Alliance/NCSA

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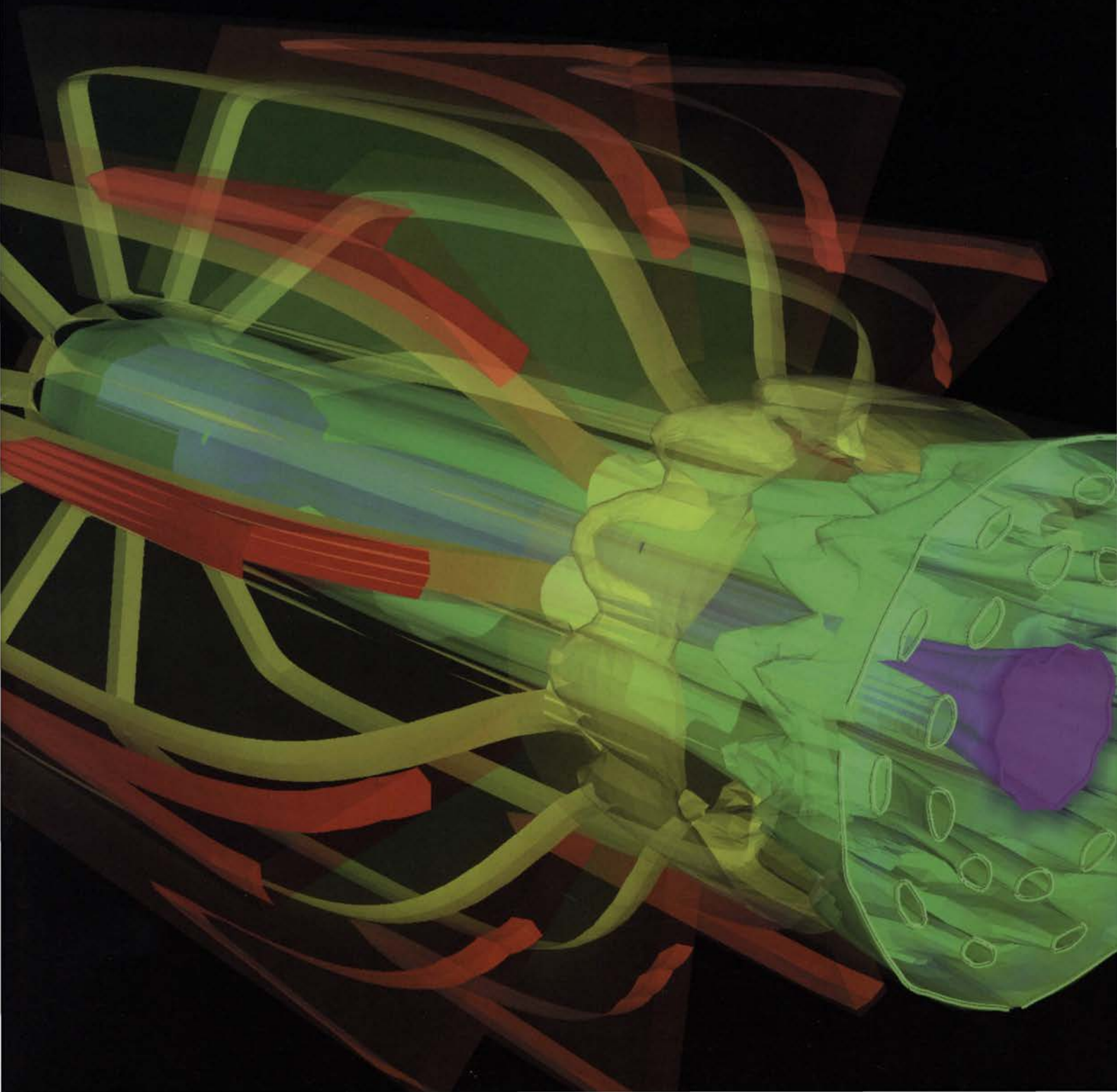
Enabling Research Using Computing, Grid, and Web Technologies



NCSA ALLIANCE

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Who we are

The National Computational Science Alliance (Alliance) is a partnership among more than 50 academic, government, and industrial organizations from across the United States to prototype an advanced computational infrastructure for the 21st century. This model infrastructure, called the Grid, will link together advanced supercomputers, visualization environments, and mass storage devices into a powerful, flexible problem-solving environment. This computing environment will be accessed via high-speed networks from anywhere in the country—eventually, the world.

The Alliance is led by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign with major support from the National Science Foundation's Partnerships for Advanced Computational Infrastructure program. Additional funding for NCSA comes from the state of Illinois, the University of Illinois, industrial partners, and other federal agencies.

Cover
Visualization of gas termperature in a space shuttle solid rocket booster. This model was created by the Center for Simulation of Advanced Rockets (CSAR) in a 10-day capability computing run on the Alliance's 256-processor SGI Origin2000 configuration at NCSA. It was visualized using CSAR's Rocketeer software.

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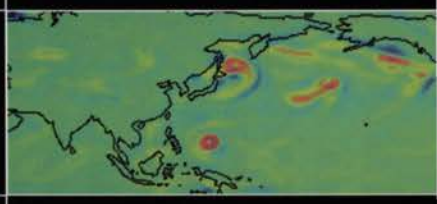
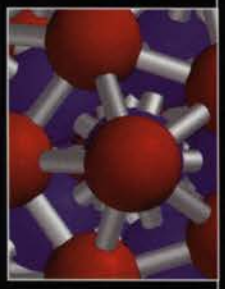




Ringing in a new era

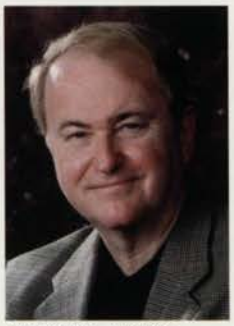
by Karen Green

The Alliance past and present. Larry Smarr, left, and Dan Reed.

After founding Director Larry Smarr became Alliance strategic advisor, Dan Reed stepped into the role of Alliance director.

Spring 2000 saw the end of one era and the beginning of another as Larry Smarr, the leader of NCSA for 15 years and the Alliance since its inception in 1997, announced a move to the University of California at San Diego (UCSD). Dan Reed, head of the University of Illinois computer science department, took over as Alliance director.

Smarr, the founding director of NCSA and a University of Illinois professor for the last 20 years, joined the computer science and engineering faculty at UCSD in July. His wife, Janet Smarr, a U of I professor of comparative literature, became a faculty member in the UCSD department of theater and dance. The Smarrs raised two sons in Urbana, IL, and with the younger starting college, the time seemed right to move on, according to Smarr.



Jim Bottum, executive director of NCSA.

"With this turning point in our lives, Janet and I thought a lot about the future," he said. "I came to realize that after 20 intense years of building at the U of I—creating first NCSA and then the Alliance—that I needed some time for renewal. The UCSD offers for both of us seemed like the right point of departure."

Smarr continues to work with the Alliance management team as Alliance strategic advisor. In this role he identifies emerging trends in high-performance computing and networking and helps integrate those trends into the Alliance's focus. With Jim Bottum, he is also co-founding a software development company that will be headquartered at the U of I. Bottum has been NCSA's deputy director since 1987 and a deputy director of the Alliance since 1997. He is now executive director of NCSA.

"The accomplishments and the reputation of both the Alliance and NCSA are the result of Larry Smarr's hard work and dedication," said Reed. "It's quite an honor to be given the chance to lead an organization that Larry nurtured from the ground up. I am looking forward to building upon his vision and insight as we move forward and begin deploying the technological advances of the Alliance."

As Alliance director, Reed has overall responsibility for the Alliance and NCSA's role as the leading-edge site for the Alliance. Reed is a respected leader in the national computer science community and among the federal agencies that support research and development in high-performance computing. For the past 15 years, he has spearheaded efforts to measure and optimize the performance of scientific applications on supercomputers. Reed continues as head of the U of I department of computer science. Rick Stevens, head of the Mathematics and Computer Science division at Argonne National Laboratory and co-lead of the Alliance's Enabling Technologies teams, assists Reed as the Alliance's new chief computer architect.

As executive director, Jim Bottum is responsible for the day-to-day operations of the center, which has a staff of approximately 275. Bottum concentrates on integrating the day-to-day operations of NCSA and ensuring a smooth linkage between Alliance partners and industrial partners in the NCSA Private Sector Program. Bottum also serves as the center's liaison with the U of I, NSF, private sector partners, and the state of Illinois.

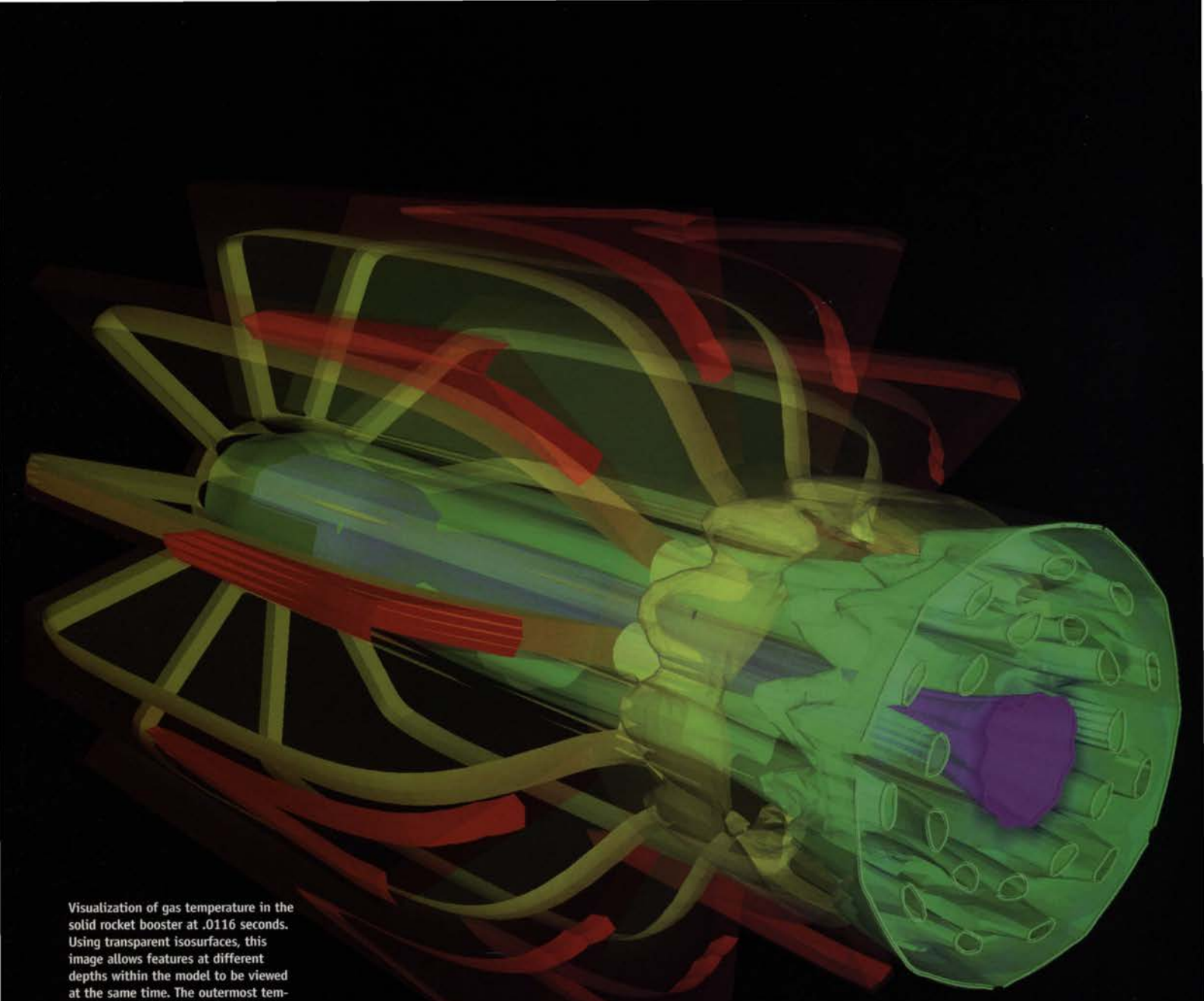
"Working with Larry Smarr over the last 13 years has been one of the most rewarding experiences of my career," said Bottum. "And I expect similar rewards working with Dan Reed. Dan brings the kind of leadership and vision that the Alliance and NCSA need at this juncture."

The new Alliance leadership team has the full backing of the NSF, which funds the Partnerships for Advanced Computational Infrastructure (PACI) program. NSF leaders also had praise for Smarr for his efforts during the last 15 years.

"All of us at NSF and in the computational science community are grateful for Larry Smarr's vision and energetic leadership," said Ruzena Bajcsy, head of the NSF's Directorate for Computer and Information Science and Engineering. "Technological advances led by NCSA have opened up entire new areas of research and changed how we do business, even as an application like Mosaic brought profound economic and cultural opportunities. I do hope and expect that NCSA will continue to build on and further this legacy."

The leadership changes come as the Alliance heads into its fourth year. The Alliance is now focusing on the creation of major new information infrastructure components, driven by collaborating with Alliance application teams. The new leadership team leads the Alliance in this important development and deployment phase.

"We are entering a new era—extraordinary advances in computing and its applications are transforming every aspect of science and society," said Reed. "The Alliance has a unique opportunity to help shape the future of computing, and in my new position I am delighted to be a key part of that future."



Visualization of gas temperature in the solid rocket booster at .0116 seconds. Using transparent isosurfaces, this image allows features at different depths within the model to be viewed at the same time. The outermost temperatures are depicted without blocking the view of additional isosurfaces inside it. Temperatures range from 331 kelvin in the purple regions to 3,588 kelvin in the red regions.

This *is* rocket science

Capability computing runs by researchers at the Center for Simulation of Advanced Rockets are creating massive computer models of solid rockets.

by J. William Bell

A solid rocket's job is simple: defeat inertia by delivering power. The two solid rocket boosters (SRBs) strapped to the space shuttle provide most of the thrust to lift a 4.5 million pound spacecraft off the ground. In the two minutes that the SRBs burn before they separate from the rest of the craft and fall away, the shuttle achieves a speed of 3,100 miles per hour and an altitude of 25 miles.

But behind this brutish task is incredible complexity—in the physics of the craft, in the materials used, and in their interactions. The SRBs are 125 feet long, but a millimeter crack can cause a failure. The amount of sunlight shining on an SRB while it's sitting on the launch pad can affect performance. And a variety of "fiendishly complex" physical processes take place during any solid rocket's firing, according to Michael Heath, director of the Center for Simulation of Advanced Rockets (CSAR).

CSAR is currently meeting all of this complexity head on, using the Alliance's SGI Origin2000 array to create massive, integrated computer models of firing SRBs.

"Our simulations will be useful as a virtual prototyping and design tool, but they will also help us understand rocket failure and improve the safety and reliability of solid rockets of all kinds," says Heath, who is also a computer science professor at the U of I and a senior research scientist at NCSA. "Sometimes simulations will save money, and sometimes they'll save lives."

The power of coupled code

In modeling incredibly complicated events, researchers often break the events down and simulate different aspects separately. One simulation may be given data from another, but they don't operate together. While CSAR uses a variety of autonomous computational codes for more basic simulations, the groundbreaking aspect of their research is that their codes are integrated and work in concert during a single run.

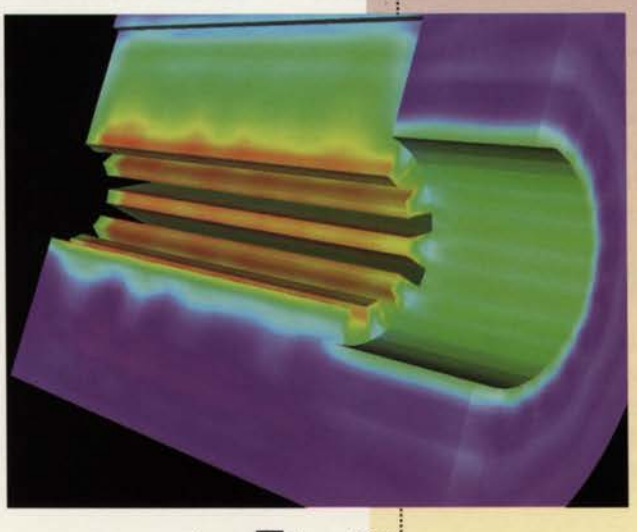
"When we run the codes separately, we have to make simplifying assumptions. With the codes coupled and constantly feeding each other data, we can simulate the whole rocket with extremely high fidelity," Heath says. "Working with the codes separately is like a football team scrimmaging and using the opposition's playbook. It's useful, but you don't know what's actually going to happen until the real game."

Shuttle SRB primer

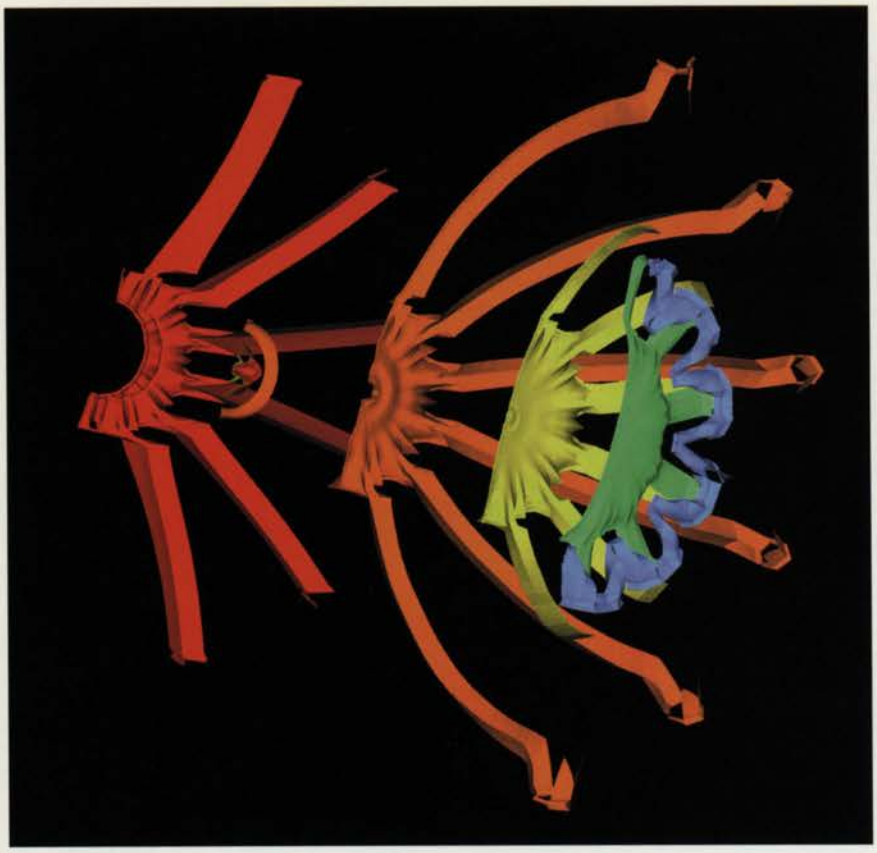
The space shuttle solid rocket boosters (SRBs) each contains about 1.1 million pounds of propellant. The propellant is a composite of powdered aluminum fuel and an ammonium perchlorate oxidizer, and its consistency is similar to that of a pencil eraser.

Each of the rocket's four sections of propellant is a cylinder that is hollow in the center. The propellant burns outward from this hollow center, and the gases produced flow down the hollow center and out the nozzle at the bottom of the SRB to produce its thrust. The head of the forward section of propellant is shaped into an 11-point star. The rest of the propellant sections are tapered toward the bottom. The 11-point star shape increases the surface area of propellant that is exposed to the burn and thus increases the amount of gas and thrust produced. This "front-loaded" burn gives the shuttle the increased thrust at liftoff necessary to defeat the inertia of a 4.5 million pound spacecraft.

At the end of the SRBs' two-minute burn, the boosters separate from the shuttle. Then the shuttle's liquid-fueled main engines, which have been burning since six seconds before launch, finish the job of pushing the shuttle to orbit. At separation, the shuttle is traveling at about 3,100 miles per hour and is about 25 miles high. After separation the SRBs float back to earth on parachutes, splash down in the ocean, and can be reused.



3D visualization of propellant stress in the space shuttle SRB at .0965 seconds into firing. Stresses range from -4.8 atmospheres in the purple regions to 31.4 atmospheres in the red regions. An atmosphere is a unit of pressure equal to the pressure of air at sea level, or about 14.7 pounds per square inch. The negative value indicates tension (in which the propellant stretches), while positive values indicate compression. The simulation was executed on NCSA's 256-processor SGI Origin2000 and visualized using CSAR's Rocketeer software.



3D visualization of gas pressure in the SRB at .0965 seconds. Pressures range from 26.8 atmospheres (purple) to 34.4 atmospheres (red).

The integrated SRB code has three component modules: ROCSOLID, which simulates the deformation of the solid propellant; ROCFLO, which simulates the pressure and velocity of the gases that create thrust; and an interface code, which allows ROCFLO and ROCSOLID to work together. Each component operates on its own, running the algorithms that represent given properties in the simulated rocket. But the components are also integral to one another and take turns influencing one another. The propellant's shape is changed by the pressure of the gases, and then the pressure is altered due to the new shape of the propellant. The result is a model that properly captures not only the processes but also their interplay.

CSAR recently had NCSA's 256-processor Origin2000 all to themselves for their first game away from the practice field. The 10-day capability computing run yielded a fully coupled, whole-system simulation of an SRB firing's first tenth of a second. Though the amount of time was incredibly brief and some complicating factors such as turbulence were not considered, the model was significantly more complex and higher in resolution than any other coupled model they had ever created.

"This model has about 10 times the resolution of our previous runs, and the previous models had only been for a tenth of a second burn as well," says Prasad Alavilli, a research scientist at CSAR. "Interesting things happen in the very, very beginning. This is when things tend to go wrong."

Matching meshes, tailoring timesteps

The coupled code is not only computationally taxing but also elaborate in its design. To model the propellant, ROCSOLID marks the cylinder of propellant with a three-dimensional mesh, a map that represents the physical design in the computational model. Likewise, to study the flow of the gases ROCFLO creates a 3D mesh of the hollow space surrounded by the propellant.

By using separate meshes researchers can study the propellant and the gases in different ways and at different scales. "Scale is a huge issue, and addressing the different scales is crucial," says Dennis Parsons, a CSAR researcher and an associate civil engineering professor at the U of I.

In the recent Origin2000 run, ROCFLO used a mesh made up of four million discrete nodes, or points on the mesh, while ROCSOLID used a mesh made up of 400,000 nodes. As a result, the resolution of the solids model is relatively coarse, while the gas model's is relatively fine. This difference allows the components to be studied at their appropriate scales and reduces the resources that must be used to compute given sections of the model. But it also complicates matters. The meshes, which have to match up where the gases and solid meet, don't do so naturally. The cells in the ROCFLO map are 10 times smaller than the cells in the ROCSOLID map.

The temporal relationship between the two codes creates a similar issue. ROCFLO advances the model by 10^{-6} seconds every timestep, while ROCSOLID advances it by 10^{-5} seconds per timestep. This difference means that for every 10 timesteps of simulated firing time that ROCFLO takes, ROCSOLID takes one.

While passing data back and forth between the codes, the interface code bridges the chasms between them, ensuring that the data are computed at the same spot and the same moment. The interface code also helps manage the parallel nature of the SRB code. Sections of each component's mesh are spread across all of the supercomputer's processors. Since pieces of the code have to pass data to one another, the interface code has to know where the data are and where they need to go.

"With two distinct meshes being calculated and each of those meshes spread across all the processors and even sharing processors, it's a great challenge even to figure out who needs to talk to whom," says Alavilli.

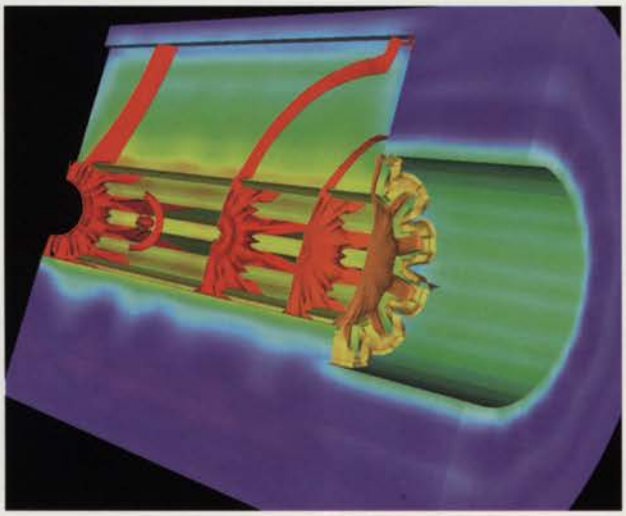
Rocketeer

Sometimes when you need the right tool, you have to build it yourself. After looking at a variety of 3D visualization software packages, the CSAR team decided that they'd develop one themselves.

"Even very expensive commercial packages did not meet all of our requirements," says Bob Fiedler, CSAR's technical program manager. So, along with his colleague John Norris, Fiedler built a new 3D visualization tool that would allow CSAR to get the most out of their detailed solid rocket models.

Dubbed Rocketeer, the software offers a number of features that make it ideal for CSAR's coupled, whole-system rocket simulations. It supports, among other things, structured and unstructured grids, the merging of multiple datafiles, and automated animation. It can also create semitransparent surfaces, slices, and isosurfaces, allowing visualizations that show features at different depths within the model. For example, a visualization of a rocket can depict the outermost temperature isosurface without completely blocking the view of additional isosurfaces inside it.

These traits, however, also make Rocketeer suitable for many complex, multicomponent datasets. "Despite the name, nothing restricts this software to rockets," says Michael Heath, director of CSAR.



Propellant stress and gas pressure in the SRB. This image combines the two previous visualizations using a single color scale.

Success is more than avoiding failures

A series of three consecutive Titan IV launch failures in the spring of 1999 cost more than $3.5 billion with the destruction of the solid rockets and their expensive payloads. The failure of one of the Space Shuttle Challenger's SRBs in January 1986 was even more costly—seven American astronauts were killed. As CSAR's whole-system simulations become ever more sophisticated, they will help designers avoid such disasters. Already CSAR researchers are working on additional modules for their modeling code that will allow them to simulate and study common solid rocket faults such as cracks in the propellant, unexpected deformations, and design flaws.

In the meantime there's a significance beyond averting failures and explosions, beyond even rockets. Daunting undertakings like CSAR's help researchers understand how to attack complex, real-world problems of any breed.

"There's a lot to be learned about our technologies and the organization of our simulations by working on such an advanced project," Heath says. "Even for those with no inherent interest in rockets, this is a concrete testbed for simulating systems with many different components, interactions, and scales."

This research is supported by the Department of Energy.

http://access.ncsa.uiuc.edu/CoverStories/RocketSimulations/

For further information:

http://www.csar.uiuc.edu
http://spaceflight.nasa.gov
http://www.csar.uiuc.edu/F_software/rocketeer

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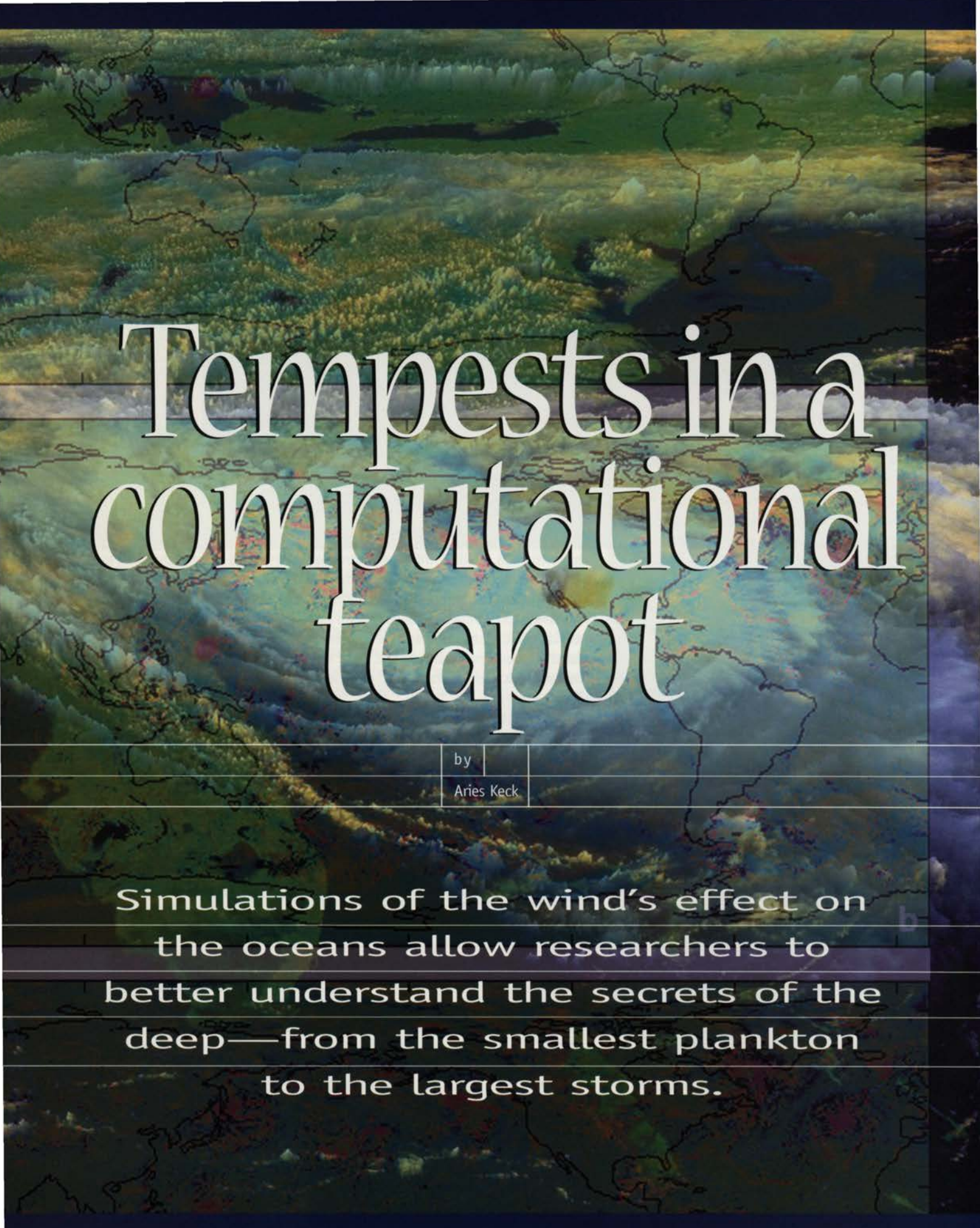


Tempests in a computational teapot

by Aries Keck

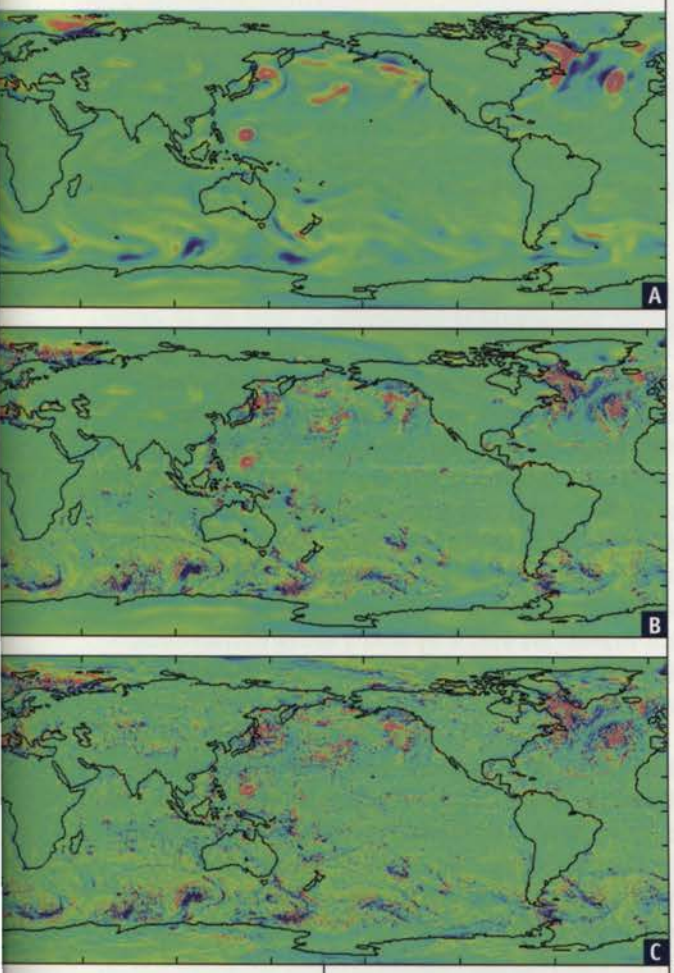
Simulations of the wind's effect on the oceans allow researchers to better understand the secrets of the deep—from the smallest plankton to the largest storms.

Capture the wind in a bottle. Then add the sea. Shake gently, and watch storms form. That's the idea behind the Spectral Element Ocean Model, a vast computer simulation of the Earth's oceans running on NCSA's SGI Origin2000 supercomputing system.

"This is the big picture," says Dale Haidvogel. "It encompasses everybody and all things." Haidvogel, a professor at Rutgers University's Institute of Marine and Coastal Sciences, leads the team that is simulating the effects of the wind on the ocean.

The wind is the main force making the oceans move. It physically changes the ocean surface in every way, from tiny riffles on the surface to massive tropical storms to worldwide weather events like El Niño. The wind also stirs the oceans, bringing cold, nutrient-rich waters up from the deep. And that creates biologically rich areas near the surface that are literally swimming with fish food. Haidvogel's worldwide ocean simulations not only model these processes but also allow other researchers to build smaller models that focus on the impact of ocean currents.

"Someone looking at the output of this model from the perspective of a pure physical scientist wants to know how the ocean is doing what it's doing," Haidvogel says. "Others are interested in the biological response to these currents, and how they ultimately affect fish. So we're building a hierarchy of nested models which will help answer these questions."

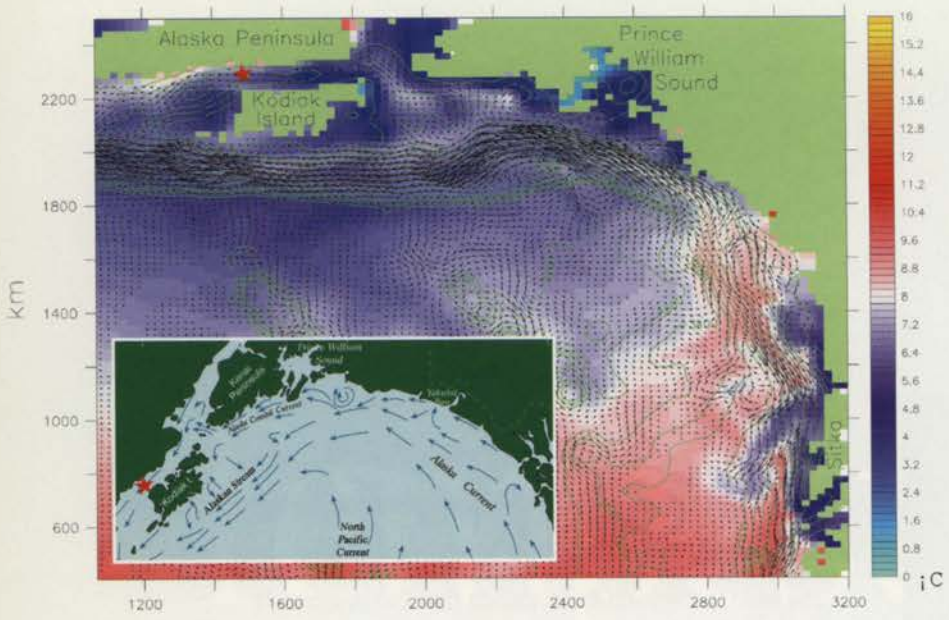


Global wind-stress curl map from December 1996. Panel A shows a 10 meter wind analysis from the National Center for Environmental Predictions. In Panel B, satellite samples from within six hours of the analysis in Panel A overlay the data from Panel A. Panel C is a blend of the NCEP and satellite data. Researchers at the National Center for Atmospheric Research use this sort of data to drive global and regional ocean circulation models.

Weathering a storm of data

To serve as the granddaddy of these nested models, the Rutgers team's massive Spectral Element Ocean Model has to be flexible enough to handle a variety of demands while maintaining the sheer power necessary to model that variety. Running on 48 Origin2000 processors, it focuses on the speed, direction, and pressure of ocean currents, using 3.5 million variables to track those features.

To grasp a system as complicated as the ocean, the body of water is broken into a grid of quadrilaterals called elements. Inside each element, the currents and pressures are computed for a set of points aligned along a mesh. The elements' orientations and sizes can be altered to fit the complicated geometries of the ocean basin and to increase accuracy. The number of points inside each element can also be adjusted.



Depth-averaged subtidal velocity in meters per second and Celsius surface temperature from a regional model of the Gulf of Alaska. Model gridpoints are roughly 22 km apart. Measurements of the water depth (bathymetry) in meters is shown in green contours. The inset map shows major observed mean circulation features.

"Essentially the elements partition the ocean into finite numbers," says Mohamed Iskandarani of Rutgers. "It's a way of breaking up a complicated equation into pieces that can be solved on a computer."

Storing and managing the data required and created by the model is quite an undertaking. For example, each element in the model has to hold 64 wind speeds. "And you need two components for the wind, one blowing north to south, and another east to west. And the model has 3,552 elements. Now, this wind field is changing every six hours. So you need new data four times a day, and you have 365 days a year. And we have data for 40 years. That's 212 gigabytes of data," Iskandarani says.

What makes it possible to compute so many pieces of data for so many elements? Iskandarani says the model only needs to notice when there's a change between two different elements. "This is a very good property if you want to do parallel computation. Calculations in each element proceed almost independently, and only edge information from a given element needs to be sent only to neighboring elements."

Data from the heavens

For all its strengths, the Spectral Element Ocean Model is completely dependent on the data fed into it. That's where Ralph Milliff and scatterometers come in. Milliff is a scientist with the National Center for Atmospheric Research, and scatterometers are instruments on NASA and European satellites that send microwave radar pulses down to the surface of the ocean. The radar pulses are scattered by little capillary waves on the ocean's surface and then recaptured by the satellites. The entire round trip is nearly 1,600 kilometers, and it all happens in the blink of an eye.

"We went from having, say, a thousand points of data from buoys," Milliff says, "Thanks to a recent series of satellite missions, we can now see the global wind field over the whole ocean, twice a day."

To determine the wind's speed, scatterometers measure the scattering of the radar pulses as they bounce off the ocean's surface. The number of tiny capillary waves, essentially riffles on the waves, tells Milliff how hard the wind is blowing. The greater the population density of these waves, the more scattering there is, and the greater the wind speed. The wind's direction, meanwhile, is found by counting capillary waves are on the faces and shoulders of larger swells.

Russian dolls and coastal models

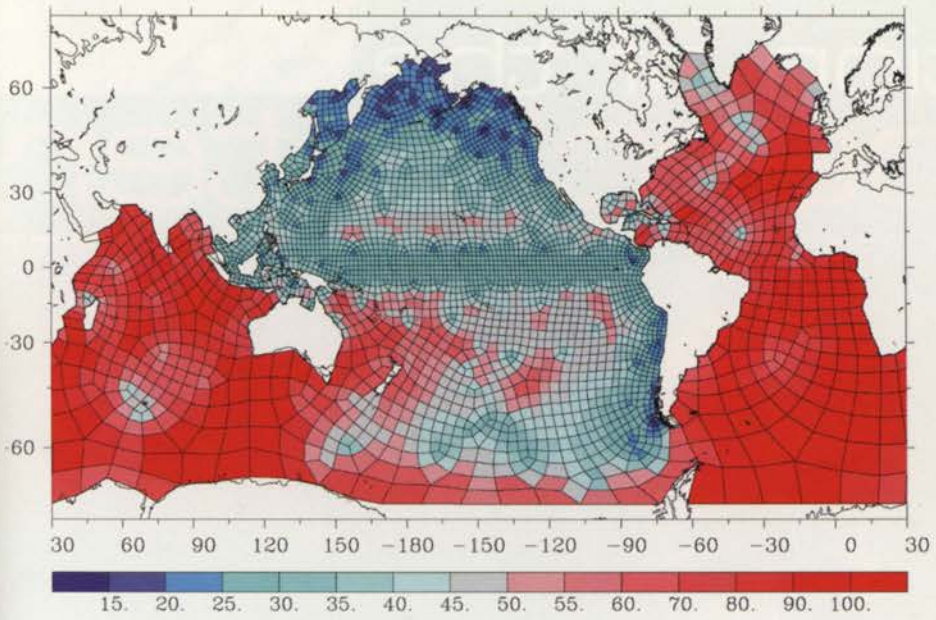
Currently the Rutgers team's model focuses on the Pacific Ocean because most of their scientific partners are studying effects on the Californian, Oregonian, and Alaskan coasts. The efforts are all part of the GLOBEC program, a National Science Foundation program that studies global ecosystem dynamics.

"The global model passes information on the state of the global ocean to coastal models," Haidvogel says. Data from those smaller physical models are then fed into even more precise biological models. It's as if they were a set of Russian dolls, each one nested inside the other, getting smaller and showing further detail along the way.

Albert J. Hermann—an oceanographer at the Joint Institute for the Study of Atmosphere and the Oceans, which is run by the University of Washington, Seattle, and the National Oceanic and Atmospheric Administration—operates some of the coastal and biological models. "We couple the output from Dale and Mohammed's Spectral Ocean Model into a more regional circulation model of the Gulf of Alaska."

Output from that physical model of the gulf is then used to drive at least two biological models. One is what oceanographers call a NPZ model. Essentially a model of fish food, N stands for nutrients, P for phytoplankton, and Z for zooplankton. Estimating the concentration of these microscopic or nearly microscopic food animals and plants can relate to fish stocks.

For example, a GLOBEC study now running looks at juvenile salmon that run along the Alaskan coastline. "We're trying to understand why these salmon populations fluctuate from year to year, and even decade to decade," Hermann says. Fishery scientists believe these natural cycles may be related to atmospheric and oceanic conditions. Knowing when and why they occur could help determine how much salmon should be fished in a year.



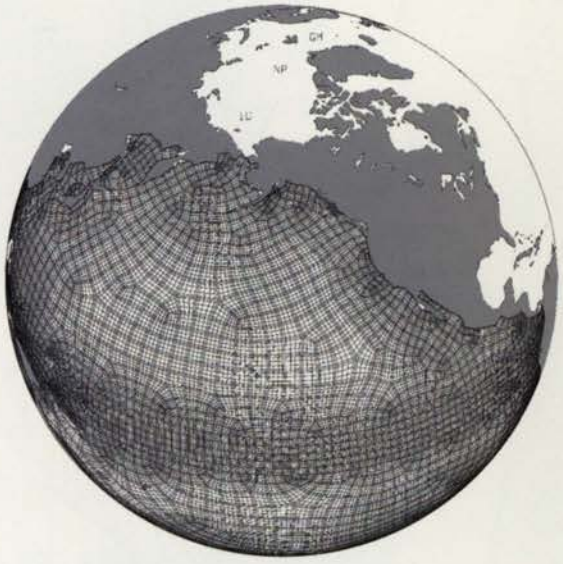
SEOM grid showing the elemental partition of the world's oceans. The grid holds 3,552 elements and has an average spacing of 20 kilometers in the North Pacific. Each element holds 64 velocity nodes and 36 pressure nodes.

Hermann says other biological models are also in the works, as are more models of the weather and other physical processes. These computer models range from a global to a fish-sized view, and the machines that run them go from massive to miniscule. The Spectral Element Ocean Model runs on NCSA's powerful Origin2000, while the fish model runs on a simple desktop workstation.

The ultimate goal for the model is what Haidvogel calls a "nowcast, a picture of what's happening in the ocean right now." Given the vastness of the ocean and the small size of the features researchers want to look at, a future nowcast will require both more data and more supercomputing strength.

"Supercomputing power has increased steadily to the point where these simulations are feasible now, but we still have a long way to go," Iskandarani says.

With the models already being used to monitor fish populations and to create maritime reports, however, the benefits already sound like a lot more than a fish story.



An example of gridding in the Pacific.

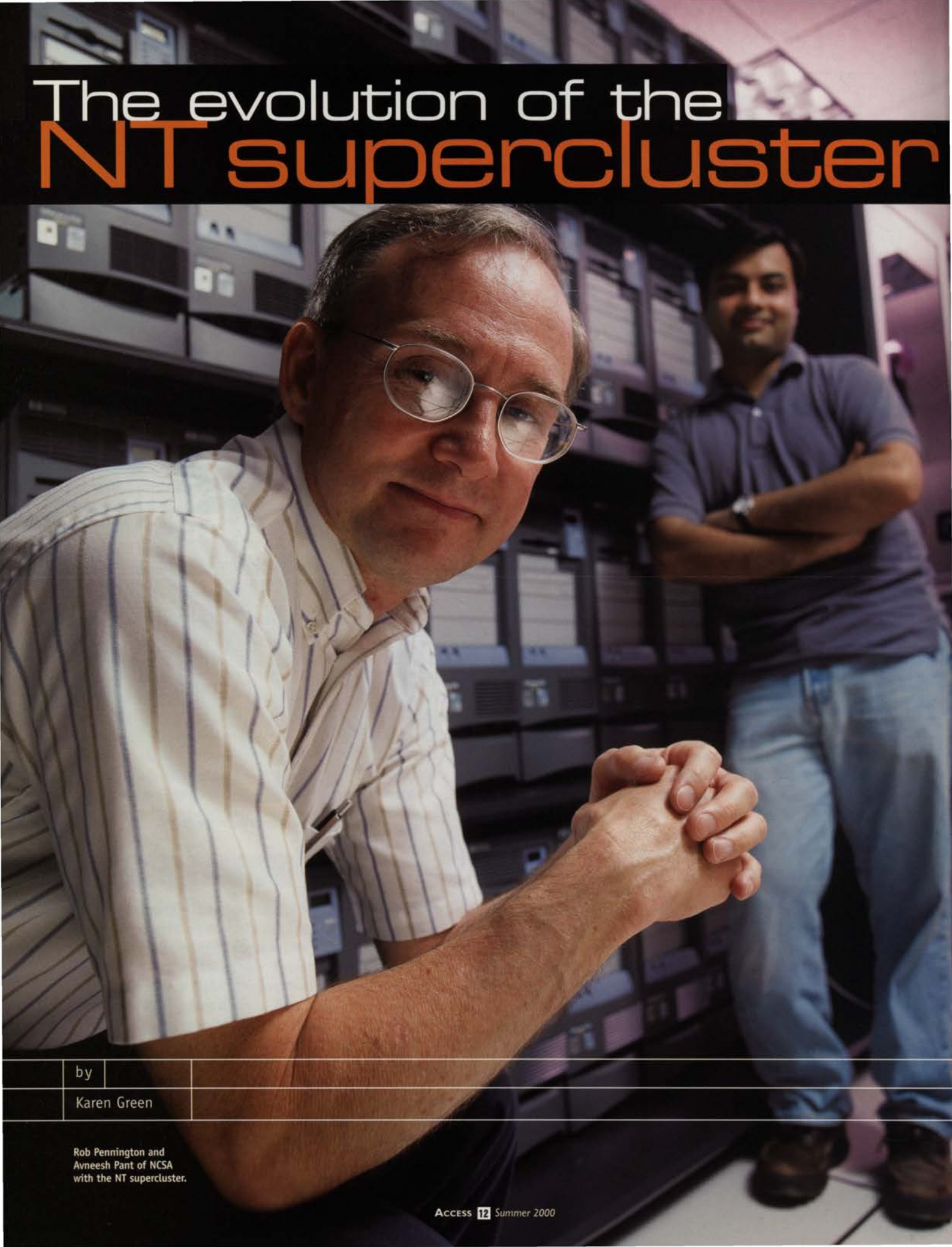
This research is supported by the National Science Foundation.

http://access.ncsa.uiuc.edu/CoverStories/OceanCirculation/

For further information:

http://marine.rutgers.edu/po/index.html
http://www.cgd.ucar.edu/
http://www.usglobec.org/

The evolution of the NT supercluster

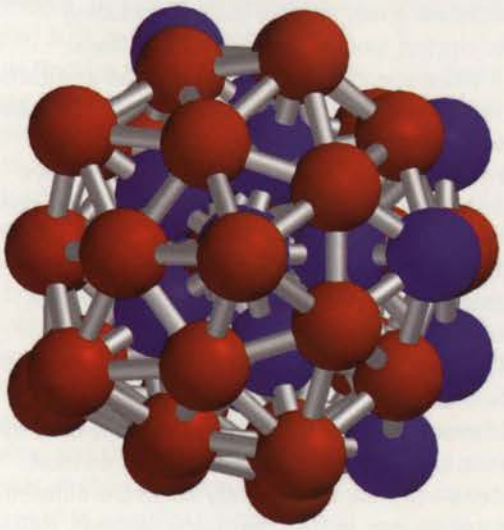


by

Karen Green

Rob Pennington and Avneesh Pant of NCSA with the NT supercluster.

NCSA's NT supercluster, though only recently put into production mode, is performing as well as or even better than more conventional supercomputing platforms.

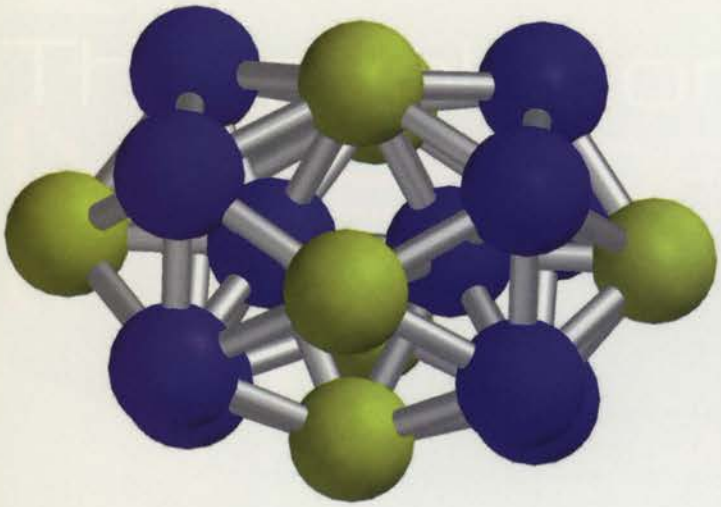


Global minimum for a molecule of 20 argon atoms and 35 xenon atoms. Argon is represented in blue and xenon in red. Potential energy surfaces of clusters and complex molecules can have a large number of local minima (often over 10^{40}), and locating the most stable of these (the global minimum) is a daunting computational task. A team of scientists at the University of Pittsburgh ran a Monte Carlo minimization code called GMIN on the Alliance's NT supercluster to efficiently locate the global minimum of this molecule. The team is led by Alliance partner Ken Jordan.

Two years ago NCSA had its first success running scientific code on a brand new hardware platform called the NT supercluster—a collection of high-end, commodity PCs running the Windows NT operating system and linked together with a fast network to operate at supercomputer performance levels.

Since then the supercluster has evolved into a system that serves a variety of NCSA and Alliance users and is ranked 207 on the latest Top 500 Supercomputer list compiled biannually by researchers at the University of Tennessee and the University of Mannheim in Germany. Between February 2000, when the NT supercluster changed from friendly user to production mode, and May 2000, 26 allocations of CPU time were granted on the cluster. The supercluster runs a variety of scientific Message Passing Interface (MPI) codes at performance levels that are comparable to, and sometimes even better than, performance levels achieved on more conventional supercomputers.

After the transition to production mode, utilization of the supercluster quickly rose to about 30 percent. That figure should double in the next few months, as more scientists are granted allocations on the system, according to Rob Pennington, head of the Alliance NT cluster development team at NCSA. "That's a very good start for production, and that figure will undoubtedly go up as more researchers are granted time on the cluster," he adds.



Global minimum for a mixed cluster consisting of 12 argon atoms and 7 xenon atoms calculated by the University of Pittsburgh team using the NT supercluster. Argon is represented in blue and xenon in yellow.

Supercluster nuts and bolts

At present the supercluster consists of more than 400 processors. A cluster of 288 Intel processors in 144 compute nodes (with one compute node equal to one dual-processor machine) is available to the scientific user community. A total of 256 of those processors—128 Hewlett-Packard machines with dual 550-MHz Intel Pentium III Xeon processors—are capable of running MPI codes using Myricom's Myrinet interconnect and software called High Performance Virtual Machine (HPVM). HPVM was developed by Andrew Chien and the Concurrent Systems Architecture Group at the University of California, San Diego. MPI codes allow communications among multiple systems, making distributed computing possible. The majority of distributed scientific codes utilize MPI for message passing. Thirty-two 333-MHz Intel Pentium II processors are available to run serial codes.

The remainder of the supercluster's processors are used for testbeds that look at a range of infrastructure and development issues and performance and portability issues with different interconnects and operating systems.

Codes that run on the supercluster include the MIMD Lattice Calculation (MILC), a parallel code used for lattice quantum chromodynamics (QCD) simulations. The MILC collaboration, led by Bob Sugar of the University of California at Santa Barbara, includes physicists from nine universities working on a Department of Energy Grand Challenge Initiative that involves using parallel computing to model QCD. The MILC code was easily ported to the NT supercluster. Since the supercluster entered production mode, MILC researchers Doug Toussaint and Kostas Orginos of the University of Arizona have used more hours on the cluster than any other allocated project to date (see sidebar).

Other codes that have been successfully ported to the supercluster include GMIN (chemistry), OVERFLOW (aeronautical fluid dynamics), Cactus (general relativity), ZEUS-MP (astrophysics), Tree Particle Mesh (cosmology), ARPI-3D (weather research), a Quantum Monte Carlo materials science code, and a polymer research code.

A fertile testbed

One of the testbeds focuses on cluster middleware called Virtual Machine Interface (VMI), developed by NCSA cluster team member Avneesh Pant. VMI makes it possible for applications to run on a cluster using different types of interconnects to communicate among processors. VMI also allows MPI applications to run between clusters, including those using different operating systems. The team has successfully run the MILC, Cactus, and ARPI-3D applications across multiple clusters, including heterogeneous clusters running Windows NT and Linux.

"Without VMI a scientist who has compiled an application on a cluster using Myrinet would have to recompile that code to use with a different cluster, such as one that had only Ethernet," says Pant. "If you compile your MPI code for systems that use the VMI layer, it will run on other types of clusters or on multiple clusters. In other words, you could have just one executable that could run on any NT cluster on the Grid, and it could also be part of a larger computation that includes a Linux cluster or other NT clusters."

The development of VMI was a consequence of the need to do performance testing on clusters, says Pennington. VMI works as middleware that allows MPICH—a tool developed by Argonne National Laboratory that implements MPI on most computer systems—to work transparently across the different interconnects and systems in the supercluster testbeds. MPICH is the standard for implementing MPI on most high-end computing systems, although it is often finetuned to the characteristics of specific computing systems. VMI allows the cluster team to tune MPICH to the supercluster environment. In addition VMI allows machines with different operating systems to work together on an application with just a simple recompilation for each operating system.

"We now have a common layer of middleware for MPI applications, so we can make direct comparisons among clusters running various applications, " says Pennington. "As a result, we can get a better idea of the performance of specific codes on different cluster systems."

Addressing the reality of the Grid

The ability to run applications on multiple clusters using different interconnects and operating systems is important as the Alliance continues to develop the concept of computing on the Grid. The PACI Grid—an experimental system that links high-speed hardware and cutting-edge applications into an efficient, persistent infrastructure—is being built by the Alliance. This Virtual Machine Room gives researchers remote access to any of the Alliance's computing resources regardless of physical location and lets resources at different locations work together as one seamless system.

"This type of technology, which can bridge multiple clusters using multiple interconnects to create a seamless system is important to the concept of Grid computing," says Pennington. "Clusters are built from commodity components, and since no single vendor supplies all the components, it is unlikely that a particular interconnect will become the standard for clusters."

The VMI middleware addresses this reality and at the same time makes the computational scientist's job easier. It is another step in the supercluster's journey from experimental system to one of the main computing platforms offered to scientific users by the Alliance.

This project is supported by the National Computational Science Alliance, with additional support from Microsoft Corp., Intel Corporation, and Myricom.

http://access.ncsa.uiuc.edu/CoverStories/vmi/

For further information:
http://www.ncsa.uiuc.edu/General/CC/ntcluster/

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Rob Pennington
Michael Showerman

QCD on the NT supercluster

The team of physicists known as the MILC (MIMD Lattice Computation) collaboration logs about 1 million CPU hours a year on supercomputers across the U.S. In February 2000, after several months of friendly user access, two members of the team began production simulations on the Alliance's NT Supercluster at NCSA. The researchers—Doug Toussaint and Kostas Orginos of the University of Arizona—have become the largest users of NCSA's NT supercluster resources.

"We quickly used up our initial 25,000-hour allocation and had to get that allocation supplemented," says Toussaint. Performance on the cluster has been about 50 megaflops per node, which is roughly the same as on NCSA's 195-MHz SGI Origin2000 processors, he notes.

"We are in the happy situation of having codes that are quite portable, so we seem to be continually moving around as time becomes available on different machines," adds Toussaint. "At this time, we are moving full speed ahead on the cluster."

The MILC collaboration studies quantum chromodynamics, or QCD, a theory that describes the strongest force in nature—the force that binds together quarks into the protons and neutrons that form the nuclei of atoms. Quarks are held together by gluons, the strongest superglue imaginable. Since quarks and gluons are among the most basic known particles in the universe, understanding the behavior of these building blocks of all matter is a key to answering some of the fundamental questions about the origins of the universe.

To conduct QCD simulations, computational researchers use a four-dimensional grid, called a lattice, that spans time as well as the three space dimensions. The finer the lattice, the more accurate the predictions that result from a QCD simulation. Unfortunately, going to a finer lattice rapidly increases the computer time needed and therefore the cost of the simulation. To get more accurate results from simulations on a relatively coarse lattice, Orginos and Toussaint use procedures known as "improved action," which are more sophisticated ways of approximating QCD theory on the space-time lattice.

The elementary particles in the strong force interactions are quarks and gluons, which have roles analogous to electrons and photons, respectively. Simulating the dynamics of gluons is straightforward, but simulating the dynamics of quarks is a very nasty numerical problem. As a result, QCD simulations make

Doug Toussaint and Kostas Orginos. University of Arizona.

compromises in dealing with the quarks, either by omitting, or "quenching," some or all of the flavors or by calculating at unphysical masses of the quarks. Quarks come in six varieties, or flavors, each with successively greater mass: up, down, strange, charm, bottom, and top. Three of these flavors—up, down, and strange—are light enough to be important in determing the physics of the most common elementary particles.

While many calculations include only two flavors of quarks (up and down), the MILC group's simulations include a third flavor—the strange quark. Adding a third quark to the simulation, says Toussaint, more realistically represents the masses and interactions among the quarks.

QCD simulations make for some of the most complex numerical calculations in science, but the team's code itself is relatively easy to port to a variety of computing platforms. Orginos worked with Rob Pennington and Mike Showerman of NCSA's NT cluster group to port the code and develop the techniques to run it on the then-experimental NT supercluster.

"In the end Kostas only had to make one change in the code to avoid one of the variants of the MPI send routines which didn't work on the cluster," Toussaint recalls. "Also, we ported the code very early in the machine's development. I imagine it would be easier now that the environment has matured."

The MILC collaboration is a Department of Energy Grand Challenge initiative that involves researchers from nine institutions: the University of Arizona, University of California at Santa Barbara, University of Colorado, Florida State University, Indiana University, University of the Pacific, University of Utah, Washington University, and the Nordic Institute for Theoretical Physics. Bob Sugar of UCSB is the collaboration's lead investigator.

This research is funded by the Department of Energy and the National Science Foundation.

Piecing it together

by
J. William Bell

Techniques and software developed at the National Center for Macromolecular Imaging will help structural biologists develop high-resolution, three-dimensional models of biological particles.

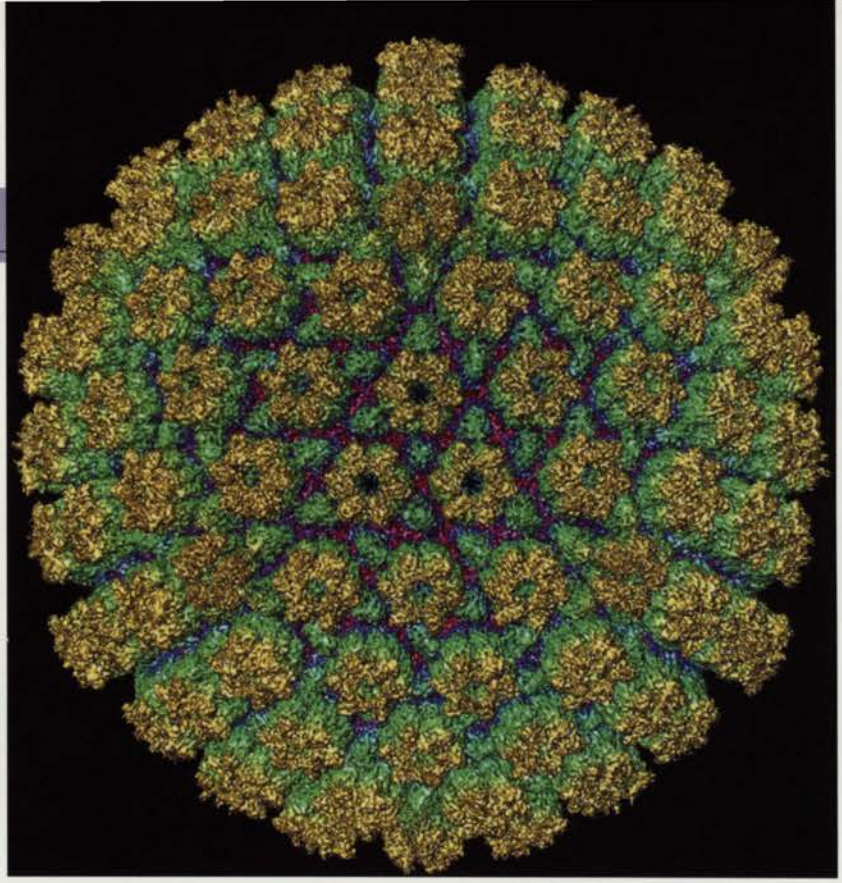
The first steps in solving a jigsaw puzzle can be among the most tedious. You pour all of the pieces onto your table, then make sure all the pieces are face up. You may even group the pieces into similar sets—all of the outside edges together, everything that's blue. Only then do you start assembling the big picture.

Structural biologists often work through similar steps. Using a transmission electron microscope to pass a beam of electrons through a specimen, researchers capture images of biological particles approaching atomic scale. With enough views of the particle—hundreds, representing tens of thousands of particles—scientists can build three-dimensional models of the particles using two-dimensional microscopic images. But creating and improving the quality of these three-dimensional models using two-dimensional microscopic images is difficult and even more labor-intensive than getting ready to put together your jigsaw puzzle.

"Structural biologists eventually want the same thing: precise and complete three-dimensional views of large and complex molecules and aggregates of molecules [called particles]," says Wah Chiu, director of the National Center for Macromolecular Imaging (NCMI) at the Baylor College of Medicine, an Alliance partner in Houston. Chiu's team is using NCSA's SGI Origin2000 supercomputer, as well as their own smaller Origin2000, to create some of the highest resolution three-dimensional models of biological particles ever produced.

Researchers at the National Center for Macromolecular Imaging in front of their new Jeol 3000SFF microscope, which allows them to collect data with near atomic resolution. Left to right: Phil Baldwin, Wah Chiu, Steve Ludtke, and Hong Zhou.

Amazing size, ambitious goals



Reconstruction of a herpes simplex virus capsid at 8.5 angstrom.

Supported by the National Center for Research Resources of the National Institutes of Health, the National Center for Macromolecular Imaging is currently working on over 25 collaborative projects with institutions all over the world, including seven Alliance partners. A few of the particles that require NCSA's Origin2000 to attain a high resolution three-dimensional model are: a lens protein of the human eye, known as alpha-crystallin that can cause cataracts as it ages; fatty acid synthase, which builds fatty acids in the human body; and the herpes simplex virus, which causes a variety of disorders such as cold sores, chicken pox, and even congenital defects.

The tiny size of these particles is amazing, and the team's modeling goals are ambitious. The herpes simplex virus is only 1,250 angstroms in diameter—an angstrom is one ten-billionth of a meter, about the size of a single atom. Earlier this year the center's researchers used their own Origin2000 to create a model of the virus with a resolution of 8.5 angstroms. Still, the team would like a model with twice the resolution. (A report on the current herpes simplex model was published in an April issue of *Science* in collaboration with Hong Zhou at the University of Texas at Houston Medical School and Frazer Rixon at the Medical Research Council Institute of Virology in Glasgow, England.)

"NCSA is going to help us get to the next step in resolution," says Steve Ludtke, a computational biophysicist at NCMI. "The herpes simplex virus requires tremendous amounts of memory and computation. Eventually we'd like to get all of the projects down to at least eight to 10 angstroms. On the herpes, we're aiming at four to five angstroms."

At only about 140 angstroms in width, alpha-crystallin is 10 times smaller than the virus. Researchers—including Phil Baldwin, Irina Serysheva, Steve Ludtke, and Florante Quiocho at Baylor College of Medicine and Mark Petrash at Alliance partner Washington University—have already created a model with a resolution of 20 angstroms and would like to increase the resolution to about 10 angstroms. At 10 angstroms, they should be able to discern not only the 24 subunits that make up alpha-crystallin but also how these subunits are arranged with respect to one another. Using this information, researchers may be able to shed some light on why degradation of the alpha-crystallin lens protein leads to cataracts.

With support from the National Science Foundation, NCMI recently installed a 300-kilovolt electron cryomicroscope, which can image biological particles with maximum contrast and at very high resolution. And the better the images collected with the microscope, the better the models that can be built from those images. The most powerful microscope of its kind in the United States, this instrument is a type of transmission electron microscope that has a highly coherent electron beam and looks at samples kept at liquid helium temperature, or about -270 C.

The amount of computing power necessary to get the kind of resolution that researchers want in their models, however, is beyond the capacity of their own 32-processor Origin2000.

"It's gotten to the point that we can't do it on our own supercomputer," says Chiu. "To push the resolution of our model of the herpes virus capsid particle from 8.5 angstroms to 6 angstroms sounds like a small improvement, but the computational task requires 50 times more effort in terms of data size."

Get the picture

To create the models, also known as reconstructions, the team uses a technique known as single-particle analysis. Particles are first selected from microscopic images, or micrographs. A single micrograph can contain hundreds of thousands of particles with random orientations, so the particles are first grouped by similar orientation. The particles within a group are then aligned to each other and averaged together. These groups represent views of the particle that are a few degrees different from one another.

From this collection of views, a preliminary three-dimensional model is built. At this point, determining the symmetry of the particle is critical. Although symmetry is not generally known, the ways in which sections of the particle

mirror one another along a given axis have a tremendous impact on the computation and refinement of the final model.

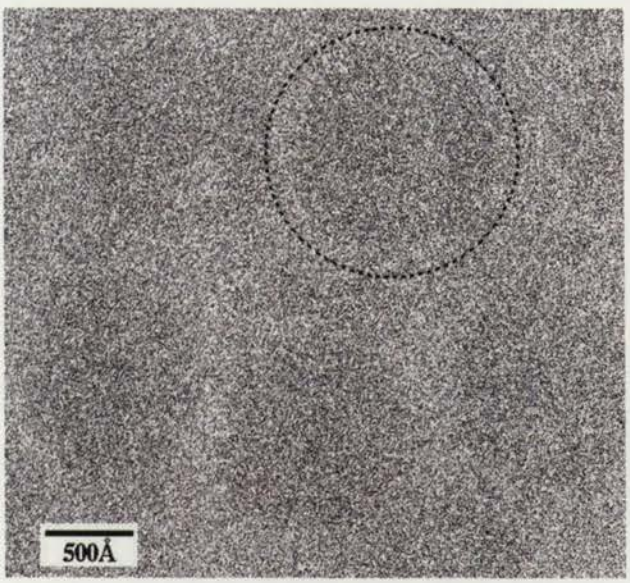
"Often the biochemistry of the particle will give you at least a hint, and generally you can get an idea based on the appearance of individual projections at a given orientation," says Ludtke. But there are also times that researchers rely on statistical techniques. "We go through a several-stage process, running refinements with several different possible symmetries to try to discover the correct answer."

Once an initial model is created, the model is refined. A version is compared to the raw data—the projections of the particle at different orientations—and adjusted. In the most computationally taxing aspect of the process, this loop continues until the data and the model match. The 20-angstrom model of alpha-crystallin, for example, required 10 refinement loops. Each loop of the model, which had no symmetry and was thus more difficult than many, took 48 hours on an eight-processor Origin2000 configuration. To get that model down to 15 angstroms, the computational requirements will go up by at least a factor of 10.

Wide open

While developing their models, the team at NCMI is also improving the field's software infrastructure. EMAN—short for Electron Micrograph Analysis—automates most of the reconstruction process, from selecting the particles to refining the three-dimensional models. The software package allows researchers to produce in 24 hours models that once would have taken a month's work.

"As a national center, we get lots of projects to work on. With existing software packages, we just couldn't get the number of projects we're working on done," says Ludtke, who developed EMAN along with the center's Philip Baldwin.



Typical electron cryomicroscopy micrograph used in the reconstruction of a herpes simplex virus capsid. The dashed circle indicates one herpes simplex virus capsid.

The first version of EMAN was released in the summer of 1999, and a new version was released in early 2000. It is provided free of charge and with open source code so that researchers around the world can use this rapidly expanding technique. At least eight research groups outside of the center are actively using the package, and there have been many more downloads.

"The open-source choice was primarily a philosophical one for us. The software should be in the public domain," Ludtke says. "There are a lot of labs around the country which have electron microscopes and can collect particle image data. But the steep learning curve and monetary expense have always been barriers to these groups doing reconstructions. We wanted to eliminate both of these barriers and get more people involved in this technique."

This research is supported by the National Center for Research Resources of the National Institutes of Health and by the National Science Foundation.

http://access.ncsa.uiuc.edu/CoverStories/ParticleReconstruction/

For further information:
http://ncmi.bioch.bcm.tmc.edu/
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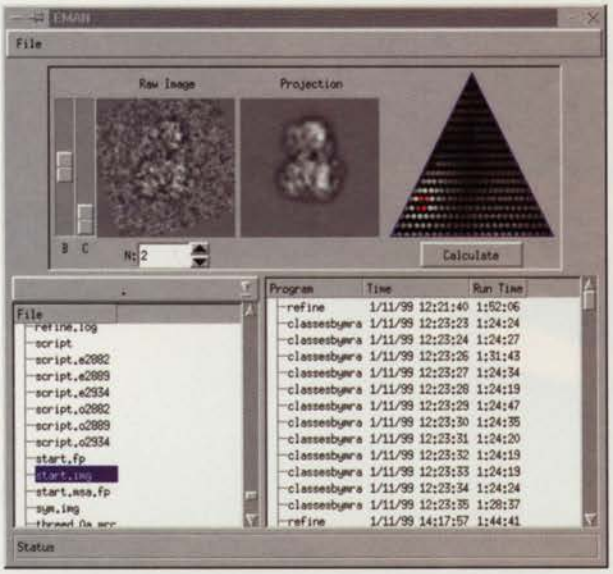
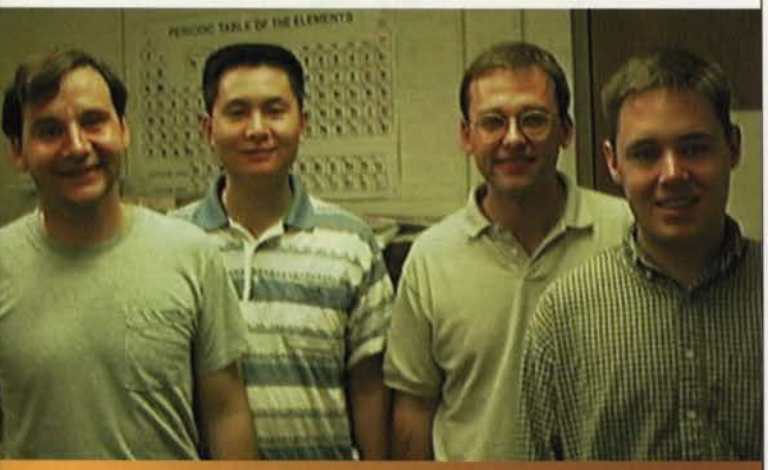


Screen shot of the EMAN software package. EMAN is already allowing researchers to perform in 24 hours particle reconstructions that formerly required a month of user-intensive work.

Puzzling proteins



Pablo Molina, Hui Li, Jan Jensen, and Ryan Minikis. University of Iowa.

by Patricia Craig

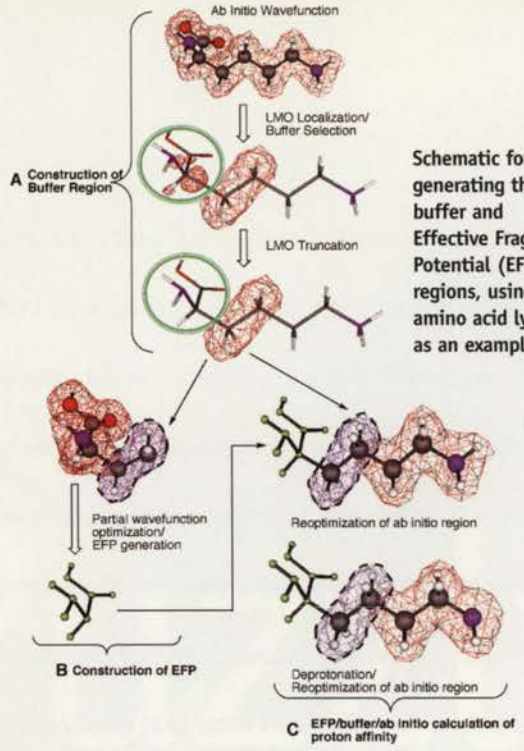
The Effective Fragment Potential simulation method being perfected using Alliance resources will help researchers overcome one of the biggest challenges in modeling proteins—size.

The thousands of proteins that exist inside cells of all living organisms are made from just 20 amino acids that must fold in very specific patterns in order to function properly. That much scientists know. What scientists don't know is precisely how these complex molecules do their jobs—how they form and break bonds to catalyze the necessary reactions that sustain life. As University of Iowa theoretical chemist Jan Jensen puts it, "We often don't know what exactly is going on inside proteins."

To Jensen, the inside of a protein is the electrostatic environment of the individual atoms and the strongly polar nature that this environment creates in the constituent amino acids. Jensen and his research group use NCSA's SGI Origin2000 supercomputer—and, previously, the IBM SP supercomputer at the Maui High Performance Computing Center, an Alliance Partner for Advanced Computational Services—to model how these electrostatic charges affect protein bonding activity.

Jensen's research team at the University of Iowa includes Ryan Minikis, Pablo Molina, Hui Li, and Visvaldas Kairys (now at the Center for Advanced Research in Biotechnology).

"We are trying to get down to the physics of how the molecules interact," Jensen says.



Schematic for generating the buffer and Effective Fragment Potential (EFP) regions, using the amino acid lysine as an example.

Atom by atom

Size may be the biggest challenge in modeling proteins. Tackling an entire protein all at once would be ideal, Jensen says, but proteins are far too big for the massive calculations required. There are two alternatives. "You can either use a very simple model for the entire protein," he explains, "or you can do what we do and use a sophisticated method for one small part and a cheaper method for the rest."

This concept lies at the heart of a simulation procedure called the Effective Fragment Potential (EFP) method. EFP is a hybrid quantum and molecular mechanical method developed by Jensen in collaboration with Mark Gordon at Iowa State University and Walter Stevens at the National Institute of Standards and Technology. The method is implemented in a molecular modeling program called GAMESS developed by Gordon and his research group and distributed to the scientific community free of charge. The EFP method makes it possible for researchers to focus on the quantum mechanics of just one small part of a protein while maintaining the bulk of the protein in a less computationally intensive state.

The process starts by assembling the model atom by atom using structural parameters derived from biochemical experiments. The protein is then cut into manageable pieces that are four to six amino acids in size. The individual fragments have regions that overlap to minimize the effect of separation. The chemistry of each fragment is then defined with first principles, or ab initio, calculations.

The first principles calculations get down to the nitty-gritty of atomic interactions, determining the location of electrons around each atom's nucleus. The charge distributions of the electrons are explicitly tailored to the arrangements of the individual amino acids and thus model the internal interactions within the local environment.

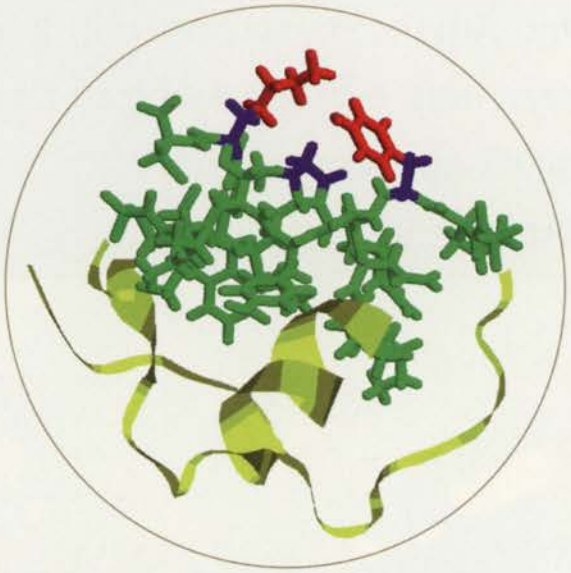
A giant puzzle

Once the fragments have been described separately, they are reassembled like a giant puzzle. Overlaps are adjusted so they are not counted twice in the final model. Now the protein is ready for researchers to study chemical reactions in a particular focus region. Because the entire protein has been described with first principles calculations, the focus region can be easily increased in size, or moved from one place to another. "That is the beauty of the program," Jensen says. "We don't have to do everything over. We just have to turn it and focus our view somewhere else."

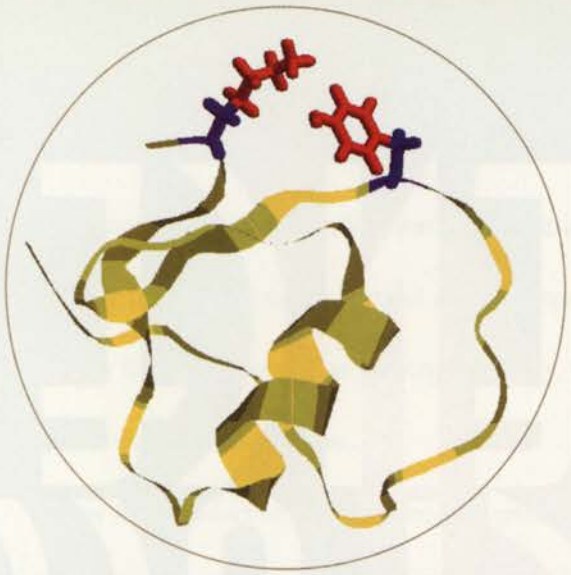
The focus region is an area only one or two amino acids in size. During a simulation, only this region is again described in quantum mechanical terms. The rest of the molecular environment, constituting the bulk of the protein, is represented in less exacting, classical physical terms extracted from the local charge density calculations. Since only the most important energy and polarization conditions are considered, this part of the model is markedly cheaper to run.

Jensen can add or remove protons within the focus region and watch what happens. The electrons, which determine the electrostatic charges and influence protein bonding, are exquisitely sensitive to such tweaking. For instance, adding a proton generates a net positive charge. To compensate, a cloud of electrons moves slightly closer.

Leaking electrons could run the simulation out of control. To prevent electrons from straying outside the focus region, Jensen adds a buffer zone of frozen electron density.



OMTKY3 protein. Red shows the regions in which ab initio quantum mechanical calculations were used. Green shows the EFP region, and blue the buffer region. The rest of the protein, which is ignored in this particular calculation, is shown as a yellow ribbon.



A focus region in the OMTKY3 protein. Two ionizable amino acid groups are shown, Lys55 (the red and blue structure on the left) and Tyr20 (the red and blue structure on the right). By studying such sites, researchers hope to understand intraprotein forces within OMTKY3.

Like a cork made of ice, the buffer zone keeps the "electron gas" from drifting into the rest of the protein. By convincing the protein that it is complete, the buffer zone also maintains a necessary link between the less precise regions and the focus region. This role is important because electrostatic charges within the entire protein can affect the chemistry of the focus region. If the model did not represent the less precise regions and convince the focus area that those regions exist, its veracity would be lost.

According to Todd Martinez, a chemist and protein modeler at the University of Illinois, Urbana-Champaign, the buffer zone is what sets Jensen's program apart from others. "Jensen concentrates on getting the boundary right between the quantum mechanics region and the rest of the protein," he says. "Even though this is a critical aspect of a realistic chemical model, it has rarely received the attention it deserves."

An experimental handle

Jensen and his colleagues are currently calibrating their modeling program against lab experiments, making sure their program faithfully represents a protein's internal environment. This is why their current work is limited to adding or removing protons. Manipulating protons is one of the few experimental handles scientists have to learn what is going on inside a protein. Comparing the energy required to add or remove a proton computationally against the energy measured experimentally helps validate the model.

Jensen's calibrating protein is a turkey ovomucoid third domain (OMTKY3). With only 56 amino acids, this protein is small but still large enough to be split into 10 fragments. Completing the first principles model for each fragment requires 10 hours on 16 processors of NCSA's SGI Origin2000.

"This is our first attempt to build a protein, and we had a lot to learn," Jensen says. "The Alliance's grant of computer time made it possible for us to develop and test our methodology in a reasonable amount of time."

OMTKY3 is an inhibitor protein that prevents a protein-eating enzyme called alpha-chymotrypsin from doing its job prematurely. Alpha-chymotrypsin normally binds to the proteins it destroys, chewing them up bit by bit. Jensen hopes to eventually understand the chemical and physical interactions that help OMTKY3 avoid destruction. He is also curious how alpha-chymotrypsin breaks down the other proteins it encounters. He and his colleagues have only recently begun using EFP to model some of these real-life scenarios.

OMTKY3 happens to be the subject of intense scrutiny in Andrew Robertson's nearby biochemistry lab at the University of Iowa. The proximity of the experiments was a major reason why Jensen chose this particular protein. He likes to interact directly with people at the bench. Robertson calls their collaboration profound. "It becomes more and more clear," he says, "that we need to understand this protein at Jensen's level—at the level of the electrons and their distributions within the protein. Jensen's approach stands to make a big contribution."

Martinez agrees. "EFP is one of the more promising methods of studying the chemistry of proteins at the atomic level."

This research is supported by the University of Iowa Biosciences Initiative Pilot Grant, a Research Innovation Award from the Research Corporation, the Petroleum Research Fund, and the National Science Foundation.

http://access.ncsa.uiuc.edu/CoverStories/efp/

For further information:

http://www.uiowa.edu/~chemdept/faculty/jensen/
http://www.uiowa.edu/~quantum/EFP.html
http://www.msg.ameslab.gov/

Team members

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Visvaldas Kairys
Hui Li
Ryan Minikis
Pablo Molina

THE SCIENCE OF GLASS

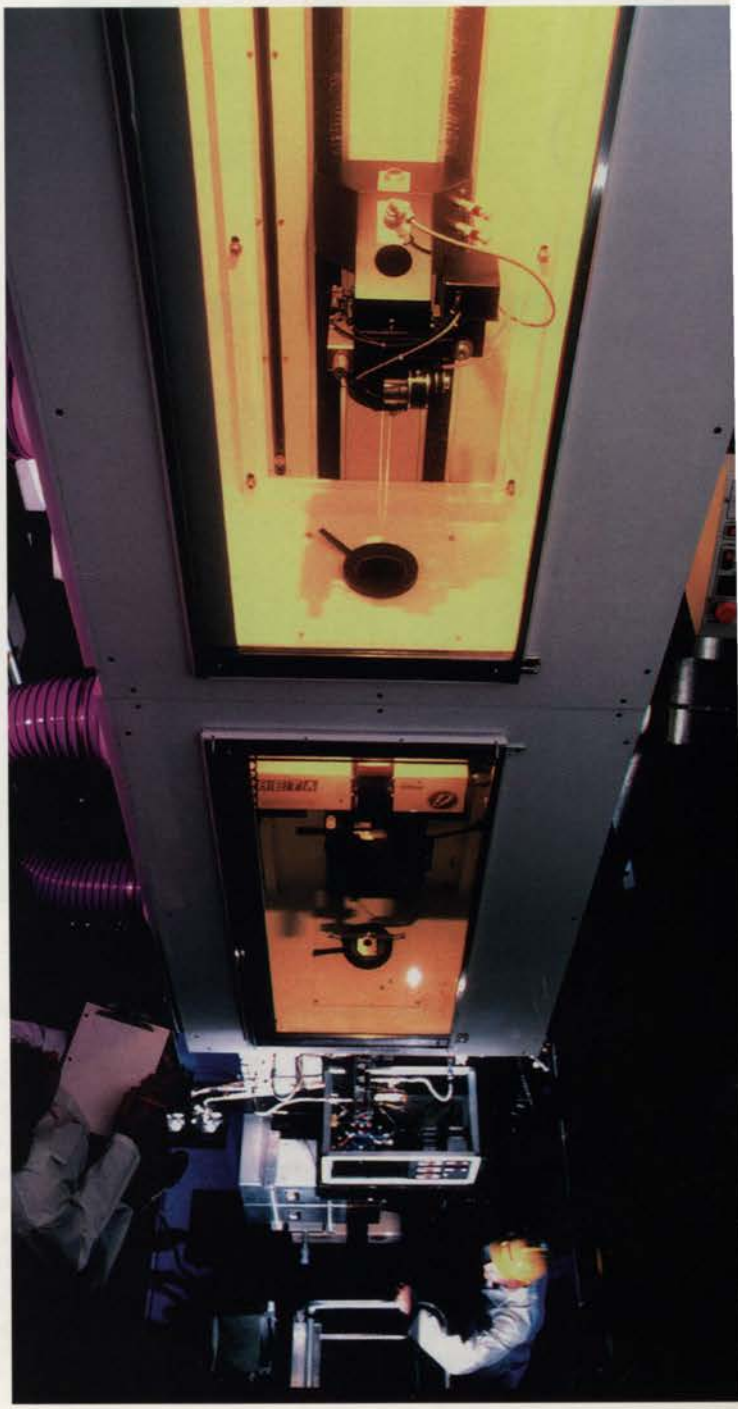
by Patricia Craig

RESEARCH AT RUTGERS UNIVERSITY IS TURNING THE PRODUCTION OF OPTICAL FIBERS, ONCE CONSIDERED AN ART, INTO A PRECISE SCIENCE WITH GUIDELINES BASED ON COMPUTER MODELS.

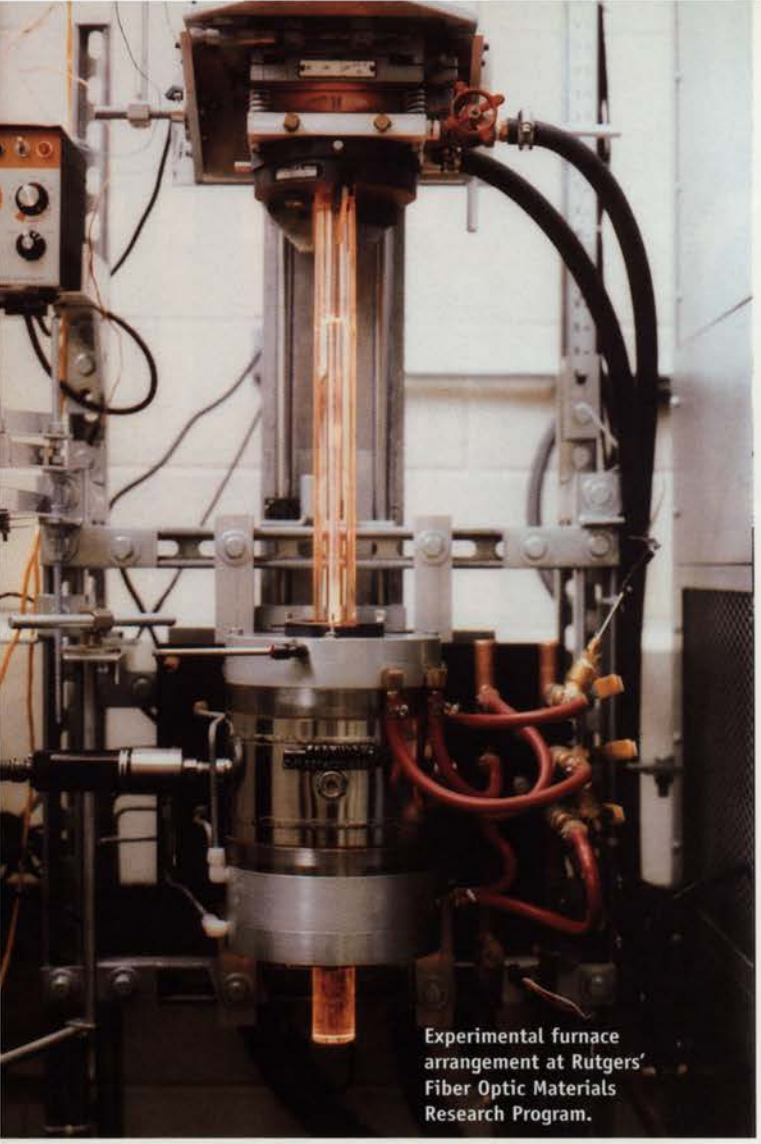
A half century ago, optical glass fibers were still a novelty, and tools of the trade were limited. Parts of one early contraption for making the fibers, also known as drawing the fibers, included discarded two-pound oatmeal boxes.

Today fiber production remains simple in principle. To begin, a cylindrical, optically pure glass rod called a preform is heated inside a small furnace to its softening point of about 1600 C. A fiber is drawn from the preform and moves along to a cooling channel, where circulating convective gases reduce the temperature to about 150 C. A coating is applied, and the plastic-bound fiber is cured in an ultraviolet oven before it is spooled around a drum. Enormous take-up spools wind fibers drawn in huge automated towers.

Despite the technological advances and the disappearance of oatmeal boxes, however, much of fiber drawing is still considered an art. Only recently, with the modeling work of such researchers as Yogesh Jaluria of Rutgers University, has it progressed toward a precise and predictable science. Using supercomputers at the University of Kentucky and Boston University, both Alliance Partners for Advanced Computational Services, Jaluria and his colleagues are establishing some of the first practicable guidelines for fiber drawing based on numerical modeling.



Typical draw tower used in the production of optical fibers.



Experimental furnace arrangement at Rutgers' Fiber Optic Materials Research Program.

The challenges of popularity

These guidelines haven't come too soon. The demand for optical glass fiber increases daily. By one account, requested telephone network capacity doubles every four months. Optical fibers gird the globe in a telecommunications network hundreds of thousands of miles long and are also increasingly used in medicine, engineering, navigation, and a host of other fields. Manufacturers respond to this demand with ever larger preforms and faster production speeds. A decade ago glass preforms averaged two centimeters in diameter and were drawn at speeds of three meters per second. Today preforms are climbing to 15 centimeters in diameter, and draw speeds are approaching 20 meters per second.

The burdens these changes place on the glass are not trivial. "Glass is a very unforgiving material," Jaluria says. "The bigger the preform and the higher the draw speed, the harder it is to obtain a uniform temperature distribution." Too often the result is a fiber with structural defects or poor transmission qualities.

Jaluria's ultimate goal is to determine optimal and feasible draw conditions for a range of draw speeds and preform sizes. Using the University of Kentucky's HP-Convex Exemplar and Boston University's SGI Origin2000, he is determining high-speed drawing guidelines for furnace length and heating-element arrangement—critical variables for maintaining an even temperature distribution in the glass. He tests the results at Rutgers' Fiber Optic Materials Research Program, where he maintains an experimental drawing facility with his colleague Costas Polymeropoulos.

Zoning and gridding

As the preform is heated and pulled, it dramatically narrows to a diameter of about 125 microns in the 10- to 15-centimeter-long "neck-down region" where the fiber emerges from the preform. The viscosity of the glass also changes radically—by several orders of magnitude—along the length of the preform and fiber.

"Even small temperature differences translate into huge differences in viscosity," Jaluria says. "It is a highly nonlinear system." Complicating all this is the cylindrical shape of the glass, the presence of inert purge gases in the furnace, and the continuous tension applied to the fiber and preform. To get a handle on the complexities, Jaluria and his colleagues use a simulation model that incorporates several aspects of heat transfer—heat transfer between the fiber and the furnace gases, convective heat transfer at the furnace walls, the radiative transfer between the furnace wall and the preform, and heat transfer in the glass itself. A quick look at just one of those aspects—radiative heat transfer—suggests the complexities the team must incorporate in their simulations.

"Very little information exists in the open literature about the radiative properties of glass, especially at high temperature," Jaluria says. Because it is transparent, glass radiates throughout its entire volume and must be modeled accordingly.

With the speed and memory of a supercomputer at hand, Jaluria and his colleagues developed a special zonal method to model the radiative properties of the glass. The volume of the preform and fiber is divided into a large number of finite zones, each of which absorbs and emits radiation. From those zones energy transport can be calculated as a function of location. Jaluria explains: "By considering two zones within the glass, it is possible to calculate the radiation between the two. This is summed over all volumes to get energy in and out of each volume."

Meanwhile, the model also calculates the viscosity of the glass. Using a strongly nonuniform gridding strategy, more grid points are placed in areas with larger temperature and viscosity variations, such as the neck-down region. For a preform 10 centimeters in diameter moving at 20 meters per second, about 100 radial points through the glass cylinder and about 300 points along its axis are used. A coordinate transformation acting in the radial direction maps the complicated neck-down region to a more easily modeled cylinder. A standard procedure in modeling complicated shapes, coordinate transformation is simply a change in the coordinate scale.

A final computing component links the separate schemes. Kinetic equations are added to predict fiber defects as functions of furnace geometry and temperature profile, preform size, and draw speed. While a complete simulation can take up to 12 hours on a single Exemplar processor, most runs use 12 or 16 processors. Depending on the operating conditions and simplifications used, multiple processors significantly reduce the time required to complete a simulation.

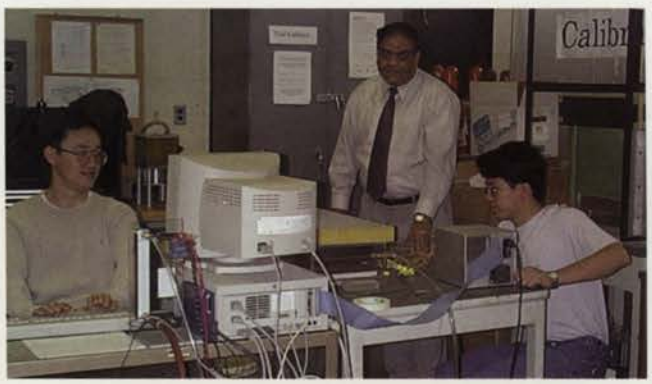
Coping with coating

As the team continues to develop guidelines for furnace configurations, they have also started to develop models of fiber coating. This effort involves a set of problems and variables quite different from those associated with the furnace in fiber drawing and requires an entirely new program.

A typical coating applicator is only two to five centimeters long. A fiber coming through at two to three meters per second has plenty of time to be adequately coated. At higher draw speeds, however, the fiber moves too fast for the coating to be uniformly applied. Too often, the interface between the glass and plastic breaks or stretches and bubbles form. This is huge problem for the industry, Jaluria says. "Most high-speed drawing today is constrained by the lack of good coating."

During the coating process, a fiber is typically drawn though an open cup or pressurized reservoir of molten plastic. As the fiber moves, the viscous shear results in a circulatory motion within the fluid. At the same time, a balance between surface tension, viscosity, gravity, and pressure results in a meniscus, or slight rise of liquid, forming at the cup entrance. Another meniscus, which forms as the fiber exits the cup though a die, affects the thickness and quality of the coating.

In order to simulate the fiber moving through this flow field, Jaluria's team must model both the upper and lower menisci, then couple these two submodels to another model of the main flow within the applicator. Then the glass' fluid properties—viscosity and temperature—can be added. The final simulation model should eventually be able to predict optimal applicator geometries, coating materials, and coating temperatures for an upper range of fiber drawing speeds.



Xu Cheng, Yogesh Jaluria, and Qinghua Wang. Rutgers University.

Though those in the highly competitive fiber optics industry give up no secrets, it's clear that they are paying close attention to Jaluria's work. Peter Simpkins, a distinguished member of the technical staff at Bell Laboratories, Lucent Technologies, acknowledges that the field needs more fundamental understanding. "A lot of the issues that Jaluria addresses, like defects in coating, are highly nonlinear and not amenable to analytical solutions. They require skillful numerical modeling." John Abbot, an engineering associate at Corning Incorporated, one of the world's leading fiber companies, echoes Simpkins. "Jaluria is doing some excellent work. There have been specific examples where his results have warranted a revisit of our assumptions."

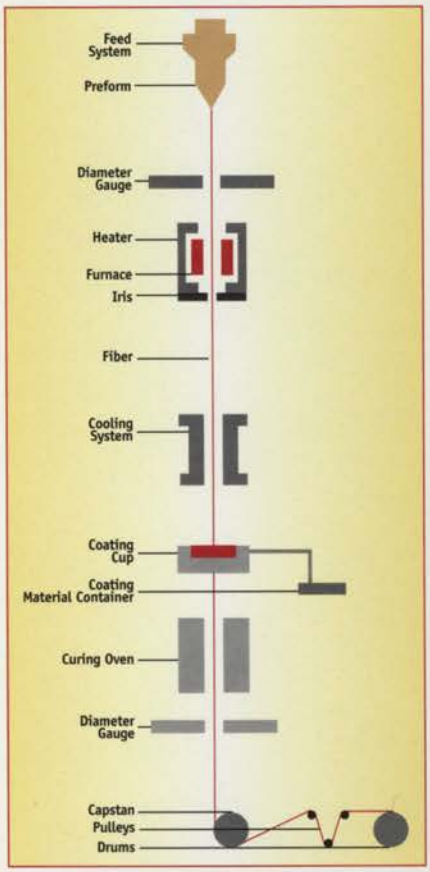


Illustration of drawing optical fibers. The Rutgers research team models the furnace length, heating-element arrangement, and the coating process in order to establish practicable guidelines for manufacturing optical fibers.

This research is supported by the National Science Foundation and the Fiber Optic Materials Research Program at Rutgers University.

http://access.ncsa.uiuc.edu/CoverStories/Optics/

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GET SMART

by J. William Bell

A UNIQUE METHOD OF MANAGING THE AIRFLOW THROUGH ENGINES MAY DRAMATICALLY IMPROVE THE PERFORMANCE OF SUPERSONIC JETS.

As Chuck Yeager and his cohorts pushed toward the first supersonic flight in 1947, nerves weren't the only bumps they encountered. Shock waves buffeted the Bell X-1, their plane of choice, on its way to Mach 1. As Tom Wolfe described it in *The Right Stuff*: "Evil and baffling things happened in the transonic zone. [Pilots reported] that the controls would lock or 'freeze' or even alter their normal function."

Supersonic aircraft have come a long way since the days of the X-1, but the aerodynamic disturbances in pressure and airflow that are caused by shock waves still hold sway over aircraft design. Most conventional supersonic designs, for example, rely on jet engines that suck in the surrounding air to oxidize their fuel. Shock waves are an integral, unavoidable, and confounding part of this process.

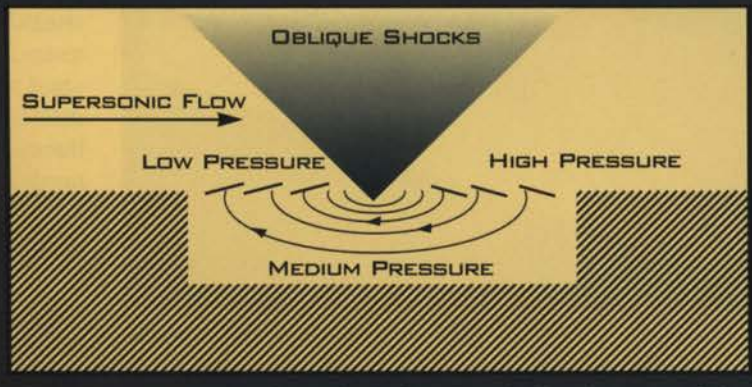
Using NCSA's SGI Origin2000 supercomputer, researchers from the University of Illinois at Urbana-Champaign, NASA, Boeing, and the United States Air Force are developing an innovative solution for the problems posed by shock waves. Known as Smart Mesoflaps for Aeroelastic Transpiration (SMAT), this system may someday greatly reduce the performance costs associated with managing airflow through supersonic engines.

Hitting the boundary

For a supersonic jet engine to operate properly, air must flow through it at subsonic speeds. Today's aircraft designs rely on, of all things, shock waves to slow the air. These shock waves are created deliberately in an inlet at the front of the engine. Even as they prove beneficial, however, the shock waves cause problems.

When air hits the surfaces of an aircraft, the velocity of the air is reduced to zero. A stream of air, known as the boundary layer, is the flow in which the velocity changes to zero. In jet engines, the smaller this layer, the better. But shock waves created to slow the air cause the flow to separate and thicken by as much as four times.

"Engines want no boundary layer at all, but that's impossible. All you can do is prevent them from becoming too large," says Eric Loth, a U of I associate professor of aeronautical and astronautical engineering.



The SMAT system. At supersonic speeds, the flaps divert the flow downstream of the shocks and reinsert the flow upstream. The flaps on one side of the shock wave bend down and allow air to flow into the cavity, while the flaps on the other side bend up and allow air to flow through the cavity and out. By wicking away air, the flaps reduce the size of the layer.

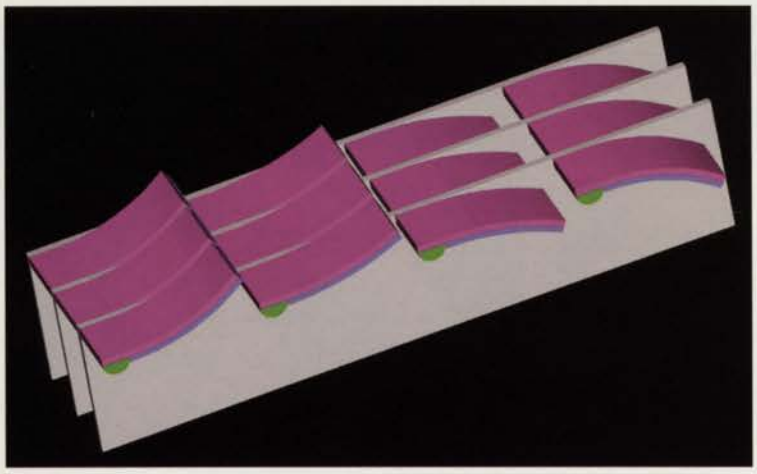
To manage the layer's size, conventional designs place a porous plate along the surface of the inlet where the shock waves hit the boundary layer. Pumps bleed air out of the layer through the plate, and a system of ducts dumps it offboard. Though this system works well, reducing the boundary layer to a size that the engine can handle, it adds weight to the craft and creates significant drag.

"Current state-of-the-art systems waste a lot of energy and weight," Loth says. "If it weighs 10 percent more, you have to make that up somewhere, and you can't fly as fast or as far. Anything above Mach 2 needs a boundary layer bleed, and the cost really starts to be a big problem at Mach 3." At Mach 3, the system may need to bleed away as much as 15 percent of the airflow ducted to the engines.

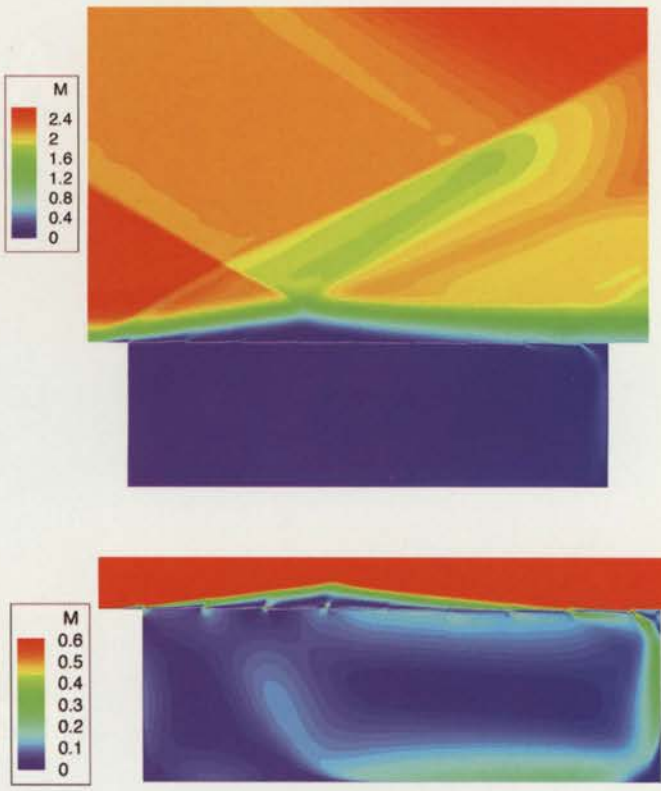
Keeping it simple

The SMAT system is simple. Instead of using a porous plate, the surfaces of the inlet where the shock waves hit the boundary layer are covered with a matrix of flaps that measure one centimeter by one centimeter. Researchers are currently studying flaps of various materials, including aluminum. Each flap is held at one end by a spar. The flap can deform up or down, bending like a reed in a hurricane. A hollow cavity runs beneath each set of flaps.

A shock wave causes a zone of low pressure on one side of its point of impact and a zone of high pressure on the other. As a result, the flaps on one side of the shock wave bend down and allow air to flow into the cavity, while the flaps on the other side bend up and allow air to flow through the cavity and out. By wicking away air, the flaps reduce the size of the layer.



Visualization of SMAT design.



Mach contours, or differences in airspeed, in a simulated SMAT system. The upper image shows the entire system, while the lower image shows increased resolution in the cavity region.

"The flaps take the flow off downstream of the shocks and then reinsert that same flow upstream, effectively recycling the air so it won't be wasted," says Loth. And the SMAT system works without any pumps or ducts. Some estimates expect the weight and cost savings to be as much as 18 percent for a plane designed to travel at Mach 3.5.

At subsonic speeds, where there are no shock waves and thus no pressure differences, the aluminum flaps lie straight. In effect, they turn themselves on only when needed. Further research will allow for even smarter flaps, though. The SMAT research team is studying thermally activated flaps made of a smart material called nitinol, a nickel-titanium alloy. The stiffness—and thus the amount they deform—of the thermally activated flaps can be changed on the fly by running an electrical current through them.

Creating a flap

The team is currently modeling their designs using NCSA's SGI Origin2000. The model considers the flaps and the airflow around them by using both a fluid dynamics code, to calculate the air's behavior, and a solids code, to calculate the flaps' behavior. The two codes are coupled, meaning that they run simultaneously and constantly pass data back and forth to one another. Variables such as flap thickness, spar shape, and wind speed can be altered to study the flaps and optimize them for peak performance.

The researchers create a mesh of about 90,000 nodes, or discrete points at which the system is modeled. The part of the mesh modeled by the fluid dynamics code is structured in the boundary layer and unstructured in the remainder of the fluid domain. The solids mesh is fully unstructured, allowing appropriate calculations in areas that require more precision, such as the rounded corners of the flaps. The unstructured mesh also prevents areas that require less precision, such as the air furthest away from the flaps, from eating up too much computing time.

The fluids code, due to its larger size and complexity, currently dominates use of the computational resources. "The bulk of the computation is in the fluid domain—about 95 percent of the CPU time is devoted to the fluids," says Philippe Geubelle, an assistant professor of aeronautical and astronautical engineering at the U of I. "This will shift back toward the solids once we begin to look at the smart materials instead of modeling the behavior of simple aluminum flaps."

The modeling of smart materials will also increase the computational resources required for the simulations. Recent efforts to parallelize the fluids portion of the code will help the model keep up. "It used to take a couple of days to run a single solution. We're getting that down to a couple of hours," according to Scot Breitenfeld, a research scientist on the project.

And a smarter code, in the end, means smarter flaps.

This research is supported by the Defense Advanced Research Projects Agency and the Air Force Office of Scientific Research.

http://access.ncsa.uiuc.edu/CoverStories/SMAT/

For further information:

http://ssm7.aae.uiuc.edu/smat/
http://www.aae.uiuc.edu/Profs/loth.html/
http://ssm7.aae.uiuc.edu/PHG_GROUP/

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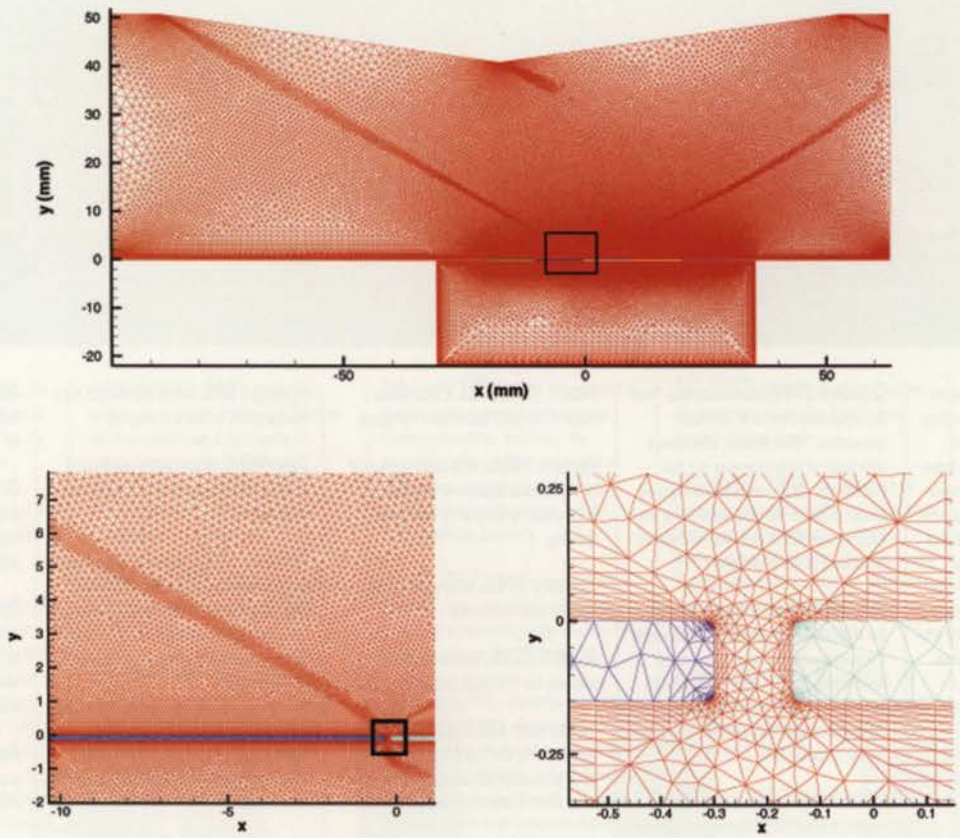


Element mesh in the coupled simulations, shown at different scales. A mesh of about 90,000 nodes is considered in the model. In parts of the fluids code, the grid created by these points is structured, meaning that all the cells are the same size. In the solids code and the rest of the fluids code, the grid is unstructured.

The achievements of the National Center for Supercomputing Applications and the National Computational Science Alliance are, in no small part, the achievements of their founding director, Larry Smarr. In March 2000, Smarr moved into the new position of Alliance Strategic Advisor and stepped down as director of the Alliance and NCSA. What better way to illustrate his unique vision than with a look at the milestones that have studded his career and the history of the center?

TWO DECADES AT THE LEADING EDGE

Smarr in the early 1980s explaining his work at the Max Planck Institute.

NCSA's first staff photo, Fall 1987.

Smarr with high-performance computing pioneer Seymour Cray in the late 1980s.

Smarr with Jim Bottum, Karl-Heinz Winkler, and Mike Norman.

Smarr working on the "black proposal," the first supercomputing center proposal to NSF in 1983.

Smarr and the astrophysics gang in 1987 with the Cray X-MP.

Smarr's wife Janet with sons Benjamin and Joseph and the Cray X-MP in 1986.

Smarr with sons Joseph and Benjamin at Fahrney Medal awards ceremony.

Jim Wilson, Smarr's computational astrophysics "guru" from Lawrence Livermore National Laboratory, with the Cray-2 in 1989.

Summer 1979. After completing his PhD in 1975 and getting top-secret nuclear weapons clearance in order to research colliding black holes using American supercomputing systems at Lawrence Livermore National Laboratory, Smarr begins computing at the Max Planck Institute for Physics and Astrophysics in Munich, Germany, studying the dynamics of extragalactic gas jets on a Cray-1 supercomputer. "My eyes were really opened when [I was asked] why it was that so many American researchers had to come to Europe to work on U. S.-built supercomputers," he says.

Fall 1979. Smarr joins University of Illinois faculty with an appointment in the astronomy and physics departments.

1980. Smarr, Bob Wilhelmson, Dick Crutcher, and Bob Haber create the Vax and Image Processing Center (VIP) in the U of I's Astronomy Building (now the Advanced Computation Building), a precursor to NCSA.

October 1982. Smarr completes "The Supercomputer Famine in American Universities." Mike Norman, who worked with Smarr at both Livermore and Max Planck, says "It was really an underground protest, a call in the wilderness. Larry was then, as now, full of new ideas and worlds to conquer. It was infectious."

Fall 1983. Smarr writes a proposal to the National Science Foundation requesting a supercomputer for the U of I campus. Ralph Simmons, then head of the physics department, travels with Smarr to hand deliver the unsolicited proposal, addressed simply "Director, NSF."

1984. NSF establishes its Office for Advanced Scientific Computing (OASC) and initiates a nationwide competition for national supercomputing center proposals.

1984. *Esquire* magazine features Smarr in a "Register of Outstanding Americans under Age 40."

March 1985. NCSA is established under a five-year, $20 million NSF grant.

August 1985. NCSA takes delivery of its first supercomputer—a Cray X-MP/24. It is housed in the U of I's Astronomy Building.

January 1986. NCSA opens to the national user community.

August 1986. Eastman Kodak becomes the first NCSA Industrial Partner.

November 1986. The Cray X-MP/24 is replaced by the Cray X-MP/48. With the jump in capacity and power, NCSA is delivering about 2,000 CPU-hours per month.

April 1987. A formal scientific visualization program begins at NCSA.

Fall 1987. NCSA Telnet, the center's first major software release, makes its debut. By 1991 it has over 100,000 users.

Spring 1988. NCSA's Hierarchical Data Format (HDF) software is released.

May 1988. NCSA's 100th employee is hired. Within a year, number 200 is added to the roster.

October 1988. The Cray-2 supercomputer is installed. It has four processors and can perform about 1.7 billion calculations per second. At the time of its installation, about 3,000 researchers are associated with NCSA.

April 1989. NCSA's Renaissance Experimental Laboratory is established with a grant of 25 SGI IRIS workstations from Jim Clark.

August 1989. The Thinking Machine CM-2 supercomputer, NCSA's first foray into massively parallel computing, is installed.

1990. Smarr is awarded the Franklin Institute's Delmer S. Fahrney Gold Medal for Leadership in Science or Technology.

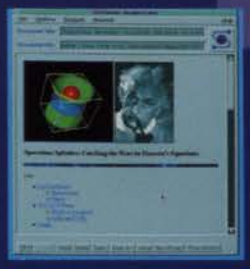
October 1990. Cray Y-MP supercomputer replaces the Cray X-MP vector computer. The new multiprocessor system has eight times the memory of the X-MP.

Spring 1991. *Fortune* magazine highlights Smarr as one of "25 Who Help the U.S. Win." The issue focuses on innovators who are helping revitalize American industry.

April 1992. A Thinking Machine CM-5 supercomputer is installed. It has 512 nodes and eight gigabytes of memory.

November 1992. Smarr delivers the keynote address at Supercomputing '92, "Grand Challenges! Voyages of Discovery in the 1990s."

NCSA



Early version of NCSA Mosaic.

Smarr with then-Senator Al Gore during Gore's first presidential run in 1988.

Smarr with the SGI Origin2000.

Smarr and Govenor George Ryan at the announcement of the VentureTECH program.

Smarr and corporate representatives of the Industrial Partners program (now the Private Sector Program), in Summer 1988 in front of the Cray X-MP/48.

Visualization from "Study of a Numerically Modeled Severe Storm" created in 1989 by an NCSA research and visualization team led by Bob Wilhelmson and Matt Arrott.

NSFNet traffic in December 1994, just before the high-speed network was decommissioned.

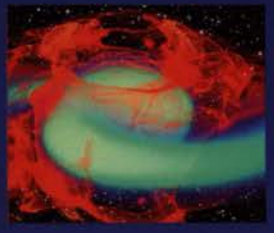
Prototyping in NCSA's CAVE virtual environment by an industrial partner from Caterpillar.

Smarr with President Clinton in 1998.

(Photo courtesy of Bill Wiegand/UI News Bureau)

Propagating jet visualization created in 1987 by an NCSA Renaissance Team led by Mike Norman and Donna Cox.

Animation showing the evolution of a distorted single black hole system created in 1992 by an NCSA research team that included Smarr.



Two neutron stars in a binary system inspiraling into one another. This visualization was created by Alliance partners at Washington University in St. Louis and the Max Planck Institute for Gravitational physics (Albert Einstein Institute) in Potsdam, Germany, using NCSA's SGI Origin2000.

Smarr with PITAC and Vice President Al Gore in 1998.

February 1993. Smarr challenges the Chamber of Commerce to build high-speed networks in Champaign County. CCNet, the Champaign County Network, is born.

Spring 1993. *Supercomputing and the Transformation of Science*, by Smarr and William J. Kaufmann III, is released.

April 1993. NCSA Mosaic, the first user friendly Web browser, is released. At the time, there are about 200 World Wide Web servers in the world. By 1994 Mosaic has several million users and has effectively given birth to the dot.com industry that is projected to be worth $1 trillion by 2001.

March 1994. Smarr is elected fellow of the American Academy of Arts and Sciences.

NCSA™

April-October 1994. Three new systems are installed. The Convex Exemplar has 8 processors and a peak speed of 1.6 gigaflops. The SGI Challenge has 32 processors, and its cousin, the SGI PowerChallenge, has 16 processors and a peak speed of 4.6 gigaflops.

February 1995. Smarr is inducted as a member of the National Academy of Engineering.

October 1996. A 128-processor SGI Origin2000 supercomputer is installed. Its peak speed is about 50 gigaflops. Today NCSA's Origin array has 1,528 processors and is the heart of the Alliance's supercomputing resources.

February 1997. Smarr is appointed to the President's Information Technology Advisory Committee (originally the Presidential Advisory Committee on High Performance Computing and Communications, Information Technology, and the Next Generation Internet).

March 1997. NSF announces that the National Computational Science Alliance, with NCSA as its leading-edge site, has been selected as one of two PACI sites.

October 1997. The Alliance becomes a reality. A partnership of some 50 institutions across the country, it is charged with prototyping the National Technology Grid. The Alliance is funded through a five-year NSF grant. "This is an unprecedented effort in which the whole is truly greater than the sum of its parts," Smarr says.

ALLIANCE

Fall 1998. Smarr is given the Chamber of Commerce's Champaign County Most Valuable Citizen Award.

November 1998. The Alliance's NT Supercluster debuts at SC98. Using the High Performance Virtual Machine software, developed by Andrew Chien, the cluster consists of almost 200 workstation processors. Today the Alliance supercluster has over 400 processors.

November 1998. Smarr, NCSA, the U of I, and Champaign-Urbana are profiled in a *Newsweek* magazine cover story, "The Hottest Tech Cities."

October 1999. More than one million hours are provided to 736 users on the Alliance's SGI Origin2000 array at NCSA. This record marks the first time that more than one million hours have ever been used in a single month on any NSF-supported high-performance computing system.

February 2000. VentureTECH—a program that includes $30 million in funding for a new building to house NCSA—is announced by the state of Illinois.

March 2000. Smarr announces that he is stepping down as director of NCSA and the Alliance and becomes the Alliance strategic advisor. At the time of the leadership change, the Alliance's five Partners for Advanced Computational Services are providing well over a million hours of supercomputing time a month to researchers around the globe.

May 2000. Smarr accepts a position on the computer science and engineering faculty at the University of California, San Diego. Relying on the national distributed computing network he has helped advance for over 15 years, he remains Alliance strategic advisor.

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