Quantum Mechanical simulation package, VASP improved for multi-core platforms by HECToR dCSE Team

Scott Woodley, University College London (UCL)
Gavin Pringle, Andrew Turner, Edinburgh Parallel Computing Centre (EPCC)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

HPC experts from EPCC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have successfully improved the efficiency of the VASP computational quantum chemistry code.

The Vienna Ab initio Simulation Package (VASP), is a quantum mechanical software package used to simulate the electronic structure of condensed phase materials. VASP is one of the most important and utilised materials science and chemistry codes in the world. VASP is currently the most heavily used single application on HECToR, consuming 20-25% of the total of the machine resource. During 2011 VASP used 267,588 kAUs on HECToR (12.65% of the overall machine and 17.61% of all jobs) and during 2012 this figure was about 651,061 kAUs (20.4% of the overall machine and 21.1% of all jobs) – equivalent to a notional cost of over £1.5 million. At that time, there were at least 63 registered HECToR users using the package from 14 different HECToR projects.

Commenting on the dCSE project success, *a representative of the materials chemistry consortium at UCL said: "The addition of more affordable hybrid functionals is of direct benefit to many of our projects and users, allowing for increasingly predictive simulations of direct relevance to experiment."*

This dCSE project has enabled VASP users to effectively double the number of cores they can now use. This will permit new science that was previously prohibited, by increasing the memory available.

"We now highlight one specific scientific project that is only possible through improved scaling in hybrid density functionals. A new class of quaternary Cu-based semiconductor based on the kesterite mineral structure have become the subject of intense interest because they are considered as ideal candidate absorber materials for low-cost thin-film solar cells."

"To further improve the solar conversion efficiencies, it is crucial to understand the basic material and device properties of these kesterite materials. Unfortunately, standard density functionals applied to CZTS result in an electronic band gap of just 0.09 eV, an error of 94% with respect to experiment. We have recently shown for the bulk system that a hybrid density functional (HSE06) can reproduce experiment exactly. The performance enhancements of hybrid density functionals will be used to model the formation of a heterostructure of this material with the CdS window layer used in real solar cell devices. This will involve the construction of a periodic superlattice of the order of a few nm, containing hundreds of atoms, and simulating the charge distribution occurring at the interface, which determines the separation of electrons and holes when light is absorbed. Having an accurate description of the electronic states is essential to understanding the interfacial electronic structure and for extracting the key physical parameters associated with the heterojunction, which can be used to model and improve photovoltaic device performance. Ultimately, these simulations, which explicitly rely on the use of hybrid functionals, could lead to improved light to electricity conversion efficiencies in next-generation devices."

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

Project Background

The objectives of this dCSE project were to produce an efficient mixed-mode version of VASP by introducing OpenMP shared memory parallelization to the distributed memory Fortran90+MPI code, improve the efficiency of the code by enabling more cores used per node, and to validate the performance and accuracy of the mixed-mode version against a set of representative test cases.

Scott Woodley of the Department of Chemistry at UCL was the Principal Investigator for the project. Gavin Pringle and Andrew Turner of EPCC carried out the 12 person-month project, in close collaboration with the NAG CSE team.

Project Results

Two new mixed-mode OpenMP+MPI versions of VASP were developed. The first employs OpenMP shared memory parallelization directives to an existing VASP 5.2.12 routine, which achieved a 50% improvement in parallel efficiency compared to the original code. Now, users of this version can double the number of cores used, thereby increasing the memory available. This development will also permit new science that was previously prohibited, as users of the new version can now double the number of cores used, thereby increasing the memory available.

The second version, which was inspired by a GPU-based version of VASP, required a complete restructuring of the Density Functional Theory / Hartree–Fock parts of the code. Furthermore, additional performance gains were achieved by replacing VASP's FFT routines with calls to the highly optimized FFTW3 library, which is now in use by HECToR users of VASP.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/vasp02/

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/