



Scalability of Materials Science Code (CONQUEST) Further Enhanced by HECTOR dCSE Team

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An HPC expert from UCL, working under NAG's Computational Science and Engineering (CSE) support service for HECTOR, the UK's national academic supercomputing facility, has successfully implemented automated partitioning and dynamic load balancing in the CONQUEST density functional theory (DFT) code, to improve scalability. The computation time taken by CONQUEST to perform certain Molecular Dynamics simulations may now be reduced by 40%-90%.

CONQUEST is a linear scaling, or $O(N)$, DFT electronic structure code developed jointly by NIMS (National Institute for Materials Science, Japan) and UCL. The code is designed to perform DFT calculations on very large systems (a system containing two millions atoms of silicon has been demonstrated). It can be run at different levels of precision, ranging from ab initio tight binding up to full DFT with plane wave accuracy. CONQUEST is currently used by academics at UCL and Imperial. It is also in use in the USA (Army Research Labs), France (University of Bordeaux) and is one of the main codes selected for optimisation on the Japanese 10PF 'K' supercomputer.

The aim of this project was to improve the linear scaling in CONQUEST by developing more efficient load balancing. This was achieved by updating the automated initial load assignment algorithm for distributing the partitions of the simulation cell to processors and furthermore, implementing mechanisms for the dynamic reassignment of simulation data.

The original partitioning of the unit cell in CONQUEST was fixed, with each atom statically assigned to the same partition during dynamics (whether molecular dynamics or geometry optimisation) regardless of its physical location. This limited efficiency for systems of 10,000+ atoms using 1,000s processing cores. Following the development of the improved partitioning mechanisms developed under this work, the computation time of certain MD simulations can now be significantly reduced.

Commenting on the dCSE project success, *Dr David Bowler of the Department of Physics and Astronomy at UCL said: "The dCSE-supported work on CONQUEST has been extremely useful indeed: in particular, the automated load balancing will allow CONQUEST to be used by a much wider group of users than would normally be the case.*

The whole project on molecular dynamics, carried out in collaboration with a team in NIMS, Japan, has enabled a new class of scientific problems to be considered: we are now able to perform several picoseconds of MD routinely, and with the unprecedented scaling of CONQUEST this will allow dynamical calculations on large systems. We are intending to apply this to problems as diverse as the gramicidinA ion channel in a cell membrane, and dopants in realistic models of silicon nanowires. For the nanowire project, we are intending to apply for ten to twenty million AUs on HECTOR, and will also use up to a million AUs via the UKCP consortium."

For a simulation with 30,000+ atoms and various shapes (i.e. bulk, slab, columns and multiple-slabs etc.), the computation time can now be reduced by 40%-90% when running on 1024+ cores, depending on the type of system.

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 XE6 supercomputer, located at the University of Edinburgh, is 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 70 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 project for CONQUEST reported here adds to these success stories with a successful performance improvement.

Project Background

The objective of this dCSE project was to improve the linear scaling in CONQUEST by developing more efficient dynamic load balancing. Firstly, the existing method of standard 3D Hilbert curves would be replaced with a more flexible and efficient Hilbert space-filling-curve method. Secondly, mechanisms for the dynamic reassignment of simulation data would also be implemented.

David Bowler of the Department of Physics and Astronomy at UCL was the Principal Investigator for the project. Lianheng Tong also of UCL carried out the 6 person-month project, in close collaboration with the NAG CSE team.

Project Results

A non-cubic compact 3D Hilbert space space-filling-curve partitioning algorithm was implemented in CONQUEST along with dynamical re-assignment. The new code with improved automatic partitioning and load balancing was then tested on systems of various sizes, including 30,000+ atoms running on 1024+ cores and shapes (i.e. bulk, slab, columns and multiple-slabs etc.).

Following this work, the partitioning process in CONQUEST is now easier to perform and control. Furthermore, the re-use of simulation data enables the computation time of certain MD simulations to be reduced by 40%-90%, depending on the type of system. During the course of this work, extended Lagrangian Born-Oppenheimer MD was also implemented. This allows stable simulations to be performed with relatively low energy tolerances, which are computationally cheap.

The developments from this project have been incorporated into the main CONQUEST source repository. The combined efforts of the CONQUEST dCSE projects as a whole have enabled wider use of the code on HECToR, e.g. during 2011 there were 5,587 kAUs used for biomolecular simulations on HECToR with CONQUEST as part of the BBSRC project "Linear Scaling Density Functional Theory for Biochemistry: Applications to Cytochrome c Oxidase" (BB/H024271/1).

A full technical report on this work can be found at <http://www.hector.ac.uk/cse/distributedcse/reports/conquest04/>

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