Usability of Oceanography Code (NEMO) Enhanced by HECToR dCSE Team

Stephen M. Pickles and Andrew R. Porter, Science and Technology Facilities Council (STFC)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

HPC experts from STFC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have improved the performance and scalability of the NEMO ocean modelling code on HECToR and other large multi-core scalar systems.

NEMO (Nucleus for a European Model of the Ocean) is an ocean modelling code of great strategic importance for the UK and European oceanographic communities. Although NEMO has been used successfully for a number of years in global and ocean basin applications, its use as a shelf-sea model is less well developed. Also, NEMO was originally designed for vector architectures, leaving room for improvement in its performance on massively parallel architectures such as HECToR. This work focused on shallow-sea problems and the performance and scalability of the code over many thousands of cores on modern architectures, by introducing more flexible domain decomposition techniques and permuting array indices to improve halo exchange performance and enable the elimination of redundant computations on land-only cells.

Commenting on the dCSE project success, *Dr Stephen Pickles of the Advanced Research Computing Group at STFC Daresbury Laboratory said "The dCSE NEMO project has improved the usability of the NEMO ocean modelling code by introducing dynamic memory allocation, so that the code no longer needs to be re-built to run on a different number of processors. It has also provided essential data to inform NERC's long-term strategy for ocean modelling within the UK through the NERC Ocean Roadmap project."*

"The dCSE programme as a whole is extremely valuable to the UK computational science community. The continued competitiveness of scientific modelling codes depends on sustained development effort. The dCSE programme fills an important gap, helping to maintain capability and expertise in High Performance Computing and software engineering, and through this, to sustain the software assets that UK scientists need in order to remain competitive on the world stage."

The code optimisations and enhancements from this project are now in a branch of the NEMO source that will be used to inform scientists to help make strategic decisions about future NEMO developments.

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 70 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 NEMO project reported here adds to these success stories with a successful performance improvement.

Project Background

The objectives of this dCSE project were to develop a set of modifications to the ocean modelling code NEMO to improve the performance, scalability, and usability of the code on very large multi-core scalar systems such as HECToR. The intended optimisations included the reordering of 3-dimensional array indices and the associated nested loops for better cache re-use on scalar processors; and to implement multi-core aware partitioning and elimination of redundant computation on land.

Project Results

The project objectives were completed on a significant subset of the NEMO source code. A general 10% saving in NEMO production work on HECToR resulted by reducing unnecessary accesses to the metadata catalogue of the Lustre high performance file system on HECToR. The optimisations and enhancements from this project are now in a branch of the NEMO source repository that will be used to inform strategic decisions about future NEMO developments.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/nemo02/

For more information 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/

HECToR – A Research Councils UK High End Computing Service