Performance of Geodynamic Thermal Convection Simulations (CITCOM) Enhanced by HECToR dCSE Team

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HPC experts from NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have enhanced the CITCOM geodynamic thermal convection model with improved multigrid implementations to achieve faster performance.

Dr van Hunen, from the University of Durham, who is both the dCSE project PI and the major user of CITCOM on HECToR, has used around 1.8 million AUs (allocation units) at a nominal cost of around £25,000 so far on HECToR. When extrapolated across future research on HECToR and other supercomputers used to run the CITCOM code, the optimizations achieved by this dCSE project could deliver significant cost savings. The key result for researchers however, is the scalability and faster convergence, thus making it possible to do new science. In particular, the significant development of local mesh refinement in combination with multigrid, and future work based on this important pioneering study, will enable CITCOM users to address much larger numerical problems.

Commenting on the dCSE success, Dr van Hunen said "*This work has provided me with an excellent basis to further optimize my code, and will allow me to work on scientific problems that were previously too large to address*".

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 XT supercomputers, located at the University of Edinburgh, are 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 nearly 40 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. This CITCOM project adds to these success stories with a valuable code enhancement and performance improvement.

Project Background

The objectives of this dCSE project were to improve the parallel performance and scalability of CITCOM by implementing new multigrid methods to improve the rate of convergence. Dr Jeroen van Hunen and Dr Charles Augarde from the University of Durham were the Principal Investigators on the project. Sarfraz Nadeem, one of NAG's HPC experts, carried out the 12 person-month project in collaboration with the NAG CSE team and the CITCOM developers.

CITCOM

CitCom (for California Institute of Technology Convection in the Mantle) is a finite element code designed to solve thermal convection problems relevant to earth's mantle released under the GNU General Public License. Written in C, the code's latest version, CitComS, runs on a variety of parallel processing computers, including shared and distributed memory platforms.
http://www.geodynamics.org/cig/software/citcoms.

Project Results

As a result of this dCSE work, CITCOM performs over 30% faster for a 2D test problem. This was achieved by improving the original multigrid methods; implementing further multigrid cycles (namely, the V-cycle, W-cycle, F-cycle or full multigrid cycle (FMG)); and implementing local mesh refinement near the high viscosity gradients.

The project also analysed the performance of four multigrid schemes, namely the V-cycle, W-cycle, FMG(V) cycle and FMG(W) cycle to develop guidance on the best schemes for given problems. The project also investigated the scaling of all multigrid schemes, which were found to be generally excellent when the identified best practice MPI configurations were used.

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

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