Project Information

Project title Quantum Monte Carlo simulations of magnetism and models in condensed matter

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Executive summary (150 words)

The researchers used high accuracy first principles quantum Monte Carlo calculations to study magnetic materials. These calculations are highly parallelizable and so could take advantage of Blue Water's high performance architecture. Blue Waters enabled the understanding of a strongly-correlated magnetic material $MgTi_2O_4$ and the design of a new experiment to further understand this material.

Description of research activities and results

Key Challenges:

The properties of materials are determined by the interactions and quantum behavior of electrons. Since there are of order 10^24 electrons in a given piece of material, we often use multiple scale models to help understand them. It has been fortunate that many important materials are actually described by simple models. One prominent example is the band structure model, which among other applications, is used to help design semiconducting devices. The parameters of this band structure model can often be calculated to reasonable accuracy using density functional theory, or more accurately using more advanced techniques such as the ones used in this work. However, as we move into more exotic materials, called strongly correlated or 'quantum' materials, with new properties, the traditional models of electron behavior and the methods to calculate them begin to fail. We are left with two major questions: how do electrons behave in these materials and how do we compute that behavior?

Why it Matters:

The ability to predict the behavior of electrons in materials can enable materials by design; using computation to help guide experimental efforts to create designer systems and quantum states with unique properties. The calculations done using this allocation were instrumental in helping to progress this field forward. We predicted the properties of several magnetic materials using quantum Monte Carlo; a long-standing challenge in the field.

Why Blue Waters:

The reliability and availability of Blue Waters enabled this project tremendously. The code performs very well on Blue Waters (Fig 1). During the course of this work, in collaboration with performance

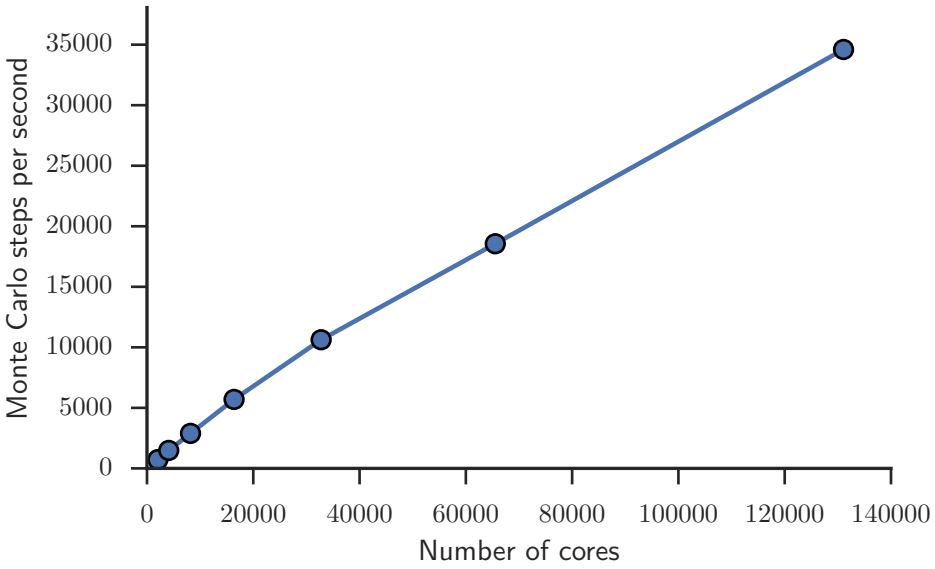

Figure 1: Scaling of our primary code on Blue Waters

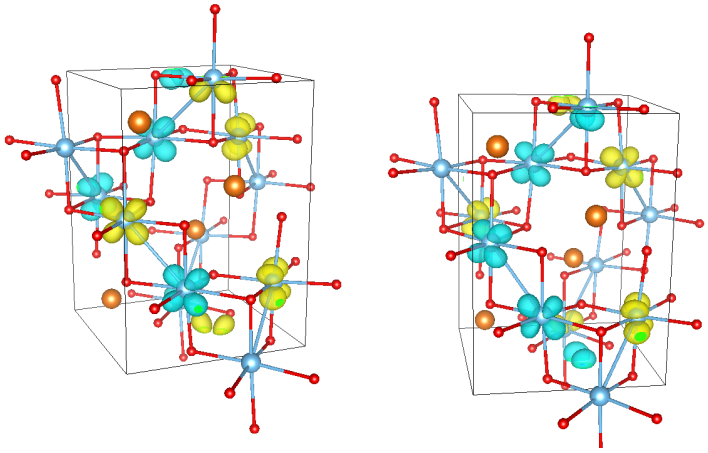

Figure 2: Spin-flip transition in $MgTi_2O_4$.

experts at Blue Waters, we discovered a few optimizations of the code that in some cases led to 20-30% increases in CPU time efficiency, and a factor of 4 in memory efficiency in some cases.

Accomplishments:

We would like to highlight an accomplishment in studying a magnetic system $MgTi_2O_4$. In this system, there is a dimerization transition, which was believed to result in the formation of spin-singlets–a case where the electron spins in a system pair up locally. However, neutron experiments by the MacDougall group did not find the excitations that corresponded to those spins. We performed first principles calculations using quantum Monte Carlo and Blue Waters and found that the excitation energy was far greater than anticipated, which put it out of the range of neutron experiments; however, it is in the range of X-ray experiments. This has helped the experimentalists design a new experiment

to probe this material.

Next Generation Work:

A next-generation system would enable not just to perform very high accuracy calculations on single materials, but on an ensemble. This opens up many new opportunities. One is the ability to 'train' simpler theories with adjustable parameters that may be more efficient for designing new materials. We have been discussing the possibility of using quantum Monte Carlo as reference data in the Materials Project, a large database and tool to study and design materials. However, the main barrier to this is just the computational cost of this study.

Publications

- "Singlet-triplet excitation in $MgTi_2O_4$ computed by quantum Monte Carlo" Brian D. Busemeyer, Greg MacDougall, Lucas K. Wagner, in progress
- "Benchmarking superexchange parameters in the monoxides using quantum Monte Carlo" Josh Schiller, Alexander Munoz, Lucas K. Wagner, Elif Ertekin, in progress.