NAG's HECToR dCSE Team Quadruple Performance of Quantum Monte-Carlo Application - CASINO

NAG HPC experts, 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.

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 the advanced supercomputers for their science. A critical benefit of NAG's 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 30 focused projects complementing the traditional HPC user support and training provided by NAG.

The dCSE projects completed so far have delivered 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. The CASINO enhancements project reported here further strengthen this.

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, carriedout the 12 person-month project in collaboration with both the wider NAG CSE team and the CASINO developers.

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, who is both the dCSE PI and a major user of CASINO, 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.

Commenting on the dCSE success, Alfè 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 is upgraded to 24 cores per node in early 2010, so CASINO will potentially run with 24x better performance due to these optimisations]. *"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.*"

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

About 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.

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.
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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