Computing the physics that links nuclear structure, element formation, and the life and death of stars

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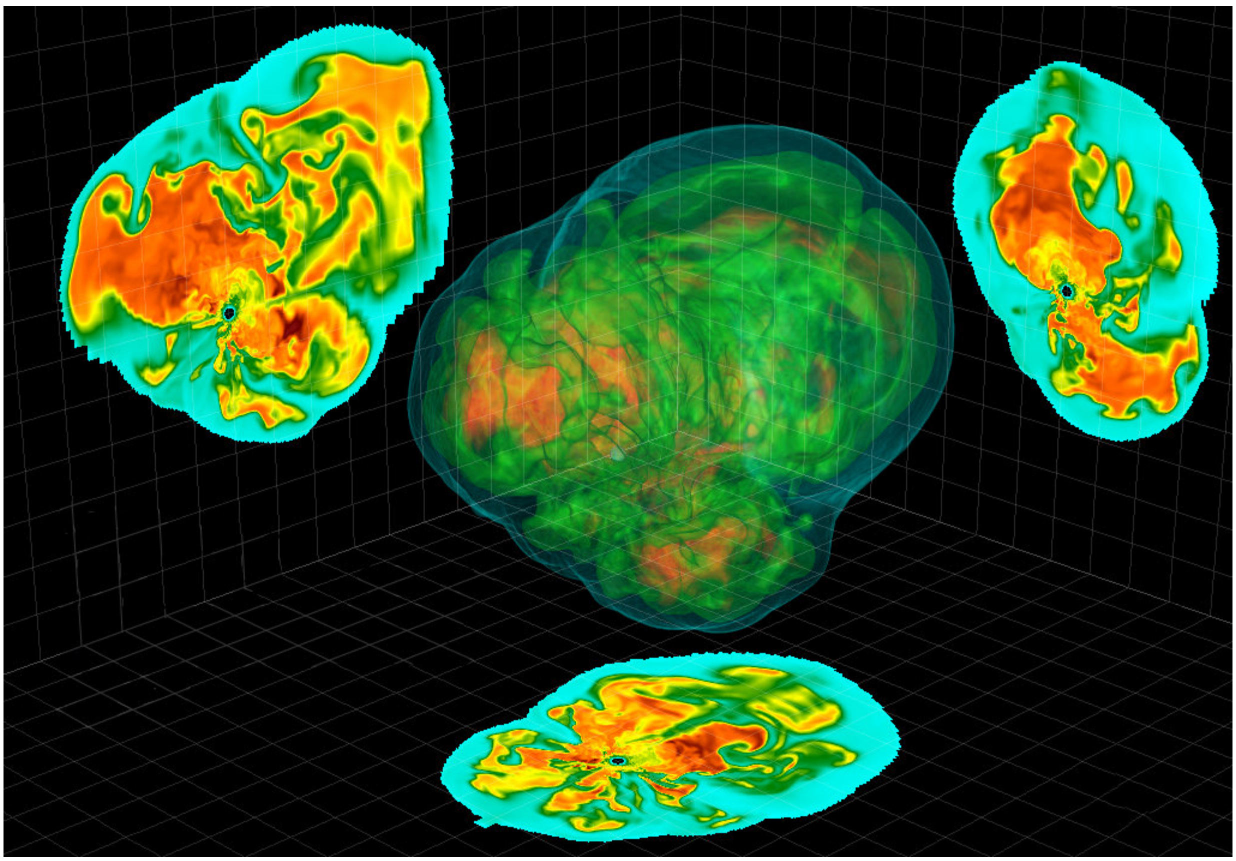

When a neutron star forms, compression creates heat that generates neutrinos. When the star's core collapses, a shock wave propagates around the star but stalls. The neutrinos reenergize a stalled shock wave, and the convection created leads to an asymmetric explosion that shoots elements into the cosmos. The heat content, or entropy, is shown, with greater entropy represented by "warmer" hues. At center is a volume rendering of the developing explosion above the newly formed neutron star (based on a simulation with the CHIMERA code); side images of orthogonal slices through the star reveal additional detail. Credit: Oak Ridge National Laboratory

The Big Bang began the formation and organization of the matter that makes up ourselves and our world. Nearly 14 billion years later, nuclear physicists at the Department of Energy's Oak Ridge National Laboratory (ORNL) and their partners are using America's most powerful supercomputers to characterize the behavior of objects, from subatomic neutrons to neutron stars, that differ dramatically in size yet are closely connected by physics.

Through the DOE Office of Science's Scientific Discovery through Advanced Computing (SciDAC) program, which concurrently advances science and supercomputing to accelerate discovery, ORNL is participating in two five-year computational nuclear physics projects.

Collaborators on the first project, the Nuclear Computational Low Energy Initiative (NUCLEI), will calculate properties and reactions of diverse atomic nuclei that are important in earthly experiments and astrophysical environments. Approximately 30 researchers at 12 national labs and universities are slated to share funding of $10 million. Joseph Carlson of Los Alamos National Laboratory (LANL) heads NUCLEI, with Stefan Wild of Argonne National Laboratory as co-director for applied math and computer science and Thomas Papenbrock of the University of Tennessee, Knoxville (UTK) and ORNL as the co-director for physics.

The second project, Towards Exascale Astrophysics of Mergers and Supernovae (TEAMS), partners 32 researchers from 12 national labs and universities. With planned support of $7.25 million, workers will simulate supernovae explosions and neutron-star mergers that create atomic elements heavier than iron and predict signatures of these cataclysms, such as gravitational waves. Raph Hix of ORNL heads TEAMS, with Bronson Messer of ORNL as the computational lead and Chris Fryer of LANL as the science lead.

"There is a nice synergy—NUCLEI is doing pure nuclear physics and TEAMS is, in a sense, doing applied nuclear physics," said Hix, a nuclear astrophysicist. "We need their nuclear physics to do our astrophysics."

NUCLEI partners will calculate the structure, reactions, interactions and decays of stable and radioactive nuclei (elements that decay to more stable states) for comparison with results of experiments at DOE facilities such as the Facility for Rare Isotope Beams (FRIB), under construction at Michigan State University. Because astrophysicists need high-quality input about how nuclei really behave, information from NUCLEI and from experiments will be used in TEAMS simulations that explore how nuclei are created under the extreme conditions of dying stars.

For both SciDAC projects, science and computing experts will start from state-of-the-art models, numerical techniques and leadership-class high-performance computers, such as Titan, ORNL's current workhorse supercomputer, or Summit, coming in 2018.

Calculating key nuclei

How does the strong force bind protons and neutrons into nuclei? How do light atomic nuclei capture neutrons to create heavier elements in stars? What is the nature of the neutrino, which plays crucial roles in radioactive decay and supernovae explosions?

These are some questions NUCLEI researchers will explore using advanced applied mathematics, computer science and physics to describe atomic nuclei. The calculations are computationally costly. "With 100 or more particles, exact solutions became exponentially costly," Papenbrock said. "New methods enable efficient performance on the fastest supercomputers."

ORNL's critical contribution to NUCLEI's scientific community is the coupled-cluster method, an efficient, systematic expansion of the nuclear wave function with a modest computational cost. Its solution provides detailed insights into the structure and decay of atomic nuclei and nuclear interactions. ORNL's lead for the NUCLEI collaboration, Gaute Hagen, also leads the development of a flagship code NUCCOR (NUclear Coupled Cluster Oak Ridge). NUCCOR provides a compromise between high accuracy and affordable computer cost.

At ORNL, Hagen, Gustav R. Jansen and George Fann will compute properties of nuclei and their decays. At UTK, a postdoctoral fellow will work with Papenbrock on the project. NUCLEI's partners at other institutions will bring their own codes, computational methods, and expertise to the project. "Atomic nuclei exhibit very different properties as one goes from the lightest nucleus with a single nucleon—a proton—to the heaviest, consisting of about 240 nucleons [protons or neutrons]," Papenbrock explained. "In this collaboration, we have complementary methods that are good for different nuclei."

Hagen said, "At Oak Ridge we developed first principles methods that can describe medium mass and heavy nuclei starting from the underlying interactions between nucleons. This is remarkable progress in the field. A decade ago we were computing the structure of oxygen-16, the oxygen we breathe, which [has] 16 nucleons. Today we just submitted a paper on tin-100, which has 100 nucleons."

NUCLEI researchers will calculate properties of key isotopes, such as calcium-60, which has 20 protons and 40 neutrons, and is therefore more exotic than the common stable isotope in our bones and teeth, calcium-40 (20 protons, 20 neutrons). "Calcium-60 has not been measured yet," Hagen said. "Nothing's known. To go to that region—and beyond—would be a major challenge for theory. But eventually we'll get there with the tools that we're developing and the computing power that will be coming available to us in this SciDAC period."

The biggest nucleus the scientists propose to compute from scratch is lead-208. Knowledge gained about what keeps its nucleons together might impact the understanding of superheavy elements beyond lead-208. Moreover, the calculations will complement both present and pending experiments.

The stars in ourselves

"Astrophysics is a quintessentially multi-physics application," said Hix, who leads the other SciDAC project in which ORNL participates, known as TEAMS. "There are so many facets of physics involved; nobody can be expert in all of it. So we must build teams."

The members of the TEAMS project will improve models of the deaths of massive stars, called core-collapse supernovae, which disperse chemical elements throughout the galaxies, as well as models of the final hours of the stars' lives that set the initial conditions for core-collapse supernovae. They will also improve models of the mergers of neutron stars, which create black holes while also dispersing newly formed elements.

Improving the TEAMS simulations will require better microscopic nuclear physics, improving our understanding of the states of nuclear matter and its interactions with neutrinos. TEAMS scientists will also study the consequences of explosions detectable by telescopes and the chemical history of our galaxy, providing observations that can be compared with simulations to validate models.

In core-collapse supernovae, massive stars (10 times the mass of our Sun) build up an iron core surrounded by layers of lighter elements—e.g., silicon, oxygen, carbon, helium, hydrogen. Eventually the iron core collapses to form a neutron star, launching a shock wave.

Since the 1960s, scientists have tried to simulate how this shock wave produces a supernova, starting with one-dimensional models that assumed the star was spherically symmetric. Simulations based on those models rarely resulted in explosions. More recently, with better understanding of the physics and faster computers, researchers started running two-dimensional, and later three-dimensional, core-collapse supernova models with improved physics.

"The behavior in two or three dimensions is completely different and you get the development of big convective regions," Hix said. "It is neutrino energy delivered to the shock wave by convective flows that ultimately powers up the explosion. The result is an asymmetric explosion that shoots out big plumes."

The power source that drives this explosion is the newly made neutron star, its Sun-sized mass compressed into a mere 30 kilometers, releasing tremendous energy that is carried away rapidly by neutrinos. Capturing just a small fraction of the escaping neutrinos reenergizes the shockwave, leading to the supernova.

The material that gets shot out into the galaxy by the supernova is available to make the next generation of stars. Elements—the oxygen in your breath, the iron in your blood—are tangible tracers of the chemical evolution of our galaxy all the way back to the Big Bang. "The story your atoms could tell!" Hix exclaimed. "Billions of years ago and thousands of light years away, parts of you have been through supernovae, neutron star mergers and other exotic events, and we can prove it because you carry all of the elements and isotopes that were made there. There's a tendency when people look at the sky to say, 'Oh, that's the universe.' But the universe is here too," he said, tapping his chest.

Provided by Oak Ridge National Laboratory

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