



Capabilities of Key Materials Science Application (CASTEP) Significantly Enhanced by HECToR dCSE Team

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HPC experts from STFC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have implemented scientifically valuable new functionality in CASTEP.

CASTEP is an electronic structure code based on density function theory used in areas such as inorganic and organic photovoltaic materials, catalytic reactions at surfaces, light-emitting polymer materials for optical displays, and femtosecond laser chemistry. CASTEP is one of the most heavily used applications on HECToR.

Commenting on the dCSE project success, Keith Refson (the Principal Investigator) said *"This project has developed a major new functionality in CASTEP, allowing the computation of excitation spectra using TDDFT. We anticipate that this will have twofold benefits in the next year, first enabling new science using the new functionality as developed, and secondly using this as a basis for further methods development for the treatment of excited states. A poster on this work presented by Dominik Jochym at the recent "Trieste Total Energy" electronic structure conference was well received by peers and potential users."*

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

Project Background

This goal of this dCSE project was to implement time-dependent density functional theory (TDDFT) in CASTEP. TDDFT has become a well-established technique for modelling excited state properties in molecular systems, and has been implemented in several quantum-chemistry codes. This project also forms the first half of the work to implement excited-state force calculations for geometry optimisations and molecular dynamics in CASTEP. The implementation of TDDFT in CASTEP will enable the UK electronic structure community to address a new range of scientific problems.

Specifically, it will enable direct modelling of experimental optical, and UV spectra and help us understand the fundamental properties of electronic excitations at the atomic level, giving detailed insight into optical properties of technologically important materials.

Keith Refson of STFC was the Principal Investigator, Stewart Clark of Durham University and Leonardo Bernasconi of STFC were co-investigators on the project. Dominik Jochym of STFC carried out the 10.5 person-month project in collaboration with the NAG CSE team and the CASTEP developers. Over 90 million AUs (allocation units) were used on HECToR since late 2009 to run CASTEP simulations.

Project Results

The dCSE project implemented TDDFT in the CASTEP code, including a parallel solver compatible with the existing parallel distribution schemes used. Good parallel efficiency was observed for the enhanced code up to 256 cores on the Cray XT4. Projects using CASTEP TD-DFT to generate new and publishable science with Durham and Oxford Universities are currently in planning. All developments within this dCSE were carefully planned to comply with CASTEP coding standards and guidelines and are expected to go into the main release.

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

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