Magnetic Modelling Code (MICROMAG) Parallelized by HECToR dCSE Team

Wyn Williams, University of Edinbugh
Chris Maynard, Edinburgh Parallel Computing Centre (EPCC)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

An HPC developer from EPCC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, has developed a new version of the MICROMAG magnetic modelling code which takes advantage of multiple processors (such as those on HECToR) to execute compute tasks in parallel, resulting in better performance.

Commenting on the dCSE project, Prof Wyn Williams of the School of Geosciences at the University of Edinburgh said: *"Over the last 20 years, micromagnetic modelling has yielded a wealth of information both on the fundamental nature of the physics of magnetic recording processes, and as a design tool for developing new forms of magnetic recording technology. Modelling codes are being developed by just a handful of researchers worldwide. It is extremely difficult to get UK funding for such initiatives through normal funding, where the focus is on the scientific outputs rather than technical developments. It is also difficult to recruit the skilled staff needed to get the code development done effectively. The dCSE awards have become a vital resource, providing scientific researchers the specialist knowledge and expertise that allows rapid development and coding of the numerical models where the researcher can focus on the scientific goals rather than the details […] of the parallelisation."*

> Significant progress has been made in developing the parallel version of MICROMAG, which will enable scientists to study new areas of interest.

Prof Williams further commented that there was a need to address two scientific issues using MICROMAG and HECToR. The first is the magnetic stability of rock particles, for which *"to match experiment, computational models require resolutions in the order of 200X the current practical limit of MICROMAG."* The second is the thermal behaviour of non-uniformly magnetised particles, where *"the availability of the new MICROMAG code and the computing resource of HECToR mean that there is now real hope of significant progress on what has eluded analytic theory for over fifty years".*

HECToR

HECToR is managed by EPSRC on behalf of the participating Research Councils with a mission to support capability science and engineering in UK academia. The Cray XE6 supercomputer, located at the University of Edinburgh, is managed by UoE HPCx Ltd. The CSE Support Service is provided by NAG Ltd and ensures users have access to appropriate HPC expertise to effectively exploit advanced supercomputers for their science. A critical feature of the CSE Support Service is the distributed CSE (dCSE) programme which, through lightweight peer review, delivers dedicated performance and scalability projects on specific codes in response to proposals from users. The dCSE programme now consists of over 60 focused projects complementing the traditional HPC user applications support and training also provided by NAG.

The dCSE projects completed so far have delivered outstanding examples of the cost savings and new science that can be enabled through dedicated CSE effort. The MICROMAG project reported here adds to these success stories with the development of an improved version of the code.

Project Background

MICROMAG is a code which models the magnetic properties of mineral systems on a sub-micometre length scale by solving the so-called Landau-Lifschitz-Gilbert equation of motion. Finite element methods are used for the spatial discretization of the equation in order to provide sufficient accuracy when modelling the magnetic grain boundaries. The application can be used to determine how the magnetic properties of a material changes with mineral microstructure over a range of timescales.

The first version of MICROMAG was a serial code, and the goal of this dCSE project was to parallelize it so that it could be efficiently run on HECToR. The project was structured in two parts: (a) development of a semi-parallel implementation which excluded optimisation of the unstructured partitioning and parallelization of the main component fields, and (b), implementation of a fully parallel version which incorporates both of these enhancements.

Wyn Williams of the University of Edinburgh was the Principal Investigator for the project. Chris Maynard of EPCC carried out the 6 person-month project, in close collaboration with the NAG CSE team.

Project Results

Prior to the start of this project, the MICROMAG code had been in existence for a number of years, and had been enhanced by several users in the absence of an overall development plan. It was felt that the code was becoming difficult to maintain, and included obsolete functionality and historical features. Accordingly, the program was first re-factored to produce an application that was much simpler, without any legacy code. The re-factoring included the use of modern coding techniques in Fortran 90 such as modules to abstract and re-use independent functional units.

Work on part (a) of the project included the incorporation of calls to the CVODE differential equation library for the solution of the time differential equation solver. This resulted in a speedup factor of 1.64 when compared to the previous version of the code. Subsequent in-depth analysis revealed, however, that the semi-parallel implementation was not going to work because of the way in which the main component fields are passed to CVODE. Discussions with NAG CSE resulted in part (a) being abandoned, and the concentration of resources on a fully parallel version. It was also suggested that the PETSc parallel library – part of which utilises an implementation of CVODE – should be used to this end.

Accordingly, the PETSc parallel data structures were incorporated into the code, allowing each iteration in time to be performed in parallel. A bug in the interface between PETSc and CVODE was then discovered, in which the CVODE solver would incorrectly report that it had completed when running on anything other than a trivially small number of processors. A patch was subsequently issued by the PETSc developers; its incorporation allowed the developers to start testing new code that they'd written in MICROMAG to perform expensive field calculations in parallel. Benchmarking on up to 16 nodes (384 cores) of HECToR revealed a subtle bug in the construction of one of the so-called stiffness matrices, and some poor scaling performance. Further work is required to fix the bug, and to investigate the cause of the poor performance (which may not be unrelated).

A full technical report can be found at http://www.hector.ac.uk/cse/distributedcse/reports/

For more information, please contact: HECToR CSE Team
The Numerical Algorithms Group Ltd, Wilkinson House, Jordan Hill Road, Oxford, OX2 8DR, United Kingdom
Telephone: 01865 511 245 Email: hector-cse@nag.co.uk Web: http://www.hector.ac.uk/cse/