important approximations can be assessed quantitatively.

The dominant approach for quantum-mechanics-based materials simulation is density functional theory[2] (DFT), which maps the many-body problem to an equivalent problem in which the electrons do not interact directly with each other. In principle, this leads to a simpler, but still exact, solution of the Schrödinger equation. However, the exact mapping (the 'functional') is not known, so approximations are required. Fortunately for researchers, the available approximations are good enough for them to model the properties of many materials, yielding predictions within a few per cent of values obtained experimentally. There are some major problems with DFT, however, including its inability to correctly reproduce the energy curve that describes the binding of a single electron shared between two protons[3]; the exact solution of this problem is easy to obtain, because with only one electron, there is no many-body problem to solve.

Despite the thousands of papers published each year in which DFT is used as a modelling tool, a fundamental paradox remains: because the methods of DFT are not exact, any predictions must be carefully rationalized against experimental results and against the properties of similar materials. The methods are therefore at their weakest when little is known about the material being modelled. Alternative approaches are needed that are exact and that systematically converge on the experimental result. Such an approach would inevitably be more computationally expensive than DFT, but the costs could be justified by the savings made from having to do less experimental validation, and by the potential scientific value of the findings.

Booth and co-workers' method — full configuration interaction quantum Monte Carlo (FCIQMC) — uses a statistical approach to solve the Schrödinger equation. Other statistical methods have previously been used to solve the Schrödinger equation for materials, but these required approximations or have not been demonstrated to work well for a wide range of materials. The version of FCIQMC used to predict molecular properties is only 3 years old[4], but it has been rapidly developed and has in the past year been used to calculate the optical properties[5] of molecules, for example.

The method tames the exponential complexity of the many-body problem to such an extent that useful results can be obtained using current computational resources. Booth *et al.* describe extensions to the method that enable it to calculate the properties of solids that have periodic arrangements of atoms. The authors demonstrate that sufficiently converged properties can be achieved — albeit with some difficulty — for some insulating materials. Until now, no exact methods have been available to predict the properties of even the simplest of solids, although some approaches have come close[6,7].

Using FCIQMC can require tens of thousands of computation hours, whereas a comparable DFT calculation might take one hour. However, if the computed properties are converged, the FCIQMC result will be exact within statistically defined error bars, whereas the error for the DFT result will be unknown. One use of FCIQMC may therefore be to help to improve approximate methods for calculating material's properties.

In this spirit, the authors tested whether the gold-standard approach used by computational chemists to predict the properties of molecules — a method known as CCSD(T) — could be extended to predict the properties of solids, by comparing its results with those from FCIQMC. Promisingly, the researchers found that the errors of the CCSD(T) results were much smaller than those of many modern DFT functionals. Although the number of calculations required for CCSD(T) scales with the seventh power of the number of atoms, a wealth of computational-chemistry techniques and efficient implementations may reduce the practical cost.

"Booth and colleagues' computational method solves the Schrödinger equation without the need for any approximations."

One major challenge will be to extend the applicability of the FCIQMC method to larger and more complex systems than those studied by Booth and colleagues. The oxides of the first row of transition metals in the periodic table would be good targets, for example, because they display structural, magnetic and electronic phenomena that are challenging to reproduce in existing computational models. Even if full convergence of the predicted properties cannot be achieved, information about the quantum-mechanical wavefunction of these compounds may be highly informative.

For now, though, Booth and co-workers' method is restricted to simulating very simple materials at a temperature of absolute zero. Improvements to the algorithm that enhance performance can be expected — even a doubling of the system size that can be modelled would be useful. One can also envisage the development of an 'embedding' method that incorporates FCIQMC results into those of a cheaper approach to increase the achievable length scales. This would give accurate results if the physical effects that determine properties of interest are strongly localized. But surfaces and defects in solids will be difficult to model using the authors' approach because they require large numbers of atoms to be considered.

Promisingly, metals might be studied using modest extensions to Booth and colleagues' method, or by using the current method in combination with brute-force application of computer power. This would enable the entire phase diagram (a graph plotting the physical state of a material at different pressures and compositions) of simple materials to be predicted with confidence. For example, DFT predictions of previously unknown phases of elemental solids have been made in the past few years[8–10]. In future, FCIQMC might be able to determine exactly the pressures at which these phases occur, removing lingering suspicions around the accuracy of the DFT results.

For Booth and co-workers' method to have the greatest impact, researchers will need to learn to interpret the results of FCIQMC calculations and use them to improve cheaper, everyday methods for modelling materials properties. The common language of FCIQMC and computational chemistry may enable the development of specialized methods for materials, with an accuracy and reliability far exceeding today's DFT approaches. By helping to establish a hierarchy of trusted and validated computational methods for materials, the new technique should help to deliver one of the great promises of computational materials science. ■

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CORRECTION

In the News & Views article 'Astronomy: Andromeda's extended disk of dwarfs' by R. Brent Tully (*Nature* **493,** 31–32; 2013), 13 dwarf companion galaxies of the Andromeda galaxy are described as lying "at distances from Messier 31 of between 35 and 400 kiloparsecs (114–1,305 light years)". The distance values in units of light years should have been 114,000 to 1.3 million.