Performance and Capabilities of Materials Science Code (CONQUEST) Enhanced by HECToR dCSE Team

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HPC experts from UCL, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have implemented performance improvements and new functionality in the density functional theory (DFT) code CONQUEST.

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 (containing tens of thousands, hundreds of thousands or even millions of atoms). 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 on the Jaguar Petaflops supercomputer at Oak Ridge National Laboratory (ORNL) and is one of the main codes selected for optimisation on the Japanese 10PF 'K' supercomputer. As well as linear scaling functionality, CONQUEST can be run with exact diagonalisation using ScaLAPACK, and optimising this part of the code for calculations on thousands of atoms for metallic systems was the target of the project.

The code performance has been improved by optimising ScaLAPACK use, and implementing K-point parallelism. Implementation of Kerker and wave dependent metric pre-conditioners has enabled calculations to achieve self-consistency that would be otherwise not possible with linear mixing. With the improvements from this work and the already excellent scaling properties, CONQUEST will become a valuable tool for large scale ab initio electronic structure simulation on metallic materials on HECToR.

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 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 over 50 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 CONQUEST project reported here adds to these success stories with a successful performance improvement.

Project Background

This goal of this dCSE project was to modify CONQUEST so that it can be used efficiently in exact diagonalisation mode for both insulators and metals by improving the Hamiltonian diagonalisation with ScaLAPACK and introducing a more efficient technique for reaching self-consistency in large systems. Specifically, by introducing Methfessel-Paxton smearing, K-Point parallelism and Kerker and wave dependent metric preconditioning.

Andrew Horsfield of Imperial College London and David Bowler of University College London (UCL) were the Principal Investigators of the project. Lianheng Tong from UCL carried out the 12 person-month project, in close collaboration with David Bowler (lead UK developer of CONQUEST), and the NAG CSE team.

Around 4-5 million AUs (allocation units) are used per year on HECToR to run CONQUEST simulations.

Project Results

The Kerker preconditioner was implemented, which allowed test calculations to achieve self-consistency that would be otherwise not possible with linear mixing. Methfessel-Paxton smearing was also implemented. This results in a 60% reduction on the number of k-points required for the test calculation to achieve the same accuracy.

The main bottleneck for the diagonalisation process has been improved by optimising ScaLAPACK to use smaller block sizes which improves load balancing to give a 10% speedup. K-point parallelism was implemented using a BLACS process grid and a 21% speedup was demonstrated on a 32 atom 13x13x13 Al unit cell.

A full technical report can be found at http://www.hector.ac.uk/cse/distributedcse/reports/
More details on CONQUEST can be found at http://www.order-n.org/

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