Unparalleled COMPUTING Allocations Guarantee REVOLUTIONARY Science

When researchers use the world's most powerful supercomputers, they allow us to understand the complex processes behind climate change, energy production and distribution, disease mechanisms, and myriad other scientific challenges. The high-performance computing systems that make such work possible are beyond the means of individual researchers and all but a few institutions. To make a dent in these challenges, researchers need access to programs such as the Department of Energy's (DOE's) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.

Computing Comes Into Its Own

Created in 2003 by Undersecretary for Science Dr. Raymond Orbach, INCITE applies the world's most powerful supercomputers to the world's most pressing and challenging computational problems. The program gives researchers the tools they need to create more accurate models of complex processes, simulate problems once thought to be impossible, and analyze an explosion of data generated by experiments. It also gives them access to staff scientists and computing experts at the INCITE centers, ensuring that research projects will make the most of these unparalleled resources. As a result, INCITE is expanding knowledge in the full range of computational science, from climate (figure 1) to fusion, particle physics, chemistry, biology, astrophysics, and materials science.

The INCITE program is pushing the limits of computer simulation, which is supplying answers to questions that cannot be posed in a laboratory. As Dr. Orbach explained to the Council on Competitiveness in January 2007:

"It is often said that science is based on two pillars, namely experiment and theory. In fact, high-end computation, especially through simulation, is the third pillar of science. It is actually a staple support as well. It gives us the ability to simulate things which cannot be done either experimentally or for which no theory exists—simulations of complex systems which are simply too hard or so far are not amenable to analytic approaches."

Indeed, computer simulations have become indispensable in most areas of science. In some fields, simulation augments experiment. Materials scientists and particle physicists often cannot observe the subatomic particles that control important processes. In these cases, computer simulation can help explain and elaborate on the data they are able to get from experiment. In other areas, simulation replaces experiment. For a climate scientist who would need a laboratory the size of the Earth or an astrophysicist who would need one the size of a galaxy, computer simulation provides the closest thing to a controlled experiment the researcher will ever see.

INCITE is also helping to ensure that big science gets access to big tools. Computational researchers are not alone in relying on large, multimillion-dollar facilities. Experimentalists are finding themselves in a similar position as they line up to use state-of-the-art particle accelerators or colossal magnets, and observationalists as they wait for large telescopes on the ground or in space.

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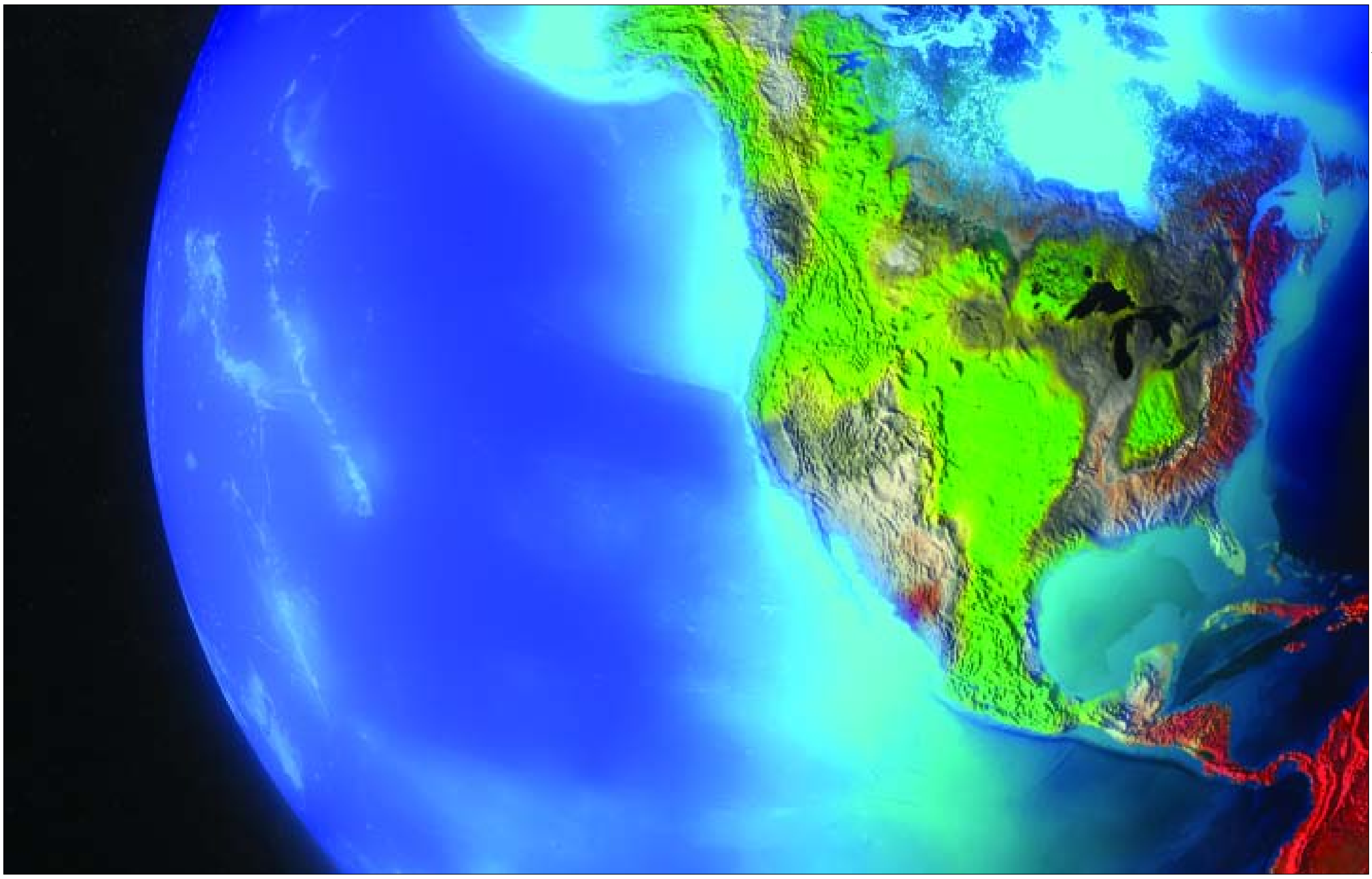


J. Daniel, ORNL

Figure 1. *In this visualization, the green areas show carbon dioxide being taken out of the atmosphere during the day, while the red areas show carbon dioxide being returned to the atmosphere at night.*

INCITE fulfills this responsibility by providing leadership and high-performance computing resources. Leadership systems are not only among the fastest in the world, they are also distinguished by the projects they host. These applications need to occupy a substantial portion of the machine, which generally hosts just a few simulations at a given time.

Examples of leadership systems can be found at the leadership computing facilities at Argonne National Laboratory (ANL) and Oak Ridge National Laboratory (ORNL). As of the June 2008 TOP500 list of the world's fastest computers, the Argonne Leadership Computing Facility's (ALCF) IBM Blue Gene/P system, known as Intrepid, was the fastest in the world dedicated to open science and the third fastest of any type. With a peak computational performance of 557 trillion calculations a second (557 teraflops), it has nearly 164,000 processing cores and 80 terabytes of memory. ORNL's Cray XT4 system, known as Jaguar, was the world's fifth most powerful system, with a peak performance of 263 teraflops. Jaguar contains 31,000 processing cores and 62 terabytes of memory. In 2009, ORNL will deploy a petascale Cray system with more than 110,000 processing cores for INCITE projects.

Big Tools for Big Challenges

The DOE Office of Science is using the INCITE program to put unprecedented computing power in the hands of world-class researchers. The payoff is discovery in the full gamut of scientific fields.

This world-class computing power is offered through the Advanced Scientific Computing Research Program and located at supercomputing centers in Tennessee, Illinois, California, and Washington states. Between them, the facilities at ORNL (sidebar "Oak Ridge National Laboratory" p23), ANL (sidebar "Argonne National Laboratory" p24), Lawrence Berkeley National Laboratory (LBNL) (sidebar "Lawrence Berkeley National Laboratory" p26), and Pacific Northwest National Laboratory (PNNL) (sidebar "Pacific Northwest National Laboratory" p30) were allocating 265 million processor hours in 2008 on systems from Cray, IBM, and Hewlett-Packard, and the allocations will more than double in 2009 to 680 million processor hours (figure 2). The largest INCITE allocation in 2008, for example, is roughly equivalent to time afforded by the aggregate compute power of 20 128-processor high-performance clusters operating 24 hours per day 365 days per year. By allocating time on some of the world's most powerful systems, the program

Source: DOE Office of Science

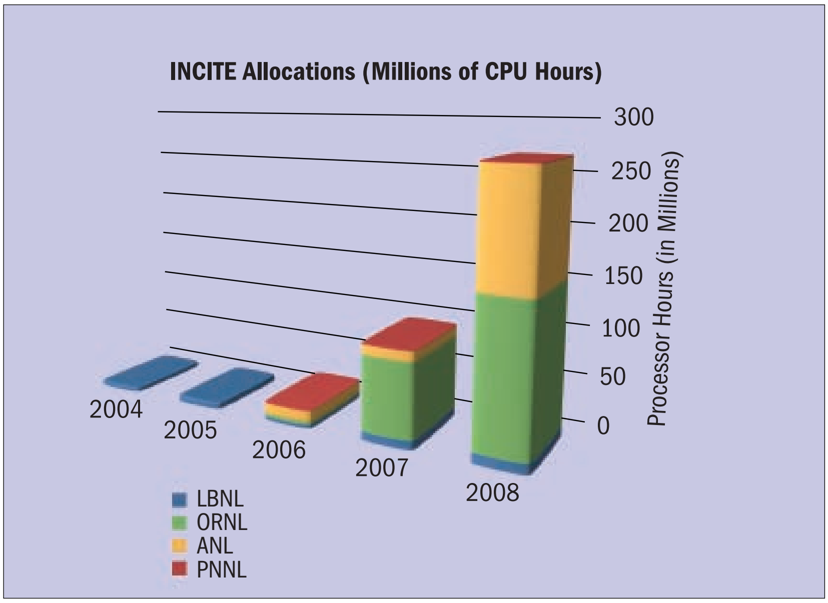


Figure 2. *INCITE allocations have grown exponentially since the program began in 2004.*

Investigators are using major INCITE allocations to study matter from the smallest scale, with explorations of the interaction of quarks and gluons and the binding properties of atomic nuclei, to the largest, with explorations of merging galactic black holes and both thermonuclear and core-collapse supernovae.

is working to overcome the world's most urgent and vexing challenges.

Climate projects are using massive computing resources through INCITE (figure 1, p21). Warren Washington at the National Center for Atmospheric Research leads a project focused on development and application of the Community Climate System Model (CCSM) with an allocation of more than 18 million processor hours in 2008 (a processor hour refers to the time run on a system for each processor; one hour on 10 processors equates to 10 processor hours). The CCSM team has achieved phenomenal results under INCITE, moving toward Earth system modeling that goes beyond the atmosphere and land models of earlier decades to include atmospheric chemistry and terrestrial and ocean biogeochemistry, including realistic formulations of the global carbon cycle.

The flip side of the climate challenge is energy assurance—the ability to produce, distribute, and consume, without costly disruption, the energy required in assured, economically viable, and environmentally benign ways to satisfy residential, commercial, and transportation needs. The INCITE program is providing tens of millions of processor hours to projects that are expanding the limits of physics, biology, and chemistry to ensure that we succeed.

Combustion scientists are perfecting the way we exploit fossil fuels, allowing us to take advantage of all the energy these nonrenewable fuels have to offer

Biophysicists are refining and making more economical the process for taking plants unsuitable for food and turning them into ethanol that can replace fossil fuels, providing a source of fuel that is both renewable and kind to the environment

Materials scientists are improving our understanding of superconductivity, providing a potentially loss-free means of electricity transmission

Fusion scientists are refining what it takes to make a plasma several times hotter than the core of the Sun, control that plasma, and use it to generate electricity, leading to an abundant, relatively clean energy that is also free of greenhouse gas emissions

Chemists are developing the catalysts that will control fuel cells, providing a source of energy free of greenhouse emissions

Nuclear engineers and physicists are probing the inner workings of nuclear reactor cores to better understand the complex fission, thermal hydraulics, heat transfer, and materials science issues involved in an effort to design safer, cheaper, and more efficient nuclear power plants

Basic science, too, is of course crucial to the INCITE effort. Just as today's researchers build on the achievements of their scientific forebears to solve contemporary problems, they also strive to expand the limits of knowledge and analysis to provide comparable tools for tomorrow's researchers. Investigators are using major INCITE allocations to study matter from the smallest scale, with explorations of the interaction of quarks and gluons and the binding properties of atomic nuclei, to the largest, with explorations of merging galactic black holes and both thermonuclear and core-collapse supernovae.

Year 1: A Star is Born

As Dr. Orbach explained in an interview with *HPCwire* in 2007, INCITE was established in 2003 to ensure that big problems were tackled with big resources.

"The problem back then was that in the U.S., we in the government were awarding computer time more to maximize the number of users, with the result that everyone got a little time. This proved not to be an efficient way to address real problems. I know from my own experience what it's like to work on challenging problems when your computer time is limited.

"We asked ourselves how discovery could advance if we gave people enough time to solve major problems and allocated the machine time based on peer review. We started with just four proposals, but when people found out we'd be allocating as much as a million hours or more per project, INCITE really caught on."

In fact, 52 proposals were received for that first year, 2004, requesting more than 130 million processor hours. Eventually three projects received nearly five million processor hours on Seaborg, an

Oak Ridge National Laboratory

The National Center for Computational Sciences (NCCS) ("Scientific Comptuting at the Cutting Edge," *SciDAC Review*, Winter 2007, p36) at ORNL was established in 1992. In 2004, it was designated—along with the Argonne Leadership Computing Facility (ALCF)—as the nation's Leadership Computing Facility, charged with developing an unclassified resource 100 times more powerful than the systems of the day.

The NCCS is hosting 30 INCITE projects in 2008 with allocations of 145 million processor hours. These projects are given time on Jaguar (figure 3), a Cray XT4 with a peak performance of 263 trillion calculations a second (teraflops), and Phoenix, a Cray X1E with a peak performance of more than 18 teraflops. Jaguar is ranked Number 5 on the TOP500 List of the world's most powerful computers (www.top500.org), while Phoenix is ranked Number 175.

Six of these projects have been awarded 10 million processor hours or more; in other words, each is twice or more the size of the entire INCITE program in its first year. For comparison, a 128-node cluster can provide just over one million processor hours if it runs 24 hours a day for an entire year.

A team led by Jacqueline Chen of Sandia National Laboratories is using 18 million processor hours to understand and control the turbulent combustion processes in next-generation internal combustion engines. A team led by Anthony Mezzacappa of ORNL is using 16 million processor hours to perform three-dimensional, multiphysics simulations to understand the elusive explosion mechanism of core-collapse supernovae, which are responsible for most of the elements in the Universe between oxygen (atomic number 8) and iron (atomic number 26) and half of the elements heavier than iron. The Climate-Science Computational End Station Development and Grand Challenge Team, led by Warren Washington of the National Center for Atmospheric Research, is using nearly 16 million processor hours to continue development of the Community Climate System Model (CCSM), with key additions such as the incorporation of land-use change and dynamic global vegetation, sulfur cycle, and aerosol feedbacks. CCSM is being used to assess climate change to the year 2030, DOE year 2000–2100 energy strategy scenarios, and coupled ice sheet control and warming scenarios. A team led by Robert Harrison of ORNL is using 10 million processor hours to promote the design of chemical catalysts using reliable prediction of the electronic structure of large molecules and surfaces. A team led by Thomas Schulthess of ORNL is using 10 million processor hours to simulate Mott insulators, high-temperature superconductors, magnetic nanoparticles, and biomolecular systems key to the future development of electric grid technologies, high-density magnetic hard drives, and biofuel production. And a team led by Jihui Yang of General Motors is using 10 million processor hours to develop thermoelectric materials that will transform the waste heat from an engine into usable electricity.

Further Information
http://www.nccs.gov

IBM SP supercomputer at LBNL's National Energy Research Scientific Computing (NERSC) Center in Berkeley, California.

A team led by Tomasz Plewa of the University of Chicago was given 2.7 million processor hours to explore the genesis of the thermonuclear explosion that leads to a Type Ia supernova. Using this allocation, the team conducted the most detailed simulations to that time of the initial stage of these events, which are among the brightest in the Universe and have been used to verify the accelerating expansion of the Universe.

According to Plewa, the large INCITE allocation made it possible for his team to move this science forward.

"None of this would have been possible without INCITE," he said. "These simulations are so computationally intensive that they do require hundreds of thousands of CPU hours per computational run. Computing centers typically do not give so much computing time to one project. So, the scale of INCITE grants was essential."

A second team, led by P. K. Yeung of the Georgia Institute of Technology, received 1.2 million processor hours to simulate fluid turbulence and mixing at high Reynolds numbers, a daunting

ORNL

Figure 3. *Oak Ridge National Laboratory's Cray XT Jaguar supercomputer.*

Argonne National Laboratory

Argonne began working with IBM and Lawrence Livermore National Laboratory in 2004 to develop a series of computing systems based on IBM's Blue Gene platform. One outcome of that collaboration is a Blue Gene/P system named Intrepid (figure 4), located at the ALCF ("Opening New Possibilities in Science and Engineering," *SciDAC Review*, Spring 2008, p42). With a peak performance of 557 teraflops, Intrepid is now the world's fastest supercomputer for open science and the third most powerful of any type.

The ALCF was established in 2006 and dedicated on April 21, 2008. The facility currently hosts 20 INCITE projects with allocations of more than 111 million processor hours. In 2009, the ALCF will provide 500 million processor hours to INCITE projects.

Five of these projects have been awarded 10 million processor hours or more. A team led by Don Lamb of the University of Chicago will use 21 million processor hours on Intrepid to validate four current models of the Type Ia supernova—the Universe's largest thermonuclear explosion (figure 5). A team led by Robert Sugar of the University of California–Santa Barbara is using nearly 20 million processor hours to deepen our understanding of how quarks and gluons combine to make up nearly all visible matter. Paul Fischer of Argonne is using 14 million processor hours to advance understanding of advanced reactors by simulating turbulent thermal transport in sodium-cooled reactor cores. David Baker of the University of Washington is using 12 million processor hours to develop computational tools for solving the structures of biologically important proteins and has exciting membrane protein structure prediction calculations under way. And David Dean of ORNL is using 10 million processor hours to perform first-principles calculations of light and medium mass nuclei and of the three-nucleon force.

Further Information
www.alcf.anl.gov

"The INCITE program is truly unique. No other agency has the resources to open their systems up to computational scientists—whether they work at a government research facility, a university, or at an industrial R&D center—and then give them access to support staff and systems to run applications at previously unheard-of scales."

Dr. Michael Strayer
DOE Office of Science

ANL

Figure 4. *Argonne National Laboratory's Intrepid Blue Gene/P supercomputer.*

computational challenge that is nevertheless key to understanding fields as disparate as combustion, propulsion, meteorology, oceanography, and environmental degradation. With his direct numerical simulation technique, Yeung and his collaborators were able to solve the exact conservation equations for mass, momentum, and chemical species concentration and mixing without approximation.

"Our INCITE award has allowed us to perform the largest simulation of fluid flow turbulence ever done in the U.S., at a level of detail and within a time frame not possible otherwise," Yeung said. "We have used as many as eight billion grid points to probe deeply into a problem arising in multiple fields of science and engineering."

The third project, led by William Lester Jr. of LBNL and the University of California, was given one million processor hours to increase scientific understanding of photosynthesis. In particular, the team simulated the process by which a plant protects itself by regulating the amount of solar energy it absorbs.

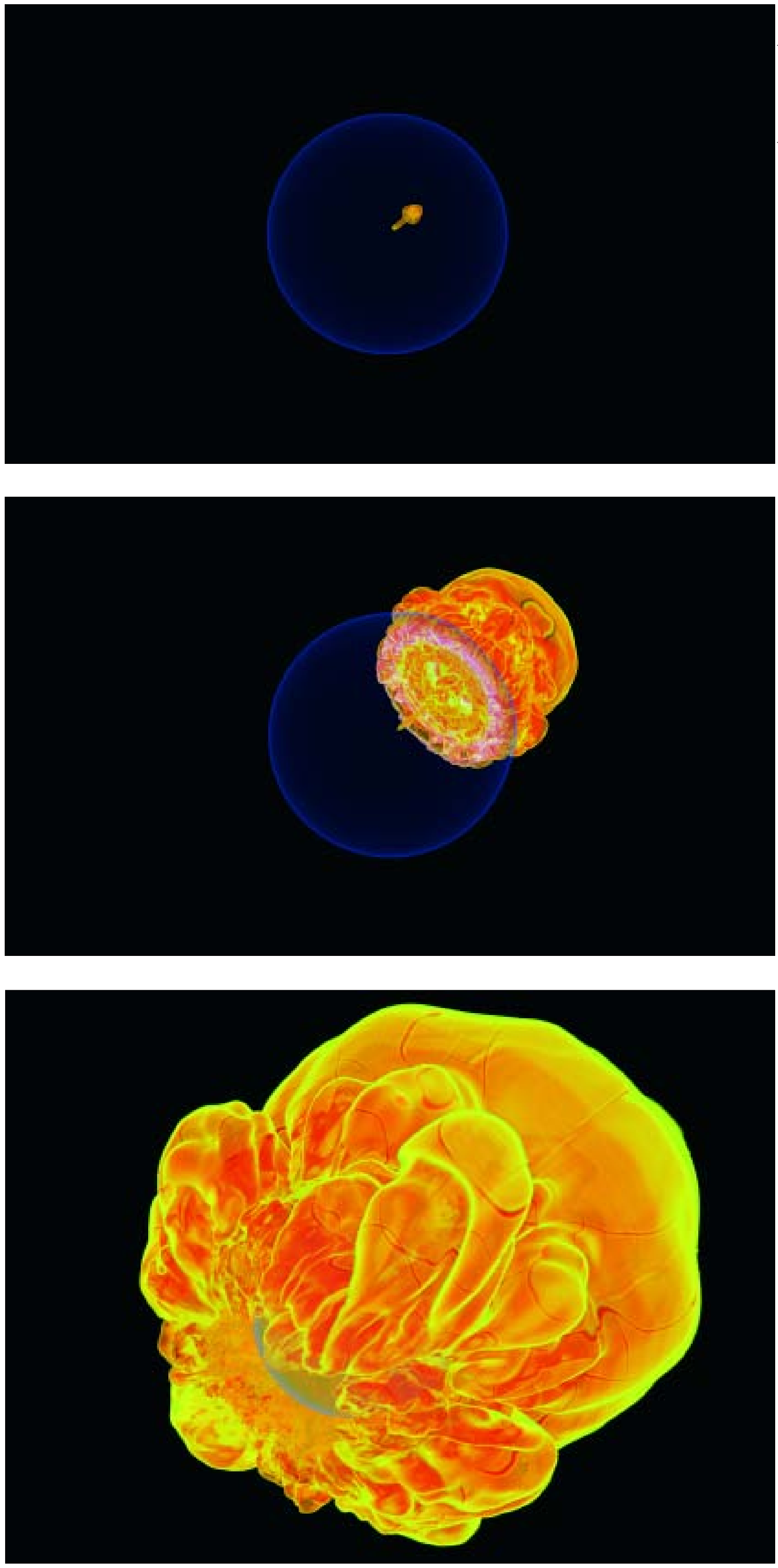
These three projects also illustrate a marked shift from previous DOE allocation programs and another guiding principle behind INCITE: projects receive allocations based on the quality of the science, the potential impact of the research, and the readiness of the project to effectively use these unique systems. They need not come from DOE researchers or DOE-sponsored projects. From the first call, INCITE invited proposals from universities and other research institutions, and by the third year it was welcoming computational scientists from industry as well.

"The INCITE program is truly unique," said Dr. Michael Strayer, associate director of the Office of Advanced Scientific Computing Research in DOE's Office of Science. "No other agency has the resources to open their systems up to computational scientists—whether they work at a government research facility, a university, or at an industrial R&D center—and then give them access to support staff and systems to run applications at previously unheard-of scales."

The program in 2005 attracted 23 proposals seeking more than 28 million processor hours. Of these, three projects were given 6.5 million processor hours on NERSC's Seaborg. A team led by combustion researcher Jacqueline Chen of Sandia National Laboratories in Livermore, California, used its 2.5 million hour allocation to conduct a three-dimensional simulation of flame for which the oxygen and fuel are not premixed, a project that promised more efficient use of jet aircraft and direct-injection diesel and gasoline engines. A team led by Fausto Cattaneo of the University of Chicago used its two million hour allocation to study processes by which the material swirling around a newly formed star or black hole becomes unstable and falls onto the central object, helping to explain the evolution of the Universe. And a team led by Valerie Daggett of the University of Washington used its two million hour allocation to create a repository of the molecular dynamics structures for protein folds, combining molecular dynamics and proteomics to promote a greater understanding of protein folding in general and the many illnesses linked to protein folding gone awry.

Industrial Strength Supercomputing

In 2006, the program expanded dramatically, with the resources allocated nearly tripling to more than 18 million processor hours. DOE made portions of all of its high-performance and leadership computing resources at ANL, LBNL, ORNL and PNNL available to INCITE researchers, and for the first time industrial users were invited into the program (sidebar "INCITE Takes Care of Business" p28). A key aspect of the INCITE program is that while the total available allocations have expanded dramatically, the number of projects have not; hence, individual project allocations have expanded in accordance with the size of the supercomputers. This fact ensures that projects have the largest



D. Lamb, the FLASH Center, University of Chicago

Figure 5. *Three phases of the gravitationally confined detonation mechanism of a Type Ia supernova. The images show the flame surface and the star (upper) at 0.5 s, soon after the bubble becomes unstable and develops into a mushroom shape, (middle) at 1.0 s, as the bubble breaks through the surface of the star, and (lower) at 1.7 s, shortly before the hot ash from the bubble collides at the opposite point on the surface of the star. These images are generated from volume-renderings of the flame surface and the density.*

Lawrence Berkeley National Laboratory

With roots in the energy crisis of 1973, LBNL's National Energy Research Scientific Computing (NERSC) Center has a long history of supporting America's energy assurance efforts. NERSC (see also "Science-Driven Supercomputing," *SciDAC Review*, Spring 2007, p36) has 3,000 users that include laboratory and university researchers, and devotes most of its computational resources to the DOE Office of Science mission, reserving 10% of its processor hours to the INCITE program. The INCITE program was established at NERSC in 2003 and was solely supported by NERSC through its first two years.

The Center's high-performance computing resources include Franklin, a Cray XT4 system with a 100-teraflop peak performance (figure 6). Franklin will be upgraded in 2008 by doubling the number of processors and increasing the peak performance of each processor to produce a 350-teraflop peak system. NERSC is hosting 11 INCITE projects in 2008 with allocations totaling 10 million processor hours and will provide 20 million hours to INCITE in 2009. The 2008 INCITE awards include a project led by John Bell of LBNL, who is using 3.4 million processor hours to enhance our understanding of the unstable flames that will be key to developing near-zero-emission combustion devices. In addition, Gilbert Compo of the University of Colorado is using 2.9 million processor hours to produce a global tropospheric circulation dataset for the 20th century, an effort that promises to be an important tool in validating leading climate models. And the Climate-Science Computational End Station Development and Grand Challenge Team is using 1.3 million processor hours to integrate the global carbon cycle into climate simulations at unprecedented levels of detail that will resolve important features of the atmosphere, ocean, and land surface.

Further Information
www.nersc.gov

allocations possible in order to break down the barriers of the unknown.

The decision to invite researchers from the private sector into the program grew out of a recommendation from the Council on Competitiveness (www.compete.org), a group of corporate executives, university officials, and labor leaders focused on strengthening the U.S. position in the global economy.

"The council's fundamental belief is that U.S. competitiveness and the nation's ability to add high-value economic activity increasingly depend on 21st-century modeling and simulation …" council President Deborah Wince-Smith told *HPCwire* in 2007. "As U.S. taxpayers, we have all invested in these HPC (high-performance computing) capabilities. The INCITE program is leveraging these investments not only to advance the nation's scientific leadership, but our industrial competitiveness and standard of living."

"We chose to collaborate with the Council in order to broaden the reach of INCITE," Dr. Orbach added, "and that choice has proven itself time and again to be the right one. Like DOE, the Council and its members care deeply about American competitiveness. Collaboration with the Council—particularly in the area of high-performance computing—is a natural extension of our mutual interest in American leadership in basic and applied research."

All in all, four industry projects were chosen for the INCITE program in 2006. A team led by Moeljo Hong of the Boeing Company used its allocation to develop and validate large-scale computational tools for flight vehicles and demonstrate the predictive accuracy of computational fluid dynamics tools in a real-life production environment. A team led by Peter Bradley of Pratt & Whitney used its time to perform computational fluid dynamics simulations to improve combustor design in gas-turbine engines. A team from General Atomics led by Ronald Waltz worked to strengthen the stability of fusion reactors by examining the interaction of turbulence at the scale of ions with the much smaller-scale turbulence at the scale of electrons. And a team led by Evan Smyth of Dreamworks Animation focused on pushing the limits of high-quality ray-tracing in real time, developing a parallel technology that could prove invaluable in such fields as medical imaging, defense simulations, and visualization in general, not to mention movie-making.

Industry interest and participation in INCITE continues to vary and grow, increasing from four industry projects in 2006 to eight in 2008. Some industries turn to INCITE to inform their in-house purchase decisions, others use INCITE for "proof-of-design" concepts running very specific tests or validations, and still others have multi-year proposals for basic research focused on a real application that could deliver results in their products. For these researchers, INCITE opened the door not only to the tools but also the expertise that would otherwise be out of their reach. INCITE centers are home to many of the world's leading experts in scientific computing.

"While Pratt & Whitney fields supercomputing resources of its own," Bradley said, "the Department of Energy through its mission, scientists, and infrastructure is uniquely qualified to operate and enable a supercomputing resource beyond the practical capabilities of a large industrial company.

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LBNL

Figure 6. *Lawrence Berkeley National Laboratory's Cray XT4 Franklin supercomputer.*

In the last two years INCITE has continued to expand, thanks in large measure to an explosive growth in computing power and a substantial investment from DOE in state-of-the-art systems.

In an ever-expanding global economy where technology leadership is critical to competitiveness, INCITE provides American industry with an engine for technological and competitive growth."

In the last two years INCITE has continued to expand, thanks in large measure to an explosive growth in computing power and a substantial investment from DOE in state-of-the-art systems. When the INCITE program was first announced in July 2003, Seaborg at LBNL was the fifth most powerful system in the world at a peak performance of just under 10 teraflops. (The world's number one system, Japan's Earth Simulator, had a peak performance of 40 teraflops.) As of summer 2008, the INCITE program had three systems more than 10 times as powerful as Seaborg: ANL's Intrepid, ORNL's Jaguar, and LBNL's Franklin system, with peak performances of over 100 teraflops.

As a result, DOE was able to continue expanding INCITE and the accomplishments it engenders. In 2007, the program awarded 95 million hours to 45 of the world's most intensive computational projects. In 2008, 55 leading projects received 265 million processor hours, more than 50 times the resources allocated just four years before. Eleven of these projects received more than 10 million processors hours, individual allocations that are more than twice the size of the program in its first year.

INCITE Delivers Groundbreaking Science

The proof of any research endeavor is the quality and impact of science it produces. In its first five years the Office of Science's INCITE program has already produced groundbreaking results across the range of computational sciences and has transformed the computational science landscape. The following are just a few of the more prominent successes achieved by research projects using INCITE resources and its expert facility staff.

Lifting the Veil on Protein Structure

A team led by David Baker at the University of Washington increased our understanding of enzyme structure and function, going as far as designing new enzymes that catalyze chemical reactions not catalyzed by any naturally occurring enzyme. In several cases, the team has predicted high-resolution structures of proteins, working only from amino acid sequences. This ability will greatly speed the interpretation of genome sequence in ongoing large-scale sequencing projects such as the Human Genome Project. The team's work was featured in the November 8, 2007 and March 19, 2008 issues of the journal *Nature* and the March 7, 2008 issue of the journal *Science*.

Stabilizing a Lifted Flame

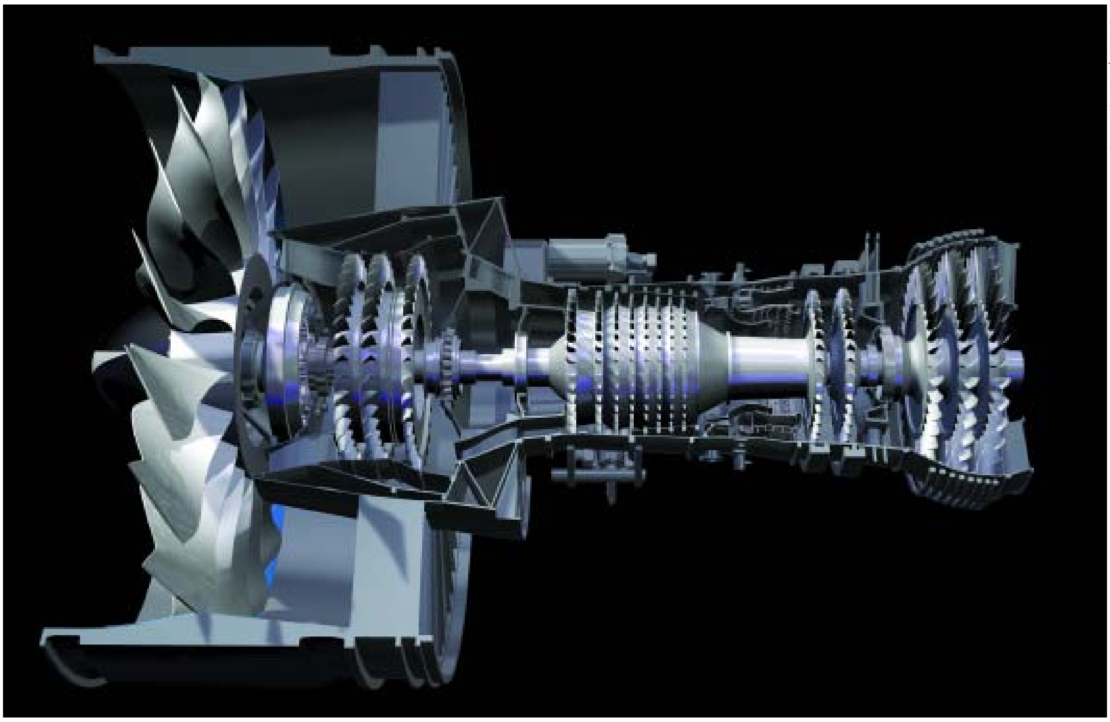
A team led by Jacqueline Chen of Sandia National Laboratories has probed and elucidated the mechanisms that allow jet flames to burn stably above a burner. Known as a lifted flame, this phenomenon is important in applications such as industrial burners for power generation, where lifting of the flame removes it from contact with the nozzle and thereby reduces damaging thermal stresses to the nozzle material. Using direct numerical simulation at resolutions of more than one billion grid points

INCITE Takes Care of Business

From the design of cars, trucks, and aircraft to the deployment of sustainable energy sources, the expansion of medical science and drug design, and the development of more effective consumer products, American businesses have come to realize the value of having the world's most powerful scientific computers at their disposal.

The INCITE program has embraced leading industrial researchers since 2006, bringing them together with both the leadership computing systems and the unparalleled expertise found at the Office of Science's INCITE centers. In that time, the program has allocated nearly 27 million processor hours to American businesses. The following is a sampling of the research being conducted by industry under the INCITE program.

- **General Motors** researchers are performing first-principles calculations of thermoelectric materials capable of turning waste heat into electricity. Using an allocation of 10 million processor hours in 2008, the team is working to capture and use some of the 60% of energy generated by an automobile's engine that is lost through waste heat. GM is hoping to exploit the properties of these exotic thermoelectric materials, which may well increase fuel economy in the next generation of vehicles.
- **Procter & Gamble** researchers have pursued a deeper knowledge of bubble formation, dynamics, and stability with 5.1 million processor hours in 2007 and 2008. INCITE allocations are allowing researchers to perform simulations at an unprecedented scale on the dissolving of soap and forming of suds. By simulating the molecular mechanisms of bubble formation, these researchers are paving the way for environmentally friendly detergents and improved consumer products with additional application to more effective chemicals for fire control and hazardous cleanup.
- **General Atomics** researchers are simulating the workings of turbulence in a fusion reactor, using 3.4 million processor hours from 2006–2008 to understand one of the most vexing problems faced by fusion researchers. Their efforts will help in predicting the performance of the international ITER reactor.
- **Pratt & Whitney** researchers are using computational fluid dynamics simulations to better understand gas-turbine engines, improve fuel efficiency, control emissions, reduce noise, and boost operability (figure 7). With allocations of more than three million processor hours from 2006–2008, the company is working to understand the impact of properly resolving turbulence scales on combustor swirler aerodynamics and to study its impact on the combusting simulation. The focus is on Pratt & Whitney's next-generation, low-emission Geared TurbofanTM engine. This groundbreaking engine will deliver unprecedented reductions in emissions, noise, and cost of ownership compared to current engines.
- **DreamWorks Animation** researchers are pushing the limits of real-time ray-tracing. The team used 1.8 million processor hours in 2006 and 2007 to develop techniques that improve the production and turn-around time of computer graphics imagery, a project with potential benefit for medical imaging, defense simulations, and visualizations in general, as well as feature films.
- **Corning Inc.** researchers are expanding our knowledge of materials, including glasses, ceramics, and polymers. With 1.6 million processor hours in 2007 and 2008, this research includes the simulation of dense suspensions and calculations of glass transition range behavior for silica and silicate glasses. Their focus is on computing the glass transition range behavior for silica and multicomponent silicate glasses and first-ever calculations of realistic glass transition range behavior for these systems. This is of very practical interest to the U.S. glass industry, since silicates account for the vast majority of all glass products in both traditional and high-tech applications.
- **Boeing** researchers are developing, correlating, and validating large-scale computational tools for flight vehicles. Allocations of 800,000 processor hours from 2006–2008 are helping these researchers demonstrate the applicability and predictive accuracy of computational fluid dynamics tools in production environments. Their focus has been building next-generation aero-elastic wing simulation capabilities (interplay between flow around a wing and its subsequent bending/flapping) and analysis of thrust-reversal flows often utilized upon landing.
- **Gene Network Sciences** researchers are simulating cardiac rhythm disturbances to help identify the underlying electrical mechanisms for dangerous arrhythmias. Using an allocation of more than 800,000 processor hours in 2008, the researchers hope to determine the effects of interventions, such as drugs, that may prevent or exacerbate these arrhythmias.
- **Fluent Inc.** researchers are testing the benefits of large-scale engineering simulation early in the process of automotive design. These researchers are using more than 300,000 processor hours in 2007 and 2008 with Fluent software to perform emerging computational fluid dynamics and thermal calculations to determine the hardware resources and software system behavior required to deliver timely results for General Motors' Global Vehicle Development Process.



P. Bradley, Pratt & Whitney

Figure 7. *Pratt & Whitney's Geared Turbofan™ engine will deliver game-changing performance, including double-digit improvements in fuel burn and environmental emissions.*

(and a jet Reynolds number of 11,000), the team revealed that by increasing the fuel or surrounding air co-flow velocity, the flame stabilized without a physical element to use for stabilization, resulting in the generation of a lifted jet flame. The position downstream of a fuel injector where a diesel fuel jet establishes a flame, the so-called stabilization point, influences the degree of premixing between the cold fuel and heated air prior to combustion, and this, in turn, affects the combustion and soot formation processes downstream. The team's accomplishments have been submitted in two different manuscripts to *Combustion and Flame*.

Understanding Water

A team led by Giulia Galli at the University of California–Davis used quantum simulations to probe the nature of water and its behavior on surfaces. The team has focused on a variety of surfaces, organic as well as inorganic and hydrophobic as well as hydrophilic. It unraveled the microscopic structure of the interface and identified the key role played by electrons in determining the arrangements of water molecules at a surface. The team also provided predictions and interpretations of what experimentalists should see when they measure the vibration of water molecules in contact with surfaces. By unraveling the properties of water at organic and inorganic interfaces, the team has enabled a more fundamental understanding of the function of biological systems and the behavior of soft and hard materials in natural environments. Such understanding allows better control of the aqueous environments found in energy systems and the environment. The team's work is featured in an upcoming edition of *Physical Review Letters* and in the July 2, 2008 edition of the *Journal of the American Chemical Society*.

Taming Turbulent Heat Loss in Fusion Reactors

A team led by W. W. Lee of the Princeton Plasma Physics Laboratory has advanced our understanding of energy loss in a tokamak fusion reactor owing to the turbulent behavior of hot plasma. Earlier simulations had overstated the loss and linked it to the length of turbulent eddies in the reactor. With access to INCITE leadership systems, however, the team was able to incorporate the complex, three-dimensional geometry of the reactor (the shaped cross-section of the toroidal system), revealing that electron thermal transport is due not to the length of the turbulent eddies but to the rapid movement of the electrons, which prevents them from being trapped by the eddies for long. This research promises to help ensure the success of the multi-national, multibillion-dollar ITER reactor (www.iter.org). The team's accomplishments are outlined in *Physical Review Letters* volume 99, and the journal *Physics of Plasmas*, volume 14.

Shining the Light on Dark Matter

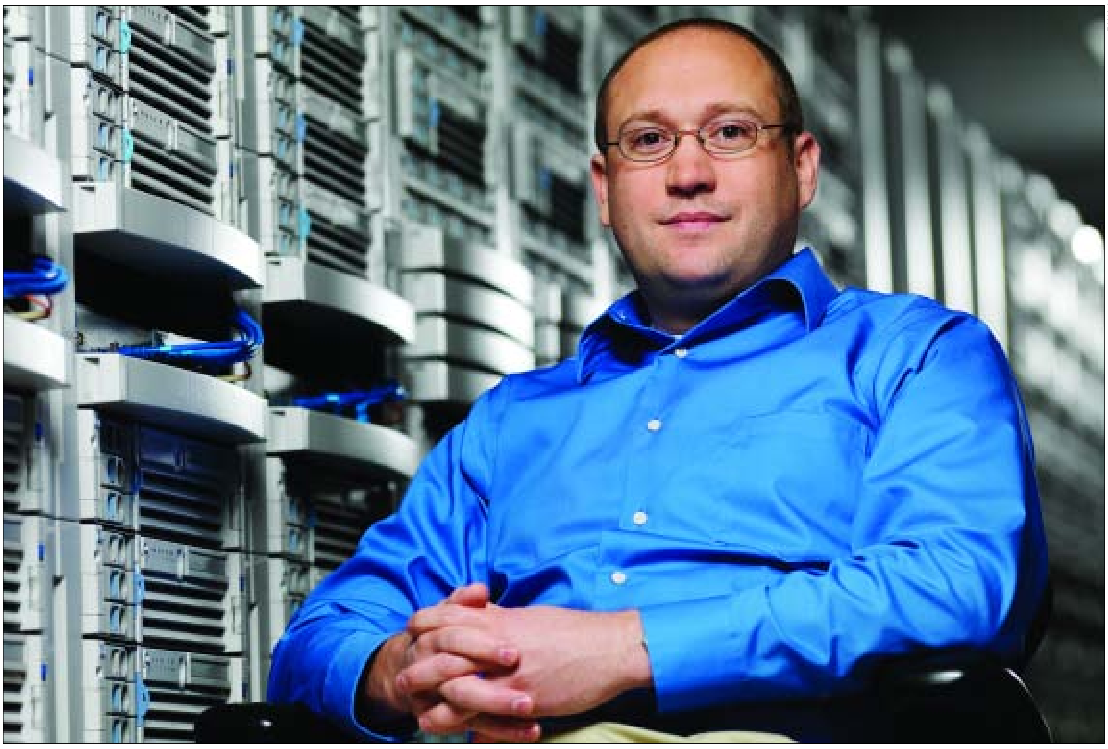
A team led by Piero Madau of the University of California–Santa Cruz provided a glimpse into the invisible world of dark matter, performing the

In its first five years the Office of Science's INCITE program has already produced groundbreaking results across the range of computational sciences and has transformed the computational science landscape.

Pacific Northwest National Laboratory

The Environmental Molecular Sciences Laboratory, a DOE national scientific user facility located at PNNL, supports a wide range of computational molecular research, including benchmark calculations on small molecules, reliable calculations on large molecules and solids, simulations of large biomolecules, and reactive chemical transport modeling.

The laboratory is participating in the INCITE program through the MPP2 system, a Hewlett-Packard supercomputer with a peak performance of 11.8 teraflops and a ranking of Number 407 on the TOP500 List (figure 8). A team led by Athonu Chatterjee of Corning Inc. is using 750,000 processor hours on this system in 2008 to examine the flow and deformation of dense suspensions, a project with processes ranging from ceramics to polymers. In addition, a team led by Peter Lichtner of Los Alamos National Laboratory is using 200,000 processor hours to model the flow of uranium in groundwater at the Hanford site in Washington state.



PNNL

Figure 8. *Pacific Northwest National Laboratory's Hewlett-Packard Chinook supercomputer pictured with Kevin Regimbal.*

largest computer simulation ever of dark matter evolving in a galaxy such as the Milky Way. The Universe is dominated by a mysterious, cold, and weakly interacting particle that appears to account for about 83% of the matter in the Universe. Revealing the nature of this dark matter is fundamental to cosmology and particle physics. The simulation divided the galaxy's dark matter halo into a billion particles and let them evolve over 13 billion years. One of its key findings is that smaller dark matter structures remain identifiable even as they are pulled into progressively larger structures, meaning that the galaxy's dark matter is decidedly clumpy. The group will be able to verify its results using the National Aeronautics and Space Administration's *Gamma-Ray Large Area Space Telescope* (*GLAST*), which will be able to detect gamma radiation produced by dark matter annihilation, and by observing the gravitational lensing exerted by dark matter within other galaxies on light from distant quasars. The team's work is featured in the August 7, 2008 issue of the journal *Nature*.

How Does a Pulsar Get Its Spin?

A team led by Anthony Mezzacappa of ORNL discovered the first plausible explanation for a pulsar's spin that fits the observations made by astronomers. According to three-dimensional simulations performed by the team, the spin of a pulsar—the spinning remnant of a core-collapse supernova—is determined by the shock wave created when the star's massive iron core collapses. The team's discovery overcomes a weakness in the previous assumption about a pulsar's spin—that is, that it comes from the spin of the original star. That explanation would explain only the fastest observed pulsars. The simulations performed by Mezzacappa's team, on the other hand, predict the

The INCITE program shows no sign of slowing as it heads to the future. The Office of Science expects to allocate more than 500 million processor hours to the program, doubling it once again.

Getting an INCITE Allocation

The INCITE program is open to research projects from industry and academia—as well as from DOE laboratories—that are advanced enough to take advantage of these leadership systems to deliver high-impact advances.

Researchers have until late summer to apply for grants in the following year's INCITE program. Successful proposals, which will be for one to three years, will describe the research in terms suitable both for specialized review in the area of exploration and for general review evaluating proposals from multiple scientific domains. Researchers submitting proposals must also demonstrate how they will be able to exploit a large fraction of a system's processing cores, which number nearly 164,000 on Argonne National Laboratory's Intrepid system.

INCITE award recipients will have access to systems at Oak Ridge, Lawrence Berkeley, and Pacific Northwest national laboratories, as well as Argonne. Lastly, for those projects requiring start-up time in order to port and test codes, start-up accounts can be provided as well.

Further Information
http://www.science.doe.gov/ascr/INCITE

The computational science community is already making plans for how it will make use of exascale supercomputers a thousand times more powerful than upcoming petascale systems.

range of observed pulsar spins. The team's work was featured in the January 4, 2007 issue of the journal *Nature*.

New Hope in the Fight Against Parkinson's
A team led by Igor Tsigelny of the University of California–San Diego combined molecular modeling and molecular dynamics simulations with biochemical and ultrastructural analysis to provide new insights into Parkinson's disease. The team showed that increases in the protein alpha-synuclein can lead to harmful pore-like structures in human membranes, while increases in another protein, beta-synuclein, can block the propagation of alpha-synuclein into the structures. Not only does this achievement pave the way for new Parkinson's therapies and potentially the first drug to fight progression of the disease, it also provides a test bed for identifying possible therapeutic interventions through computational modeling. Laboratory studies with mice have shown the effect predicted by the INCITE studies. The team's work is featured in the February 2008 issue of *Nature Methods* and on the cover of the *Federation of European Biochemical Societies Journal*, volume 274, issue 7.

Promises for the Future

The INCITE program shows no sign of slowing as it heads to the future. The 2009 INCITE call for proposals was issued on May 13, and the Office of Science expects to allocate more than 500 million processor hours to the program, doubling it once again. Projects for 2010 (sidebar "Getting an INCITE Allocation") are likely to exceed two billion hours as the planned petascale system—able to perform thousands of trillions of calculations a second—at ORNL becomes available to INCITE users. In five years, INCITE allocation awards have increased a hundred-fold (from five million to 500 million hours), roughly similar to the growth of the power of top computing systems.

The computational science community is already making plans for how it will make use of exascale supercomputers a thousand times more powerful than upcoming petascale systems. Materials scientists are likely to understand the quantitative differences in the transition temperatures of high-temperature superconductors. Climate scientists will predict future climates based on scenarios of anthropogenic emissions using integrated and coupled models for ocean, sea ice, land, atmosphere, carbon/water cycles, and biogeochemistry. Chemists will be able to simulate select liquid–liquid and gas–liquid interfaces with accurate thermochemistry and spectroscopy. And the list goes on. •

Contributors: Staff from the DOE Office of Advanced Scientific Computing Research, the ALCF (ANL), the Environmental Molecular Sciences Laboratory (PNNL), the National Center for Computational Sciences (ORNL), and the NERSC Center (LBNL)

Further Reading: More information on the scientific accomplishments made possible by the INCITE program, see "Top Breakthroughs in Computational Science" (p32) in this issue, especially the following sections: "Scientists Model the Molecular Basis of Parkinson's Disease" p34; "Astrophysicists Discover Supernova Shock-Wave Instability and a Better Way to Spin Up Pulsars" p36; "Designing Proteins at Atomic Scale and Creating Enzymes" p38; "First-Principles Flame Simulation Provides Crucial Information to Guide Design of Fuel-Efficient Clean Engines" p40; "Breakthrough Fusion Simulation Sheds Light on Plasma Confinement" p42; "Closing In on an Explanation for High-Temperature Superconductivity" p44; "A Billion-Particle Simulation of the Dark Matter Halo of the Milky Way" p48; "Exploring the Mysteries of Water" p50