



Performance of CRYSTAL Materials Modelling Code Enhanced by HECToR dCSE Team

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HPC experts from NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have implemented performance improvements for the CRYSTAL materials science code. The compute time for the application now scales with system size in a more efficient manner which, in turn, enables scientists to model larger, more complex, systems without increasing their spend on computing resource. In addition, further efficiencies in the code's performance are currently under investigation as the new mechanism for distributing the calculation across processors is being implemented in other parts of CRYSTAL.

Commenting on the dCSE project, Dr Barbara Montanari of the Computational Science and Engineering Department at the Rutherford Appleton Laboratory, STFC said: *"This dCSE project allows CRYSTAL to exploit fully the resources of HECToR and to apply advanced density functionals – such as hybrid exchange – to systems that have previously been impossible to study. The first work to benefit has been in renewable energy where extensive surveys of bulk and surface structures are now underway: applications include the photovoltaic production of hydrogen, solid oxide fuel cells and lithium ion batteries.*

The dCSE software development programme has been very effective in producing a novel development of CRYSTAL performed in close collaboration with the high end computing support [...] at the Rutherford Appleton Laboratory who provide long-term and in-depth support for the CRYSTAL suite of codes."

Larger systems can now be studied, which opens up new problem areas which can be tackled using this program. The parallelisation techniques are also being applied to other parts of the code.

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

Project Background

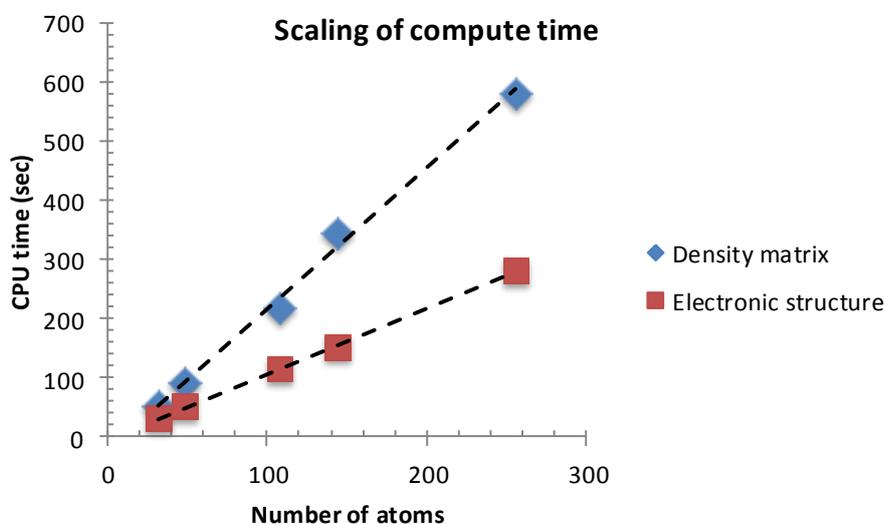
CRYSTAL is a program which computes a material's electronic structure from first principles, and then uses this to determine its properties. CRYSTAL is an important resource for UK materials chemists, and it is necessary to continue its development to ensure it makes best use of HPC resources such as HECToR. For large system sizes, a significant amount of time in codes of this type is spent in the diagonalisation of the Hamiltonian matrix, an operation which scales $O(N^3)$ with N , the number of atoms in the system. The goal of this dCSE project was to improve the performance of CRYSTAL (thereby allowing it to be applied to larger systems) by implementing a so-called divide and conquer strategy – which scales $O(N)$ – when diagonalising this Hamiltonian.

Barbara Montanari of the Computational Science and Engineering Department at the Rutherford Appleton Laboratory, STFC was the Principal Investigator for the project. Daniel Jones, one of NAG's HPC experts, carried out the 18 person-month project, in close collaboration with the NAG CSE team.

Around 200,000 kAUs (thousands of allocation units) are used per year on HECToR to run calculations using CRYSTAL and other materials modelling codes.

Project Results

The divide and conquer strategy exploits the effective short-ranged interaction between electrons in a many-electron system by spatially decomposing the system into constituent pieces which are decoupled from each other. The electronic structure of each piece can then be determined independently (which, in turn, allows the pieces to be processed in parallel) before the subsystems are reconnected, and the total energy of the system determined. The figure shows how the new strategy results in linear scaling with system size for two parts of the calculation – specifically, the computation of the so-called density matrix, and for the setting up and computation of the electronic structure for all subsystems. The mechanism for farming the separate subsystems out to multiple processors has been implemented in a general fashion, and is currently being used to improve the performance of other parts of the CRYSTAL code.



The new code shows linear scaling of compute time with system size for both the computation of the electronic structure of the subsystems and the reconstruction of the density matrix.

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

More details for CRYSTAL can be found at <http://www.crystal.unito.it/>.

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