Who we are
The National Center for Supercomputing Applications (NCSA) opened its doors in January 1986. NCSA earned and maintains an international reputation in high-performance computing and networking and in developing innovative software applications—like NCSA Mosaic, the first readily-available graphical Web browser. Since 1997, NCSA has been the leading-edge site for the National Computational Science Alliance (Alliance), one of two partnerships of the NSF’s Partnerships for Advanced Computational Infrastructure program. The Alliance is a partnership among about 60 academic, government, and industrial organizations from across the United States.

In August 2001, NCSA---as part of a four-institution team---was tapped by the National Science Foundation to build one of the world’s first computational grids and put it to use. It will be the most comprehensive grid yet deployed for open scientific research, spanning the country and providing the backbone from which tomorrow’s global grid can grow. With software developed to make it all work in concert, this TeraGrid will offer the fastest unclassified supercomputers as well as an unparalleled array of visualization tools, sensors and instruments, and mass storage devices. These resources will be linked via a network four times faster than today’s fastest.

Major support for NCSA and the Alliance is provided by 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
Six 1,3-cyclohexanedione molecules bridged by hydrogen bonds (white) between neighboring oxygens (red). They surround a single benzene ring (center) in a nearly two-dimensional plane. This simulation was created by researchers at Syracuse University using NCSA’s IBM p690 system and visualized with the Visual Molecular Dynamics software.
Coal-burning power plants spew toxic mercury into the atmosphere, but a researcher at the University of Arizona aims to better understand mercury reactions in order to develop effective emission controls.
Toward computing crystal forms

by Katherine A. Caponi

A team of scientists from Syracuse University uses periodic quantum chemical calculations to figure the limits of molecular quantum theory in describing molecular crystal properties.

Six 1,3-Cyclohexanadione molecules bridged by hydrogen bonds (white) between neighboring oxygens (red). They surround a single benzene ring (center) in a nearly two-dimensional plane. Visualizations produced with Visual Molecular Dynamics (VMD).
Chemists make many compounds that can be prepared in crystal form, three-dimensional solids arranged in a repeating pattern. The physical and chemical properties of those compounds, or crystalline solids, depend on two factors: the type of molecules that they are composed of and the arrangement of those molecules.

Unfortunately, there is no accurate method for predicting the arrangement that those molecules will take, which currently makes it impossible for scientists to design crystalline solids with useful traits. This difficulty must be overcome to make synthetic organic chemistry a practical tool for materials engineering.

One much-discussed example of this problem is a type of crystal that converts laser light from one color to another. For the crystalline solid to have that ability, the arrangement of molecules within the smallest repeating unit must be asymmetrical. However, there are many possible ways the molecules may arrange themselves when forming crystals. Scientists are trying to find a way to predict what conditions must be present in order for a particular arrangement to occur so that they can produce crystals with that quality in the lab.

Bruce Hudson and a team of scientists from Syracuse University are trying to break down such barriers. Because computational methods for studying crystals have only recently become widely available, chemists have not previously studied them with these methods. The Syracuse team uses NCSA's IBM p690 and now-retired SGI Origin2000 and other supercomputers to evaluate the accuracy of solid-state quantum chemical theory in comparison to experimental methods that investigate crystals and the quantum chemical methods commonly employed to examine isolated molecules.

Hydrocarbons

The project has several goals. The first is to see how reliable current computational methods are for certain molecules that have very weak intermolecular bonds, such as hydrocarbons. Hydrocarbons are simple compounds that contain only hydrogen and carbon. Since these molecules have weak interactions that stabilize their orientations, many of them, when surrounded by other molecules just like them, form crystals that retain the arrangement of atoms that they had as isolated molecules.

In those cases, scientists usually think of the crystalline solid as composed of molecular building blocks linked together. If the molecules don't change their structure when surrounded by other like molecules, scientists treat them as an oriented gas, a collection of molecules with fixed relative orientation, spacing, and properties. Because the arrangement of the individual molecules is not altered by strong chemical interactions with surrounding molecules, their traits will be expressed in the whole crystalline solid. Scientists can then predict the properties of the crystalline solid based on the traits of the individual building blocks by using quantum chemical methods called oriented gas approximations.

On the other hand, some molecules—even some hydrocarbons—do change their structure when surrounded with other like molecules. The properties of those crystalline solids are different than the properties of the individual molecules, and oriented gas approximations fail. In those cases, Hudson says, "the assembly of the crystalline solid with the desired properties may not be as simple as the independent packing of the building blocks but rather a cooperative process of different chemical reactions working together when each molecule interacts with the ones surrounding it."

The team found that the best way to look for failure in quantum theoretical methods like the oriented gas approximation was to experimentally test the vibrations in the molecular structure. The bonds between atoms in a molecule are a lot like springs. By exciting a molecule with energy, you can learn a lot about its structure and the strength of its bonds based on the way those springs vibrate.

Hudson's team did this by shooting a beam of neutrons into a highly symmetric hydrocarbon molecule called dodecahedrane, using an experimental method called inelastic neutron scattering (INS) spectroscopy. The intensity with which the neutrons scattered upon interaction with the nuclei of particular molecules was computed from knowledge of which atoms were moving like they normally would absent the beam of neutrons. The team then compared the results of this experimental method on both isolated crystal molecules and a sample of the crystalline solid.
Damian Allis, a graduate student working on the project, says, "Molecules feel the same physical constraints from crystal packing that someone on the subway would from other passengers. If you take that person on the subway and put them on a bumpy track, where they move and how far they move will be determined by where everyone else is. Their restricted motion on a crowded subway will look very different to an observer than their motion on a bumpy track if the car was empty of other people. We see those differences when comparing vibrational spectra of isolated molecules with crystalline solids and, therefore, learn about the environment of the molecule in the crystal."

The team found that quantum theoretical methods currently used by scientists described the vibrations observed in the isolated molecule fairly well. However, when looked at in detail, the methods used for isolated molecules did not accurately describe the molecular structure of many molecules forming a solid, showing that the arrangement of dodecahedron atoms relative to each other changes slightly when surrounded by other like molecules. New quantum chemical methods applicable to solids correctly predict this molecular deformation.

**Hydrogen-bonded crystals**

Another aspect of the team's project was to study the accuracy of quantum theoretical methods when dealing with crystals that contain hydrogen bonds. "Hydrogen bonding is one of the major bonding mechanisms that lead to large-scale crystal architectures," says Hudson. "In chemistry, hydrogen bonding is like molecular Velcro—or some type of rearrangeable glue. It forms bonds that can come apart at room temperature because they have an energy that is not much larger than thermal energy."

Because hydrogen bonds can form and come apart easily, they are quite forgiving with respect to the orientation of the atoms forming them. That the bonds form easily is useful in the engineering of crystals because the hydrogen-bonding molecules will self-assemble rather than requiring a specific reaction to make each attachment between molecules. That the bonds come apart easily is also useful because they are just weak enough that when one forms incorrectly, there is a good chance that it will be jostled apart by other molecules and reformed correctly.

However, the fact that hydrogen bonds act as molecular Velcro instead of superglue also has a downside: polymorphism. Polymorphism is a characteristic of many molecular compounds whereby they can form distinct crystals with more than one arrangement because of the forgiving nature of hydrogen bonds.

While organic chemists can produce many molecular species, they cannot yet predict which polymorphic arrangement a crystal will form. In fact, the molecules of the compound may convert from one arrangement to another in time, and one polymorphic form may disappear in favor of another form with minor changes in crystallization conditions. In some cases, different polymorphic arrangements may coexist within a batch of crystals all grown from the same solution.
The arrangement of the molecules in these polymorphic crystals will cause variances in the traits that they display—such as the rate at which the substance dissolves. This results in differences in drug diffusion rates and is therefore a problem for the pharmaceutical industry.

To learn more about the molecular arrangements of hydrogen-bonded crystals, Hudson's team performed INS spectroscopy experiments on crystalline 1,3-cyclohexanedione. INS spectroscopy proved a particularly valuable method for testing hydrogen-bonded crystals because hydrogen atoms are known to scatter the neutrons much more strongly than other atoms. This feature made it simple to find where the hydrogen bonds were located in the structure of the sample material and therefore easier to pinpoint the arrangement of the whole molecule.

The team applied standard quantum mechanical methods to both individual molecules and "cluster" models of the crystalline solid to examine how being surrounded by others of the same molecule would affect the arrangement of the atoms in the crystal-forming molecules. The major point of interest is how the molecular structure changes as the cluster chain length used to model the crystal becomes longer. From these computations, they found that hydrogen bonding between molecular units results in significant changes in molecular structure with increasing chain length. This effect is cooperative, meaning that the effect observed on bonding one molecule to another depends on whether either of those two molecules is already bonded to a third. The hydrogen bonding process is not simply additive.

The team then compared its experimental results and the known crystal structure with results from new periodic quantum theoretical computations. This assessment showed that the full three-dimensional model corresponds well to what is extrapolated for the finite chain cluster and also to what is observed for the crystal.

The vibrational spectra computed using the same methods agree very well with the observed INS spectrum, meaning that the solid-state calculations are providing a reliable description of the energy of the solid. Further to the point, the vibrational spectrum measured or calculated at a very low frequency is important in establishing the relative thermodynamic stability of two crystals, which is the first step in understanding and controlling polymorphism.

The team hopes that someday its findings will help scientists use the theoretical methods tested on NCSA supercomputers to predict what arrangement crystals will make. "One of our ultimate objectives is to be able to compute the relative free energies of crystals so as to be able to predict the relative stability of observed or proposed crystalline structures. This may permit crystal engineering in a proactive sense," Hudson states. Instead of using quantum chemistry merely as a way of describing the arrangements of the molecules in a lab, scientists may be able to predict what arrangements will form and even produce compounds with specific molecular arrangements and thus specific properties.

This project is supported by the National Science Foundation, the U.S. Department of Energy, and Syracuse University.

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For further information:
[http://hudsonlab.syr.edu/](http://hudsonlab.syr.edu/)

Team members
- Damian Allis
- Jenn Ciezał
- Hegui Hu
- Bruce Hudson
- Tim Jenkins
- Mark Kosmowski
- Yanmei Lan
- Chris Middleton

Hudson's team of students at Syracuse University.
TOIL AND BUBBLE

Hydrosystems research on NCSA’s Titan cluster aids the U.S. Army Corps of Engineers as it chooses aeration systems for a pair of massive reservoirs.

by
J. William Bell
About 25 million people visited Chicago’s World Columbian Exposition in 1893. They streamed in from around the world, arriving by ship, locomotive, and “L” train. Because of the city’s dubious drinking water and fear of a dysentery outbreak, their water was piped in from a Wisconsin spring.

Chicago still faces its share of water woes more than a century later. The Metropolitan Water Reclamation District of Greater Chicago serves more than three million people with a combined sewer system. Rain water and the sanitary sewer share a single set of pipes, tunnels, reservoirs, and treatment plants. Though the facilities can treat about two billion gallons of water a day, a single large rainstorm can produce more than five billion gallons before a single sink is turned on or toilet is flushed, according to data from the water reclamation district.

On the wettest days, the treatment plants can’t keep up. Sewage is diverted into the area’s waterways, and the Environmental Protection Agency levies fines. People go home to flooded basements. To avoid these problems, the U.S. Army Corps of Engineers and the water reclamation district are building a pair of reservoirs that will bring the district’s total storage capacity to 15.6 billion gallons. (A third reservoir, with a capacity of more than 325 million gallons, is already complete.)

The plan certainly holds water. But it’s not without drawbacks, especially in a metropolis with an average of 12,000 people per square mile. “The reservoirs are in residential areas,” says Heather Henneman, a Corps of Engineers hydrologist working on the project. “Can’t be helped. Everything’s populated in Chicago.”

The longer the water sits in open reservoirs, the more it begins to smell. Aeration systems, not unlike the one in your aquarium, can be used to oxygenate standing water and reduce odor. But an 87-acre reservoir is no mere fish tank.

“Aeration at this scale is not common,” says Fabián Bombardelli.

As part of his PhD work at the University of Illinois at Urbana-Champaign, Bombardelli used NCSA’s Titan cluster to model the plumes of air bubbles produced by aeration systems. The models are the first of their kind to consider not only the physics of aeration but also the amount of oxygen consumed by organic particles in the wastewater. They are used in conjunction with an existing Corps of Engineers model to help the Corps make decisions about the final design of the reservoirs.

Bombardelli worked with Marcelo García, the Chester and Helen Siess Professor of Civil and Environmental Engineering at the University of Illinois, and Professor Gustavo Buscaglia of the Instituto Balseiro and Centro Atómico Bariloche in Argentina. An early description of the model can be found in the November 2002 edition of the International Journal of Multiphase Flow.

An aerobic exercise

Given the opportunity, organic matter in a reservoir will begin to break down via aerobic reactions, which generate carbon dioxide, carbonates, and other innocuous chemical species. In the absence of oxygen, anaerobic reactions take place. Products such as methane and sulfide hydrogen—which, in sufficient amounts, are sure to annoy the neighbors—result.

Aeration is a simple way to prevent anaerobic reactions. Just blow air bubbles into the reservoir. The bubbles carry a high concentration of oxygen. The water that surrounds them carries a lower concentration. The process of mass transfer forces oxygen out of the bubbles and into the water. Provide enough oxygen, and you get nothing but aerobic reactions.
The Corps of Engineers is comparing two possible means of aeration, one submerged and one that sits on the surface. Bombardelli's models help the Corps hash out the fine points of a submerged system.

Under their current scheme, the 7.3-billion-gallon McCook reservoir would include a total of 2,140 submerged diffusers, each blasting between 16 and 23 cubic feet of air per minute into the water. The Corps of Engineers has to position the diffusers, decide when to turn them on and off, and reckon how the resulting plumes of bubbles will interact. They also want to know how efficiently the system will operate when the reservoir is filled to different levels. This figuring currently relies on relatively small-scale experiments, historical data, and educated guesswork.

"Most mass transfer experiments are limited to the depth of storage tanks at sewage treatment plants," which are typically less than half the depth of the Chicago reservoirs, according to Henneman. With the computer models, however, the Corps of Engineers can analyze various design configurations in greater detail.

"They are asking very ambitious questions," says Bombardelli, who is now an assistant professor of civil and environmental engineering at the University of California at Davis. By the end of the year, the Corps of Engineers intends to use answers to those questions to pick which type of aeration system it will use in the reservoirs.

Losing some bulk

Early bubble models in environmental engineering were not very sophisticated affairs. They showed only the bulk parameters of the plumes and only on a vertical axis. "You saw how the plume spread and how fast but comparatively little about the bubbles themselves," Bombardelli says.

His new simulations, however, rely on a set of submodels to create a much more complicated picture. After months of experimenting with different turbulence models and comparing the quality and efficiency of their results to experimental data, Bombardelli can now create some of the most-detailed, highest-resolution views of bubble plumes available. It takes about seven hours of computing time on 20 processors of NCSA's Titan cluster to simulate nine seconds of action.

The models track the buoyancy, drag, and turbulent dispersion of bubbles in three dimensions as the bubbles collide, break apart, and coalesce. The mass transfer of oxygen and nitrogen out of the bubbles is also replicated. Finally, a biochemical oxygen demand model simulates how much oxygen is consumed by organic material in the water, how this demand varies in different parts of the plume, and how it changes over time.

All of these features are critical to understanding the rate and degree of oxygenation caused by the aeration process, and all give the Corps of Engineers information that it can't easily derive from experiment.
Snapshots of velocity magnitude in the aeration simulations.

"And [computational models] are odorless, which is an accomplishment in this field," says the University of Illinois' Marcelo Garcia. Joking aside, he is pleased with the way the team has been able to build a new, powerful tool by combining knowledge from a variety of fields. "We've borrowed from chemical engineering, nuclear engineering, computer science, and mechanical engineering and brought them all into environmental engineering."

This research is supported by the U.S. Army Corps of Engineers.

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For further information:
http://cee.uiuc.edu/research/mhgarcia/index.htm
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http://www.lrc.usace.army.mil/

Team members
Fabian Bombardelli
Gustavo Buscaglia
Marcelo Garcia
Butterfly bending and other delicate

by

Kathleen Ricker

A University of Kentucky professor investigates how some of the reactions that sustain life might depend on the interactions of a few electrons.

The enzyme nitroreductase, the focus of Miller's study. Nitroreductase is composed of two identical monomers, colored different shades of grey. An FMN molecule (shown in a stick model) is bound to each monomer or individual protein macromolecule at its interface with the other monomer. The cleft in which the substrate binds against the face of the FMN is revealed as a cut-away in the surface. (Image courtesy of Anne-Frances Miller.)
The chemical reactions that make up metabolism are accelerated and controlled by catalysts known as enzymes. Composed mostly of protein, enzymes also often contain a cofactor. The cofactor can be made of metal ions, such as iron, or can be a vitamin derivative, such as a flavin (a derivative of riboflavin, also known as vitamin B2).

The flavin may accelerate a reaction by brokering electron transfers between reagents to convert them to product. For example, flavins are crucial for metabolism of fatty acids. Flavin enzymes allow a kind of controlled burn, in which the fatty acids are oxidized, allowing the energy released to be captured for use by the body. "Flavin enzymes play many crucial roles in human metabolism," says Anne-Frances Miller, an associate professor of chemistry and biochemistry at the University of Kentucky. "Deficiency with regard to one of the flavoenzymes essential for fatty acid metabolism has been implicated as a possible cause of sudden infant death syndrome."

It is their versatility that makes flavins especially interesting to biochemists like Miller. "Although many different enzymes contain flavins, and as a class, they do a wide variety of chemistry," says Miller, "a given enzyme catalyzes a unique reaction. So, somehow or other, the flavin cofactor is being used for different purposes in different contexts."

Two types of flavin cofactors are most common: flavin mononucleotides (FMN) and flavin adenine dinucleotides (FAD). "The flavin is rather a beautiful molecule," says Miller. "It's an intense, brilliant yellow. The optical properties are yet another reflection of the very versatile electronic properties of the flavin ring."

This versatility makes it both important and challenging to understand the flavin's exact mechanism and reactivity. How the mechanism and reactivity are determined by active sites—the protein environments in which a given chemical reaction occurs—is also critical. Different enzymes may apply the same flavin to different types of reactions, and, according to Miller, the interaction between the flavin and a given protein may be correlated with the resulting chemistry.

How flavins bond

Flavins are generally not covalently bound to enzymes. Rather, proteins generally hold and control them via constellations of weaker non-covalent interactions, including charge-charge interactions and partial sharing of labile protons. Miller hypothesizes that the function a given flavin performs may be determined by the unique non-covalent chemical interactions occurring at a given active site and that recurring patterns or sets of interactions will be found in enzymes that use their flavins in similar ways. These interactions, she says, might shape the flavin's reactivity by changing the distribution and energy of the flavin's valence electrons.

To test this hypothesis, Miller is running a series of high-level calculations on the Alliance's HP Superdome cluster at the University of Kentucky. She is focusing on two very specific kinds of non-covalent interactions that take place between the flavin and the enzyme: hydrogen bonding (H-bonding) and butterfly bending. A hydrogen bond consists of a hydrogen ion (H+) bound between two electron-rich atoms, such as oxygen or nitrogen. Thus, both groups are drawn together by the partial sharing of the H+. 

Ribbon diagram of the structure of nitroreductase, showing the folding of the protein chain. (For simplicity, amino acid side chains are omitted.) The two shades of grey distinguish the two monomers. The two FMN cofactors are shown as green stick models with red oxygen and blue nitrogen atoms. (Image courtesy of Anne-Frances Miller.)
A butterfly bend is somewhat more unusual. "The flavin looks like three sections of a honeycomb or three hexagonal bathroom tiles," explains Miller. "If you were to fold the central segment right down the middle, the two outside rings would look a little like the wings of a butterfly. It's not a butterfly that can sit on a branch and fold its wings right up so that the tips actually touch—it will only bend by some 25 degrees. The wing tips do not come close to each other, but the ring system ceases to be flat, and that is crucial." This bending is important because it is associated with reshaping of the valence orbitals, and it generates tension of a sort that can translate into chemical reactivity.

Although the flavin butterfly doesn't have a large range of motion, significant electron density movement can be achieved by H-bonding taking place along the edge of the "wings" as well as bending. Miller likens this phenomenon to what happens when a standing wave is created in a small space. "If you sat in a bathtub and pushed yourself with your feet from one end, so that your body slid up to the other end, a big wave of water would follow you," she explains. "The wave would hit the back of the bathtub behind you and would then sweep you forward again toward the faucet. In this case, the water is the electron density, and it's pretty fluid—it does have the possibility of moving back and forth in the flavin system."

The flavin electron density doesn't really slosh back and forth in time, Miller points out, but it is spatially spread out over the whole flavin ring system just as the standing wave makes use of the whole tub even though the crest itself is only in one place at a time. But the extent to which the valence electron density is able to run the full length of the tub is related to how bent the ring is, and the extent to which the valence electron density will prefer to stay at one end of the tub depends on the H-bonding at that end.

For different cases of hydrogen bonding and butterfly bending, Miller calculates the ionization potentials, or energy required to remove an electron from reduced forms of the flavin. Her team also calculates what effects these interactions will have on the nuclear magnetic resonance shielding experienced at each carbon and nitrogen atom of the flavin ring. Finally, they compare the computational results with sets of experimental results obtained by nuclear magnetic resonance (NMR) spectroscopy, which provides information about the distribution of electrons in a molecule. Thus, her group validates calculations of electron density distributions in the flavin ring and uses them to predict and understand reactivity.

**Chemistry in small spaces**

Miller's research showcases the advantages of integrating computational and experimental biochemistry. However, both the subtlety of the interactions involved and the large variety of enzyme functions which the flavins assist are especially challenging. "In order to capture the particulars of an enzyme active site," she explains, "you need to include a few of the surrounding [protein] groups." It is crucial to identify features that are important to the flavin behavior without including inessential detail that will tend to blunt the focus of the conclusions and enormously increase the computational cost.

Another concern is the ability of existing experimental methods to support the extraordinarily fine structural detail needed to correctly compute electron density distribution. Miller says that typical current crystallographic structures available for proteins, at 1.8 angstrom resolution, do not have sufficient resolution for studies of flavin electron density.
"That accuracy is as good as is available for proteins, but it's still very crude for quantum mechanical calculations. 0.1 angstrom makes a huge difference in the energy and the electronic structure calculated."

The reward of all this careful calibration and concentration on the infinitesimal world of flavin enzyme electron density, Miller hopes, will be a greater understanding of how the versatile flavins operate—and how they can be engineered to perform yet more useful tasks. "We would like to be able to design changes in an existing enzyme in order to make a new version that would catalyze desired chemistry," she explains. Engineered flavin enzymes are being used in the areas of drug metabolism and waste detoxification treatment and could even provide new gene therapies for congenital birth defects.

In the end, such essential biological processes come down to the valence electrons.

This research was supported in part by the provost's office at the University of Kentucky and now by the National Institutes of Health.

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[http://www.chem.uky.edu/research/miller/](http://www.chem.uky.edu/research/miller/)

**Team members**
- **University of Kentucky**
  - Anne-Frances Miller
- **National Cancer Institute**
  - Joseph Walsh
- **University of Pennsylvania**
  - Ronald Koder
Searching for a pollution solution

Coal-burning power plants spew toxic mercury into the atmosphere, but a researcher at the University of Arizona aims to better understand mercury reactions in order to develop effective emission controls.

by Trish Barker
The modern age is marked by a nearly insatiable hunger for electricity, and more than half of that power is generated by burning coal. But that electricity is doing more than lighting our homes and driving our computers; its production is also generating toxic mercury. Coal-burning power plants are the largest source of human-generated mercury emissions in the United States.

Scrubbing the hazardous mercury from power plant emissions is not easy. In its elemental form, mercury is not soluble in water and is not readily absorbed by solids, traits that allow it to elude current techniques for trapping dangerous flue emissions. Recent research, however, has demonstrated that CDEM (a product derived from recycled pulp and paper mill waste) can capture 100 percent of the mercury in flue gases if the mercury is oxidized. Elemental mercury can react with the other components of flue gases, such as chlorine, to form oxidized compounds.

Putting this knowledge to use is complicated by the fact that the mechanisms that change elemental mercury into various oxidized forms are largely unknown. Paul Blowers, an assistant professor of chemical and environmental engineering at the University of Arizona, uses NCSA's two-teraflop IBM p690 to study these reactions in the hopes that a better understanding of them will enable the design of improved strategies for capturing mercury to protect our air, water, and food supplies and our health.

From power plant to dinner plate

The concentration of mercury in power plant emissions is low, but because of our ceaseless demand for electricity the total amount of mercury released from power plants mounts. The total is now about 48 tons per year in the United States alone.

Power plants are equipped with a variety of devices to control other dangerous emissions—from fabric filters to catch particulate matter to wet and dry scrubbers that absorb sulfur dioxide and other chemicals. “None of the environmental remediation techniques that are typically used work for mercury,” Blowers explains.

This mercury pollution can linger in the atmosphere for up to two years before precipitation pulls it down into our rivers, lakes, and oceans. Microorganisms convert some of the elemental mercury into highly toxic methylmercury, the form that is most readily absorbed by living things. Small organisms absorb the methylmercury and are then eaten by animals higher in the food chain. Because mercury can never be eliminated from the body, large animals—particularly large predatory fish—retain all of the mercury contained in a lifetime of meals in a process called bioaccumulation.

At the pinnacle of this food chain, humans sitting down to dine on swordfish, shark, tuna, or salmon can also unwittingly ingest a large dose of mercury. Mercury can damage the nervous system, liver, and kidneys. Developing fetuses are particularly vulnerable, and studies have found that eight percent of American women of childbearing age have unsafe levels of mercury in their blood.

Even a small amount of mercury escaping from a power plant can be hazardous. According to the National Wildlife Federation, as little as 1/70th of a teaspoon of mercury can contaminate a 25-acre lake, rendering all of its fish unsafe for human consumption.
Studying the smokestack

Because of the dangers, the Environmental Protection Agency is proposing the first ever federal regulations on mercury emissions from power plants. The EPA plan calls for a 70 percent reduction in mercury emissions by 2018. Reaching that goal will mean implementing new techniques in the smokestack.

With that in mind, Blowers began to question how mercury interacts with the other components of flue gases, including chlorine, ozone, oxygen, and even soot particles. "What can happen to mercury in the smokestack? Can we maybe drive it into a form that's water soluble?" he wonders.

The questions aren't simple ones to answer. "We don't understand how mercury reacts in the gas phase," Blowers says. "And if you're trying to figure out how fast reactions will happen and what products will be produced, we just can't do that experimentally."

Finding a quantum method

Blowers instead relies on quantum chemistry calculations to try to build a model of how mercury reacts in the superheated environment of a power plant's smokestack.

Quantum chemistry examines the world at the atomic and subatomic level. Given just a system's elements and molecules as a starting point and working with the basic laws of quantum mechanics, it is possible to predict molecular structures, heats of formation, vibrational frequencies, and activation energies. This information then can be used to calculate the reaction's rate constant, reaction rate, and kinetics. However, even a slight error in a predicted activation energy can lead to reaction rates that are off by several orders of magnitude.

Designing a mercury control mechanism

Burning coal produces harmful byproducts, including fly ash emissions, sulfur dioxide (SO2), oxides of nitrogen (NOx), and elemental mercury (Hg, Hg+1, Hg+2).

A variety of devices (see "Today's pollution solutions") reduce the amounts of these byproducts in power plant emissions, but no current device is designed to capture mercury. As a result, U.S. plants send about 48 tons of mercury into the atmosphere each year.

Research suggests that an effective mercury cleanup system will first require oxidation of the mercury. The difficulty lies in devising a safe, effective technique for forcing the elemental mercury into an oxidized state (meaning it has lost one or more electrons). Currently, the reactions through which elemental mercury is converted into oxidized compounds—such as HgCl2 and HgO—are not well understood.

Oxidized mercury compounds such as HgCl2 and HgO can be captured completely by CDEM, a product derived from recycled pulp and paper mill waste.
At the quantum scale, there are many complex forces and interactions that must be taken into account. All quantum chemistry methods seek a solution to the Schrödinger wave equation for the given molecular system, but even with today's powerful supercomputers the equation is a challenge to solve for a real system. Therefore, scientists use various levels of theory and approximations (such as treating an atom’s inner electrons as an averaged potential rather than as individual particles) to simplify the quantum model and reduce the computational costs while still returning useful results.

Blowers' first step, therefore, was to determine which computational method would generate the most accurate results, so he started his research with a reaction for which known experimental data could be compared to theoretically derived rate constants. He calculated rate constants for the reaction in which chlorine atoms oxidize elemental mercury using seven combinations of methods and approximations.

He found that the most accurate results—within an order of magnitude—were generated by the combination of the QCISD method and a basis set developed in 1992. The QCISD (quadratic configuration interaction with single and double excitations) method optimizes the structural geometries of a system at a higher level than other methods. The 1992 basis set, which is a set of mathematical functions that are combined to approximate the wavefunctions for electrons, contains more valence electron basis functions than other basis sets.

Combining both makes for a computationally intensive method, and Blowers has used 45,000 hours of compute time on NCSA’s systems over the past four and a half years.

Charting new territory

With the methodology demonstrated (and an article describing it recently published in the journal Fuel Processing Technology), Blowers has gone on to predict rate constants for reactions for which there is no experimental data.

“We’ve measured or predicted rates for some reactions that no one has ever measured or predicted before,” he says.

An article published in Environmental Science and Technology reports on the use of quantum chemistry methods to investigate the reaction in which hydrogen chloride oxidizes mercury, and another study used the technique to estimate the heat of formation for HgO. In the latter case, the heat of formation found by Blowers accorded well with other high-level quantum chemical estimations but was much higher than the experimental values frequently used by other researchers.

“We’ve given modelers what we think are more accurate rates to put in their models,” he says.

Blowers next plans to examine mercury’s reactions with O2 and sulfur and is considering the other aspects of the flue environment.

“One of the things that intrigues me is, what is the soot particle doing to mercury? Experimentally, that is a black hole,” he says. It is possible that the smokestack interaction between particulate matter and mercury could provide an opportunity for improved emissions control. “We’re still open to the idea that water scrubbing won’t be the solution,” he says.

As the reactions occurring in flue gases are better understood, scientists will be able to experiment with techniques to steer the reactions in a way that enables the capture of mercury and safeguards the environment.

This research is supported by the U.S. Environmental Protection Agency.

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For further information:
http://blowers.chee.arizona.edu/
http://www.epa.gov/ebtpages/pollairpolmercury.html

Team members
Aaron Bennett
Paul Blowers
Jennifer Wilcox
Nianliu Zhang
Xiaobo Zheng
Matters of reflection

by

J. William Bell

A global team gauges the capability of a laser pulse to control the shock structures in high-speed aircraft engines.
The three-pronged attack has always been a staple of military planning—sometimes ending in victory, sometimes in disaster. The Soviet Union used the tactic to great effect in Europe at the close of World War II. George Custer and his men, on the other hand, didn’t fare so well on the plains of Montana in 1876.

For an international group of aerospace engineers using NCSA computing resources, there’s no Little Bighorn in sight. The team is making a successful attack on Mach reflections, unusual high-speed airflows that are a bane to airplane designers. They have found that lasers can diminish or eradicate these confounding events when they crop up in the inlets at the front of supersonic engines.

Two members of the team, Hong Yan of Rutgers University and Dmitry Khotyanovsky of the Russian Academy of Science’s Institute of Theoretical and Applied Mechanics (ITAM), are running calculations on NCSA’s Platinum cluster. Though they are modeling identical systems, Yan and Khotyanovsky use different codes to get the job done. The University of Illinois at Urbana-Champaign’s Gregory Elliott represents the third prong in the team’s battle plan and conducts experiments on the system in a wind tunnel.

“It is critical to make sure that our final results are not a numerical artifact caused by the influence of...errors present in any [particular] shock-capturing scheme,” Khotyanovsky says. “The cross comparison of our results gives us confidence.”

**Take the good, fight the bad**

Air traveling through an engine at many times the rate of sound doesn’t mix readily with fuel injected into the engine, resulting in unburned fuel and inefficient combustion. To combat this situation, designers typically place an inlet in front of the engine. “The inlet creates shock waves, which lower the air’s speed and allow for good mixing with the fuel. Otherwise, it blows past too fast,” explains Yan. She is a research assistant professor in Rutgers’ mechanical and aerospace engineering department.

When shock waves intersect, what are known as regular reflections typically form. These reflections result in minimal energy loss and thus have little detrimental impact on engine performance. Under very turbulent conditions caused by extreme acceleration or unusual maneuvering, however, shock wave intersections can instead form Mach reflections. These reflections decrease total air pressure and degrade engine performance.

Using a laser pulse or other source of heat, engineers have found that they can turn Mach reflections into regular reflections as they form. At the spot of the temperature increase, the air expands and a subsonic region develops. This change deflects one of the shock waves responsible for the Mach reflection, which eliminates, or at least momentarily reduces the size of, the Mach reflection.
Small scale, big impact

Yan and Khotyanovsky are modeling tiny versions of such a system. Air moves at Mach 3.45 between two wedges pitched 22 degrees off the top and bottom of the simulated domain. The entire domain is less than six inches across. Despite the small size and the fact that an inlet would only have one wedge and the flat aircraft body instead of two wedges, the simulation represents with great fidelity what would occur inside a real engine inlet.

"This is a common and widely used model for experiments on shock wave reflection," Khotyanovsky says. It allows the team to discount the effects of the boundary layer, a viscous airflow that runs along the body of the aircraft and weakens the resulting shock waves. Introducing the boundary layer into the simulations would "greatly complicate the problem," he says, without much of an upside.

Whether the simulation is run by Yan, who uses the commercial GASPex software, or by Khotyanovsky, who uses a code developed by ITAM's Alexey Kudryavtsev, the simulations begin by calculating the initial flow. The domain is separated into millions of cells of varying sizes, with smaller cells in the areas of the domain that are most relevant. GASPex automatically groups cells that will be calculated on the same computer processor depending on the amount of memory and number of processors available for the calculations. The Euler equations, which determine the motion of the flow, are solved for each cell over and over until a Mach reflection appears and the flow reaches a steady state.

Energy equal to that of a 10-nanosecond, 215-millijoule laser pulse is then introduced into the system, raising the temperature of the targeted area to 8,000 K for a matter of microseconds. The flow is recalculated, and the team can watch the laser pulse's impact.

Meanwhile, Greg Elliott recreates the entire system in a miniature wind tunnel. "The simulations are [looking at a system] exactly the same size of the wind-tunnel experiment," Yan says. The air blasts through the system at the same speed, and the laser pulse is of the same power and duration, too.

Though the goal is simple comparison and confirmation, as Khotyanovsky explained previously, there are other benefits to combining experiment and simulation.

"The different approaches verify one another, and both allow us to understand the system's fluid dynamics," says Elliott, an associate professor of aerospace engineering at the University of Illinois. "With the combination, though, we can also see what's the best use of our resources. Some changes to the wind tunnel model can be made in a matter of seconds to probe for an optimal solution. The flow field can then be computed, which may take a much longer time, to obtain details of the flow so that the reason for changes in the flow characteristics can be better understood."

Cleaning up, moving on

The team has completed a series of simulations using both GASPex and the ITAM code. The correlation of the results from the two codes is very tight, according to the team. The team has also tested GASPex at two different levels of detail, running some simulations with 1.5 million cells and others with a more taxing 5 million cells. These simulations, which required as many as 64 processors on NCSA's Platinum cluster, also had very similar outcomes.
In every case, the laser pulse caused the detrimental Mach reflection to change into its more innocuous cousin. Details of these results were published in the journal *Shock Waves* in 2003.

To date, however, results from the experiments don’t quite match up. Instead of being eradicated, the Mach reflection in the wind tunnel is only reduced to 30 percent of its original size. While this decrease is still a testament to the ability of the laser to influence and improve a supersonic inlet’s aerodynamics, it is also a discrepancy that the team would like to overcome. The most likely cause of the inconsistency is additional turbulence created by the wind tunnel itself.

“In the wind tunnel, there is additional turbulence in the supersonic free stream [the moving air that creates the flow and shock waves around the wedges] that is not present in a perfectly clean flow. In the simulations, they can obtain a free stream without the effects of turbulence,” Elliott says. Soon, he hopes to be able to run the experiments in a tunnel that generates less unintended turbulence. This “quieter” tunnel will allow for an improved comparison between the experiments and computations.

The simulations will move forward in the coming months as well. Yan and Khotyanovsky plan to embellish their fundamental models. Among other things, they will move the location of the laser’s thermal spot and introduce multiple spots—and, of course, study the impact those alterations have on the Mach reflections.

But even without these additional efforts, the work is considered a success. “These are the first such simulations of their kind,” according to Doyle Knight, another Rutgers professor who studies aerodynamics using NCSA resources. “They’ve shown how you can do this—how you can take a Mach reflection when it appears and flip it back into a regular reflection using a laser pulse.”

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[http://www.rci.rutgers.edu/~hoyan/](http://www.rci.rutgers.edu/~hoyan/)

Team members
Gregory Elliott
Mikhail Ivanov
Dmitry Khotyanovsky
Doyle Knight
Alexey Kudryavtsev
Hong Yan
Forecasting with chemicals

NCSA supercomputers help predict and resolve fleeting reaction details that puzzle organic chemists.

by

Kathleen M. Wong

Transition structures of an intramolecular aldol cyclization catalyzed by the amino acid phenylalanine. In the preferred pathway (green), the molecule forms the transition structure with the lowest energy barrier (right), yielding more of one stereoisomer than the other.
1926 was a very good year for science. Physicists Werner Heisenberg, Paul Dirac, and Erwin Schrödinger independently came up with mathematical ways to predict the locations of the electrons whirling about an atom's nucleus.

The discovery was a critical one for chemists. The positions of electrons, and the ways they can be shared with other atoms, determine how atoms link into molecules and how molecules react with other molecules to form new substances. Describing these interactions is particularly important for organic chemists, who study the behavior of molecules containing carbon. Organic molecules can link into astonishingly intricate structures that can include multiple rings, side chains, lattices, and polymers. In nature, organic molecules form the basis of hormones and steroids, pheromones and poisons. In industry, they are synthesized into medicines and plastics, flavorings, pesticides, and much more.

Despite the help provided by quantum mechanics, many fine-grained details about organic chemistry still remain a black box. In 1929, Dirac wrote that with the discovery of quantum mechanics, "the underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

But solving such cumbersome equations is finally within reach. The computational obstacles presented by quantum mechanics equations, says professor of chemistry Kendall Houk of the University of California at Los Angeles, are tailor made for the number-crunching talents of supercomputers. For nearly two decades, he has depended on NCSA's supercomputing resources to analyze the intricacies of organic reactions.

Quantum computations

Most chemists work amid shelves filled with bottled solutions and bubbling beakers. But Houk and his 30-strong research group labor largely in cyberspace. "NCSA's resources are extremely valuable to us. Almost every one of our projects has some really big calculations in it," Houk says. "In principle, you could study anything locally, but you might get answers that were so inaccurate they were not useful. With more powerful resources, you can get a better, more accurate answer." After doing rough approximate calculations on local workgroup computers, Houk and his colleagues have routinely turned to NCSA resources over the years. Today, they rely on the center's IBM p690 to conduct their more realistic but time-consuming computations.
The results have grown progressively more rewarding. "Over the last century, we have pretty much been explaining things after the fact, but we're getting to the point where we're able to predict things of interest to explore in experiments," Houk says. Computing speeds, in other words, are finally catching up to real-time chemistry.

Most of the Houk group's efforts are aimed at building computer models of what happens in the proverbial beaker. Though visions of molecules swinging this way and that might come to mind, their simulations are typically far more abstract. "One molecule has to crash into another and disrupt its otherwise happy, stable structure. It takes energy to break existing electron bonds and make others. Quantum mechanics can tell us what those energies are quantitatively, so we can compare competing reactions," Houk says. The more energy it takes to create a given structure, the more slowly the reaction is likely to proceed—and the less likely that structure is to be formed.

Computational chemistry offers many advantages beyond not requiring lab coats and goggles. Researchers can quantify the relative amount of energy it takes to produce different reaction products; study any transition products formed along the way; and even learn larger lessons about organic chemistry theory, such as why a particular catalyst works with some compounds but not others.

**Predictions without palmistry**

Houk and his group often collaborate with experimental chemists—the traditional lab-coat kind—on interesting problems they've come across in their work. One recent opportunity was provided by Benjamin List of the Max Planck Institute in Muelheim, Germany. List studies the production of chiral molecules—molecules that, like our two hands, are mirror images of one another. Such stereoisomers can have distinct chemical or bioactive properties, so chiral catalysts, which favor the production of one stereoisomer over another, can be very valuable. List challenged the Houk group to predict the relative quantities of four different stereoisomers that could be produced by the amino acid catalysts proline and phenylalanine.

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Energy required to complete an intramolecular cycloaddition reaction with various substrate molecules. The Houk team determined that for this type of reaction to proceed, the energy barrier must be less than 13.5 kilocalories per mole. Below this energy threshold, the desired reaction occurs faster than the competing intermolecular dimerization reaction. These calculations explain why substrates with higher reaction energies provide only low yields.
Houk doctoral student Sami Bahmanyar took on the problem. Bahmanyar took three months to calculate the energies required to produce all possible transition states, products, and pathways—a process called mapping out the potential energy surface—and reported her relative yield predictions to Houk. When compared to the experimental results, her computed forecasts were astonishingly accurate. "We were able to predict the major products in all cases. The only time we were not exactly right, it was a difference of less than three percent," Houk says. "This should give people some confidence that this method is appropriate for studying these kinds of reactions."

Postdoctoral researcher Fernando Clemente used similar quantum mechanical calculations to explain the catalytic properties of proline and phenylalanine. Proline serves as a better catalyst in some cases, while phenylalanine is more effective in other situations. He and his fellow postdoc Christophe Alleman and graduate student Paul Cheong made a variety of predictions about these catalysts that should prove valuable to chemists.

At present, it takes far longer to churn out predictions than experiments. But the difference may not stand for long; faster computers should mean shorter calculation times with every passing year. "At some point it will be possible to use theory to screen a lot of potential catalysts," Houk predicts, "to run through a list of 1,000 in a few weeks and pick out a few promising candidates for intensive experimental study."

### Genie in a bottle

In another recent study, Houk graduate student Kelli Khuong helped Boston College chemistry professor Marc Snapper explain the apparently capricious behavior of a group of reactions. Snapper’s experiments were conducted with variations of groups connecting an alkene to the highly reactive molecule cyclobuta diene. In about half of the reactions, the cyclobuta diene reacts with the alkene to which it is tethered. The result is the desired Diels-Alder adduct, which contains a new cyclohexene ring. In the other reactions, very similar versions of cyclobuta diene tend to form dimers—the chemical equivalent of conjoined twins—instead. Snapper wanted to know what caused the differences.

Khuong restudied all the reactions computationally, exploring the reaction pathways and determining the lowest energy—and most likely—pathways for each reaction. It’s a feat that’s nearly impossible in real life, because cyclobuta diene reacts far too quickly. But with a computer simulation, says Houk, "we can essentially put in a bottle something that cannot ever be observed by experimenting, inspect it, and determine what it is about the geometry that makes some of these very easy to achieve, why some are distorted and have atoms crashing into each other and reacting, and why some have high energies and are not easily achievable."

Understanding why chemicals with some structural variations react, while others don’t, is the kind of theoretical information that is transferable to other problems. Multi-ring carbon molecules are found in many natural products, and learning to efficiently synthesize variations on these chemicals could some day add drugs to our medicine chests or new flavorings to foods. And for theoretical chemists like Houk, shining a light on the black boxes of organic chemistry is what it’s all about.

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**Team members**

Christophe Alleman  
Sami Bahmanyar  
Paul H.-Y. Cheong  
Fernando Clemente  
Kendall Houk  
Kelli Khuong  
Benjamin List  
Marc Snapper

The Houk research team at the University of California at Los Angeles.
Tuning in tumors

by Trish Barker

A new understanding of nuclear magnetic resonance could lead to better techniques for detecting cancer.
Magnetic resonance imaging is one of the most valuable diagnostic tools available to today's physicians. MRI gives medical practitioners highly detailed views of the inside of the human body and aids in the diagnosis of a wide range of diseases and injuries.

A revised understanding of nuclear magnetic resonance that has developed over the past decade holds the potential to make MRI an even more sensitive tool, one that can provide unprecedented contrast and resolution and could potentially detect tumors at an earlier, smaller stage. A team of researchers led by Warren S. Warren, of Princeton University and the University of Pennsylvania Medical School, is using computational modeling on NCSA's IBM p690 system to support unusual experimental results that have added an important new chapter to established NMR theory.

Minuscule magnets

The technique of nuclear magnetic resonance was first developed in the 1940s and is based on the quantum mechanical property of spin. Spin makes particles—protons, electrons, and atomic nuclei—behave like miniature magnets.

In NMR, a strong magnetic field is applied to a sample (water, for example, or the tissues of the body in the case of MRI). In response to this magnetic field, the nuclei in the sample align either with the field or in opposition to it. A radio frequency pulse is then applied, which knocks some of the nuclei into a new position, their spins askew. The axis of each tipped nucleus rotates, or precesses; the speed of the rotation varies depending on the type of nuclei and the strength of the fields that are involved.

The minute magnetic fields of these nuclei oscillate because of this rotation, and this creates a radio frequency current. These NMR signals can be detected and harnessed to create detailed images of the interior of the human body.

How NMR produces images

The human body is full of hydrogen atoms, which are ideal subjects for MRI because they have a strong tendency, termed magnetic moment, to line up in the direction of a magnetic field. The magnet in an MRI machine forces those hydrogen atoms to line up either in sync with or in opposition to its magnetic field.

For the most part, the alignments of these atoms cancel each other out—for each one aligned toward the patient's head another will be aligned toward the feet. But out of the millions of hydrogen atoms in the body, some will not be canceled out. These "extra" atoms are those that will produce the MR images.

A radio frequency pulse is applied to the area of the body to be examined. The pulse pushes the "extra" atoms to spin in a different direction and at a particular frequency. When the radio frequency pulse is turned off, these atoms slowly begin to return to their former state, releasing a signal as they do so. This signal is detected and is converted, through a mathematical operation known as a Fourier transformation, into an image.

A shift in NMR theory

That was the understanding of NMR and the state of MRI technology until the early 1990s, when Warren noticed experimental results that didn't fit the established theory. Simple pulse sequences that NMR theory predicted would generate no signal instead produced strong signals. The results were so unexpected, they initially were labeled "crazed" experiments, but continued experimentation established that the signals were no fluke. Instead, Warren realized that a key assumption of NMR theory was wrong.

Scientists had long known that two spins within the same molecule could sometimes react to a magnetic field in tandem, precessing differently as a pair than they would independently. This phenomenon is known as multiple-quantum spin coherence. Warren realized that the strange signals he had found were the result of spins from widely separated molecules teaming up. He labeled this new phenomenon intermolecular multiple-quantum coherence (IMQC).

"Ordinarily you assume that individual molecules don't interact with each other. That is where we found the mistake," he explains. Because of Warren's experiments, NMR theory was adjusted to include the IMQC phenomenon.

Comparison of conventional MR images (left) with images produced using intermolecular multiple-quantum spin coherence (right). The top images are of a rat brain; the spin coherence image gives a much clearer view of the tumor. The bottom images of a human brain also show the enhanced contrast of the spin coherence method.
Creating sharper images

In addition to this shift in NMR theory, Warren's discovery also presented opportunities for improved MRI techniques.

The frequency of the signal received from teamed spins correlates with the amount of oxygen in the sample, which is a key indicator of what processes are occurring there. Tumors are often oxygen guzzlers, so a detailed map of tissue oxygenation could provide a precise technique for cancer detection.

Spin coherence could also help MRI technicians create more detailed images at a higher resolution. In standard MRI, NMR signals are detected from blocks of tissue that are a few millimeters in height, width, and depth. But by leveraging IMQC, technicians may soon tune MRI machines to detect signals from spins that are separated by as little as 100 micrometers. This capability translates into more refined images, which could enable physicians to detect tumors that are too small to be found with standard MRI technology. Earlier detection means treatment can begin sooner and increases the chances of recovery.

The new imaging technique could also provide a more precise map of a tumor's position and shape, information that could help physicians and pharmaceutical researchers target tumors more effectively.

"The problem with targeted medicine is you need to be able to see the target," Warren explains. The enhanced MRI technique could be extremely valuable in the drug development process because researchers would be able to determine at a molecular scale whether or not the drug being tested was having an effect.

Warren's research group is now trying to "tune in" the finer resolution by determining which pulse sequences produce the sharpest images. "The basic issue is trying to find methodologies that do a better job of telling you something at the molecular level," Warren says.

The research team uses an NMR simulation program to test pulse sequences; the code models how various sequences will affect a fat-water system that is similar to human tissue. The goal is to determine which pulse sequences yield the most useful information and the most detailed images.

Warren's research group had been running the simulations on a workstation at Princeton University and the University of Pennsylvania Medical School. While on a research sabbatical with Warren's group, Lakkaraju worked on parallelizing the simulation program and porting it to NCSA's p690 cluster, where the group has an allocation of 20,000 hours. "What it will take is running a large number of datasets," Warren says.

This research is supported by the National Institutes of Health.

Access Online http://access.ncsa.uiuc.edu/CoverStories/NMR/

For further information:
http://www.princeton.edu/~wwarren/

Team members
Prasad Lakkaraju
Motohiro Mizuno
Louis Serge-Bouchard
Warren S. Warren
Dark matter in a Lambda CDM universe

About five years ago, cosmologists discovered that the universe is accelerating in its expansion. These findings were contrary to the behavior of matter in Einstein's well-tested theory of general relativity, which predicted that the universe's expansion would slow with time. They forced cosmologists to contemplate the possibility that, besides dark matter, the universe also contains "dark energy," which experiences gravity as a repulsive force and thus speeds expansion. The cosmological constant is one type of dark energy model, originally considered by Einstein, in which the cosmic repulsion is built into the fabric of spacetime.

This volume visualization shows the distribution of cold dark matter in a model of cosmic structure formation that incorporates the effects of a cosmological constant (Lambda) on the expansion of the universe. The simulation contains 17 million dark matter particles in a cube of model universe that is 300 million light-years on a side. It was performed on NCSA's Platinum cluster as a test of an expanded version of the adaptive mesh refinement code FLASH by Paul Ricker, an NCSA research scientist and assistant professor of astronomy at the University of Illinois at Urbana-Champaign.

FLASH was developed by a team of researchers including Ricker at the Department of Energy-funded ASCI Center for Astrophysical Thermonuclear Flashes at the University of Chicago. Though FLASH was originally intended to simulate supernova explosions, Ricker led an effort to enhance it with self-gravity, expansion, and the ability to track particles. These modifications have extended FLASH's capabilities to cosmological simulation.

The visualization was created by NCSA's Dave Bock, using a custom volume-rendering system called Visualization Shading.

For further information on the project, see http://www.astro.uiuc.edu/~pbricker/research/codes/flashcosmo/.