Book of Abstracts

The Second HPC-GA Workshop, Bilbao, 11-15 March, 2013

Title: Modeling Earthquake Dynamics in Realistic 3D Media with an hp-Adaptive Discontinuous Galerkin Method: Toward Physics Based Seismic Hazard Assessment

Authors: Josué Tago Pacheco (ISTerre, France / UNAM, Mexico), V. M. Cruz-Atienza, E. Chaljub, V. Etienne, S. Day and J. Virieux

Abstract: We introduce a novel scheme, DGCrack (Tago et al., JGR, 2012), to simulate dynamic rupture of earthquakes in three-dimensional visco-elastic media based on an hp-adaptive discontinuous Galerkin method. We solve the velocity-stress weak formulation of elastodynamic viscous equations on an unstructured tetrahedral mesh with arbitrary refinements (h-adaptivity) and local approximation orders (p-adaptivity). Our scheme uses a generalized Maxwell body to incorporate the anelastic attenuation of seismic waves through the specification of Q, the rock quality factor, with any frequency dependency. For modeling the dynamic source we consider second-order fault elements (P2) where dynamic-rupture boundary conditions are enforced through *ad hoc* fluxes across the fault. To model the Coulomb slip-dependent friction law, we introduce a predictor corrector scheme for estimating shear fault tractions, in addition to a special treatment of the normal tractions that guarantees the continuity of fault normal velocities. We verify the DGCrack by comparison with several methods (e.g. spectral elements, boundary integrals and finite differences) for spontaneous rupture tests (i.e. SCEC code-verification problems) and visco-elastic wave propagation in complex 3D basin models (i.e. Euroseistest in Volvi, Greece), finding excellent agreement. The DGCrack method reveals convergence rates close to those of well-established methods and a numerical efficiency significantly higher than that of similar discontinuous Galerkin approaches. The effect of mesh-refinement rates and unstructured meshes are quantified and analyzed carefully. We apply the method to the 1992 Landers earthquake fault system in a layered medium, considering heterogeneous initial stress conditions and mesh adaptivities. Our results show that previously proposed dynamic models for the Landers earthquake require a reevaluation in terms of the initial stress conditions that take account of the intricate fault geometry. Other interesting simulation results are presented for rupture scenarios close to 3D heterogeneous basin models with extreme velocity contrasts and attenuation properties.

Title: Verification of 3D Numerical modeling of earthquake ground motion in sedimentary basins: insights from the E2VP Project

Author: *Emmanuel Chaljub (*ISTerre, France)

Abstract: Numerical simulation is playing a role of increasing importance in the field of seismic hazard by providing quantitative estimates of earthquake ground motion, of its variability, and its sensitivity to geometrical and mechanical properties of the propagation media. Continuous efforts to develop accurate and computationally efficient numerical methods, combined with increasing computational power have made it technically feasible to calculate seismograms in 3D realistic configurations and for frequencies of interest in seismic design applications. Now, in order to foster the use of numerical simulation in practical prediction of earthquake ground motion, it is important to evaluate the accuracy of current numerical methods when applied to realistic 3D applications, where no reference solution exists. This process of verification, which is a necessary prerequisite before to confront numerical predictions to observations, is the main focus of this talk. I will present an investigation of the capability of numerical methods to predict earthquake ground motion through the ongoing Euroseistest Verification and Validation Project (E2VP). The project focuses on the Mygdonian basin (northern Greece), which has been a subject of extensive geophysical and geotechnical investigations for more than two decades. Numerical-modeling teams from Europe, Japan and USA employ the finite-difference method (FDM), finite-element method (FEM), global pseudospectral method (GPSM), spectral-element method (SEM) and discontinuous Galerkin method (DGM). The problem configurations include elastic and viscoelastic rheologies, basin models built from smooth velocity gradients or composed of three homogeneous layers with varying thicknesses, and a series of five 3D canonical cases. Numerical predictions for frequencies up to 4 Hz are compared using quantitative time-frequency envelope and phase goodness-of-fit criteria. It is shown that the numerical representation of models with fast variations (e.g. discontinuities) may vary strongly from one method to the other and may become a dominant source of inaccuracy, especially for seismic waves which are the most sensitive to those variations (e.g. guided or surface waves). A suggestion to temper this source of misfit is to resort to consistent homogenization (a.k.a. up-scaling) of the propagation model before to run and compare the simulations, and ideally during the construction of the model itself.

Title: Asymptotic Models for Geophysical Applications.

Author: Victor Peron **(INRIA, Pau, France)**

Abstract: In the context of the HPC-GA project, we are interesting in the mathematical modeling of Earthquakes. Thus, we must take into account the coupling of elasto-acoustic waves in complex media (Earth, ocean, atmosphere).

Asymptotic models and Equivalent boundary conditions have become classic notions in the mathematical modeling of wave propagation phenomena. They are used for instance for scattering problems from thin obstacles. The general idea is to replace an "exact model" inside the obstacle by approximate boundary conditions. This idea is pertinent if the boundary condition can be easily handled numerically, for instance when it is local.

In this talk, we present equivalent models for diffraction problems of elasto-acoustic waves. First, we consider solid obstacles coated with a thin layer of fluid medium. This problem is well suited for the notion of equivalent conditions: due to the small (with respect to the wavelength) thickness of the coating, the effect of the layer on the solid medium is as a first approximation local. We present 3D equivalent models for the elasto-acoustic problem: acoustic waves propagating in water are represented by an equivalent boundary condition. This approach leads us to solve only elastic equations. We discuss also the influence of a layer with a variable thickness. The mathematical models are rigorously justified. Then, we consider the case of a solid obstacle coated with a thin layer of fluid medium, and surrounded by a third medium. We can thus take into account the influence of the atmosphere in the modeling. We present also 3D equivalent models.

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Title: Aspects of Ocean Waves Modelling

Author: Leandro Farina (UFRGS, Brazil / BCAM, Basque Country)

Abstract: Some works on the modeling of ocean waves will be presented. The global model WAM is used to simulate ocean waves in the South Atlantic from June 2006 to July 2007 with high resolution in time. The four leading modes of the significant wave height, swell, wave peak period and surface wind velocity based on the EOF and SVD methods are computed and analysed. The results show a number of specific characteristics present in the short-scale regime, which emphasise, and in some cases, reduce some of the aspects of the global wave climate.

The interaction between atmosphere and ocean has been found in several fields and modes examined and a relationship with tracks of extratropical cyclones are observed. Particular strong coupled modes of variability are detected between swell and peak period and a region of a swell shade, observed in the global wave climate are reinforced and evidenced. Some recent findings on the local low dimensionality of global ocean waves dynamics will also be presented.

Title: Past, Present and Future Wave Climate: Global, Regional and Local Scales

Author: Fernando J. Mendez (Environmental Hydraulics Institute "IH Cantabria", Universidad de Cantabria, Spain)

Abstract: The term "wave climate" refers to the assessment of the statistical distribution of sea state parameters in a given ocean location (i.e., wave height, wave period, and direction). Wave climate varies at spatial scales (from the opean ocean to a beach) and temporal scales (wave-by-wave, seasonality, interannual variability, long-term changes). This topic involves different disciplines: ocean engineering, oceanography, climatology, statistics, computer science, remote sensing, among others. The success in the estimation of wave climate at a particular site strongly depends on the correct combination of measurements, atmospheric models, data analysis, wave propagation models, statistical models and on the knowledge of the time scales involved. In this talk, a review of all these components will be analyzed, showing examples at different spatial and temporal scales.

Title: Does High-Throughput Genome Analyses pose a challenge for High Performance Computing?

Author: Ana M. Aransay (CIC bioGUNE, Basque Country, Spain)

Abstract: Since 2004, when the first so called next-generation-sequencer was sold by Roche, there has been a growing demand of High Performance Computing approaches dedicated to the analyses of the vast amount of data generated at each project of this kind. The aims of massive-sequencing projects are very diverse, being for instance committed to study DNA variants associated with certain disease, tissue gene expression patterns under different biological conditions or epigenetic modifications related to particular cell types.
From small core facilities to big Genomics centres, all had to fit their infrastructures not only to the massive-sequencing equipment, but also to computing hardware and software requirements. The latter comprises acquisition of multiple-core servers and data storage capacity, establishment of faster networks as well as hiring skilled people in informatics and bioinformatics. Potential solutions for small core facilities, such as Cloud-computing, are being considered in order to reduce the costs of the host institutions acquiring computing equipment. However, we still have to face some challenges related to data format conversion of the outputs of some tools to be used as inputs of subsequent software in order to set up standard analysis workflows, in addition to the bandwidth necessities for the transfer of the "*heavy-weighted*" files yielded by this sort of research.

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Title: High Performance Computing at BCAM: Overview

Authors: Eneko Perez (BCAM, Basque Country)

Abstract: The overall goal of the presentation is to give an overview of the High Performance Computing available resources in BCAM, the work performed by different research groups using these resources and collaborations with industry that require HPC technologies to solve problems.

Title: High Performance Computing at BCAM: Simulating Complex Systems at various scales

Author: Elena Akhmatskaya and Bruno Escribano (BCAM, Basque Country)

Abstract: We present an overview of three ongoing scientific projects aiming at modelling and simulation of behaviour of real physical systems at various temporal and spatial scales:

1. Investigation of the mechanism of binding and release of Aluminium by serum Transferrin (atomistic scales)
2. Dynamic modelling of morphology development in multiphase waterborne polymers (meso-scales)
3. Computational study of polymorphism in drugs (multi-scales)

The studies are based on the original computational models and simulation methodologies developed in BCAM, and employ highly parallel open source and in-house software packages implemented on high performance computers. The computational models and their multi-level parallel implementations are discussed. Parallel performance of two software codes used in the studies, GROMACS and GSHMC-GROMACS (BCAM) is analysed.

Title: Status of porting BRGM's simulation software on top of INRIA Bordeaux's StarPU runtime

Authors: David Michea (BRGM, France), Olivier Aumage ((INRIA Bordeaux), Fabrice Dupros (BRGM, France).

Abstract: Ondes3D is a 4th order Finite difference code that simulates seismic wave propagation in an elastic medium. This code has been previously parallelized using MPI and OpenMP and successfully ported on hybrid GPU-CPU clusters using CUDA and MPI.

The StarPU runtime system developed in the Runtime Team is dedicated to heterogeneous architectures. Such architectures are made of both generalized processors and specialized processors. Applications submit elementary tasks to the StarPU runtime. StarPU is then responsible for scheduling these tasks on the available processors in a way that minimizes the execution time of the application. StarPU has already been used to schedule some basic stencil-like computations.

We are therefore interested by the comparison of the stencil based Ondes3D application performance between the static only GPUs or CPUs approach we used before and the dynamic and hybrid approach StarPU offers. That's why we have ported Ondes3D for the StarPU runtime system. We will discuss about the implementation and analyze the results.

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Title: Performance optimization of Numerical Simulation of Waves Propagation in Time Domain and in Harmonic Domain using OpenMP Tasks

Author: Giannis Ashiotis (INRIA, Grenoble)

Abstract: The numerical simulation of acoustic waves is a very important tool for the oil industry. When used together with data recovered from a series of on-site measurements, it can help in the discovery of oil deposits. Such a tool is the Hou10ni program which uses the Interior Discontinuous Galerkin Method to solve the wave equations. My task was to optimize the code by rearranging the order of the operations and the form of the data structures, together with reordering the input data, to create code that would display good cache behaviour, with remote memory accesses kept to a minimum. Moving on ready to be parallelized using OpenMP Tasks. The resulting code was parallelized using OpenMP Tasks, making it ready to have the Kaapi be integrated in it, giving it control over the parallelization. In this report, I make a summary of the changes made in order to achieve that, together with the resulting change in performance.

Title: Scalability issues of elastodynamics equations on multicore architectures. Early results with libKOMP runtime system

Authors: F.Dupros (BRGM, France), H.T Do (BRGM, France), F.Broquedis (INRIA, Grenoble)

Abstract: Owing to its simplicity and numerical efficiency, the finite difference method is one of the most popular techniques to solve the elastodynamics equations and to simulate the propagation of seismic waves.

Most of the parallel implementations for x86 cores are based on a distributed memory assumption and rely on the MPI library for coarse-grained parallelism with a possible use of OpenMP directives to distribute the triple nested loops corresponding to the discretization in space.

In spite of the regularity of the algorithm and the good speedups usually reported, the performance levels obtained with standard implementations on multicore nodes remain poor and far from the peak performance.

In this talk, we evaluate the impact of multicore architectures on standard implementation of the elastodynamics equations. We will therefore comment some preliminary results on the use of OpenMP tasking model in such a case. These experiments rely on LibKOMP runtime systems developed by the Inria Moais research team.

Title: Porting Ondes 3D to Adaptive MPI

Authors: Rafael Keller Tesser (UFRGS, Brazil), Víctor Matínez (UFRGS, Brazil)

Abstract: Ondes 3D is a simulator of three-dimensional seismic wave propagation.
Because it simulates a finite computational domain, it needs artificial conditions to absorb the outgoing energy. This results in extra operations near the lateral and bottom edges of the simulated geometry. Therefore, Ondes 3D can benefit from load balancing techniques. In the context of the HPC-GA project, it was proposed the modification of Ondes 3D, to take advantage of the load balancing mechanisms provided by the Charm++ framework. As a first step towards this goal, we ported a MPI implementation of Ondes 3D to use the Adaptive MPI (AMPI) framework. AMPI uses the same underlying mechanisms as Charm++. In our presentation, besides discussing the porting, we will show an performance evaluation of the AMPI port of Ondes 3D, using load balancing strategies.

Title: Toward Physics-Based Earthquake Modelling for Hazard Assessment

Authors: Victor Manuel Cruz-Atienza *(UNAM, Mexico)*, J. D. Sanabria, J. Tago, V. Etienne, V. Hjörleifsdóttir, J. Virieux, and E. Chaljub
Abstract: Applying computational methods for understanding earthquakes requires solving a diversity of fundamental problems. Besides having a sufficiently accurate description of the wave propagation media (e.g. including anelastic energy-dissipation properties), capabilities of the methods must be suitable for insuring the numerical accuracy of the wavefield propagation throughout these models, which may exhibit intricate geometries and extremely high velocity contrasts. The computational challenge to this purpose relies in both the extreme wavelength modulation within the model (e.g. from ~6,000 to ~200 m) and the wavefield excitation from the source, which should account for realistic prestress conditions and constitutive relationships over the fault (i.e. friction laws).

One of the most challenging earthquake-modelling problems worldwide is to understand the seismic response in the Valley of Mexico, where Mexico City is located above a large sedimentary basin; to major subduction earthquakes that take place more than 300 km away, along the Pacific coast. In this work we present preliminary results on the h-adaptive tetrahedral meshing of a basin model (i.e. 90 x 80 x 22 km^3) that includes topography and the intricate 3D geometry of the sediment layer. Wave propagation in this model is illustrated with double-couple point sources by means of an hp-adaptive discontinuous Galerkin method, namely DGCrack, developed by Etienne et al. (2010) and Tago et al. (2012). Additionally we present a set of realistic finite-source rupture models in the Guerrero Gap subduction segment within a 2.5D tomographic velocity model (Iglesias et al., 2010) from which the ground motion is analysed through several metrics as Peak and Spectral Ground Accelerations. These results allow assessing the size of the computational challenge in this kind of simulations. Furthermore, the exercises may help to point out the directions toward which our computational developments should move to tackle the large final applications considered in the last stage of the HPC-GA project.

References:

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Title: An example of the use of computational seismology in observational seismology: Moment-tensor inversions of intermediate-size earthquakes in Mexico

Authors: Vala Hjorleifsdottir (UNAM, Mexico), Oscar O. de la Vega Cabrera (UNAM, Mexico), Arturo Iglesias (UNAM, Mexico), Víctor M. Cruz-Atienza(UNAM, Mexico)

Abstract: Observational seismology is inherently linked to computation. For even the most basic earthquake locations we calculate travel times through simple one- dimensional structures. To estimate the moment tensors of earthquakes we calculate synthetic seismograms for one-dimensional Earth models and compare to observed data. Due to the relatively simple structure of the mantle, using one-dimensional models of the Earth works very well when looking at body waves at large distances and long-period surface waves, that spend most of their time in and are most sensitive to, respectively, the mantle. However, small earthquakes do neither excite body waves that are observed at large distances, or long-period surface waves, and have to be observed nearby, looking at waves that travel through the Earth's highly heterogeneous crust. As a result one-dimensional Earth models are not as effective for the study of intermediate-size earthquakes in a regional setting as they are for larger events in a global setting.

In this presentation we will present our ongoing work of estimating moment tensors for moderate size earthquakes in Mexico using shorter-period surface waves. We use a grid-search based algorithm developed for Southern California (Liu et al 2004) that allows for the use of 3D synthetic seismograms in the source inversions. The synthetic seismograms are calculated using a spectral element method, (SPECFEM3D_GLOBE, Komatitsch and Tromp, 2002a, 2002b). Currently we are using a global velocity model that combines crustal model Crust 2.0 (Bassin et al 1999) and mantle model S362ANI (Kustowski et al 2008). We will demonstrate that the use of this model provides some advantages over a one dimensional Earth model, however, many of the observed seismograms are still poorly matched at periods of 40 seconds and shorter, which are the ones strongly excited by intermediate-size earthquakes. As part of the HPC-GA project, we are starting to implement a regional velocity model based on the modeling of surface-waves phase velocities, down to periods of 5 seconds (Gaite et al 2012), into SPECFEM3D_GLOBE. The model includes thick sediments, mainly in the western part of the Gulf of Mexico, that we expect will need to be meshed very finely to accurately account for. An adaptive meshing scheme might be needed for efficiency.

We will also briefly present how synthetic seismograms can be effectively used for detection of earthquakes using surface-waves.

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Title: Computational Challenges on Wave Propagation

Author: Enrique Zuazua (BCAM, Basque Country)

Abstract: Flow control is an important topic for its many applications, in particular in aeronautic shape design. The theories of Control and Optimal Design face difficulties when addressing these issues because of the possible presence of singularities on solutions, making classical computational approaches fail. In this lecture we shall briefly review the work of the team in this context and indicate some interesting open problems and computational challenges.

Title: Task parallelism with the libKOMP runtime system

Author: François Broquedis (INRIA, Grenoble)

Abstract: Task parallelism has become a commonly-adopted paradigm to program HPC shared memory platforms. Several parallel environments have evolved to support tasking, considering tasks as the right entity to express fine-grain dynamic parallelism. OpenMP, the de-facto standard for shared memory parallel programming, is about to introduce data-flow extensions to its tasking model, granting the programmer the ability to express dependencies between tasks. In this talk, I will present the libKOMP OpenMP runtime system developed by the MOAIS research group in Grenoble, giving insights on the way we efficiently implement these data-flow extensions and the impact they will have on the way we develop parallel applications. Another part of this talk will focus on ongoing research developments related to the topics of the HPC-GA project, like controlling tasks execution on NUMA platforms and speeding-up the execution of visualization applications thanks to the VTKSMP parallel plug-in we also develop in Grenoble.

Title: IZO-SGI SGIker, Scientific Computing at the UPV/EHU

Authors: Jose M. Mercero , (UPV/EHU, Basque Country), Eduardo Ogando (UPV/EHU, Basque Country)

Abstract: The IZO-SGI SGIker provides High Performance Computing (HPC) resources and human support not only to the UPV/EHU researchers but also to the Basque country scientific community. In the present talk we will describe the Service and we will summarize some of the research that is being done using our resources.

Title: Liquid water from first principles

Author: Emilio Artacho (CIC **nanoGUNE, Basque Country)**

Abstract: The understanding of liquid water at molecular scale and its interactions with other fluids or solids is of enormous importance in the geosciences, from the formation of clathrates in sediments, to chemical reactions on or in water droplets in the atmosphere, including a very vast part of geochemistry, be it homogeneous (reactions of species dissolved in water) or heterogeneous (at the interface between a solid and a mineral). Liquid water itself is an enormously intriguing system, displaying around 17 anomalies in its thermodynamic and dynamic behaviour, as compared with conventional fluids, floating ice being the best known of them. Very substantial insights into its behaviour has been obtained from molecular dynamics simulations based on relatively simple empirical forces among molecules. They capture the essential interactions and fit their few free parameters so as to reproduce key thermodynamic properties of water, obtaining extremely successful description of water and its anomalous behaviour, including clues on the speculated liquid-liquid phase transition, related to two fluids of different density that are supposed to coexist at temperatures below freezing.

It is however very hard if not impossible to reproduce that level of success in the simulation of water in interaction with other systems, especially if reactive. The number of fitting parameters shoots up and becomes unwieldy, and the simple force expressions themselves become too rigid and blunt to describe subtle electronic effects.

It is thus important to be able to describe such systems from first principles. Pure liquid water from first-principles has a history of more than two decades, based mostly on molecular dynamics for classical nuclei using density functional theory (DFT) for the electrons.

I will show recent progress in the description of liquid water with recent developments in approximate density functionals, most importantly, the inclusion of dispersion interactions from first principles.

We have performed first-principles molecular dynamics based on DFT using the Siesta program. It is a DFT code that uses finite-support atomic orbitals as basis sets and which is aimed for efficiency, allowing for calculations that scale linearly with system size instead of the customary cubic scaling.

We will see how it affects (improves) properties as the equation of state (equilibrium density, compressibility) and the diffusivity. We will also see how the fine balance in the interactions in the liquid is shifted by the presence/absence of dispersion, in the direction of the high-density / low-density liquid component of the supercritical liquid room-temperature water is proposed to be.

Title: Non-conforming meshes withe curved elements and local-time stepping for the simulation of wave propagation in elasto-acoustic media

Authors: *Julien Diaz, Ángel Rodriguez-Rozas (INRIA, Pau, France)*

Abstract: We propose to design and to implement a finite element method for coupling elastodynamic and acoustic wave equations, which could accurately describe the transmission phenomena occuring at the interfaces between the surface. This is crucial in order to model seismic wave propagation between oceanic and continental crusts, but also in order to improve offshore seismic imaging. Since the depth of the ocean is very thin compared with the size of the subsurface, the meshes are composed of very fine cells in the water. In order to improve the performance of the numerical methods, it is thus necessary to consider non-conforming meshes. This is not a major difficulty when the interface between the ocean and the subsurface is plane. However, when the interface has a strong topography, it is no longer possible to generate non-conforming meshes that are perfectly matched to the interface. To overcome this difficulty, we propose to represent the interface using splines and to use curved elements. Since we use explicit time schemes, the difference between the size of cells impacts severely the stability condition of the time scheme which is much more restrictive in the fluid than in the solid and it will be necessary to consider a local time stepping method,

This talk will be composed of three parts. In the first part, we will present the solution strategy we have chosen for constructing the non-conforming meshes and the first results we have obtained. Then, we will describe the local-stepping method and finally we will discuss the difficulties induced by implementation of the algorithms in a HPC framework.

Title: Tectonic evolution at mid-ocean ridges: geodynamics and numerical modeling

Author: *Edie Miglio (Politecnico di Milano, Italy)*

Abstract: Tectonic evolution at rift zones is commonly considered symmetric along mid-ocean ridges, when modeling with relative plate motions and steady-state processes. However, the bathymetry of rift zones is generally asymmetric, being the eastern flank in average slightly shallower (100-300 m) than the western one. Also, based on surface wave tomographic models, shear wave velocities in the upper mantle indicate a difference between the western and eastern flanks of an oceanic basin. A better way to understand dynamics of the lithosphere at rift zones, and lithosphere/mantle interactions corresponds to absolute plate kinematic analyses, i.e., with respect to the mantle, modeling time-dependent tectonic processes. We performed numerical simulations of plate-driven mantle flow beneath mid-ocean ridges and we considered a time-dependent flow induced by the relative motion of overlying rigid plates in an incompressible viscous mantle.

In mantle reference frames, a net "westward" rotation of the lithosphere relative to the mantle can be observed, and we used velocities obtained in the hotspot reference frame, as boundary conditions. This implies that plates along a ridge, and the ridge itself, move toward the west but with different velocities, relative to the mantle, and the separation between plates triggers mantle upwelling.

Numerical solutions for viscosity flow beneath plates that thicken with increasing age are presented. The mantle can be modeled as a viscous fluid, and its dynamics can be described using the Stokes equations. At a first approximation the fluid is considered Newtonian. A further step in the description of the phenomena would require the inclusion of thermal effects: in this case the fluid viscosity and density have to be considered as a function of the temperature.

For solving both the Stokes equations and the thermal effects, a finite element approach has been adopted. Results show an asymmetric thickening of plates along the ridge, as suggested by geological a geophysical observations, and provide useful relationships between mantle temperature and thickness of the oceanic lithosphere.