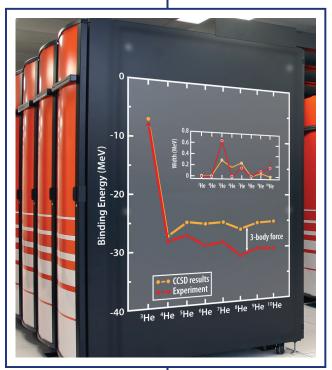
NATIONAL CENTER FOR COMPUTATIONAL SCIENCES



Beyond the Valley of Beta Stability Researchers probe the nature of fleeting nuclei

Protons and neutrons go together inside an atom's nucleus just so. Each time you add a proton -- the tiny, charged particle that determines what element an atom will be -- you need just the right number of uncharged neutrons to make the nucleus stable.



Supercomputers enable nuclear calculations that were impossible only a few years ago. The graph above shows the first-ever ab initio computation (yellow) of weakly bound nuclei in coupledcluster theory which was enabled by ORNL's Jaguar (above).



Being held together by the same force that binds even smaller quarks to make protons and neutrons in the first place, the nucleus is very picky about how it's arranged. Start out with one proton and you have hydrogen. Add a proton and you have helium, but you need one or two neutrons to balance the two protons. Add another proton and you have lithium, but you need three or four neutrons there as well.

The process continues up the roster of elements. Through about nickel, with 28 protons, the number of neutrons in stable nuclei will just about match the number of protons. Moving farther up the roster, the number of neutrons will exceed the number of protons; the platinum in your ring, for instance, has 78 protons but 116 neutrons. Still, if you were to put the numbers on a chart, the journey through the stable nuclei would move up the chart in a continuous line. This line is known as the Valley of Beta Stability, and it encompasses the nuclei that make up the world we encounter.

Not all nuclei are stable, just the ones that last. Most of the elements in the universe are produced by exploding stars known as supernovas, and most of these new nuclei are unbalanced, having far too many neutrons or protons to be stable. As a result, these very unstable nuclei sometimes last only a tiny fraction of a second.

Add too many neutrons or protons and the nucleus will do what it must to become stable. Near stability this means the nucleus will go through a process known as beta decay. Either a neutron emits a negatively charged electron and a small, uncharged particle called a neutrino, turning the neutron itself into a positively charged proton, or a proton emits the positively charged version of an electron -- known as a positron -- along with a neutrino and becomes an uncharged neutron. Farther from stability -- in a region known as the "drip line" -- the process might involve the nucleus expelling excess neutrons, protons, or alpha particles.

"When these very neutron-rich nuclei are made within a star, they go through all kinds of different physical processes, and then they become half of the heavy elements in your body," explained Oak Ridge National Laboratory physicist David Dean. "We like to understand how those things happen."

Dean and a team of researchers from the University of Tennessee, Argonne National Laboratory, and Iowa State University are using the National Center for Computational Sciences' Cray XT4 Jaguar supercomputer to probe the nature of these fleeting, unstable nuclei in an effort to better understand all nuclei, stable and unstable alike. The team's work ultimately promises to help make nuclear power generation more stable and reliable as well as to ensure the effectiveness of America's nuclear stockpile.

The work will also help us understand ourselves and the world in which we live a little better.

Dean discusses his work in the November issue of Physics Today, published by the American Institute of Physics.

"What we've found over the last decade is understanding the stable nuclei isn't enough," Dean explained. "We know what happens in stable nuclei pretty well -- there are only 300 of them -- but when you add neutrons to the nucleus, you isolate and amplify different aspects of the underlying interactions within the nucleus. You can make a better theoretical description of all nuclei by understanding the very neutron-rich nuclei."

By pursuing unstable nuclei, the team has expanded its list twentyfold, from around 280 stable nuclei to 6,000 possible nuclei. It is pursuing its calculations on Jaguar using several techniques, depending on the size -- and therefore complexity -- of the nucleus.

Three of these approaches are ab initio calculations, relying on the specific properties and interactions of individual particles. While these techniques provide the most accurate information possible, the calculations become overwhelming as the team pursues everlarger nuclei. Nevertheless, one of these techniques has scaled more successfully than the others. The team has successfully applied coupled-cluster theory, as the technique is known, to medium-mass nuclei. A fourth technique, known as density functional theory, is able to calculate the properties of larger nuclei by relying on the density of particles interacting with each other. "You get different kinds of physics depending on how many particles you have in the nucleus," Dean said, noting that members of his team are world leaders in nuclear density functional theory. "With just two particles you never see the kind of effects that you have with 100 particles or 200 particles."

As it moves forward, the team also needs the help of experimental facilities. Physicists are discovering that exotic nuclei far from stability have unexpected properties, and computational scientists must be able to validate their calculations. On the other hand, it is both expensive and time consuming to explore these nuclei using accelerators. The Facility for Rare Isotope Beams under consideration by the Department of Energy and the National Science Foundation, for example, would cost half a billion dollars to construct and would not be available for years.

"At some point you won't be able to do all experiments on nuclei," Dean explained. "What experiments do for you is to enable you to benchmark your theory, to say, 'Ah, I know what my theory is doing in this region.'

"What we're doing is calculating the whole mass table -- all 6,000 nuclei -- and once you calculate that you can compare the ones that are measured -- maybe 2,000 -- to experiment."

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