Contract n. RII3-CT-2003-506079 - Supported by the European Commission Access to Research Infrastructures Action

HPC-Europa

Pan-European Research Infrastructure on High Performance Computing

WELCOME to the March issue of HPC-Europa newsletter. This issue is edited by the Barcelona Supercomputing Center (BSC), and focuses on the research that one of BSC's HPC-Europa visitors has performed using one of the most advanced computing architectures available today: MareNostrum, the most powerful supercomputer in Europe and the fifth in the world.

Next closing date for applications: 15th May 2007

NEWS

- The TAM - Workshop 2007 will held in June in Bologna. All the past visitors will be contacted in a short time. More detail will appear on the HPC-Europa web site.

- The Transnational access sites are working in order to guarantee the access to research infrastructures also after the end of 2007.

- During the third year, 303 applications were made to the Transnational Access programme. The selection panel offered places to 201 user-projects, with an acceptance rate of 66%. A total of 211 visitors took part in HPC-Europa with an average visit length of 7.2 weeks. These users spent 349.9 visitor-months at the six different infrastructures, and used 4,597,186 Allocation Units (AUs). An Allocation Unit is equivalent to a processor running at 1 sustained Gflop during1 hour.

- The Spanish Ministry of Education and Science has created the Spanish Supercomputing network that consists of a distributed structure of supercomputers in order to provide support to the supercomputing needs of the different Spanish research groups. The initial nodes of this network are located at the BSC, in the CesViMa (Centro de Supercomputación y Visualización de Madrid), in the IAC (Instituto de Astrofísica de Canarias) as well as in the Spanish Universities of Cantabria, Málaga and Zaragoza.

About the Barcelona Supercomputing Center

In 2004 the Ministry of Education and Science, the Generalitat de Catalunya and the Technical University of Catalonia took the initiative of creating a National Supercomputing Center in Barcelona (BSC). The BSC was officially constituted in 2005. BSC manages MareNostrum, the most powerful supercomputer in Europe.

The BSC is a research center focusing on Computer Sciences, Life Sciences and Earth Sciences. As a result of this multidisciplinary approach, BSC brings together a critical mass of researchers, high performance computing experts and cutting-edge supercomputing technologies in order to foster scientific progress.

More information: *www.bsc.es/hpc-europa*
E-Mail: *hpc-europa.hosting@bsc.es*

Edited by Barcelona Supercomputing Center – Centro Nacional de Supercomputación

contact

staff@hpc-europa.org
access@hpc-europa.org

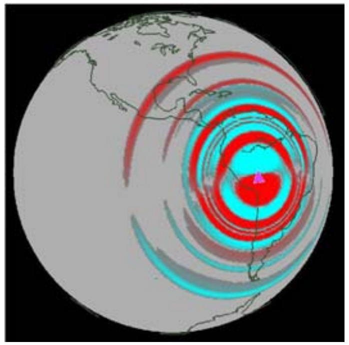
CORDIS

Transnational Access

Barcelona Supercomputing Center – Centro Nacional de Supercomputación

SPECTRAL FINITE ELEMENT METHOD IN THREE DIMENSIONS

Dimitri Komatitsch (dimitri.komatitsch@univ-pau.fr)



Seismic waves propagating around the Earth after a large earthquake in Bolivia, computed on MareNostrum using the SPECFEM3D software package

In the last thirty years, several numerical methods have been used to solve the seismic wave equation in order to calculate synthetic seismograms in complex geological models. The spectral element technique that I developed to solve this problem is based on a variational formulation of the wave equation and combines the flexibility of a finite element method with the precision of a global pseudospectral method to propagate the seismic waves, as illustrated in the picture. The method is implemented on parallel computers based on message-passing (MPI) to handle communications. The corresponding software package, SPECFEM3D (Spectral Finite Element Method in Three Dimensions), is currently used by more than 150 research groups worldwide.

For this HPC-Europa project we proposed a "grand challenge" for which MareNostrum could allow us to break a barrier and be able to improve our knowledge of the effects of the anisotropic structure of the Earth on seismic wave propagation following large earthquakes. To give an idea of the difficulty of the problem, quasi-analytical solutions for a 1D spherically-symmetric Earth are limited to low frequencies in practice. Therefore, if we manage to perform our 3D simulations on MareNostrum, we will be in the unusual situation of having gone beyond quasi-analytical solutions with a fully 3D numerical solution.

The goal of the first part of the project was to install the SPECFEM3D source code on MareNostrum, fix any possible portability problems and measure scaling. Another goal was to see if the order of the processors assigned to the code (sorted or not sorted machines in the Myrinet network) had an effect on performance and if activating trace recording (for analysis with ParaVer) slowed down the code. The conclusions are that the code worked fine on MareNostrum with only minor portability adjustments, and that processor order and trace recording have a negligible impact on performance.

The main goal of the second part of the project was to generate traces for several runs of SPECFEM3D using different mesh configurations and analyze them with ParaVer, and then modify the source code based on the conclusions of the ParaVer analysis in order to adapt it to the grand-challenge case considered. From the ParaVer analysis it quickly became clear that load balancing was relatively poor using the initial source code, since two groups of processors performed much more work than the others. There was also a large variance between processors due to cache misses. At the end of the project we found a theoretical explanation for these two problems, and possible solutions: we need to modify the way in which we generate the mesh, and we need to sort mesh elements using the Cuthill-McKee sorting algorithm to reduce the number of cache misses. Once these two improvements are implemented (which will take us a few months, considering that each modification affects several thousand lines of the source code), we hope to have excellent load balancing and return to Barcelona to be able to solve the Grand Challenge problem that we initially proposed.

The full source code of our software package SPECFEM3D is freely available for non-commercial academic research through *www.geodynamics.org*

Curriculum

Dimitri Komatitsch is a Professor of Geophysics at University of Pau in France and is the Director of the Department of Modeling and Imaging in Geosciences. He holds a Ph.D. in Geophysics from Institut de Physique du Globe de Paris, France, 1997. His HPC-Europa visit was done with BSC's Earth Sciences Group led by José Mª Baldasano.

"My research interests include the numerical study of seismic wave propagation in geological structures, and the study of associated site effects related to steep topography and strong lateral heterogeneities. I use a variational formulation of the equations of elastodynamics, and solve it in three dimensions (3-D) using the so-called spectral-element method, a high-order version of the finite-element method, which can be shown to be very accurate at low cost, and particularly well suited to an efficient implementation on parallel computers."

Personal webpage: *www.univ-pau.fr/~dkomati1*