Laser-driven double-ionisation: the HELIUM code on HPCx

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Laser-driven helium is a scientifically crucial physical system which provides a first opportunity for the study of non-equilibrium two-electron quantum mechanical wavepackets. Knowledge and understanding of these multi-dimensional multi-electronic wavepackets and their properties is beginning to emerge through our ab-initio work, in close contact with complementary laboratory experiment on this system.

In moving from the Cray T3E architecture of the CSAR service to HPCx we considered it essential to re-engineer our HELIUM code so as to minimise inter-processor communication. We accomplished this over the period from October 2002 to March 2003 by changing from domain decomposition in angular momentum space to a configuration space domain decomposition. Moreover in this new decomposition we could, through exploiting a quantum mechanical symmetry, reduce, for any given problem, our memory and CPU demands by approximately 50%. We estimate overall that the re-engineered code is a factor of 5 more efficient on HPCx than the previous version.

With this re-engineered code, we have been able to make the world's first successful ab-initio calculation of double-ionisation of helium by high-intensity light from the most widely used laboratory short-pulse laser source, namely the Ti:sapphire laser operating at its fundamental wavelength of 780 nm. We are currently performing calculations of energy-resolved double-ionisation helium wavepacket spectra resulting from exposure of the atom to frequency-doubled Ti:sapphire light (ie 390 nm wavelength light). Such energy-resolved work for 780 nm is beyond the capability of phase 2 HPCx. This work is being carried out in close contact with world-leading experimentalists at Ohio State University in the USA making complementary measurements on helium at this laser wavelength.

The figure displays a typical energy-resolved two-electron ionisation wavepacket spectrum we have obtained, in this case for a laser peak intensity of 9.0×10^{14} W cm^{-2}. The figure was obtained through integration of the Schrödinger equation for the laser-driven 2-electron helium atom, a 5-dimensional time-dependent partial differential equation. Successful calculation of the physics of double-ionising wavepackets has required a numerical integration to 12 significant figures of accuracy. The colour scale runs from red indicating highest probabilities through yellow, green to blue at the lower probabilities. The axes plot magnitude of momentum carried by each electron, with the result that circular arcs in the figure occur at fixed kinetic energy shared between the two ionising electrons. A striking aspect of the figure is the succession of such circular arcs each separated in energy by the energy carried by a 390 nm photon. In this particular case it is possible to discern no less than 38 such rings. This very large number together with the strong probability density spread over individual rings indicates the highly non-perturbative strongly correlated character of the double ionisation process at this important laser wavelength. These complicated but fascinating dynamics are caused by three forces (of widely disparate geometries), ie laser-electron, electron-electron and electron-nucleus all coming into play to a comparable extent.

Given that twenty-five 390 nm photon absorptions are required to achieve initial ionisation of the 2 electrons, the figure represents a double-ionisation process involving at least 63 photon absorptions. Our closest competitors (in various countries around the world)

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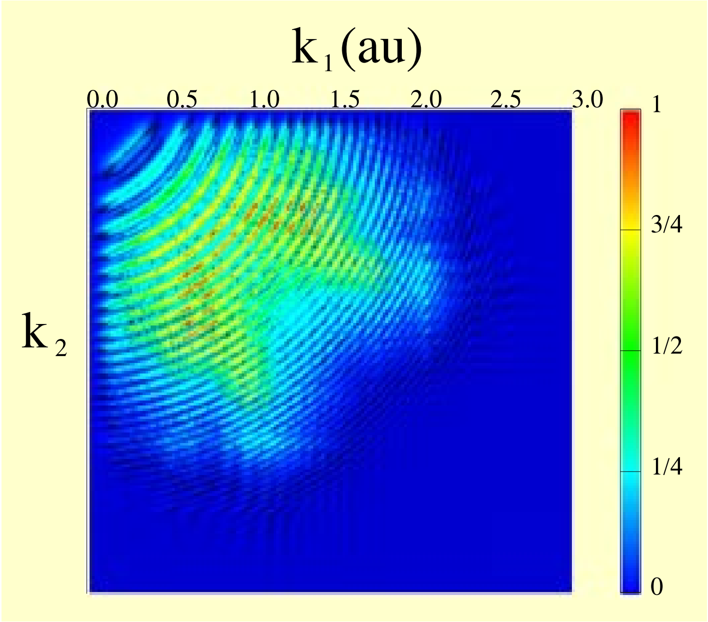

Figure 1. Probability density distribution of doubly-ionizing electrons in radial momentum space at the end of a 7-cycle 390 nm laser pulse of 9.0×10^{14} W/cm^2 peak intensity. The colour scale linearly maps probability density values from 10^{-4} (red) down to 0 (blue), with the colour legend in units of 10^{-4}.

SC2004: bridging communities

Lorna Smith and Andrew Sunderland, HPCx Terascaling Team

The world's largest conference on high performance computing took place in Pittsburgh in November last year. Alongside 169 vendors including the usual industry heavyweights, over 100 universities, laboratories and other research groups were present. The conference is always a good place to find out about new and emerging technologies. One of the biggest splashes was made by IBM's new BlueGene L system, which topped the top 500 list with a peak performance 70 Tflops/s, displacing the Earth Simulator.

Field programmable gate arrays (FPGAs) also hit the exhibit floor with companies such as SGI and Cray demonstrating FPGAs closely integrated into HPC architectures, promising exceptional performance gains on critical components of an algorithm.

Edinburgh and Daresbury were busy at the event promoting HPC activities in the UK. Members of EPCC and Daresbury Laboratory (DL) jointly looked after the HPCx booth which featured highlights of the scientific and engineering-based research undertaken on HPCx. From the IBM stand Andrew Sunderland from DL gave a more detailed overview of scientific activities to the delegates with his presentation on Capability Science from the HPCx IBM p690+ Cluster in the UK.

EPCC presented a tutorial on performance scaling on constellation systems. It was particularly timely as constellation systems, or clustered symmetric multiprocessing (SMP) systems, have clearly become more prominent in the HPC market, most notably NASA's new SGI Altix 3700 cluster which clocks in at an impressive 51.87 Tflop/s. We focused on the tools and techniques required to achieve optimal performance and scaling on these systems, looking at topics such as optimising inter- and intra-node communication, such as overlapping communication, cluster aware message passing, mixed mode programming and processor mapping.

EPCC's Neil Chue Hong was selected to make a presentation in the HPC Software Challenge, which honours participants working to improve the productivity of HPC software developers and the quality of HPC software. Neil talked about OGSA-DAI, a highly successful UK project involving Edinburgh, Manchester and Newcastle universities, with industrial participation by IBM and Oracle. The project has developed middleware to assist with access and integration of data from separate data sources via the grid.

Other highlights included SC Global 2004, the Access Grid-enabled component of SC2004, which included a first-ever demonstration of a simultaneous connection of AG nodes from all six inhabited continents. All in all a successful event was had by all, with a good UK presence. Seattle beckons for 2005.

Laser-driven double-ionisation

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are capable of calculating no higher than two-photon absorption double-ionisation processes. They are consequently limited to weak-field calculations for laser wavelengths of the order of 30 nm which are not yet experimentally feasible. Current developments in Free Electron Lasers (FELs), however, should make experiments involving few-photon double ionisation of atoms possible shortly.

The physics of 2-electron atoms in intense laser radiation is currently a hot topic world-wide, with the experimental study typically performed at the laser wavelengths we alone can seriously address with ab-initio theory, ie with the ubiquitous Ti: sapphire laser at a wavelength of 780 nm or frequency doubled Ti: sapphire at a wavelength of 390 nm. The computational difficulty encountered in the theoretical analysis scales as the wavelength cubed. Integration of Schrödinger's equation to obtain energy-resolved doubly-ionising wavepackets for a laser wavelength of 390 nm, for instance, is $13^3 \approx 2000$ times more computationally demanding than the corresponding 30 nm calculations performed by our competitors. Similarly 780 nm is $2^3 = 8$ times more demanding than 390 nm.

The present energy-resolved calculations at 390 nm require a minimum of 861 HPCx processors, each using its maximum user-available memory. The calculation represented in the figure required 50 wall-clock hours on 861 HPCx processors. Future calculations for the corresponding energy-resolved response to 780 nm laser light will require the re-engineered HELIUM code exploiting the full capability of an upcoming HECToR service.

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