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HPC-Europa

Pan-European Research Infrastructure on High Performance Computing

Beginning with this issue, the HPC-Europa Project partners have agreed to publish this newsletter more frequently. We hope, that you like this new approach to keep you always up to date about the HPC-Europa Community. A new feature is also that the newsletter will be edited everytime from a different HPC-Europa access centre. We hope, that you can get a better insight of HPC-Europa and the community.

This newsletter was edited by HLRS, and we would like to use this oppurtunity to introduce you to Molecular Dynamics within HPC-Europa and to HLRS. We hope you enjoy reading this newsletter.

HPC-Europa offers a way to get access to HPC resources taking advantage of the knowledge of the staff of the HPC-centre and using the latest tools.

Next Closing Date: 15th November 2006

+++ News +++

On Friday, the 19th of October, the HPC-Europa partners held another lecture in the series of the so-called "AccessGrid Surgeries", a Powerpoint-enabled Video-conferencing. For this surgery, Mr. Uwe Küster from HLRS gave a presentation on “Single-Processor Optimization techniques”. Despite a few technical difficulties, AccessGrid allowed the HPC-Europa guests and staff from the involved centres to better communicate with the lecturer and to participate in an interactive "virtual" lecture .

The next HPC-Europa Surgery will be held by Cineca on the 28th of Nov.

About HLRS:
For a whole decade the High Performance Computing Center (HLRS) has been following its mission by providing its users with systems, tools, and expertise to achieve top international positions in their research field. The show-piece of our machines is the 72-node vector machine NEC SX-8.

HLRS is one of 11 partners and one of the HPC-centres providing “Transnational Access” within HPC-Europa. We are as well involved in several research and networking activities.

More information: *http://www.hlrs.de/hpc-europa*
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CORDIS

Transnational Access

MD @ HLRS

CPMD
The **CPMD** consortium has been established in 2001. The CPMD consortium is coordinated by Prof. Michele Parrinello (ETH Zurich) and Dr. Wanda Andreoni (IBM Zurich Research Laboratory).
The CPMD code is a plane wave/pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics. Its first version was developed by Jurg Hutter at IBM Zurich Research Laboratory starting from the original Car-Parrinello codes.
The current version, 3.11.1 is installed on the clusters cacau, strider and a optimized version for NEC SX-8.
More information: *http://www.cpmd.org/*

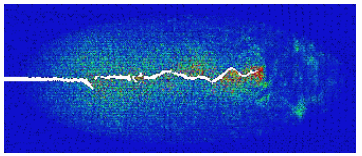
Molpro:
Molpro is a complete system of ab initio programs for molecular electronic structure calculations, designed and maintained by H.-J. Werner of the University of Stuttgart and P. J. Knowles.
As distinct from other commonly used quantum chemistry packages, the emphasis is on highly accurate computations, with extensive treatment of the electron correlation problem through the multiconfiguration-reference CI, coupled cluster and associated methods.
Various versions of Molpro are installed on the NEC SX-8.
More infomation: *http://www.molpro.net/*

Amber:
The Amber-suite, developed mainly for the simulation of biomolecules, consists of roughly 50 programs. There are many force-fields available in the package, visualization for various windowing systems is available as well.
The programs antechamber, LEaP, sander, etc. of the Amber-8 package are installed on the clusters cacau and strider.
More information: *http://amber.scripps.edu/*

MD at other HPC-Europa Centers:
Besides HLRS, all other HPC-Europa Access Centre provide several MD applications on their installed systems. If you want to find out more about the available applications, feel free to write a mail to: *staff@hpc-europa.org*

Custom MD Codes:
Last but not least, you always have the possibility to compile your own code on the machines available at the HPC-Europa Access Centres. The staff of the centres has a lot of experience with the installed hardware, as well as with installed compilers, MPI-libraries, optimisation and performance measurements of codes. You may get a better speed-up out of an omptimized code, and fast machines.

Further Activities relating to Code Development and Execution:
Please contact the HPC-Europa team for further information about the following additional activities:
JRA1: Performance Optimization using Paraver
JRA2: Single-Point of Access to any HPC-Europa Platform
NA2: AccessGrid Video-Conferencing with your HPC-Centre / Host



Molecular Dynamcis:
Molecular dynamics (MD) is a form of computer simulation where atoms and molecules are allowed to interact for a period of time under known laws of physics. Because in general molecular systems consist of a large number of particles, it is impossible to find the properties of such complex systems analytically. MD simulation circumvents this problem by using numerical methods. It represents an interface between laboratory experiments and theory and can be understood as a virtual experiment.

Molecular dynamics is a multidisciplinary field. Its laws and theories stem from mathematics, physics and chemistry. MD employs algorithms from computer science and information theory. It was originally conceived within theoretical physics in the 1950's, but it's mostly applied today in materials science and biomolecules.

(Wikipedia)