Physicists wipe away complexity for a clearer view of heavy nuclei

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Despite advances in experimental nuclear physics, the most detailed probing of atomic nuclei still requires heavy doses of advanced nuclear theory. The problem is that using theory to make meaningful predictions requires massive datasets that tax even high-powered supercomputers.

In a March 16 *Physical Review Letters* article, researchers from Michigan State and Central Michigan universities report dramatic success in stripping away much of this stubborn complexity. The advance, which slashes computational time from days or weeks to minutes or hours, may help address one of the most important questions in nuclear physics today: what is the structure of heavy atomic nuclei?

At the heart of this question is the devilish difficulty in modeling any system with multiple particles that interact via the nuclear force. One way to tackle this so-called many-body problem is to first construct mathematical functions that describe each particle, and then start multiplying these functions together to get some idea as to the underlying physics of the system.

It’s a brute force approach that works well enough to describe light nuclei but is a computational nightmare when it comes to heavier elements, which have greater numbers of protons and neutrons.

Describing each particle, which can exist in any number of quantum states, is complicated enough. But when modeling a system composed of several dozen or more of these particles, each of which potentially interacts with every other particle, the computational complexity quickly becomes astronomical in magnitude.

For example, applying this approach to Nickel-56, the isotope with 28 protons and 28 neutrons that is the subject of the research, effectively means solving an equation with 1 billion variables. The result is "a huge computational effort, which has become feasible only recently," the authors note.

Chemistry researchers face a similar problem in studying molecules with many dozens of interacting electrons. Yet all electron interactions are not created equal, and for decades scientists have relied on this fact to build streamlined models that stem the tide of quantum data that needs to be computed.

The key is correlation, the idea that some pairs of electrons are strongly linked and related. Correlations are what make it possible to rely on a modicum of data to make predictions about a complex system like a molecule, an atomic nucleus or even the nightly crowd at a restaurant.

To decide how to make the best use of a limited supply of tables, restaurant owners don't need to think of every potential customer as likely to interact with every other customer and move freely from table to table. Rather, most maitre d's can anticipate seeing customers who show up in pairs or small groups and tend to stick together during any given evening. Observing similar behavior in electrons, quantum chemists have worked for decades to build and refine the coupled cluster theory, which today has emerged as the preeminent approach to explaining complex molecular systems.

Correlations also loom large in current theory of atomic nuclei. For several years, scientists have known that focusing on the behavior of pairs of nucleons – the generic term for protons and neutrons – goes a long way to painting an accurate picture of the entire atomic nucleus. But until now, no one had used coupled-cluster theory with heavy atomic nuclei.

The researchers first relied on the MSU High Performance Computing Center and the CMU Center for High Performance Scientific Computing for the weeks-long task of solving the billion-variable equation describing Nickel-56, in effect generating a yardstick by which to measure their more abbreviated model. Next they compared their energy and wave function data to those generated by the computationally expensive alternative.

Coupled-cluster theory produced near identical results and the time spent crunching the numbers – on a standard laptop – was often measured in minutes or even seconds.

"Sometimes it took longer to input the information than to run the calculation," said Piotr Piecuch, one of the authors and a professor in the MSU Department of Chemistry and the MSU Department of Physics and Astronomy and at National Superconducting Cyclotron Laboratory.

Other MSU authors include Alex Brown, NSCL professor; Marta Wloch, a research assistant professor in Chemistry in Piecuch's group; and Jeff Gour and Maricris Lodriguito, doctoral students in Chemistry in Piecuch's group. The lead author is Mihai Horoi, associate professor in the Department of Physics at Central Michigan University. Horoi and Brown did the daunting supercomputing work of solving the billion-term equation and analyzing the results, while Gour, Wloch, Lodriguito and Piecuch performed the coupled-cluster calculations.

Their research bodes well for next-generation nuclear science. Because of existing and planned accelerators around the world, the next few decades promise to yield a panoply of heavy isotopes for study.

Theoretical models will need to keep pace with this expected avalanche of experimental data. To-date, many such models have treated the nucleus as a relatively undifferentiated liquid, gas or other set of mathematical averages – all of which tends to gloss over subtle nuclear nuance.

In contrast, coupled cluster theory may be the only manageable and scalable model that takes a particle-by-particle approach.

"We're really starting to see the nucleus from a microscopic perspective," said Piecuch. "This gives us a way to start with particles, in this case nucleons, build an equation and then solve it – and to do so in a way that is computationally efficient.

Several of the authors are active in the MSU Mesoscopic Theory Center, a focal point for collaborations between nuclear and condensed matter physicists, chemists, mathematicians and scientists from other disciplines. Created in fall 2006, the center seeks to understand the emergence of complexity from interactions of elementary constituents. The work of Piecuch and his colleagues suggests that generic solutions to these mesoscopic problems may be at hand.

"What's most exciting may be broad applicability of the model," Piecuch said. "Coupled cluster theory grew up in chemistry but seems to work equally well in nuclear physics, where the physical dimensions and forces are hugely different."

Source: Michigan State University