanol. Recent cost estimates of these processes conducted at the National Renewable Energy Laboratory suggest that, with existing technology, a gallon of ethanol can be produced for **$2.24** using the biochemical approach and **$2.08** using the thermochemical approach. Technology improvements are needed to reduce these costs to $1.31 per gallon to make cellulosic ethanol economically sustainable.

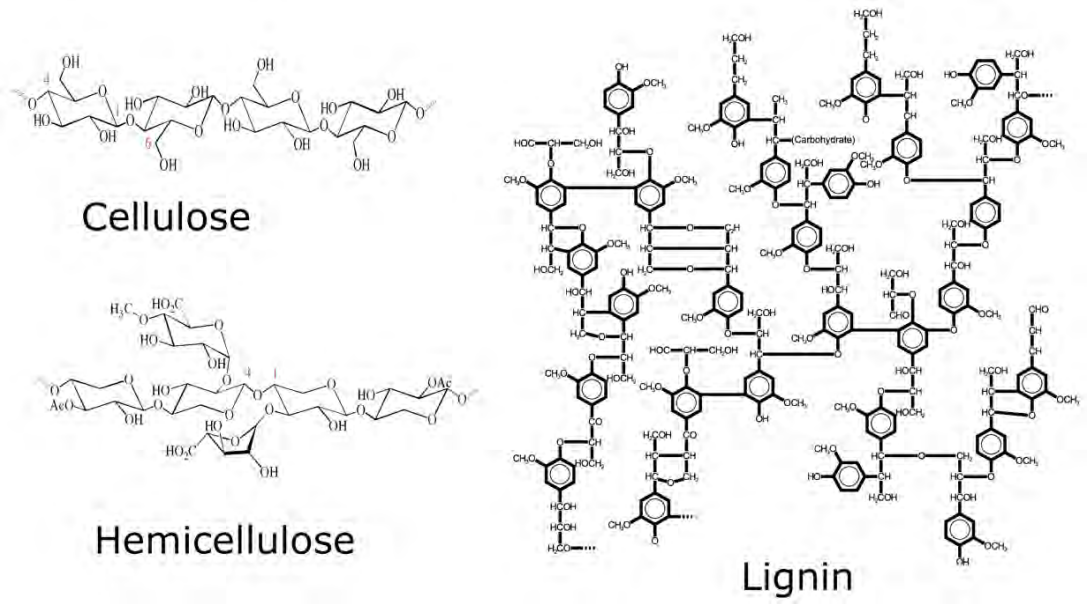
THERMOCHEMICAL TECHNOLOGIES

The economics of thermochemical technologies are largely determined by the production of unwanted chemical by-products, often in trace quantities. With gasification technologies, these by-products include recalcitrant tars (largely aromatic compounds), methane, sulfur compounds, and trace metals. These species deactivate fuel-synthesis catalysts, and their formation requires costly conditioning steps. Pyrolysis is capable of producing an inexpensive liquid that can potentially be used by existing petroleum refineries. However, the acidity and instability of these liquids make them unacceptable. Both of these technologies have been studied extensively using engineering and empirical approaches. Reduction of the by-products will require a more fundamental understanding of the chemistry of the thermal decomposition of biomass.

COMMON THEMES

The biomass conversion problem has been intractable and faces challenges not represented in other bioresearch efforts. The scale of the problem is much larger than most others (acres, gallons) and must tackle issues of biomass complexity and heterogeneity with a rudimentary understanding of fundamental details. Computation uniquely provides a multiscale framework of understanding to guide and interpret experimentation on complex biological systems [Baker 2004]. The complexity of bioenergy systems exceeds the complexity of current computational modeling, and experimental data capacity is already exceeding our ability to handle it effectively. We will rapidly need new systems of multiple models to deal with multiscales and multiphysics and smart agents for systems assembly and auto-query; data-intensive computing with the ability to handle massive and disparate data sets, error, uncertain or missing data, and noise; new theories and algorithms for interfaces; information-extraction algorithms; interfaces between models and data; efficient inference techniques for dynamic systems; self-updating

Plant Structure



Biomass is made up of roughly 38%–50% cellulose, 23%–32% hemicellulose, and 15%–25% lignin.

systems; network inferences that simplify the burden of analysis, similar to visualization, image analysis, and pattern recognition problems; and high-performance computing (HPC) hardware and software, including the migration and scaling of existing tools and the development of alternative algorithms more amenable to massively parallel computing and molecular dynamics (MD) for modeling at biological times and scales, and studying rare events.

The priority research directions identified in the Biomass Conversion Breakout Session, each summarized below, include:

- Understanding lignocellulosic biomass depolymerization and hydrolysis
- Chemical energy extraction from heterogeneous biomass.

UNDERSTANDING LIGNOCELLULOSIC BIOMASS DEPOLYMERIZATION, HYDROLYSIS, AND CONVERSION

ABSTRACT

Alternative and renewable fuels derived from lignocellulosic biomass offer the potential to reduce our dependence on imported oil, support national economic growth, and mitigate global climate change [Kamm et al. 2006]. However, technological breakthroughs are needed to overcome key barriers to the development and commercialization of these fuels [Aden et al. 2002]. These barriers include pretreatment processes that improve the yield of fermentable sugars while minimizing the formation and release of toxic by-products; the high cost of the enzymes that hydrolyze crystalline cellulose; and microbial biocatalysts that enable rapid and efficient fermentation of the mixed sugars in hydrolysate streams [McMillan 1992; Wyman et al. 2005]. Overcoming these barriers on a commercial scale will require the development of high-energy-content feedstocks and microbial processes that deconstruct complex biomass feedstocks and then ferment the derived sugars to ethanol or other some other biofuel. Computational science can provide the depth of understanding required to enable lignocellulose biorefineries by providing knowledge-based solutions to key processing challenges. Specific computational science needs include the development and improvement of force-field parameterization of polymers and matrices found in plant cell walls; scalable and efficient algorithms and dynamic simulation tools; models for transport and diffusion of enzymes acting on insoluble substrate surfaces; mesoscale codes applicable to complex cell wall deconstruction models; and analytical tools for interface to experimental data.

EXECUTIVE SUMMARY

Biomass sugars are locked in a complex composite of polymers exquisitely recalcitrant to biological and chemical degradation. A key barrier to the emerging biofuels industry is to understand how the complex chemical and physical structure of the plant cell wall can be deconstructed and converted to fermentable sugars by thermochemical and enzymatic pretreatments. Developing a fundamental understanding of the architecture of plant cell walls at the cellular, molecular, and atomistic scales is essential to accelerate improvements in the chemical and biological conversion processes. A systematic understanding of enzyme interactions with the plant cell wall architecture may allow us to predict plant-tissue response to hydrolytic attack as a first step to improving the specific activity of hydrolytic enzymes. Computational strategies will be key to acquiring new levels of understanding of cell wall conversion science. These strategies will enable us to build and validate simulation models of biomass, from cellulose to cell walls; to develop spatial/temporal models for the dilute acid and alkaline pretreatment processes; to develop a detailed understanding of the biomass hydrolysis process, focusing on enzymes, substrates, cell walls, cells, and plants using quantum mechanics (QM) [Gao 1995], molecular mechanics (MM)[Leach 2001], combined QM and MM (QM/MM) and mesoscale modeling; and to describe the role water plays in cell wall hydrolysis reactions. Indeed, this new computational science can direct improvements in biomass conversion-to-sugars processing steps necessary to achieve the near-term (2012), mid-term (2017), and long-term (2030) objectives of DOE.

SUMMARY OF RESEARCH DIRECTION

Understanding energy plant cell wall structure

Research is needed to increase our understanding of the fundamental principles regarding the synthesis, structure, and function of the plant cell wall at the level of the elementary microfibrils. Developing a fundamental understanding of the architecture of plant cell walls at the cellular, molecular, and atomistic scales is essential to accelerate improvements in the biological conversion processes.

Understanding depolymerization and hydrolysis of plant cell walls

To reduce the costs of this process, research is needed to increase our understanding of the factors governing the rates of cellulose hydrolysis. Furthermore, a systematic understanding of enzyme interactions with the plant cell wall architecture may allow us to predict plant-tissue response to hydrolytic attack as a first step to improving the specific activity of hydrolytic enzymes. This knowledge will also aid us in reducing the loadings of enzymatic catalysts.

Understanding and engineering biological systems for biomass conversion

Work is needed to improve the efficiency and capabilities of microbial strains used for production of fuels from biomass sugars. Whereas the central metabolic pathways that produce biofuels are well known, we now recognize the need to understand and engineer complex metabolic networks and regulatory structures to optimize biomass conversion to biofuels.

SCIENTIFIC CHALLENGES

A key challenge to the emerging biofuels industry is to understand how the complex chemical and physical structure of the plant cell wall is synthesized, can be deconstructed, and can ultimately be converted to fermentable sugars by thermochemical and enzymatic treatments. The technology challenges for development of efficient biological lignocellulose conversion processes are outlined below.

Understanding energy plant cell wall structure

Economical conversion of lignocellulosic biomass to fuels requires harsh pretreatment steps to liberate the hexose and pentose sugars from the complex polysaccharide matrix before they can be fermented by microbial biocatalysts. Furthermore, these pretreatment steps also generate substantial amounts of acetate and other compounds that inhibit the subsequent fermentation process. The feedstock represents the largest component of the operational cost for producing biomass-derived liquid fuels, so maximizing the yield of fermentable sugars from these feedstocks is essential for a commercially feasible process. However, lignocellulosic biomass is highly recalcitrant to most current industrial treatments. Developing an understanding of the mature cell wall requires that we first understand its synthesis, an approach that could also contribute to the design of species that would be more conducive to industrial degradation processes [Somerville et al. 2004].

Understanding depolymerization and hydrolysis of plant cell walls

Commercial glycosyl hydrolases are now used to hydrolyze the polysaccharides in the plant cell wall to fermentable monosaccharides. However, the high loadings of expensive cellulases that are currently needed to achieve the necessary hydrolysis yields are cost-prohibitive. Despite many attempts, the specific activity of cellulases has not been improved after more than 30 years of research. A better understanding of the structure/function relationships governing the activity of soluble enzymes on insoluble polymeric substrates is essential to break this bottleneck. Work at NREL, ORNL, and other institutions funded by the DOE Biomass Program and the DOE Biological and Environmental Research Program, in collaboration with the DOE Advanced Scientific Computing Research Program, is leading the way with currently funded projects aimed at gaining such understanding of cellulase function on plant cellulose and microfibrils. However, an equivalent level of understanding is required for noncellulases acting on plant cell walls and microfibrils, including hemicellulases, pectinases, and lignin-carbohydrate esterases.

Understanding and engineering biological systems for biomass conversion

We have a critical need to characterize microbial and plant systems at the molecular and biochemical level to ultimately understand and engineer organisms for an efficient conversion of biomass to bioenergy. New and emerging technologies in systems and synthetic biology permit the integration of biological datasets that capture information at the genomic, proteomic, transcriptomic, and metabolomic levels. These technologies use computational approaches to address issues such as growing complexity, dynamics, heterogeneity, and noise in the data. Optimization of high-performance computer hardware and software is needed to cope with the explosion of genomic data. The potential impact on bioenergy conversion is the possibility to pioneer new technologies for biomass conversion into biofuels by providing deep insights into the metabolic capabilities of diverse organisms involved in lignocellulosic degradation in a variety of environments.

We need to establish first principles for designing algorithms to investigate metagenomic and genomic data for finding new genes and pathways needed for biomass conversion. First, we need to establish systematic approaches to understand, at the molecular and biochemical level, microbe-mediated plant cell wall deconstruction in a wide variety of environments, including an extensive taxonomic representation of microbes involved in the process. Second, there is a need to extract design principles from natural systems valuable for optimization of biomass conversion. This research goal will allow the identification of mechanisms for the rational design of enzymes, metabolic pathways, and gene regulatory networks to obtain desired phenotypes in natural or synthetic organisms. Third, we must improve the tolerance of bioconversion processes to inhibitory substances generated during biomass pretreatment.

Metagenomic computational research goals include developing efficient genome assembly algorithms for new sequencing technologies (comparative sequence assembly techniques are especially valuable); methods for post-processing metagenome assemblies, including binning methods to discriminate between species; and computational methods for accurate phylogenetic description and taxonomic assignments of complex communities.

NEEDS FROM COMPUTATIONAL SCIENCE

Modeling the cell wall

Computational science can provide the depth of understanding required to enable lignocellulose biorefineries by providing knowledge-based solutions to key processing challenges. The problem of understanding the structure of the cell wall is huge and intractable when it is treated as a monolithic problem, and there are no modeling tools available at present to do this. Even subsets of the problem, such as the structures of the true cellulose microfibril, hemicellulose, and lignin complexes, are currently outside the reach of molecular modeling techniques. These simulations, however, will be treatable in the near future as mesoscale modeling techniques, programs, and parameterizations are being created. Nevertheless, a large contribution can be made to the understanding of biomass hydrolysis to usable sugars with current and emerging techniques and software applied to small- and moderate-sized systems. The computational limitations of these studies are due largely to a lack of resources and (somewhat) to a lack of methods. The time-to-solution of these mid-range problems is severely hampered by insufficient resources dedicated to them, even though more scientific productivity, publications, and scientific insight results from these studies.

Modeling cell wall-degrading enzymes

Specific computational science needs for enzymatic cell wall deconstruction include atomistic models with hundreds of thousands to millions of atoms and long reaction times and models for transport and diffusion of enzymes acting on insoluble substrate surfaces. These tools will enable us to develop a detailed understanding of the biomass hydrolysis process, focusing on enzymes and cell walls using QM/MM and mesoscale modeling and describe the role water plays in cell wall hydrolysis reactions. Computational modeling of the plant cell wall (see Figure 1) will also aid our understanding of the obstacles that its structure and chemistry present to cell wall polymer-degrading enzymes and microorganisms.

Modeling metabolic pathways

Computational approaches will be needed for the automated generation, curation, archiving, and prototyping of metabolic models for microorganisms and plants with relevance to biomass conversion. The elucidation of regulatory information (transcriptional, allosteric, and beyond) and incorporation in metabolic models will be required to improve their predictive capabilities. Additional enhancements include modeling of non-steady-state behavior of metabolic models by incorporating kinetic information whenever available and the incorporation of cellular structure topology information. Testing and improvement of metabolic model predictions will depend on the use of flux measurements using labeled isotopes (MFA) requiring the development of computational approaches to support flux elucidation and experimental design for large-scale metabolic models. Given this modeling infrastructure, reliable algorithms will need to be developed to identify engineering strategies that lead to the targeted biomass conversion target. Approaches must be responsive to the inhibitory effect of the by-products of biomass pretreatment to the subsequent enzymatic conversion processes and potential toxicity of biofuels to microbial production systems. Approaches will be needed for pinpointing patterns/signatures in omics data that give rise to desired phenotypes. Computational approaches will be needed not

only for constructing complex biological models, but also for driving the design of future experiments so as to maximize their information content and relevance to biofuels production.

COMMON THEMES

The biomass conversion problem has been intractable and faces challenges not represented in other bioresearch efforts. The scale of the problem is much larger than most others and must address issues of biomass complexity and heterogeneity with a rudimentary understanding of fundamental details. Significant computational challenges are expected to arise from this lack of molecular structural detail in regard to the plant cell wall as well as the enzyme action site. For metabolic modeling, the anticipated metabolic model size (thousands of reactions in multiple compartments) and combinatorial nature of procedures are aimed at correcting inconsistencies with experimental data (e.g., gene essentiality experiments and flux measurements) and strain optimization. Non-steady-state descriptions and spatial dimensions will further compound the combinatorial challenge, requiring multiscale distributed mathematical descriptions and customized-solution procedures. To this end, leveraging high-performance computations will become a priority.

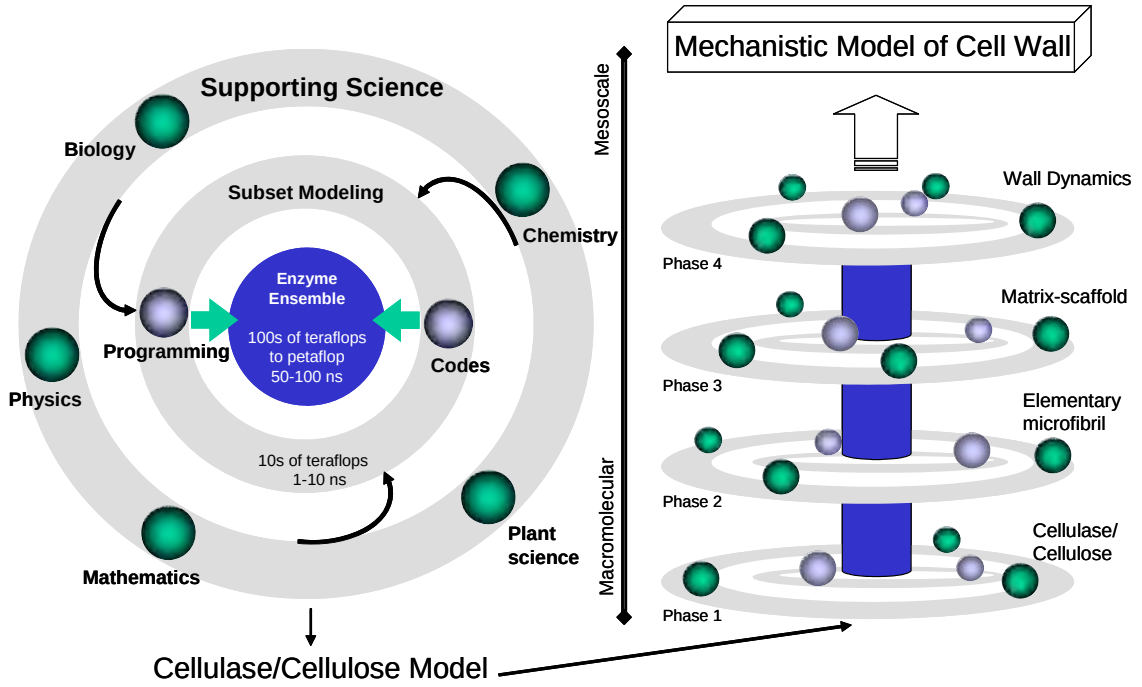


Figure 1: Depiction of a multiscale approach to modeling the plant cell wall, where the problem is parsed in subsets solvable in the near term, followed by combinations of subsets into ensemble problems studied as advanced codes and computers become available.

Specific computational science needs include the development and improvement of force-field parameterization of polymers and matrices found in plant cell walls; atomistic models with hundreds of thousands to millions of atoms and long reaction times; scalable and efficient algorithms and dynamic simulation tools; models for transport and diffusion of enzymes acting

on insoluble substrate surfaces; mesoscale codes applicable to complex cell wall synthesis and deconstruction models; and analytical tools for interface to experimental data. Currently, most large computational facilities favor large-scale computational tasks of the few users and projects that utilize large portions of high-performance computers, on the order of thousands to hundred of thousands of processors, and do not provide for the multitude of users who need long simulations of smaller systems that use smaller fractions of the machines. The need is for some method of reallocating the existing resources, or to make available computer resources that will supply the demand for high-performance computing at the hundreds-of-processors level and serve many users.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

In December 2005, the DOE Biological and Environmental Research within the DOE Office of Science and the DOE Biomass Program within the DOE Office of Energy Efficiency and Renewable Energy jointly sponsored a Biomass-to-Biofuels Workshop in which more than 50 scientists convened to define the barriers and challenges to the emerging biofuels industry. The workshop produced a roadmap to help make biofuels cost-competitive by 2012, with the potential to displace up to 30% of the nation's current gasoline use by 2030 using a systems biology approach exploiting a new generation of biological and genomic research tools to expedite the development and implementation of the required technological breakthroughs. It has since become apparent that successful implementation and execution of this systems approach requires the concurrent development and application of advanced scientific computing capabilities. Realizing the potential of lignocellulosic biofuels now requires the application of a new generation of biological research and genomic tools. The Biomass Conversion breakout session of this workshop addressed the computational research needed to accelerate the development of cost-effective processes for the conversion of lignocellulose to fuels.

TIME FRAME

One to 20 years.

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EXTRACTION OF CHEMICAL ENERGY FROM BIOMASS

ABSTRACT

Overcoming key barriers to the effective extraction of chemical energy from biomass requires a more thorough understanding of the chemistry and transport of important chemical and thermochemical processes. Computational science support is needed to provide scalable, integrated, multiscale modeling tools for application, data management, and visualization; predictive tools for biomaterial properties, including kinetics, thermodynamics, and physical properties; data management across scales with a user-friendly interface; and uncertainty quantification. These tools will enable the prediction of chemical kinetics, thermodynamics, and physical parameters, such as heat and mass transfer coefficients; build chemical kinetics model networks; and formulate multiphase models to describe transport and chemistry from the complex structure of plant cell walls to device scale.

Chemical Extraction Technologies

Pretreatment involves the deconstruction of biomass in aqueous solution in order to hydrolyze hemicelluloses and make the cellulose more accessible to enzymatic hydrolysis. The sugars liberated from this process can be used as a fermentation feedstock to make fuels and chemicals. The temperature for this process is usually between 100° and 250°C and often includes the addition of base, acid, or other catalysts.

Pyrolysis is conducted without added water or air and uses temperatures up to 600°C. Light gases and oils are produced, which can be used as fuels or feedstocks for further processing.

Gasification is conducted at high temperatures (up to 900°C) and produces primarily syngas (a mixture of CO, CO_2, and H_2). Syngas is a source of hydrogen, or it can be used as a feedstock for catalytic production of liquid transportation fuel.

EXECUTIVE SUMMARY

Extraction of the chemical energy available in biomass using thermal technologies presents unique and important challenges for the development of a sustainable supply of energy. This is owing to the chemical composition of biomass and the complex structures found in plant material. Because it is composed largely of polysaccharides, thermal deconstruction and decomposition of biomass will likely require different approaches than have traditionally been used for coal or oil. To fully understand chemical and thermal treatment of plant matter, it is necessary to characterize the chemical reactions of the biopolymers that occur among heat and mass flow restrictions resulting from complex structures that exist at multiple spatial scales. In addition, the processes occurring at these different scales will have widely different time constants and will require different physical treatment. Thus, understanding biomass treatment becomes a multiscale/multiphysics problem.

Thermal treatment technologies can be classified by three categories based on an increasing level of severity: (1) pretreatment, (2) pyrolysis, and (3) gasification. For all of these approaches, the chemical and structural complexity of biomass presents difficult challenges that could be directly addressed using computational modeling.

SUMMARY OF RESEARCH DIRECTION

Pretreatment

To reduce the costs of this process, research is being conducted to increase the rates of hemicellulose hydrolysis while reducing the rates of sugar loss. Work is also being conducted to determine how pretreatment conditions improve the digestibility of the resulting material.

Pyrolysis

Work is under way to reduce the formation of aldehydes, ketones, and acids. These species contribute to the acidity and instability of the oils. It is also important to maintain low viscosity by reducing polymerization.

Gasification

Gasification research is being conducted to maintain a high efficiency while reducing the formation of tars, methane, sulfur compounds, and metals.

SCIENTIFIC CHALLENGES

Although the technologies for extraction of chemical energy appear diverse, the three technology areas listed above face many common technical challenges. These challenges center largely on the complex chemical composition and reactivity of biomass and its structure. To make significant progress, detailed fundamental understandings are needed. These are outlined below.

Chemistry

The mechanisms of thermal decomposition of polysaccharides in plant cell walls are at best superficially understood, and much work is needed to describe the chemical processes occurring in pretreatment, pyrolysis, and gasification. Typically, these materials deconstruct to form anhydrous sugars and oligomers. For example, cellulose is the most abundant material in plant matter; during gasification and pyrolysis, it is likely that a significant amount of cellulose forms levoglucosan [Shafizadeh 1982]. However, the mechanisms and kinetics of levoglucosan formation and destruction are not clearly established. Furthermore, the yield of levoglucosan is highly influenced by the presence of alkali metal compounds that exist in biomass [Shafizadeh and Lai 1972; Evans and Milne 1987]. Establishing the chemical mechanisms and kinetics of the decomposition of polysaccharides such as cellulose is critical in devising strategies to control the production of unwanted by-products. For pyrolysis, we would like to optimize the formation of anhydrosugars and oligosaccharides, while minimizing the decomposition to smaller products. For gasification, the decomposition of these compounds to syngas, as opposed to aromatic

compounds, is critical. Because of the complexity of pyrolysis and gasification, studying the chemistry of these processes has been difficult. Computational modeling that characterizes the chemical kinetics of thermal degradation in the presence of heat and mass-transport phenomena is essential to understanding thermal conversion and improving performance.

The chemistry of biomass pretreatment is better understood, but it is not fully characterized. It is important to determine the kinetics of oligomer hydrolysis and monomer dehydration. The kinetics of these reactions will help determine optimal operating conditions. In addition, the kinetics hydrolysis of other linkages in hemicellulose and the reactions of lignin are important. The rate of hydrolysis of acetate groups on the sugars is important because the released acetic acid is a toxin for many fermentation organisms. The hydrolysis of hemicellulose linkages to lignin carbohydrate complexes (LLCs, i.e., ferulic acid) is also critical, as are the chemical reactions of other biological compounds such as proteins and lipids. The mechanisms and kinetics of these competing reactions are often difficult to determine experimentally, and there is a need for computational modeling to address these issues.

Mesoscale methods

The basic mesoscale building block involved in the chemical extraction from heterogeneous biomass is an interface depicted in Figure 2. This prototype problem is a multiscale, multiphysics problem involving four distinct physical processes: fluid motion (F), reactant species transport (T), fluid-wall interaction (W), and wall chemical reactions (C). Each process involves characteristic time and length scales that evolve with local thermodynamic and chemical conditions. Generally speaking, processes F and T can be considered to be macroscopic, W is intermediate, and C has microscopic character and chemical-reaction-dependent timescales. The relevant F timescales are the advective and momentum-diffusion times, whereas the T timescale is related to mass-diffusion time of the species. The W process and, especially, the C process, are at the time step of chemical wall transfer and chemical reaction on the substrate, which are several orders of magnitude smaller than the former two. The methods that can be used to model this system are the mesoscale Lattice Boltzmann Method (LBM), which is suitable for modeling multiphase reacting flows with low Mach numbers, and the microscale Kinetic Monte Carlo (KMC) for modeling of chemical reactions on the catalytic surfaces along with a suitable method to couple these methods. The reaction barriers for the KMC can come from density functional theory or other electronic structure calculations.

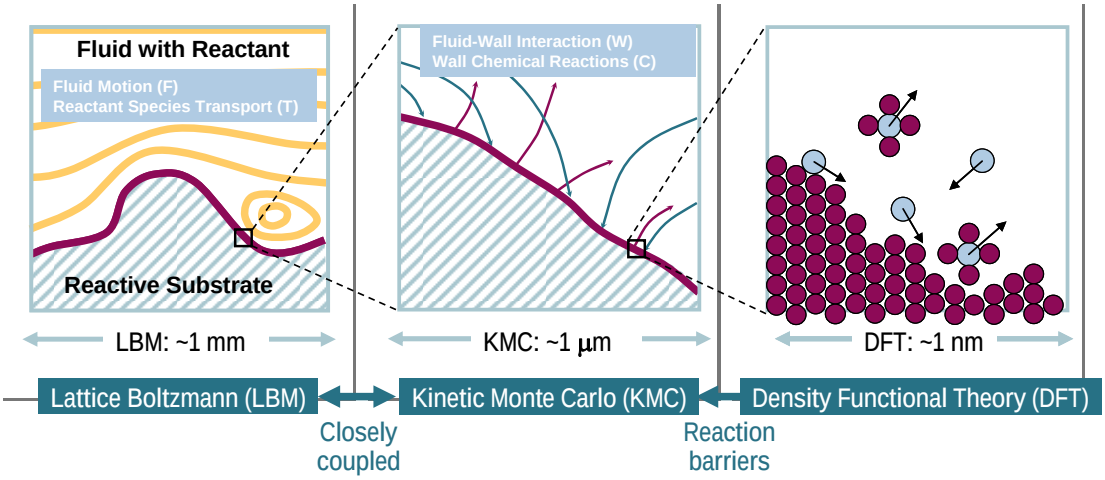

Figure 2: Illustration of the combined multiscale Lattice Boltzmann Method (LBM)/Kinetic Monte Carlo (KMC) scheme. In the LBM regime, the system length scale is ~1 mm, and the description is in terms of hydrodynamic fluid flows (gold lines). In the KMC regime, the scale of the cell is ~1 μm, and the description is in terms of fluxes of reactants (blue arrows) and reaction products (beige arrows) determined by the diffusion, advection, and chemical reactivity rates [Succi *et al.* 2001].

NEEDS FROM COMPUTATIONAL SCIENCE

Quantum mechanical modeling of large molecules

It is clear that this research effort needs to span the interfacial regime from solid surfaces to complex, solution-phase chemistry and cover a range of time and length scales. Thus, one important focus of the overall computational science effort must be an understanding of the linkages between different temporal and spatial scales. No matter how many details of the physics are included in the reactive-mass-transport models, if the critical underlying physical, chemical, and biological data are missing or unreliable, the accurate predictive capability of such models will be lessened. Computational molecular science can provide the thermodynamic, kinetic, and structural properties data needed for the models, and can provide data that are difficult, or at times even impossible, to obtain in the laboratory or in the field because of the cost of the experiment. In addition, computational molecular science allows the complex systems to be decomposed into the individual contributing reactions and allows for accurate information to be generated regarding the feasible reaction paths.

The calculation of interactions of chemicals, including those containing biological living species, is incredibly complex and will require sustained petaflops to begin to reliably predict the molecular interactions of chemicals with environmental systems and to provide the underlying data needed for transport models. High-quality data are needed—often within 1 kcal mol^{-1}—and great care must be taken to minimize the errors in the calculated underlying data used in a sophisticated environmental or chemical process model so that errors in the data do not accumulate, propagate, and ultimately invalidate the macroscopic-scale model. There is a time criticality in the need for the data that a computational molecular science effort will provide. Computational molecular science can also be used to aid in the design of new processes, for example, the design of new compounds for efficient breakdown of cellulose with minimized formation of undesirable by-products. Here, computational molecular science not only provides

needed data, but can also be used to provide new insights and answer "what if" questions raised by scientists and engineers. Improving the response time to answer such questions will dramatically shorten the design and development time for new experimental strategies. In summary, theory can, at enormous but feasible computational expense, reliably and safely predict the chemical and physical properties of biomass-related substances, often more cost-effectively than performing an experiment.

Several clear software and method development needs must be met to have the desired impact on solving DOE's and the nation's energy problems:

- Improved methods for the inclusion of environmental effects such as solvents in electronic structure calculations
- Much improved quantum mechanic/molecular mechanics integration, methodology, and usability to enable the examination of reactions in large, complex systems and environments
- Faster MP2, CCSD(T), and CCSDT methods with improved scaling (better than current N^5 to N^7 methods), including 1st and 2nd derivatives for large molecules/basis sets to allow for the efficient computation of energy transfer
- Improvements in density functional theory, especially to the exchange/correlation functionals
- Efficient methods for the optimization of large molecules with floppy modes with electronic structure methods (e.g., small proteins and sugar complexes)
- Efficient statistical sampling methods to determine reaction barriers in complex environments
- Improved molecular dynamics timescale methods to examine processes involving short and long time processes
- Correlated spectroscopic properties including IR, UV-vis, and NMR to easily compare with experimental information
- Improvements to combined molecular dynamics and electronic structure calculations (Car-Parinello approaches)
- Improved methods for treating chemical kinetics for complex reactions with high accuracy and lower computational cost.

Each of these theoretical/model developments will require significant algorithmic work to be performed efficiently on petascale computers. This level of scalability will be required for the very large computations needed to solve the energy transfer of biomass. Each of these algorithms is built on a cache-blocked architecture; therefore, cache latency, bandwidth, and size are important to performance and scalability. Also key to performance is the ability to interweave computation, communication, and input/output (I/O) operations (e.g., use of asynchronous I/O, use of nonblocking communication operations). These algorithms will also need to be cognizant of the underlying architecture of the machine. For example, replicating some of the data may provide more scalability than fully distributing the data. Also, different parts of the computation may need to be delegated to subgroups of processors and then brought back together to proceed to the next step. The communication software must be able to handle these situations in an efficient and flexible manner that is easy for the software developer to use.

The complexity of the algorithms and the software will require a much-improved level of usability to allow researchers to actually perform the required simulations. This will require improved data management, input development, and output visualization methods.

Multiphysics/multiscale coupling

Coupled processes involving various multicomponent interactions are common in chemical energy extraction processes; this is especially true with heterogeneous biomass as a source. These interactions typically exhibit an unusual degree of complexity across a large range of spatial and temporal scales. Not only do we have to deal with orders of magnitudes in differences in time and length scales, we also have to deal with different governing equations and/or constitutive relationships for the same process at different scales. Addressing all these complexities calls for novel multiscale computational frameworks and architectures that can consistently feed relevant information across scales (both upscaling and downscaling) to simulate coupled process dynamics efficiently. This requires the development of multiscale and multiphysics mathematics to address needs in various disciplines, including building a general multiphysics framework for energy processes involving chemical reactions [Frantziskonis et al. 2006] and that eventually integrates various multiphysics simulations as shown in Figure 3. This development and new algorithms for petascale and exascale applications would give us tremendous capability to integrate coupled simulation components at scale. These algorithmic developments, along with accelerated hardware acquisition for

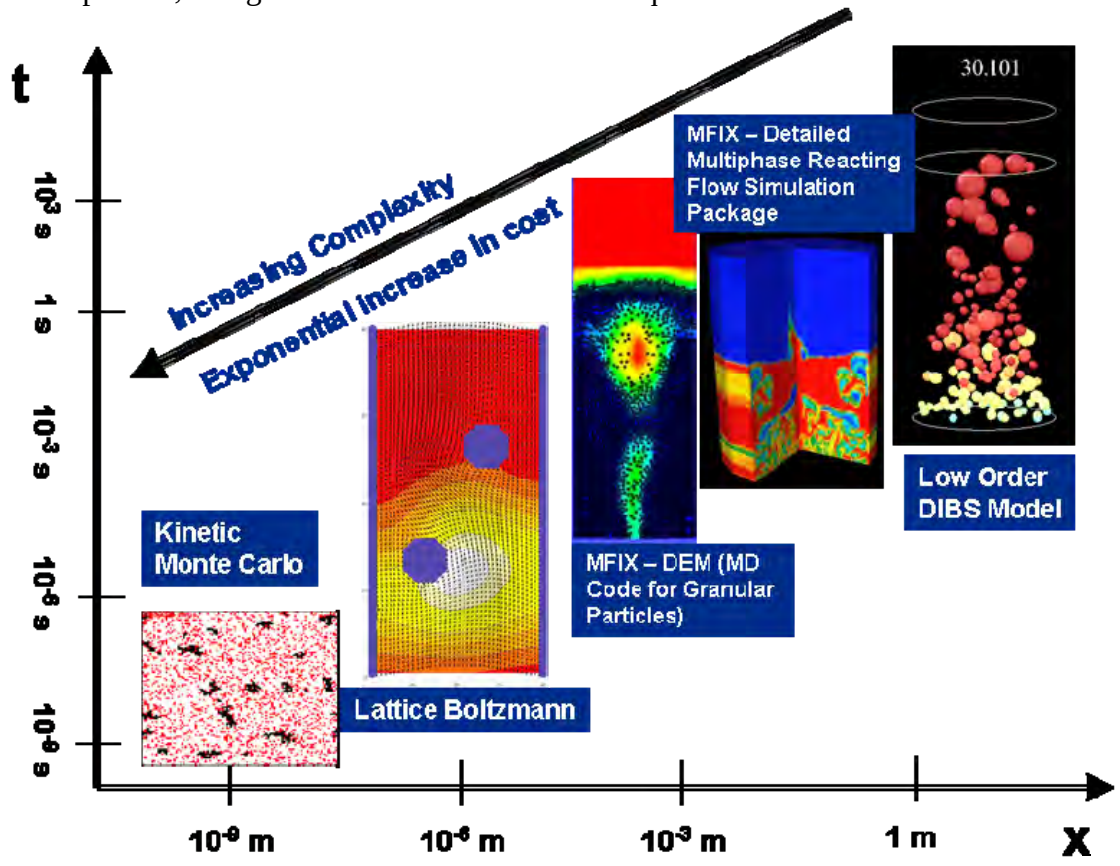

Figure 3: Multiphysics heterogeneous chemically reacting flows for energy systems

petascale/exascale computing in the next decade, would give unprecedented tools to engineers to revolutionize the design of chemical extraction processes.

Related to the needs of developing the above models, it is critical that the data and knowledge from one scale are made easily and readily available to other scales. For example, accurate and reliable thermodynamic and reaction rate information from the molecular scale is necessary to drive the mechanism generation and reduction. Detailed information from the mechanism generation will drive development of accurate molecular scale models and the associated computations with those models. Even at a given scale, significant informatics challenges exist. For example novel mechanism-reduction algorithms need extensive mechanism information that must be clearly annotated with many details such as reproducibility, reliability, and error information. The complexity of the data that will be generated in heterogeneous biomass must be transformed into a knowledge base that will be essential in understanding the chemical energy that can be extracted from the varying processes.

To enable this exchange of information and knowledge, the chemical community will need advanced collaboration and metadata-based data management technologies to develop a multiscale informatics toolkit that enables cross-scale data discovery, viewing, comparison, transformation, and exchange while facilitating community formation, communication, and data development. This toolkit must also include tools for browsing cross-scale data dependencies and mechanisms to integrate custom and community resources into active research projects. The data must be distributed across many sites (federated databases) because many of the individual research groups will want to maintain their own data.

This effort must be more than just data management. While fully accessible and searchable metadata including pedigree and ontologies will be essential to the success of this effort, tools must be developed that will transform that information into useful knowledge. This will require interactive and batch mode access from and to application codes through an advanced collaboration environment. There must be a significant ability to allow—and indeed encourage—the interplay between application and data models. This is required to enable additional processing, exchange, prediction, extrapolation, and reduction of information into required knowledge. Looking forward, it will be necessary to enable data assimilation or data fusion into this collaborative capability. This will require the ability to include instructions with the data and to allow on-demand data analysis capabilities. With these capabilities available to the researcher, the next step is to develop advisory capabilities so that new, required computations will be as efficient and effective as possible. For example, if a particular mechanism requires molecular rate information, but the reduction model shows that the mechanism does not need the information at a particularly accurate level, an advisory capability could recommend (or even launch) a reasonable calculation to obtain the result. Likewise, the advisor could recommend a highly accurate calculation if the mechanism required it.

Intricately tied to these capabilities is the ability to visualize the data and cross-data connections, both at any given scale as well as between scales. With the huge amount of data that will be generated, the mining and visualization of information will be required for human cognitive skills to grasp novel solutions or problems within the models.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

An increased understanding of the chemistry and transport in energy extraction from biomass will immediately lead to improved methods for designing and optimizing these renewable processes. Since government and privately funded pilot plants using gasification, pyrolysis, and pretreatment are now being built, this type of research is timely. The knowledge developed from this type of computational modeling can be immediately transferred to practitioners to help reduce the risks in developing new industrial plants.

TIME FRAME

One to 15 years.

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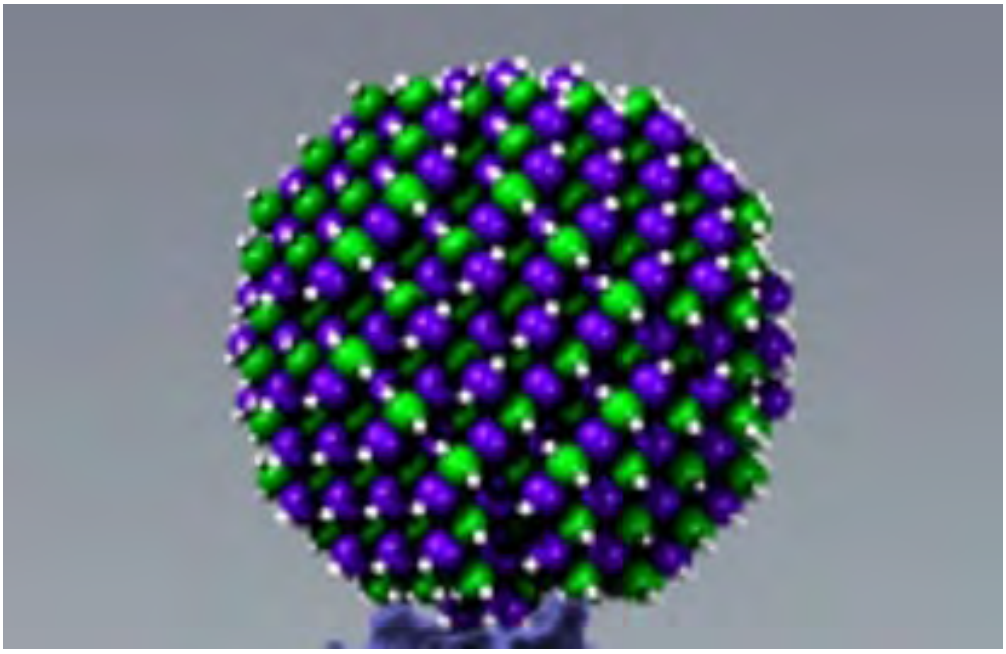
RENEWABLE ELECTRICITY — PHOTOVOLTAIC SOLAR ENERGY CONVERSION



Quantum dots are nanoscale photovoltaic crystals that can be "tuned" to particular wavelengths by varying their size, leading to potentially far greater efficiency than bulk materials.

CHARGE TO PANEL

Sunlight is, by far, the largest of all potential carbon-neutral energy sources. More energy from sunlight strikes the Earth in one hour than all the energy consumed on the planet in a year. However, solar electricity currently provides only a very small fraction of our total electricity supply. Thus, a grand challenge in energy research is to harness solar energy efficiently, economically, and reliably into useable forms such as electricity. In particular, we need the cost of delivered photovoltaic electricity to decrease by two to four times to make solar cost competitive with traditional sources. Solar energy can also be converted to electricity using solar thermal and other technologies, but the charge to this panel was to focus on photovoltaic electrical generation.

The charge to the members of the Solar Energy breakout session was to identify Priority Research Directions in photovoltaic technology related to:

1. Accurate quantitative prediction and design of material properties for various applications in solar-energy conversion systems. Properties include: electronic structure, excited states, light absorption, defects and nonradiative recombination, carrier transport, heat transport, and thermoelectric properties.
2. Computational models focused on improved performance in terms of efficiency, cost, and lifetime, not just for the active material but also for the nonphotoactive parts that contribute to a substantial fraction of system cost
3. Accurate modeling and design of nanoengineered materials with novel properties for enhanced solar-energy conversion efficiency
4. Detailed modeling and simulation of complex systems to understand interactions of macro molecules and other surfaces, thus helping organic photovoltaics realize its potential
5. Computational support for combinatorial and high-throughput experimental techniques
6. Modeling the use of nonlinear optical, photon recycling, and/or other efficient and economical conversion mechanisms to transform a broad spectrum of sunlight into a narrow one tailored for efficient photovoltaic conversion
7. Theoretical identification of a physical photovoltaic system that could achieve conversion efficiency approaching the thermodynamic limit
8. Modeling of advanced optics and subwavelength optics for solar concentration that enable the integration of optics and photovoltaic cells in a robust, economic manner.

SESSION BREAKOUT LEADERS

Victor Batista, Yale University
Jerry Bernholc, North Carolina State University
Kai-Ming Ho, Ames Laboratory
Mark Hybertsen, Brookhaven National Laboratory
Tim Kaxiras, Harvard University
Jim Misewich, Brookhaven National Lab
Lin-Wang Wang, Lawrence Berkeley National Laboratory
Shengbai Zhang, National Renewable Energy Laboratory
Zhenyu Zhang, Oak Ridge National Laboratory

INTRODUCTION AND BACKGROUND

Solar energy is abundant, but costs need to be brought down by two to four times to be practical. A key goal of the national Advanced Energy Initiative is to "reduce the cost of solar photovoltaic technologies so that they become cost-competitive by 2015." To achieve this goal, the DOE Office of Energy Efficiency and Renewable Energy (EERE) outlined a strategy of "conducting accelerated research and development to improve the materials performance and reduce the cost of advanced photovoltaic (PV) systems and developing new manufacturing technology to lower process costs and increase throughput for enabling expanded U.S. manufacturing capability." Our panel examined computational research needs and opportunities that will support these goals. The panel was well attended, having some 35 panel members who exhibited great enthusiasm and excitement on the subject of photovoltaic solar electricity.

OVERVIEW OF SOLAR PRIORITY RESEARCH DIRECTIONS

Five priority research directions resulted from extended discussion among panel members. The priorities can be divided into three main areas: three are in the area of materials properties prediction and design, one is in the area of system integration and design, and another one is in the area of materials processing simulations for industrial-scale synthesis and manufacture. The three material properties priorities can be related to different classes of solar PV materials with different physical processes dominating performance/cost in different systems.

Materials optimization in inorganic PV

Current inorganic PV materials are either cheap or efficient, but not both. Defects are often a significant limiting factor that leads to detrimental processes such as recombination at defect sites and/or grain boundaries, low mobility, and materials degradation under illumination or environmental stress. Computational capabilities in prediction and design will make a strong contribution toward improving the performance of these materials.

Organic polymerics and small molecules and inorganic nanostructure PV

Current PV cells made of these materials suffer from low efficiency and fast degradation. Many fundamental properties are still being worked out and scientific computing can make important contributions. Prediction and design in these systems will focus on the behavior of strongly localized excitons and carriers.

Design and optimization of complex, biomimetic, and hybrid materials for solar-electric energy conversion

The third priority in materials prediction and design gives attention to materials that have heterogeneity and more complex interactions. These systems pose considerable challenges in reliable and effective predictions of the material structure and morphology stability, excited states, electrical transport, as well as the interplay between thermal and electrical transport.

System- and device-level integration and design

In this area, we note that novel solar cell architecture has huge potential to improve cost and efficiency. Fast and efficient scientific computing can significantly shorten the cycle for device development and optimization.

Processing simulations for manufacturing PV materials

In this area, we highlight that linking manufacturing processes to material characteristics and performance is important to developing cost-effective processing. Effective process-simulation tools have a direct impact on accelerating the development of new manufacturing technologies.

MATERIALS OPTIMIZATION IN INORGANIC PV

ABSTRACT

Current inorganic PV materials are either cheap or efficient, but not both. Defects are often a critical factor limiting a particular type of material from reaching its potential, due to detrimental processes such as recombination at defect sites and/or grain boundaries, low mobility, and materials degradation under illumination or environmental stress. We need to understand and predict carrier transport at interfaces and grain boundaries in these systems. Computational research in this area will focus on the development of methods for accurate determination of band gap, defect level positions, and efficient algorithms for structure determination of very large systems.

EXECUTIVE SUMMARY

Despite the range of different inorganic PV materials, they pose unified materials challenges: understanding and predicting defect thermodynamics, stability, diffusion, defect levels, generation mechanisms, and doping efficiency vs. recombination. Predicting defect properties—both for single defects and assemblies of defects—gives materials designers the basic tools needed to control those defects. At the same time, we wish to find what dopants can maximize the efficiency of PV devices. Prediction at this level requires accurate treatments of bandgap engineering and carrier transport, both in the bulk and through interfaces. PV devices often make use of tandem structures to maximize efficiency, but these structures can induce their own defects. We need computational approaches to study these complex systems to tailor new devices around such limitations.

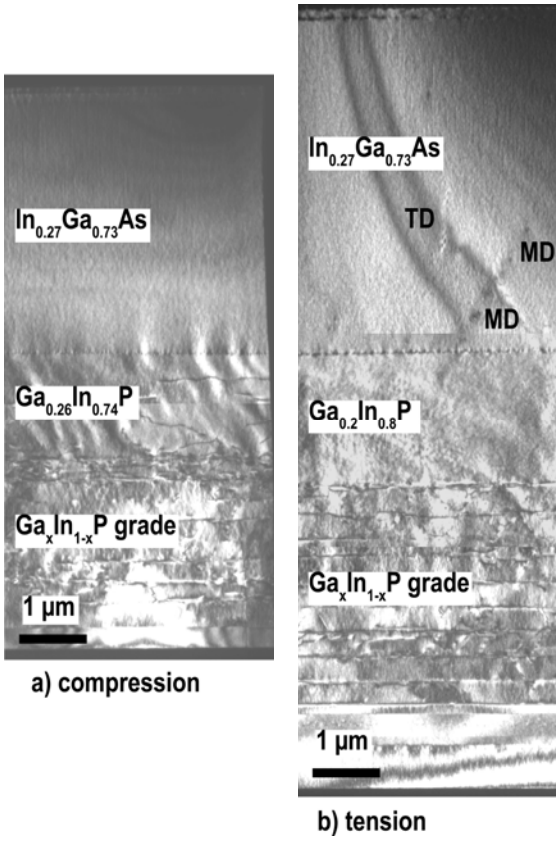


Figure 1: Dislocation densities in inverted, lattice-mismatched III-V tandem solar cell structures are greater under tensile strain than under mild compressive strain. (Courtesy: John Geisz and Andrew Norman, NREL)

Addressing these broad problems in inorganic PV materials requires substantial progress on several fronts in computational science. Density functional theory methods require improved scaling to reach systems involving many thousands of atoms. Simulating even higher length scales requires new accurate semi-empirical methods with heretofore unseen transferability between material environments. New methods are needed to predict bandgaps and defect levels accurately and efficiently, which include many-body and lattice-relaxation effects. Quantum molecular dynamics

and accelerated dynamics approaches are needed to reach to physically important timescales in devices. All of these methods must be scalable to the even larger computational architectures coming on line in the next decade.

SUMMARY OF RESEARCH DIRECTION

Three key research directions are as follows:

- Accurate prediction of thermodynamic properties of defects and defect complexes
- Prediction of doping conditions to maximize PV efficiency and minimize recombination
- Accurate prediction of bandgap engineering via alloying or lattice-mismatched epitaxy.

SCIENTIFIC AND MATERIALS CHALLENGES

Defects and impurities cause problems in PV materials and devices in a number of ways: (1) They can be the source of recombination centers that cause the photo electron-hole pairs to recombine; (2) Defects, especially the charged ones, also act as strong scattering centers that decrease the mobility of the charged carriers; and (3) They are the sources for many of the photo-catalyzed or chemically catalyzed material instabilities due to continued illumination or environmental stress.

The electronic and optoelectronic properties of the PV materials are controlled entirely by defects and impurities through intentional doping. The equilibrium concentrations of dopants and defects in semiconductors have been extensively studied in the last decade, and a general theory of doping efficiency was formulated [Zhang 1991]. It has recently been extended to surfaces and interfaces, allowing for calculation of segregation coefficients and equilibrium concentrations of defects and impurities in heterostructures [Boguslawski 2006]. Such heterostructures form the basis of modern devices, including solar cells. Segregation can also occur during growth, altering the distribution of dopants, separating the constituents of the growing layers, and also affecting the number and kind of native defects.

RESEARCH GOALS

Accurate prediction of thermodynamic properties of defects and defect complexes

The Holy Grail of inorganic PV is to find a material that has high performance while tolerating a great amount of defects and stress. Current PV materials include crystalline and amorphous materials such as Si, III-V semiconductors, and various semiconductor alloys. Some of the highest-efficiency solar cells have been achieved using the well-established crystalline semiconductors and high-quality semiconductor processing techniques; however, the cost per watt is currently relatively high. Amorphous semiconductors have significantly lower efficiency and suffer during use from degradation known as the Staebler-Wronski effect [Staebler 1977]. Polycrystalline materials suffer from defects at grain boundaries, which need to be made electrically inactive and benign. A thorough understanding of the thermodynamics of defect formation, doping mechanisms, and doping energetics, as well as defect and impurity-induced recombination, would vastly increase the efficiency and cost performance of solar cells.

Among the existing thin-film PV materials, $CuInSe_2$ (CIS) is especially promising as a low-cost inorganic photovoltaic material. Its defect physics shows three very unusual effects [Zhang 1998]: (1) Structural tolerance to large off-stoichiometry up to many percent; (2) The ability to be doped only by native defects; and (3) The electrically benign nature of its structural defects. While polycrystallinity in Si and other ordinary III-V semiconductors leads to a high concentration of electrically active defects with detrimental effect on the performance, polycrystalline $CuInSe_2$ is as good an electronic material as its single-crystal counterpart. A 19.5%-efficient $CuIn_{1-x}Ga_xSe_2$ solar cell has already been achieved, despite the many nonstoichiometric defects [Ramanathan 2003].

CIS is particularly interesting due to what appears to be a self-assembled nanostructure which likely is a significant contributor to its high tolerance [Yan 2005]. It would be useful to understand the physics behind this and to be able to manipulate it. To understand the performance of $CuInSe_2$ PV, one needs accurate predictions of the stability of an assembly of defects and impurities that inherently interact, sometimes creating new defects while annihilating old ones. This requirement will become even more acute as new low-cost inorganic PV materials emerge. The major goals are to understand defect generation and diffusion mechanisms, and to provide an accurate description of the electronic energy levels of defects and impurities, as well as the excitation energies. In addition, grain boundaries and other extended defects are often pitfalls to first-principles calculations due to their complexity and lack of sufficiently detailed experimental information.

Prediction of doping conditions to maximize PV efficiency and minimize recombination

Doping in PV applications critically affects the design of PV architecture. Doping is an artificial manipulation of the electron Fermi level, which has a strong effect on the formation energy and concentration of the charged defects. These defects, in turn, can affect the position of the Fermi level. Electronic properties of a defect can also strongly couple to its structural properties, further complicating accurate prediction. For example, in the case of a small (localized) polaron, such a coupling causes asymmetric atomic displacements. Although small polarons [Schirmer 2006] have been observed experimentally in ZnO, local density approximation (LDA) calculations within density functional theory fail to predict them due to the unphysical self-interaction. The accurate prediction of the impact of dopants and defects on the Fermi level of existing and new PV materials—to find the most effective and cost-efficient control of carrier concentration—is a crucial piece in developing PV devices with reduced cost and increased efficiency.

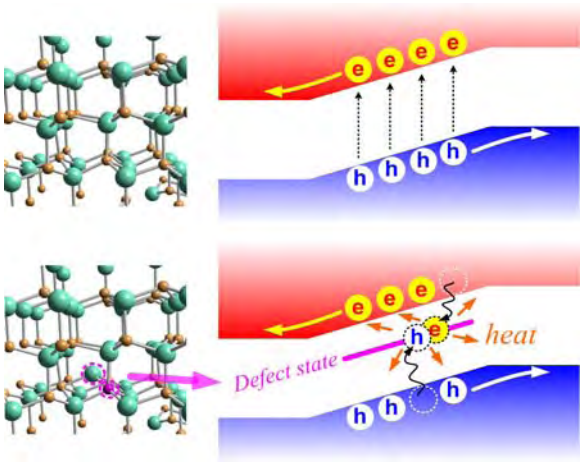


Figure 2: Separation of charged carriers is generally required in photocurrent generation. Deep-level defect states, however, work as non-radiative recombination centers, trading current for the generation of heat, which is an undesirable loss. (Courtesy: Sukit Limpijumnong, NREL)

Nonradiative carrier recombination at defects and impurities (as a result of doping) is often the limiting factor for PV devices. Most inorganic PV devices are minority-carrier devices. In such devices, a relatively small amount of (unpassivated) recombination-active defects (as low as 10^{13} cm^{-3} [Davis 1978] can lead to detrimental PV efficiency loss. A better understanding of which defects are not passivated, as well as recombination mechanisms, is vital to future improvements of inorganic PV. Aside from detrimental recombination, one needs to better understand carrier transport. The flow of current in PV devices is governed by the timescale for the separation and collection of photo-generated carriers. For real devices, we need to model transport not only in the bulk, but also across the various interfaces in a real device and—for lower-cost materials—across grain boundaries.

Accurate prediction of bandgap engineering via alloying or lattice-mismatched epitaxy

Ultra-high efficiency in PV devices can be achieved in semiconductor tandem solar cells that are lattice-matched, but with different bandgaps. GaAsN alloy is one such candidate for III-V PV [Kurtz 1997]. The large size mismatch between substitutional N atoms and the GaAs host profoundly alters the electronic properties of the semiconductor, both for desirable optical absorption and for undesirable recombination from defects induced by the internal stresses. The accurate prediction of changes in the bandgap and lattice constant with defect alloying is thus important for physics-based design of complex architectures from new and existing PV materials.

However, alloying GaAs with nitrogen is not easy. Considerable attention has recently shifted to using lattice-mismatched gap engineering, such as growing GaAs on silicon or InN on GaN. The great challenge here is managing the propagation of dislocations induced during growth and their associated electronic defects, without causing undesirable degradation [Wanlass 2005]. Other candidate bandgap engineering systems include GaAlInP/GaAs/GaInAs and amorphous semiconductor alloys, e.g., a-Si:H and a-SiGe:H.

In all of these candidate systems, quantitative computational prediction of electronic structure in complex alloyed and layered systems provides a route to accelerate the development of new materials for PV devices.

THEORETICAL METHODS

Current status

Ab initio methods that do not use any empirically or experimentally derived quantities are particularly useful in predicting the properties of new materials. For a given configuration of atoms, density functional theory (DFT) accurately predicts the distribution of electrons through the solution of Schrödinger-like Kohn-Sham equations. Defect formation energies depend on the LDA bandgap. In the notorious case of ZnO, the LDA gap of 0.8 eV is considerably smaller than the experimental value of 3.4 eV [Zhang 2001]. More sophisticated approaches include self-interaction correction, GW theory, and Bethe-Salpeter electron-hole equations to account for excitonic effects. The latter two approaches are generally considered to be reliable, but are currently limited to about 100 and 30 atoms, respectively, and atomic relaxations are often not

accounted for in such calculations. Clearly, additional methodological developments to both increase the system size and the accuracy, are sorely needed. New methods using the two-electron Green's function, which scales O(N) and O(N log N) with guaranteed finite accuracy, are just beginning to show promise.

In parallel with methods that allow larger systems to be studied using free surface or periodic boundary conditions, the use of new "embedded" or "flexible" boundary condition methods provide more efficient structure optimization in the core of defects. Efficient use of material response to strain fields and atomic forces — extracted from DFT calculations — for long range to atomistic-scale can provide a way to reduce the region of interest in a defect calculation to those atoms with the largest changes in local environment. Embedded approaches require a careful coupling of the long length-scale displacement due to a defect with the core of a defect in a consistent fashion. Further development of flexible boundary condition methods combined with improved scaling techniques for DFT will allow many more defects structures to be studied in a larger array of materials.

Challenges

The above scientific challenges require further substantial progress in theoretical methods and in their implementation on petascale computers. The following methodological research directions will broadly benefit the development and simulation of PV materials and devices:

- Linear-scaling DFT and/or hybrid DFT methods capable of handling 10^3 and more atoms
- Quantum molecular dynamics and accelerated dynamics methodology that will approach the timescale for real physical processes
- New accurate and efficient methods for calculating excited states and bandgaps, scalable to large systems
- Accurate semi-empirical methods with unprecedented transferability between systems
- Theory of multicomponent, multilayered, and amorphous materials
- New mathematical and computational methods, capable of high sustained performance on petascale and exascale systems.

The outcome of this research would be a suite of simulation tools to enable transformational research in solar materials. The emerging petascale and exascale hardware will dramatically enhance their impact in speeding up the search for novel materials and device design, and lead the quest for new, environmentally friendly processes and technologies.

Developing and adapting such tools to the petascale level is a highly non-trivial task that most likely requires interdisciplinary teams to answer challenges that require expertise in multiple areas:

- *Quantum simulation methods*: The most accurate methods are prohibitively expensive for large systems and they scale poorly with system size [up to $O(N^7)$]. Interdisciplinary expertise is required to develop multiscale methods that will provide sufficient accuracy at acceptable cost, while performing well for grand-challenge-size problems at the petascale level.
- *Existing codes and algorithms* perform well on current terascale systems, but need major performance tuning and adaptation for petascale systems. This requires use of advanced

profiling and optimization tools, and additional development of these tools to adapt them to different petascale architectures, with different memory hierarchies, latencies, and bandwidths.

- *New or improved algorithms* can greatly decrease time to solution without sacrificing accuracy and stability. Very large problems often exhibit "slow down" of convergence, requiring "coarse-level" accelerators adapted to the particular algorithm. Algorithmic changes to decrease bandwidth or latency requirements may also be necessary. In time-dependent simulations, sophisticated variable time-stepping, adaptive implicit methods, and interpolation methods can greatly increase the "physical time" of the simulation, enabling the discovery of new phenomena. Algorithmic research at this level requires broad expertise in applied mathematics.

POTENTIAL IMPACT

The potential impact is for high-efficiency solar cells that are close to the thermodynamic limit. In addition, these solar cells will be inexpensive, exhibiting tolerance to defects. This work will feed forward into device simulation and pilot projects, allowing comparison to experimental results.

TIME FRAME

New methods are expected in 2 to 5 years. Computed material properties coupled with processing and device modeling are expected in 2 to 5 years. And the impact on materials selection and design of inorganic PV devices is expected in 3 to 5 years.

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ORGANIC POLYMERICS AND SMALL MOLECULES AND INORGANIC NANOSTRUCTURE PV

ABSTRACT

Organic polymers and inorganic nanostructures offer inexpensive means of synthesizing solar cells. For example, a solar cell consisting of a blend of C_{60} and conjugated polymer can be rolled out from a machine as a plastic thin film. Unfortunately, current solar cells made with polymers have efficiencies in the range of 1%–3%, and they usually degrade after a short period in the sun [Huynh 2002]. Dye-sensitized cells can have a power efficiency of 6%, but they also suffer from instability [O'Regan 1991]. To have a major impact in the energy market, the efficiencies of such cells need to be higher than 8%, and devices need to be stable for a few years under sun and air exposure. To achieve these goals, we need to understand the efficiency bottleneck of these devices and find ways to overcome them. We also need to know what causes the degradation of the polymers, and whether they can be chemically modified to improve stability.

EXECUTIVE SUMMARY

A common theme in this priority research direction is the strongly localized character of excitons and carriers. Although PV cells made of these materials are inexpensive, they suffer from low efficiency and fast degradation. Many fundamental properties are still being worked out and scientific computing can contribute greatly. Research directions include exciton transport and dissociation, carrier transport and collection, the effects of nanostructures and surface proximity on the electronic and optical properties and carrier dynamics, the mechanism of materials degradation under solar radiation and environmental stress, charge separation and recombination processes, and the mechanism of multi-exciton generation. Needs from computational science include accurate prediction of the excited state, exciton binding energy, trap states, surface states, scalable methods for aperiodic systems, linear-scaling [O(N)] methods, theory and computational methods for charge transport in complex/disordered systems, and better modeling for chemical reactivity.

SUMMARY OF RESEARCH DIRECTIONS

The four key research directions are:

- Exciton generation, transport, and dissociation
- Carrier transport and collection
- Electronic structure, optical property, and carrier dynamics in nanosystems
- Mechanism of radiation-induced performance degradation.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

To use organic molecules as the active material for a solar cell, the first issue is to have a broad absorption spectrum to cover the light spectrum of the sun. Most organic molecules have a narrow absorption spectrum. Current organic solar cells solve this problem by stacking different

molecules together. But it would be ideal to have a single molecule that can absorb most of the sunlight.

A common feature of organic polymer and inorganic nanostructures is the localization of their excited excitons and carriers. In bulk inorganic PV, the exciton binding is small compared with the room-temperature kT. As a result, the excited carriers can be considered as free carriers. In contrast, in organic molecules, polymers, and nanostructures, the excited carriers are physically localized in a small space and there is a lack of efficient dielectric screening in organic systems or outside a nanowire. As a result, the electron-hole Coulomb binding energy is large, usually in the range of 0.1–0.4 eV [Knupter 2004]. Due to this large electron-hole interaction, how to dissociate the excited exciton into separated electron and hole carriers is a fundamental bottleneck in organic and nanostructure solar cells.

Exciton transport is another important issue in organic and nanostructure solar cells [Lin 2006]. Because of the large exciton binding energy, exciton dissociation often happens at interfaces where a type II band alignment exists: at such interfaces, the electron and hole will reside on opposite sides of the interface, which reduces their Coulomb binding energy and facilitates the break up of the exciton. For this to happen, the exciton must move to the interface from the location where it is created. If the light absorption happens in the nanostructure, exciton transport in the nanostructure (e.g., rods or wires) would be straightforward. However, if the active material is the organic material, then the transport situation can be complicated. The transport might be sensitive to the morphologies of the polymers. For example, if the polymer chains align together, forming a semicrystal in one region, the mobility in that region could be orders of magnitude larger than in the very disordered regions. Exciton transport is important for the newly created exciton to move quickly to the dissociation interface, before it recombines to give away its energy. Another mode of exciton transport in nanocrystal assembly is via fluorescence resonance energy transfer (FRET). The exciton can jump from one quantum dot to another via FRET due to dipole coupling.

Besides exciton transport, single-carrier transport is another major issue [Nakamura 2005]. For example, for many organic or organic/inorganic hybrid solar cells, the holes are transported in the p-type polymers. Compared to the other part of the device, the hole has a very small mobility in the polymer, and this often becomes another bottleneck. The hole transport process is also very complicated. Very often, it is unclear what is the right picture to use in describing the hole mobility: is it a hopping transport, or a free-carrier-like transport, or a tunneling transport? The necessary theoretical tools might also vary, from electron-phonon interaction, to Marcus' charge-transfer theory, to quantum-elastic transport, to direct-electron and atomic dynamics.

Nanostructures present their own challenges in the areas of electronic structures, and electron-electron, electron-phonon, and electron-photon interactions. The electronic structures and wavefunction localizations of nanocrystals and nanocrystal composites are complicated by quantum confinement effects, band offsets, strain effects, and piezoelectric effects. For example, even the issue of the possible internal electric field in a simple quantum dot is not completely settled. Apparently, an internal electric field might play an important role, for instance, for the mobility in a nanowire. A bent nanowire might produce a transverse electric field across the diameter of the wire, significantly reducing the conductivity of that wire [X. Wang 2006]. The

exciton wavefunction and binding energy in a simple or composite nanostructure is another major problem. In addition, multiple exciton generation in nanocrystals due to the Auger effect provides the potential for a highly efficient solar cell. However, to truly understand such processes, one needs to calculate and understand electron-electron interactions (Auger effects), electron-phonon interactions (hot-carrier cooling), and electron-photon interactions (exciton generation). To understand the carrier dynamics and possible quantum coherence effects, it might be necessary to carry out direct time-dependent simulations simultaneously for both the electron and atom. Computationally, this is very challenging, and the corresponding theoretical formalism to carry out such simulation is still being developed.

A major bottleneck for solar cells made of organic components is light-induced performance degradation [Kawano 2006]. Often, this is due to chemical reactions in the excited state. Thus, excited-state chemical reaction paths and the corresponding barrier heights need to be investigated. Sometimes, however, we might not have detailed ideas of specific chemical reactions and reaction paths. In such cases, direct *ab initio* dynamics in the excited state might prove to be a useful simulation approach.

POTENTIAL COMPUTATIONAL SCIENCE IMPACTS

The availability of large-scale computation will change the paradigm on how research is done in this area. Current theoretical investigations suffer from two problems: (1) in many cases, it is unclear what the right model is and formalism for a specific problem and (2) the computational task is beyond the capabilities of current computers. These two problems are obviously coupled: with increasing computer capabilities, the computational formalisms often change accordingly.

There are many different ways to calculate the wavefunctions and binding energies of excitons. Methods range from variational wavefunction calculations, to the GW Bethe-Salpeter equation (which is a Green's function method with a screened Coulomb interaction) [Grossman 2001], to the excited-state quantum chemistry method [Dreuw 2005] and quantum Monte Carlo method (which deals directly with the many-electron Schroedinger equation) [Williamson 1998]. But many of these high-end methods are limited to a small number (a few tens) of atoms. They often scale badly with the size of the system, e.g., the Bethe-Salpeter equation scales as N^6, and the coupled cluster quantum chemistry method also scales as N^6. Thus, in order to increase the amenable system size to experimentally relevant sizes, increase of computer power has to be complemented by development of new methodologies. With widespread availability of petascale computing, reliable exciton wavefunction and binding energy calculations should be possible in the near future. When such calculations become routine, we will gain much-needed insights about the exciton dissociation processes in organic systems, nanostructures, and at their interfaces.

One main challenge to study carrier transport in organic systems is to determine the right physical model for such transports. For a complex system such as a blend of organic polymers, it is unclear whether any of the available simple models are correct. In that case, a more fundamental approach may be necessary. The approach may be to follow the quantum-mechanical electron dynamics along with the atomic dynamics, simply to see what happens at the end and what picture is correct. The computational demand for such calculations is

tremendous. It requires following the time-dependent Schrodinger's equation to a timescale of perhaps a few nanoseconds. The time step for Schrodinger's equation is a thousand times smaller than the molecular dynamics time step (which is typically a femtosecond). Thus, to reach to nanoseconds, there will be 10^9 time steps. Here again, development of new temporal acceleration scheme is critical. For example, one might want to solve the eigenstates of the Schrodinger's equation at a given time, then follow the time evolution of these eigenstates at a longer time. There are also unsolved fundamental physical issues for such simulations, e.g., how the quantum states collapse into eigenstates (the "quantum dephasing problem").

Nevertheless, increased computer power and its widespread availability will help us to get into such research paradigms. Currently, such simulations are extremely rare—only having been performed for very small systems for a short period of time on one of the largest supercomputers in the world (the "earth simulator") [Tejima 2005]. To have a true scientific breakthrough, such single proof-of-concept simulation is not enough. It must become widely available, so there will be a sustainable effort and research community working on similar problems.

The challenges for electronic structure calculations for nanostructures stem mainly from their large sizes. A typical colloidal quantum dot contains a few thousand to hundreds of thousands of atoms. Despite their large sizes, atomistic simulations are often necessary due to the importance of impurities, surface states, and possible heterostructures. With traditional density functional theory, the computational timescales as N^3. It is impractical, as well as unnecessary, to use such methods to calculate systems with hundreds of thousands of atoms. Instead, a linear scaling O(N) method must be developed. There can be a variety of linear scaling methods. It could be a total-energy calculation method, such as the localized orbital [Mauri 1993] or truncated density matrix method [Li 1993], or the divide-and-conquer method [Yang 1991]. But it could also be a method just for electronic structure calculations, such as the folded-spectrum method [L.W. Wang 1994] or the charge-patching method [L.W. Wang 2004]. Developing such methods should emphasize the linear scaling with the size of the system, but should also emphasize the parallelizability of the algorithm on future massively parallel petascale computers.

Another challenge for nanosystem simulation is the atomic structure at the surface and interface. Due to the lack of such information, the role of surface states is often unknown. This also makes the electronic structure calculation very difficult. To solve such problems, one might like to perform an *ab initio* molecular dynamics (MD) simulation. With current computers and algorithms, one can only do such MD simulation for systems with about one hundred atoms for a few picoseconds. It will be much more helpful to do simulations for a few thousand atom systems to a few nanoseconds. Future computers and algorithms might help us realize this dream.

To study radiation degradation of organic solar cells, we must study atomic structures and chemical reactions induced by photon absorption. The current approach for such studies is based on intuitions for possible chemical reactions and pathways. Theoretical calculations are used to confirm or disapprove pre-selected hypotheses. Such an approach may miss some important reactions. With a significant increase in computer power, another possible approach is to do molecular dynamics for excited states to find out the possible reactions. *Ab initio* molecular dynamics is a time-consuming simulation, and there are different ways to do excited-state

molecular dynamics, from the occupation-constraint LDA method, to the expensive GW Bethe-Salpeter equation excited-state MD method [Ismail-Beigi]. All these methods will have a big impact only when a large-scale computer is available for many people to use.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

Solar cells made of organic polymers and nanostructures are a potentially very promising future solar technology for large-scale deployments due to their relatively low cost. Currently, their power efficiency is only around 1%–3%. To make a big difference, their efficiency needs to be increased to 8%, and they must have a reliable lifetime of at least a few years. These are major challenges for organic/nanostructure solar cells. Experimentally, many of the critical properties such as exciton and carrier transports, as well as atomistic structures, are difficult to measure. This makes theoretical studies and simulations critical. Only by understanding these basic physics processes is there hope for improving the efficiencies and reliabilities of these devices. The old experimental trial-and-error approach will not be good enough to develop next-generation solar cells in a timely fashion. To accelerate the developments of such solar cells, we need to use the next generation of supercomputers to help solve the critical problems listed in this section.

TIME FRAME

With the availability of computer time and funding to develop the corresponding algorithms and codes, there will be a visible impact in the understanding of the above basic problems in 5 years. To have a device that will make a commercial impact will probably take 10 to 15 years.

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DESIGN AND OPTIMIZATION OF COMPLEX, BIOMIMETIC, AND HYBRID MATERIALS FOR SOLAR-ELECTRIC ENERGY CONVERSION

ABSTRACT

Promising developments for solar-to-electric energy conversion have emerged with the discovery of solar cells based on complex nanostructured materials. These include biomimetic PV cells that harvest light with molecular antennas and directly convert photon energy into electricity by electron-hole pair separation (e.g., Graetzel cells) (see Figure 3) and direct solar-thermal cells that first create a temperature gradient and then use mechanical heat engines to generate electricity (see Figure 4). However, the large-scale use of solar cells based on these general approaches remains prohibitively expensive. Further design and discovery of new nanostructured materials are essential to achieving the necessary efficiency breakthroughs that would make the next generation of solar cells economically viable solutions to current energy concerns.

EXECUTIVE SUMMARY

Materials in this section are heterogeneous and have more complex interactions. Hybrid materials such as P3HT-Fullerenes and Graetzel systems involve organic, polymeric, and inorganic components interfaced with each other. Different interactions—from covalent to polar to van der Waals—determine structural stability and degradation. In thermoelectric materials, a complex mixing of compositional and structural disorders at the nanoscale is important for optimizing device performance. Novel biomimetic materials also have complicated structures. In all these systems, there exist considerable challenges in reliable and effective predictions of the material structure and morphology stability, excited states, electrical transport, as well as the interplay between thermal and electrical transport. Computational research directions include accurate prediction of level alignment at heterojunctions and contacts, photon conversion processes, new methodologies for determining carrier and thermal transport in complex structures, structural defects, disorder, and surface passivation, and accelerated *ab initio*-based molecular dynamics.

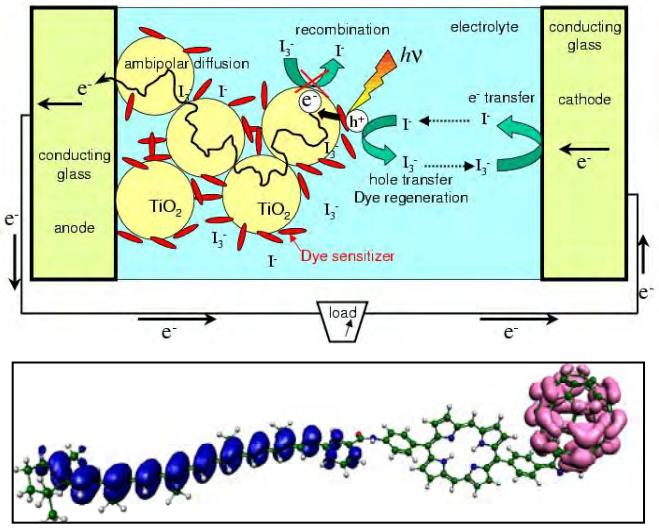

Figure 3: PV solar cell and biomimetic antenna for light harvesting and e^{-}-h^{+} pair charge separation proposed for nanostructured molecular components.

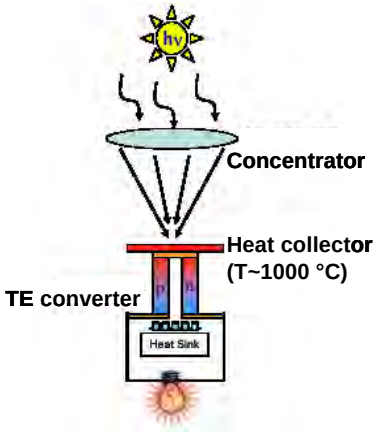

Figure 4: Diagram of a solar-thermal cell.

SUMMARY OF RESEARCH DIRECTIONS

The three key research directions are:

- Structural prediction and stability assessment
- Impact of structural defects, disorder, and surface passivation in nanoscale heterogeneity
- Predictions of photon conversion, charge, and thermal transport in complex and nanostructured bulk materials and interfaces.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

In these heterogeneous systems, the detailed mechanisms and interplays between nanostructure size, shape, and composition with materials chemistry are still poorly understood. It is necessary to develop, assemble, and further integrate density-functional-based and other efficient mean-field electronic-structure computational tools for the multiscale simulation of charge and heat transfer in the nanoscale. In fact, our current limited ability to calculate the lattice thermal conductivity and electronic relaxation dynamics in complex and nanostructured materials remains a significant barrier to progress in the field.

The strong nanoscale heterogeneity inherent to these systems results in a high density of electronically active inorganic-organic interfaces, which are responsible for fundamental steps in energy conversion processes such as charge transfer and resonance energy transfer. Fundamental properties intimately connected to the efficiency of these interfaces, such as absorption, interfacial exciton formation and (non-adiabatic) dynamics, electronic alignment, and carrier transport are often dominated by significant many-electron effects that are not included in standard (e.g., density functional theory) electronic structure approaches.

In principle, transport properties, including thermal conductivity, can be obtained from dynamical simulations by using the Green-Kubo formalism, or direct calculation of diffusivities. However, at present, simulations for sufficiently long times are not practical, except for relatively simple materials or with simplified classical models that are often difficult to construct for complex materials. For example, it is now possible to apply Boltzmann transport theory to calculate the thermoelectric power of simple bulk materials with periodic boundary conditions. However, large-scale electronic structure simulations and new computational methodologies are needed to extend these types of approaches to nanostructured materials. In addition, new computational methods are required to estimate trends in electron phonon scattering and other processes that affect carrier mobility. The required developments include significant improvements in performance of first-principles dynamics methods and computational tools for calculating electronic scattering rates from point and extended defects, as well as electron phonon scattering in complex structures. When combined with Kubo or other transport formalisms, these methods would enable computations of thermal and electric conductivities. These methods could also play an important role in calculations of thermopower in some temperature ranges.

Software developments would benefit from rigorous validation and verifications focused on specific types of materials for PV and thermoelectric cells, with emphasis on the relatively wide class of molecular-based materials showing promise to be inexpensive, robust, cost effective, and

environmentally friendly. For example, promising materials for PV devices include semiconductor surfaces functionalized with biomimetic light-harvesting molecules, organic layered compounds consisting of pentacene-based molecular donors and fullerene-based acceptors, and systems containing metal pthallocyanines. Such materials could integrate the necessary structural and functional properties of the cell with molecular components that have either one or multiple functions (e.g., chromophores or light absorbers, antennae-like appendages to funnel light energy from the chromophore, the ultimate donor/acceptor pairs to provide initial charge separation or the defects, and dopants at the interface to promote efficient charge injection from the leads). Computational needs, common to all of these materials, are fully atomistic computational modeling techniques that could calculate electron excitation energies and transition rates, energy transfer rates (such as Foerster and Dexter processes) [Jang 2004] and coherent and incoherent charge-transfer rates. Strategies aimed at multiple-exciton generation and possibly infrared-induced vibrational-electron transfer also depend on the same underlying matrix elements.

Given the complexity of these systems, considerable developments in both quantum and classical computational approaches are absolutely necessary to predict and rationalize structural aspects that determine morphology, degradation, and durability of hybrid materials. Some of the important challenges include the development of force fields and coupled quantum mechanical/molecular mechanical (QM/MM) methods for handling weak (e.g., van der Waals and non-covalent) and strong interactions (breaking/formation of chemical bonds) on the same footing. In addition, new coarse-grained and empirical potential models are also required to address structure, formation dynamics, stability, durability, and related morphological questions. Furthermore, accurate, efficient methods for computing electronic structure (e.g., electronic excited states, electron-phonon coupling, nonequilibrium electronic and thermal transport) for realistic systems, systems with a large number of atoms, require urgent development. Although accurate approaches exist for the electronic structure of small molecules and bulk solids, they are simply computationally intractable for predicting many of the key properties of nanoscale-model structures with many thousand atoms. In fact, the development of new methods and algorithms that would allow for accurately determining excited-state electronic relaxation processes in realistic model nanostructures represents a grand challenge for theory and simulation.

Massively parallel computational software for prediction of structure-function relations and transport properties in hybrid nanostructured and biomimetic systems

Studies of new materials for PV devices would greatly benefit from developing computational software for accurate computations of excited-state energies in vacuum and in the polarizable dielectric environment provided by a solution or spectator molecules. Particularly for charge-transfer excitations, standard DFT and time-dependent density functional theory (TDDFT) methodologies must be extended to properly account for the electron-hole interaction energy [Casida 2000; Dreuw 2004]. We need systematically improvable methodologies that efficiently correct for this interaction and simultaneously address or bypass the computational problem related to oscillations between occupied and unoccupied states. Self-interaction corrections for the occupied manifold are also important for many of these cases [Pederson 1984; Perdew 1981]. Many-body perturbation theory (GW, BSE) and QMC methods are promising for providing accurate energy alignments/electron-hole interaction, as possible complementary approaches to

DFT [Grossman 2001]. In addition, it is important to develop a computationally efficient means for including corrections to the excited-state energy that arises when the surrounding medium polarizes in response to a charge-transfer-induced change in the dipole moment of a molecular system [Baruah 2006]. Such methods should eventually be able to determine how the interactions modify transition rates, how to broaden the transition energies, and the timescale on which the environment can relax or dissipate energy after an electronic excitation.

Simultaneously, studies of complex hybrid biomimetic materials would benefit from the development of fully atomistic computational packages integrating the description of electronic and nuclear relaxation in quantum-classical dynamics, with emphasis on describing excitations including electron-hole separation and carrier-trapping mechanisms critical for the overall efficiency of carrier collection [Abuabara 2007; Abuabara 2005; Rego 2005; Rego 2003]. The simulations must account for quantum effects and interactions between a bath of incident solar photons and the vibrational and polaronic states of the system. Although initial optical absorption effects will generally be fast, the relatively rare cascade of these states into longer-lived trapping states and metastable excited states are of significant importance, as well. Actual lifetimes of such states will depend on the nature and distribution of material defects, as well as on two-photon processes, the spin-orbit-based mixing between singlet and higher spin states, and phonon-assisted processes. A computational toolbox must also include methods for calculating and eventually tailoring such lifetimes.

In addition to computational methods for describing the electronic structure and dynamics of electronic relaxation, new methods are required to account for van der Waals interactions that determine the density in PV systems composed of macromolecules, high-symmetry nanoclusters, and quantum dots [Park 2006; Rydberg 2003]. The attractive dispersion interactions are outside the validity of standard mean-field treatments, and methods for calculating such interactions are required. Another important area is the development of computational tools to predict electron and hole mobilities and how they are affected by band structures, phonons, defects, and interfaces.

Large-scale simulations of phonon thermal conductivity, stability, and formation of nanostructured and complex materials

Experiments have shown that high efficiency of solar-thermal cells, as determined by large values in thermoelectric figures of merit (ZTs), results mainly from the reduced phonon thermal conductivity of nanostructured materials. In fact, increasing values of ZT have been reported in recent years for various superlattices [Chen 2003; Harman 2002; Venkatasubramanian 2001] and nanostructured bulk materials [Hsu 2004]. However, reliable computational tools for predicting the thermal conductivity of complex nanostructured materials are yet to be established. Currently, there are several frameworks being developed for thermal conductivity prediction, but each has its own limitations. Classical molecular-dynamics simulation based on equilibrium Green-Kubo formalism can predict the thermal conductivity of bulk materials by using periodic boundary conditions, but cannot be adapted to nanostructures due to computation limitations. In addition, empirical potentials exist only for a limited number of materials. Nonequilibrium molecular dynamics is similarly limited to empirical potential and very small system size. Boltzmann equation or Monte Carlo (MC) simulation techniques can be applied to mesoscale

structures, but typically rely on the relaxation-time approximation. In addition, the Boltzmann equation or MC approaches for nanostructures require phonon reflection and transmission coefficients at realistic materials interfaces. We need simulation tools for phonon-scattering processes at realistic material interfaces and simulation tools with predictive power for realistic nanostructures.

Accurate and efficient methods for modeling the stability and the development of nanostructures under various material synthesis and processing conditions are required to optimize the performance of existing materials and to design novel nanostructured thermoelectrics. This requires new computational methods for the solution of a hierarchy of problems—from thermodynamics of homogeneous bulk materials to the analysis of the equilibrium shape and structure of nano-precipitates, and the actual kinetics of the nanostructure development. An integral approach applying efficient methods to all these problems is needed, with accuracy comparable to that of direct first-principles calculations. A study of thermodynamics and kinetics of nanostructured materials can then build on top of a cluster expansion by adding the direction-dependent strain and hopping activation-energy barriers for nanoscale analysis and kinetic Monte Carlo (KMC) studies. This requires extending the existing cluster-expansion methods to include strain and KMC treatment in multicomponent systems (beyond the case of quasi-binary alloys), and incorporating the distinct state-of-the-art methods in an integrated computational framework suitable for large-scale nanostructure simulations of the nanostructure geometry. Finally, tools are required to connect the results of the nanostructure geometry simulations to calculations of phonon and electrical transport. With these components in place, we could achieve the ultimate goal of the theoretical search for materials composition and processing conditions resulting in materials with optimal energy conversion performance.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

Advancing the state-of-the-art performance of PV cells and thermoelectric materials represents a major technological challenge that would greatly benefit from an integrated experimental and computational effort, because the fundamental processes that determine the overall efficiency of solar cells remain poorly understood. These developments thus require new computational tools capable of providing insights into the influence of structure and composition on photoabsorption and transport properties that are essential to achieve high performance.

In the long term, progress in this field will provide a molecular-level understanding of structure/function relationships and physical principles that are essential for engineering suitable materials for efficient solar-to-electric energy conversion cells.

TIME FRAME

In the intermediate (~3-year) term, we need to develop widely available, massively parallel computational software for predicting structure-function relations and transport properties of complex nanostructured materials. In the longer (~5–10-year) period, large-scale computational studies of complex nanostructured materials would provide fundamental scientific insights on the structural principles that determine the overall efficiency of solar-to-electric energy conversion, and reliable guidance to synthetic work and engineering developments.

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SYSTEM- AND DEVICE-LEVEL INTEGRATION AND DESIGN

ABSTRACT

Third-generation PV systems require innovations on every scale—from nanostructured materials through device designs to light-harvesting and photon-management architectures. Optimal performance and cost-effective implementation depend on rational design of the integrated system. However, the design space is complex with significant interdependence between subsystems. Fast and efficient scientific computing with physics-based models integrated into system-level simulations can significantly shorten the cycle for device development and optimization. Achieving this goal poses substantial challenges in developing the required hierarchical physical models, solving the resulting nonlinear coupled equations that describe the system, and performing efficient design optimization using the simulations.

EXECUTIVE SUMMARY

Bridging the significant gap between present-day PV system efficiency and thermodynamic limits with cost-effective technologies requires innovations across all scales. Examples of promising research areas include nanostructured materials for multiple-exciton generation, exploitation of plasmonics to control energy flow, high internal-surface-area organics to improve charge-collection efficiency, and new architectures for efficient light management. However, each innovation must be embedded in a device or system architecture that increases power output efficiency. Success must be measured in terms of total system performance and cost.

Semiconductor electronics and photonic systems for communications represent more mature technologies that have demonstrated the power of multiscale hierarchical, physics-based computer-aided design (CAD) tools. The semiconductor electronics industry follows a design paradigm that relies heavily on simulation at every level—from materials fabrication processes through integrated-chip layout and performance. In the photonic systems area, simulation tools aid design at every scale—from active devices such as lasers, to passive devices such as waveguide routers, and finally, fiber-optic system performance. The current state of the art grew out of significant research and development investments in physical model development, computational algorithm development, and model verification. This investment has resulted in new companies that market CAD tools, and it has been a key enabler of exponential advances in semiconductor electronics and photonic communications systems.

In the near term, tools and methodologies from electronics and photonics technologies provide a valuable, initial platform to attack the new design problems unique to the solar PV challenge. Encouraging closer collaboration between PV research groups and experts in photonic device and system simulation will lead to improvements in design and performance.

In the longer term, further substantial research is essential to overcome significant challenges and to realize the full benefit of CAD for PV systems. Models that capture the behavior of nanostructured materials and complex organic materials need to be developed and integrated into device simulation capabilities. New fast and efficient multiscale solvers for the Maxwell equations are needed to model critical photonic processes for light harvesting (e.g., multiple scattering, plasmonic effects, and excited media). System simulation requires integration of the

Maxwell equations with the models for electronic behavior (e.g., carrier generation and transport). The resultant coupled equations are nonlinear and need to be represented in a form amenable to stable algorithms for efficient solution. Advances are needed in algorithms for hierarchical optimization over the complex and large design spaces inherent to PV systems. Finally, validation of the physical models used in simulation tools is crucial for their utility and to support widespread use. The validation process will be facilitated by close working collaboration between simulation and experimental groups.

SUMMARY OF RESEARCH DIRECTION

Semiconductor device equation framework. Many device concepts including organic, amorphous, and nanostructured materials face severe limitations due to low carrier mobility. Further complications are introduced by solar concentration and multijunction concepts. As the solar spectrum is divided into progressively smaller units for conversion in each junction of a multijunction solar cell, the recombination in each junction becomes a limitation to performance of the whole. Solar concentration boosts the carrier generation rate differently in the various junctions so that performance needs to be optimized as a function of concentration. Modeling recombination processes requires a detailed understanding of the capture of both electrons and holes by individual defect states. A multiscale model, combining fundamental device physics with the equations describing the steady-state device operation and time-dependent transient effects, is needed to understand experimental results and to design new devices.

Sophisticated and flexible semiconductor device simulation capabilities from the electronics and photonics technologies give a strong platform for further research to address these issues [Algora 2004; Letay 2006; Li 2007]. Research questions for PV devices focus on implementing key physical models with validation, developing and adapting models for novel materials such as organics, and accurately treating interfaces and recombination centers. For integration with light trapping and other photon-management architectures, the light intensity will vary with position, and simultaneous simulation of the local photon modes will be needed.

Kinetic modeling. In organic semiconductors, charge separation occurs selectively at interfaces, underlying the importance of kinetic modeling of transport in organic solar cells. The role of nanostructured materials for improved solar cell performance—for example, via multiple exciton generation—also supports the importance of a kinetic approach. Modeling organic or nanostructured solar cell devices must therefore incorporate the desired sequence of light absorption, exciton generation and dissociation, electron/hole transport and extraction, as well as various loss mechanisms, including recombination and trapping. A discrete event approach can be adopted in which the device is represented by a lattice with appropriate materials species at each site. A population of particles (exciton, electron, hole) evolves according to rate laws derived from underlying physics models of individual processes. Initial results for nanostructured organics illustrate the potential of this approach [Marsh 2007]. Significant research is necessary to incorporate accurate models for the underlying kinetic processes and to extend the scale of implementations. A key advantage of the kinetic approach is its broad applicability to different materials, e.g., semiconductor nanocrystal arrays embedded in a semiconducting host. An important alternate line of attack on these problems is a hybrid approach in which critical regions are treated with kinetic models while the rest of the device is treated with continuum techniques.

Nanostructured Materials: Opportunities in Solar Energy Conversion

Structured materials with different regions of nanometer-scale extent defined by interfaces exhibit significant changes in electronic and optical properties, revealing phenomena that present important opportunities for solar energy conversion. Two examples illustrate the potential.

Semiconductor nanocrystals: In conventional semiconductor PV, the *excess energy* $h\omega - E_g$ of absorbed photons above the semiconductor bandgap is lost to heat, instead of being used to generate additional electron-hole pairs. This is fundamental to the Schockley-Queisser limit to solar cell efficiency [Schockley 1961]. A new concept for solar cells overcomes this limitation to efficiency: high-energy photons at the blue end of the solar spectrum can generate multiple electron-hole pairs By "impact ionization," instead of thermalizing by phonon emission [Werner 1994; Nozik 2002]. Efficient production of multiple low-energy electron-hole pairs by high-energy photons—multiple-exciton generation (MEG)—has recently been observed in semiconductor nanocrystals [Schaller 2004; Ellingson 2005]. For example, MEG Efficiencies as high as 700% have been reported in PbSe nanocrystals [Schaller 2006]. As illustrated in Figure 5, exploiting MEG can fundamentally change limits [Schaller 2006]. The application of MEG to functioning solar-cell devices will require a careful selection of quantum-dot materials and geometries, and the development of solar-cell architectures specifically designed to efficiently extract the carriers from the nanostructures.

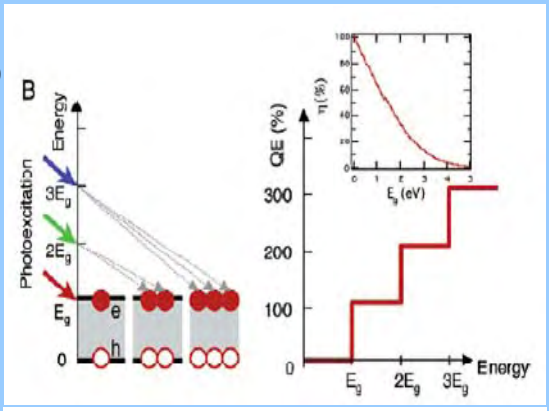

Figure 5: Exploiting multiple-exciton generation can fundamentally boost PV efficiency limits.

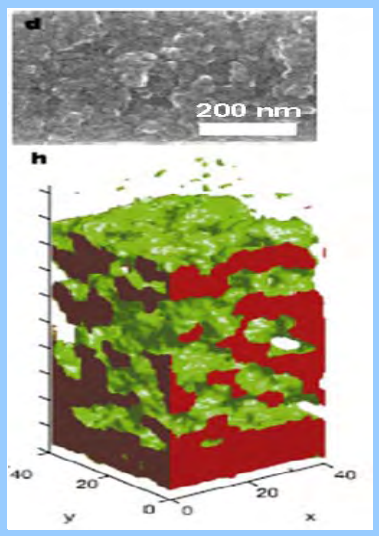

Figure 6: Nanostructured mixtures can significantly enhance the area of the donor-acceptor interface, which shortens the necessary exciton diffusion length, thus improving PV efficiency.

Nanostructured Organic Interfaces: Research directed to use of organic layers to form wide-area PV focuses on unique problems that affect efficiency. Low carrier mobilities, short exciton diffusion lengths, and large exciton binding energy drive designs that focus on multilayer structures with an interface between donor- and acceptor-type materials. Excitons diffuse to the interface where the electron and hole are separated for subsequent collection at the respective contacts. The external quantum efficiency depends on absorption, carrier collection, and exciton diffusion $\eta_{EQE} = \eta_A \times \eta_{CC} \times \eta_{ED}$ through [Peumans 2003]. Through new developments in material deposition and processing, nanostructured mixtures significantly enhance the area of the donor-acceptor interface, as illustrated in Figure 6 [Peumans 2003]. This shortens the necessary exciton diffusion length, resulting in improved PV efficiency. Further improvements depend on understanding and optimizing both the materials processing and transport through the resulting nanostructured layers.

Multiscale simulation of photonic architecture

There is a significant mismatch between the scale for solar energy collection (light harvesting) and the operation of PV devices. Efficiency considerations and cost-effective utilization of materials require new photonic architectures to optimize energy extraction from the solar flux. While some of these novel architectures have been adopted into existing solar cells, most of the concepts are relatively new and much research remains to be done. Because of the large number of design possibilities, fast and efficient scientific computing is invaluable for fast and cost-efficient design and testing of novel concepts and architectures to shorten the device development and optimization cycle.

Maxwell's equations provide an accurate description of electromagnetic waves. However, existing simulation tools have deficiencies in treating active media containing excited optical subsystems, gain, and nonlinear response. Furthermore, a broad range of length scales must be resolved, e.g., for photonic crystal or plasmonic concepts with field concentration at a small fraction of the wavelength, while significant variation in the optical fields across critical elements of the photonic architecture may span 1 to 10 micrometers or even longer scales. Accurate tools such as those based on finite-difference time-domain (FDTD) methods do not easily span the necessary length and time scales, while more approximate methods need to be adapted to capture the local field effects. There is a need for fast, efficient algorithms that can be used repetitively to examine a large number of cases required in the device design/optimization process. Finally, it must be feasible to integrate the solvers with models for carrier generation and carrier transport to predict complete system performance.

Integrated system modeling and optimization

There are distinctive challenges associated with model integration for PV system performance simulation. First, to simulate devices with nanostructured regions or centers with discrete populations, local kinetic processes need to be embedded within a continuum model. Second, to investigate light-trapping or concentrating architectures with active regions, Maxwell's equations need to be integrated with the kinetic or continuum model of those regions. Furthermore, it is necessary to simulate the generation of carriers by incoming light and simulate the electron and hole transport and photo-generated current in a complex solar architecture including interference effects. Although more frequently used one- and two-dimensional simulations are computationally much more tractable and provide important insight, predicting solar cell performance requires simulation of multi-dimensional structures.

The true power of validated, physics-based simulation of the system performance is realized through design optimization. The design space involved is complex and interdependent. Internal to a multijunction cell, each layer absorbs different regions of the solar spectrum, and it is necessary to accurately model the different materials and interfaces, as well as transport processes. External to the cell, the system optimization includes such processes as solar concentration, antireflection coating, photonic crystal light diffraction, and random scattering from textured surfaces. Performance of the system is strongly linked between the internal and external design parameters. Capturing these disparate design parameters with accurate physical models in an integrated simulation of system performance is essential for optimization.

Photon Management Architectures

Solar energy arrives in the form of light waves with relatively low intensity that necessitates harvesting the light from large areas. Design of the architecture of solar cells for optimal harvesting of solar energy is a significant challenge. Two strategies are illustrated here.

Optimal absorption of incident light: In additionto the common strategy of minimizing reflection of incident light through surface texturing or antireflection coatings, absorption can be enhanced by increasing the dwell time inside the device by light-trapping architectures or use of multiple scattering to lengthen the light path. Novel solar cell architectures incorporate a diffraction grating [Heine 1995; Eisele 2001]. As illustrated in Figure 7, a photonic crystal can be combined with an all-angle-and-wavelength antireflection coating. For the back-side reflector, a loss-less distributed Bragg reflector combined with a grating has been demonstrated for crystalline Si layers [Zeng 2006]. A similar scheme has been predicted to enhance the absorption of near-infrared photons in thin-film noncrystalline absorber layers [Biswas 2007]. The applications of loss-less photonic crystals [Joannopolous 1995] within solar cell architectures are just emerging.

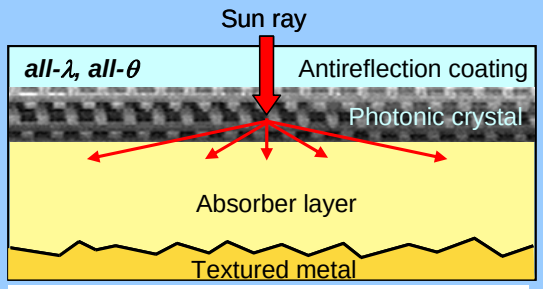

Figure 7: A photonic crystal can be combined with an all-angle-and-wavelength antireflection coating.

Solar concentration and spectrum conversion: Concentrating solar light reduces the area of PV materials used in energy conversion and makes the deployment of more-expensive high-efficiency solar cells economical. Passive designs (without mechanical tracking of the sun) that collect diffuse, as well as direct, sunlight offer significant advantages of cost and maintenance [Herman 1982]. Furthermore, the sun has a broad spectrum, whereas most solar conversion devices operate optimally in a narrower frequency region. The efficiency of PV cells can be increased by converting photons in parts of the solar spectrum to other parts of the spectrum for efficient use. Down-conversion/ shifting can be achieved by absorption and reemission (e.g., using phosphors). As Figure 8 illustrates, the solar input is concentrated and focused onto a perfect absorber that heats up a selective emitter to 1000°–1500°C. A photonic crystal is one example of a highly efficient emitter that provides a narrow band emission in the infrared wavelength (λ = 1–2 μm) [Lin 2003]. Using this approach, an optical-to-electricity conversion efficiency of >50% has been predicted in a one-dimensional model calculation [Walsh 2007].

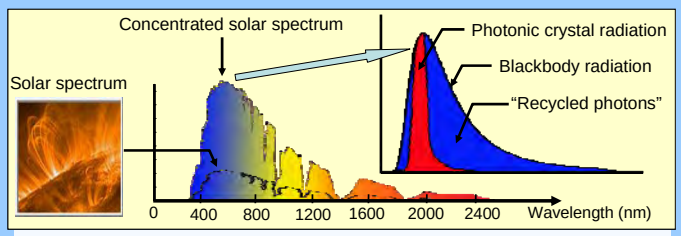

Figure 8: The solar input is concentrated and focused onto a perfect absorber that heats up a selective emitter to 1000°–1500°C.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

The research directions contain scientific challenges embedded above, as well as several cross-cutting computational challenges.

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Multiscale solvers for Maxwell's equations

Approaches with controlled accuracy, such as FDTD, rely on solutions on a real space grid. However, solar cell architectures exhibit very dissimilar length scales. Applications of FDTD to general, three-dimensional nanoplasmonic research problems already require large-scale, parallel computations [Sukharev 2007]. An efficient solver must be developed to simultaneously handle (1) plasmonic, photonic crystal and local field effects (10–100-nm length scale); (2) random scattering from a textured metal (0.1–5 μm); and (3) absorption within the thin film of the absorber (tens of micrometers). Furthermore, the solver must be adaptive enough to handle the computational needs of a whole variety of solar cell optical components. At the same time, it is critical to identify a comprehensive set of basic building blocks of optical devices that are to be included in the solver.

Stable algorithms for solution of integrated model equations

The solution of highly coupled nonlinear equations resulting from models described above requires efficient robust solution algorithms if they are to be useful for system-level design optimization. The self-consistent solution of the semiconductor device equations is typically achieved with an iterative Gauss-Seidel scheme based on accurate calculation of the Jacobian [Bank 1983]. This has been extended to include local populations confined to quantum wells, as well as the nonlinear coupling to photon populations in semiconductor lasers [Alam 2000]. These methods can be extended to include more complex kinetic models coupled to the device equations. The Maxwell equation solutions for the few active modes in typical semiconductor lasers have been integrated into the self-consistency and modal changes tracked dynamically [Liu 2003]. However, the higher complexity in system geometries may pose additional computational challenges in extending these algorithms to solar cell applications.

For example, extending the kinetic modeling described above to realistic simulations of PV cells (size and carrier densities) involves a significant increase in the number of local populations in the model. This petascale computing problem demands a parallel implementation. However, developing large-scale parallel discrete event simulators is a highly challenging parallel processing problem [Perumalla 2006]. One of the main challenges is that fine-grained synchronization of event execution across processors is nontrivial. Correctness of results requires that events are executed to preserve *global* timestamp order among all events.

Algorithms for multiscale optimization

Optimization of hierarchical systems coupling multi-physics, multiscale mathematical, and computational models is as yet an unsolved problem for complex nonlinear systems. Further

research is needed to develop efficient algorithms, including heuristic ones, for the special cases of mixed, nonlinear hierarchical optimization problems such as those discussed here.

Adjoint models provide an attractive approach for addressing several of the above issues. Adjoint models allow us to *efficiently* calculate the sensitivity of system properties to parameters [Cao 2003]. These are exactly the derivatives needed to perform efficient gradient-based optimization. Furthermore, such models allow use of powerful duality-based optimization methods. Adjoint-based methods are also at the heart of recent developments in *a posteriori* error estimation, which is a powerful and efficient manner for including adaptivity in simulation codes [Estep 2000]. However, significant research efforts, both in mathematics and computer science, are still required to properly extend these methods to complex, multiphysics, multiscale problems. The key research lines include treatment of multiscale adjoint models, incorporation of multiphysics problems with "black-box" subsystems and coupled stochastic-deterministic models.

Another direction involves the explicit recognition and management of the approximations inherent in multiscale models for purposes of optimization. In this technique, a search is made more efficient by repeated alternation between partial optimizations on coarse scales and approximate-refining calculations on fine scales. For example, this technique has been shown to be effective for derivative-free optimization of systems described (in part) by eigenvalue problems [Graf 2007]. Methods such as this that can explicitly exploit the multiscale nature of the underlying physical models must be further developed.

Extensible software to support multi-physics modeling

Simulation of novel devices is a large-scale software development undertaking. Systems for modularizing code, such as broker/component architectures [Kumfert 2006], abstract parallel simulation interfaces [Mascarenhas 1995], and parallel programming, must be brought to bear. Several categories of simulation "middleware" must be developed, which include tools integrating the details of novel device physics into existing abstract interfaces. Also, they include software embodiment of problem-specific multiscale modeling methodologies such as effective quantum-classical and discrete-continuous coupling [Park 2004] and effective medium methods [Fishchuk 2001], as applied to the particular types of physical systems and simulations domains envisioned here.

POTENTIAL COMPUTATIONAL SCIENCE IMPACT

The types of optimization problems described here epitomize the frontier of optimization research: highly nonlinear, with nonlinear constraints, a mixture of discrete and continuous variables in large domains with complex structure, multiple spatial and temporal scales, multiple objectives, multiple-physics models, large and disparate underlying component simulations, and derivatives often unavailable. The need to solve large-scale optimization problems with mixed continuous and integer variables will have a tremendous impact on optimization research required to address the well-known problems with mixed-integer nonlinear programming (MINLP). There are mixed-integer *linear* problems that current state-of-the-art algorithms cannot solve today, even using the top-of-the-line available computers. The types of hierarchical optimization problems arising in the applications described here will also help direct

optimization research. Indeed, algorithms for the solution of nonlinear hierarchical optimization problems may well prove to be necessarily heuristic in nature since even the linear bilevel programming problem is NP-hard in that the number of local minima is exponential in the number of variables [Dempe 2003].

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

As exemplified in the electronics and photonics industry, fast and efficient scientific computing with physics-based models integrated into system-level simulations significantly shortens the cycle for device development and optimization. Extensible software and simulation support environments are critical to make the transition to widespread use of CAD tools by the scientists and engineers directly engaged in PV research and development. Successful execution of research directed to the challenges outlined here can have a significant impact on third-generation PV systems.

TIME FRAME

Pilot research projects that encourage closer collaboration between the PV research community and experts in photonic device simulation could result in systematic improvements in first- and second-generation PV systems in the relatively near term (~4 years), with accelerating benefits as the research and development community more widely adapts to the use of CAD methodologies. Robust models and algorithms with adequate validation for the novel materials and architectures proposed for third-generation PV systems will take longer to develop, with significant impact in 6 to 8 years.

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PROCESSING SIMULATIONS FOR MANUFACTURING PV MATERIALS

ABSTRACT

An extraordinary amount of time and money is spent—almost exclusively through experimental trial and error—to design and engineer the manufacturing processes of PV devices with the desired performance characteristics. Numerical simulation can significantly impact and reduce the design time by predicting the possible successful procedures and parameters, but also by optimizing the anticipated large-scale manufacturing processes. These processes are described by multiscale and multi-rate phenomena that span orders of magnitudes in time and space, and by theories bridging atomistic to continuum, and from quantum to classical. To realize such numerical simulations will require developing and implementing robust, accurate, and scalable mathematical methods, algorithms, and software to enable accurate and applicable multiscale simulations on petascale and exascale computers.

EXECUTIVE SUMMARY

Significant advances in materials research, manufacturing processes, and computer simulations are required for PV energy production to be competitive with traditional non-renewable energy sources. Currently, an extraordinary amount of time and resources are spent connecting the desired PV device properties to the manufacturing process—almost exclusively through experimental trial and error. Numerical simulation can significantly reduce the time to design and engineer the production processes, as well as to optimize the manufacturing procedures by predicting optimal design and control strategies. In addition, computer simulations can contribute to basic research by elucidating the fundamental relationships of these multiscale systems.

The grand challenge is to develop accurate, robust, and scalable computational tools to support the basic research, engineering, and manufacturing processes of PV. The simulation tools must link *manufacturing process variables* at the reactor scale to the *material properties* and *performance* described by electronics structure, microstructure nucleation, and evolution models at the mesoscales, nanoscales, and atomic scales.

Research for PV manufacturing systems are required in chemical vapor deposition, crystal-melt growth, sol-gel synthesis, and polymer-extrusion processes associated with first-, second-, and third-generation solar cell technology. The physics of these systems spans multiple time and length scales, which create a number of difficulties.

There are five areas of scientific and computational challenges:

- Accurate, stable, and fast methods for representing operators and functions to evolve in time and to rigorously connect the multiple time, space, and theoretical models
- Scalable and fast differential algebraic equation and iterative linear equation solvers with preconditioners for the multiple-scale models
- Improved microstructure evolution algorithms and associated front-tracking algorithms for modeling multicomponent complex devices

- Fast and stable algorithms for coupling the continuum and microscale models derived from reactor and microstructure models
- Scalable analysis tools for run-time optimization of large parameter sets (e.g., eigenvalue analysis and bifurcation analysis).

SUMMARY OF RESEARCH DIRECTION

This priority research direction focuses on developing computational tools to support basic research and related manufacturing processes of PV associated with first-, second-, and third-generation solar cell technology. The goal is to (1) provide simulation tools that link *manufacturing process variables* at the reactor scale to the *material properties* and *performance* described by models at the mesoscales, nanoscales-, and atomic scales, and (2) to provide accurate and scalable algorithms and methods to aid in the optimal design and control of manufacturing processes and to elucidate fundamental physical insights into the processes.

Reactor scale

Manufacturing process variables are typically described with reactor-scale models. Important manufacturing techniques for solar cell technology that could potentially benefit from numerical simulation include chemical vapor deposition (CVD), crystal-melt growth, sol-gel synthesis, and polymer extrusion. CVD is used to produce thin-film PV materials for first- and second-generation technology including polycrystalline and amorphous Si, and compound semiconductors such as CdTe or CuInSe. CVD processes are designed to produce films with desired properties and uniformity across the substrate. These characteristics are controlled by the operating conditions (e.g., inlet species concentrations, inlet flow rates, pressure, temperature, plasma power) and the geometry of the reactor. Identifying the correct procedures and operating conditions to construct the desired film is a major challenge—especially as the material complexity increases, the size of the substrates continues to increase, and the desired final thickness of the film decreases.

Traditionally, CVD processes are developed using carefully executed design of experiments. This approach is slow, expensive, and does not provide insight between process parameters and film properties. This lack of insight results in the need for additional experiments each time a new property is desired. Numerical simulation of the CVD process can lead to unique insight into the complex coupled chemistry, energy, multi-species transport, and flow patterns that determine the film characteristics [Salinger 2004]. Such research can lead to a revolutionary science-based optimization of the reactor design to address long-standing issues of film uniformity.

Crystal melt growth manufacturing process (for crystalline substrate material including Si for PV) faces similar technical challenges. Growth processes are also similarly developed via costly design of experiment. Because the final crystal properties are highly sensitive to both growth and subsequent annealing (cool-down) processes, equipment design deficiencies may prevent the desired properties, even with the most thorough experimental process-development activities. Advanced modeling and simulation capabilities have the potential to improve material quality by improving the understanding of furnace operational programs (control strategies) during the

material growth and annealing processes [Sonda 2005]. As material specifications become more challenging, simulations are needed to both optimize the design and operation of the growth apparatus. Difficulties to address include control of melt contaminants, resolving necessary length scales ranging from characteristic crystal-lattice dimensions (nm to μm) up to furnace dimensions (m), scalable coupling of the physics, and capturing the solidification and evolution of materials described at the microscopic level. A science-based approach to process and hardware design can result in higher-performing materials and increased yields that have the potential to significantly reduce the cost of PV devices, thus making them competitive with non-renewable energy sources.

For third-generation PV systems, process-simulation tools would potentially have the greatest impact. These systems—for example, polymer/nanoparticle hybrid dye-sensitized solar cells, or quantum-dot or nanowires-based solar cells—show great promise [Mao 2007], but cannot be made on a larger scale using conventional semiconductor manufacturing processes. These systems will likely be made via a combination of disparate unit operations involving advanced materials processing techniques such as high-throughput plasma or sol-gel synthesis of nanoparticles and more mature manufacturing operations such as polymer blending and extrusion. For some components of third-generation PV systems, there is no high-throughput route yet—this scale-up has not yet been performed. Although many operations can be simulated for other manufacturing processes, once the same types of operations are performed with nanomaterials (e.g., polymer blending), key phenomenological relationships may not apply. Thus, developing quantitative process models for these operations based on atomistic-to-continuum approaches will be essential to perform necessary scale up and process integration.

Meso/nano/atomic scales

As noted above, to accurately describe PV processing, models should be extended to the meso-, nano-, and atomic levels. For example, polycrystalline thin-film deposition processes require knowledge of the microstructure evolution. This includes a description of the nucleation and growth of individual grains during deposition, as well as understanding their subsequent evolution, leading to strategies to control/direct these processes. This requires applying electronic structure techniques (e.g., DFT) to assess relevant atomic-scale interactions, using these or model interactions in MD simulations targeted to explore key dynamical processes; developing statistical mechanical models to follow structure development and evolution on the nano- and mesoscale (as well as on the relevant timescale); and using such treatments to inform more versatile and efficient coarse-grained modeling of mesoscale structure and morphology.

SCIENTIFIC AND COMPUTATIONAL CHALLENGES

Scalable differential algebraic equation solvers for process modeling

CVD and crystal-melt growth systems are typically described at the reactor level by large sets of high-index differential algebraic equations (DAEs). The physics involves flow (Navier-Stokes), energy, and species transport coupled to complex chemical-reaction mechanisms. The timescales can range from $1x10^{2}$ to $1x10^{-12}$. The scientific challenge for these systems is to build fast and robust DAE solvers to enable the analysis of large parameter spaces. Difficulties center on

developing stable and accurate discretizations in both time and space and developing O(N) scalable solvers for multiprocessor and multicore architectures.

The disparate spread of time and length scales makes implicit, semi-implicit, and operator-split time integration appealing to follow the timescales of interest. Time-integration research into global error estimation for high-index DAE systems is virtually nonexistent and should be addressed. Stable and accurate operator-splitting methods are lacking for the systems of interest. Fast iterative linear solvers that scale to tens or hundreds of thousands of processors are required for implicit and semi-implicit solvers. An important path to scalability is the development of better preconditioning techniques such as physics-based and multilevel algorithms.

Efficient and scalable micro-structure evolution modeling

To illustrate the challenges for electronic structure/MD/stat mech/coarse-grained modeling, we return to the example of describing microstructure in polycrystalline thin films. Tremendous advances have been made in predictive modeling of homoepitaxial and low-misfit defect-free heteroepitaxial thin-film growth [Evans 2006]. However, such a level of treatment of polycrystalline thin films will be far more difficult and computationally demanding—although efforts have begun to apply multiscale modeling to more complex thin-film deposition systems [Baumann 2001], and there has been some assessment of strain evolution on polycrystalline films [Floro 2001]. To achieve this goal for thin-film PV systems, atomistic-level studies of substrate structure, substrate-film interactions, grain nucleation and growth, and grain-boundary evolution might be incorporated into (or at least guide) coarse-grained mesoscale modeling. For the latter, phase-field methods could potentially capture both grain morphology and growth dynamics incorporating strain effects, as well as complex deposition and diffusion dynamics including compositional heterogeneity. For nucleation control, modeling of deposition on pre-patterned substrates might be explored.

Robust multi-physics coupling

Coupling models between the microstructure and reactor scale and between different physics can critically impact the simulation. Naive couplings/operator splittings can produce a numerically unstable model that can fail to converge to a solution [Ropp 2004; Yeckel 2006]. Complexities to address include the influence of the strength of interaction between models, enforcing conservation across model interfaces, and accuracy and efficiency of the techniques.

Scalable analysis tools

The ability to simulate a manufacturing process in itself is not enough to make a simulation tool useful to designers. For systems with large numbers of design parameters, the number of runs to adequately cover the design space can be intractable. Advanced analysis algorithms can reduce or eliminate the need to explore the entire parameter space by directly computing the optimal quantity of interest, resulting in a run-time analysis that can be orders of magnitude faster.

Scalable and efficient optimization algorithms are required to address *control and design* (maximizing system performance) and *inverse problems* (fitting parameters to minimize

deviation from experimental data). For example, a designer wanting to achieve a specific doping profile or morphology via CVD [Choo 2005] could use multiparameter optimization to directly calculate the required operating conditions and geometry of the reactor. This will require further research into more efficient (and typically more invasive) algorithms: for example, full-space methods, reduced-space sequential quadratic programming, interior-point methods, and adjoint computations (required for estimating Hessians and for sensitivity analysis) [van Bloemen Waanders 2002].

Scalable eigenvalue analysis is an invaluable tool for designers. For example, CVD reactors have been shown to generate buoyancy-driven instabilities/oscillations that can ruin film uniformity [Pawlowski 2001]. Eigen analysis can help users determine if the operating regime is unstable. Once instabilities are identified, algorithms that map out high-dimensional manifolds in phase space can show designers stable regions of operation. A challenge will be to build robust and scalable tracking algorithms.

POTENTIAL COMPUTATIONAL SCIENCE IMPACT

Over the course of developing the simulation tools, significant progress in algorithms development will have to occur to make the problems tractable for designers. Research into discretizations, multi-physics coupling, time integration, linear solvers, eigensolvers, bifurcation analysis, and optimization will have to be advanced. Although targeting solar PV systems, the algorithms developed are general enough to be leveraged by other scientific fields.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

Overall, numerical simulation can help transition solar energy technology to be a competitive energy source. Significant R&D investment in developing process simulation tools for PV materials manufacturing will have an impact—from materials discovery in the laboratory to large-scale manufacturing. For rapid adoption of new higher-efficiency PV systems, it is critical to be able to identify the best material, but also**,** the lowest-cost path to the marketplace.

In the manufacturing of first-generation PV materials, there is an opportunity for impact via science-based optimization to improve manufacturing efficiency. Second-generation PV systems based on more-complex compound-semiconductor architectures have higher conversion efficiencies**,** but are presently cost-prohibitive to manufacture. Process simulation could have significant impact in reducing the cost to manufacture these systems. Third-g**e**neration PV systems have the greatest potential for impact. Scale-up for production and handling of nano-materials in manufacturing processes both remain open issues. Finally, a full process-simulation capability could also be used in conjunction with life-cycle analysis to down-select materials systems/manufacturing processes that are the most sustainable with respect to environmental impact.

TIME FRAME

The time frame to impact renewable energy ranges from 6 to 10 years. Depending on funding levels, algorithms research can range from 3 to 5 years. Additional time (probably another 3 to 5 years) will then be required for the algorithms to be integrated into either existing or new codes.

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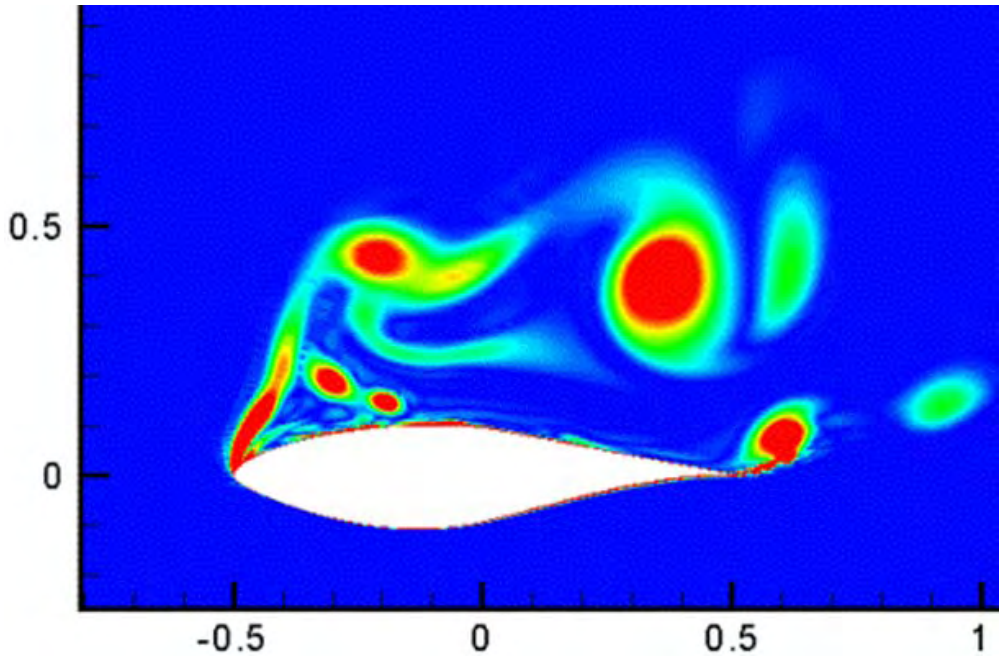
RENEWABLE ELECTRICITY — WIND ENERGY



A two-dimensional section extract of a wind turbine flow field developed with computational fluid dynamics modeling; the intricate structure of the flow field is responsible for powerful aerodynamic loads and complex aeroacoustic emissions. Graphic courtesy of P. Morris, L. Long, and K. Brentner, Pennsylvania State University.

CHARGE TO PANEL

Advanced computational modeling will be crucial to achieving the massive penetration targets for wind energy established by the current administration. Accurate physics-based aerostructural and aeroacoustic models will be needed to reliably predict the energy capture, structural loads, and radiated noise of turbines.

The charge to the members of the Wind Energy breakout session was to identify priority research directions in this area related to the following:

1. Aeroacoustic and aerostructural modeling for design and operational assessment
2. Computational wall-clock times, including gridding, convergence, and post-processing
3. The need for experimental and test data for assessing accuracy
4. Model verification and validation requirements and related issues.

SESSION BREAKOUT LEADERS

Larry Carr, U.S. Army Aeroflightdynamics Directorate (retired)
Earl Duque, Intelligent Light and Northern Arizona University
Scott Schreck, National Renewable Energy Laboratory

OVERVIEW AND BACKGROUND

By 2030, wind energy technologies have the potential to generate 20% of total U.S. electricity production. The U.S. Energy Information Agency estimates that our nation's electricity demand will rise by 39% in the years 2005 to 2030, and will reach 5.8 billion megawatt-hours (MWh) by 2030. To produce 20% of that electricity, U.S. wind power capacity will need to exceed 300 gigawatts (GW), corresponding to an increase of more than 290 GW over 2006 levels. A recent analysis by the U.S. Department of Energy (DOE), National Renewable Energy Laboratory (NREL), and the American Wind Energy Association (AWEA) demonstrated the technical feasibility of expanding the U.S. wind industry to this level. While the 20% wind scenario is not a prediction of the future, it does represent a plausible scenario for the role of wind energy in the U.S. electricity generation portfolio.

Scalable Wind

By 2030, wind energy technologies have the potential to generate 20% of total U.S. electricity production. Further advances in wind-turbine design enable this technology to generate ever-increasing amounts of power per unit surface footprint. Higher unit capacity turbines also facilitate grid integration, making it possible to achieve the 2030 goal.

In 2006, wind energy production costs ranged from 5 to 8.5 cents/kWh (before any reduction by the Production Tax Credit, at 1.9 cents/kWh in 2006). Since 2004, turbine costs have increased due to strong demand for new wind equipment, commodity price increases for materials such as steel and copper, and the weakening U.S. dollar. Clearly, current turbine technology has enabled wind to become and remain a viable power source in today's energy market. However, wind energy still provides less than 1% of total U.S. electricity generation. Improving turbine technology by reducing capital cost, increasing capacity factors, and mitigating risk through enhanced system reliability has the potential to increase wind energy's contribution to the nation's generation portfolio. Appropriately applied, advanced computational predictive capabilities hold strong potential for improved turbine designs and reduced performance uncertainties.

Producing 20% of the nation's electricity from wind technology presents a daunting challenge. To meet this challenge, several wind turbine technological advances are in active development, and several others are entering the development process. However, the risk associated with introducing new technology at the same time that manufacturing production is scaling up and accelerating to unprecedented levels will be substantial. Before turbine manufacturers can stake the next product on a new feature, the performance of that innovation needs to be firmly established and the durability needs to be characterized as well as possible. These risks are mitigated by research and development (R&D) investment, including extensive component and prototype testing before deployment. Because of tightening resource constraints and compressed timelines in product development, physics-based computational modeling has the potential to achieve importance comparable to that of test and experimentation—provided that research is begun promptly and vigorously pursued to establish requisite foundational capabilities.

Ultimately, investment in wind technology R&D aimed specifically at improving machine technology holds the potential to save billions of dollars in energy costs annually with an electricity portfolio that includes 20% wind technology generation. Various risks threaten the U.S. wind industry's ability to meet this challenge. Wind-farm performance, in terms of revenues and operating costs compared with the estimated revenues used in plant financing, will drive the risk level of future installations. The consequences of these risks both *directly* affect the revenues of wind equipment manufacturers and wind farm operators, and *indirectly* affect the continued growth of investment in wind. Direct impacts include increasing operations and maintenance (O&M) costs, poor availability driven by low reliability, and poor wind-farm array efficiencies. Indirect impacts include increased cost of insurance and financing, slowing or stopping development, and loss of public support.

WORKSHOP CHARGE FOR WIND ENERGY

Advanced scientific and engineering computational modeling will be crucial to reliably achieving the future 20% target for wind energy penetration. The charge to the members of the wind energy breakout session was to identify priority research directions in wind energy specifically related to aerodynamics, aeroelasticity, and aeroacoustics.

OVERVIEW OF WIND PRIORITY RESEARCH DIRECTIONS

The three priority research directions identified during four breakout sessions are summarized below. These three areas were highlighted because of potential impact to wind energy cost effectiveness and deployment, as well as complex scientific and engineering issues that can be uniquely addressed using high-performance computation. Overall, these three areas define a continuum of temporal and spatial scales, and they represent a progression that begins with scientific research and culminates in engineering application.

Reliable aerodynamics/acoustics prediction

This research direction will use computations to clearly understand the physical details underlying turbine aerodynamics and aeroacoustics, and thus, it will establish a rational basis for subsequent work. Spatial scales will extend across nine orders of magnitude, from microns (turbulence scales) to a kilometer (extreme wake length). In connection with associated temporal scales, this will imply large mesh sizes and extended execution times. Computational efficiencies will be enhanced by automatically adapting both meshes and algorithms, and wall-clock times will be reduced by advances in scalability. Converged data sets will grow into the petascale range and will require data-mining techniques for full exploitation.

Robust design and performance

This research area will develop and validate accurate, reliable methodologies for wind-turbine design and performance prediction. The general aeroservoelastic problem thus addressed will entail predictions encompassing aerodynamics, structures, and controls. To accomplish this demanding task within time constraints imposed by industrial design timelines, a hierarchical

suite of aerodynamics, structures, and controls models will be developed. This will allow designers to flexibly balance accuracy and detail with computational intensity and turnaround time. Ultimately, this suite of aerodynamics, structures, and controls models could be coupled using appropriate methodologies to yield a multidisciplinary design-optimization capability.

Turbine reliability and longevity

Nominal 20-year lifetimes projected for wind turbines, combined with the impossibility of controlled atmospheric testing of full-scale machines, have drastically limited knowledge of turbine component wear and failure modes. Computational strategies will be developed to address pressing issues concerning machine reliability and failure under both long-term routine operation and infrequent episodes of extreme loading. These strategies will include methodologies specifically suited to simulating complex aerodynamic loads and nonlinear structural responses over extended physical times. Because of the lengthy physical times involved, methods likely will involve reduced-order algorithms constructed using results from the first research direction above for guidance.

RELIABLE AERODYNAMICS AND ACOUSTICS PREDICTION

ABSTRACT

Reliable physics-based aerodynamics and acoustic prediction tools are needed to enable the advanced designs that can provide low-cost wind energy and provide the confidence needed for greater market penetration. Wind-turbine analysis benefits from a range of computational tools developed for rotorcraft and other aerospace applications, but those tools are not well suited for the unique aspects of the wind-turbine operation—namely, extensive dynamic stall, gusts, rapid changes in wind direction, and uncertainty of the complete range of operating conditions that will be experienced during the operational lifetime. What is needed are wind-turbine-specific enhancements to available physics-based tools and the development of adaptive tools that are scalable to a large number of processors.

EXECUTIVE SUMMARY

The aerodynamic flow field around large wind turbines is the driver that determines the structural loads experienced by the turbine blades and tower, and the torque transmitted through the drive train to the generators. The unsteady aerodynamic loading is also a primary source of noise generated by the turbine. A thorough understanding of the complicated, unsteady, 3-D flow fields is critical for cost-effective design and efficient operation. The flows encountered in wind-turbine operations are unique among rotor operations because rapid flow-direction changes, inflow turbulence, and flow transition can result in large transient loading fluctuations. Current empirical analysis tools have significant uncertainty that ultimately results in high maintenance cost, reduced turbine lifetime, and higher energy costs with less market penetration.

The primary way to reduce the uncertainty in operating conditions, loads, efficiency, and effectiveness is to develop a first-principles prediction capability for the aerodynamics and acoustics. Such capabilities have not been developed for wind turbines. Although wind turbines benefit from theoretical and computational advances made for rotorcraft and other aerospace applications, the range of variability, rapid changes in flow direction, and extreme operating conditions (e.g., gusts) are beyond the current state of the art. The development of large eddy simulation (LES) or hybrid LES tools is necessary to account for the flow separation, dynamic stall, blade loading, and broadband noise prediction. Such predictions are critical for quantifying and mitigating uncertainty and developing more advanced reduced-order models such as Blade Element Momentum (BEM) and Proper Orthogonal Decomposition (POD) that can be used for advanced wind-turbine designs.

Uncertainty quantification and reduction will lead to less unscheduled maintenance and increased investment and market penetration. Continued improvement of the physics-based tools will lead to improved reduced-order models that can be used in design, while representing the flow much more accurately than those today. As confidence increases, and as the tools mature, this increased confidence should lead to increased wind-energy penetration into the market—ultimately reaching the 20% goal by 2030.

SUMMARY OF RESEARCH DIRECTION

The aerodynamic flow field around large wind turbines is the driver that determines the structural loads experienced by the turbine blades and tower, and torque transmitted through the drive train to the generators. The unsteady aerodynamic loading is also a primary source of noise generated by the turbine. A thorough understanding of the complicated, unsteady, 3-D flow fields is critical for cost-effective design and efficient operation. The flows encountered in typical wind turbine operations are unique among rotor operations because rapid flow-direction changes, inflow turbulence, and flow transition can result in large transient loading fluctuations. Operator data collected by the National Wind Technology Center indicate that state-of-the-art wind turbines are already quite capable, offering 98% availability and 80% of the maximum theoretical rotor efficiency. However, there is significant uncertainty in operation of these machines because the designs are based on an empirical understanding of the flow and operating conditions in which the turbines will operate. One outcome of this uncertainty is that the current generation of machines may encounter conditions outside the design specifications and the lifetime will be substantially less than originally planned. The uncertainty also may lead to substantial overdesign or high maintenance costs—both resulting in significantly higher energy costs than originally estimated.

The primary way to reduce the uncertainty in operating conditions, loads, efficiency, and effectiveness is to develop a first-principles prediction capability for the aerodynamics and acoustics. Such capabilities do not currently exist for wind turbines. Although wind turbines benefit from theoretical and computational advances made for rotorcraft and other aerospace applications, the range of variability, rapid changes in flow direction, and extreme operating conditions (e.g., gusts) are beyond the state of the art. Furthermore, the range of spatial and temporal scales that must be predicted for large wind turbines ranges from turbulence in a blade boundary layer (which can be as small as microns) to the extent of the wake of the turbine and the acoustic propagation to nearby communities (which may be kilometers).

The tools are also needed to model special devices and characteristics of modern wind turbines. Some of the devices of great interest include: new advanced airfoils, such as flat-back airfoils, which have extensive unsteady separated flow; flow-control devices, such as deployable microtabs, which control the boundary layer and circulation around the airfoils; and elastically tailored blades that incorporate capabilities such as bend-twist coupling.

The development of first-principles aerodynamic tools to capture the unique unsteady, separated 3-D flow fields with turbulence and transition that drive wind turbines—and the resulting aerodynamic loading and acoustic fields—is critical for quantifying and mitigating uncertainty, and for developing reduced-order models that can be used for advanced turbine designs.

SCIENTIFIC CHALLENGES

Reliable aerodynamics and acoustics prediction faces the two major challenges described below.

Current techniques cannot accurately predict performance or lifetimes of wind turbines

Current state-of-the art tools, which have been primarily developed for aerospace applications, have difficulty in accurately predicting turbine rotor aerodynamics, even in the ideal conditions found in a wind tunnel [Simms et al. 2001]. Currently, empirical modeling is used extensively in both aerodynamics and aeroacoustics. This is necessary mainly because the aerodynamic tools used in the design process must be relatively fast. Industry needs to run a large array of computations to analyze each rotor design—all of which must be completed in about two days in order for designer to evaluate all the configurations typically studied in developing a new design. The array of computations is large because a wind turbine must operate over a wide range of wind conditions, and there is significant unsteadiness at each nominal condition that must also be modeled.

Figure 1: Unsteady Aerodynamics Experiment modeled with computational fluid dynamics, showing the wake from the turbine tower and the vortex from a blade tip. (Graphic courtesy of Fredrick Zahle, Risø National Laboratory)

Although current "fast" tools are available and are used, these empirically based tools are not assured to be particularly accurate—especially for significant departures from current design (i.e., significant increases in size). Furthermore, current certification requirements specify "extreme conditions" for which the turbine must be designed, but it remains uncertain whether these conditions are in fact extreme, because these are based on test data that are limited in resolution, as well as duration. A "50-year" event may actually occur much more often or be more severe in magnitude, leading to higher-than-anticipated loads and failure rates. In fact, current utility-class horizontal-axis wind turbines have been experiencing premature gearbox failures. This is a unique problem to wind turbines because similar-sized drivetrain technology is used in other applications without such failures. It is likely that the aerodynamic loading and transient loads transmitted from the rotor to the gearbox are outside the expected values in the design (or they occur more frequently than the designers anticipated).

Some new turbine designs are planned to be significantly larger than the current 2.5–3 MW devices in operation, especially for offshore deployment. These turbines will have diameters well over 120 m. Such large rotor blades will necessarily be very flexible structures that will be extremely challenging from both a static and dynamic viewpoint. It is also desirable to operate

new machines at higher tip speeds to increase the efficiency. But noise considerations and incomplete understanding of the noise currently limit the maximum operating speeds.

Physics-based methods need to be developed and validated to replace existing inadequate models for wind applications

Physics-based methods are needed to provide an understanding and quantitative assessments of new designs that are significantly outside the current design practice. Once validated, the physics-based models can become "truth models" that provide the details necessary to develop reduced-order models that are more accurate and reliable, but still fast enough for use in design. Furthermore, physics-based models should be capable of predicting extreme events such as dynamic stall, rapid flow-direction changes, and gusts, which are unique in wind-turbine operations. These conditions will require computational fluid dynamics with either large-eddy simulation (LES) or hybrid LES to account for the flow separation, dynamic stall, and broadband noise prediction. (The widely used Reynolds-Averaged Navier-Stokes equation with one- or two-equation turbulence models will not be sufficient.) Structural analysis codes are currently sufficient for blade analysis and design. But the anticipated large, flexible blades—which may be composed of multiple segments—will require additional tool development. Also needed is coupling between computational fluid dynamics and computational structural dynamics.

Computational fluid dynamics (CFD), computational aeroacoustics (CAA), and computational structural dynamics (CSD) tools have been developed for rotorcraft and other aerospace applications. However, they do not address the unique aspects found in wind applications. Nevertheless, the wind-energy research community can leverage these tools and extend their capabilities.

NEEDS FROM COMPUTATIONAL SCIENCE

To meet the technical challenges, several computational science developments are needed.

Develop techniques to model and quantify flow physics across 10^9 scale range (e.g., microns to kilometers)

To accurately compute the flow field and associated blade loading, it is necessary to compute the flow over a very large range of scales—from the small-scale turbulence in viscous boundary layers to the scale of the rotor wake, which is on the order of several rotor diameters. The combination of high grid resolution to capture the smallest details and the large extent of the computational domain leads to very large computations (large memory and run time). Such computations cannot currently be done by "brute force" even on the largest parallel machines. But they are necessary to capture the flow separation, transition to turbulence, and dynamic stall—all of which have a strong impact on rotor loads and noise.

Develop techniques to adapt grids and models

One way to reduce the computational effort without loss of accuracy is to dynamically adapt the grids such that high resolution is used only in the regions where it is needed. This can significantly impact the total number of grid points used in the computation, but it makes

algorithm development and load balancing on parallel computers difficult. Another way to improve computational efficiency is to adapt the computational model in limited regions of the flow such that higher accuracy but more computationally expensive models, such as LES, are only used in regions such as boundary layers, wakes, and regions of separation. Less computationally expensive models, such as Reynolds-averaged Navier-Stokes or detached eddy simulation can be used in the vast majority of the flow field, thus saving substantial computational effort.

Develop techniques to improve scalability of algorithms

Current CFD codes used for rotorcraft and wind-turbine applications (e.g., OVERFLOW) do not currently scale well with large numbers of processors. Future high-performance computing (HPC) tools will need to use the emerging high-performance computing clusters; hence, new codes will have to be able to run as efficiently (i.e., balancing communications and computation costs) on thousands of processors. The Department of Defense HPC Institute for Advanced Rotorcraft Modeling and Simulation (HI-ARMS) at the Army's Aeroflightdynamics Directorate is developing new codes specifically to address many of the scaling, grid-generation and adaption, and coupling issues for rotorcraft (http://www.hpcmo.hpc.mil/Htdocs/INSTITUTES/index.html). It would be valuable to leverage this work by adding the capabilities needed for wind turbines.

Develop techniques to mine petascale data sets

Long-term, well-resolved computational characterizations are needed to accurately capture the range of gusts, wind-direction changes, and other conditions in which wind turbines operate. Such computations, done on billion-node grids for million time-step durations lead to overwhelmingly large petascale data sets. A thorough understanding of these large data sets and the ability to find the critical information are needed to help provide understanding and remove uncertainty. However, due to the nonlinear, time-dependent nature of wind-turbine flow fields, flow structures and events that control important aerodynamic loading episodes may be spatially and/or temporally compressed, and thus, not readily detected. Automated data-mining methodologies will be required to interrogate these large data sets efficiently, identify key flow structures and events reliably, and arrive at a thorough comprehension of key machine loads.

Advances are needed in data comparison between coupled CFD-CSD-CAA and experiments. Also needed are more-effective case and data management techniques for computations and experiments.

Figure 2: Wind-tunnel testing achieves inflow control, but constrains turbine size.

Validate and verify methods

It is important to validate the physics-based tools developed in this effort. However, the extremely fine spatial and temporal resolution of which these tools are capable will pose significant challenges for validation, requiring either adaptation of existing measurement techniques or development of new ones. In addition, the dilemma will remain that pits dynamic parameter matching against inflow control, because full-scale turbines cannot be wind-tunnel tested, but field testing surrenders inflow control. Well-designed experimental measurements of critical flow features and operating conditions are required to validate the tools. Furthermore, it will be necessary to try to understand the flow physics of extreme cases to aid in developing and verifying models. Both wind-tunnel tests and field tests are needed. Ultimately, greater understanding furnished by improved computational models will likely help to provide the needed improvements to wind-tunnel and field-measurement capabilities.

Expand computational resources

Physics-based tools will be computationally expensive—both in terms of computer memory and computer time. LES computations for a full rotor will nominally require hundreds of processors for problems with several hundred million grid cells for a single run. Substantial HPC cluster resources will be required.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

The success of computational science focused on the needs of wind energy will have several potential impacts.

Improved aerodynamic and acoustic prediction will enable improved turbine designs necessary for high penetration

Accurate physics-based aerodynamic and acoustic predictions will reduce the uncertainty in the operational environment in which a turbine must operate and will reduce the dynamic machine loading. This, in turn, will lead to efficient and robust structural and control design. Quantifying and reducing uncertainty will lead to less unscheduled maintenance and increased investment and market penetration.

This fundamental work will provide the basis for improved design capability

The physics-based tools will support the development of robust design and performance prediction tools. Fundamental understanding of the aerodynamic loading will enable the accurate prediction of turbine longevity and reliability. One way to think of this is if we can drive up the tip speeds without increasing acoustics, then we can build lighter machines that are more cost-effective. The overall metric is low cost of energy.

TIME FRAME

Reliable aerodynamics and acoustics predictions are time critical to enable 20% penetration by 2030

During the first five years following project inception, tool development will have limited direct impact on the design of new turbines. But it is likely that as fundamental understanding is developed (e.g., what is causing premature gearbox failures in current-generation machines), it can be applied. Improved understanding should lead to substantial improvements in new designs in the 5–10-year period. Continued improvement of physics-based tools will lead to improved reduced-order models that can be used in design, while representing the flow much more accurately than those today. Increased confidence and more mature tools should lead to increased wind-energy penetration into the market—ultimately reaching the 20% goal by 2030.

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ROBUST DESIGN AND PERFORMANCE

ABSTRACT

Achieving 20% of U.S. energy production from wind by 2030 will require accurate prediction and enhanced performance under design-condition wind and a dramatic increase in the confidence of predicting the lifetime and survivability of extreme events. Current trends toward improving modeling capacity will not achieve these objectives without the bold steps in developing hierarchical fluids and structures models, and improved coupling not only between the fluids and structures, but also, flow control and optimization techniques that can simultaneously balance performance with survivability of extreme events. These developments will draw on and heavily integrate with ongoing developments in computational science, including massively parallel CFD and CSD solvers, parallel, anisotropic mesh adaptation, adaptive model selection, reduced-order models, scale-linking models, and verification and validation procedures, together with being highly coordinated with experiments.

EXECUTIVE SUMMARY

Achieving 20% of U.S. energy production from wind by 2030 will require accurate prediction and enhanced performance under design-condition wind and a dramatic increase in the confidence of predicting the lifetime and survivability of extreme events. Current trends toward improving modeling capacity will not achieve these objectives without the following bold steps: (1) developing hierarchical fluids and structures models, including hybrid models that combine strengths of two or more modeling levels, (2) developing improved coupling between the fluids and structures, but also recent advancement in flow control that hold promise of responding to the inherently dynamic wind environment, and (3) developing optimization techniques that bring these developments into a design environment that can simultaneously balance performance with survivability of extreme events. These developments will draw on and heavily integrate with ongoing developments in computational science, including: (1) massively parallel CFD and CSD solvers, (2) parallel, anisotropic mesh adaptation guided by discretization error estimation, (3) adaptive model selection that selects a model based on a regions estimate of its modeling error, (4) reduced-order models derived from and/or calibrated against high-fidelity simulations, while also contributing to modeling-error estimates (e.g., confidence level of a model for a particular class of flow), (5) scale-linking models that define the information that must be exchanged between hybrid models at two different scales to maintain accuracy, and 6) verification and validation procedures. Finally, focused experiments that are highly coordinated with the numerical simulations will be required to achieve this vision. If these developments are carried out by 2012, the petascale simulation tools that are scheduled to be online at that time will enable the design of wind turbines with high performance and long life, thereby raising the reward-to-risk ratio—and subsequently, the investor confidence—to a level necessary to achieve 20% penetration of the energy market by 2030.

SUMMARY OF RESEARCH DIRECTION

Develop hierarchical fluids and structures models

Fluids and structures models have varied fidelity: they range from very simplified models that neglect complicated physics and can be performed quickly, to more-complete models that require extensive computational resources. Although a hierarchy of models for both fluids and structures is known, there remain considerable challenges to effectively leverage the hierarchy in a way that yields the best modeling capacity for very complex fluid-structure interactions encountered in wind-turbine design. Even ignoring coupling (which is considered below), there are grand challenges in simply modeling the fluid dynamics around a perfectly rigid wind turbine due to the unsteady and spatially irregular nature of the Earth's (turbulent) boundary layer, the very high Reynolds number flow created by a large turbine blade, and the complex fluid mechanics associated with smooth separation, stall, and tower-wake interactions. Even using petascale computers, the 100-m span of wind-turbine blades will preclude [Spalart 1997] application of the highest two levels of continuum fluid models: DNS (Direct Numerical Simulation, or no model) and LES (Large-Eddy Simulation, or model only the smallest scales). Simpler models such as RANSS (Reynolds-Averaged Navier-Stokes Simulation), which average out all of the turbulent fluctuations, are known to be incapable of predicting smooth separation, which is of critical importance for flow over turbine blades. Therefore, the hierarchy developed must include hybrid models that apply RANSS models to the regions where these models are accurate, but switch over to LES in regions where the higher fidelity is required. The physics of this "switch over" is beginning to be understood for statistically stationary flows [Lund 1998; Araya 2006]. But there remain grand challenges to extend it to the dynamic environment of wind turbines, where the location of the "switch over" varies with rotor rotation and wind conditions. The structural hierarchy is somewhat more mature, but has similar issues [Bauchau 2007].

Hybrid models apply high-fidelity models only where required, simple models elsewhere, and manage "switch-over" in between (S_3 interior data augments S_1 model boundary data).

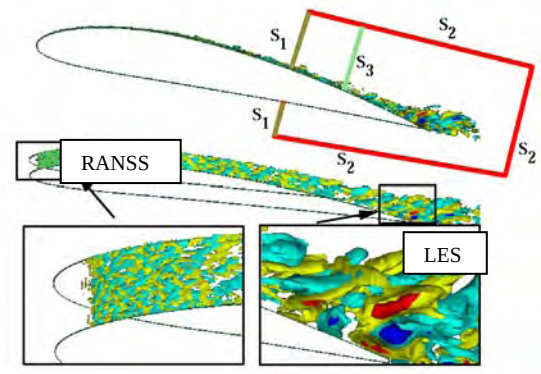

Figure 3: Vorticity contours from LES of a narrow section of an airfoil superposed with potential hybrid model developments.

Develop aeroservoelasticity capabilities that couple fluids, structures, and controls to predict blade deflections and loads

The coupling of the aforementioned fluids and structures modeling hierarchies with controls is required to predict and manage blade performance and mitigate wind-turbine damage. This will be achieved only with accurate and efficient coupling of the various physics models. For example, synthetic jets [e.g., Glezer and Amitay 2002; Amitay and Cannelle 2006] have been shown to be capable of "aero-shaping" the blade (creating well-controlled separation regions that dynamically change the flow path, and thus, the pressure distribution) to either increase or decrease its lift [e.g., Amitay and Glezer 2002; Bales et al. 2003; Glezer et al. 2005; Seifert et al. 1996]. Such a process, responding to onboard sensing, could extract maximum power out of variations around the "design condition" wind. But perhaps more important, it could decrease lift in gust conditions that create dangerous unsteady loads on the blade that are transmitted through the structure. This highly dynamic interaction of the structure, primary fluid flow, and flow control requires the development of coupling beyond current fluid-structure interaction (FSI) to include the coupling with controls to realize this vision. Furthermore, experimental efforts that complement the computational developments in the controls area will be required for guidance and validation. The design of the aeroservoelastic coupling (e.g., tight vs. loose) must be guided by stability, accuracy, and efficiency of the complete system.

Develop optimization approach for wind-turbine design

With the hierarchy of models in both structures and fluids coupled together with robust control models, the next stage of research would include optimization techniques to accelerate and raise the confidence in wind-turbine design. The unsteady nature of the problem and the wide variety of conditions pose great challenges. Specifically, although performance should be optimized for common wind conditions, a hard constraint is the survivability of a variety of extreme events already part of the certification process.

SCIENTIFIC CHALLENGES

Current techniques cannot accurately predict performance and seriously overpredict lifetimes of wind turbines

Current approaches to design and certification use very simplified models that do not account for enough physics to accurately predict turbine performance. Of greater concern, the unsteady nature of loads on the rotors appears to be poorly represented, leading to a high failure rate in the gearboxes, despite already substantial factors of safety.

Develop and validate predictive capabilities for turbine design and performance incorporating fluid-structure interactions

Developing, verifying, and validating the fluid-structure interactions with controls as described above can substantially improve the performance, lifetime, and operations cost of wind turbines, thereby making them more viable financially.

NEEDS FROM COMPUTATIONAL SCIENCE

Develop massively parallel, scalable, adaptive computational algorithms

Only a few of the currently available CFD and CSD solvers scale to the level required to carry out the simulation required. And even these solvers do not yet include all the capabilities described above. As these developments come on line, there will be a need to continuously improve their parallel performance. Furthermore, the flow physics will require the use of highly anisotropic grids—with the degree of anisotropy depending strongly on spatial location, but also, on time (e.g., rotational position of the rotor). Because a priori grid-size selection would be impossible, this suggests a strong need for development in massively parallel anisotropic mesh adaptivity guided by error estimation/indication. In addition to mesh adaptivity, model adaptivity will also be required to define the aforementioned "switch over" locations for models. This requires a new and different model error estimation/indication where the confidence of a given model is characterized. Achieving this vision will require developing and validating reduced-order models from the higher-fidelity predictions. Recursive application of this approach between successive levels is required to develop the coupled hierarchical suite of models appropriate for design and performance prediction. To be clear, this comparison of solutions between scales identifies the confidence level that a given model can achieve under particular conditions, but it also is useful in identifying the type of information that must be transferred to accurately "switch over" at the hybrid model boundaries. In the sidebar above, vorticity isosurfaces are shown from an LES applied to a very narrow (5% of chord to maintain a tractable computation) section of the domain. This type of simulation, although not representing the complete geometry, provides guidance to RANSS models and a check on the correctness of hybrid models of the boundary S_1 between the LES region (inside the box) and the RANSS region (outside the box).

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

Dramatically improve confidence in the design of lighter, larger, more-efficient wind turbines

The fully coupled, hierarchical suite of fluid-structure-controls models proposed to be developed will accurately reflect the unsteady, turbulent environment that wind turbines must perform in. They will thereby accurately reflect the unsteady loads and forces throughout the turbine design, and potentially, using flow control, a substantial reduction in the intensity of the unsteadiness. This 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.

TIME FRAME

Research fruition must substantially precede 2012 to enable 20% penetration by 2030

The development of fluids and structures modeling hierarchy is under way, but needs to be substantially accelerated and directed toward wind-specific needs as soon as possible to achieve

the goal of 20% penetration. Much can be learned from the significant Army, NASA, and DARPA investments in rotorcraft. But much work remains to be done because of the lack of massive parallel scalability, absence of parallel anisotropic mesh adaptivity, limited hybrid modeling, and ITAR restrictions (which turbine manufacturers identify as unacceptable) on the codes. Furthermore, coupling of the fluid, structure, and flow-control models—together with the experiments required for validation—cannot be delayed. Clearly, there is a substantial effort in massively scalable algorithm development, mesh and model adaptivity, and error estimation within the DOE that can be leveraged. But some focusing on the particular needs of wind engineering is critical. Without a change to the more-advanced modeling paradigm outlined above, the currently primitive modeling effort employed in the wind engineering community runs the risk of having high gear and turbine-blade failures and less-than-optimal performance yields—thus painting a picture that wind is not commercially viable due to uncertain performance and uncertain cost of ownership.

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TURBINE RELIABILITY AND LONGEVITY

ABSTRACT

Better design tools for predicting wind-turbine reliability and lifetime are needed to reduce the cost of energy for these systems. The current generation of tools grossly overestimates the observed lifetime of most turbines and is unable to predict dominant failure modes. High-fidelity models of dynamic loading and structural response are needed to correctly predict dominant failure modes, while better statistical models of long-term loading are needed to predict turbine response to rare and extreme wind events. Better tools will allow for more-narrow design margins and less-uncertain lifetime estimates, both of which will dramatically reduce the costs of turbine designs.

EXECUTIVE SUMMARY

Predictions of wind-turbine reliability and machine lifetime are necessary components of the design cycle and also major contributors to the overall cost of energy. In the current wind-turbine fleet, many machines experience major failures well before their predicted lifetimes. This suggests that the current methods used to predict failure and lifetime are inadequate.

To improve reliability prediction methods, two approaches are needed. The first approach is to introduce higher-fidelity modeling for complex systems, such as the wind-turbine blades and gearboxes. By fully coupling structural finite-element codes with complex aerodynamic and multi-body dynamic simulation tools, designers will be able to model the failure modes of these systems more reliably. The second approach is to improve statistical models of the long-term response of wind turbines operating in constantly varying and sometimes extreme wind events. This approach will use high-throughput computing to run large Monte Carlo simulations, which will model all possible scenarios of wind-turbine operation over a design lifetime. Once the detailed long-term response of the wind turbine is better understood, design margins can be reduced, along with associated costs. Improvement and integration of existing models should also result in more reliable wind-turbine designs that dramatically improve the confidence of the operators, developers, and investors. These combined factors will enable 20% wind-energy penetration by 2030.

SUMMARY OF RESEARCH DIRECTION

The reliability and longevity of wind turbines is a key component in the cost of wind energy. Being able to predict wind-turbine reliability and lifetime is necessary for manufacturers designing for a minimum of 20 years of operation. To create such robust structures, manufacturers follow internationally developed design standards and use somewhat-standard simulation tools. The design standards have been evolving over decades and have resulted in more-reliable designs, to the point where most in the wind community believe them to be sufficient. However, as is evidenced by a continuing large number of turbines failing before their design life, the tools used to satisfy the standards are thought to be woefully inadequate. The tools used in turbine design that directly affect reliability can be divided into two areas:

high-fidelity models that can predict the detailed physical aspects of turbine operation, and long-term statistical models that reflect the stochastic nature of turbine loading over long periods of time.

High-fidelity models are needed to model the behavior of complex systems such as the wind-turbine gearboxes or turbine blades, which, because of their importance to the system as a whole, govern wind-turbine lifetime. The current generation of design tools for predicting loads on blades and gearboxes is simplistic in that they calculate the average steady behavior of these systems at a macroscopic level. To predict typical failure modes that affect reliability, more fine detail in dynamic situations will be required. Improvements in the areas of atmospheric turbulence, aerodynamic response, and structural loading are most important at present, as well as coupling between these areas of modeling.

Long-term simulations are needed to characterize the loading behavior of wind turbines operating in highly varying winds. These simulations will need to be run over time periods as long as 50 years to properly model the full statistical range of operation. As with higher-fidelity models, these simulations should run quickly compared to a typical design cycle, which is on the order of a week.

SCIENTIFIC CHALLENGES

Designers using present computational techniques cannot accurately predict reliability, which leads to serious overprediction of wind-turbine lifetimes. Turbines are typically designed for a 20-year lifetime, but many are failing after about five years of operation, according to an analysis by Steisdal and Madsen [2005]. This fact limits the viability of wind energy by reducing investor confidence and also indirectly increases the cost of energy through heightened risk.

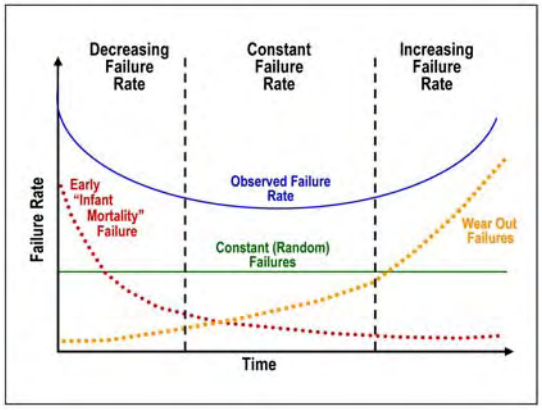

Figure 4: Typical reliability curve for machinery (Wikipedia 2007).

The typical failure rate of a generic piece of machinery can be seen in Figure 4. Usually, failures occur at the greatest rate at the beginning of operation and also near the design lifetime. According to Steisdal and Madsen, observed turbine failures are not currently following this expected shape. This is because a large number of turbines are experiencing wear-out failures well before the design lifetime. The authors attribute this observation to a lack of maturity in the wind-turbine design process, which is unable to predict early failures. To ensure further maturation and growth in the wind industry, it is essential to model failures and mitigate them in the design process. However, because of the simplicity of design tools, the physical mechanisms for these failures are not entirely well understood. The use of advanced computing tools to analyze these turbine failures should provide important insight.

Another problem in the design process is a lack of understanding of the environment in which the wind turbine operates over an entire lifetime. Often, wind turbines are designed for extreme weather events that occur once every 50 years. However, because modern turbines have only existed for several decades, the true nature of these extreme events is uncertain, as well as turbine responses to these events. And because of their infrequent nature, it is difficult to measure these events reliably on a time frame necessary for turbine design. Therefore, advanced statistical tools and simulations are essential in predicting both the extreme events and the turbine response to these events.

NEEDS FROM COMPUTATIONAL SCIENCE

The needs from computational science to fully address these challenges are vast. They involve a large range of time and spatial scales that, in a simulation environment, translate to large computational hardware and software requirements. For example, turbine blades are now larger than 60 m in length, but cracks in the blade structure can occur on microscopic levels. Similarly, turbine response must be estimated for events as fast as a few milliseconds, as well as over a period of decades.

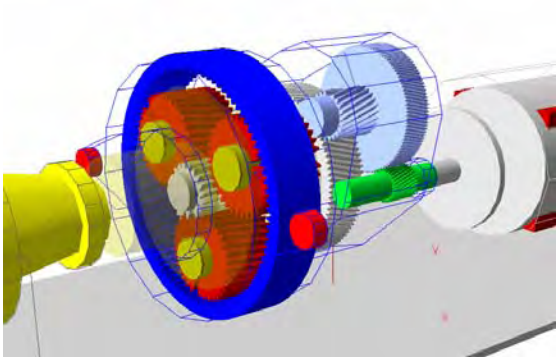

Figure 5: IMPACK gearbox simulation model (Schlecht et al. 2004).

Two examples of how reliability can be improved are better modeling of blades and gearbox performance. Currently, many turbines worldwide are experiencing gearbox bearing failures [Musial *et al.* 2007], even though these gearboxes have been designed using standard design practices and tools. More-complicated analyses of the issue (e.g., see Figure 5) have revealed that standard design practice may be insufficient in capturing important dynamics that may influence gearbox loading. And even the current generation of advanced models may be insufficient to fully characterize the problem. In this instance, current gearbox simulation codes such as SIMPACK [Schlecht *et al.* 2004] will need to be integrated with finite-element analysis (FEA) codes to capture the dynamic effects of loading on the stresses encountered by gearbox bearings. Also, because of the stochastic nature of the problem, Monte Carlo simulations of gearbox configuration operation will have to be performed to create a reasonable statistical set of bearing loading over a 20-year lifetime.

Similarly, wind-turbine blade failures will have to be modeled over a large range of scales, from the microscale of the blade materials to the response of entire blades to large gusts. Future computational models will start with advanced FEA codes capable of modeling composite structures used in blades. These models will then be integrated with high-fidelity computational fluid dynamics (CFD) codes to predict the full aeroelastic response of the blade operating in a turbulent wind environment.

One other challenge for computational science will be to develop models used in stability analysis of large turbines. As turbines continue to grow in size, their stability during operation becomes increasingly important given the increased flexibility and also greater energy absorbed

from the atmosphere. Stability models will depend on FEA, CFD, and dynamics models that incorporate the turbine control system into the analyses. Ultimately, these tools can be used to predict the unstable regions of turbine operation and also the potential failure modes for increasingly complex turbine configurations.

All these models must also run quickly enough so that a researcher will be able to execute them over long periods of time to fully quantify the uncertainty of the turbine response to stochastic winds and rare extreme events. The challenge to computational scientists in this regard will be increased scalability of codes and algorithms to run on increasingly large processor count machines.

The data-handling issues of all these problems will also become paramount. As designers produce highly detailed data over long periods of time, the size of data sets will be on the order of petabytes. Being able to analyze, manipulate, and store such data sets will be a great challenge for computational scientists.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE ENERGY

Improved models for turbine reliability will substantially improve cost of energy for wind by eliminating much of the risk inherent in the turbine design process. Examples of factors driven by risk are overdesigned blades that account for current uncertainties in the blade design process, or rising warranty costs to cover gearboxes that fail before their design lifetime. More-accurate tools will enable designer to lower these risks and associated costs. Success in this area will also dramatically improve the confidence of the operators, developers, and investors and will lead to greater penetration in the energy market.

TIME FRAME

Research into improved methods of reliability will have a near-term impact on turbine designs, particularly those involving gearbox failures. Many of the computational tools can be developed by integrating and modifying existing tools over the next five years (by 2012). Research after this time period should continue to ensure refinement of the tools and continued improved accuracy. These improved capabilities should enable 20% penetration by 2030.

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ENERGY DISTRIBUTION — GRID FUTURES AND RELIABILITY

Many transmission lines of the future electrical grid may look similar to those of today, but they will likely carry information as well as energy, allowing the control of electrical appliances and electrical generators to better match the real-time needs of the system.

CHARGE TO PANEL

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. It serves over 500,000 industrial and commercial customers and well over 125 million residential customers, distributing approximately one terawatt (TW) of electrical power across the United States during peak periods [Energy Information Administration (EIA) 2007a]. 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. (Using publicly available 2005 NYISO market data, PNNL calculated congestion costs by subtracting wholesale electricity costs from the lowest wholesale system price.) Furthermore, the existing grid structure and centralized control philosophy do not rapidly incorporate significant penetration of renewable and alternative energy sources. Advances in managing and delivering electrical energy must occur.

The charge to the members of the Grid Futures and Reliability breakout session was to identify priority research directions in this area as it relates to the following:

1. Advanced materials for electric energy storage
2. Digital power controllers
3. Nanotechnology transmission lines
4. Management of the Smart Grid (e.g., equivalence to Internet routing protocols, real-time load redistributions)
5. Threat simulations and optimizing techniques.

These topics were addressed from a grid integration perspective, since discussions in the other breakout sessions covered research directions to advance many of the specific technologies. This session considered the impacts of such technologies on the overall power grid.

SESSION BREAKOUT LEADERS

Ross Guttromson, Pacific Northwest National Laboratory
Ian Hiskens, University of Wisconsin-Madison
Phani Nukala, Oak Ridge National Laboratory
Dora Yen-Nakafuji, Lawrence Livermore National Laboratory
Ellen Stechel, Sandia National Laboratory

BACKGROUND

The need for a sustainable electrical grid or "Smart Grid"

The Smart Grid

…will manage and deliver bulk electrical energy through a combined centralized and distributed system, in which many nodes are capable of producing, consuming, and storing electrical energy. Managing transactions on this network will involve extensive communications networks and distributed, hierarchical control schemes.

DOE's Energy Information Agency (EIA) has projected that electricity demand in the United States will increase by nearly 50% over the next 20 years [EIA 2007b]. Transmission expansion is already struggling to keep pace with this demand growth, and investment actually declined over the last two decades [EIA 2007c]. The reasons for the shortfall include the cost of transmission infrastructure, land access, and public opposition. Exacerbating these issues is deregulation, which has separated the roles of generation, transmission, and distribution in many regions, resulting in decreased coordination. The goals emerging from increasing national and statewide attention on renewable and energy policies will require renewable and alternative energy sources to supply a large proportion of the increased demand. In addition, limitations on transmission and distribution (T&D) growth coupled with increasing requirements for power quality will drive growth in the use of distributed generation technologies. Another trend calling for the grid to transform and modernize shows increasing stress and reliability failures with associated large economic costs according to the Electric Power Research Institute. The existing grid structure, combined with the centralized control philosophy, is ill suited to accommodate significant levels of flexible and distributed energy resources without dramatic changes in operations, infrastructure, and development strategy.

As illustrated in Figure 1, today's electrical demand typically undergoes large fluctuations varying with time of use. Utilities must size their grids for sufficient capacity to meet the peak demand, as shown in the evening peak hours in Figure 1. This approach, however, leaves the grid underutilized during large portions of the day, especially at night under minimum load conditions. With increasing penetration of renewable generation, finding ways to manage resources in a way that would reduce the ratio of peak to average power demand, thereby effectively increasing the total energy capacity of the grid, provides an opportunity to partially address the capacity challenge. Reducing the ratio of peak to average demand may be achievable by actions such as:

- Placing distributed storage near loads (including the possibility of utilizing the batteries in hybrid or all-electric vehicles in a grid-controlled manner)
- Placing distributed generation near loads including on-site generation (e.g., photovoltaics, fuel cells) with net metering
- Incorporating smart loads capable of shifting their demand in response to price or other control signals

- Shifting existing loads to alternative, non-utility-connected sources
- Implementing new regional market pricing strategies and incentives integrated with demand
- Placing large storage capacity associated with wind generation, which tends to peak at minimum load conditions
- Placing large storage capacity near solar generation, which misses the evening peak.

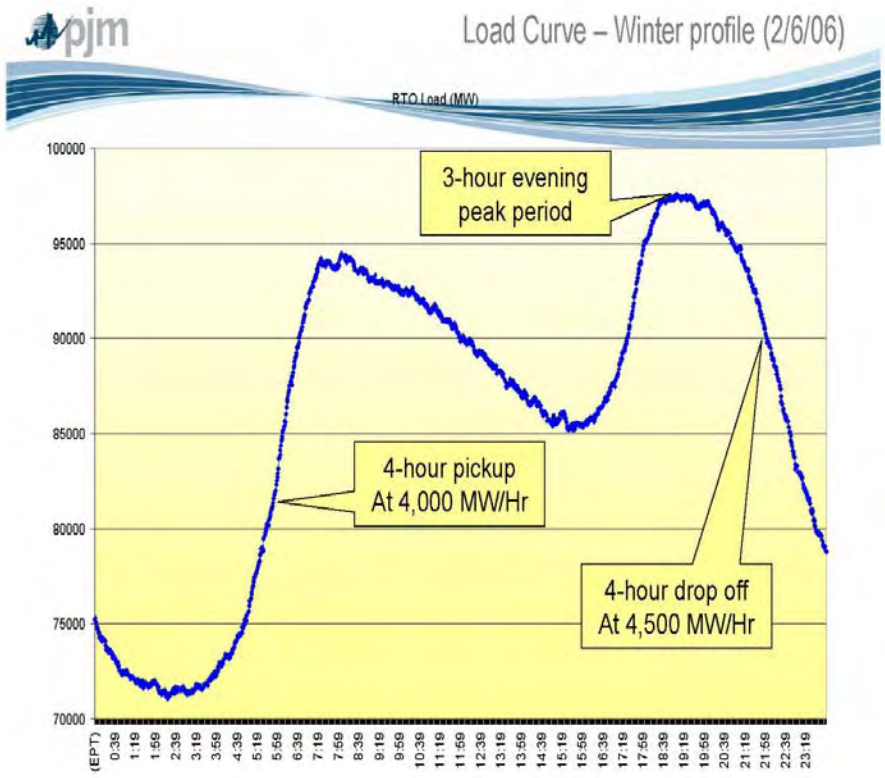

Figure 1: Diurnal Load Shape for the PJM System
(Diagram courtesy of PJM Interconnect, LLC www.pjm.com/markets/market-monitor/downloads/20070521-pjm-overview.pdf)

Incorporating significant levels of highly variable energy resources and/or widely distributed resources requires advanced, interactive control infrastructures that monitor and correct power imbalances in real time. These controls must be able to communicate with and dispatch alternative sources and utilize advanced grid management technologies, including storage, in order to smooth the effective output of low-carbon, renewable, and alternative energy sources. These alternative resources, likely placed near loads, suggest that the control infrastructure will need to include real-time distributed response and decision-making throughout the grid. The nonlinearity of the power grid, the introduction of smart loads and distributed generation sources, and the desire for and advantages of load leveling in an environment with limited predictability, make this a truly challenging problem.

Moreover, technology transformation is rapidly taking place under existing market forces, making resulting power management issues even more critical to address. For example, Toyota recently announced that it would be offering plug-in hybrid electric vehicles (PHEVs) by 2010 [Maynard 2008]. Pacific Gas and Electric (PG&E), a California based utility, became the first utility in the nation to publicly demonstrate the possibility of electric vehicles to supply homes and business with electricity at a Silicon Valley Leadership Group event in April 2007 [PG&E 2008]. A recent DOE study suggests that the current "idle" capacity in the grid (0.1-0.2 TW) could be enough to recharge approximately 158 million (73% of the light duty fleet) plug-in hybrid electric vehicles (PHEVs) using off-peak power [Kintner-Meyer 2007]. In addition, studies suggest that PHEVs are the best near-term option to reduce dependence on petroleum

[Gaines 2007]. Yet the current U.S. grid is not equipped to respond to the operational needs that would follow from the widespread adoption of this technology. Appropriate infrastructure, control algorithms, and technology performance metrics are required to ensure that the electrical supply or demand created by PHEV is properly integrated into the dispatch schedule for all major stakeholders. Without such management, PHEVs may aggravate dispatch problems, especially during system extremes— peak demand or minimum load. Consider, for example, the system impacts of a concentration of PHEVs all recharging immediately after their evening commute. This extra load concentrated at a weak point on the grid would in fact further exacerbate the difficulties of satisfying the evening peak demand.

Despite the significant benefits arising from a future of net-metering, load-control technologies, grid-connected storage, and new but highly variable generation capacity, there will be significant barriers to achieving such a future if the added complexity of the new grid compromises attributes critical to consumer satisfaction—namely, safety, security, reliability, quality, and affordability. In addition, future grids will be judged by their capacity to support sustainable development. Hence, the requirements will include the ability to:

- Operate and maintain assets for efficient and effective utilization of resources and capacity
- Accommodate all types of generation and storage options, including dynamic availability of distributed generation and storage
- Enable innovative and efficient market mechanisms to enhance resource effectiveness for consumers, producers, and service providers
- Provide variable power quality and reliability that matches the variable demand for quality and reliability
- Resist and recover from natural and human-induced disruptions (both cyber and physical "attacks")
- Self-correct, be information-rich, and operate interactively with users via automated controls and advanced system-wide visualization.

Maintaining an adequate portfolio of generation (conventional and renewable) capacity to meet growing electrical demand, maintaining reliability, managing reserves and costs will become ever more challenging with increasing adoption of variable (intermittent) renewables and continuing trends to cancel base load coal power plants due to environmental concerns. Even at 10-15% penetration, intermittency issues are raising resource adequacy concern among system operators especially during system extremes. This is amply evident through the recent state and utility-led integration studies that cite integration issues and potential cost with varying levels of wind penetration.

The current grid

To understand the challenges of incorporating smart loads, distributed generation, and variable sources such as solar and wind, one must have an understanding of the physical behavior of the electricity network and electrical flow.

The electricity network operates in a load-following mode; in other words, as a just-in-time delivery system (i.e., limited reserve inventory), generating, transmitting, and consuming

electrical power virtually instantaneously. Operators adjust for system conditions and large shifts in loads over timescales from minutes to hours, by increasing or decreasing the generation. Within an interconnected power system (there are three interconnects in North America), the power flows from generators to loads through transmission and distribution lines. Though the electrical grids for Alaska and Hawaii are not interconnected to the rest of the nation, they exhibit similar and more serious resource integration and control issues, as their grids are relatively more distributed because of their remote or island locations. The current system of centralized generation supports the stability of the grid. Furthermore, the frequency and phase must remain within narrow margins. (In normal operating scenarios, the frequency variation is controlled to within ±0.01%; see, for example, *Basic Research Needs for Electrical Energy Storage*, BES Workshop Report, April 2007.) Should the instantaneous generation (the supply) not match the instantaneous loads (the demand), the frequency will drift.

Grid Reliability

We must "keep the lights on," independent of natural or deliberate disturbances.

With solar and wind generators, the instantaneous electrical generation is variable on a relatively fast time scale; and therefore, it is effectively nondispatchable from the standpoint of the current grid. Furthermore, to transport power from one node to another, power will flow over *all* connected paths between them. This can and does lead to some unexpected and not easily controlled behavior, especially in unregulated markets. To avoid damage, each transmission line must operate below its rated capacity. If a transmission line becomes overloaded, it could trip out of service, overloading adjacent lines that could also subsequently trip. This might lead ultimately to a widespread outage [Albert 2004; Motter 2004]. In fact, even without the introduction of renewables, the 15-year-time-series transmission-system-blackouts data provided by the North American Electric Reliability Council suggests that blackout sizes follow a power law with significant economic impact. It is estimated that such power interruptions introduce an annual national cost of approximately $80 billion [Hamachi-LaCommare 2004].

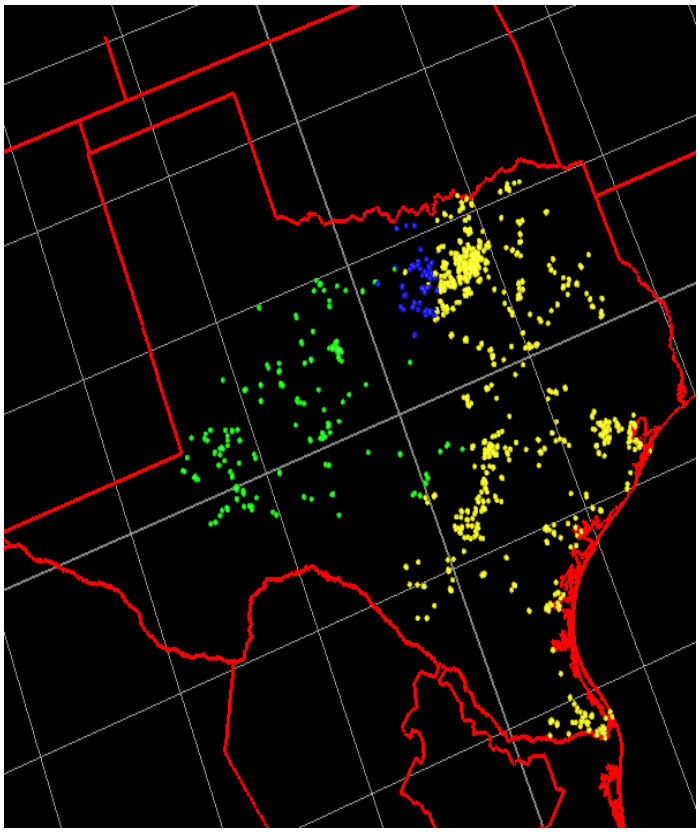

Figure 2. Simulation results show how cascading failures would break the Electric Reliability Council of Texas system into three independent islands (each shown in a different color) leading to blackouts.

Therefore, computer simulation of electrical grid failures is a key tool for understanding and preventing cascading

failures leading to blackouts of electrical grid systems. In these computer simulations, the electrical grid is represented as a network of transmission lines and buses (generators and loads). During service conditions, each of the lines and buses operates below a specified rated capacity. However whenever the lines or buses are overloaded, they trip out of service, which could lead to a cascade of tripping events in the neighboring lines or buses.

Figure 2 presents a simulated scenario of such a cascading failure of the Electric Reliability Council of Texas (ERCOT) system, where each of the dots in the figure refers to a bus (or node) in the ERCOT system, which, while perhaps still operating, is isolated from nodes of other colors. Figure 2 was developed by combining National Oceanic and Atmospheric Administration National Geophysical Data Center data and geographical coordinates of ERCOT buses. This simulation clearly shows how cascading failures of transmission lines and buses break the ERCOT system into three independent islands (each shown in a different color) leading to a blackout [Phani Nukala and Srdjan Simunovic, unpublished]. Understanding the progression of cascading events allows us to develop control strategies to prevent or mitigate the effects of power blackouts. To simulate such events for larger systems such as the entire eastern interconnect or to simulate multiple, interconnected systems will require high-performance computing capability.

The U.S. electric power grid is one of the most complex systems of any type in the world. This system has evolved over the past 100 years and currently includes an array of technologies and architectures. To achieve the control needed, the system has a hierarchical structure consisting essentially of four levels:

- Physical protection for equipment (generators, lines, components)
- Local regulating feedback controls (sensors, switches, monitors)
- Automated and computer-assisted controls, including Supervisory Control and Data Acquisition (SCADA), Energy Management Systems (EMS), Automated Generation Control (AGC), and Wide-Area Monitoring and Control
- Markets and regional reliability.

In the coming years, control systems and strategies must evolve (although this will require more than evolutionary advances) in order to operate in an environment consistent with the envisioned changes that were identified earlier. New systems and strategies will also ensure that security and reliability standards are met and potential vulnerabilities are identified.

The underpinnings of power system operation are extensive analyses of system conditions to ensure compliance within standards and to indentify vulnerabilities. As generation becomes more variable (from increased penetration of renewable and alternative energy sources) and loads become more flexible (because of enhanced controllability and local storage, possibly including PHEVs), the ability of existing analysis tools to faithfully replicate actual system behavior will diminish. Future grids will require new analysis concepts and technologies to accurately assess system stability and security and formulate control actions. In terms of computational needs, the goal is to develop new high-performance computational resources and algorithms necessary to expand today's model from its current state to a potential case of 100 million distinct nodes in a multi-scale centralized and distributed system. Within this context, the panel convened to

identify priority computational research directions to enable the necessary transformation and modernization of the electrical grid.

SUMMARY OF COLLECTIVE PRIORITY RESEARCH DIRECTIONS

Grid Evolution

As diverse, end-user-based energy generation, storage, and consumption technologies develop that offer advantages to the consumer, the grid will evolve from its current centralized generation and control structure to a more distributed system, especially if transmission capacity continues to grow at a rate that cannot keep up with the demand growth.

The Energy Distribution – Grid Futures and Reliability Panel convened to discuss the necessary evolution of the current grid to a future, more controllable, "greener" grid. This would be one that can effectively incorporate new forms of electricity generation, storage, and consumption in order to capitalize maximally on investments in and benefits from renewable energy generation and distributed load-management technologies. The addition of renewable and distributed energy resources to the overall energy mix poses challenges to the management of the current grid infrastructure. Specifically, the panel identified five fundamental challenges:

- Dramatic movement toward further decentralization of grid management and toward a larger, more complex, more diverse system of distributed energy resources significantly alters the operation and the structure of the grid. The challenge will be to develop and install new capabilities to monitor, assess, and control the power grid in a way that ensures its overall reliability.

- Policy instruments can and will have a strong influence on the rate and degree to which the grid decentralizes and diversifies. The challenge will be to develop capabilities to assess impacts and provide decision support for various policy instruments.

- The use of price signaling, net metering, and other market strategies has the potential to produce a very large and time-variable customer response function. The challenge will be to develop a highly adaptive transactional network in order to effectively manage these emerging market strategies in a manner that promotes reliability, efficient operation, and effective integration of new technologies.

- Grid reliability remains essential. Estimated costs based on momentary and sustained power interruptions on U.S. electricity customers (commercial, industrial and residential) range from $23 billion to over $119 billion [Hamachi-LaCommare 2004]. As the electrical grid moves toward a more distributed and diverse system, the challenge will be to strategically invest in a robust grid, to mitigate issues such as intermittency (from sources of variable generation) and to develop a capability to manage generation and load more effectively. Intermittency forecasting has shown to provide improved management potential for accommodating increasing levels of variable resources.

- For certain parts of the grid, substantial penetration of intermittent renewable sources of generation can raise system stability issues if not properly planned. The challenge is to develop new paradigms for managing flexible resources and maintaining system stability despite independent and potentially rapidly varying generation and load. Geographic diversity of wind and solar generation provides some smoothing of their variable nature, however events in both the US and Europe suggest that depending on the transmission interconnects and flexibility of other resources on the grid, challenges still remain.

The overarching goal of each of the identified priority research directions described here is to apply advanced computational resources to maintain grid robustness while managing increasing levels of renewable and alternative energy resources. In other words, future grids must continue to operate reliably through any credible (natural or deliberate) disruption. As the world makes the transition from traditional fossil fuels to more environmentally friendly energy alternatives, decision makers will need better scenario-based planning capability, control/response, and integration tools (i.e., models, sensors, new reliability metrics, high-resolution data) befitting emerging technologies. Likewise, for clean distributed energy resources (including distributed generation and demand response), further research, development, and demonstration will be needed to improve the technology, to inform industry planners, and to help decision makers transform markets and policies. Ultimately, however, all of these decisions, plans, and generating, storage, and end-use technologies must come together to motivate the critical need for methods of better managing the production, distribution, and use of electricity while ensuring the overall reliability of grid operations and enabling sustainable development.

We emphasize that effective, reliable management of the grid is critically important to achieve the benefits provided by new sources of renewable and efficient energy generation. Simply put, the impact of the large-scale introduction of nontraditional alternative and renewable resources has no historical precedence. The grid will likely be a large, complex, multi-scale network requiring dynamic feedback on a far greater scale than the one that currently exists. Thus, there is a strong need to develop new algorithms to characterize the system and to forecast future behavior (near-term and long-term) under various scenarios. There is also a strong need to develop better software and visualization packages that will move the management of the grid to a real-time automated state. Finally, there must be continued research into the properties of advanced materials and devices to drive technology innovations such as large-scale energy storage, low-loss electrical transmission, and distributed, adaptable technologies.

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EVALUATING THE EVOLUTION OF GRID INFRASTRUCTURE AND IMPACTS ON GRID RESPONSE UNDER VARIOUS MARKET AND POLICY INFLUENCES

ABSTRACT

The existing power grid is saturated, stressed, and not readily capable of accommodating large amounts of distributed sources of new electricity generation or load management. Furthermore, existing power systems, which have evolved over the past half-century, were never designed to support significant levels of renewable or bidirectional distributed resources. The regulatory and planning process to interconnect various new sources of generation (both central and distributed) will have a profound effect on the evolution of grid infrastructure as the grid strives to distribute ever-increasing amounts of power. This change requires the development of new tools and methodologies to understand and evaluate the forces transforming the system (and the consequent changing characteristics), to assess potential impacts, and to generate options (which can help inform investment and policy decisions).

The existing system is complex and composed of a multitude of components, communication devices, sensors, and control structures. The current state of modeling must simplify the system in both scale and complexity. For study purposes, the representation of high-voltage transmission systems within the Western Interconnect used 14,000 nodes [Albert 2004]. In reality, the total number of nodes in this interconnect is several orders of magnitude higher. Practical analysis has had to omit the details within the distribution system. Clearly, there is a need for new and higher fidelity methodologies and efficient computational algorithms in order to capture the essential details of existing grid conditions, let alone model their behavior under new market and policy influences, and as the grid evolves to an even more complex structure.

EXECUTIVE SUMMARY

Building a sustainable and resilient electricity infrastructure to incorporate new alternative and renewable resources and technologies and meet ever-growing demand remains a challenging task. If not properly considered, this challenge will result in detrimental consequences not only to our economy but also to our national security. With the growing worldwide need for electric power, diminishing fossil resources, and increasing concern over security and the environment, there is a clear case for adopting alternative and indigenous energy-generating resources and optimize their integration onto the power grid. (“Indigenous resources” are those available locally or regionally and not globally, such as wind, biomass [including municipal solid waste and wood], geothermal, solar, or related industry by-products of heat.) One particular need is a framework or system of computational models with which to simulate the temporal evolution of the future grid with enough fidelity to inform critical decisions. This represents a crucial element to avoid unintended, damaging, and unforeseen interactions. This framework must be capable of reliably modeling various possible future grid scenarios in a dynamically scalable manner. It also needs to identify strategies to implement alternative and renewable resources and technologies that support various policy goals.

SUMMARY OF RESEARCH DIRECTIONS

With the widespread incorporation of alternative and renewable energy sources, including those on the scale of individual households, the grid would be composed of more than 1×10^8 individual nodes. Each individual node might be able to buy or sell electricity at any given time and respond to different efficiency and optimization objectives; thus, the new grid must be able to accommodate a variety of simultaneous load-response strategies. Moreover, there is a need to construct accurate models of the grid in order to evaluate many different "what if" scenarios. For example, policy makers and industry might want to know the effect of supplying wind-generated electricity at a 10%, 20%, or 30% share of total generation [California Energy Commission 2007] and know if any effects depend on other critical factors, in addition to the percentage. Other drivers of "what if" scenarios are various policies for energy distribution and production, particularly as they relate to market or policy incentives for the customer and the service provider. A simple example is a plug-in hybrid electric vehicle or PHEV [Pacific Gas and Electric Company2007; Letendre 2002]. In principle, a PHEV gives the consumer devices that can act as local electrical storage in addition to providing energy for mobility. Acknowledging that policy will encourage the technologies driving energy efficiency, what would be the effect of a given policy on the overall energy system and what are the interdependencies with other policy or market actions? One example would be to evaluate the effects of large numbers of PHEVs in several scenarios. Due diligence in encouraging the widespread adoption of this technology, via policy incentives, will be necessary to avoid overstressing existing grid infrastructure. These distributed technologies represent a dramatically different way of operating the grid. They have the potential to provide tremendous benefits in the overall performance of the grid, yet they come with an equally important obligation to ensure appropriate integration strategies to avoid detrimental effects. In addition, models will have to be able to capture critical dependencies on existing infrastructure, human actors, and outside market responses, as they attempt to simulate the grid-evolution under forcing functions arising from various technology and policy scenarios [Parsons 2006].

Power system operation is becoming increasingly dependent upon modern information technologies to solve management and control problems in the distributed electric power grid. The transient dynamics and information processing mechanisms embedded within the complex interconnected electric grid could already benefit from more fundamental understanding, but current state-of-the-art models for cascading failures and distributed behaviors consider only smaller systems that are simplified steady-state network models. The resulting change in scale from the current state-of-the-art (order 1×10^5 nodes) and the introduction of complexity resulting from realistic modeling of disruptive technologies, policies, market mechanisms, and human/market forces requires the development of simulations capable of taking advantage of leadership class computers. More specifically, we can define the main computational challenges by the following elemental needs:

- To create a capability to model human and market responses in order to understand the likely effectiveness and impact of different choices among technology development, investment strategies, and policy instruments
- To create a capability to model the integrated dynamics of social, technology, economic/market, and environmental impacts with a large number of diverse and interdependent elements

- To create discovery-based tools to explore “known unknowns,” as well as to reveal unknowns that cannot yet be contemplated (“unknown unknowns”)
- To develop a fundamental knowledge base to underpin the development of control strategies to maintain stability, security, reliability, affordability, and sustainability.

The priority research directions described below capture different aspects important to enabling a smooth transformation and modernization of the electrical grid.

- Planning, informing key stakeholders, and guiding the evolution of the grid
- Considerations for operating and managing complexities in the future grid
- Considerations for implementation to ensure interoperability between diverse elements of the grid and between existing and future elements
- Exploratory and discovery-based tools to understand the fundamentals determining performance attributes, to elucidate potential unexpected or perhaps emergent behavior, and to uncover vulnerabilities within possible future grid states and topologies
- Advancing technology innovations to enable the future grid.

Trends and needs are driving the electrical grid to a networked system with no previously explored analog. The combined flow of electrons, information, and instructions makes this network-based system far more complex than the Internet. The electrons must be consumed as they are created; the information is rapidly varying, heterogeneous, and distributed; and the instructions are of numerous types and depend on past and existing states. The system is not only complex, but is also complex-adaptive and a system of systems; the sciences of complex adaptive systems and of systems of systems are both in their infancy.

COMPUTATIONAL NEEDS

A power system model that integrates generators, loads, transmission lines, control processes, and packet-switching data networks is an example of a hybrid system (some continuous flows and some discrete events.) The behavior of physical systems is describable with differential-algebraic equations, with some discrete dynamics that result from circuit breakers, relays, and other types of local response mechanisms. In contrast, packet switching networks are best describable as discrete event systems with a dynamic behavior represented by chains of significant events. What is required are modeling and simulation capabilities that support such hybrid systems at large scale and high fidelity as a core set of capabilities [Hiskens 2000]. The computational challenges in this area include not only a sophisticated model construction that can combine complex, continuous, and discrete representations but also credible validation methodologies to build confidence in the results.

Given the high degree of uncertainty in modeling all the key phenomena, uncertainty analysis, and the ability to detect high consequences (even if low probability states) will be essential [Hiskens 2006]. This requires a forward model that is able to predict with reasonable confidence the system response to specific stimuli; however, the real goal is to identify both short- and long-term responses on multiple temporal and spatial scales. Pursuing this goal requires studying inverse models [Hiskens 2004] and, possibly, radically new approaches in representing the

forward problem underlining the importance of studying nonlinear systems with discrete and continuous interfaces.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE RESOURCES AND TECHNOLOGIES

With all the benefits of renewable resources, the realities of large-scale integration of such resources present technical as well as economic challenges for our electrical system as it stands today. For example, in many parts of Europe and the United States, wind generation is becoming a dominant renewable resource, leading to, because of the variability, a compounding of pre-existing grid quality issues [IEA 2007]. Variable and remotely distributed resources are posing significant grid integration and operational challenges for the current electricity infrastructure. Predominately because of the variability of the wind resources and the lack of operational confidence at high renewable penetration levels, there is a sense of "uneasiness" in pushing for more renewables. The lack of advance forecasting and planning tools that can utilize reliable data (both temporal and spatial) and new sources of data befitting the new technologies contribute to the discomfort and uncertainty experienced throughout our nation's utility industry. Other alternative and renewable resources and technologies such as biomass, biobased fuels, and solar (PV, CPV, and CSP) face similar source-to-sink issues as a result of the lack of transmission capacity and operational experience. Thus, it is essential to develop grid planning tools or modes of simulation that can more easily accommodate with confidence these new but variable sources of electricity generation without unintended consequences.

Finally, this priority research direction enables the exploration of technologies under different policy and market influences, providing the ability to evaluate strategies without compromising the the security, economics, or reliability of the grid while ensuring the realization of the intent of the strategy. It will provide the tools to reduce risk and enable informed decision making regarding our future infrastructure.

TIME FRAME

The grid is transforming under natural forces and policies are being implemented without any reliable tools to assess whether the results will be consistent with the goals. Hence, the need exists now and will continue for at least a decade or longer.

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EVALUATING AND INTEGRATING AUTOMATION AND SCALABLE OPERATING STRATEGIES INTO THE FUTURE GRID

ABSTRACT

As the grid becomes more complex as a result of increased demand, limited capacity, new market mechanisms, and new technologies, the management of this complexity in near-real-time becomes an increasingly arduous task.

There is a need to develop a set of tools that will enable real-time operational management of the future grid — including decision making, associated with generation and load management, ancillary services, distributed generation, select markets, and grid reliability. Real-time operation and distributed decision-making capabilities will be critical enablers in any future grid that is able to better accommodate distributed technologies and variable generation capacity; this requires the use of new tools.

EXECUTIVE SUMMARY

There is a growing concern that the aging grid infrastructure is at risk of becoming more vulnerable to system-wide failures by naive integration of alternative and renewable resources and technologies. More important, grid sustainability and reliability require ancillary services such as frequency regulation, transmission voltage support, and spinning reserves. As new load and generation technologies are integrated, it will be necessary to address these ancillary services separately. It is no longer appropriate to assume they are automatically available as part of these new technologies as they were with legacy generation.

Experienced utility dispatchers and system engineers currently manage these issues; however, the characteristics of renewable sources and distributed load management differ enough from conventional operating paradigms, thereby creating a need for new operating paradigms to prevent local failures from cascading into system-wide blackouts. The anticipated complexity will require movement toward intelligent/automated management of the grid.

SUMMARY OF RESEARCH DIRECTIONS

The essence of this priority research direction is to identify new models and algorithms to enable real-time management and distributed decision-making in the absence of precise knowledge of the structure of the future grid. In fact, developments here could materially affect the outcome of the grid's evolution.

Existing standards might need modifications, and new standards might need to be developed, in response to the findings from various simulations studying system transformations. A crucial aspect of meeting this challenge lies in the ability to perform rapid state assessments of the operating grid and the ability to represent that state in a form that is an easily accessible and understandable visual interface [Power World Corporation; Overbye 2001].

Operational training on simulator modeling would provide an extremely useful mechanism for both the operator and the engineer to understand the behavioral characteristics of the grid and to have the ability to determine, effectively and efficiently, appropriate methods of interaction. Development of a visually enhanced, grid simulation capability with diverse and distributed data sources will undoubtedly require significant algorithmic development to quickly assess normal versus abnormal operation anywhere in the grid, make the appropriate decision, and signal the appropriate corrective action, as needed, all in real-time, despite the complexity of the system. Development and validation of such capabilities will be practical only by using high-performance computing platforms.

Industry standards exist to protect equipment integrated into the grid and to ensure an adequate level of reliability for consumers and industries. U.S. electric power grid reliability requirements are implemented and enforced by the North American Electric Reliability Company (www.nerc.com), and they are overseen by the Federal Energy Regulatory Commission. Standards include those developed by the Institute of Electrical and Electronics Engineers. Utility managers maintain a balance between electricity supply and demand using the availability of generation resources and demand technology in order to "keep the lights on." With the likely increase in the number of distributed elements, which react to load and generation imbalances within the overall network, grid management must become more automated, resulting in systems within systems. The operator function thus would move closer toward managing control systems rather than managing individual grid components. This trend is becoming more evident in today's grid, where grid operators' responsibilities now include the management of wide-area control systems, referred to as Remedial Action Schemes (RAS) or Special Protection Schemes (SPS).

The blackout of August 2003 in North America demonstrated that a fault in one part of the power system can ripple and cascade to ultimately disrupt neighboring transmissions [Wald 2005]. The post-disturbance analysis and report highlighted the clear need for wide-area situational awareness. Human operators in the loop are currently unavoidable for the reliable management of the power grid, since the robustness of automation is not at a level where the system can allow autonomous operation. A utility's supervisory control and data acquisition (SCADA) network monitors the balancing authority's status. Increasingly, however, operators require visibility into the grid beyond their own area. Thus, the wide-area system now requires an overarching layer that can collect information and provide operators with a broader context of the state of the grid.

Existing power system operating strategies exploit the predictability and periodicity of daily load variations. Increased utilization of renewable generation will result in generation and load patterns that are much more sensitive to weather conditions and hence exhibit greater variability. Other technological changes, such as distributed generation, price-responsive loads, direct load control, and vehicle-to-grid concepts will tend to further reduce the predictability of operating strategies. Operating strategies will always require some predictive capability, though, to account for time delays and rate limits that are inherent in rescheduling large generators. Research is required to establish operational requirements that are suited to this new, more dynamic environment. Compensating for less intrinsic predictability is achievable through increased awareness of the current state of the system and improved predictive modeling of components. This implies a need for both capabilities for vastly more extensive state estimation and algorithms for significantly faster and more reliable calculations.

Power system emergency operation, following a large disturbance, is largely operator-initiated and responsive. Some special protection schemes (also known as remedial action schemes) have been established to assist operators. But even they offer limited flexibility, responding to preset triggering conditions in a predetermined way. As power systems become more heavily loaded and approach stability and security limits, the effectiveness of such responsive control efforts will diminish. The future grid will require control schemes that incorporate short-term predictive capabilities. The underpinnings for such schemes will be fast, reliable, and accurate capabilities to create situational awareness. Disturbances will be quickly detected, along with the estimated system state used for predicting a range of possible transient responses. The event-detection process will need to be capable of assessing, in real-time, the proximity of the system to the boundary of the stable, secure operating region. The control algorithm will use this predictive capability to determine actions that minimize the maximum disruption. This min-max objective implies a need for algorithms that solve large-scale games.

Such predictive control is dependent upon system models that are sufficiently accurate—the required level of accuracy is itself an open question. Maintaining the appropriate level of accuracy will require an online model validation process that is continuously monitoring system behavior and updating model descriptions.

Although we cannot completely know, at this time, all the operational components of any future grid, it will nevertheless likely include the following:

- A hierarchical control structure consisting of centralized coordinating controls and distributed decision making, with two-way information flow between the levels
- Integration of real-time communication infrastructure to accommodate wide-area monitoring and real-time control of the grid
- Real-time situational awareness of the system state, consisting of order 1×10^8 independent and sometimes autonomous generators, storage, and loads. This awareness would likely be produced using visualization technologies that incorporate tools to filter out irrelevant background data. Decision management tools, helping the operator to determine the optimal robust path forward, depending on the situational awareness
- Closed loop, wide-area, adaptive control algorithms
- Real-time load-leveling and distributed load-management, including the ability to turn loads both on and off varying dispatch orders, as needed, to smooth intermittent resources such as wind or solar generation
- New methodologies for self-diagnostics, design, and assessment of operational health.

COMPUTATIONAL NEEDS

The sheer quantity of transactions required for supporting real-time monitoring and control makes the priority research direction a major computational challenge, in terms of both the computational capacity needed and the subsequent information network required to support decision making. There is a need for large-scale, real-time, spatio-temporal situational awareness tools for monitoring and state estimation of the grid.

Deregulation of electricity markets, compounded with the introduction into the grid of alternative and renewable resources and technologies, further enhances the transactional and pricing complexity of electricity markets [Joint Western Public Utility Commission 2007; Geerli 2003]. Development of models and algorithms for efficient transactional management of electricity, especially in the presence of alternative and renewable resources, becomes necessary for the seamless integration of alternative and renewable sources into conventional electricity markets. Internet and/or banking traffic models may be reasonable surrogates to address this issue [University of Oregon Route Views Project 2005]. In addition, game-theory based models may play a role in addressing the large numbers of transactions arising as a result of the increasing number of market-participants associated with distributed energy resources.

State estimation, dispatch optimization, real-time predictive modeling (which continually predicts the future state of the grid), and contingency analysis are complex tasks, especially in a large, heterogeneous network with renewable generation. Combining these complex tasks and including market optimization will require impressive breakthroughs in algorithmic development and solution methods.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE RESOURCES AND TECHNOLOGIES

Identifying needs for tools that will enable real-time management techniques is a critical first step toward a robust and efficient future grid that is able to manage the complexity resulting from the large penetration of alternative and renewable resources.

To date, a number of utilities have distributed generation and distributed energy resource programs and have gained considerable “behind the meter” experience, but the penetration and the technology are limited. Although transmission and distribution infrastructure planning for the future grid is happening now, it lacks good scenario-based system evaluation tools. Such tools will be very useful in guiding and informing major infrastructure transformation investment and policy decisions, and they could even accelerate the decision-making process.

TIME FRAME

This is not something solvable in one pass. In the face of these new complexities, it will be important that new control paradigms be explored, options developed, and the best concepts allowed to mature to commercialization. This is likely a decade-long endeavor, and efforts must start as soon as possible.

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MAINTAINING CONTINUITY AND INTEROPERABILITY AS THE GRID TRANSFORMS

ABSTRACT

It cannot be emphasized too strongly how critical and difficult it will be to ensure continuous, reliable, and secure operation of the power grid during periods of changing technology and infrastructure to a qualitatively different, more sustainable grid, and to do so in a timely manner. The ability to evolve the grid requires continued or enhanced interoperability among all of its constituent parts and players.

EXECUTIVE SUMMARY

Renewables and the integration of new technologies into the existing electrical infrastructure are causing a number of operational and reliability concerns for the grid. This is in part because the characteristics of most renewable and demand management technologies are different enough from their legacy counterparts, but more fundamentally, the existing infrastructure was never designed to accommodate such diverse and distributed technologies or rapid controls envisioned for the future [Tomsovic 2005]. The electricity grid is undergoing a rapid transformation, but there are important lessons from our current and past experiences. It will also be important to ensure a smooth transformation that does not compromise system performance yet will promote competitive engagement by industry.

SUMMARY OF RESEARCH DIRECTIONS

The priority research direction in this section focuses on utilizing current knowledge of the system and extracting that knowledge to maintain a high degree of grid reliability as grid technologies undergo change.

Because of the evolutionary development process, our current grid and grid management and business processes have inherent strengths and weaknesses at various levels. These processes are specific to certain infrastructures and locations—design, communication, operation, controls, and technology. As change continues, our understanding of the existing infrastructure becomes more disparate and incomplete as personnel change, resources diversify, and incremental changes occur in the grid. At the most basic level, this priority research direction captures the need to ensure that standardized communication taxonomies be maintained for cross-platform interoperability. Similar to managing computer infrastructure changes from mainframe-based computing to client-server based platforms, control algorithms and standard communication protocols are needed to convert from a legacy structure to more flexible data exchange methods. There is a need to adapt smart technologies and control algorithms to legacy platforms while the grid makes its transition from its current state to a smart grid. From the system design point of view, this requires the development and implementation of standardized communication taxonomies. One such industry entity that exists solely to address this grand challenge is the GridWise Architecture Council [2007a]. Their mission, as they defined by their vision statement, is to do the following:

> Weave together the most productive elements of our traditional infrastructure with new, seamless plug-and-play technologies. Using advanced telecommunications, information, and control methods, we can create a "society" of devices that functions as an integrated, transactive system. [GridWise Architecture Council 2007b]

At a more functional level, transformation to new grid technologies requires that we maintain "institutional" memory and the links that are unique to other interdependencies, including location constraints, unique architectural designs, generation portfolio management, co-located resources, and other community considerations. The expert knowledge currently held by system operators and planners needs to be captured, assessed, and utilized to simulate functional designs for grids of the future [Kontogiannis and Safacas 2004]. The ability to transcend quickly from micro to macrosystem perspectives is the essence of the research challenge. Approaches to capturing this information, and the sheer volume of information to organize for further assessment, makes this a priority research direction.

COMPUTATIONAL NEEDS

The objective of this priority research direction is to develop, test, and implement knowledge and data capture, data control, and exchange principles that serve to maintain the continuity of the current grid as its components evolve to form the future grid. Methods to capture expert knowledge and maintain interoperability among old and new components will be necessary to ensure smooth grid operations [Zheng et al. 2006]. This includes trending and assessment of existing system operations and effectiveness of control [Tullis and Albert 2008] (especially during system excursion times or out of limit operations). Simulation training for utility operators can be expanded not only to include historical events but also to research methods of operation using new tools, effective tools, and technologies to see how they respond to out-of-normal operations when significant penetrations of alternative and renewable technologies have been integrated with the grid.

The computational challenges involved include the following:

- Ensuring interoperability between legacy controls and generation technologies and new platforms; this requires large-scale, high-resolution modeling of power system components to develop valid choices of standards and their potential impact on market adoption of innovative new technologies and strategies
- Developing system simulation models to capture details down to the power distribution level and integrate cross-dependencies (renewable technology, market, and policy influences) to ensure the ability to uncover potential but unexpected incompatibilities after incorporation
- Maintaining user confidence in real-time management and situational awareness tools
- Addressing data standards, protocols, annotation, archival storage, and access control issues for legacy data, future data, and derived data captured
- Integrating advanced visualization, knowledge discovery, and data analysis to identify new extremes for operations during the transformation period in the operating grid.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE RESOURCES AND TECHNOLOGIES

As more renewable and alternative energy resources penetrate the grid, implementation strategies need due diligence to ensure interoperability with other infrastructural elements. Whether modifications to existing practices will be incremental or will require fundamental shifts in operating paradigms is a current debate among many; however, considerations of interoperability and the effect on operations need to be addressed today in order to ensure maximal benefit from these technologies. Implementation strategies also need to be sound to ensure reliable delivery of power. Computational capability exists from the research community for visualization and knowledge discovery. These tools can be leveraged, and further adapted, and then applied in support of the transforming grid. They can also establish confidence in the adoption of new innovative technologies and strategies.

TIME FRAME

As the grid is already undergoing rapid change, and as policies to promote change are increasing in popularity—for example, a number of states have already adopted renewable portfolio standards—addressing issues of interoperability and implementation to avoid catastrophic disruptions of electric service is pressing. Hence, the time is now and will continue at least for a decade.

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EXPLORING COMPLEX BEHAVIORS IN GRID SCENARIOS

ABSTRACT

Complex and emergent behavior is the surfacing of a systemic pattern not characteristic of the components that comprise the system. This presents a unique challenge within the evolving power grid. Designing benign control systems such as automated demand response controls into a residential house may not be benign at all when vast numbers of homes exhibit the same behavior. Understanding what will happen when a large population starts to use a new technology is critical before deploying the technology in large numbers. If emergent behavior would result from large-scale implementation of a particular technology, and not identified before integration into the grid, then cascading effects could occur. Identification beforehand presents an opportunity to develop mitigation strategies to retain the principally desirable benefits while eliminating any propensity to cause detrimental emergent behavior and hence, safe incorporation into an electric power grid. Similarly, emergent behavior could result from crossing a threshold in a changing topology as added resources incorporate at nodes or edges of the grid network. Identification beforehand again presents an opportunity to develop mitigation strategies to guide growth to eliminate any propensity to cause detrimental emergent behavior through naïve growth.

EXECUTIVE SUMMARY

In the future grid, we can reasonably expect a variety of different behaviors to emerge from the interaction between demand response, distributed resource technologies, and the topology of the electric system as a whole. These unanticipated emergent behaviors can arise from interactions between infrastructural elements within the energy system.

Discovering emergent behavior (whether beneficial, benign, or harmful) requires highly credible models of the grid in order to detect anomalies that might represent any unusual behavior and be confident that it is not an artifact of the model. These models must be detailed enough to capture subtle interactions, large-scale feedbacks, and low-level but amplifying changes in component, system behavior, and traffic (power and information flow).

SUMMARY OF RESEARCH DIRECTIONS

There are vast numbers of potential drivers for emergent behavior (e.g., sunrise on a PV farm, wind picking up on a wind farm, consumers postponing usage until prices drop) that can alter the flow of power to different regions of the country. These small-scale perturbations and the interaction among the nodes of the grid that amplify these perturbations need to be clearly understood under a variety of “what if” scenarios in order to identify potential forms of overall grid-emergent behavior. Furthermore, the ability to model emergent behavior allows for identification and possible mitigation of behavior or growth patterns that are detrimental to the grid’s performance. Thus, early indicators of emergent behavior need to be formulated, methods for identifying the most important components influencing the behavior need to be developed, and strategies for limiting the impact of the behavior need to be tested. This requires identifying

and assembling the relevant data that might serve as critical indicators of any impending problem and having the capacity to rapidly communicate this information to planners and grid operators. The need for visual or graphical representation of the grid as it approaches the critical behavior may require new computational and information architectures suitable for efficient portraying of models that are capable of representing these emergent behaviors [Foster].

In order to understand emergent behavior, power system models will need added sophistication to include components on many scales and as fine as down to the consumer level. The resulting model dimension will increase by several orders of magnitude, making traditional solution approaches infeasible. When market effects, weather effects, and policy effects are included, the model will become even more complex.

A few models exist that characterize the overall emergent behavior of a complex system. However, these models are still in their infancy and are limited to small, idealized networks with simple interactions among the agents that make up the network. Algorithms that can extend to real networks with hybrid (continuous and discrete) interactions are needed to explore emergent behavior in grid systems. Furthermore, significant challenges exist in the proper mathematical description of the model, designing new algorithms for simulating the model, and designing tools to extract useful information and knowledge from the simulations.

COMPUTATIONAL NEEDS

The computational challenges associated with this priority research direction include:

- Identifying methodologies to characterize the grid system (electron flow, information, and transactions) on various temporal and spatial scales
- Applying appropriate model construction to represent a wide range of possible grid structures and topologies
- Developing new algorithms to simulate various possible grid structures and topologies with a goal of exploratory and discovery-based investigations of the relationship between structure and performance attributes; find and elucidate patterns and unusual behaviors to promote or to avoid
- Developing new algorithms to treat the possible grid structures and topologies as complex adaptive systems or a system of systems and uncover key characteristics that lead to robustness, resiliency, and sustainability
- Acquiring and using current system data to validate, improve, and refine simulation models
- Designing data analysis tools to extract information and knowledge from current and simulation-based systems.

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE RESOURCES AND TECHNOLOGIES

Energy security and environmental concerns are placing significant investment in alternative and renewable resources; however, it will be important to have reliable capabilities to assess the performance characteristics of resulting new grid topologies, depending on various incorporation strategies, as some naïve strategies can increase renewables on the grid yet decrease reliability or even increase greenhouse gas emissions. The efforts identified will enhance our ability to identify hidden incompatibilities or hidden interdependencies that these different technologies might induce in the grid to characterize their behavior in the future grid and to provide requirements for new controls and information strategies in the grid.

TIME FRAME

As demand increases and the market responds and as policies promote the incorporation of new resources the nation is at significant risk of unanticipated consequences from the creation of an ever-increasing complex grid and limited understanding of its fundamental characteristics. Hence, it will be important to see efforts in the next one to two years and grow those efforts over *the* next decade or more.

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DEVELOPING AND INTEGRATING INNOVATIVE COMPONENTS AND PROCESSES FOR THE NEW GRID

ABSTRACT

Advanced computational materials research and validation remain crucial to component research for the future grid. New materials will allow increased grid capacity through, for example, high-temperature superconducting or nanotechnology transmission lines, demand-leveling of the grid through electrical storage, and the use of distributed generation technologies such as advanced fuel cells.

EXECUTIVE SUMMARY

The development, design, deployment, use, and characterization of advanced materials and technology components can benefit enormously from computationally based research in order to enhance the adoption of renewable and alternative resources by accelerating development, reducing technology risks, and generally building confidence. Specifically, the deployment of potentially large amounts of electrical storage, enabled by the development of new materials, will require impact analysis, integrated testing facilities, and new controls to facilitate robust integration into the future grid. Thus, adopting new materials for transmission lines, such as high-temperature superconducting lines and nanotechnology (e.g., carbon nanotubes for transmission lines) may, without proper planning and integration, create new challenges for managing the grid. As an example, one objective of the current grid design is to sustain an outage of at least a single element without propagating a failure; however, superconducting transmission lines will carry a disproportionate amount of electricity, and if a contingency were to occur on one, it might increase the probability of a cascading outage. The design of appropriate scalable markets needs consideration, because devices need to be engineered to perform robustly in response to market signals (e.g., price), enabling a complex market where devices may be polled periodically and each may have the option to buy or sell electricity or do nothing for some period of time. Such transactions must be accurately recorded; modeling or running such a system is a distributed petascale data management and processing challenge.

SUMMARY OF RESEARCH DIRECTIONS

New industry facets will likely emerge, centered on the computational requirements to design, manage, and process grid information envisioned for the future. Advances in material and computational research offer the possibility of using superconducting materials for transmission and storage and the utilization of advanced computational resources to properly characterize and design respective technologies as well as aid in their testing; however, building off other scenario-based priority research directions, the focus of this research area is to derive new knowledge of system functionality and need. With that knowledge base, researchers can then use extracted information to guide the design of new grid components and properly parameterize the system conditions to aid the design of technology solutions (e.g., advanced electrical storage, transmission, generation capacity, conversion, or system management and control to integrate PHEVs, market signals, other distributed technologies, and so on).

There is also a critical need for significant advances in materials research to create effective, low-cost solutions to the electrical storage problem such as batteries, supercapacitors, superconducting magnetic energy storage, and high-speed flywheels. Thus, significant research into electrical storage and properties of new materials, which operate safely, is crucial to an efficiently operating energy infrastructure.

In addition, each unique technology brings with it a need to control it as an integral element of the grid. For example, if all devices on the network were polled every second, approximately equivalent to using the SMS protocol, the data rate could be as large as two terabits per second continuously. Managing the grid using this data set would require new algorithms and high-performance computing.

These new operational paradigms—such as managing versus preventing interruptions with distributed electrical storage and generation, demand response, and high capacity transmission—will require new methods and algorithms for robust control.

COMPUTATIONAL NEEDS

Computational needs include:

- Improving the accuracy of numerical physics-based models that deal with chemical, material, fluid, and thermodynamic processes—basic science, engineering and design tools
- Utilizing system knowledge extracted to inform the design and characteristics of components intended for specific grid enhancements (speed, efficiency, decarbonization, real-time processing, alternative operations during extreme conditions by applying game theory,, chaos theory or other types of behavior-based processes)
- Exploring market infrastructures and other infrastructure models (banking internet) and seeing if there are complementary platforms (i.e., communication, controls) to maximize grid operations (not only electricity but coupled with natural gas and water management).

POTENTIAL IMPACT ON ALTERNATIVE AND RENEWABLE RESOURCES AND TECHNOLOGIES

The exact layout of the future electric grid is unknown at this time. The grid will continue to evolve with technology, policy, and market forcing functions; however, our ability to shape future designs and future grid requirements is dependent on what we can envision today based on anticipated needs to improve reliability and security, reduce costs, and to incorporate renewables and environmentally friendly alternatives. To make those visions a reality, findings of simulation-based scenario analyses are essential in shaping the design and characteristics of technologies that complement needs.

One of the biggest promises of alternative and renewable resources and technologies lies in their potential ability to become a controlled source of electricity to the grid. A typical house could have many forms of energy generation—some in the form of more traditional generation such as rooftop PV or hydrogen fuel cells. Another type of energy generation is simply the controlled

ability to curtail load. Finally, electric storage, including PHEVs, might serve the grid. Enabling these energy technologies, and controlling them in a manner to aid both the electric power grid as a whole and the local communities they serve is a key component to meet this realization.

TIME FRAME

To maximally impact the modernization of the grid, the next three to five years and then ongoing ones will be important, noting that the technology will continue to evolve.

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APPENDICES

APPENDIX 1: WORKSHOP PARTICIPANTS

Computational Research Needs in Alternative and Renewable Energy

Hilton Rockville
Rockville, Maryland
September 19-20, 2007

Srinivas Aluru	Iowa State University
Katherine Andrews-Cramer	Sandia National Laboratories
Dan Arvizu	National Renewable Energy Laboratory
Tom Autrey	Pacific Northwest National Laboratory
Sam Baldwin	U.S. Department of Energy
Sergey Barabash	University of California at Los Angeles
Matthew Barone	Sandia National Laboratories
Victor Batista	Yale University
Miroslav Begovic	Georgia Institute of Technology
John Bell	Lawrence Berkeley National Laboratory
Dale Berg	Sandia National Laboratories
Jerry Bernholc	North Carolina State University
Rana Biswas	Ames Laboratory and Iowa State University
Greg Bothun	University of Oregon
Jim Brainard	National Renewable Energy Laboratory
Kenneth Brentner	Penn State University
David Brown	Lawrence Livermore National Laboratory
Howard Brown	National Renewable Energy Laboratory
Mark Bryden	Iowa State University and Ames Laboratory
Lawrence Carr	U.S. Army Aeroflightdynamics Directorate
Lali Chatterjee	U.S. Department of Energy
Gang Chen	Massachusetts Institute of Technology
Joseph Cleary	San Diego Supercomputer Center
Bruce Clemens	Stanford University
Scott Collis	Sandia National Laboratories
Terence Critchlow	Pacific Northwest National Laboratory
Michael Crowley	National Renewable Energy Laboratory
Vince Dattoria	U.S. Department of Energy
Brian Davison	Oak Ridge National Laboratory
Matt DeJongh	Hope College
Gennady Denisov	J. Craig Venter Institute
Patrik D'haeseleer	Lawrence Livermore National Laboratory
Lori Diachin	Lawrence Livermore National Laboratory
Julie Dickerson	Iowa State University
David Dixon	The University of Alabama
Earl P.N. Duque	Intelligent Light and Northern Arizona University
Phillip Duxbury	Michigan State University

Sheryl Ehrman	University of Maryland
Ted Einstein	University of Maryland
James Evans	Ames Laboratory and Iowa State University
George Fann	Oak Ridge National Laboratory
Steven Fernandez	Oak Ridge National Laboratory
Barbara Fossum	Purdue University
Alberto Franceschetti	National Renewable Energy Laboratory
Marv Frazier	J. Craig Venter Institute
David Gao	Tennessee Tech University
Al Geist	Oak Ridge National Laboratory
Brandon Gerber	General Electric
Steven Gianoulakis	Sandia National Laboratories
David Goodwin	U.S. Department of Energy
Peter Graf	National Renewable Energy Laboratory
Susan Gregurick	U.S. Department of Energy
Ross Guttromson	Pacific Northwest National Laboratory
Steven Hammond	National Renewable Energy Laboratory
Jorgen Hansson	Software Engineering Institute
Michael Heben	National Renewable Energy Laboratory
Mike Himmel	National Renewable Energy Laboratory
Ian Hiskens	University of Wisconsin-Madison
Kai-Ming Ho	Ames Laboratory
Roy Hogan	Sandia National Laboratories
Zhenyu Huang	Pacific Northwest National Laboratory
Mark Hybertsen	Brookhaven National Laboratory
Kenneth Jansen	Scientific Computation Research Center
Purusottam Jena	Virginia Commonwealth University
Duane Johnson	University of Illinois Urbana Champaign
Gary Johnson	U.S. Department of Energy
Wesley Jones	National Renewable Energy Laboratory
Bonnie Jonkman	National Renewable Energy Laboratory
Yosuke Kanai	University of California
Peter Karp	SRI International
Efthimios Kaxiras	Harvard University
Neil Kelley	National Renewable Energy Laboratory
Moe Khaleel	Pacific Northwest National Laboratory
Song-Charng Kong	Iowa State University
Norman Kreisman	U.S. Department of Energy
Teja Kuruganti	Oak Ridge National Laboratory
Bernard Lesieutre	University of Wisconsin-Madison
Shawn Lin	Rensselaer Polytechnic Institute
Mark Lusk	Colorado School of Mines
Costas Maranas	Pennsylvania State University
Leonardo Marino-Ramirez	National Institute of Health
Dmitry Matyushov	Arizona State University
Jeffrey Mazer	U.S. Department of Energy

Clare McCabe	Vanderbilt University
George Michaels	Pacific Northwest National Laboratory
Michael Minion	University of North Carolina
James Misewich	Brookhaven National Laboratory
Patrick Moriarty	National Renewable Energy Laboratory
James Muckerman	Brookhaven National Laboratory
Jayathi Murthy	Purdue University
Habib Najm	Sandia National Laboratories
Jonathan Naughton	University of Wyoming
Jeffrey Neaton	Lawrence Berkeley National Laboratory
Mark Nimlos	National Renewable Energy Laboratory
Phani Nukala	Oak Ridge National Laboratory
James Nutaro	Oak Ridge National Laboratory
Ruth Pachter	Air Force Research Laboratory
Ellen Panisko	Pacific Northwest National Laboratory
Sreekanth Pannala	Oak Ridge National Laboratory
Eleftherios Papoutsakis	University of Delaware
Edward (Ned) Patton	National Center for Atmospheric Research
Roger Pawlowski	Sandia National Laboratories
Mark Pederson	Naval Research Laboratory
Joerg Petrasch	ETH Zurich (Swiss Federal Institute of Technology)
Stephen Picataggio	Synthetic Genomics
Alex Pothen	Old Dominion University
Tijana Rajh	Argonne National Laboratory
Jennifer Reed	University of Wisconsin-Madison
Angus Rockett	University of Illinois
Michael Sale	Oak Ridge National Laboratory
Andy Salinger	Sandia National Laboratories
Russell Schmehl	Tulane University
Scott Schreck	National Renewable Energy Laboratory
Thomas Schulthess	Oak Ridge National Laboratory
Eric Schwegler	Lawrence Livermore National Laboratory
Mark Sears	U.S. Department of Energy
Radu Serban	Lawrence Livermore National Laboratory
Rekha Seshadri	The J. Craig Venter Institute
Andrew Shabaev	George Mason University
John Shadid	Sandia National Laboratories
Mallikarjun Shankar	Oak Ridge National Laboratory
Mark Shephard	Rensselaer Polytechnic Institute
Abhijit Shevade	Jet Propulsion Laboratory
Blake Simmons	Sandia National Laboratories
David Singh	Oak Ridge National Laboratory
Jeremy Smith	Oak Ridge National Laboratory
Philippe Soucaille	Metabolic Explorer
Ranjan Srivastava	University of Connecticut
Ellen Stechel	Sandia National Laboratories

G. Malcolm Stocks	Oak Ridge National Laboratory
Galen Stucky	University of California
Tatiana Tatusova	National Institute of Health
Jeremy Templeton	Sandia National Laboratories
Robert Thomas	Cornell University
Donald Thompson	University of Missouri – Columbia
Jean-Francois	Tomb DuPont
David Trebotich	Lawrence Livermore National Laboratory
Dallas Trinkle	University of Illinois
John Turner	National Renewable Energy Laboratory
Jeffrey Varner	Cornell University
Ross Walker	San Diego Supercomputing Center
Cai-Zhuang Wang	Ames Laboratory
Lin-Wang Wang	Lawrence Berkeley National Laboratory
Theresa Windus	Ames Laboratory and Iowa State University
Boris Yakobson	Rice University
Dora Yen-Nakafuji	Lawrence Livermore National Laboratory
(Alan) Qi Yuan	Purdue University
Shengbai Zhang	National Renewable Energy Laboratory
Yong Zhang	National Renewable Energy Laboratory
Zhenyu Zhang	Oak Ridge National Laboratory
Yufeng Zhao	National Renewable Energy Laboratory

APPENDIX 2: WORKSHOP PROGRAM

Tuesday, September 18, 2007		
6:00pm	Working Dinner for Organizing Committee, Breakout Leaders, and DOE Program Managers Location: Madison Room on the first floor of the Hilton. Cash bar available outside Madison Room 5:30-7:30pm	
Wednesday, September 19, 2007		
7:00-8:00am	Working Breakfast and Introduction	Gary Johnson
8:00-8:15	ASCR Workshop Goals and Welcome	Michael Strayer
8:15-8:30	EE Workshop Goals	Sam Baldwin
8:30-9:15	Renewable Energy Opportunities and Challenges	Dan Arvizu
9:15-9:45	Break	
9:45-11:45	Parallel Working Sessions Led by Breakout Leaders • Renewable Fuels - Hydrogen • Renewable Fuels - Bioenergy Conversion • Renewable Electricity - Wind Energy • Renewable Electricity - Solar Energy Conversion • Energy Distribution - Grid Futures and Reliability	
11:45-12:45pm	Working Lunch	
12:45-1:30	Can Energy Production Scale? Choices and Challenges from the Current Century	Greg Bothun
1:30-3:20	Parallel Working Sessions (Continued)	
3:20-3:50	Break	
Reports on Panel Working Sessions		
3:50-4:10	Renewable Fuels - Hydrogen	Breakout Leads
4:10-4:30	Renewable Fuels - Bioenergy Conversion	Breakout Leads
4:30-4:50	Renewable Electricity - Wind Energy	Breakout Leads
4:50-5:10	Renewable Electricity - Solar Energy Conversion	Breakout Leads
5:10-5:30	Energy Distribution - Grid Futures and Reliability	Breakout Leads
5:30-5:40	Closing Remarks	Michael Strayer
7:00-9:00	Writing Time for Breakout Leads	

Thursday, September 20, 2007		
7:00-8:15am	Working Breakfast	
8:15-9:00	Computational Advances in Predicting Molecular Properties for Alternative Energy Solutions Dave Dixon	Dave Dixon
9:00-9:30	Break	
9:30-12:00	Parallel Working Sessions Led by Breakout Leaders • Renewable Fuels - Hydrogen • Renewable Fuels - Bioenergy Conversion • Renewable Electricity - Wind Energy • Renewable Electricity - Solar Energy Conversion • Energy Distribution - Grid Futures and Reliability	
12:00-1:00pm	Working Lunch	
1:00-3:20	Parallel Working Sessions (Continued)	
3:20-3:50	Break	
Reports on Panel Working Sessions		
3:50-4:10	Renewable Fuels – Hydrogen	Breakout Leads
4:10-4:30	Renewable Fuels - Bioenergy Conversion	Breakout Leads
4:30-4:50	Renewable Electricity - Wind Energy	Breakout Leads
4:50-5:10	Renewable Electricity - Solar Energy Conversion	Breakout Leads
5:10-5:30	Energy Distribution - Grid Futures and Reliability	Breakout Leads
5:30-5:40	Closing Remarks	Michael Strayer
7:00-9:00	Writing Time for Breakout Leads	
Friday, September 21, 2007		
7:00-8:00am	Working Breakfast	
8:00-12:00	Writing time for Breakout Leads	
12:00pm	Adjourn	