RMT Method for Schrödinger Equation Solutions Implemented by HECToR dCSE Team

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An HPC expert from QUB, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, has successfully demonstrated that a highly parallelized implementation of the RMT method (R-Matrix incorporating time-dependence) for solving the time-dependent Schrödinger Equation is both computationally stable and highly efficient. RMT is a new method for addressing multi-electron atomic and molecular systems in intense short laser pulses.

General R-matrix methods successfully model multi-electron atom-laser and molecule-laser interactions, but only in the time-independent limit. HELIUM, which has been in heavy use on massively parallel machines for over 15 years, successfully models time-dependent atom-laser interactions, but is limited to 2-electron atoms. RMT removes both of these limitations. Significant performance and load balancing optimizations to the RMT code make it possible to achieve a 30% speed-up using 8192 cores.

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Commenting on the dCSE project success, *Professor Kenneth Taylor of the Department of Applied Mathematics and Theoretical Physics at QUB said: 'dCSE support for software development has underpinned the success of the RMT code (R-Matrix incorporating Time). RMT is a large complex parallel code that exploits the high accuracy and high efficiency of the finite-difference and time-propagation methods of HELIUM. RMT is capable of handling laser interactions with many-electron systems at a level quite impossible before. HELIUM is a well-established HPC code for calculating such laser interactions with two-electron systems and has been developed in Belfast over the past 20 years.'*

'The time-independent R-matrix code (RMATRX) coupled in has again been (largely) developed in Belfast over several decades and combining the two codes (HELIUM and RMATRX) successfully was a project demanding several years of work by researchers intimately familiar with the scientific domain, the specialized numerical methods, and parallel programming methods. RMT has now been applied with success to ab initio calculation and analysis complementary to recent experimental measurements of attosecond time-delays in the photo-emission from the outer sub-shells of neon, and to calculations of high-harmonic generation in helium. Additional application areas of RMT include the study of inner shell excitations and decays in complex atoms, and intense-field atom-laser interactions at XUV frequencies generated by the new free-electron x-ray lasers. Preliminary research in several of these domains is now being moved from small computers to HECToR for large scale production runs.'

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

Project Background

The objectives of this dCSE project were to develop and test a series of improvements to the RMT model for efficient load balancing, as well as optimizations to the MPI communications to enable improved scaling for up to 10,000 cores.

In addition, a new RMT code for the calculation of High Harmonic Generation processes was developed and tested. A speedup of up to 50% for up to 1056 cores was achieved for a small model of the helium atom.

One of the goals of RMT is to enable theoretical analysis of experimental advances with a degree of reliability that would be impossible using other methods. Such analysis includes time-resolved studies of ionization events on attosecond time-scales, studies of time-delays between the ejection of electrons in double-ionization, inner shell excitations and decays in complex atoms, intense-field atom-laser interactions in the XUV limit using the new free-electron x-ray lasers, and harmonic generation in atoms and molecules.

Kenneth Taylor of the Department of Applied Mathematics and Theoretical Physics at QUB was the Principal Investigator for the project. Jonathan Parker of QUB carried out the 12 person-month project, in close collaboration with the NAG CSE team.

Project Results

Optimizations to the RMT code and algorithms significantly improved load balancing and MPI communications on HECToR, enabling up to a representative 30% speedup.

Additional coding developments to the RMT code were made for High Harmonic Generation processes.

The HELIUM and RMT codes were tested independently of each other – results for the dipole and the acceleration methods of calculating the energy spectrum of High Harmonic Generation processes agreed over a range of 9 orders of magnitude. In addition, improvements to the design of the numerical propagator yielded an 80% speedup.

Full technical reports on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/rmt/ and http://www.hector.ac.uk/cse/distributedcse/reports/rmt2/

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