Supercomputer simulations provide new insights into calcium-48's controversial nuclear magnetic excitation

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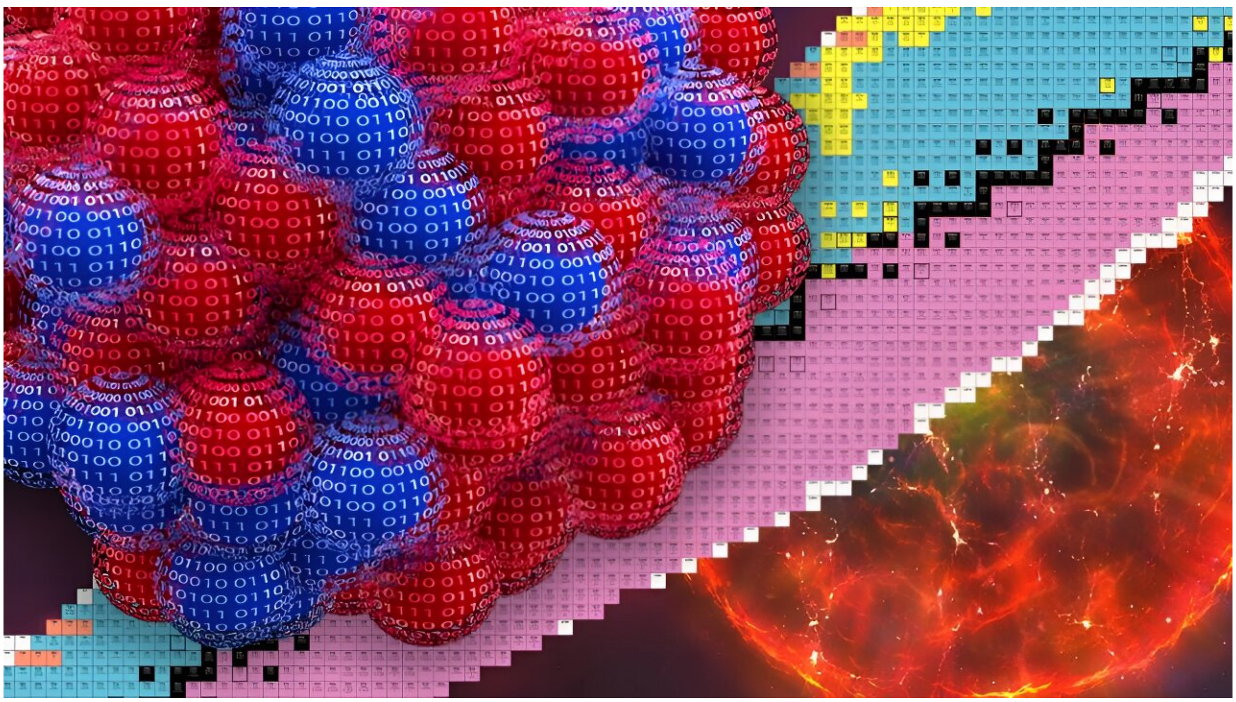

The Frontier supercomputer simulated magnetic responses inside calcium-48, depicted by red and blue spheres. Insights into the nucleus's fundamental forces could shed light on supernova dynamics. Credit: ORNL, U.S. Dept. of Energy

The world's most powerful supercomputer is helping resolve conflicting research results that have puzzled scientists for more than a decade, which could also shine new light inside collapsing stars.

Nuclear physicists at the Department of Energy's Oak Ridge National Laboratory recently used Frontier, the world's most powerful supercomputer, to calculate the magnetic properties of calcium-48's atomic nucleus. Their findings, published in the journal *Physical Review Letters*, will not only provide a better understanding of how magnetism manifests inside other nuclei but will also help to resolve a decade-old disagreement between experiments that drew different conclusions about calcium-48's magnetic behavior. Additionally, the research could provide new insights into the subatomic interactions that happen inside supernovae.

"The calcium-48 nucleus has an excited state that decays quickly because it has strong magnetic interactions and one of the highest transition strengths," said Gaute Hagen, a computational physicist at ORNL. "We're very interested in the rules that govern how nuclei are made. Simulating the fundamental forces inside calcium-48 will help us better understand how it's created and perhaps also give us some insight into what other nuclei could exist."

Calcium-48 is an important isotope used for scientific research. Its nucleus is composed of 20 protons and 28 neutrons—a combination that scientists call "doubly magic." Magic numbers—such as 20 and 28—are specific numbers of protons or neutrons that provide stability by forming a complete shell within the nucleus.

The strong binding and simple structure of calcium-48 also makes it an interesting test subject for studying the strong and weak nuclear forces that hold particles together or break them apart.

Like flipping a light switch, scattering electrons or photons off calcium-48 energizes and excites the nucleus, causing it to become magnetic and flip. This action, called the magnetic dipole transition, is dominated by the spin flip of a single neutron.

What happens in that precise moment is what Hagen and his colleagues are seeking to understand—a query that has puzzled the scientific community for more than a decade.

The decade-old disagreement

In the early 1980s, scientists studied calcium-48's magnetic dipole transition by bombarding the isotope with different beams of protons and electrons. The beams energized the nucleus with approximately 10 megaelectron volts, or MeV—just enough to spark a magnetic signature.

They determined the strength of the magnetic transition to be 4 nuclear magnetons squared. Magnetons are units of measure used in nuclear physics to describe the magnetic behavior of a nucleus.

But in 2011, nearly three decades later, researchers obtained significantly different results after studying the isotope with gamma rays and exciting the nucleus to the same energy level. They measured a magnetic transition strength that was almost two times stronger than what was previously recorded.

"As nuclear physicists, we compute nuclei from scratch based on state-of-the-art theoretical models of nuclear forces," said co-investigator Thomas Papenbrock, ORNL physicist and joint faculty member at the University of Tennessee, Knoxville. "The discrepancies between the different experiments motivated us to find out what result we would get if we used those theoretical models to study the magnetic transition."

Unleashing Frontier

The Frontier supercomputer—managed by the Oak Ridge Leadership Computing Facility, a DOE Office of Science user facility located at ORNL—is the world's first exascale machine and can perform more than a quintillion, or a billion-billion, calculations per second. The system's incredible computing power enabled Hagen's team to conduct simulations with remarkable efficiency and precision.

The team used a model called chiral effective field theory to connect nuclear phenomena to the fundamental theory of the strong nuclear force—the theory of quantum chromodynamics. They used a powerful numerical method called the coupled-cluster method to compute the properties of the calcium-48 nucleus. The approach provides a compromise between high precision and detail and computational cost, making it an ideal task for Frontier.

The simulations showed that calcium-48's magnetic transition strength was consistent with the results of the gamma ray experiments.

But shedding light on the magnetic dipole transition wasn't all they did. They also investigated other factors such as so-called continuum effects that describe how the nucleus interacts with its surroundings. Additionally, they examined how pairs of nucleons—the particles found within the nucleus of an atom—interact inside the nucleus during the transition and how they contribute to the overall electromagnetic properties.

The simulations showed that continuum effects reduced the magnetic transition strength by about 10%. And, contrary to previously held beliefs that nucleon pair interactions significantly suppress or weaken the magnetic transition strength, the simulations showed that in some cases, these effects slightly increased the magnetic transition strength.

"Hopefully, this will inspire experimentalists to reexamine their approach and make important adjustments. Or, perhaps, in time, we could learn that the lower values recorded in the 1980s experiments were in fact correct," said Hagen. "That would mean the theory we are using is incomplete, which would also be a shock in so many ways. But, either way, we will learn a lot from this."

"What we expect is that the computations will stimulate new discussions between the theorists and the experimentalists," added Papenbrock. "For now, this puts the ball back in the experimentalists' court."

From subatomic to astronomic

Bijaya Acharya, the study's first author, is a postdoctoral fellow in ORNL's Theoretical and Computational Physics group. One of Acharya's primary responsibilities was developing the algorithms that allowed the team to study many of the higher-order quantum effects in the simulations. He specializes in studying neutrinos—tiny particles created from exploding stars that travel through space at nearly the speed of light. Neutrinos are generated by nuclear fusion reactions in the sun's core and are also produced by nuclear reactors on Earth.

"We see the abundance of calcium-48 deep inside the core of a collapsing supernova, where there's also a large neutrino exposure," said Acharya. "The physics that describes the magnetic transition strength in calcium-48 also describes how neutrinos interact with matter.

"That suggests that larger transition strengths also imply that neutrinos are more likely to interact with matter. So, if the value of the magnetic transition strength is larger than previously thought, that means that reheating and other factors associated with neutrino interactions in supernova explosions would also be larger, and vice versa for smaller values. And that would, of course, greatly influence our understanding of these massively large systems."

Stars are like alchemists, explained ORNL nuclear astrophysicist and group leader Raphael Hix. The star dust emitted from supernovae contains a wide range of newly created nuclei, including calcium-48 in some cases, and these new heavy elements seed the creation of new generations of stars and planets.

"You can't understand how Mother Nature does that in a star unless you understand the rules that she has for putting nuclei together. That's fundamentally what Hagen's calculations are about," said Hix. "And like alchemy, someone will turn these calculations into interesting reaction rates, and then those reaction rates will be turned into astrophysics calculations to help us better understand the universe."

More information: B. Acharya et al, Magnetic Dipole Transition in ^{48}Ca, *Physical Review Letters* (2024). DOI: 10.1103/PhysRevLett.132.232504. On *arXiv*: DOI: 10.48550/arxiv.2311.11438

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