The Next Best Thing

INCITE Awards Give Scientists Predictive Powers for Nuclear Structure and Core-Collapse Supernovae

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They are exotic and fleeting; rare and mysterious. They die spectacular deaths with drama and brilliance. They fascinate scientists even as they deftly elude them. Yet there are tools—supercomputers to be exact—that give physicists the ability to simulate evasive particles and events. Using rapid and powerful computation, they can, for example, predict how rare isotopes are put together and how they behave; or how stars die in violent explosions. That is exactly what UTK physicists will do with their collective 103 million processor hours on the supercomputers Jaguar (at Oak Ridge National Laboratory) and Intrepid (at Argonne National Laboratory). Through the U.S. Department of Energy INCITE (Innovative and Novel Computational Impact on Theory and Experiment) program, they have won time with these premier scientific resources to study nuclear structure and core-collapse supernovae.

Jaguar at ORNL

The proposal "Nuclear Structure and Nuclear Reactions" features a seven-person cast including UTK Physics Professor Witek Nazarewicz as a co-investigator. They've been allotted 28 million hours on Jaguar and 15 million on Intrepid to dig into the secrets of nuclei. Of the nuclei comprising the mass of matter around us, more than 99.9 percent are stable—meaning they essentially live forever. Remarkable as these are in terms of longevity, the unstable nuclei are even more fascinating. They're the ones with unusual combinations of protons and neutrons—the ones that dwell farther and farther from the edge of stability, where the rarest and most exotic isotopes live only briefly before disintegrating into decay. A comprehensive description of all nuclei, stable and not, will give scientists a reference point for how they are structured and how they interact. Via simulations, supercomputers make it much easier to assemble that catalog, especially in the realm of the most exotic nuclei where direct experimentation is either not an option or would be subject to large uncertainties. A clear and decisive map of nuclei is relevant for fields like nuclear medicine, where radioactive substances can help diagnose and treat disease; or nuclear astrophysics, where rare nuclei play a key role in the element production within stars.

Stars, or to be more precise, their violent demise, are exactly what UTK-ORNL Joint Faculty Professor Tony Mezzacappa has in mind. He is the principal investigator on "Three Dimensional Simulations for Core Collapse Supernovae," which won 60 million hours on Jaguar through INCITE. He and five co-investigators will use their supercomputing currency to perform 3-D simulations of how stars more than 10 times the mass of our sun meet their end in stellar explosions known as core-collapse supernovae. The fireworks are impressive in their own right, but even more significant is that these astrophysical events are the dominant source of elements in the universe—all those between oxygen and iron and half the elements heavier than iron—elements required for life to exist. At present there are no sufficiently realistic 3-D models of these supernovae, a void this proposal seeks to fill.

The DOE Office of Science supports the INCITE program, which, through the combined assets of Jaguar and Intrepid, provides computing capabilities equivalent to 135,000 laptops with four processers each. The 2011 awards, announced in November, support 57 projects in academia, commercial research, and industry. Collectively they will receive 1.7 billion processor hours, the largest total to date.

Along with Nazarewicz, other scientists working on the nuclear structure proposal include James Vary of Iowa State University (principal investigator), Joseph Carlson of Los Alamos National Laboratory, Pieter Maris of Iowa State University, Hai Ah Nam of Oak Ridge National Laboratory, Petr Navratil of Lawrence Livermore National Laboratory, and Steven Pieper of Argonne National Laboratory. They have recently completed the third year of an INCITE proposal (2008-2010), and the new 2011 award represents a 7.5 percent increase from their previously allotted computing time.

Mezzacappa's group has had an INCITE allocation since the inception of the program in 2003 (ranking among the top three from 2005-2009), with the fifth largest allocation this year. The collaborative team includes additional UTK personnel Joint Faculty Assistant Professor Christian Cardall , Joint Faculty Associate Professor Raph Hix, and Adjunct Professor Jirina Stone, all of whom are based at Oak Ridge National Laboratory. They are joined on the proposal by John Blondin of North Carolina State University and Stephen Bruenn of Florida Atlantic University.