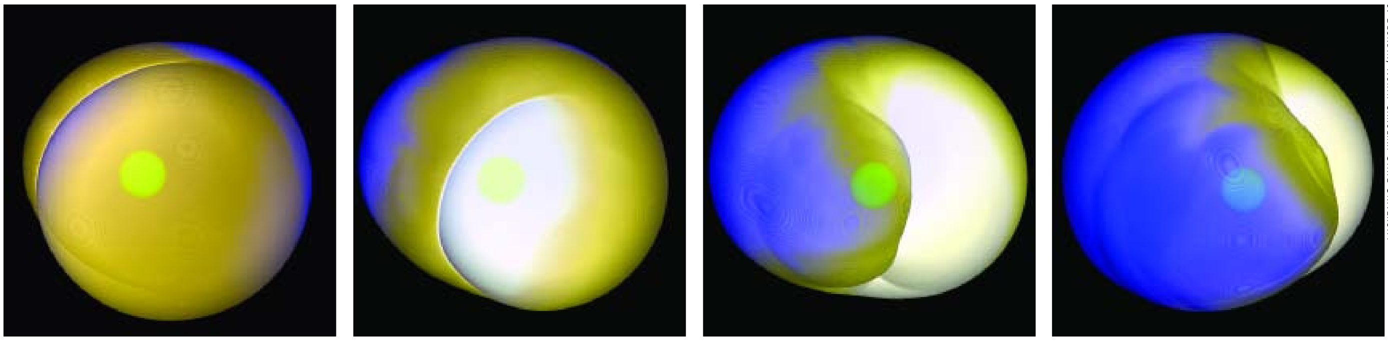
Science Accomplishments

Results from SciDAC's Supernova Project

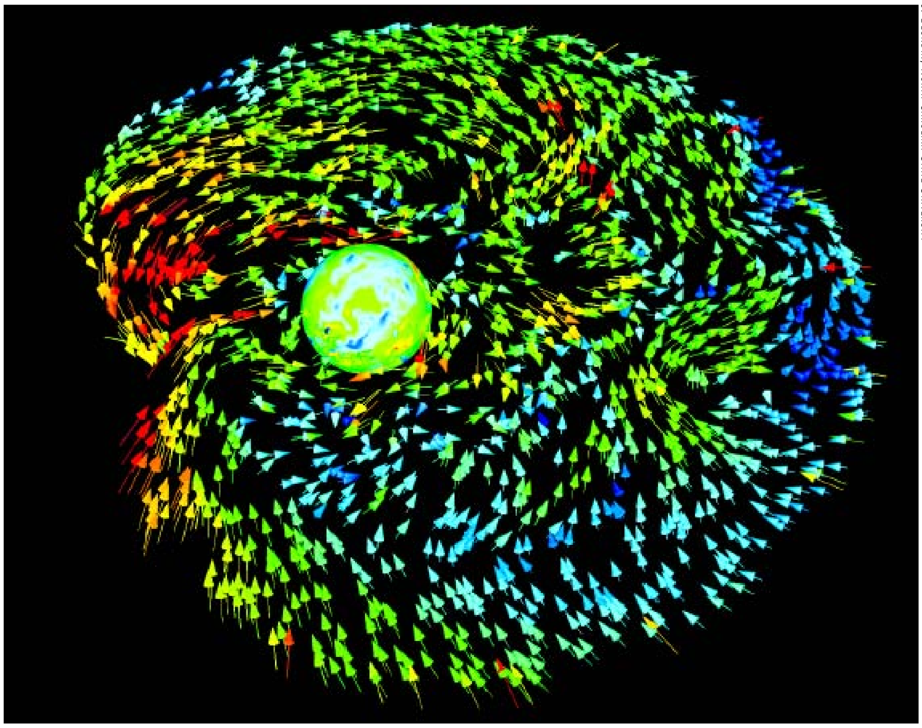


J. Blondin, North Carolina State University

Figure 1. *Four steps from a simulation of supernova accretion shock evolution.*

In core-collapse supernovae, neutron stars are born spinning at a rate of dozens of times per second. Current theoretical models hold that the high rotation rate of these radio pulsars is the result of the conservation of angular momentum during the collapse of rotating stellar cores. According to these models, pulsar spin is thus directly correlated with the progenitor star's rotation. Problematically, however, these models predict neutron star rotation rates that are only consistent with the fastest known radio pulsars.

Researchers Dr. John M. Blondin of North Carolina State University and Dr. Anthony Mezzacappa of ORNL have recently challenged the conventional assumptions about pulsar rotation. In the January 4, 2007 issue of *Nature*, Dr. Blondin and Dr. Mezzacappa proposed a new explanation for the generation of neutron star spin which, for the first time, matches astronomical observations. Their results are based on simulations run on the Leadership Computing Facility Cray X1E at ORNL as part of the SciDAC TeraScale Supernova Initiative, a multi-institution collaboration between astrophysicists, nuclear physicists, applied mathematicians, and computer scientists headed by Dr. Mezzacappa.



J. Blondin, North Carolina State University

Figure 2. *Flow vectors elucidate two rotational flows.*

During the collapse of a massive star's core, the outward-directed shock wave, meeting the infalling gas of the stellar implosion, stalls at a radius on the order of 100 km. This stalled-shock phase lasts for less than one second, after which an as-yet undetermined mechanism revives the shock wave and triggers the supernova explosion. Two-dimensional simulations have shown that this quasi-steady shock is subject to the stationary accretion shock instability (SASI), a phenomenon first described by Dr. Blondin in 2003. Simulations in two dimensions, however, were not able to take into account the rotation of the accretion flow. Now Dr. Blondin and Dr. Mezzacappa have performed a series of three-dimensional simulations through which they have determined that the SASI is characterized by a non-axisymmetric spiral flow pattern.

The research team explains that the spiral SASI can be understood as a growing acoustic wave propagating around the periphery of the region between the proto-neutron star (PNS) and the accretion shock (figure 1). This robust instability creates two strong counter-rotating flows in the vicinity of the PNS (figure 2), fueling the deposition of angular momentum onto the PNS.

Simulations were run using different initial perturbations, both with and without a moderately rotating progenitor star. In every case, the research team found that the SASI spiral mode became dominant. This dominance was achieved more quickly when the progenitor star was rotating. They also found that the spiral flow pattern generated by the distorted accretion shock had a marked effect on the protoneutron star. The magnitude of the angular momentum deposited onto the PNS was set by the flow pattern of the spiral SASI wave, not by the angular momentum of the infalling gas above the accretion shock.

Likewise, the research team found that the net angular momentum deposited onto the PNS as a result of the spiral SASI had a profound effect on the spin rate of the neutron star left behind after the supernova. For a progenitor star that is not rotating or rotating slowly, the SASI—not the progenitor core spin—will be the dominant source of angular momentum in the remnant neutron star, producing spin rates consistent with observational data for pulsars. Dr. Blondin and Dr. Mezzacappa's results demonstrate that progenitor core spin and neutron star spin are not as simply correlated as prevailing stellar evolution models suggest. Their results also indicate that progenitor core rotation rates may actually be significantly lower than currently predicted.

According to Dr. Blondin and Dr. Mezzacappa, the final spin rate of a neutron star is determined by how long the SASI spiral mode was dominant during the core collapse. This in turn depends on how soon the spiral SASI began after the creation of the shock wave as well as on how long the stalled accretion shock lasted before the explosion was triggered. Although the research team's model is only valid for the stalled-shock phase, and three-dimensional models need to be developed which are sufficiently realistic to allow scientists to follow the entire supernova explosion process, Dr. Blondin and Dr. Mezzacappa's results nevertheless confirm the robustness of the spin-up induced by the spiral SASI, and provide the first plausible explanation for the generation of pulsar spin.

Contributors:

Dr. John Blondin, North Carolina State University; Dr. Anthony Mezzacappa, ORNL

Further Reading:

J. M. Blondin and A. Mezzacappa. 2007. Pulsar spins from an instability in the accretion shock of supernovae. *Nature*, **445**: 58–60.

Forthcoming Conference

SciDAC 2007 in Boston, MA

The next SciDAC annual meeting is to be held in Boston, MA from June 25–28, 2007. For the third straight year, the annual meeting will be expanded from a working meeting of SciDAC principal investigators to an exposition of scientific results obtained using high-end computing and some of the general purpose mathematical and software infrastructure that enables them.

The Scientific Discovery through Advanced Computing Program has begun its second round of projects (see "SciDAC-2: The Next Phase of Discovery," p16), after a wealth of successful projects spanning its first five years. Joining the Office of Science of the U.S. Department of Energy over the next five years in key aspects of SciDAC are the National Nuclear Security Administration (NNSA) and the National Science Foundation (NSF). This hallmark of the SciDAC program is the joining together of computer scientists, applied mathematicians, and computational scientists across many application domains, from universities and national laboratories, in vertically integrated collaborations. As a result, the computational state-of-the-art in many fields has advanced significantly, and the program has enabled studies that could only be dreamed of in the recent past.

While the purpose of SciDAC is scientific discovery, due to the multiscale nature of complex phenomena this is tantamount in many areas of science to harnessing new levels of performance on data sets of new scale. Computational platforms at the petascale should be coming on line in 2008, and our mathematical and software infrastructure must target this scale—millions of processor cores—in anticipation. Consequently, a major theme of SciDAC 2007 will be the identification of challenges for specific leading applications at the petascale, and approaches for overcoming these challenges. Application experts will be asked to focus on performance and scaling issues. Enabling technologies experts will be asked to focus on petascale applications and architectures.

Approximately three hundred researchers from across the SciDAC program and related endeavors will assemble in Boston. Through invitation-only talks and posters, they will offer updates that span the diverse areas of SciDAC. SciDAC 2007 will also celebrate the achievements of computational science worldwide. Computational science leaders from abroad will join in offering additional updates in important areas relevant to understanding our universe on its largest and smallest scales, from understanding Earth's climate to developing new energy sources. Astrophysics, biology, combustion, fusion, materials, nanotechnology, particle physics, and subsurface flows are among the applications that will be featured. Enabling technologies presented at the meeting will include mesh generation for complex geometry, advanced discretizations, problem adaptability, partitioning and balancing tools, optimal solvers, data archiving and data mining, software componentization, performance engineering, and compilation techniques for advanced architectures.

The four-day technical program will be preceded and followed by programs in the use of SciDAC software. The "CompFrame" workshop on common component architecture will be held on June 23–24. A tutorial program aimed at new users, with hands-on consulting for existing users, of popular SciDAC enabling technology software will be offered on June 29, at MIT.

Beyond the reporting on existing projects and tools, SciDAC 2007 should provide an enviable critical mass for fruitful discussions of the future of computational science.

Contributor:

Dr. David Keyes of Columbia University is the SciDAC 2007 conference chair and the author of this news item

Further Reading

http://www.scidac.gov/Conference2007/

Innovative and Novel Computational Impact on Theory and Experiment

DOE INCITE Program Awards 95 Million Hours

Supercomputers are playing an increasingly important role in scientific research by allowing scientists to create more accurate models of complex processes, to simulate problems once thought to be impossible, and to analyze vast amounts of data generated by experiments. Scientists engaged in such pursuits can never have access to too many computational resources. Needless to say, the demand for computing hours on powerful machines far exceeds the supply of supercomputing time.

For some scientists, however, time is now on their side. As part of the 2007 Innovative and Novel Computational Impact On Theory and Experiment (INCITE) program, DOE has awarded 45 projects a total of 95 million hours of computing time on some of the world's most powerful supercomputers. DOE's Under Secretary for Science Dr. Raymond Orbach presented this year's awards on January 8 at the Council on Competitiveness in Washington, DC.


COURTESY OF COUNCIL ON COMPETITIVENESS

Figure 3. *Front row, left to right: Dr. Raymond L. Orbach, Under Secretary for Science, DOE; Deborah L. Wince Smith, President, Council on Competitiveness. Back Row, left to right: Suzy Tichenor, Vice President, Council on Competitiveness; Michael Garrett, Director, Airplane Configuration, Integration & Performance, Boeing Commercial Airplanes; Dr. Robert Fisher, Deputy Astrophysics Group Leader, Flash Center, University of Chicago; Dr. Benoit Roux, University of Chicago; Tom Lange, Director, Modeling and Simulation Corporate R&D, Procter & Gamble; Dr. Michael Strayer, Associate Director of Science for Advanced Scientific Computing Research, Office of Science, DOE.*

"The Department of Energy's Office of Science has one of the top ten most powerful supercomputers in the world and four of the top 100 and we're proud to provide these resources to help researchers advance scientific knowledge and understanding," Energy Secretary Samuel W. Bodman said. "I look forward to witnessing the promise of these efforts as some of the world's greatest thinking minds use some of the world's greatest thinking computers."

Launched in 2003, the INCITE mission is to advance American science and industrial competitiveness. The awards further that mission by supporting computationally intensive, large-scale research projects with large amounts of dedicated time on supercomputers at DOE's Leadership Computing Facilities at ORNL and ANL, the National Energy Research Scientific Computing Center at LBNL, and the Molecular Science Computing Facility at Pacific Northwest National Laboratory. The projects were chosen based on the potential scientific and engineering impact of the research and the projects' suitability for supercomputer use.

"One of the most important aspects of the INCITE program is that the resulting knowledge will largely be available, so that the information and technologies can be used by other researchers, further broadening the impact of this work," Dr. Orbach said. "Our scientific leadership underpins nearly every aspect of our economy and by making these resources available to a broad range of science and engineering disciplines, we believe the resulting work will make us more competitive in the years and decades to come."

Research areas to be addressed in 2007 include accelerator physics, astrophysics, chemical sciences, climate research, computer science, engineering physics, environmental science, fusion energy, life sciences, materials science, nuclear physics, and nuclear engineering. The research will have a wide range of practical applications including designing quieter cars and better commercial aircraft, advancing fusion research, studying supernovae and global climate change, understanding nanomaterials, and investigating the causes of Parkinson's disease.

Among the award recipients are researchers at Auburn University, Fisk University, Northwestern, the University of Alaska–Fairbanks, the University of California campuses at Davis, Los Angeles, San Diego, and Santa Cruz, the University of Chicago, the University of Colorado, the University of Michigan, the University of Rochester, the University of Washington, and the University of Wisconsin–Madison. DOE scientists receiving awards this year conduct research at ANL, LBNL, LANL, ORNL, SNL, the Thomas Jefferson National Accelerator Facility, the Princeton Plasma Physics Lab, and the Stanford Linear Accelerator Center. Awards were also made to researchers at the National Center for Atmospheric Research, NASA's Goddard Space Flight Center, the National Oceanographic and Atmospheric Administration, and the Max Planck Institute for Quantum Optics in Germany.

Nine of the projects selected for 2007 INCITE awards are from industry, doubling the number from last year—a clear indication that U.S. industry has realized the potential benefits of our nation's investment in high-end computing. Firms receiving awards for the first time include Corning Inc., Fluent Inc., General Motors, and Procter and Gamble. Firms with renewed awards are DreamWorks Animation, Pratt and Whitney, The Boeing Co., and General Atomics.

Advanced Scientific Computing Advisory Committee

New ASCAC Members Invited

Figure 4. *Invited ASCAC members, from left to right, Dr. Horst D. Simon, Dr. Rick L. Stevens, and Dr. Thomas Zacharia.*

Last year, Energy Secretary Samuel W. Bodman invited three new members from the research community to join DOE's Advanced Scientific Computing Advisory Committee (ASCAC). Dr. Horst D. Simon, Dr. Rick L. Stevens, and Dr. Thomas Zacharia are scheduled to be sworn in as members of the committee on February 27, 2007.

Established on August 12, 1999, ASCAC provides DOE with valuable and independent advice on a variety of complex scientific and technical issues related to its Advanced Scientific Computing Research program. ASCAC offers recommendations on long-range plans, priorities, and strategies in order to address more effectively the scientific aspects of advanced scientific computing, including the relationship of advanced scientific computing to other scientific disciplines, and the appropriate balance among elements of the program. The committee, which formally reports to the SC Director, is primarily composed of representatives of universities, national laboratories, other federal agencies, and industries involved in advanced computing research. Particular attention has been paid to obtaining a diverse membership for ASCAC, with a balance among scientific disciplines, institutions, and geographic regions.

Dr. Simon received his Ph.D. in mathematics from the University of California–Berkeley. He joined LBNL in 1996 as director of the newly formed National Energy Research Scientific Computing (NERSC) Center, DOE's flagship supercomputing facility for unclassified research funded by SC. Dr. Simon is also the founding director of LBNL's Computational Research Division, which conducts applied research and development in computer science, computational science, and applied mathematics. In 2004, Dr. Simon was named Associate Laboratory Director for Computing Sciences at LBNL. His research focuses on sparse matrix algorithms for eigenvalue problems and for sparse linear systems, and his current interests include applications of eigenvalue techniques to computational chemistry and biology, and spectral methods for dynamic load balancing of unstructured CFD computations. Dr. Simon is also involved in a number of benchmarking and performance evaluation projects, and is a regular contributor to the TOP500 reports.

Dr. Stevens is Professor of Computer Science at the University of Chicago. He is also the Associate Laboratory Director for Computing and Life Sciences at ANL, where he heads an advanced computing initiative targeting the development of petaflop computing systems. In addition, he is Leader of ANL's Computing and Communications Futures Laboratory, a group he started in 1994 to investigate problems in large-scale scientific visualization and advanced collaboration environments. His group in the Futures Lab developed the widely deployed Access Grid collaboration system. Dr. Stevens' research interests include advanced collaboration and visualization environments, high-performance computer architectures including Grids, and computation problems in the life sciences, most recently with an emphasis on the problems arising in systems biology. He also teaches courses on computer architecture, collaboration technology, virtual reality, parallel computing, and computational science.

Dr. Zacharia received his Ph.D. in engineering science from Clarkson University. He joined ORNL in 1987, and in 1993 formed ORNL's Materials Modeling and Simulation Group, serving as Group Leader until 1998, when he was made division director of the Computer Science and Mathematics Division. He also served as Deputy Associate Laboratory Director of High Performance Computing from 2000 to 2001. In 2001 Dr. Zacharia was named Associate Laboratory Director for ORNL's newly formed Computing and Computational Sciences Directorate. He is the author or co-author of more than 100 publications on high-performance computing for manufacturing processes, including superplastic forming, casting and solidification, and the stamping process.

SciDAC Connection

2006 Gordon Bell Prize

The prestigious Gordon Bell Prizes were awarded last November at the SC06 conference in Tampa, FL. Dr. Francois Gygi led a winning team, which also includes Dr. Bronis de Supinski. Both researchers are also members of SciDAC project teams.

Titled "Large-Scale Structure Calculations of High-Z Metals on the BlueGene/L Platform," the entry won in the "peak performance" category, judged on sustained floating point operations per second. Such research on heavy metals is of interest to scientists with the National Nuclear Security Administration's (NNSA) Stockpile Stewardship Program.

Dr. Gygi's team used the first principles molecular dynamics (FPMD) code called Qbox to achieve simulations of unprecedented scale and detail. A sustained peak performance of 207.3 TFlop/s was measured on 65,536 nodes, corresponding to 56.5% of the theoretical full machine peak using all 128,000 CPUs.