HECToR dCSE Team Enhances Speed and I/O Performance of Oceanography Code - NEMO

The UK's national supercomputing facility, HECToR, is used by scientists needing capability supercomputing resources. A substantial part of the Research Councils' six-year (2007-2013) funding for HECToR is devoted to the Computational Science and Engineering (CSE) support provided by NAG and especially to the distributed CSE (dCSE) programme which, through lightweight peer review, funds focused multi-month performance and scalability projects in response to proposals from users. The first dCSE projects to complete are providing excellent examples of what can be achieved through dedicated CSE effort, with dramatic improvements in code performance and scalability which could potentially save millions of pounds and allow significant new science to be undertaken.

Project Background

The objectives of this dCSE project were to improve the performance of the NEMO (Nucleus for European Modelling of the Ocean) code for scalar MPP architectures and reduce the amount of storage resource required. NEMO is a modelling framework for oceanographic research, operational oceanography seasonal forecast and climate studies. The key tasks of the project were (a) to address the potential I/O bottleneck arising from the more complex models, higher spatial resolutions and larger numbers of processors needed by the researchers; and (b) to investigate the performance of nested models in NEMO (which enable different parts of the ocean to be modelled with different resolution within the same global model).

Dr Andrew Coward of The National Oceanography Centre, Southampton (NOCS) was the Principal Investigator on the project. Dr Steven Alderson and Mrs Beverly de Cuevas, also from NOCS, were the Co-Investigators. NAG contracted Dr Fiona Reid of EPCC at the University of Edinburgh to carry out the work in collaboration with both the wider NEMO team and the NAG CSE team.

Project Results

The investigations into gridding and the removal of land-only cells performed under this dCSE project resulted in significant reductions to the Allocation Unit (AU) usage (notional cost) for a given simulation, by as much as 25% at larger processor counts, and a reduced runtime. NEMO has been converted to use netCDF 4.0 for its main output files resulting in a reduction in output file size of up to 3.55 times relative to the original netCDF 3.x code. It is expected that a production length research simulation should benefit in reduced run time also, due to fewer I/O bottlenecks resulting from the reduced I/O data sizes.

Dr Andrew Coward, who is the manager of the Global Ocean Modelling Consortium on HECToR, estimated that their group used around 6M AUs running NEMO last year. Reducing the wall clock time of NEMO by up to 25% could result in a saving in notional cost of AUs by as much as £95,000 per year (up to £400,000 for the remainder of the service), for only six months of person effort.

Other consortia using NEMO on HECToR have used around 40M AUs over the same period. If the code modifications are accepted into the main code base, then these other users could benefit too, leading to the possibility of multi-million pound savings overall.

Commenting on the future wider applicability of the dCSE success, Andrew Coward said "*The NEMO code is constantly evolving with two major releases a year. Fiona's work will certainly inform our decisions on how best to run the code on HECToR but changes for particular architectures aren't guaranteed to make it into the base code unless a general benefit is evident. More groups are moving away from the vector parallel machines (mainly NECs) to MPP scalars so the code structure should begin to evolve in our favour.*"

The other NEMO users on HECToR, NCAS (National Centre for Atmospheric Science) can only use code that has firstly been filtered through the main NEMO developers and the UK Met Office, which will take some time. Dr Coward has switched permanently to using the new netCDF4 I/O option. Disk space is a valuable and limited resource and this dCSE enhancement allows him to save a considerable amount. It also allows either more or longer time series to be kept on-line for analysis by the wider Ocean modelling community.

A full technical report on the NEMO dCSE can be found at http://www.hector.ac.uk/cse/distributedcse/reports/nemo/.

About NOCS
The National Oceanography Centre, Southampton is the national focus for oceanography in the UK. It delivers a diverse mission spanning those of both NERC and the University of Southampton. The Centre is also specifically charged with working inclusively with the wider science community to provide strategic leadership, coordination and facilitation for the whole of the UK marine and related earth sciences.

About NEMO
NEMO (Nucleus for European Modelling of the Ocean) is a state-of-the-art modelling framework for oceanographic research, operational oceanography seasonal forecast and climate studies. The framework allows several ocean related components e.g. sea-ice, biochemistry, ocean dynamics, tracers etc to work either together or separately. Further information on NEMO and its varied capabilities can be found at http://www.nemo-ocean.eu.

About HECToR
HECToR is the UK's front-line national supercomputing service, managed by EPSRC on behalf of the UK Research Councils. Its mission is to support capability science and engineering in UK academia. HECToR's Cray XT supercomputers are located at the University of Edinburgh, managed by EPCC. Computational science and engineering (CSE) applications support, including training and documentation, is provided by NAG Ltd.
HECToR – A Research Councils UK High End Computing Service. http://www.hector.ac.uk

About NAG
The Numerical Algorithms Group (NAG) applies its unique expertise in numerical engineering to deliver high-quality computational software and high performance computing services. For almost 40 years NAG experts have worked closely with leading researchers in academia and industry to create powerful, reliable and flexible software which is relied on by tens of thousands of users, as well as numerous independent software vendors. NAG serves its customers from offices in the UK, USA, Japan and Taiwan and through a global network of distributors. http://www.nag.co.uk

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