



New tools from DEISA training

The 1st DEISA training organized in the beginning of July in Paris gathered together 30 participants interested in HPC and Grid computing. In this session, first a global introduction to the DEISA infrastructure and its general middleware services were given.

Then, the focus of the training was put on highly scalable parallel applications. HPC specialists presented tools and techniques for achieving optimal scaling on a large cluster of shared memory nodes. These presentations covered all the main aspects of optimisation work, from some algorithmic aspects to the usage of performance analysis tools to detect the bottlenecks in the applications, and to various techniques to optimize especially communications and I/O. Then, scientists from the fields of cosmology, climate modeling, fluid dynamics, and plasma physics report-

ed on their experience on highly scalable parallel applications on the DEISA infrastructure through use case presentations. For instance, one speaker explained how he succeeded to reach nearly optimal scaling properties up to 4000 processors, switching to a completely different decomposition domain strategy then working on the optimization of the new code. All the presentations of this training session are available at <http://www.deisa.org/training>.

According to the feedback received, the participants were very satisfied with the training session. The scientists felt that the training had had a positive contribution in support to their research activities. In particular they appreciated the lectures on new techniques in supercomputing and the opportunity to exchange ideas with researchers from different scientific disciplines.



The first DEISA training was organised in July.

The next DEISA training session will be organized in Jülich, Germany, on October 23-25, 2006. The program for this session will be communicated in early September, as well as the opening of the registration.

UK national supercomputer joins DEISA infrastructure

Initially, the UK's flagship supercomputer, HPCx, was not integrated into the DEISA computational network. However, in January 2006, HPCx started to contribute to the shared pool of resources operated jointly by the DEISA partners.

The UK's Engineering and Physical Sciences Research Council, EPSRC, funds HPCx and recently Hugh Pilcher-Clayton, head of High-End Computing at EPSRC, announced: "EPSRC has recently agreed that 5% of HPCx resources should be donated to DEISA, [which] demonstrates the UK's commitment to working in Europe in the area of High Performance Computing"

HPCx comprises 96 IBM POWER5 eServer nodes, i.e. 1536 processors, delivering 9.2 TFlops peak, or up to at least 6 TFlops sustained. This will increase to 12 TFlops sustained by December, 2006. The system is equipped with 3.2 TByte of memory and 36 TByte of disk.

In January 2006, HPCx donated 5% of its cycles to the DEISA pool. Indeed, HPCx has already successfully completed its first DECI project, Supernovae, and is currently running



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its second, GIMIC, exercising the DESHL. Both of these share RZG as their home institution but are from two separate research consortia.

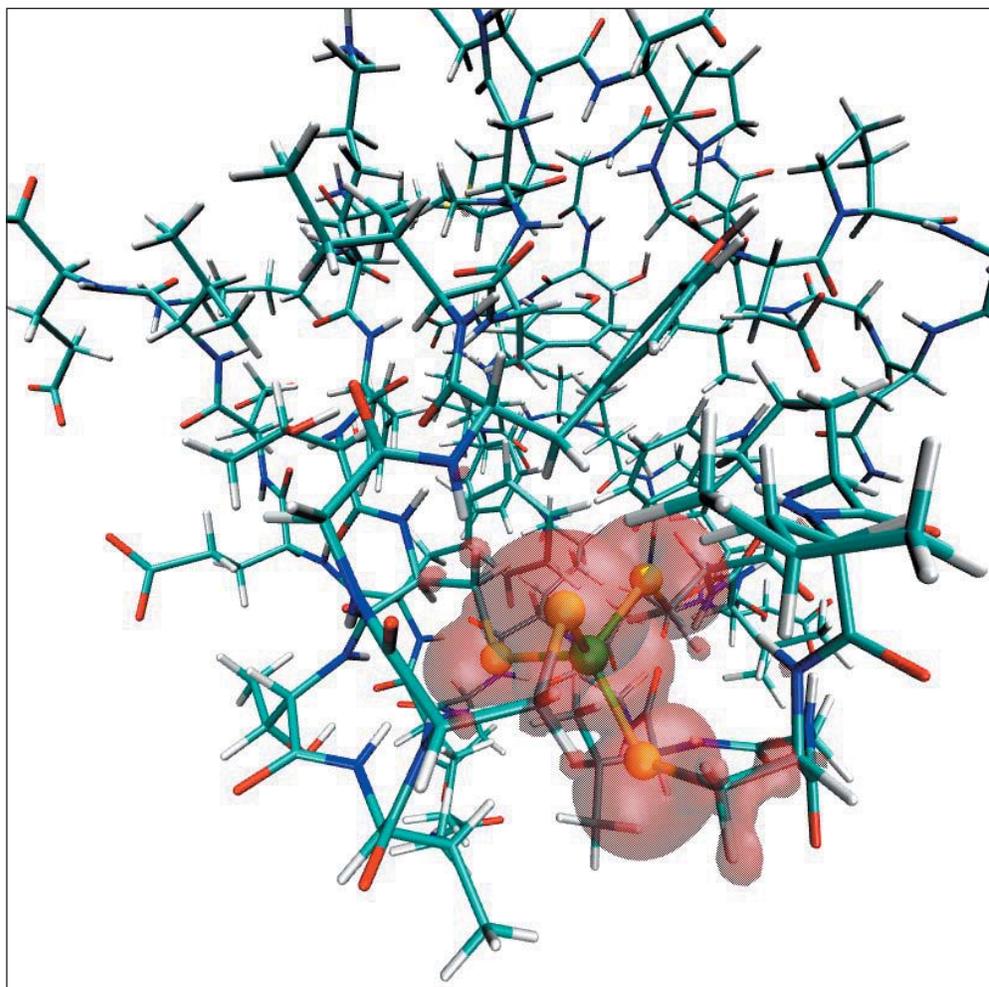
The staff at HPCx has installed UNICORE to provide access to the system in the same way as the other DEISA sites and is currently completing the installation of the necessary soft-

ware to adhere to DEISA's Common Production Environment, or DCPE.

Plans are underway to connect HPCx to the rest of the DEISA sites through the dedicated 10 Gb/s network. Once this is in place HPCx will then join the MC-GPFS infrastructure. The goal is for HPCx to be part of DEISA's AIX super-cluster.

BET: First-Principles and Mixed quantum classical QM/MM Simulations of Biological Electron Transfer

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Isosurface enclosing the 95% of the total spin density (difference of the up and down electron densities) in the oxidized form of the rubredoxin from *Clostridium Pasteurianum*. The iron center is represented by a green sphere, whereas the four sulphur ligands (four cysteines) are drawn as yellow spheres. All of the other atoms are represented as colored sticks (carbon: cyan; oxygen: red; nitrogen: blue; hydrogen: grey). The *ab initio* (DFT) calculation of the electronic wave function explicitly took into account all of the atoms and their valence electrons (included those of the solvent and of the counterions which are not shown for sake of clarity) were explicitly taken into account at *ab initio* (DFT) calculation of the electronic wave function.

Electron-transfer (ET) proteins are crucial for the life of organisms. They serve as electron carrier and/or as catalyst in biochemical ET reactions. As such they are responsible, for instance, of the respiration and the photosynthesis. A detailed understanding of the involved molecular mechanisms is thus of prominent interest from a fundamental point of view as well as for the potential design of highly efficient bio-inspired optoelectronic devices and solar cells.

The study of ET proteins at full atomic and electronic level represents a new challenge

for computational biochemistry. These proteins contain one or more metal ions in the active site, such as iron and copper. During the ET process the metal changes oxidation state (i.e., Fe(III/II) and Cu(II/I)) and this is usually accompanied by a reorganization of the environment surrounding it. It has been largely recognized for a long time the importance of a molecular description of the solvent and the proper inclusion of the polarization medium around the metal center. As yet, these effects limited the applicability of standard computational schemes.

We have used state-of-the-art first-principles electronic-structure techniques to perform the first *ab initio* investigation of entire electron-transfer proteins in aqueous solution. We exploited a combined approach, which used empirical force field based molecular dynamics coupled to full quantum mechanics (linear scaling density functional theory) and hybrid quantum mechanics/molecular mechanics (QM/MM) calculations, to get insights on the nature of the drastic decrease of reorganization energy for metal ions in the protein frame and to calculate the tendency of these proteins to acquire electrons (i.e., the redox potential) [J. Phys. Chem. 122 (2005) 234505].

We focused on a copper protein (azurin from *Pseudomonas Aeruginosa*) and two iron-sulfur proteins (rubredoxin from *Clostridium Pasteurianum* and from *Pyrococcus Furiosus*). The calculations were carried out at Idris Centre in Paris and at CINECA in Bologna with the codes CPMD [www.cpmc.org] and CP2K [cp2k.berlios.de]. The full *ab initio* (mixed Gaussian and Plane Waves) CP2K calculations performed on rubredoxin, which represented the most expensive part of our study, took explicitly into account the entire protein, 700 water molecules, and 9 counter ions, for a total of 2825 atoms (the Gaussian basis set for the wave functions included 11334 primitives). For this system, each electronic wave function optimization required 4.5 hours on 128 processors of the IBM-SP4 at the Idris Centre. To have reliably converged quantities, hundreds of such calculations were required.

Our study shows that full *ab initio* calculations on bio-molecules at physiological conditions are now possible by exploiting modern quantum chemistry protocols and today's large-scale supercomputing facilities, like those made available through the DEISA initiative, effectively.

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