Performance of Atmospheric Chemistry Simulations (GLOMAP/TOMCAT) 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 restructured key parts of the GLOMAP-mode TOMCAT application and enhanced multicore performance allowing researchers to achieve four-fold reduction in runtimes, thus enabling new science, including the possibility of running simulations at higher resolutions.

Dr Graham Mann of the University of Leeds, who is both the dCSE Principal Investigator and a major user of GLOMAP/TOMCAT, estimated that users of GLOMAP-mode consumed around 3.2 million AUs (allocation units) of resources over a 15 month period on HECToR with a notional cost of £44,000. When extrapolated across future research on HECToR and other supercomputers used to run the GLOMAP-mode TOMCAT code, the optimizations could deliver significant cost savings. The key result for researchers however, is the reduction in CPU-time per model time-step, thus making it possible to do new science.

Commenting on the dCSE success, Dr Mann said "*The optimization work by the NAG dCSE team means the code runs 15-20% faster in general and, importantly for us, delivered much more economical scaling to 256 cores on the XT4. This improved scaling means we can achieve significantly reduced runtime per timestep, thus enabling the investigation of scientific scenarios requiring many more timesteps*". Mann also noted that "*NAG's addition of another level of parallelism to the code via OpenMP will also enable more efficient use of the XT6 (Phase 2b) supercomputer, with its much greater number of cores per node*."

HECToR

A Research Councils UK High End Computing service, HECToR is funded for six-years (2007-2013), providing capability supercomputing resources for researchers. A substantial portion of the funding is devoted to the CSE support service provided by NAG, which 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 support and training 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 GLOMAP-mode project reported here adds to these success stories with a valuable code restructuring and performance improvement.

Project Background

The objectives of this dCSE project were to enable the TOMCAT atmospheric science code, and especially the GLOMAP aerosol process, to better utilize large supercomputers with multicore nodes. The goal was to make higher resolutions feasible through reduced solution times; and by improving multicore performance, to enable more cost-efficient use of resources. Graham Mann of The University of Leeds was the Principal Investigator on the project. Mark Richardson, one of NAG's HPC experts, carried out the 10 person-month project in collaboration with both the wider NAG CSE team and the GLOMAP developers.

Project Results

The project was initially focused on the quad-core XT4 system. The data access in the pure-MPI code was restructured enabling up to 12% faster performance for the same number of processors. Then OpenMP parallelism was introduced to allow the code to extract additional performance from the multicore nodes on HECToR when scaling. With hybrid parallelism, the code was able to run 4 times faster using additional nodes. These optimizations mean that the GLOMAP-mode TOMCAT application is much better placed to achieve good cost-performance and turnaround times on the 24-core per node XT6 system now in place at HECToR.

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

About GLOMAP
Aerosol affects the climate by scattering and absorbing solar radiation and by affecting the properties of clouds. Aerosol 'forcing' of climate is one of the largest uncertainties in the quantification of climate change over the last 150 years. GLOMAP is a global atmospheric aerosol and chemistry model with a comprehensive treatment of aerosol microphysical and chemical processes. The model is being used to study the global lifecycle of aerosol and the impact of aerosol on climate. GLOMAP runs within the TOMCAT Chemical Transport Model and the UKCA aerosol-chemistry-climate model.
http://www.env.leeds.ac.uk/research/icas/clouds/current/glomap.htm.

About HECToR
HECToR is the UK's 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.

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