NERSC NEWS

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Berkeley Lab

Office of Science
U.S. DEPARTMENT OF ENERGY

MARCH 2007

Star Power

NEW PURSUIT AIMS TO DECODE FORCES BEHIND HIGH-MASS STAR FORMATION

After presenting powerful evidence to cast doubt on one of two current theories on star formation, Richard Klein and his collaborators Mark Krumholz and Christopher McKee have embarked on a project to be the first in the world to carry out calculations that fully characterize the formation of high-mass stars.

Klein and his collaborators, who have relied on NERSC to generate important findings in the field of star formation, are eager to solve a crucial question about the birth of stars: What are the effects of proto-stellar winds along with radiation on the creation of a star that can be 100 times more massive than the sun? High-mass stars with masses greater than eight to 10 solar masses eventually explode as supernovae and produce most of the heavy elements in the universe. In fact, these stars inject energy into the interstellar medium of galaxies through supernovae, stellar winds and UV radiation. By injecting both heavy elements and energy into the surrounding medium, massive stars shape the evolution of galaxies.

"We want to solve the entire problem of the formation of high-mass stars, not just with the effects of radiation, which we've already shown," said Klein, an adjunct professor of astronomy at UC Berkeley and a researcher at the Lawrence Livermore National Laboratory.

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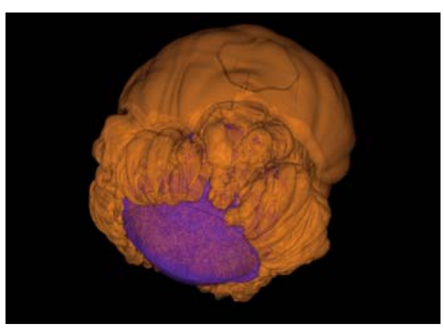
Blow It Up

SCIENTISTS COMPUTE DEATH THROES OF WHITE DWARF STAR IN 3D

University of Chicago scientists have achieved a breakthrough by creating three-dimensional models to simulate the detonation of a white dwarf star, a feat they presented publicly for the first time at the "Paths to Exploding Stars" conference in Santa Barbara on March 22.

The research, led by Don Lamb, director of the university's Center for Astrophysical Thermonuclear Flashes, used NERSC to develop the simulations in January this year.

"I cannot say enough about the support we received from the high-performance computing team at Lawrence Livermore and Lawrence Berkeley national laboratories," said Don Lamb, who received 2.5 million computing hours at NERSC under DOE's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. "Without their help, we would never have been able to do the simulations."



In this image from a simulation of an exploding white dwarf star, the orange represents the flame that nuclear ash follows as it pops out of the star while the blue approximately marks the surface of the star. The star is approximately the size of the Earth, but contains a mass greater than the sun's. Image courtesy of Cal Jordan/University of Chicago Flash Team.

White dwarf stars pack one and a half times the mass of the sun into an object the size of Earth. When they burn out,

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Electric Science

FUEL CELL RESEARCH COULD MAKE CLEAN ENERGY AFFORDABLE

A team of NERSC users is investigating innovative catalytic materials for engineering cheaper and more efficient fuel cells, research that could make the alternative energy production technology commercially viable and help reduce the world's dependence on oil.

Manos Mavrikakis, a professor of chemical and biological engineering at the University of Wisconsin-Madison, is heading this timely project to understand the mechanisms for accelerating the desirable chemical reactions in fuel cells in order to improve their power output and make them affordable to consumers.

His work addresses several key problems in developing more productive low-temperature fuel cells, which can operate at 80 degrees Celsius and are a good alternative for powering cars and portable and other consumer electronics.

A fuel cell generates power when the catalyst-coated anode causes hydrogen to

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Material World

ORNL NANOSCIENCE GROUP MAKES BIG PROGRESS AT NERSC

Theory, modeling and computation are playing an increasingly important role in nanoscience, which is producing discoveries that will lead to more complex, powerful, and energy-efficient electronics, scientific instruments and other devices.

That is why Peter Cummings is mining resources at NERSC to carry out simulations in molecular dynamics and explore novel nanostructured materials. Aside from these two projects, Cummings, the John R. Hall professor of chemical engineering at Vanderbilt University, is also the director of the Nanomaterials Theory Institute (NTI) within the Center for Nanophase Materials

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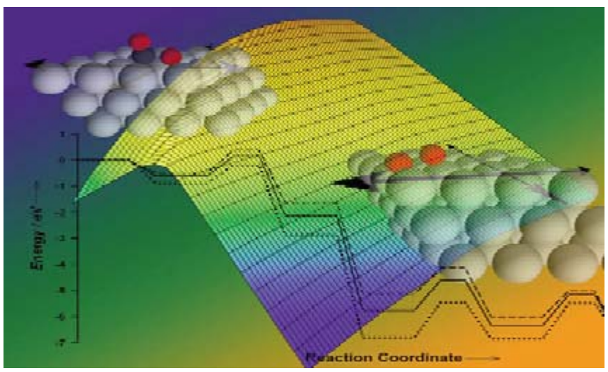
split into hydrogen ions and electrons. The electrons flow through an external circuit and provide electricity before reaching the cathode. Meanwhile, the hydrogen ions move through the electrolyte and meet up with oxygen at the other end, where the catalyst-coated cathode is located. The hydrogen ions, oxygen and the electrons then combine to produce water.

Mavrikakis's research explores the use of cheaper materials in order to reduce the reliance on expensive platinum as a catalyst while speeding up the oxygen reduction reaction rate (ORR), which can cause a 60-percent energy loss during power generation. Another challenge is to increase the anode's resistance to carbon monoxide, present in hydrogen-based fuels, because carbon monoxide impairs platinum's ability to speed up the electrochemical reaction.



Lattice strain plays a key role in determining catalytic activity of platinum, the current state of the art catalyst used in fuel cells. The effect of strain on the oxidation of CO, a reaction catalyzed by the anode of fuel cells, has been demonstrated by using density functional theory calculations at NERSC. This image appeared in the cover of Physical Chemistry Chemical Physics (Issue 26, 2006).

"Personnel at NERSC have always been very helpful with efficient handling of CPU requests, and with porting and testing our codes on ever-improving computational platforms," Mavrikakis said.

His team runs a density functional theory-based code on a NERSC supercomputer for modeling the step-by-step interactions of various catalytic materials with hydrogen fuel. By fully characterizing the behavior of these materials, which are coated on anode and cathode in the fuel cell, scientists can design catalysts to accelerate the desired chemical reactions.

Mavrikakis's work has been published extensively, including a 2006 issue of Physical Chemistry Chemical Physics that featured his work on the cover. His research team includes undergraduate, graduate and post-doc students at the university: Lars Grabow, Anand Nilekar, Rahul Nabar, Peter Ferrin, Falk Eichhorn, Faisal Mehmood, Denise Ford and Kate Bjorkman.

The team's research already has yielded results that will enable cheaper and better fuel cell designs. For example, in Angewandte Chemie, International Edition and the Journal of American Chemical Society in 2005, Mavrikakis and collaborators illustrated an alternative method for increasing the ORR and reducing cost by paving a layer of a different conducting material underneath a single atomic layer of costly platinum.

Instead of using only pure platinum nanoparticles, fuel cells that use a monolayer of platinum deposited on cheaper palladium can increase the ORR by 30 percent. Further calculations have led Mavrikakis to theorize that the use of other metallic compounds in conjunction with platinum and palladium could loosen hydroxyl's (OH) bond to platinum, thereby lessening its ability to degrade the catalyst's performance, and increase reaction rates by a factor of four. Mavrikakis' team has worked with Radoslav Adzic's experimental group at Brookhaven National Laboratory to verify their results.

"Computational chemistry has become a respectable partner to experiment, guiding inorganic materials nano-synthesis community towards synthesizing promising nanocatalysts, which will play a central role in solving energy and environment related problems," Mavrikakis said.

Mavrikakis's research aligns closely with the public and private interest in developing alternative energy. Funding for his work partly comes from the Hydrogen Fuel Initiative launched by the government in 2004.

In the private sector, automakers and a slew of alternative energy firms have been experimenting with different fuel cell technologies, searching for the least expensive and most efficient method of producing clean energy.

Although the results of his research can be useful for various kinds of fuel cell technologies, he is particularly interested in direct methanol fuel cells. The research investigates the mechanism for methanol (MeOH) decomposition on various platinum-based alloys. The findings could lead to better anode materials and hydrogen production from methanol in liquid or gas form.

Learn more about Mavrikakis's work at http://manos.engr.wisc.edu and http://www.nersc.gov/news/annual_reports/annrep05/research-news/08-talent.html.

Job Well Done

NERSC users gave kudos to the High Performance Storage System (HPSS), Jacquard uptime and Bassi Fortran compilers in recently published results of a survey to solicit feedback about their experiences using NERSC resources in 2006.

The annual survey enables NERSC staff to gauge their successes and make improvements. The survey asked researchers to rate their overall satisfaction with the hardware, software and services. It also posed more specific questions about these tools and services and invited users to share their thoughts. On a scale of 1 to 7, with 7 being "very satisfied," survey respondents gave an average of 6.3 for the question about their overall satisfaction with NERSC, an improvement from 2005 and 2004.

"We take feedback from our users very seriously, whether it is in the form of day to day interactions, through the NERSC User Group meetings or via our annual survey," said Bill Kramer, General Manager of NERSC. "We work very hard to bring any low scores up and to keep the overall satisfaction high in all areas. I want to thank all the users who took the time to provide this valuable feedback."

About 13 percent of the active NERSC users, or 256, took the online survey. The respondents represented all six programs within the DOE Office of Science.

Areas with the highest user satisfaction in 2006 included account and consulting services, DaVinci C/C++ compilers and net-

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Material World

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Sciences (CNMS) at Oak Ridge National Laboratory (ORNL). In addition to allocations for his chemical sciences and materials sciences research from the Basic Energy Sciences (BES) program at the DOE Office of Science, he also has also secured an allocation at NERSC for NTI users.

"The NERSC facilities are a great choice for projects that require more resources and/or higher interconnect speed than clusters can provide, but are not demanding to the point of needing leadership class computing," Cummings said. "The fact that NERSC has installed and professionally maintains many of the codes we and NTI users need is also a big plus. Finally, the user-oriented production environment at NERSC and the user support services make it straightforward for my students and postdocs to use the facilities."

Nanoscience is an emerging multi-disciplinary field that is garnering strong government backing and efforts in the private sector for developing cutting-edge technologies for the industrial and consumer market. Investigating sciences at the atomic scale will have to rely heavily on theoretical work that is backed by hefty computational resources, Cummings said during a keynote speech at the SIAM Computational Science and Engineering conference in Costa Mesa, California, last month.

"Unlike bulk systems, large-scale manufacturability of nanoscale systems will require deep theoretical understanding, since the functional properties of nanostructured materials depend critically on size and structure, which must both be then tightly controlled during manufacture" said Cummings.

During his talk, he outlined the role of the institute, part of CNMS at Oak Ridge. Built in 2005, CNMS is the first of five national nanoscience research centers, which include the Molecular Foundry at Berkeley Lab. The number of user projects at the CNMS is now nearing 200; the number at NTI has grown from 11 in 2005 to about 45 now.

Cummings also cited reports he co-authored with two scientists at Berkeley Lab—Paul Alivisatos, Associate Lab Director of Physical Sciences, and William McCurdy in the Chemical Sciences Division—in describing the work that contributed to the creation of national nanoscience initiatives and the computational nanoscience initiative at DOE.

Aside from being an advocate for scientists supported by NTI, Cummings also carries out research exploring new materials and the processes for manufacturing them.

Using NERSC resources, Cummings and fellow researcher Clare McCabe have generated simulations of composites based on polyhedral oligomeric silsesquioxane (POSS) molecules, a hybrid of silicon and oxygen molecules that can enhance the strength and heat resistance in ordinary plastic. Cummings and McCabe, a chemical engineering professor at Vanderbilt, published two papers on these nanostructured materials in the Journal of Physical Chemistry B and the Journal of Chemical Physics in 2006.

As part of this NERSC project, Cummings and graduate student Christina Payne (a DOE Computational Science Graduate Fellow) along with ORNL collaborators are creating molecular simulations of DNA transport for a proposal to design a high throughput/low cost genomic sequencing device.

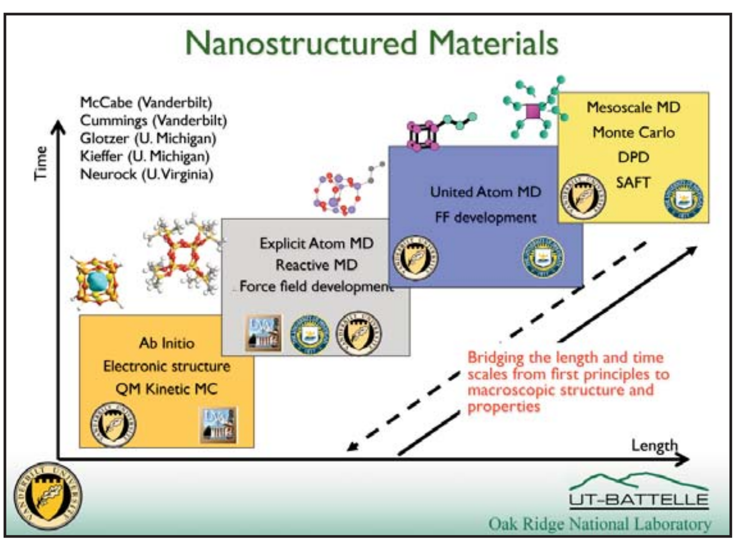
Cummings's second project strives to bridge fundamental disagreements between experiment and theory in the design of molecular electronic devices. This field holds the promise to develop the next-generation, cheaper and more powerful computers and intelligent gadgets that are not possible with the current semiconductor and electronic manufacturing technologies.

The research aims to solve issues such as the integration of molecular electronic systems with semiconductor technology and the self-assembly of novel materials that form the basis of electronic circuits.

Cummings and fellow researchers are using newly developed computational tools, including the finite-bias non-equilibrium simulations as well as electron-electron and electron-phonon coupling, to conduct their work. Aside from Cummings, the team includes Vincent Meunier, Xiaoguang Zhang and Robert Harrison, all from ORNL, and Jerzy Bernholc at North Carolina State University. BES and ASCR (Advanced Scientific Computing Research) in the Office of Science jointly funded this research.

The research already has produced results that addressed quantum transport problems in two areas. One is the modeling of a novel non-volatile memory element designed by the team. The other area deals with the tunneling effect in oxide ferroelectric materials placed between two metallic electrodes, a research that could lead to the development of an improved switching mechanism.

Learn more about Cummings's research at http://flory.vuse.vanderbilt.edu. Information about the Nanomaterials Theory Institute can be found at http://www.cnms.ornl.gov/nti/nti.shtm.



The chart shows the range of scales and methods used in a research on polyhedral oligomeric silsesquioxane (POSS) molecules.

Star *continued from page 1*

Klein, Krumholz and McKee's work has been published in many journals, including Nature.

The research, which Klein began with McKee, a physics and astronomy professor at UC Berkeley and Krumholz, now a post-doc at Princeton University, paved the way to an understanding that had eluded theoretical astrophysicists for decades. For a long time, scientists have understood that stars form when interstellar matter inside clouds of molecular hydrogen undergoes gravitational collapse, but problems remained of how strong radiation generated in the process wouldn't prevent the proto-stars from growing in size to become high-mass stars.

The question has led to two competing theories on how massive stars come into being, starting with a turbulent interstellar cloud that can be several light years across. In the "competitive accretion" theory, the cloud gravitationally collapses to produce clumps containing small cores. These cores are the seeds which undergo growth by gravitationally pulling in matter from around them, competing with other cores in the process and often gaining many times their original mass. In this sense, the theory is a "bottom up" theory

The rival "direct gravitational collapse" theory that Krumholz, McKee and Klein subscribe to contends that the cores already are large when they are first developed in clumps and do not undergo the snowballing effect championed by supporters of the competitive accretion theory. After these high mass cores collapse to form fragments, the fragments continue to accrete the remaining matter from the embryonic core to become a high mass star. This is a top down theory.

Klein, McKee and Krumholz refuted the competitive accretion theory when they completed the first three-dimensional simulations demonstrating why the theory isn't backed by observations from several star-forming regions in the galaxy.

"Our work was the first attempt with fully three-dimensional simulations to show how high-mass stars are formed, and it dealt a serious blow to the competitive accretion theory," said Klein, who with Krumholz and McKee carried out the simulations at NERSC and the San Diego Supercomputer Center. "This kind of three-dimensional simulation can only be done on multiprocessor platforms like those at LBNL."

The key to unlock the mystery of why competitive accretion appears to work in the simulations that others have done lies in the turbulence swirling inside the gas cloud. In order for simulations buttressing the competitive accretion theory to work, the researchers found that two factors have to be present in the simulations: a parameter (the ratio of kinetic energy of the gas to the gravitational energy) representing the turbulence in the clumps must be small, and the clumps in which the cores are formed also must be small (a few solar masses). For a small parameter representing the turbulence to remain small, simulations would have the turbulence taper out quickly in the star-forming process.

Krumholz, with McKee and Klein then asked the question: did these two conditions necessary for competitive accretion exist? After reviewing observations of eight star-forming regions in the galaxy, Klein and his team found no observational evidence to support the two assumptions. In general, the turbulent parameter is not at all small and the

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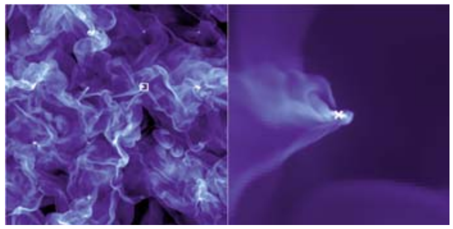
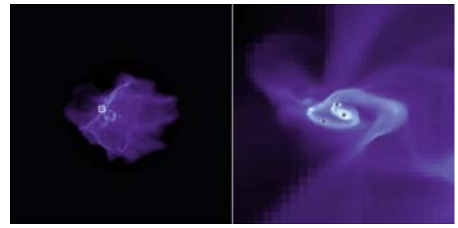
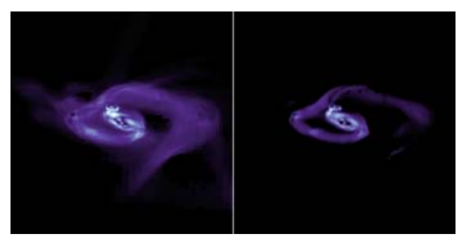


This image shows a column density 2D projection of the 3D simulation of stars forming by gaining mass from a turbulent gas cloud by a process called Bondi-Hoyle accretion in a turbulent medium. The left panel is a slice of the entire cloud and shows brightened regions where newly formed protostars are attracting surrounding gas. The right panel zooms in on one of the newly-formed protostars (x in the right panel that is zoomed in from the boxed region in the left panel) surrounded by a turbulent wake. A key finding of the simulations is that the turbulent wake prevents the star from gaining much mass, lending strong support to the direct gravitational collapse model.



This image shows a column density 2D projection of the 3D simulation of a high mass turbulent core after 27,000 years of evolution. The core initially has 100 solar masses. The left panel shows the entire simulation box which is 0.6 parsecs across (1.81 10e18 cm., approximately 121,000 AU where an AU is the distance of the earth to the Sun). The structure of the turbulent core reveals multiple intertwined filaments, some of which are channeling mass into the newly formed high mass star in the boxed region. The right panel shows a zoomed-in region revealing the formation of an accretion disk 3000 AU in size. The location of newly formed stars in the disk is shown by the three stars present. The primary star forming near the center of the disk is a high mass star with 8.3 solar masses. The disk itself has about 3 to 5 solar masses. The formation of two additional low mass stars are visible in the spiral arms of the disk with 1.8 and 0.05 solar masses. A fourth low mass star that may be forming is shown near the outer left edge of the large spiral arm surrounding the disk.



This image is a simulated beam-smeared image of the brightness temperature emitted in two rotational transitions of the methyl cyanide molecule from the accretion disk (See first figure above) that the future submillimeter telescope ALMA would observe. The left panel shows the molecular line emission at a rotational frequency of 220.7091 gigahertz, and the right panel shows the line emission at 220.6411 gigahertz. These simulated ALMA images will help distinguish between the two theories of high mass star formation: direct gravitational collapse and competitive accretion. These simulations predict that ALMA will detect disks around young high-mass protostars of about 1000 AU in size. The competitive accretion theory would predict that disks around newly formed high mass protostars would be smaller than 30 AU and not be detectable.

Where the Time Goes

NERSC's high-performance computers will enable research from a variety of disciplines this year. DOE has budgeted 92 million computing hours, with projects in fusion energy, chemistry and material sciences winning some of the largest allocations in fiscal 2007 (see Table 1). Most of the hours are going to projects funded or otherwise supported by the six DOE Office of Science programs, including SciDAC projects (see Table 2). Meanwhile, the High Performance Storage System (HPSS) also will play host to valuable data and results this year. Nuclear physics, astrophysics and climate research are disciplines that have received the most storage hours, which come from a separate pool of DOE allocation.

Although DOE has budgeted 92 million hours for fiscal 2007, not all the hours have been distributed. Here is a breakdown of the 66.9 million hours allotted so far (see charts 1-3). For current storage allocations, measured in Storage Resource Units (SRUs), see charts 4-6.

TABLE 1

Allocation Category	Hours (in millions)
INCITE	9.2
NERSC Special Programs	9.2
Office of Science Director	9.2
DOE Base & SciDAC	64.4
Total	92.0

TABLE 2

Breakdown of DOE Base & SciDAC Allocation (64 million hours) by DOE Program Offices

ASCR	3.1%
BES	25.7%
BER	12.2%
FES	26.0%
HEP	14.2%
NP	8.7%
Not yet allotted	10.9%

CHART 1

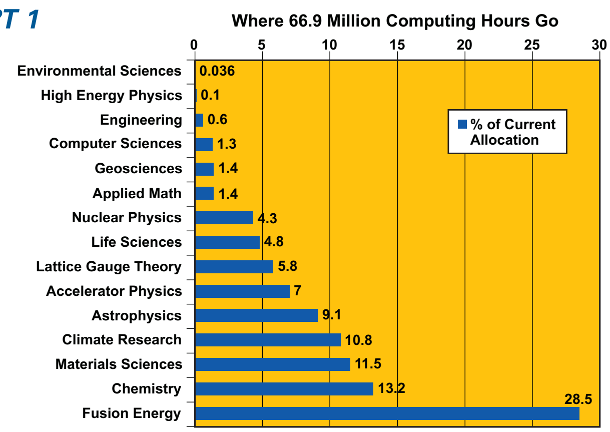


CHART 2

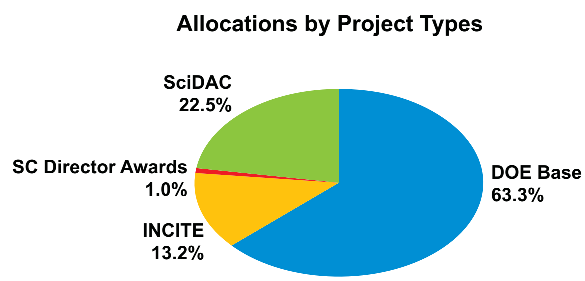


CHART 3

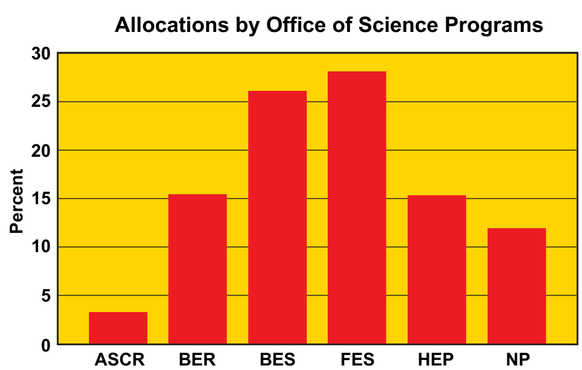


CHART 4

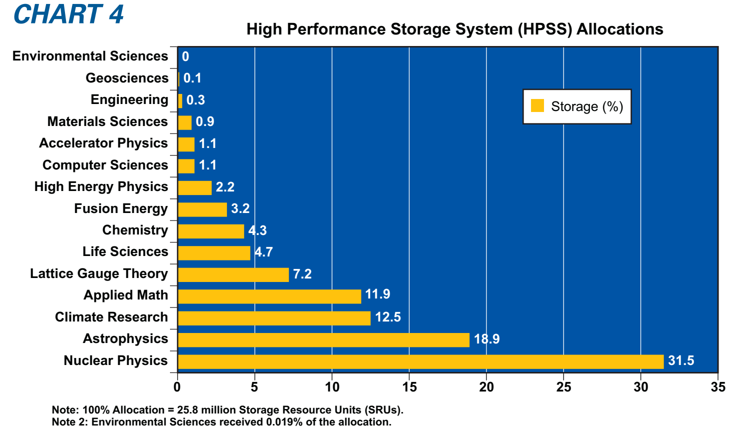


CHART 5

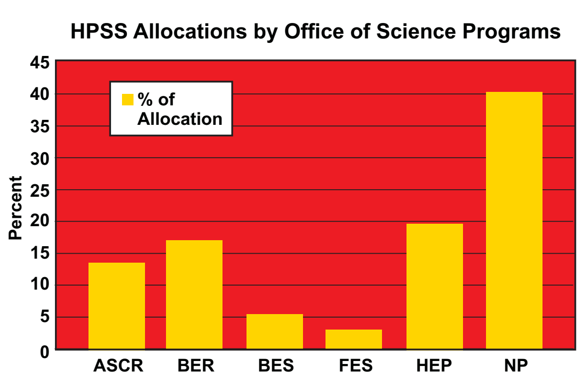
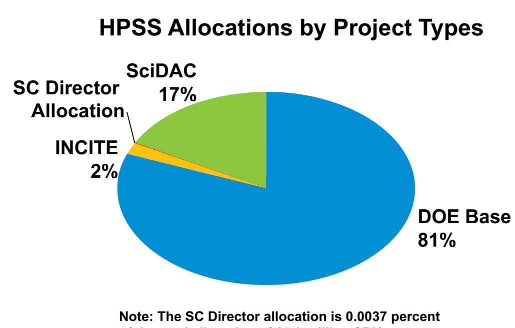


CHART 6



Star *continued from page 1*

clumps tend to have several thousand solar masses. Their breakthrough was published in the November 17, 2005 issue of Nature.

"Every observation of these large clouds indicates that a mechanism, perhaps proto-stellar winds, must be present that keep stirring the clouds to keep the turbulence around," Klein said. Carrying out simulations that take fully into account the effects of these winds will be the next goal for Klein, Krumholz and McKee.

Klein's work wouldn't have been possible without tools developed by other scientists in the 1980s. He cited Phil Colella and John Bell, both scientists in the Computational Research Division of Berkeley Lab, for developing a key technique that allowed scientists to do three-dimensional, large-scale simulations over an enormous range in spatial scale.

The technique was adaptive mesh refinement (AMR), and Colella worked with one of the original AMR developers, Marsha Berger, to put this method for numerical analysis into a code. Klein and McKee then worked with Colella to make the code applicable to the astrophysics problems in 1994.

"It enabled us for the first time to cover the full dynamic range with numerical simulations on a large scale not just in star formation but in cosmology," Klein said. He and McKee, along with then graduate students Mark Krumholz and Robert Fisher, further modified their code called Orion to make it more applicable to their star formation research by taking into account physical processes such as gravity, magnetic fields and radiation transfer. Researchers Jeff Greenough and Louis Howell of Livermore Lab collaborated on aspects of this work.

By late 1990s, they were ready to take on research that had not been possible before. Klein and McKee went on to found the Berkeley Astrophysical Fluid Dynamics Group in UC Berkeley's astronomy department around the same time. More information about their high-mass star formation research can be found at http://astro.berkeley.edu/~cmckee/bafd/research/highmass.html.

Survey *continued from page 2*

work performance within the NERSC center.

The largest increases in satisfaction over the 2005 survey were for the Jacquard Linux cluster, Seaborg batch wait times and queue structure, NERSC's available computing hardware and the NERSC Information Management (NIM) system.

Despite the improvements, however, Seaborg batch wait times received a low average score compared with assessments about other systems and services. Other areas that received lower scores included PDSF disk storage, interactive services and performance tools, analytics facilities and Bassi and Seaborg visualization software.

The survey gave users an opportunity to pen their own thoughts about using NERSC. The question "What does NERSC do well?" drew answers from 113 users. Among them, 87 stated that NERSC gave them access to powerful computing resources without which they could not do their science; 47 mentioned excellent support services and NERSC's responsive staff; 27 highlighted good software support or an easy-to-use user environment; and 24 pointed to hardware stability and reliability.

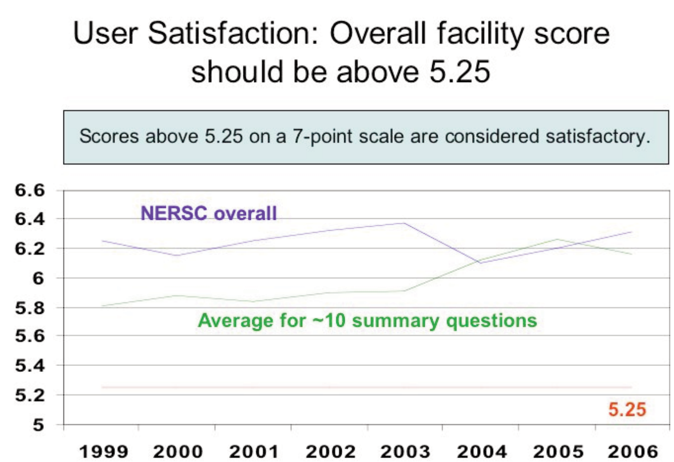
"NERSC runs a reliable computing service with good documentation of resources. I especially like the way they have been able to strike a good balance between the sometimes conflicting goals of being at the 'cutting edge' while maintaining a high degree of uptime and reliable access to their computers," wrote one user.

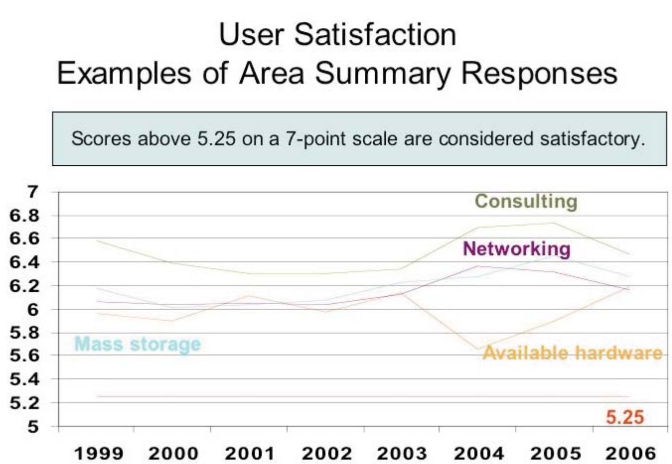
In previous years, queue turnaround and job scheduling issues were areas of the greatest concerns. NERSC has made many efforts to acquire new hardware, to implement equitable queuing policies across the NERSC machines and to address queue turnaround times by adjusting the duty cycle of the systems.

These efforts have clearly paid off. In 2004, 45 users reported dissatisfaction with queue turnaround times. In 2005 this number dropped to 24. In 2006 only five users made such comments.

Improvements to Jacquard's computing infrastructure and the deployment of the NERSC Global File System also addressed shortcomings voiced by users in previous years. Although job scheduling remained a concern in 2006, NERSC users pointed to new challenges for NERSC staff. Researchers said they would like more compute cycles and software fixes.

The complete survey results can be found at http://www.nersc.gov/news/survey/2006/.





SPOTLIGHT

NUGEX ELECTION RESULTS

Members of the NERSC Users' Group have selected 13 people to fill vacancies on the 24-person executive committee (NUGEX). The committee directs the Users Group's activities, works with NERSC management to identify problems and finds solutions. NUGEX also runs a semi-annual membership meeting. The newly elected members will serve a three-year term and represent six program offices within the DOE Office of Science. The newly elected are:

ASCR	Kirk Cameron	Virginia Tech
	Mike Lijewski	Berkeley Lab
	Ravi Samtaney	Princeton Plasma Physics Lab
BER	David Beck	U. Washington
	Adrianne Middleton	National Center for Atmospheric Research
BES	Bas Braams	Emory U.
	Eric Bylaska	Pacific Northwest Lab
	Thomas Miller	UC Berkeley
FES	Andris Dimits	Livermore Lab
HEP	Frank Tsung	UCLA
NP	James Vary	Iowa State
AT LARGE	Jerry Potter	Livermore Lab
	Xingfu Wu	Texas A&M

For a complete list of NUGEX members, click https://www.nersc.gov/about/NUG/nugex_members.php. Twenty-eight candidates ran in the election. Each candidate's short bio and statement can be found at https://www.nersc.gov/about/NUG/elections.

NEW DUTY

David Paul

At the winter SP-XXL meeting on February 5-9, **David Paul**, Seaborg system lead and member of the NERSC Computational Systems Group, was elected to serve as Secretary on the Board of Directors and to chair a newly formed security working group. SP-XXL is a self-organized and self-supporting user group for organizations that have large installations of IBM equipment.

Paul's responsibilities as a board secretary will include compiling the yearly report to IBM that details requests for improvement, highlights deficiencies and provides suggestions for IBM's technology roadmap. The voting members of each site prioritize each item, and the report is then provided to IBM for their response, which is typically delivered at the summer SP-XXL meeting. The efforts of SP-XXL have resulted in a number of software improvements, changes to the hardware roadmaps, and improvements to service and support of large IBM HPC sites.

Given the current security-sensitive climate, SP-XXL decided to form a separate security working group, which Paul will chair, to give the topic more focus. (Security was formerly covered by the system administration working group.)

There are currently 29 member organizations in SP-XXL. The focus of the group is on large-scale scientific and technical computing using IBM hardware, covering areas such as applications, code development tools, communications, networking, parallel I/O, resource management, system administration and training. More information on the group can be found at http://www.spxxl.org/new_website/html/index.html.

Dwarf *continued from page 1*

the ensuing explosion produces a type of supernova that astrophysicists believe manufactures most of the iron in the universe. But these Type Ia supernovae may also help illuminate the mystery of dark energy, an unknown force that dominates the universe.

Scientists for years have attempted to blow up a white dwarf star by writing the laws of physics into computer software and then testing it in simulations. At first, the detonations would only occur if inserted manually into the programs. Then the Flash Center team naturally detonated white dwarf stars in simplified, two-dimensional tests, but "there were claims made that it wouldn't work in 3D," Lamb said.

But in January, the Flash Center team for the first time naturally detonated a white dwarf in a more realistic three-dimensional simulation. The simulation confirmed what the team already suspected from previous tests: that the stars detonate in a supersonic process resembling diesel-engine combustion.

Unlike a gasoline engine, in which a spark ignites the fuel, a diesel engine relies on compression to trigger ignition. "You don't want supersonic burning in a car engine, but the triggering is similar," said Dean Townsley, a research associate at the Joint Institute for Nuclear Astrophysics at Chicago.

The temperatures attained by a detonating white dwarf star make the 10,000-degree surface of the sun seem like a cold winter day in Chicago by comparison. "In nuclear explosions, you deal with temperatures on the order of a billion degrees," said Flash Center research associate Cal Jordan.

The new three-dimensional white dwarf simulation shows the formation of a flame bubble near the center of the star. The bubble, initially measuring approximately 10 miles in diameter, rises more than 1,200 miles to the surface of the star in one second. In another second, the flame crashes into itself on the opposite end of the star, triggering a detonation.

"It seems that the dynamics of the collision is what creates a localized compression region where the detona-

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Dwarf

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tion will manifest," Townsley said.

Telescopic images of the two supernovas closest to Earth seem match the Flash Center team's findings. The images of both supernovas show a sphere with a cap blown off the end.

"In our model, we have a rising bubble that pops out of the top. It's very suggestive," Jordan said.

This process plays out in no more than three seconds, but the simulations take considerably longer. The Flash Center team ran its massive simulation on two powerful supercomputers at NERSC as well as Lawrence Livermore National Laboratory. Just one of the jobs ran for 75 hours on 768 computer processors, for a total of 58,000 hours.

"We have it set up so that if something goes wrong, text messages are sent out instantaneously to everyone," said Flash Center scientist Robert Fisher. "It's like being a doctor on call 24/7."

Astrophysicists value Type Ia supernovas because they all seem to explode with approximately the same intensity. Calibrating these explosions according to their distance reveals how fast the universe has been expanding at various times during its long history.

In the late 1990s, supernova measurements revealed that the expansion of the universe is accelerating. Not knowing what force was working against gravity to cause this expansion, scientists began calling it "dark energy." The Flash Center simulations may help astrophysicists make better calibrations to adjust for the minor variation that they believe occurs from one supernova to the next.

"To make extremely precise statements about the nature of dark energy and cosmological expansion, you have to be able to understand the nature of that variation," Fisher said.

Aside from INCITE, the research has received funding and computing time from DOE's Advanced Simulation and Computing program.

Learn more about Lamb's work at http://www.asci.uchicago.edu/website/home. The Flash Center's 2D simulations were described in the 2004 NERSC Annual Report: http://www.nersc.gov/news/annual_reports/annrep04/html/adv-comp-sci/02-big-flash.html.

Foreign Exchange

Jim Craw (left), head of NERSC's Computational Systems Group, gave Thomas Lippert (right) a tour of the supercomputer room.

Thomas Lippert, director of the Central Institute for Applied Mathematics at Research Center Juelich in Germany and head of the Jon van Neumann Institute for Computing, spent a day with NERSC staff on March 6 and held thoughtful discussions on performance and benchmarking of scientific computing systems. Like NERSC, the institute is a national user facility providing supercomputers for the Helmholtz Association of German Research Centres and about 250 research groups at German and European universities. Lippert also gave a talk outlining activities at Juelich to scale codes on the IBM Blue Gene installed last year in order to support more demanding simulation projects in areas such as plasma physics, biosciences and nanomaterials. He discussed Juelich's role as a founding member of DEISA (Distributed European Infrastructure for Supercomputing Applications), which aims to enhance scientific discovery through collaborations among Europe's supercomputer centers. After touring NERSC's machine room at the end of his visit, he said, "NERSC is a model of how high-performance computing should be done."

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