NUCLEAR PHYSICS

A historic match for nuclei and neutron stars

Bayesian history matching is a statistical tool used to calibrate complex numerical models. Now, it has been applied to first-principles simulations of several nuclei, including ^{208}Pb, whose properties are linked to the interior of neutron stars.

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Nuclei are strongly-interacting many-body systems formed of N neutrons and Z protons; their sum equals the mass number A. The first-principles modelling of these complex systems is known as the ab initio approach and has brought significant advances to nuclear physics in the last decade. From predictions of nuclear masses and radii to fusion and decay modes, a wide range of phenomena have been addressed starting with neutrons and protons as degrees of freedom and including their interactions through a systematically improvable Hamiltonian. Despite the recent advances of ab initio nuclear theory, the developments have seemingly come to a halt in the last couple of years, with crude uncertainty estimation schemes and the largest simulations limited to isotopes up to mass numbers around *130*[1]. Now, writing in Nature Physics, Baishan Hu and colleagues have presented a set of statistically meaningful predictions for ^{208}Pb with a mass number of *208,* thus overcoming — at once — several of the issues that were hampering the ab initio approach[2]. Their method can also be applied to the nuclear matter found in the interior of neutron stars.

Solving the many-body fermion problem is not easy, but in the last decade practitioners have shown that several methods exhibit an increase in computational time that is polynomial in A. With enough time on high-performance computers, one could — in principle — have tackled heavy nuclei, such as lead, a while ago. So why did ab initio approaches stall at a mass number around *130*? A key problem was the mere size of the interaction matrix elements associated with three-nucleon forces, which can reach tens to hundreds of terabytes. A recent breakthrough, published in the beginning of 2022 by some of the authors involved in the present study, introduced a novel storage scheme that reduced the size of these files to a few tens of gigabytes. This opened the door to ab initio simulations of heavy nuclei[3].

In addition to the issues associated to many-body simulations, a different hold-up was rooted in the nuclear Hamiltonian itself. Current state-of-the-art nuclear Hamiltonians use effective field theories, which are linked to quantum chromodynamics. These effective theories are built term by term, using the most general Lagrangians that are compatible with the symmetries of the system, according to a power counting scheme that works below a certain momentum scale[4]. Each term is multiplied by a so-called low energy constant (LEC), which parametrizes its strength. These LECs are either fitted to experimental data or inferred from high-energy, lattice quantum chromodynamics simulations. When it comes to the LECs associated to interactions among neutrons and protons, Hu and colleagues used data from nucleon–nucleon scattering experiments and the properties of selected nuclei to fit a total of 17 LECs. While some of these constants are associated with interactions between pairs of nucleons, others quantify the strength of genuine three-nucleon forces.

A key struggle of ab initio nuclear theory was the quantification of uncertainties associated with these LECs. In the early days, individual subsets of LECs were often chosen based on their performance on reproducing nuclear properties at the ab initio level. Theoretical errors were typically estimated using a few of these subsets, as shown in the left panel of Fig 1. This is, most likely, a statistically-biased assessment of uncertainties, but is computationally inexpensive. In contrast, a meaningful uncertainty quantification scheme requires the propagation of LEC central values, their individual statistical errors, and correlations into the many-body domain. In principle, this calls for an exploration of a 17-dimensional space coupled to ab initio many-body simulations — a very ambitious program that would consume massive computing resources.

Hu and colleagues managed to overcome these limitations with the help of recent innovations. First, rather than performing computationally expensive ab initio simulations of several isotopes, they created a set of numerical emulators. These emulators efficiently capture the LEC dependence of ab initio simulations at a fraction of their computational cost. The uncertainties caused by the emulation process are relatively small and can be included into the uncertainty quantification scheme.

While the use of emulators accelerated the scheme, the LEC search in a 17-dimensional space was still necessary. Hu and colleagues borrowed from research in other fields — most notably oil reservoir modelling — and applied Bayesian history matching[5] algorithms to constrain the search in a computationally tractable way. In history matching, computer model predictions are compared to experimental values to exclude areas of the parameter space that are statistically implausible. Hu and colleagues achieved this in five consecutive waves of theory–data comparisons. The first wave made use of data from neutron–proton scattering. The input of the second to the fourth wave was from increasingly heavier systems starting from nuclei with a mass number of two in the second wave. In the third and fourth waves, nuclei with mass numbers up to four and eventually *16* were included, and all the data was used in the final wave. Thanks to history matching, the parameter space search was reduced from 10^9 samples to as few as 34 non-implausible samples in the 17-dimensional LEC space.

To gauge the quality of these 34 samples, Hu and colleagues performed simulations for the well-known mid-mass isotope ^{48}Ca. By comparing with experimental data in this nucleus, where the LECs have not been fit, one can calibrate the quality of not just one, but several ab initio models, providing statistically meaningful weights to each of the 34 samples. In other words, with this technique one obtains not only LEC sets, but also the posterior distributions of LECs conditioned on the calibration data of ^{48}Ca (see right panel of Fig. 1).

Finally, in a true tour de force of ab initio methods, Hu and colleagues computed the heaviest doubly closed-shell isotope, ^{208}Pb, with these 34 LEC parameter sets. As explained above, up to a few months ago, it looked as if such heavy isotopes were out of reach for ab initio methods. Armed with the importance-sampled distributions, Hu and colleagues were able to predict the properties of ^{208}Pb together with their associated posteriors. Among several quantities of interest, they looked into the so-called neutron skin thickness, which is the difference between the average radius of the 126 neutrons and the 82 protons in this isotope. The neutron skin thickness was recently measured in parity-violating electron scattering experiments at the Thomas Jefferson National Acceleration Facility[6], providing much-debated results in the community. The ab initio simulations of Hu and colleagues prefer rather "thin" values for the neutron skin, with thicknesses between 0.14 and 0.20 fm, compared to the recently measured value of (0.283 ± 0.071) fm. The tension is at the 1.5σ level, and the theoretical results by Hu and colleagues are closer to previous indirect measurements of the neutron skin thickness using electromagnetic and hadronic probes.

Importantly, the very same methods applied to the study of ^{208}Pb can also provide predictions for an entirely different system: neutron stars. These astrophysical compact objects can be observed with a variety of tools ranging from radio telescopes to gravitational wave detectors. Future precise measurements of the radii and masses of neutron stars could potentially be used to discern between different nuclear Hamiltonians. In fact, Hu and colleagues confirmed a well-known correlation between the neutron skin of lead and the equation of state of neutron matter in the interior of neutron stars. Bayesian history matching has thus not only allowed for the first uncertainty-quantified, wide-ranging simulations of isotopes with mass numbers from 2 to 208, but it has also allowed practitioners to reach for the stars.

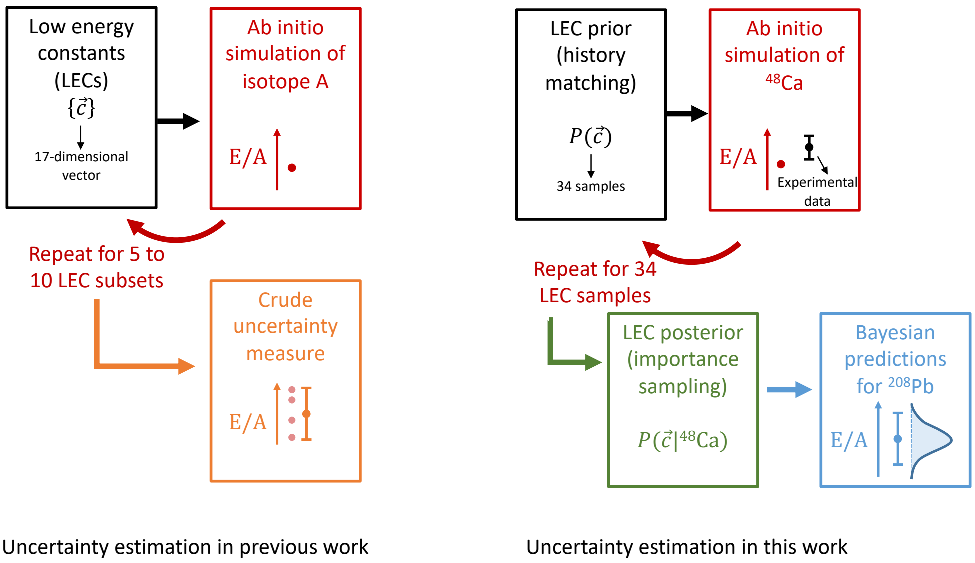

Fig. 1: Uncertainty estimation methods. (Left) In most previous studies, different low energy constant subsets were used to repeatedly compute the properties of a given isotope. Averages and standard deviations over these results were often used as model uncertainties. The illustration focuses on a single observable, the energy per particle of a given isotope. (Right) In contrast, Hu and colleagues used Bayesian history matching to find a prior distribution of low-energy constants. This is then calibrated on known properties of ^{48}Ca to obtain Bayesian posteriors, which can then be used in the predictions of the properties of ^{208}Pb.

COMPETING INTERESTS

The author declares no competing interests.

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