DEISA Newsletter

DISTRIBUTED EUROPEAN INFRASTRUCTURE FOR SUPERCOMPUTING APPLICATIONS

Vol. 1, 2010

EuQuake project develops earthquake scenarios in Europe

Sanna Pyysalo

Seismic hazards and ground motion amplitudes will be better estimated in the future thanks to the EuQuake project. Its research results were achieved using supercomputing resources offered by DEISA. The project started in June 2008 and ended in August 2009.

Seismic waves generated by earthquakes carry a wealth of information on the Earth's interior structure and the behaviour of the earthquake's source. The aim of the EuQuake project, carried out by the Section of Geophysics of the Department of Earth and Environmental Sciences at the Ludwig Maximilian University of Munich, Germany, was to calculate theoretical seismograms for given three-dimensional velocity models and earthquake sources. The research group was led by **Dr. Martin Käser** and used new numerical algorithms and high-performance computing (HPC) to achieve this goal. The project was largely funded by the Emmy Noether Programme of the German Science Foundation. Numerical simulation algorithms are the central tool for modelling and explaining field observations at seismological stations on the European continent. By minimizing the difference between synthetic and observed seismograms it is also possible to recover information on the physical properties of the subsurface structure below Europe.

"Improved understanding in this field will allow us to better estimate seismic hazard, ground motion amplitudes and the consequences of ground shaking after earthquake events, for example via real-time earthquake parameter determination in early-warning systems," says Dr. Käser.

Many steps towards the goal

The main goal of the EuQuake project was to create a simulation software tool to be run on large supercomputers in order to produce accurate synthetic seismic data sets for earthquake scenarios on the European continent.

In the first part of the project, the technical prerequisites for large-scale simulations had to be met, and the necessary input data provided.

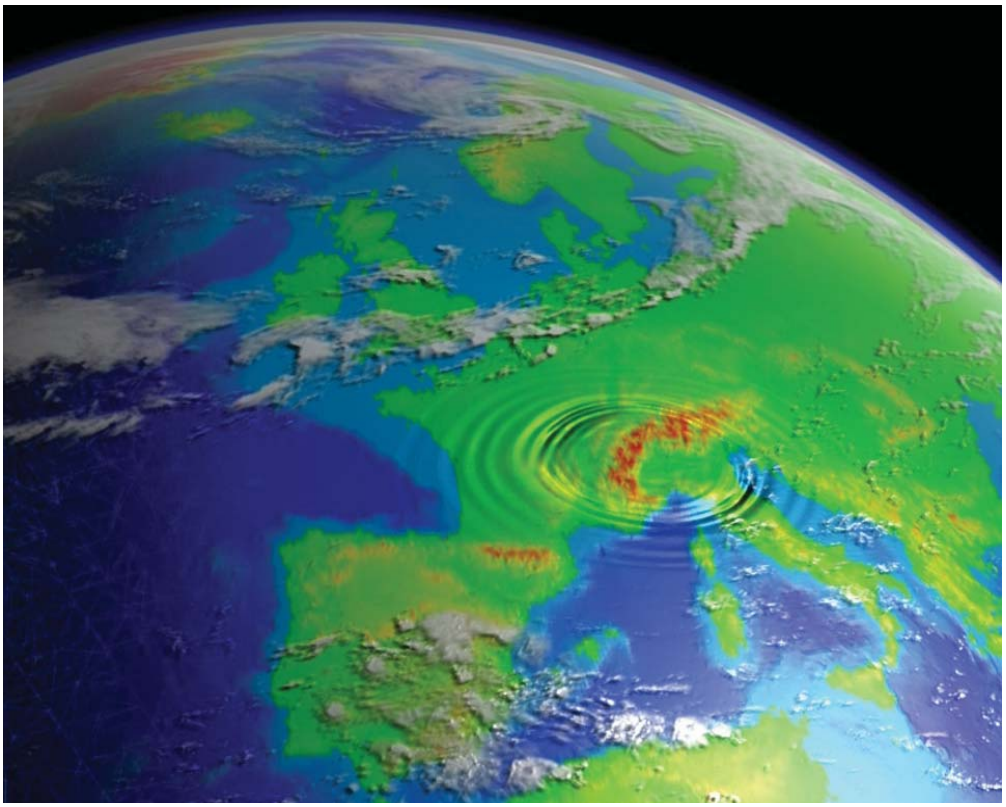

Fig.1. Schematic visualization of the propagation of earthquake waves at the Earth's surface where the faster P and S body waves have travelled further than the Love and Rayleigh surface waves that produce much higher amplitudes.

"Next, wave field calculations were carried out for past earthquakes for which observations are available. In the future, it is envisaged that these calculations will be performed on a semi-automatic basis, as soon as an earthquake occurs," Käser explains.

After the simulation, the waveforms are stored a format compatible with observational data in order to allow the application of the same processing tools to both empirical and synthetic results.

Models of the Earth´s crust are necessary

The main finding of the EuQuake project was that the crustal structure of the Earth has an enormous influence on arrival times of earthquakes and on seismic wave forms in particular, even though the layers it consists of are remarkably thin when compared to the dimensions of the European continent and the wavelengths of the propagated waves.

"We were able to show that we are still dependent, to a high degree, on the simplification of crustal models in order to represent the crust in numerical simulations. The automatic generation of accurate 3-D simulation setups for the ´on-demand´ computing of large synthetic data sets is only in its infancy," notes Käser.

Furthermore, the research group found that a quantitative measure for the frequency-dependent effects of the fine-scale structure of the crust is crucial to successful simulation setups.

"Only with such a systematically evaluated error analysis can we create appropriate discretized models and give a quantitative quality measure to our synthetic seismograms."

>>>

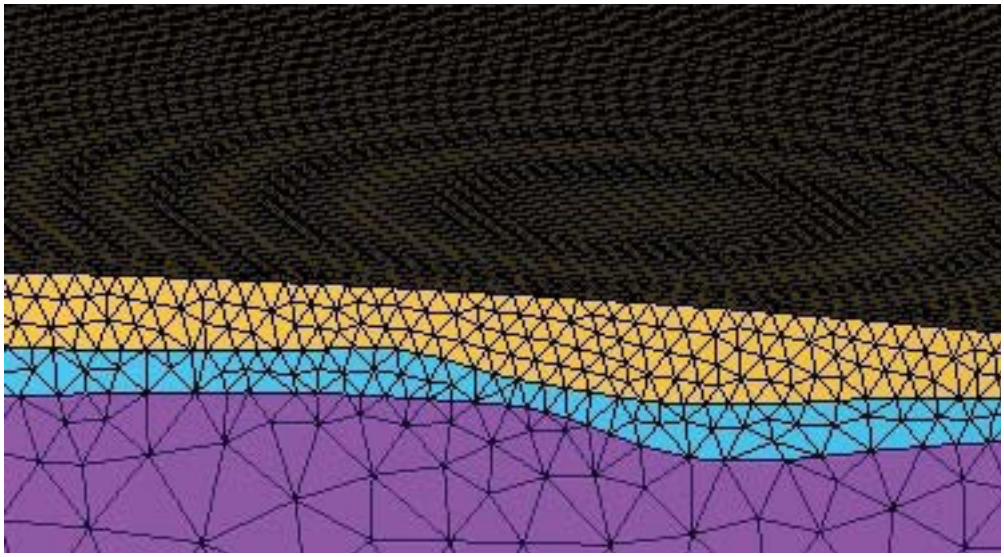

Fig.2. Color-coded discretization of the Earth's crust and upper mantel (purple) using an unstructured tetrahedral mesh. The geometrical flexibility of the mesh allows for the correct incorporation of major discontinuities such as the interface between the upper (yellow) and lower (blue) crust and the Moho-discontinuity.

Significant results for earthquake research

Numerical and computational methodologies have dramatically improved in the past few years. Nevertheless, due to the complicated nature of elastic wavefields and the long propagation distances of the waves, these calculations are computationally extremely expensive.

"Our research was unique, because we tried to consider with high levels of accuracy the geophysical and geometrical properties of the Earth's crust – the first 5–60 kilometres just below the Earth's surface," Käser says.

This is particularly challenging because the top layer consists of highly heterogeneous geological material both vertically and laterally, is of variable thickness and has the dominant influence on the shape, strength and arrival time of the seismic signals and, therefore, on ground shaking.

The EuQuake project was very significant for international research into earthquakes.

"It clearly showed that there is still a lot of work to be done towards the validation of the new European crustal models that are continuously being put forward. Much research effort is being put into the integration of more and more geophysical data into the creation of new seismic velocity models."

However, most modern simulation technologies still seem unable to take the resolution of these models fully into account, especially in the vertical direction. This means that accurate seismic wave propagation simulations after earthquake events are still limited to rough approximations of the crustal velocity models on a continental scale. Therefore, the ability to reliably predict ground motion in any given scenario is currently not dependent on the availability of missing information or the resolution of the velocity models, but rather on the validation of these models and the corresponding discovery of their weaknesses or errors.

"EuQuake has shown that we only can overcome these problems by investing in even more efficient and accurate simulation technology, which will require close and long-term collaboration between seismologists, computational geoscientists, numerical mathematicians, software engineers and computer experts from the most powerful HPC sites worldwide," Käser states.

DEISA´s help was essential

Developments in the field of seismology in recent years have highlighted the need for massively 3-D simulation technology in order to understand and explain the information from an ever-increasing stream of seismic observations.

"We as computational seismologists are absolutely dependent on the supercomputers as provided by HPC infrastructure of DEISA, with its distributed resources on huge parallel supercomputing systems," emphasizes Käser.

In other words, studies like those of the EuQuake project would simply be impossible without DEISA.

"This is why we believe that DEISA should play an important role in establishing a new working model for our CPU-intensive applications in the Earth sciences. We intend to embed the work started during the EuQuake project within further EU-wide initiatives and, in particular, to make efforts to establish an e-infrastructure for Earth sciences on an international scale."

Technical box:

Computations for the EuQuake project were performed on HLRB II in Garching, Germany, MareNostrum in Barcelona, Spain, and Huygens in Amsterdam, The Netherlands. There were several test and production runs, which used from 128 to 2048 CPU cores per simulation. A total of approximately 600 000 CPU hours were invested in these simulations. To construct the discretized models, commercial software packages like ANSYS ICEM CFD and GAMBIT were used on local computers. The simulations were carried out by the in-house developed solver "SeisSol" for seismic wave propagation problems, coded in Fortran90 using MPI for parallelization. Output visualization and data analysis were performed on local computers using MATLAB, PARAVIEW, and BLENDER.

More information: www.deisa.eu/science/deci/projects2007-2008/EuQuake

Fig.3. Dr. Martin Käser

Distributed European Infrastructure for Supercomputing Applications — PRACE

DEISA PRACE SYMPOSIUM 2010

10-12 MAY, CASA MILÀ, BARELONA

Registration and more information:
http://www.deisa.eu/news_press/symposium

PROGRAMME

Monday, May 10

12:00 Registration and lunch
14:00 Welcome
14:10 "World-wide Perspectives 1"

Montserrat Torné, Director General for International Cooperation and Institutional Relations, Ministry of Science and Innovation, Spain
Kostas Glinos, Head of Unit, DG INFSO, European Commission
José Muñoz, Acting Director, Office of CyberInfrastructure, National Science Foundation, US

16:30-18:30 "World-wide Perspectives 2"

Akira Ukawa, Vice President, University of Tsukuba, Japan
Thomas Zacharia, Deputy Director, ORNL, Department of Energy, US
Catherine Rivière, GENCI, France, European Exascale Software Project EESP

Tuesday, May 11

9:00 "DEISA and PRACE Updates"

Thomas Lippert, FZJ, Germany: *"PRACE Implementation Phase"*
Hermann Lederer, RZG, Germany: *"DEISA Extreme Computing"*

9:30 "Challenges in Computational Science 1"

Astrophysics:
Wolfgang Hillebrandt, MPI for Astrophysics, Germany: *"Modelling Cosmic Explosions"*

Materials Science:
Thomas Schulthess, ETHZ & CSCS, Switzerland: *"Ab initio Calculation of Free Energies in Nanoscale Systems"*

11:10 "Challenges in Computational Science 2"

Earth Sciences:
Jose Maria Baldasano, Earth Sciences Dep, BSC, Spain
Fusion for Energy:
Laurent Villard, EPFL, Switzerland: *"HPC Simulations of Magnetic Fusion Plasmas"*
Life Sciences:
Ivo Gut, Centro Nacional de Analisis Genomico, Spain

14:30 "Extreme Computing 1"

Richard Kenway, University of Edinburgh, UK: *"Solving the Mysteries of Quarks"* (Particle Physics / QCD)
Ilpo Vattulainen, Helsinki University of Technology, Finland: *"Physics of biological systems"* (Life Sciences)
Stephan Stellmach, University of Muenster, Germany: *"Turbulent transport in buoyancy-driven geophysical flows"* (Earth Sciences)
Roel Verstappen, The Netherlands: *"Regularizing isotropic turbulence"*(Engineering)

16:40-18:00 "Technology for the Future"

Jesus Labarta, BSC, Spain: *"Programming models and tools"*
Ana Bela Dias, NCF, The Netherlands: *"Access to PRACE systems"*
Herbert Huber, LRZ, Germany: *"Emerging and future technologies"*

20:30 Conference Dinner

Wednesday, May 12

9:00 "Using DEISA/PRACE & TERAGRID"

Peter Coveney, University College London, UK *"Towards Accurate and Precise Patient-specific Treatment Using Large-Scale Free Energy Calculations"*

9:30 "Extreme Computing 2"

Marco Bernasconi, Università Milano Bicocca, Milano, Italy: *"Ab-initio study of GeSbTe phase change alloys"* (Materials Science)
Stefan Gottloeber, Astrophysical Institute Potsdam, Germany:*"The Small Scale Structure of the Universe"*(Astrophysics)
Philip Eric Hoggan, CNRS, France: *"Slater Type Orbital Project for Quantum monte carlo large molecule simulations"* (Molecular Quantum Chemistry / QMC)

11:30 "Extreme Computing 3"

Patrick Joeckel, DLR, Germany: *"Coupling the Chemistry in Earth System Models on multiple Scales"* (Earth Sciences)
Vassilis Theofilis, Universidad Politécnica de Madrid, Spain: *"Global instability Analysis of Turbulent Separated flows"* (Engineering)
Sandor Katz, Department of Theoretical Physics, Eötvös University, Hungary: *"Lattice QCD thermodynamics with improved dynamical fermions"* (Particle Physics / QCD)
Michael Martinez, Klaus Tschira Fund, EML Research GmbH, Heidelberg, Germany *"Multiscale simulation of membrane associated multiprotein complexes"* (Life Sciences)

13:05 Closing remarks and lunch

DEISA TRAINING

Next training courses at University Collage, London on 5-6 May 2010

- Introduction to High Performance Computing

- Introduction to the DEISA Infrastructure

DEISA is running two training courses at University College, London, in early May 2010. Both will be based around a number of practical programming exercises. No prior knowledge is assumed for either of the courses.

The first course on Wednesday 5th May is an "Introduction to High Performance Computing". It will cover the fundamentals of modern HPC architectures and the two major parallel programming models: shared variables and message passing. Practical sessions will involve running existing parallel programs to investigate issues such as performance and scalability.

The second course on Thursday 6th May is an "Introduction to the DEISA Infrastructure". This will cover the basic aspects of the DEISA distributed supercomputer environment and the software tools that are used to access it, including the Application Hosting Environment (AHE). Practical sessions will involve installing software on the desktop and using it to access the DEISA systems.

Courses are available free for academic attendees. If the courses become over-subscribed, preference will be given to members of the Virtual Physiological Human Network of Excellence.

Those attending are encouraged to use their own laptops for both courses.

To register, please fill in the form at:

www.epcc.ed.ac.uk/training-education/course-registration-form/

DEISA Extreme Computing Initiative (DECI) Attracts Record Number of Proposals

Europe's HPC infrastructure DEISA announced that the number of proposals received for the DEISA Extreme Computing Initiative (DECI) had jumped this year by 62% to a record 122 applications. Proposals submitted this year involve researchers from 30 countries - 22 in Europe and eight from the continents of America, Asia, and Australasia. More than half a billion compute-hours have been requested, an over-subscription by a factor of ten.

Researchers applying to DECI are hoping to be given access to Europe's most powerful supercomputers at one or more of the 13 DEISA partner sites which operate fifteen of the Top 100 supercomputers in the world. For the first time this year, national supercomputers in Switzerland and in Sweden will be available via DECI, in addition to the national supercomputers in Germany, UK, France, Italy, Spain, the Netherlands and Finland.

Through DECI, now in its sixth year of operation, scientists from 35 countries have tackled a wide range of scientific challenges in materials science, astronomical science, particle and plasma physics, earth sciences, biological sciences and engineering. Successful projects are chosen for their potential to achieve groundbreaking scientific results through the use of supercomputers, enabling them to run more detailed and accurate simulations of scientific problems than was previously possible. Staff from DEISA work closely with the researchers on each project, providing specialist applications support to optimise the scientific codes and deploy them on the most appropriate architecture.

Alison Kennedy, Coordinator of DECI said, "DEISA is delighted that the computational science community has demonstrated how much it values the important role which DECI plays in enabling collaborative European computational science. The response to the latest call has been overwhelming, in terms of both the quantity and quality of proposals received. We hope to support as many projects as possible."

Jukka Heikkinen from Finland is one of the scientists who has participated in several collaborative DECI projects. He said, "Realization of fusion energy for future requires today a vast amount of simulations of microscopic plasma turbulence at real size of the burning fuel. This is possible only with massively parallelized kinetic particle codes which can be only run in world's top supercomputers. DECI has made some of the best European supercomputers available to the fusion scientists developing the plasma turbulence codes. It has helped, in particular, in characterization of turbulence in several tokamak experiments and in understanding the plasma energy confinement transition at the tokamak plasma edge. In addition to providing flexibility and quickness in distributing the runs on several computers, speeding up thus the science making, the DECI scheme has enforced the harmonization of the user solutions for coding and library use. The latter has made the codes more independent of the computer architecture, helping thus the world-wide integration of the codes."

CPU-h requested and awarded in previous DECI proposals