Performance of Quantum Monte-Carlo Application (CASINO) Quadrupled by HECToR dCSE Team

Dario Alfè, University College London (UCL)
Lucian Anton, Numerical Algorithms Group Ltd (NAG)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

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 optimised a Quantum Monte-Carlo application for multicore architectures, resulting in a performance increase of a factor of four, potentially saving £760k in computing resources for a single one year research project.

Commenting on the dCSE success, Dario Alfè (the Principal Investigator and a major user of CASINO) said "*The new shared memory facility is effectively speeding up the code by a factor equal to the number of cores per node for large jobs, i.e. a fourfold increase with the current quadcores, but clearly set to increase in the future*". [Note HECToR was upgraded to 24 cores per node in 2010]. "*The new second level of parallelism will allow an efficient use of at least 4 times as many cores as previously possible, therefore increasing the scalability of the code to well over 100,000 cores. Finally, the rewriting of the checkpointing routines (that were found to choke on more than 10,000 cores) allows us to cut restart times from over 1 hour to a few seconds. This work has helped CASINO to affirm itself as a modern code, well capable of exploiting current and future massively parallel machines.*"

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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. The CASINO project reported here adds to these success stories with a successful performance improvement.

Project Background

The objectives of this dCSE project were to enable the CASINO Quantum Monte Carlo code to effectively use the multicore processors of HECToR's Cray XT supercomputer and thus model more complex physical systems with greater efficiency. Dario Alfè of University College London was the Principal Investigator on the project. Lucian Anton, one of NAG's HPC experts, carried out the 12 person-month project in collaboration with the NAG CSE team and the CASINO developers.

CASINO and Quantum Monte-Carlo simulations

Quantum Monte Carlo (QMC) methods are accurate numerical tools used for computing the properties of physical models that contain a relatively large number of atoms, e.g.: crystals, nanoclusters or macro-molecules. Although QMC computing time has the advantage of scaling with second or third powers of the system size, very precise results require the need to process large samples of phase space configurations and therefore the most challenging QMC problems require use of the most capable computers and available algorithms. CASINO is a QMC software package developed and maintained over the last 10 years at Cavendish Laboratory, Cambridge University.

Project Results

Shared memory techniques were introduced to allow larger models to be computed with greater efficiency by enabling multiple MPI processes on a single node to share common data set, thus reducing the number of nodes needed for a given simulation. Further work including hierarchical parallelism with OpenMP and I/O optimisations improved the scalability of the code, enabling CASINO to run 60-80% faster for simulations using more than 10,000 cores. Following NAG's work, the scientists were able to run on 40,000 cores of the Jaguar Petaflops supercomputer at Oak Ridge National Laboratory.

Alfè estimated that this dCSE work saved around 12 million AUs (allocation units) for a one year research project on HECToR, representing a saving in notional cost of AUs by as much as £760k, with several million pounds of savings when applied to future research on HECToR and other supercomputers used to run CASINO.

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

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/

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