Performance and Functionality of HELIUM Code Enhanced by HECToR dCSE Team

Kenneth Taylor, Jonathan Parker, Michael Lysaght, Laura Moore, Queen's University Belfast (QUB)
Edward Smyth, Numerical Algorithms Group Ltd (NAG)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

HPC experts from QUB and NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have enhanced the performance and extended the functionality of the HELIUM code. These improvements have enabled scientists to investigate novel areas of physical science which are fundamental to practical applications.

> The functionality extensions have improved scientists' ability to analyse laser-atom interactions, whilst the code now runs more efficiently due to the performance enhancements.

Commenting on the dCSE project, Professor Kenneth Taylor of the Department of Applied Mathematics and Theoretical Physics at QUB said: *"dCSE support was essential to the successful development of several very large and complex HPC parallel programs. Each of these projects required months to years of full-time attention by someone who was both a specialist in the science, and had experience developing software for parallel processors. In each case the software packages enabled calculations that cannot to our knowledge be performed elsewhere. A generalized version of HELIUM for crossed and circularly polarized laser fields was developed and tested with dCSE support. We now have the ability to integrate the helium-laser Schrödinger Equation in its full generality (essentially 6-spatial dimensions plus time integration). This ability is unique in the world. The code has been used to search for failures in reduced dimensionality models of atom-laser physics. Full exploitation of this high dimensional code awaits HECToR's successor for reasonable performance. A particularly successful outcome of the HELIUM dCSE project was the development of post-processing code that calculates the energy spectrum of double ionization. It has recently been used to provide a high-integrity analysis of an experiment that has been controversial for several years. dCSE support and the full performance of HECToR were both vital to the success of this 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 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 HELIUM project reported here adds to these success stories with a successful performance improvement.

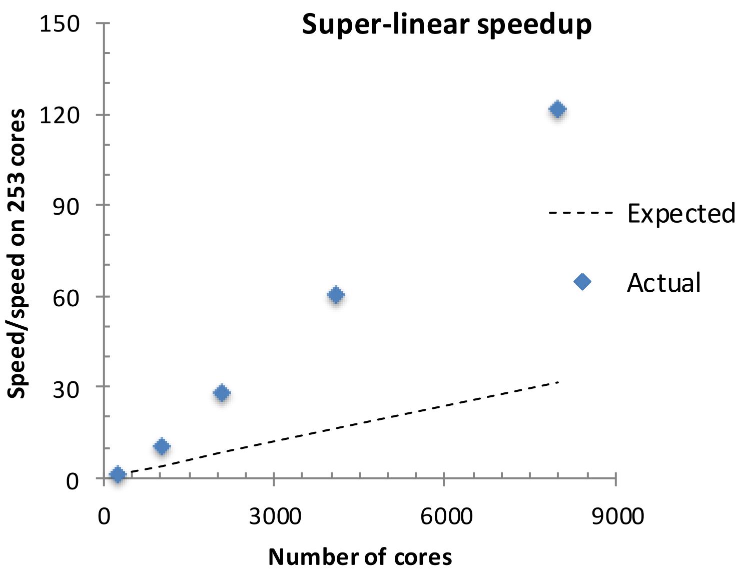
Project Background

HELIUM is a program which solves the non-relativistic time-dependent Schrödinger equation for a two-electron atom or ion exposed to intense laser radiation. Applications include the study of electron dynamics on atto-second time-scales, intense field interactions with XUV radiation generated by free-electron lasers, and the behaviour of atoms exposed to laser light at Ti:sapphire wavelengths. These phenomena are all also being studied by experimentalists, whose results complement those of HELIUM; the combination is advancing discovery in important fields such as quantum computing and quantum cryptography.

This dCSE project was aimed at improving the performance of HELIUM on many-core architectures (such as HECToR), and also extending its functionality to systems interacting with crossed laser fields, and those containing more than two electrons. Kenneth Taylor of the Department of Applied Mathematics and Theoretical Physics at QUB was the Principal Investigator for the project. Jonathan Parker, Michael Lysaght and Laura Moore of QUB, together with Edward Smyth at NAG carried out the 44 person-month project, in close collaboration with the NAG CSE team.

Project Results

The new code enabling calculations with crossed laser fields exhibited super-linear scaling on HECToR (see figure), because of the way that arrays could be distributed over larger numbers of cores and fitted into faster cache (for smaller numbers of cores – for example, 253 – the arrays spilled out of the cache into slower memory). The extension to multi-electron systems was performed by developing new routines using the so-called R-matrix method for electron scattering. It is expected that this enhancement will have an impact on the prediction of physical phenomena occurring in laser-atom interactions in which multiple electrons participate.



The expected relative speedup of HELIUM (obtained by extrapolating from its performance on 253 cores) is about a quarter of the actual speedup.

Other enhancements to HELIUM included the implementation of hybrid MPI-OpenMP parallelism, the development of new parallel postprocessing code to transform the application's output from spherical to cylindrical geometry, and the implementation of new methods for the transformation of the final-state wavefunction from configuration to momentum space. These extensions have enabled scalability to higher core counts for a given problem size, and a more efficient usage of memory per core. For example, the new momentum space methods have shown speedup factors of up to twenty (running on 8,001 processors in HECToR) when compared to the methods used in the previous version of HELIUM.

A full technical report can be found at http://www.hector.ac.uk/cse/distributedcse/reports/
More details for HELIUM can be found at http://web.am.qub.ac.uk/ctamop/ili_1.html.

For more information, please 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/