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Dancing in the Dark: Berkeley Lab Scientists Shed New Light on Protein-Salt Interactions

Posted By lcyarris On August 11, 2010 @ 12:08 pm In Feature Stories | Comments Disabled

Simulation of the interaction between triglycine and dissolved sodium sulfite in water shows the long chain-like triglycine molecule (center) interacting directly with sulfite anions (tripods of yellow and red atoms) while also interacting via multiple hydrogen bonds (thin red or blue lines) with the surrounding water molecules (red and white sticks).

To study nanostructures in real environments, Berkeley Lab scientists have combined theoretical and experimental approaches to glimpse into a protein's interaction with simple salts in water. Enabled by x-ray absorption simulation software developed at Berkeley Lab's Molecular Foundry, these findings shed new light on how salts impact protein structure at the atomic level.

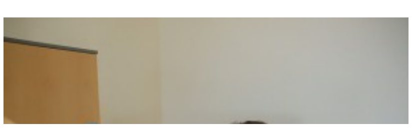
Traditional crystallographic techniques, such as x-ray diffraction, provide a profile of ordered materials with static structures. However, for dynamic or complex systems in which the atomic structure is rapidly changing, more sophisticated methods are needed. Now, Berkeley Lab scientists have applied x-ray absorption spectroscopy to study a model protein, triglycine – a short chain of three molecules of the simplest amino acid, glycine. By simulating this molecule's x-ray absorption spectrum the team has show how its chain kinks and straightens in response to ions in solution.

"Watching a molecule in solution is like watching a marionette—you can see it bending in response to making and breaking of hydrogen bonds," said David Prendergast, a staff scientist in the Theory of Nanostructures Facility at the Molecular Foundry. "A concrete knowledge of how ions influence this behavior comes from using molecular dynamics simulations, which show persistent differences in structure on nanosecond timescales. From this data we can generate x-ray absorption spectra which can then be compared with experimental results."

In a specialized x-ray absorption experiment called near edge x-ray absorption fine structure (NEXAFS), x-rays are used to probe the chemical bonding and environment of specific elements in a molecule or nanostructure, such as the nitrogen atoms in a triglycine molecule. Coupled with a liquid microjet technology developed at Berkeley Labs, NEXAFS has been previously used to examine how proteins dissolve and crystallize in the presence of various ions [1].

Prendergast's software can now simulate NEXAFS data by averaging a series of snapshots taken from a molecular dynamics simulation of a given molecule. This software is a critical tool for interpreting NEXAFS data from complex, dynamic systems, as the probe times in these measurements are too slow—seconds rather than nanoseconds—to reveal structural differences at the nanoscale.

"Previous studies from our group have shown the development of x-ray absorption spectroscopy of liquid microjets provides a new atom-sensitive probe of the interactions between aqueous ions, but it is the advent of this new theory that provides the first reliable molecular-level interpretation of these data," said Richard Saykally, a Berkeley Lab chemist and professor of chemistry at the University of California at Berkeley. "Here we see this new combination of theory and experiment applied to one of the most important problems in biophysical chemistry."



Prendergast says his molecular dynamics technique can be used to model x-ray spectra of a biological system with known structure to determine its local interactions, what causes it to form a particular structure, and why it takes on a particular


[2]

David Prendergast

conformation—all by simulating the spectra of a series of individual snapshots and comparing with experimental results. These simulations are computationally intensive and rely heavily on the large-scale supercomputing infrastructure provided by Berkeley Lab's National Energy Research Scientific Computing Center (NERSC).

"Although these effects are a fundamental part of nature, they are still poorly understood," said Craig Schwartz, a researcher working with Prendergast and Saykally, whose graduate work led to this publication. "The experimental sensitivity of NEXAFS, coupled with a breakthrough in theory, gave us new insight into how these molecules interact."

The researchers anticipate demand from other groups exploring water (or other solvent) interactions, as well as both soft materials (such as polymers) and inorganic materials (oxides and metal surfaces) that are directly relevant to energy-related applications in catalysis, battery technology and photovoltaics. In addition, as x-ray free electron laser sources become available to scientists, a richer experimental data set will be available to augment theoretical findings.

A paper reporting this research titled, "Investigation of protein conformation and interactions with salts via X-ray absorption spectroscopy," appears in Proceedings of the National Academy of Sciences and is available to subscribers online [3]. Co-authoring the paper with Schwartz, Prendergast and Saykally were Janel Uejio, Andrew Duffin, Alice England and Daniel Kelly.

This work at the Molecular Foundry and Advanced Light Source was supported by DOE's Office of Science. Computational resources were provided by NERSC, a DOE advanced scientific computing research user facility.

The Molecular Foundry is one of the five DOE Nanoscale Science Research Centers (NSRCs), national user facilities for interdisciplinary research at the nanoscale, supported by the DOE Office of Science. Together the NSRCs comprise a suite of complementary facilities that provide researchers with state-of-the-art capabilities to fabricate, process, characterize and model nanoscale materials, and constitute the largest infrastructure investment of the National Nanotechnology Initiative. The NSRCs are located at DOE's Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge and Sandia and Los Alamos National Laboratories. For more information about the DOE NSRCs, please visit http://nano.energy.gov.

Berkeley Lab is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California. Visit our website at http://www.lbl.gov.

Additional Information

For more information on the research of David Prendergast go here http://nanotheory.lbl.gov/people/prendergast.html [4]

For more information on the Molecular Foundry go here: http://foundry.lbl.gov/ [5]

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[1] proteins dissolve and crystallize in the presence of various ions :
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dissolve-and-crystallize/
[2] Image: **http://newscenter.lbl.gov/wp-content/uploads/david_prendergast1.jpg**
[3] online: **http://www.pnas.org/content/107/32/14008.abstract**
[4] http://nanotheory.lbl.gov/people/prendergast.html:
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California Is the Primary U.S. Stop for LHC's ALICE Data

Contact: Linda Vu, lvu@lbl.gov , 510-495-2402

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July 30, 2010

For approximately one month a year, the nuclei of lead atoms traveling near the speed of light will collide in the Large Hadron Collider's (LHC) ALICE experiment, generating a fireball about 100,000 times hotter than the core of our Sun. At these temperatures protons and neutrons dissolve into a "particle soup" of quarks and gluons, known as the quark-gluon plasma—a state of matter that first occurred in nature at the birth of our Universe almost 14 billion years ago, a few millionths of a second after the Big Bang. By watching this "soup" cool, physicists hope to better understand the nature of matter, which makes up everything from galaxies to humans.

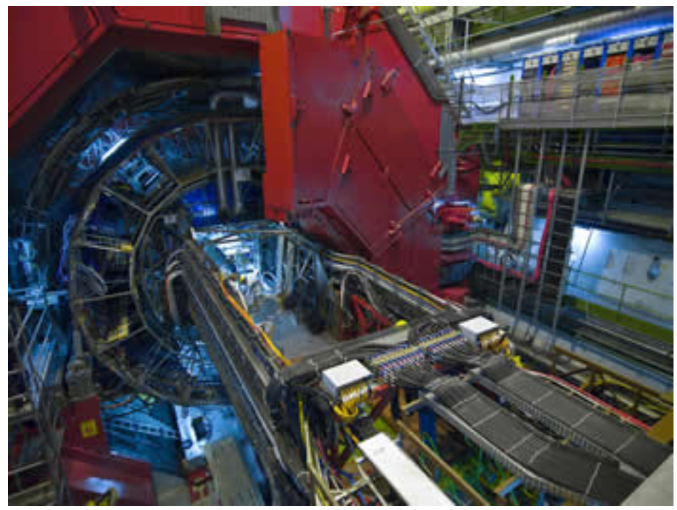

Photo courtesy of CERN

The first door of the L3 magnet in the ALICE experiment

For the month that these lead ions collide, the ALICE experiment will collect over 10 terabytes of data per day, equivalent to the amount of information that could be stored on 20,000 DVDs. About 10 percent of this data will travel from the LHC in Switzerland to the National Energy Research Scientific Computing Center (NERSC) at the Lawrence Berkeley National Laboratory (Berkeley Lab) and to Lawrence Livermore National Laboratory (LLNL) in Northern California via the Department of Energy's (DOE's) Energy Sciences Network (ESnet). These facilities will provide the primary computing and storage resources for the ALICE collaboration in North and South America.

A Dedicated Link Between Europe and California

ALICE data will flow from Europe to California on ESnet's Science Data Network (SDN), which is optimized for large data transfers. This strategy allows the ALICE researchers to leverage ESnet's On Demand Secure Circuits and Reservation System (OSCARS) protocol to set up multi-domain, virtual circuits for guaranteed end-to-end transfers.

"ESnet has been facilitating large, distributed scientific collaborations like ALICE since its inception and has the finely tuned infrastructure and a knowledgeable staff eager to assist with the transfer of these massive datasets," says Steve Cotter, who heads ESnet. "Our high speed networking architecture is finely tuned to guarantee the performance of these temporal data flows. The OSCARS system which manages bandwidth allocations on the Science Data Network is specifically designed for this purpose."

In the last year, DOE's Office of Nuclear Physics funded a significant expansion of NERSC's PDSF platform to handle the ALICE data processing and analysis. The U.S. ALICE collaboration also secured a storage allocation of about 600 TB on the NERSC's High Performance Storage System (HPSS) for 2010. The team recently made these computing and storage resources available to more than 1,000 collaborators worldwide via the ALICE Grid.

"Storage is very important for the ALICE experiment. Thousands of scientists from around the globe will be looking for different things in the same dataset and building on the results of other collaborators; so in addition to duplicating and storing raw data, we also have to copy and archive it at many different stages of the analysis," says Jeff Porter, computing project manager for the U.S. ALICE project and member of the ALICE Grid Task Force. He is also a member of the NERSC Outreach, Software & Programming Group.

The international ALICE Grid connects computing and mass storage resources across 31 countries, and facilitates science by allowing researchers all over the world to submit computing jobs to a single queue. Supercomputing centers connected to this grid run software that locates the data needed to complete a job, determines which systems can perform the job's tasks and where the results will be archived in order to submit and run the computing job. All of these complex procedures are transparent to individual researchers. Later this year LLNL's Green Linux Collaborative cluster will be added to the ALICE Grid. This system will also be funded by DOE's Nuclear Physics office.

The U.S. portion of the ALCE Grid leverages the existing Open Science Grid, which relies heavily on the ESnet networking infrastructure and operations.

"The LHC computing problem is so vast that CERN alone cannot handle all of this data, it requires an international collaboration," says Peter Jacobs, a senior scientist in Berkeley Lab's Nuclear Science Division. He also leads the team of ALICE collaborators based at Berkeley Lab.

He notes that the nature of ALICE data analysis is "embarrassingly parallel," meaning each task requires its own CPU to reconstruct independent collision events in addition to disk storage so it can efficiently access the very large event samples. Because the PDSF and HPSS systems at NERSC have a track record of providing these types of resources to similar experiments, the center was a prime candidate for serving as a Tier-2 facility to handle ALICE data.

"The Lawrence Berkeley and Livermore Laboratories have a history of supporting ALICE science. Researchers from both labs have already collaborated to design and build the experiment's electromagnetic calorimeter detector; and the partnership between NERSC and Green Linux Collaborative to provide computing resources is an extension of that tradition," says Ron Soltz, a researcher at LLNL and coordinator of the ALICE U.S. Computing Project.

According to Soltz, the different strategies that NERSC and LLNL use to procure hardware will be highly beneficial to the ALICE collaboration, providing both optimal pricing through large volume purchases and continuous upgrading of the combined system to keep pace with the growth of ALICE computing requirements with time. This is accomplished by LLNL purchasing all of its new hardware approximately every three years with NERSC upgrading its PDSF system in a more incremental fashion every year.

"Computing is a very important part of this scientific process. You can build a world-class accelerator like ALICE, but you can't do the science without computing," says Soltz.

For more information about computing sciences at Berkeley Lab, please visit: **www.lbl.gov/cs**

About NERSC and Berkeley Lab: The National Energy Research Scientific Computing Center (NERSC) is the primary high-performance computing facility for scientific research sponsored by the U.S. Department of Energy's Office of Science. Berkeley Lab is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California for the DOE Office of Science.

About ESnet
ESnet **www.es.net** is a high speed network serving thousands of DOE scientists and collaborators worldwide, funded by the DOE Office of Science to support the agency's mission to further energy and climate research. Managed and operated by the ESnet staff at Lawrence Berkeley National Laboratory, ESnet provides high bandwidth network connections to all major DOE sites, and via comprehensive connections to the world's research and education networks, to essentially all U.S. and international R&E institutions. As such, ESnet is one of the most widely based and successful cooperative research efforts within the U.S. federal government. ESnet is comprised of two networks, an IP network to carry daily traffic to support lab operations, general science communication, and science with relatively small data requirements, and a circuit-oriented Science Data Network to transfer massive data sets and enable scientific collaborations.

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HOME

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Jobs and Fellowships
Berkeley CSE
Safety and Health
CS Newsletters

NERSC
News & Publications
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Simulations Show That "Sweaty" Flowers Cool the World

Contact: Linda Vu, lvu@lbl.gov , 510-495-2402

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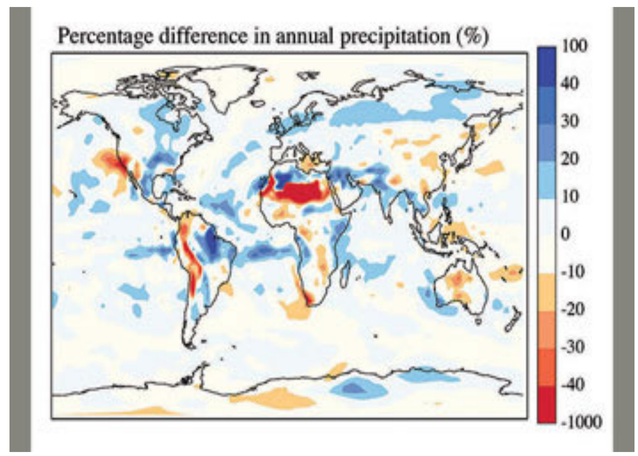
July 19, 2010

The world is a cooler, wetter place because of transpiring flowers, say University of Chicago researchers who ran more than a million lines of code on the National Energy Research Scientific Computing Center's (NERSC's) IBM Power5 "Bassi" system last year. They found that this effect is especially pronounced in the Amazon basin, where 80 percent of ever-wet rainforest area would not exist without flowering plants. These findings were published online on June 16, 2010 in *Proceedings of the Royal Society B.*



The blue regions of this world map show where annual precipitation is higher because of the presence of flowering plants, according to NERSC supercomputer simulations.
(Courtesy of C.K. Boyce and J.–E. Lee)

"The vein density of leaves within the flowering plants is much, much higher than all other plants," said the study's lead author, C. Kevin Boyce, Associate Professor in Geophysical Sciences at the University of Chicago.

He notes that the higher vein density in the leaves means that flowering plants are very efficient at transpiring water from the soil back into the sky, where it can return to the Earth as rain. "That whole recycling process is dependent upon transpiration, and transpiration would have been much, much lower in the absence of flowering plants. We can know that because no leaves throughout the fossil record approach the vein densities seen in flowering plant leaves," says Boyce.

To see what the world would look like without flowers, Boyce teamed up with Jung-Eun Lee, an atmospheric scientist at the University of Chicago and long-time NERSC user. At the time Lee was working on a Department of Energy (DOE) sponsored project with Inez Fung, of UC Berkeley, to understand how soil moisture feeds back into climate through energy, water and carbon exchanges. She realized that similar simulations could contribute significant insights to Boyce's research as well.

For these projects, Lee adapted the NCAR-DOE Community Climate Model to simulate air motion over the entire globe at a resolution of 300 square kilometers (approximately 116 square miles). The results showed that by replacing flowering plants in eastern North America with non-flowering plants, rainfall in the region would be reduced by 40 percent. And replacing flowering plants in the Amazon Basin with non-flowering plants would delay onset of the region's monsoon season from October 26 to January 10.

According to Lee, the atmosphere, land surface and oceans exchange energy, water and trace substances on all space and time scales. The exchange is dependent on, and in turn determines, the states of the atmosphere and biosphere themselves. "The motion of the air is dependent on temperature distribution, and the temperature distribution depends on how heat is distributed. Evapotranspiration is very important in this equation, that's why we have plants in the model," she adds.

In total, Lee used approximately 20,000 computer processor hours at NERSC to run these simulations, and recently submitted a companion paper to the Journal of Geophysical Research. The Community Climate Model was developed with some funding from DOE's Scientific Discovery Through Advanced Computing (SciDAC) program.

Meanwhile, the Energy Department's Office of Biological and Environmental Research supports Inez Fung's climate research. After more than four years in production, NERSC's Bassi system was replaced in April 2010 with another IBM system called "Carver."

This story was adapted from a **University of Chicago press release** written by **Steve Koppes.**

For more information about computing sciences at Berkeley Lab, please visit: **www.lbl.gov/cs**

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Berkeley CSE
Safety and Health
CS Newsletters

NERSC

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Image Gallery
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Berkeley and Princeton Scientists Watch Stars Explode in 3D

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September 16, 2010

For scientists, supernovae are true superstars—massive explosions of huge, dying stars that shine light on the shape and fate of the universe. Recorded observations of supernovae stretch back thousands of years, but only in the past 50 years have researchers been able to attempt to understand what's really happening inside a supernova via computer modeling. These simulations, even crude ones, can lead to new information about the universe's size and eventual fate and help address longstanding problems in astrophysics.

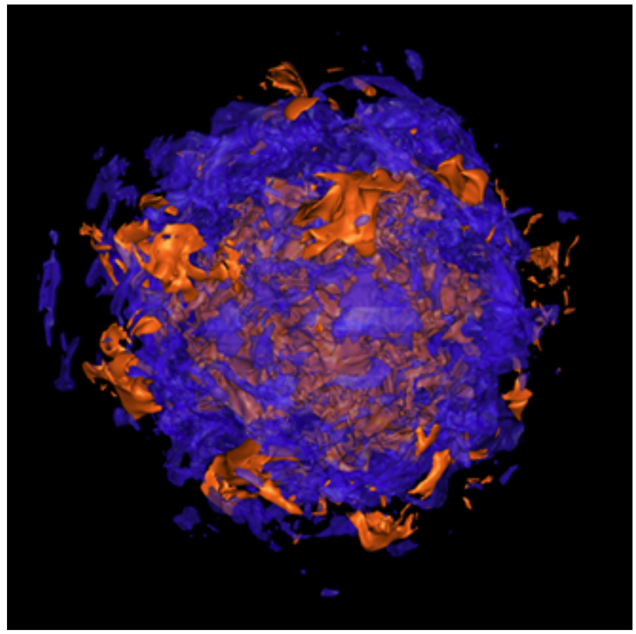

Image credit: Jason Nordhaus and Adam Burrows, Princeton University

This image is a slice of a 3D supernova model. The colors show different entropy values. At this snapshot in time, the star is exploding and the shockwave is propagating.

Now, researchers from Princeton University and the Lawrence Berkeley National Laboratory have found a new way to make computer simulations of supernovae exploding in three dimensions. The new simulations are based on the idea that the collapsing star itself is not sphere-like, but distinctly asymmetrical and affected by a host of instabilities in the volatile mix surrounding its core.

Writing in the Sept. 1 issue of the Astrophysical Journal, Jason Nordhaus and Adam Burrows of Princeton University, and the Lawrence Berkeley National Laboratory's Ann Almgren and John Bell report that the new simulations are beginning to match the massive blow-outs astronomers have witnessed when gigantic stars die.

The team performed these 3D simulations with approximately 4 million computer processor hours on the National Energy Research Scientific Computing Center's (NERSC) Cray XT4 "Franklin" system. The simulations were run using a sophisticated computer code called CASTRO, the development of which was led by Almgren and Bell of Berkeley Lab's Center for Computational Sciences and Engineering.

"I think this is a big jump in our understanding of how these things can explode," said Burrows, a professor of astrophysical sciences at Princeton. "In principle, if you could go inside the supernovae to their centers, this is what you might see."

In the past, simulated explosions represented in one and two dimensions often stalled, leading scientists to conclude that their understanding of the physics was incorrect or incomplete. Using supercomputers many times more powerful than their predecessors, this team was able to create three-dimensional supernovae simulations, revealing multidimensional instabilities.

"It may well prove to be the case that the fundamental impediment to progress in supernova theory over the last few decades has not been lack of physical detail, but lack of access to codes and computers with which to properly simulate the collapse phenomenon in 3D," the team wrote. "This could explain the agonizingly slow march since the 1960s toward demonstrating a robust mechanism of explosion."

Birth of a supernova

Supernovae are the primary source of heavy elements in the cosmos. Their brightness is so consistently intense that supernovae have been used as "standard candles" or gauges, acting as yardsticks indicating astronomical distances. Most result from the death of single stars much more massive than the sun.

As a star ages, it exhausts the hydrogen and helium fuel at its core. With still enough mass and pressure to fuse carbon and produce other heavier elements, it gradually becomes layered like an onion with the bulkiest tiers at its center. Once its core exceeds a certain mass, it begins to implode. In the squeeze, the core heats up and grows even denser.

"Imagine taking something as massive as the sun, then compacting it to something the size of the Earth," Burrows said. "Then imagine that collapsing to something the size of Princeton."

"Visualization is crucial. Otherwise, all you have is merely a jumble of numbers. It allows one to diagnose the dynamics, so that the event is not only visualized, but understood. "

—Adam Burrows, Princeton University

What comes next is even more mysterious.

At some point, the implosion reverses. Astrophysicists call it "the bounce." The core material stiffens up, acting like what Burrows calls a "spherical piston," emitting a shock wave of energy. Neutrinos, which are inert particles, are emitted too. The shock wave and the neutrinos are invisible.

Then, very visibly, there is a massive explosion, and the star's outer layers are ejected into space. This highly perceptible stage is what observers see as the supernova. What's left behind is an ultra-dense object called a neutron star. Sometimes, when an ultramassive star dies, a black hole is created instead.

Scientists have a sense of the steps leading to the explosion, but there is no consensus about the mechanism of the "bounce." Part of the difficulty is that no one can see what is happening on the inside of a star. During this phase, the star looks undisturbed. Then, suddenly, a blast wave erupts on the surface. Scientists don't know what occurs to make the central region of the star instantly unstable. The emission of neutrinos is believed to be related, but no one is sure how or why.

"We don't know what the mechanism of explosion is," Burrows said. "As a theorist who wants to get to root causes, this is a natural problem to explore."

Multiple scientific approaches to solve the problem

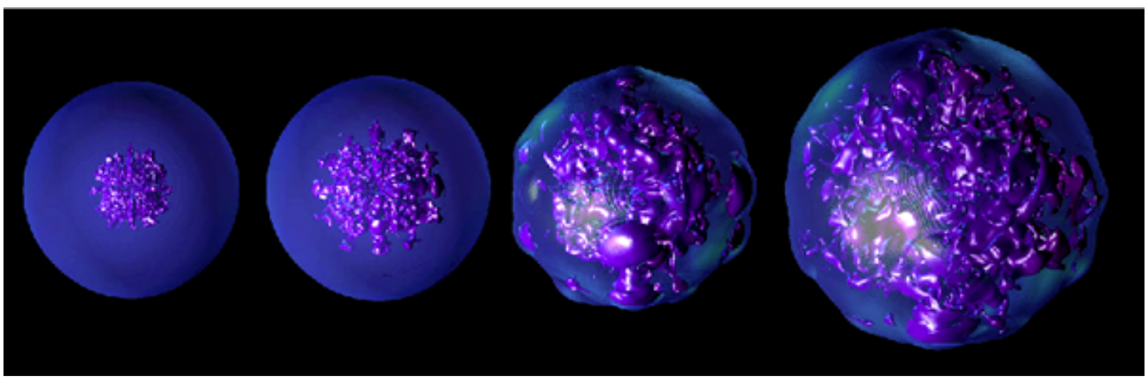

Image credit: Jason Nordhaus and Adam Burrows, Princeton University

This image shows a 3D time series of the development and expansion of the supernova shock. Time is

increasing as you move from left to right. The purple surface is an isocontour of entropy while the blue/green surface is an isocontour of density.

The scientific visualization employed by the research team is an interdisciplinary effort combining astrophysics, applied mathematics and computer science. The endeavor produces a representation, through computer-generated images, of three-dimensional phenomena. In general, researchers employ visualization techniques with the aim of making realistic renderings of quantitative information including surfaces, volumes and light sources. Time is often an important component too, allowing researchers create "movies" showing a simulated process in motion.

To do their work, Burrows and his colleagues came up with mathematical values representing the energetic behaviors of stars by using mathematical representations of fluids in motion -- the same partial differential equations solved by geophysicists for climate modeling and weather forecasting. To solve these complex equations and simulate what happens inside a dying star, the team used an advanced computer code called CASTRO that took into account factors that changed over time, including fluid density, temperature, pressure, gravitational acceleration and velocity.

The calculations took months to process on supercomputers at Princeton and Berkeley Lab.

The simulations are not ends unto themselves, Burrows noted. Part of the learning process is viewing the simulations and connecting them to real observations. In this case, the most recent simulations are uncannily similar to the explosive behavior of stars in their death throes witnessed by scientists. In addition, scientists often learn from simulations and see behaviors they had not expected.

"Visualization is crucial," Burrows said. "Otherwise, all you have is merely a jumble of numbers. Visualization via stills and movies conjures the entire phenomenon and brings home what has happened. It also allows one to diagnose the dynamics, so that the event is not only visualized, but understood."

To help them visualize these results, the team relied on Hank Childs of the Berkeley Lab's Visualization Group. Nordhaus noted that Childs played an important role in helping the team create 3D renderings of these supernovae.

"The Franklin supercomputer at NERSC gives us the most bang for the buck," said Nordhaus. "This system not only has enough cores to run our 3D simulations, but our code scales extremely well on this platform. Having the code developers, John Bell and Ann Almgren, nearby to help us scale our simulations on the supercomputer is an added bonus."

This research is supported in part by the Department of Energy's Scientific Discovery through Advanced Computing Computational Astrophysics Consortium led by Stan Woosley of the University of California, Santa Cruz.. The National Science Foundation also provided additional support for this work.

This story was adapted from a **Princeton University press release** written by Kitta MacPherson. Click here to read the paper in **Astrophysical Journal**. For more information about computing sciences at Berkeley Lab, please visit: **www.lbl.gov/cs**

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