Particle interactions on Titan support the search for new physics discoveries

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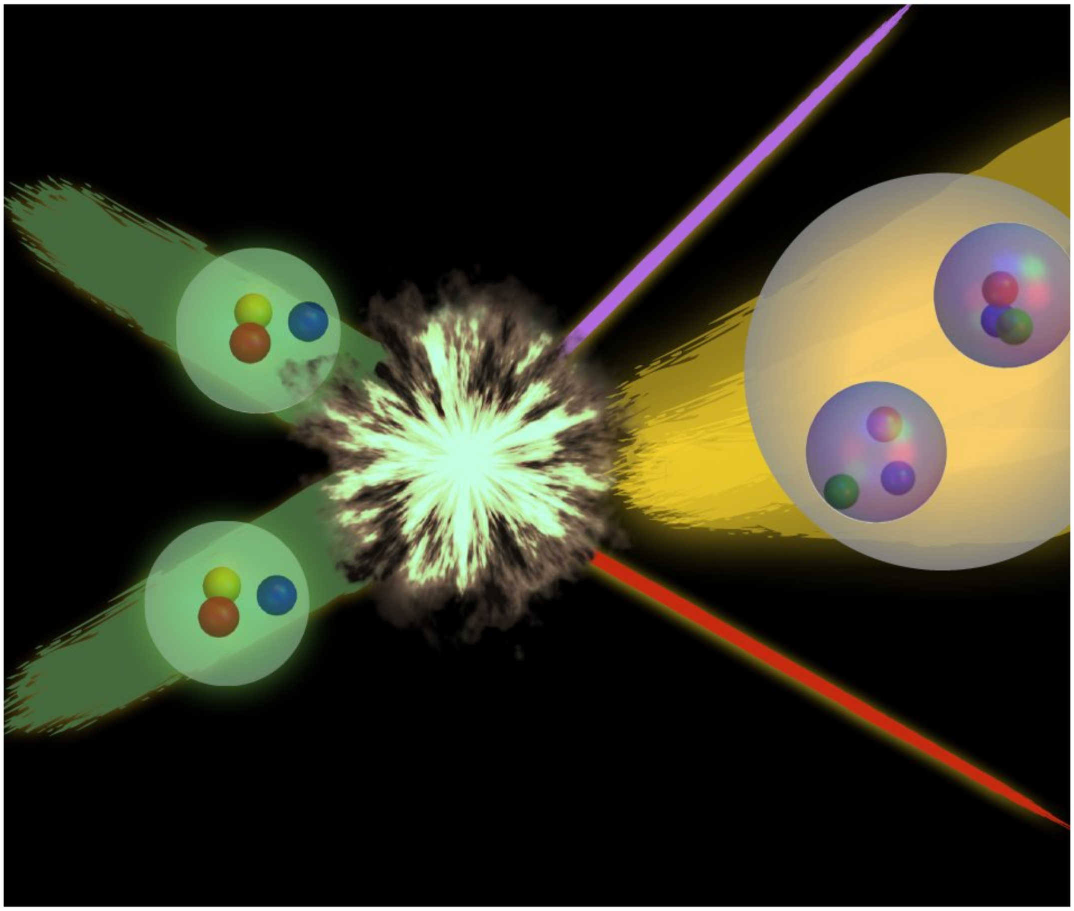

A conceptual illustration of proton-proton fusion in which two protons fuse to form a deuteron. Credit: William Detmold

Nuclear physicists are using the nation's most powerful supercomputer, Titan, at the Oak Ridge Leadership Computing Facility to study particle interactions important to energy production in the sun and stars and to propel the search for new physics discoveries

Direct calculations of these nuclear processes can contribute new and fundamental information to the fields of high-energy physics, nuclear science, and astrophysics, including how matter formed in the early universe and its relation to dark matter and the large-scale structure of the universe.

The research team using Titan, including principal investigator William Detmold of the Massachusetts Institute of Technology, is calculating proton-proton fusion—a process that powers the sun and other stars in which two protons fuse to form a deuteron—and double beta decay, a rare process which occurs when an unstable nucleus decays by emitting two electrons with or without neutrinos (subatomic particles with near-zero mass).

Although double beta decay with neutrinos has been observed in experiment, the team is focused on neutrinoless double beta decay—a type of double beta decay predicted by theory in which no neutrinos are emitted, only electrons. Yet to be observed, this neutrinoless process is of great interest to physicists because it could lead to new discoveries beyond the current model of particle physics known as the Standard Model.

The Standard Model, a description of all the known subatomic particles and fundamental forces in the universe except for gravity, has held up in experiments time and again. However, the Standard Model is not complete because it cannot fully explain what scientists observe at the cosmic scale.

Based on observations of galaxies, supernova, and other phenomena, researchers estimate that the universe consists of very little ordinary matter (only about 5 percent) and is mostly unseen dark matter that exerts a gravitational pull on ordinary matter (about 25 percent) and dark energy (about 70 percent). Yet scientists do not know what makes up dark matter or in what ways it may interact with ordinary matter other than gravitationally.

To help answer these and other cosmic questions, experiments are being built around the world to probe particle interactions at new scales and energies, and supercomputers are being used to simulate rare or theoretical interactions. By modeling the interactions of simple nuclei, physicists can understand the kind of experiments they need to build and what they may expect from experimental data.

On Titan, Detmold's team used complex lattice quantum chromodynamics (QCD) calculations to predict the reaction rate—the probability that nuclear fusion or decay will occur—of proton-proton fusion and an important part of the theoretical rate of neutrinoless double beta decay.

"We're showing that you can see the bound states of nuclei using quantum chromodynamics," Detmold said. "From there, we're calculating the simplest nuclear processes that happen."

Modeling space-time

Nuclear fusion of hydrogen—the lightest element consisting only of a proton and electron—powers stars for millions to billions of years. Detmold's team calculated the proton-proton fusion cross section on supercomputers because this interaction plays a critical role in solar energy production.

"We can't experimentally probe proton-proton fusion that well," Detmold said. "Even if you take a proton target and irradiate it with a beam of protons, the protons will just scatter, not fuse, so this fusion process is very rare in the laboratory."

In this process, two protons overcome their electromagnetic repulsion between like charges and interact through the short-range, subatomic force known as the weak force.

Lattice QCD calculations represent how the fundamental particles that make up protons—quarks and gluons—interact in the volume of space-time in which proton-proton fusion occurs. Quarks are the smallest known constituents of matter, and gluons are the force-carrying particles that bind them. Named for the 4-D grid (the lattice) that represents space-time and the unique "color charge" (chromo), which refers to how quarks and gluons combine rather than to actual colors, lattice QCD calculations are intensive computations that can require supercomputing power.

Efficiently using Titan's GPU-accelerated architecture, Detmold's team used the Chroma lattice QCD library (developed primarily by Robert Edwards and Balint Joò of Thomas Jefferson National Accelerator Facility) with a new algorithm to include weak interactions important to proton-proton fusion and QUDA, a lattice QCD library for GPUs (developed primarily by Kate Clark of NVIDIA). The calculations generated more than 1,000 snapshots of the 4-D lattice with 10 million points of calculation per snapshot.

"These are the first QCD calculations of the proton-proton fusion rate," Detmold said.

Researchers used the same lattice QCD algorithms to calculate another weak interaction process, tritium beta decay, which has been studied experimentally and was used to verify the calculations.

Narrowing the search

Researchers also calculated subprocesses that contribute to double beta decay rates, including theoretical rates for neutrinoless double beta decay.

A rare particle event, double beta decay was first predicted in 1935 but not observed in experiments until the 1980s. This type of decay can occur naturally when two neutrons decay into two protons inside a nucleus, emitting two electrons and two neutrinos in the process. Although rare, double beta decay occurs in some isotopes of heavy elements as a way for the nucleus to stabilize its number of protons and neutrons.

Neutrinoless double beta decay, also predicted over half a century ago, has never been observed. However, this potential process has gained much more significance in recent years since physicists discovered that neutrinos have a small mass. Because the neutrino has a neutral charge, it is theoretically possible that it is its own antiparticle—a particle of the same mass but opposite charge. Antiparticles exist in nature and have been created and observed in experiment, but matter particles are much more dominant in nature.

A particle that is its own antiparticle, known as a Majorana particle, could help explain the mechanism by which matter took precedence over antimatter in the universe, which is one of the great outstanding questions in cosmology.

Many experiments across the globe are trying to observe neutrinoless double beta decay, which would confirm the existence of a Majorana neutrino. Such a discovery would, for the first time, provide an unambiguous signature of the violation of lepton number conservation—the principle that describes balance between certain types of matter particles and their antiparticles.

Experiments such as the MAJORANA Demonstrator at the Sanford Underground Research Facility cool heavy elements in underground laboratories to temperatures colder than empty space. In their remote locations with heavy shielding, neutrino detectors like the MAJORANA Demonstrator are enabling scientists to narrow their search for rare neutrino interactions.

Because neutrinoless double beta decay is theoretical and, if real, still very rare, researchers must make extremely refined predictions of its reaction rate. The smaller the reaction rate, the less likely experiments will be able to capture the process and the bigger the experimental detector needs to be. The Titan calculations help researchers understand potential decay rates.

"Ultimately, what we are trying to determine is how likely an experiment of a given size is going to be able to see this process, so we need to know the reaction rate," Detmold said.

Current neutrino experiments are pilot scale, using tens of kilograms of a heavy element medium (germanium crystals in the case of MAJORANA). Future detectors could be built at ton scale, and it is important to know that such an experiment would be sensitive enough to see neutrinoless double beta decay if it exists.

The team's calculations of double beta decay on Titan provide the kind of theoretical support experimentalists need to develop experiments and analyze data.

But proton-proton fusion and neutrinoless double beta decay are only two nuclear processes of many that can be gateways to new discoveries in physics.

With next-generation systems like the OLCF's Summit supercomputer, which will come online later this year, these calculations will be taken to a new level of accuracy, and researchers can begin to study the decays and interactions of more complex nuclei.

"Now that we've shown that we can control these few nucleon processes, we can start calculating more complicated processes," Detmold said.

More information: Phiala E. Shanahan et al. Isotensor Axial Polarizability and Lattice QCD Input for Nuclear Double- β Decay Phenomenology, *Physical Review Letters* (2017). DOI: 10.1103/PhysRevLett.119.062003

Martin J. Savage et al. Proton-Proton Fusion and Tritium β Decay from Lattice Quantum Chromodynamics, *Physical Review Letters* (2017). DOI: 10.1103/PhysRevLett.119.062002

Provided by Oak Ridge National Laboratory

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