Performance of VASP Materials Science Code Optimised by HECToR dCSE Team

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HPC experts from EPCC and NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have optimised the performance of the Vienna Ab initio Simulation Package (VASP). VASP is the most heavily-used application on HECToR, and the improvement in its performance enables scientists to study systems of interest in a more efficient fashion, obtaining more accurate results for system properties without increasing their expenditure on computing resources.

Commenting on the dCSE project, Dr Ricardo Grau-Crespo of the Department of Chemistry at UCL said: *"Recent progress in the development of the VASP code has made possible a very accurate description of the electronic structure of some types of solids (e.g. transition metal and rare earth compounds) for which traditional methods fail. This opens the opportunity for new research in fields like catalysis and electronics. The remaining limitation is in the computational cost of these calculations, in particular given the need to comply with short job completion times on HECToR. Achieving good scalability in the parallelisation of the code is therefore essential in order to take advantage of these new developments. This DCSE work has significantly expanded the scalability of the VASP code in HECToR by exploiting k-point parallelism, and exciting new research in computational materials science will now be possible thanks to this work."*

The optimisation has improved the efficiency of the package, enabling the more accurate determination of material properties, particularly for small and medium sized systems.

In addition, Dr Aaron Walsh of the Department of Chemistry at the University of Bath commented: *"k-point parallelism will be of major impact in facilitating both the utilisation of more cores and new science. This will remain the case for HECToR Phase 3 and any other HPC 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 60 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 VASP project reported here adds to these success stories with a successful performance improvement.

Project Background

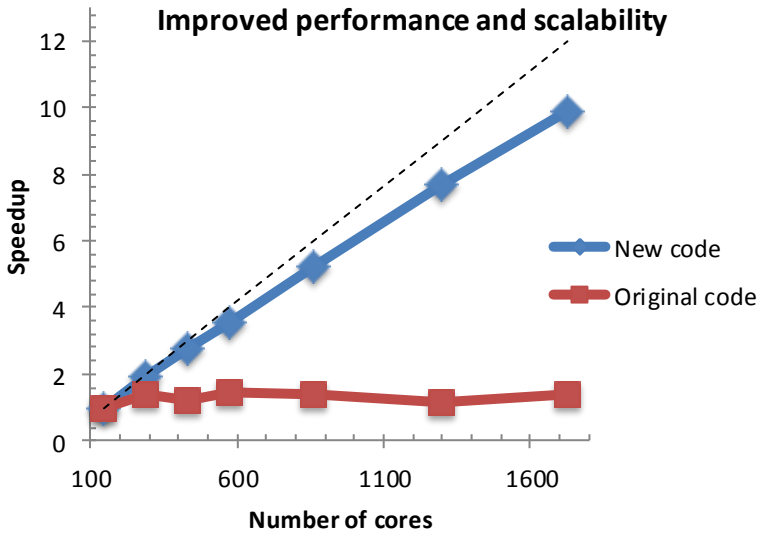
VASP is a program which performs atomic-scale materials modelling (for example, electronic structure calculations and quantum-mechanical molecular dynamics) from first principles. It has an extensive international user base (including a large community in the UK) and is the most heavily used package on HECToR. In spite of this, VASP does not perform well on this machine – especially for smaller system sizes – because of the way it scales poorly with number of cores. This dCSE project was aimed at improving this by (a) determining the optimum distribution of tasks to run in parallel, and (b) introducing a new level of parallelism into the code.

Richard Catlow and Scott Woodley of the Chemistry Department at UCL were the Principal Investigators for the project. Andrew Turner at EPCC carried out part (a) and Asimina Maniopoulou at NAG implemented part (b), in close collaboration with the NAG CSE team. Part (a) required 4 person-months, which was half the resource needed for part (b)

During 2011, VASP calculations consumed approximately 320,000 kAUs (thousands of allocation units) on HECToR.

Project Results

Part (a) involved the determination of recommended values for the VASP parameter NPAR (which controls the distribution of parallel tasks) for a set of widely-used test cases, followed by the incorporation of routines from the ScaLAPACK library for dense linear algebra operations. The optimisations improved the scalability of the code by providing a speedup factor of between three and twelve for calculations using more than 128 cores. Part (b) implemented a new level of parallelism in VASP – specifically, over so-called k-points, which exploits translational symmetry in the system under study. This resulted in a speedup factor of between two and seventy for a series of test cases [different from those used in (a)]. The figure shows the improvement in scalability for one of the test cases which resulted from the implementation of k-point parallelism. This work has been published (A. Maniopoulou, E.R.M. Davidson, R. Grau-Crespo, A. Walsh, I.J. Bush, C.R.A. Catlow and S.M. Woodley. Introducing k-point parallelism into VASP. Computer Physics Communications 183, 1696-1701, 2012). The new version of VASP is available on HECToR, and the source code is being released to the UK's Materials Chemistry Consortium.



Speedup of VASP relative to its performance on 144 cores, before and after implementing k-point parallelism (the dashed line represents ideal linear scaling).

A full technical report can be found at http://www.hector.ac.uk/cse/distributedcse/reports/
More details for VASP can be found at http://www.vasp.at/.

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