

LEADERSHIP COMPUTING AT DAK RIDGE NATIONAL LABORATORY

Center for Computational Sciences

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With the emergence of simulation and modeling as the third leg of science, joining theory and experiment, comes the opportunity to accelerate scientific progress by applying highperformance computing and computational sciences to our most challenging research problems. This opportunity is one for which the Oak Ridge National Laboratory is uniquely prepared.

ORNL is strategically positioned at the intersection of nanoscale science and engineering, high-performance computing and computational sciences, and systems biology—which, for convenience, we call the "nano-info-bio" nexus. As the Department of Energy's largest multidisciplinary science laboratory, ORNL conducts cutting-edge theoretical and experimental research across the scientific disciplines anchored in the nanoscale. It serves as the steward for a set of highly sophisticated facilities that support experimental investigations of complex questions. And, as described in this document, ORNL develops state-of-the-art resources in high-performance computing, manages them effectively, and applies them to pressing scientific questions.

The highlights featured here clearly show how rapidly the field of computing and computational sciences has evolved. Over the past 15 years, we have seen astonishing increases in processing power, exponential growth in the size of data sets, and a remarkable expansion in connectivity. These highlights also show that ORNL has consistently taken advantage of advances in computing and computational sciences—and has overcome the challenges of working at the "bleeding edge"—to deliver scientific breakthroughs and new technologies with the potential to meet the Department of Energy's mission needs, contribute to our nation's security, and improve the standards of living and health for all. I have every confidence that ORNL will continue to set the standard for leadership computing, with exciting results that will expand the frontiers of science and fuel the innovation needed to solve our most challenging problems.

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Since its creation in 1992, the Center for Computational Sciences (CCS) has participated in many of our nation's most important scientific insights and discoveries, working in areas such as climate research, astrophysics, combustion, chemistry, global climate change, fusion energy, accelerator design, and materials. The CCS goal is to remain a world leader in computational science. Currently, our Cray XT3 system is the most powerful system in the world for open science applications. In 2008, a supercomputer able to perform 1,000 trillion calculations in a single second will be delivered. Known as a "petascale" system, it will be more than 25,000 times more powerful than the foremost supercomputer at the time the Center was founded.

These systems—and the advances they demand in areas such as storage, software development, and facilities—require an enormous commitment of will and resources. In 2004, the Department of Energy announced the creation of a National Leadership Computing Facility, to be housed at ORNL. In conjunction with that announcement, UT-Battelle committed to building a \$72 million, privately

financed structure for CCS, and the State of Tennessee provided another \$10 million for a neighboring facility, the Joint Institute for Computational Sciences, which is shared by ORNL and the University of Tennessee.

The reward for these commitments will be the new science made possible. This report presents breakthroughs achieved by our talented users and staff since the creation of CCS; we are committed to expanding those accomplishments into the coming years.

Computation is now synonymous with scientific discovery, and preeminence in high-performance computing is indispensable to maintaining U.S. leadership in science and technology. CCS is excited to be instrumental in pushing computational science in the United States to new levels.

Thomas Lacharia

AT THE BEGINNING...

From the early years of the emerging field of computational science, ORNL helped lead the development of hardware, software, and scientific models. The Laboratory installed its first distributed memory parallel computer-a 64-processor, 2-megaflops (2 million calculations per second) Intel-in 1985 and tested other early "supercomputers" through the 1980s. In 1986, ORNL researchers released VPF, a tool for developing supercomputing algorithms. By 1990, ORNL was testing a 128-processor computer with a blistering speed of 7.7 gigaflops (7.7 billion calculations per second). That same year, materials calculations performed at ORNL won the Gordon Bell award and several other honors; ORNL released TORT, the first publicly available 3-dimensional radiation transport code; and the Atmospheric Radiation Measurement Archive was established at ORNL. Parallel Virtual Machine (PVM) software, which laid the foundation for grid computing, was released by ORNL in 1991.

> PICS PAVED THE WAY FOR ORNL TO BECOME A MAJOR PLAYER IN SCIENTIFIC COMPUTING.

Also in 1991, ORNL joined with three other national laboratories and seven universities to submit the Partnership in Computational Science (PICS) proposal to the Department of Energy. PICS paved the way for ORNL to become a major player in scientific computing. It proposed, among other things, that DOE's Office of Science fund a high-performance computer to be located at a Center for Computational Sciences that would be established at ORNL. The new center made it possible for ORNL researchers to tackle "grand challenge" science, develop software and other supercomputing tools, and mentor the next generation of highperformance computational scientists.





Participating in a ribbon-cutting ceremony for the opening of the Center for Computational Sciences in 1992 are (L to R): Jim Glimm, State University of New York at Stony Brook; Larry Dowdy, Vanderbilt University; Jack Dongarra, University of Tennessee–Knoxville; Justin Rattner, Intel; Dave Nelson, DOE-HQ; Bill Appleton, ORNL; Clyde Hopkins, Martin Marietta Energy Systems; Joe LaGrone, DOE-OR; Al Trivelpiece, ORNL Director; Jim Decker, DOE-HQ; John Marburger, State University of New York at Stony Brook; Billy Stair, State of Tennessee; and Ed Masi, Intel.

Yene Recognition and UAnalysis Internet Link (GRAIL) is part of DOE's Human Genome Project, an effort to shed light on the role of genetics in human health. GRAIL sifts through the mountain of material in a DNA sequence to identify the proteins that make up the blueprint of all living things. This revolutionary application points to the genes responsible for specific diseases, enabling researchers to explore possible cures.

Eventually, it will allow us to view the entire human genome. Much of the work conducted at

the National Institutes of Health will use the early work of GRAIL at ORNL as the model. GRAIL will go on to win an R&D 100 Award, one of many for ORNL and CCS.

- SC92 (1992 Supercomputing conference) Challenge: PVM wins "Most Heterogeneous"
- Kendall Square Research system upgraded to KSR1-64
- 512 GP node Intel Touchstone Sigma installed

CCS has its origins in the federal High-Performance Computing and Communications Initiative. After ORNL submits a successful Partnership in Computational Sciences proposal to DOE's Office of Scientific Computing, CCS is established as a high-performance computing research center. The proposal stressed the importance of supercomputing in climate, materials, and groundwater research. The Intel Supercomputer Systems Division, with its Paragon computers such as the XP/S-35 (below), becomes the first major computer supplier.

L to bring new computing power to three especially difficult scientific challenges: groundwater transport, materials properties, and fundamental physics. More powerful computer models are needed to elucidate how harmful pollutants are transported in groundwater, which supplies much of the country's potable water. Mathematical models clarify how underlying electronic structure affects mechanical properties of materials, but much greater computing power is needed to expand the types of materials phenomena that could be simulated. Phys-

ics studies of the fundamental

The PICS proposal seeks

structure and dynamics of matter on microscopic scales have outgrown the computing capabilities available, and access to massively parallel machines is needed to enable major breakthroughs. **PICS** demonstrates the need for a supercomputing infrastructure to retain U.S. leadership in science and

technology and proposes a plan to build it.

SC93 Challenge: XPVM wins "Most Elegant Interface"

> HPSS development begins

CCS has a long history of breakthrough materials research. The Paragon XP/S-35 is used to validate the KTHNY theory, which illustrates how solids melt in two dimensions (surprisingly, there was no accepted vision of how solids melted at the atomic level). Researchers also use high-performance computing to balance the weight and safety of materials for automobile development (inset). While prototype crash testing does yield useful information, computer modeling saves time, money, and lives. Other advances are achieved in giant magnetoresistance for data storage, quasi-crystals for use in the electronics industry, and superconducting materials (shown above).

Parallel Virtual Machine (PVM) enables a series of computers to mimic a single parallel processor by working on a problem simultaneously. PVM links computers of varying architectures and sizes through a network and allows a user to "see" and

operate the whole collection as a single computer. Researchers who need to solve a large problem but have no access to a supercomputer can link several ordinary computers via PVM and use their combined power and memory. PVM can also link multiple supercomputers in different locations in a huge computational grid to attack grand-challenge problems such as climate modeling. PVM is easy to install, easy to use, and available free from ORNL.

Researchers at CCS run hundreds of groundwater simulations on the Intel Paragon and Kendall Square Research computers. These new computationally intense models describe concentrations and movements of specific contaminants in groundwater (see image above), allowing researchers in the field to better evaluate their options when dealing with contaminated groundwater supplies. By using larger and more detailed grids, running more simulations under different conditions to evaluate remediation options and determine uncertainty, and developing more complete computational models of physical processes, CCS revolutionizes groundwater research and aids in more rapid and thorough decontamination projects.

PVM wins R&D 100 IBM SP-2

installed

The Paragon XP/S-150 (shown below) is delivered in January. The new system features 1,024 computing nodes for a total of 3,096 processors, offering a peak performance of over 150 billion calculations per second (150 gigaflops). Its performance is due in part to its processors' being connected by a high-speed communication network and to the processors' ability to trade and organize data via message passing. The XP/S-150 would later be used in modeling internal combustion engines, climate prediction (which involves unusually large data sets), simulating interactions of magnetic atoms and the melting of solids (which validated a long-standing theory), and automobile impact and collision simulations.



ORNL Paragon networked to Sandia National Labs Paragon

First T170 climate run continuously to 1 year



ORNL participates with Argonne National Laboratory and the National Center for Atmospheric Research in the Computer Hardware, Advanced Mathematics, and Model Physics Program (CHAMMP), which seeks to rapidly advance the science of climate prediction over decade and longer time scales. By joining the latest technologies in highperformance computing with efficient and accurate climate prediction models, this project generates 72 terabytes of data for a single 100-year climate simulation (shown above).

Then a group of scientists at different locations are collaborating to run a simulation over a network, each one must be able to observe the simulation in progress and exert some control over it. CUMULVS is developed at ORNL to coordinate "steering" of applications by multiple users. Using CUMULVS, each collaborator can view a running simulation at his/her location, look through all the data fields being computed, and make adjustments while the calculation is in progress. CUMULVS also provides for automatically restarting failed tasks without losing the data accumulated. The tool revolutionizes highperformance computing, enabling researchers to fine-tune their calculations

as they are being run. It is a boon to applications such as the simulation of airflow over a jet airplane wing (inset).

> SC96 Challenge: Metacomputing wins gold for Concurrency

Giant magnetoresistance wins DOE award for Outstanding Scientific Accomplishment

Giganet OC-12C board wins R&D 100

ORNL is part of a consortium that links supercomputers from three sites across the country to solve scientific problems too large for a single computer. The project links an Intel Paragon at ORNL, two Paragons at Sandia National Labs, and a Cray T3D at Pittsburgh Supercomputing Center—a total of 3,872 processors. The PVM software, developed at ORNL, is used to connect the four computers through high-speed networks. Initially, the system is used for three tasks: analyzing the behavior of NiCu alloys; predicting the response of a nuclear weapon to a nearby explosion; and linking atmospheric, oceanic, and sea ice models to study the climate system.

Data explosion, data tsunami, drowning in data—Google any of those terms and you'll get pages of links, indicating how the computing community is struggling to manage the outpouring of information

from large computer systems and complex calculations. HPSS usage will grow steadily to 100 terabytes archived between 1997 and 2002 and then climb steeply to more than 400 terabytes by 2004 and almost 700 by 2005. According to ORNL's Al Geist, "The problem is getting exponentially worse. There is no resolution in sight. Computers and highenergy physics experiments continue to generate more data than we can store or analyze." Despite many competing attempts to address the data explosion in high-performance computing, HPSS continues to be the most successful approach to archiving large volumes of data scalably (robotic tape library shown in inset).

- HPSS wins R&D 100
- ORNL-Sandia create first high-performance computational grid
- Real CTH runs using PVM on 1,024 nodes each of ORNL / Sandia Paragons



CCS'S High-Performance Storage System (HPSS), capable of managing petabytes of data on disks and libraries (above), is developed to archive and manage the massive quantities of data generated by larger computers and simulations. Like the computers it serves, HPSS is parallelized—there are parallel data paths both into and within the system for scalable bandwidth, and multiple networks, disks, and tape drives are used to sustain bandwidth. As more bandwidth is needed, servers and tape drives can be added. HPSS was developed by a consortium of Oak Ridge, Sandia, Lawrence Livermore, Lawrence Berkeley, and Los Alamos National Laboratories and IBM Government Systems.



A team led by ORNL's Malcolm Stocks launches the first application to sustain 1 teraflops, winning the Gordon Bell Prize. The team uses the 45,000-line LSMS code to model magnetic materials in multilayer storage and read-head devices (visualization above). "Details of the magnetic structure . . . could not have been predicted without the full machinery of first-principles spin dynamics and the use of massively parallel computing," Stocks says. The team will also be nominated for the 2000 Computerworld Smithsonian Award, the most prestigious award for information technology, guaranteeing that materials from the project will be archived in the Smithsonian's Permanent Research Collection.

team A from ORNL's Computer Science and Mathematics Division develops Terminal **Repeller Unconstrained** Subenergy Tunneling, or TRUST. Though its application has broad appeal, TRUST is used primarily by the petroleum industry to improve faulty seismic image focusing, thus reducing exploration costs. This groundbreaking tool goes on to win ORNL an R&D 100 Award, given by R&DMagazine each year to the most innovative products to enter the marketplace. (CCS and its users will go on to receive numerous R&D 100 Awards in recognition for their pioneering research.)

> CCS team wins Gordon Bell prize for first science application to sustain 1 teraflops

Regional Climate Prototype Center established at ORNL In the early 1990s, a wave of massively parallel processors began to appear, enabled by improvements in microprocessors and chip technologies. In 1990, supercomputer speed and memory were measured in gigaflops and in gigabytes; by 1999, the measures are teraflops and terabytes; by 2006, CCS would be on the verge of petaflops and petabytes, a million-fold increase over 16 years. The evolution and growth of computing technology has been truly astonishing. Computational science is having a transformational effect on scientific disciplines such as physics, genetics, environmental modeling, materials science, and astrophysics, says Jack Dongarra of ORNL and the University of Tennessee. Whole disciplines can explore mathematical theories on a large enough scale to test them against observation and experiment. In addition, high-end computing is starting to affect everyday life by enabling more accurate, detailed predictions of trends in fields from weather forecasting to transportation planning.

The ATLAS and NetSolve projects, which involve software developed by Jack Dongarra of ORNL and the University of Tennessee, win R&D 100 Awards. ATLAS (Automatically Tuned Linear Algebra Solver) automatically generates an optimized version of system-critical operations. It can replace months of labor-intensive hand coding to achieve the same result. NetSolve is a client-server system that aggregates the hardware and software resources of any number of computers connected through a network, uses them to solve problems, and returns the results to a user through a familiar programming interface. Dongarra is internationally



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known for several efforts, particularly his annual list of the 500 fastest computers in the world.

> IBM 0.4-teraflops SP installed

Green's function derived at CCS for heat conduction in functionally graded material

Come of the world's Alargest-ever climate simulations are run on the new IBM Power4 supercomputer, known as Cheetah. Researchers from the National Center for Atmospheric Research succeed in running century-long climate models to simulate global climate change from 1870 to 2170, using several different greenhouse-gas scenarios. A joint effort involving multiple laboratories and institutions, the Parallel Climate Model simulates interactions among the atmosphere, oceans, and land (inset shows climate simulation in the CAVE virtual reality theater).



New world record for data transfer set at CCS

 HPSS storage volume hits 1 terabyte per week

PVM and Electronic Notebook win Energy 100 awards **The** installation of the Eagle supercomputer (shown above) is a significant milestone: The IBM Power3 is the DOE Office of Science's first teraflops computer and is the 10th-fastest computer in the world. The IBM RS/6000 has 176 Winterhawk-II thin computing nodes, each with four 375-MHz Power3-II processors and 2 gigabytes of memory. Researchers use Eagle to explore problems in climate prediction, astrophysics, biology, computational chemistry, fusion, and materials science. At the dedication of Eagle, Ernie Moniz, then DOE undersecretary, calls such computers "extraordinary tools for extraordinary science." Eagle would continue operating until June 2005.



DOE launches its SciDAC program (Scientific Discovery through Advanced Computing) to enable scientists to harness the power of supercomputers as a tool for scientific research. SciDAC focuses on developing new computing infrastructure—equipment, software tools, and methods—to ensure U.S. leadership in the use of simulation as a research tool. It encourages partnerships among discipline scientists, computer scientists, and mathematicians as models for performing research. It also provides funding for computational research in several scientific fields—including climate change, fusion (visualizations below and in inset), combustion, astrophysics, and chemistry—and for the development of improved tools for high-performance computing. ORNL scientists are principal investigators for 12 of the first round of SciDAC projects funded in 2001.

Work begins on a SciDACfunded initiative to use CCS's Eagle supercomputer, upgraded to 4 teraflops, to predict the behavior of radio waves in fusion plasma. A



team headed by ORNL's Don Batchelor, building on previous fusion research at ORNL, proposes to simulate the interactions of the radio waves and the plasma in two and three dimensions rather than the one dimension possible with lesser computers. The multidimensional simulations can handle equations of increasing complexity to provide a more detailed, accurate model of wave activity across a cross section of plasma. The ultimate goal is to control the flow of plasma inside a fusion reactor, leading to a clean, abundant energy source.

Cheetah (IBM Power4) installed

PROSPECT and PAPI software win R&D 100s

> CCS chosen as primary computing resource to SciDAC

The year 2002 sees breakthroughs in fusion and astrophysics. Memory efficiency improvements allow for a faster TORIC fusion code, while Adaptive Data Reduction greatly enhances the speed of the TSI astrophysics codes, paving the way for faster, improved simulations. CCS provides a staff of computational scientists who assist users with all aspects of the facility, from scaling and porting their codes to increasing the speed and efficiency of their applications.

> Partnership with Cray on X1 begins; first X1 cabinet installed

- Network sets record for data transfer between ORNL and Berkeley
- Climate model doubles resolution on Cheetah





Two SciDAC chemistry projects are under way at CCS. Researchers use simulation



of molecular groups to provide insight into how to build and control molecular electronic devices (MEDs) through selfassembly of molecules on surfaces. MEDs could make electronics faster, smaller, and more powerful by replacing conventional semiconductors such as silicon. A second SciDAC project focuses on developing and using multiscale methods for fast, accurate numerical solutions to electronic structure problems (see image above). The principal investigator for this project, Robert Harrison, had received the Sidney Fernbach Award from IEEE in 2002 for his role in developing NWChem, the first computational chemistry code designed specifically for use on massively parallel supercomputers.

- Supernova shock wave instability discovered
- Spin dynamics simulations resolve decades-old physics controversy
- SNS target simulations, IPCC runs on Cheetah

ORNL completes construction of the most advanced facility in the country for unclassified scientific computing (shown below). The National Center for Computational Sciences is designed specifically for leadership-class computer systems. Inside the 300,000 ft² building is a 40,000 ft² computer center, a high-bay visualization theater, labs, and training areas. The building provides 12 MW of power and 3,600 tons of cooling capacity. Its networking capabilities include 10 Gbit/s connections to ESnet, TeraGrid, and Internet2 and direct high-speed links to Internet hubs in Atlanta and Chicago. There is ample physical space, cooling capacity, and electrical power to upgrade and add computers. The facilities will be ready as the Center advances the boundaries of science with petascale systems and beyond.





Cimulations conducted On the Cray X1 (left) at CCS resolve a key physics question about the forces that influence electron flow in high-temperature superconductors. They are the first to solve the 2-dimensional Hubbard model-the model most often used to study the physics of high-temperature superconductivityon a scale adequate to describe high-temperature superconductors. The calculations show that the electron pairing that underlies superconductivity at higher temperatures can result from strong electronic correlations rather than the lattice vibrations that produce low-temperature superconductivity (visualization shown in inset below).

- CCS provides bulk of IPCC 4th assessment
 - SCI Altix "RAM" (installed
- Network of protein vibrations in cyclophilin A discovered



IN May, DOE announces CCS will lead a project to build the world's most powerful supercomputer by 2007, maintaining the standing of the United States as the world's leader in high-performance computing. ORNL is commissioned to build a machine that will be able to sustain 100 teraflops (TF) in 2006 and 250 TF in 2007. Plans are to install a machine capable of 1,000 TF—a petaflops—in 2008. ORNL's role in this project can be seen as a long-term outcome of its leadership of the Partnership in Computational Science proposal 13 years earlier.

Jaguar and Phoenix provide unprecedented levels of computing power and speed to researchers. Recordbreaking calculations and scientific breakthroughs occur in several fields as a result. For example, calculations using the AORSA (All-Orders Spectral Algorithm) solver

With the commissioning of the new flagship supercomputer, dubbed "Jaguar," CCS comes into full production. The first time allocations for Jaguar and the newly upgraded Phoenix are awarded to research teams exploring fusion, combustion, astrophysics, chemistry, and accelerator design. In 2005, Jaguar and Phoenix perform some of the largest, most detailed, most accurate simulations ever completed in those fields. Jaguar, a 5,212-processor Cray XT3 (shown below), has a peak performance of 25 teraflops. It is the fastest machine available for open scientific computing in the United States. Phoenix, a Cray X1, is upgraded to an 18.5-teraflops X1E. With 1,024 multistreaming vector processors, it is the largest vector processing supercomputer in the country.



enable the first full-wave simulations of mode conversion in ITER, the international reactor experiment designed to test controlled fusion. **Combustion researchers** working at CCS run some of the largest, most accurate combustion simulations ever completed. In addition, 3-dimensional simulations of a core-collapse supernova contribute fundamental new insights into astrophysics theory. In 2005, CCS holds its first users meeting for scientists representing the 22 projects with time allocations for 2006. Participants discuss their research goals and attend workshops focused on CCS resources and support services (see inset).

UltraScienceNet
operational

 Largest fusion simulation using AORSA code

5 major SciDAC projects running on CCS systems Leadership computing science enters a new era in 2006, with 22 allocations in nuclear fusion, high-energy physics, astrophysics, biology, chemistry, climate, and materials. The focus shifts

to large-scale models and simulations that test the limits of modern computing power, such as the gyrokinetic toroidal code, which runs faster on Jaguar than on any other computer in the world. Projects include combustion simulations (top), biological modeling (second from top), fusion plasma turbulence (second from bottom), and astrophysics (bottom).

CCS'S tradition of scientific endeavor and advancement continues in 2006. Materials research is exploring colossal magnetoresistance in manganites, which could revolutionize data storage; fusion simulations are unlocking the mysteries of turbulent transport in tokamak reactors, bringing the world one step closer to a cleaner and more abundant energy source; and breakthrough simulations of molecular motors will lead to a better understanding of human health and nanotechnology. CCS's new visualization facility, EVEREST (below), makes it possible for researchers to view their data in real time with unprecedented resolution.



More than 300 scientists from across the nation carry out grand-challenge research using CCS resources



INTO THE FUTURE...

By the end of 2007, Jaguar will be capable of a peak operating power of 250 teraflops. A contract is in place with Cray to install a petascale computer by the end of 2008 (prototype shown in inset). This aggressive schedule recognizes how indispensable scientific computing has become to research. High-performance computing will spur dramatic scientific breakthroughs that can alter the conditions of human life all over the world.

The needs of the scientific community drive advances in computing capability. Researchers in all areas are eager for more power; materials science, climate modeling, biology, astrophysics, fusion, and chemistry, particularly, are already poised to take advantage of petascale machines. Climate modelers, for example, need more capacity to couple land, sea, ice, and atmosphere models to simulate how different variables impact global climate.

Chemists want to simulate properties of materials that do not yet exist. Astrophysicists need the power and speed to conduct 3-dimensional simulations of supernova explosions. To take full advantage of the power of petascale and beyond computers, scientists also must have new software and algorithms that will scale to more than 100,000 processors.

CCS scientists and engineers are already at work on meeting those challenges. In its early days, CCS pioneered the development of high-performance scientific computing; 15 years later, it leads the drive to petascale and beyond.









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