By Jacob Berkowitz

Supernova Express

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A WHITE DWARF IS EXPLODING. **This carbon-oxygen star, slightly smaller than our sun, has been gradually accreting hydrogen, helium and other atoms from a neighboring star. This siphoning-off has doomed it. As the white dwarf grows in mass, its temperature and density rise without bound as it approaches the Chandrasekhar limit. Then the carbon atoms ignite.**

Trillions of high-energy protons careen through the star's supercharged atmosphere. The result is a runaway thermonuclear explosion that will completely obliterate the star.

Peter Nugent watches this Type Ia supernova on his computer screen at Lawrence Berkeley National Laboratory's National Energy Research Scientific Computing Center (NERSC). The explosion process wasn't exactly what he was expecting. Which is fine, because he created it.

A staff scientist with NERSC's scientific computing group, Nugent is at the forefront of a new realm of supercomputer-based computational astrophysics. He grew up looking at the stars in his Easton, Pennsylvania, backyard through a Newtonian telescope given to him by his grandfather. Now he's using an IBM RS/6000 SP, the world's second-most-powerful unclassified supercomputer, to virtually model solar phenomena that would otherwise be impossible to test experimentally in the lab.

The Dawn of a New Era of Supernova Science

When Nugent graduated with a PhD in physics from the University of Oklahoma in 1996, he was on the cusp of a revolution in Type Ia supernova research.

Three years earlier, the Carnegie Institution of Washington's Mark Phillips demonstrated that these supernovae are remarkably accurate beacons of cosmic distance. Since they all explode with about the same amount of mass, in a near-uniform fashion, their spectra and light curves represent 'standard candles' which vary with distance and time.

The new understanding of the value of Type Ia supernovae to cosmology was quickly bolstered by two major technological advances in astronomy: the launch of the Hubble Space Telescope and the development of the charged coupling device (CCD). As a space-based telescope, the Hubble is able to capture the fainter light of ancient high-redshift supernovae, unobservable from Earth-based observatories. As digital imaging systems, CCDs enable electronic computational subtraction of two images taken at different times.

This confluence of theoretical and technological advances led to the creation of the Supernova Cosmology Project (SCP), led by Saul Perlmutter of Berkeley Lab's physics division. The project's goal is to use high-redshift Type Ia supernovae in exploring a bevy of cosmological questions. The group pioneered the automatic detection of supernovae through using CCDs.

Nugent's doctoral thesis, on the modeling of Type Ia supernova spectra, made him a perfect addition to the Supernova Cosmology Project.

"When I graduated, the Project didn't have anyone to interpret their data and push the envelope by suggesting better ways to take measurements," says Nugent, who was hired as the Project's first theoretician, starting out as a post-doctoral researcher in Berkeley Lab's physics division.

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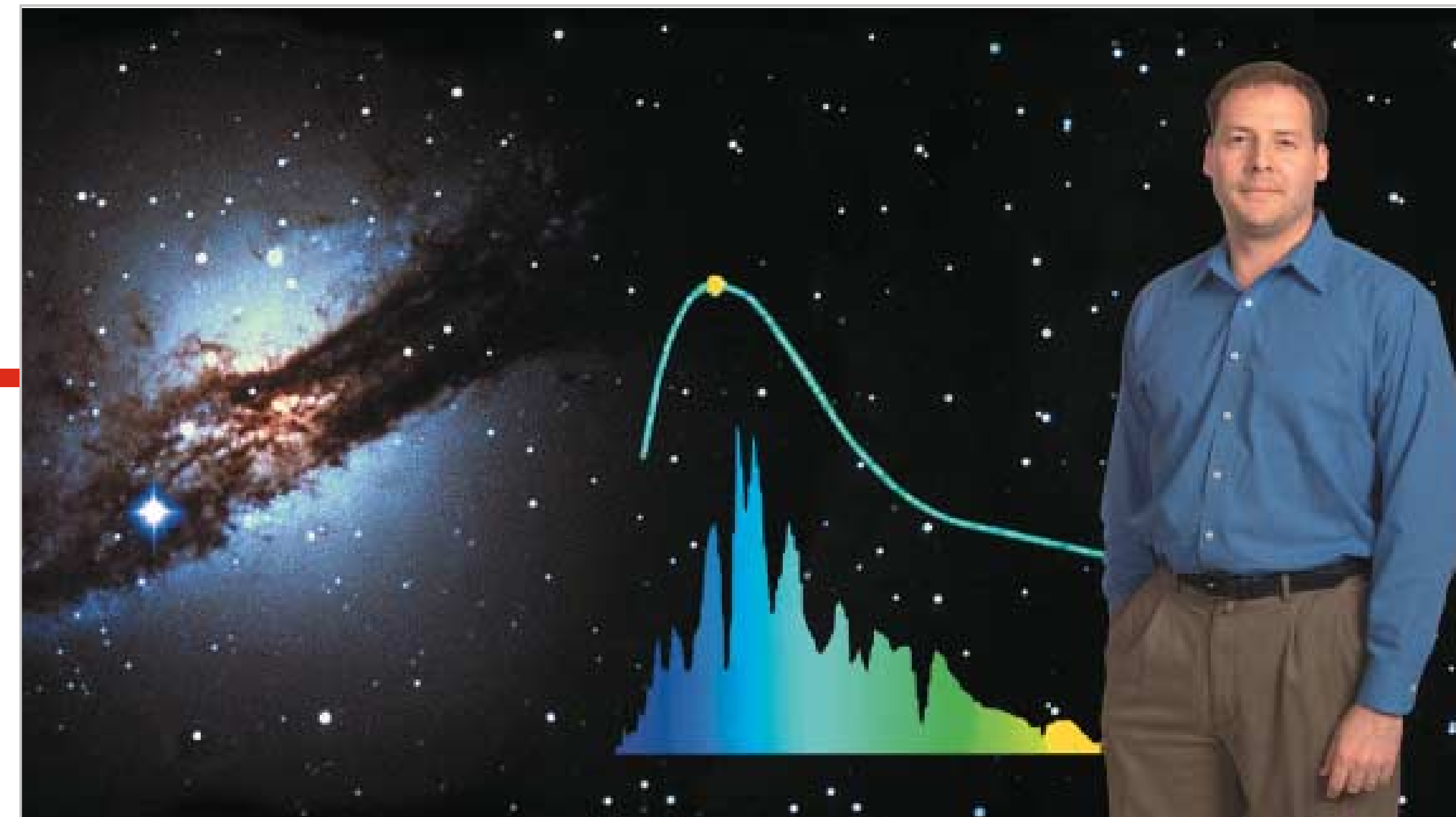


Peter Nugent studies supernovae to answer basic questions about the nature and destiny of the universe.

"There's a great synergy between observations and theory in this field. For me it's a very exciting one because there's a lot of contact between the theorists and the observers. What we do with the modeling is create a theoretical spectrum and then compare that model with observed data. We then frame questions in ways that people can do data analysis and say, 'The models are telling us that if these parameters change then we'd expect to see this signal,'" says Nugent.

This joint observational and computational modeling approach has already led to what the journal *Science* called the "Breakthrough of the Year for 1998". Using dozens of supernovae at distances greater than four billion light years, the SCP and their competitors, the High-Z Supernova Search Team, were able to determine that the universe is expanding at an accelerating rate.

It's an observation that implies the existence of a mysterious, anti-gravity property of space called "dark energy".

Two years later, using data from SN 1999ff, the most distant Type Ia supernova ever found, Nugent and Adam Reiss of the Space Telescope Science Institute were able to roughly determine when the expansion of the universe began to accelerate.

Modeling the Insanely Big

Like genomics and climate modeling, creating virtual supernovae deals in the realm of the mind-numbingly large and complex. In short, it's a job for a supercomputer.

Modeling the spectrum of a Type Ia supernova means recreating a combination of millions of spectral lines. Each line represents an atomic type within the exploding star's rapidly evolving atmosphere. These include sulfur and silicon, with hundreds of thousands of lines representing iron in various transition states. The spectral lines are in turn strongly dependent on temperature and density in the various zones of the star's atmosphere.

Mimicking the observational data, the models begin at about one second after ignition and continue to 20 days, at which time the supernova reaches peak brightness.

"The memory requirements are incredibly large," Nugent says. "The atomic data we feed in to do our calculations is about a gigabyte of data. It's handled differently for 100 different zones of the atmosphere, so that makes for more than 100 gigabytes of I/O. And then we model each of the atoms."

PETER NUGENT

Peter Nugent graduated from Bowdoin College in 1990 and attended the University of Oklahoma, where he received his PhD in Physics (concentration in Astronomy) under Eddie Baron and David Branch in 1996. From there he started a post-doc at Lawrence Berkeley National Laboratory (LBL), working for the Supernova Cosmology Project under Saul Perlmutter. In 1998 the group shared the journal *Science* 'Breakthrough of the Year Award' for the discovery of the accelerating universe. In 2001, Peter became a scientist at the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory and that summer was an integral member of the group that discovered the most distant supernova to date. He has recently been appointed to the Hubble Space Telescope User's Committee and is a lead member of the Supernova Acceleration Probe and Supernova Factory.

Further Reading

K-corrections and Extinction Corrections for Type Ia Supernovae, P. Nugent, A. Kim & S. Perlmutter, Publications of the Astronomical Society of the Pacific, 2002, vol 114, pg. 803.

The Farthest Known Supernova: Support for an Accelerating Universe and a Glimpse of the Epoch of Deceleration, A. Riess, P. Nugent et al. Astrophysical Journal, 2001, vol 560, pg. 49.

Measurements of Omega_M and Omega_Lambda from 42 High-Redshift Supernovae, S. Perlmutter et al., Astrophysical Journal, 1999, vol. 517, pg. 565.

Contact:
Peter Nugent
nugent@panisse.lbl.gov

Moving to 3-D

Until recently, his supernova models were created in one dimension. Now the work is about to get a lot harder.

"We're just about to go to 3-D with our code, and this will cube the time and memory requirements and exhaust the amount of computing time I have to run a couple of simulations. So I want to make sure I'm doing this in the best possible fashion," Nugent says.

The move to 3-D models is part of the SCP's efforts to move beyond spectral analysis to gain even more detailed understanding of these stars' behavior.

One key element of this is study of the polarization spectra. As Nugent puts it, when a Type Ia explodes, is it aspherical like a football or relatively round like a basketball?

Addressing this question entails modeling very small polarization differences (in the range of half of one percent) in the flux spectrum. And this in turn requires a model that involves a much greater number of photons, and requires more memory, in order to produce a statistically significant result.

To make the move to 3-D, Nugent is drawing on NERSC's computational science expertise to create ever-smarter simulations.

And it just so happens that one of the best ways to model a supernova is to physically mimic it within the computational hardware.

"We divvy up our atmosphere between the processors. The way you can think of it is that the photons are making their way through the supernova atmosphere by traveling from processor to processor," says Nugent.

With more than 3,000 processors, NERSC's IBM RS/6000 SP is ideal for this modeling, which requires rapid communication between processors and large amounts of memory. The processors are distributed among 184 compute nodes with 16 processors per node. Each node has a common pool of between 16 and 64 Gbytes of memory.

Yet even with this computational workhorse, there's still the question of how to best divide up the atmosphere to maximize the computational efficiency.

"You could have a very low-density chunk of your atmosphere where there are very few interactions. So if a photon comes in, it basically leaves immediately, you do very little with it. So you'd like to have just a few processors handle all those parts of the atmosphere," he says. Nugent is working with NERSC computational scientists Osni Marques and Tony Drummond to assess questions of load balancing, as well as exploring ways to use dynamic allocation of the processors for on-the-fly reallocation of processing power.

Dynamic reallocation could play a particularly important role when it comes to creating 3-D visuals. Nugent is collaborating with NERSC's science visualization staff to finesse both the processing and data representation of these models.

"At some point we're going to get simulations that will take days to run and we may want to go into the middle of a simulation and look at the data in a visual way and ask: 'Is this going anywhere near the result we want? And if not, let's just stop it right now and start down another path, so we don't waste all our time on the supercomputer.' So they would help us interact with the supercomputer," says Nugent.

The role of computational supernova simulations will be increasingly important as the SCP shoots for its next goal: SNAP — the SuperNova Acceleration Probe. This multi-agency, multi-institution proposal, led by Saul Perlmutter and Michael Levi of Berkeley Lab's physics division, is for the creation of a space-based, 2-meter telescope with the largest and most sensitive CCD ever.

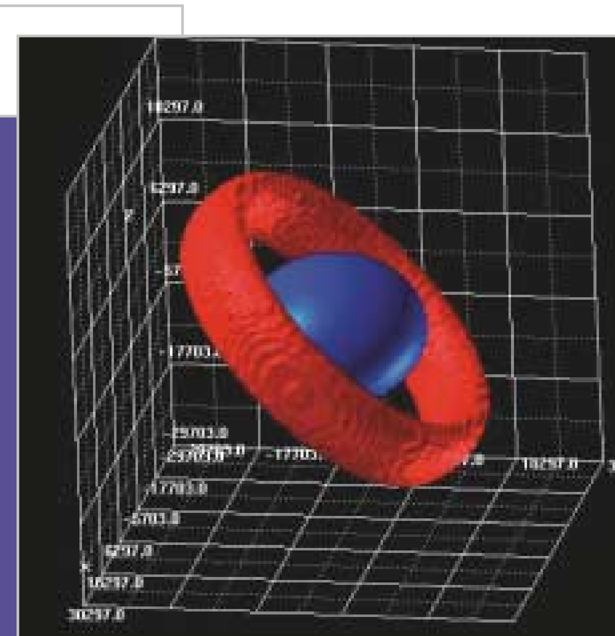
Unlike even the biggest ground-based telescopes — such as the Keck 10-meter telescope in Hawaii — currently used to detect and take high-redshift supernova spectra, SNAP will be able to detect and take spectra of the faint light (especially in the infrared) from the most distant and ancient high-redshift supernovae. The data would be essential to helping us understand the nature of dark energy, says Nugent. It will help not only to confirm that the so-called cosmological constant is nonzero, but also to answer questions as to whether it has changed over time.

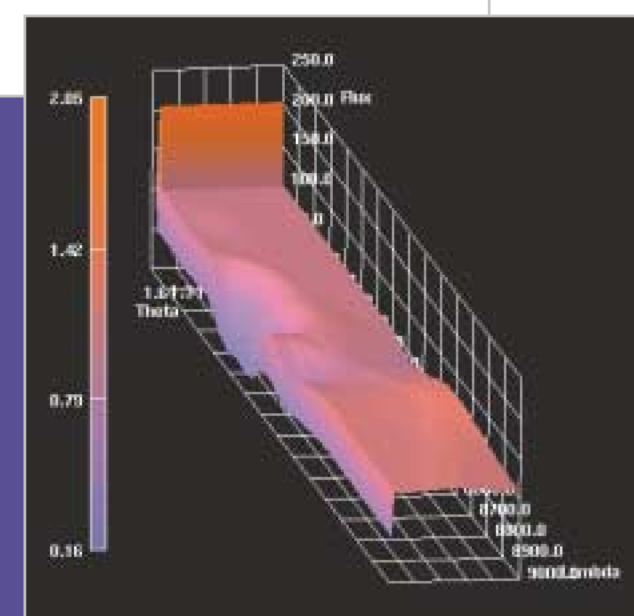
According to Nugent, theoretical modeling will help guide what SNAP actually snaps images of. The plan is for the probe to take images in batch mode and probably find thousands of supernovae. The question would be which ones to focus on so as to capture their spectra.

Nugent plans to use simulations to create a comparative grid of both Type Ia and Type II supernova data. It will enable observers to use the initial handful of data they receive to select the supernovae they want to follow.

"Right now we're sitting at a point very much like Einstein at the turn of the last century. We're trying to detect things that we have no idea what they are — dark energy. It has huge importance for understanding the universe and basic physics. Getting that data into a form so that theorists can understand it will come about through supercomputing."

Here we present a spectrum synthesis calculation of a supernova atmosphere surrounded by a toroid. The layout of the atmosphere is presented on the right while at the left we have a graph of the flux vs. wavelength vs. viewing angle. As the viewing angle shifts towards the toroid, the strength of the absorption increases dramatically. Data that confirm such a model would for the first time put strong constraints on the progenitors of Type Ia supernovae.





WHY THE DOE FINDS ITSELF AT HOME IN THE STARS

>> Supernova research brings together the really big and the really small. And in the process it demands an astronomical amount of collaboration, says computational astrophysicist Peter Nugent.

"There has always been a tie between astrophysical phenomena and work in nuclear physics. With both there's a whole range of energies, temperatures and densities that are inaccessible in the laboratory," says Nugent, a staff scientist with the Department of Energy's National Energy Research Scientific Computing Center (NERSC) based at Lawrence Berkeley National Laboratory.

Nugent notes that physicist Hans Bethe is perhaps best known for his role in the Manhattan Project. However, Bethe's 1967 Nobel Prize in physics was awarded for his contribution to the theory of nuclear reactions, especially as it related to his discoveries concerning energy production in stars.

The intersection of elementary-particle and nuclear physics with observational and computational astrophysics means that supernova research requires a high degree of interdisciplinary cooperation. A collaborative approach is also motivated by the need to use a variety of telescopes and staff to identify, track and record spectra from supernovae during the course of their visible lives (about 3 months from Earth-based telescopes).

In 1999, Nugent was one of 32 authors — from the observers to the data processors and interpreters — on a superno-va journal article for which he had provided the computational analysis.

Says Nugent: "With these cosmological observations, astronomy and particle physics are coming together in a way in which, if you understand cosmology, then you certainly have great insights into fundamental particle physics. Because we're pushing back to exactly what came out of the Big Bang and what are the equations which govern the physics of the universe. In that, many people believe there will be great insights into particle physics."