Scalability of Ocean Modelling Application (Fluidity-ICOM) Dramatically Improved by HECToR dCSE Team

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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 transformed the scalability of the ocean modelling application Fluidity-ICOM (Imperial College Ocean Model). As a result of this project, the Fluidity-ICOM now scales to run efficiently on 4096 cores of the Cray XT4 at HECToR.

Fluidity-ICOM is built on top of Fluidity, an adaptive unstructured finite element code for computational fluid dynamics. It consists of a three-dimensional non-hydrostatic parallel multi-scale ocean model, which implements various finite element and finite volume discretisation methods on unstructured anisotropic adaptive meshes so that a very wide range of coupled solution structures may be accurately and efficiently represented in a single numerical simulation without the need for nested grids.

Commenting on the dCSE project success, the co-Investigator Dr Gerard Gorman (Imperial College London) said "*Achieving excellent strong scaling up to 4096 cores broke new territory for Fluidity-ICOM. Moving from computational platforms of the scale available at universities to HECToR allowed scientists to "think big". For many complex physical problems resolution is a key limiting factor to what can be simulated. Indeed, a lot of physics has to be parameterised in crude ways in order to allow simulations to execute within a given computational platform. Using HECToR with this dCSE improved code greatly increases the accuracy to which the physics can be captured.*"

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 over 50 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 Fluidity-ICOM project reported here adds to these success stories with a successful performance improvement.

Project Background

The goal of this dCSE project was to develop Fluidity-ICOM from being a state-of-the-art workstation and cluster based code to become a model able to run efficiently on the largest supercomputing platforms, which will also help Fluidity-ICOM make the transition from local research software to high quality community software. The project covered profiling and optimisation, the scalability of mesh adaptivity and parallel I/O. Mike Ashworth of STFC was the Principal Investigator on the project, with Gerard Gorman of ICL as co-Investigator. Xiaohu Guo of STFC carried out the 12 person-month project in collaboration with the NAG CSE team and the ICOM developers. Usage of Fluidity-ICOM on HECToR has exceeded 2 million AUs (allocation units) in 2009.

Project Results

The dCSE project covered a wide range of developments, including: increased portability; optimisation of the matrix assembly code (with blocked sparse storage); implementation of interleaved I/O; code re-factoring; profiling to highlight and resolve performance bottlenecks; and implementation of an index renumbering method for parallel linear solver performance (provided via the PETSc interface). Also, as Fluidity-ICOM has relatively complex dependencies on third party software (as many as twenty external packages are used), several modules were provided to HECToR users to allow them to easily set their software environment and install Fluidity-ICOM. A key part of this work was to recommend the optimal compilation flags. A scalability analysis of both the parallel mesh optimisation algorithm and of the complete GFD model was performed.

This work has been in the main development branch so will become part of the main Fluidity release. Dr Gorman also said "*Projects like this, which are vitally important to enable the science objectives, are generally not possible to fund under standard research grants. The dCSE has ensured that effort has not been directed away from the science*."

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

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