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HPC-Europa

Pan-European Research Infrastructure on High Performance Computing

WELCOME to the January issue of HPC-Europa Newsletter. This issue is edited by EPCC at the University of Edinburgh, and is focused on the research that two of EPCC's HPC-Europa visitors have performed using one of the most advanced computing architectures available today: IBM Blue Gene.

We would also like to take this opportunity to wish all our visitors and hosts a very Happy New Year 2007!

Next Closing Date for HPC-Europa applications: 28 February 2007

NEWS

MareNostrum installed at the Barcelona Supercomputing Centre doubles its calculation capacity and is ranked again as the most powerful supercomputer in Europe which will allow to successfully run more scientific projects

HLRS have installed future hardware architectures such as multi-core clusters and the Cell processor. The machines will be available to HPC-Europa guests with the specific need for these kinds of platforms.

HPCx supercomputer at EPCC underwent the final upgrade and has substantially increased its performance to over 12 TFlops (sustained)

EPCC is one of the Europe's top high performance computing and technology transfer centres and one of the 11 HPC Europa partners.

EPCC's facilities include a 52-processor SunFire E15K (Lomond), a 2560-processor IBM Power 5 system (HPCx) and a 1024-node BlueGene/L(BlueGene).

At EPCC, we research and develop novel computing solutions, write software, manage computing systems and provide HPC training.

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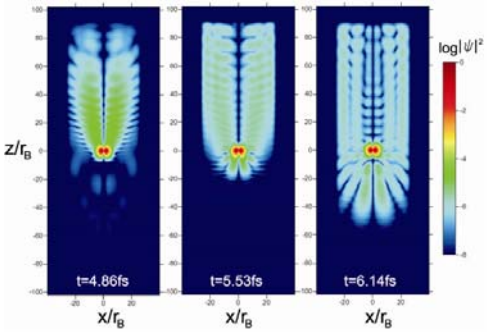
CORDIS

Transnational Access

BlueGene in femtosecond physics

By Teodora Baeva, HPC-Europa visitor to Department of Chemistry, University of Edinburgh



The dynamics of electrons during the interaction of atoms and molecules with laser pulses used in experiments (wavelength $\lambda = 800nm$ and duration $\tau \approx 10 - 100fs$) is confined to an area of a few hundred Bohr radia ($1rB \approx 10^{-10}m$) on a typical time scale of about hundred femtoseconds ($1fs = 10-15s$). For the visualization of the electron motion and the processes of ionization and scattering on the atom or molecule numerical simulations are extremely important.

Fig 1: Dynamics of the electron wave pulled out of a molecule by an intense laser and pushed back to re-combine and re-scatter.

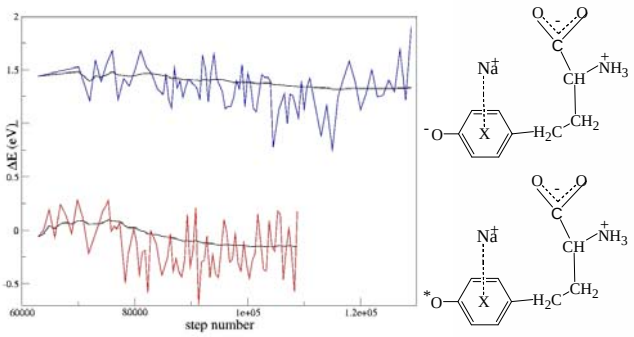
Although the lengths and times connected with these processes are so small compared to world of objects we have around us, simulations of the electron dynamics are quite time consuming. Indeed, on a single CPU a physical time interval of $1fs$ consumes roughly 9 days of calculation time. In addition to this problem of performance, there is also a problem of memory: the computational grid for such calculations often does not fit into the memory of a single computer.

Simulations with BlueGene allowed observing in detail the electron dynamics in 3 dimensions. In a numerical experiment of laser-molecule interaction one can follow the re-scattering of an electron pulled out of the molecule and then pushed back by the laser field to re-combine.

Study of redox reactions involving tyrosine complex in solution by ab initio MD

By Francesca Constanzo, HPC-Europa visitor to Department of Chemistry, University of Edinburgh

The motivations for applying to HPC-Europa were the need to use High Performance facilities and to look for scientific support and collaboration. My research project dealt with ab initio simulations of the redox active tyrosine complex. I ran CPMD simulations on a large number of processors to measure the redox potential of tyrosine complexes with alkali metal cations namely M+(Tyr*)/M+(Tyr-) where M+ is Na+ or K+.



During the HPC-Europa visit, we (EPCC staff and myself) were able to install the CPMD code on HPCx and Bluegene. Vertical transition energies for the oxidized and reduced form of the Na+(Tyr), K+(Tyr) and Tyr in gas phase were calculated. The system in solution was prepared using a cubic box containing 50 water molecules.

The host group I visited at the University of Edinbirgh was very friendly and helpful. I had nice discussions with Prof. Madden and Dr. Carole Morrison.

Fig1 : Vertical transition energies calculated for the Na+(Tyr) in the anion and radical state as shown in the figure on the rght