Electron-Molecule Scattering Inner-Region Code, UKRMol-in Parallelized by HECToR dCSE Team

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HPC experts from The Open University and NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have parallelized and ported to HECToR, a significant part of the inner region programs of the electron-molecule scattering suite UKRMol.

UKRMol-in is a suite of codes that are used to model electron- and positron- molecule scattering processes for the inner region. These codes use *ab initio* methods (from quantum physics first principles) to solve the time independent Schrödinger equation and are based on R-matrix theory for electron scattering. The UKRmol-in suite solves the problem in a (small) inner region where it is essential to describe the interactions accurately. The solution of the outer region part of the problem is carried out by the programs belonging to the UKRMol-out suite. The overall aim of this project was to enable much larger R-matrix calculations by implementing a distributed parallel version on HECToR.

Scalability to several nodes on HECToR is now achievable and much larger problem sizes may now be investigated.

Commenting on the dCSE project success, *Dr Jimena Gorfinkiel of the Department of Physical Sciences at The Open University said: "The dCSE project allowed us to carry out development work that would have been extremely difficult to perform otherwise. By providing the funds and mechanism to hire an experienced developer to work intensively on this specific task (the parallelization of the Hamiltonian construction and diagonalization) it enabled us to carry out this work effectively and to a high standard."*

"The DCSE work will allow several groups in the UK (at UCL, Open University and QUB) to perform new science in the very near future. In the short term:

- *Electron collisions with DNA constituents: we will run significantly improved calculations for electron scattering from biologically relevant molecules containing 40+ electrons and 10+ nuclei. This work is essential to understand how low energy electrons damage DNA.*
- *Electron collisions with molecular clusters: in order to model the effect of the medium in electron scattering from biological material in the cell, experimental and theoretical studies of collisions with small molecular clusters need to be carried out. Again, the DCSE work will allow us to do this for cluster of, for example, a DNA base and several water molecules.*
- *Positron-molecule collisions: it is essential for these calculations to be accurate that a good description of the polarization of the target is achieved; we do this by including enough pseudostates in the calculations.*

In the medium term, and together with software development begin carried out under the EPSRC UK-RAMP grant, the developments will allow us to describe the multi-electron response of polyatomic molecules to intense short laser pulses. The software in development will be world-leading in this very active area of research."

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 UKRMol-in project reported here adds to these success stories with a successful performance improvement.

Project Background

The objective of this project was to enable much larger R-matrix calculations (i.e. greater than 500,000 x 500,000), by developing a distributed parallel version of UKRMol-in. This would be achieved by implementing an efficient parallel matrix construction and diagonalization routine within SCATCI , which is the code from the UKRMol-in suite used for the construction and diagonalization of the Hamiltonian.

Dr Jimena Gorfinkiel from the Department of Physical Sciences at The Open University was the Principal Investigator for the project. Michael Lysaght of The Open University and Paul Roberts of NAG carried out the 12 person-month project, in close collaboration with the NAG CSE team.

Project Results

A scalable parallel version of UKRMol-in was developed for use on HECToR and other large HPC resources. Further improvements to load balancing and performance of the parallel code were made, achieving scalability to several nodes on HECToR, with the result that much larger problem sizes can now be investigated with UKRMol-in. This work is now available to UKRMol-in users on HECToR, and has been submitted to CCPForge for distribution to the wider scientific community.

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

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