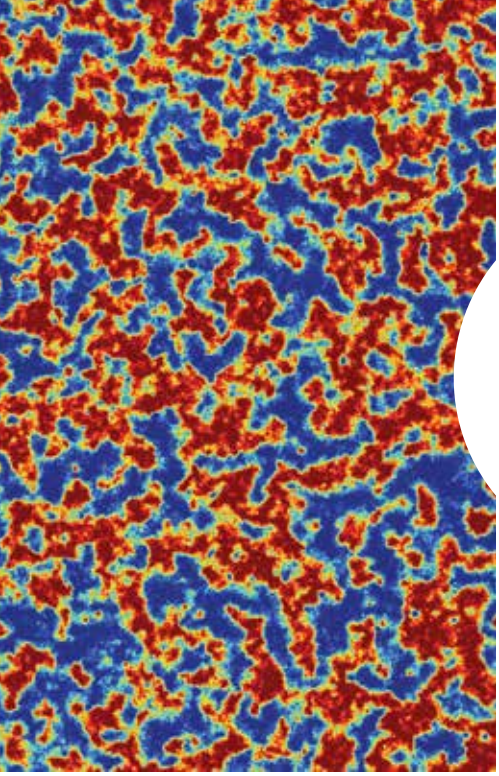

BILLION-ATOM SIMULATIONS OF MAGNETIC MATERIALS

Magnets are extremely useful in a wide range of industries. In our daily lives, there are magnets in our fridges, headphones, computers, and many more everyday objects. In the industrial world, magnets are key components of many medical imaging devices, data storage technologies, and power generators.

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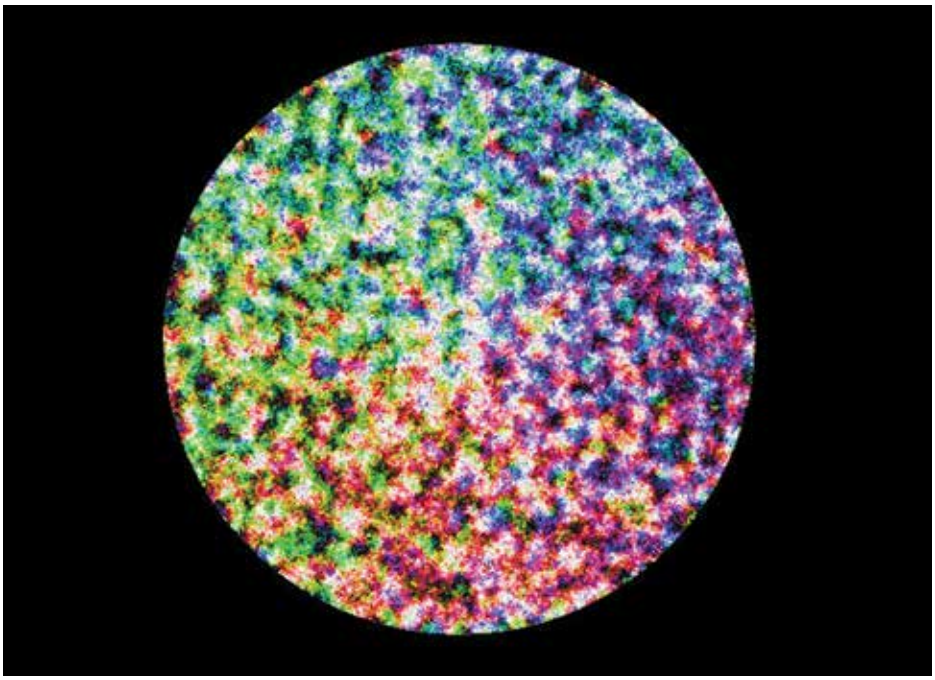
Due to the many uses of magnets, we are always looking for new, better magnetic materials to improve the technologies they enable. This has been difficult, however, as the simulation tools we use to model magnetic materials are limited. Before this project, atomistic magnetic modelling software was only capable of simulating a few million atoms at a time and it was impossible to manage and process the huge amounts of information generated by larger simulations. This was a fundamental barrier to performing large scale device and materials simulations needed to develop new magnetic technologies and devices.



In this project, an open source software package called VAMPIRE was used. This software is designed to simulate magnetic materials by modelling the interactions of atoms within the material, treating each atom as possessing its own localised spin magnetic moment. This allows the simulation of a range of complex properties such as phase transitions, laser heating, and magnetization dynamics in complex systems such as nanoparticles, surfaces and interfaces.

The goal of the project was to improve the VAMPIRE code so it would be able to be used for simulations of up to a billion atoms. The improved code enables a new class of magnetic materials simulation containing between 10,000,000 and 1,000,000,000 atoms. The ability to perform such large simulations gives us unprecedented insight into to the behaviour of complex magnetic materials for realistic situations.

Scientific benefits

Prior to this project, simulations of this scale were completely impractical, which was a major issue when designing new materials. This project has had a transformative impact on the code and enabled a new, state of the art, capability for large scale atomistic simulations of magnetic materials. It is now possible to simulate complete magnetic devices at the level of atoms. This will enable researchers to gain an unprecedented understanding of these materials' physical properties and operation. Effects which can now be simulated include temperature effects, atomic disorder, crystal defects, interface mixing, surface effects, and impurities. Understanding the role of these effects can lead to new optimised devices and materials with better performance and engineered from the atom up.

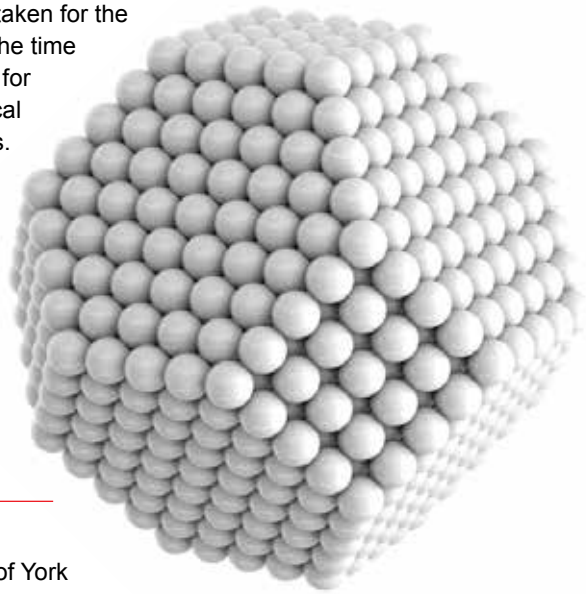
The code can now also be used to simulate more fundamental aspects of magnetic materials such as ultrafast laser induced magnetization dynamics or domain wall effects considering the role of atomic defects which often have a dominating effect on the physical behaviour. Eventually, this could lead to new kinds of magnetic devices and technologies - such as all-optical magnetic data storage or race track memory, which would be capable of storing thousands of times more data than present technologies.

Computational benefits

The improvements made to the VAMPIRE code during this project are significant, enabling a whole new area of simulations. Where previously only a few million atoms at a time could be simulated, the updated code allows for simulations from ten million to one billion atoms to be performed in a reasonable time frame.

The input/output code was refactored during the project to enable more sustainable development of new code features. This will save significant developer time for all future I/O code enhancements, which is a major benefit. The addition of a compile option for the code on ARCHER greatly simplifies the installation process for end users of the code. The implementation of parallel output routines now enables the code to efficiently use the parallel file system on ARCHER.

In terms of the amount of time taken for the simulation, before the project, the time taken was too long to measure for large core counts. It had a typical output bandwidth of a few MB/s. After the enabling work done by the project, however, the time taken has decreased dramatically, to the point where these simulations are now feasible. The typical output bandwidths are in excess of 10 GB/s, a 10,000 times improvement over the previous method.



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Acknowledgement:

Atomistic spin model simulations of magnetic nanomaterials
R. F. L. Evans, W. J. Fan, P. Chureemart, T. A. Ostler, M. O. A. Ellis and R. W. Chantrell
J. Phys.: Condens. Matter 26, 103202 (2014)

About ARCHER

ARCHER is the UK National Supercomputing Service. The service is provided to the UK research community by EPSRC, UoE HPCx Ltd and its subcontractors: EPCC and STFC's Daresbury Laboratory, and by Cray Inc. Laboratory.

The Computational Science and Engineering (CSE) partners provide expertise to support the UK research community in the use of ARCHER, and researchers can also apply for longer-term software development support through the Embedded CSE (eCSE) programme. The ARCHER CSE partners are EPSRC and EPCC at the University of Edinburgh.

The Case Study Series

The ARCHER service facilitates high quality science from a broad range of disciplines across EPSRC's and NERC's remits. The outcome is science that generates significant societal impact, improving health and overall quality of life in the UK and beyond. This science influences policy and impacts on the UK's economy.

This case study is one of a series designed to showcase this science. It has been produced as part of the ARCHER CSE service, supported by EPSRC research grant No EP/N006321/1.

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