Frontiers in Computational Geophysics: simulations of mantle circulation, plate tectonics and seismic wave propagation

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1 Introduction

Geophysics differs from other scientific disciplines in its focus on processes one can neither repeat nor control. Examples include the nucleation of an earthquake as brittle failure along faults, or the dynamic processes of ductile (creeping) flow in the earth's interior which give rise to plate tectonics and the endogenic (internally driven) geologic activity of our planet. The inherent experimental limitations and the indirect nature of our observations explain in part why there is such a remarkable impact and success of high-performance computing (HPC) in this field. And indeed many a geophysical observable are only interpretable through the use of sophisticated modelling tools. Another reason for the prominence of HPC lies in the recent crossing of long standing thresholds in capacity and capability computing. This allows us today to implement models having in excess of 1 billion grid points. The development makes it feasible for the first time to overcome in three dimensional (3D) models the great disparity of length scales which characterises important geophysical phenomena: an earthquake rupturing a fault segment over a distance of some 100 km while emanating seismic energy throughout the planet (10,000 km), or the peculiar nature of plate tectonics with deformation concentrated along plate boundaries of 10-100 km width separated by plates of dimension 1,000-10,000 km serve as example. Before we address challenges and recent successes in global geophysical modelling, let us take a brief look at the gross structure and inherent dynamic time scales of our planet.

The earth's interior is complex, consisting of three distinct regions. Starting from the outside there is first the cold lithosphere, which is dominated by brittle behaviour. It then follows the solid mantle, which deforms slowly over geologic time by a mechanism known as ductile creep. Finally near the earth's centre there is the (mostly) liquid core. As a result of convective and other forcings, all three regions are in motion, albeit on different time scales.

On the longest time scale solid state convection (creep) overturns the mantle once in about every 100-200 million years [8]. This overturn is the primary means by which our planet rids itself of primordial and radioactive heat. Tectonic processes operate on shorter time scales, up to a few million years or so. They include rapid variations in plate motions, which are revealed by the recent arrival in the earth sciences of highly accurate space geodesy techniques, such as the global positioning system GPS [11]. On still shorter time scales of perhaps 1-1000 years convection of the liquid iron core generates the earth's magnetic field through a complicated dynamo process that probably operated throughout much of earth's history [18]. Only recently have geophysicists been able to study dynamo action in sophisticated magneto-hydrodynamic models of the core. We will not concern ourselves with these models and refer to the recent review by [15]. On a time scale of hours to seconds both the core and the mantle are traversed by seismic sound waves, and seismologists are now turning to computer models to study seismic wave propagation through our planet [21].

2 Mantle Flow and Circulation Modelling

The mantle comprises approximately 70 % of the earth's volume and convects with surprising vigour. Its thermal Rayleigh number, estimated at 10^6 to 10^8 [10] exceeds the critical value at which convection begins by a factor of 10^3 to 10^5, yielding flow velocities of 1-10 cm/year and an upper thermal boundary layer (known as plates) of thickness of 50-100 km depth. The advent of powerful computers allows us to resolve the flow in realistic 3D spherical geometry, and a number of high-resolution, parallelised mantle convection models are now available. The models have provided crucial insight into key parameters governing the behaviour of global mantle flow, such as the effects of mantle phase transitions, a depth-wise increase in viscosity and the partitioning of internal (radioactive) and external (core derived) heating, [37, 6, 41, 35].

Mantle convection can mathematically be modelled by a coupled system of three equations, see e.g. [29, 35], describing the conservation of mass, momentum and energy. These differ from the standard Navier-Stokes system of convection driven fluid dynamics in that respect that due to the high Prandtl number (on the order of 10^{24}) inertial terms in the momentum equations can be dropped. This reflects the creeping nature of the flow. Note also that for similar reasons Coriolis and centrifugal forces may safely be neglected.

Mass conservation is a constraint on the velocity field of the Stokes problem, and the coupled system of mass and momentum conservation, after discretisation by standard techniques like finite-element and finite-volume approaches, give rise to a saddle-point problem, which one solves for a velocity field satisfying the divergence-free condition. Most mantle convection codes adopt Uzawa-type algorithms for this purpose, see e.g. [1], often employing conjugate gradients for the outer and multigrid for the inner iteration. Multigrid employs a hierarchy of nested computational grids, so that near-and far-field components of the momentum balance are effectively solved at once. We show the nested structure of the icosahedral grid adopted in the Terra code [7] as an example in Fig. 1.

Similarly one often treats the energy equation through mixed finite volume, finite difference methods for the advected and conducted heat flux. The Péclet number of the mantle is large (in the range of 10-100), that is heat transport in the mantle is controlled primarily by advection outside of thermal boundary layers. This makes finite volume methods, which are conservative and easily adapted to unstructured meshes, an effective solution approach.

It is common to use the term *circulation* to describe the motion of the mantle, in analogy to the general circulation of the oceans and atmosphere. A number of mantle circulation models (MCMs) have been constructed recently, [8, 4, 27], and a representative MCM at high numerical resolution (about 100 million grid points) is shown in Fig. 2. MCMs differ from traditional convection models in that they include geologic information on the history of subduction [8]. This allows them to make explicit predictions on the large-scale thermal structure of the mantle, which is an essential component if one wants to assess the force balance of plate motion.

In general MCMs compare well with tomographic mantle models, [33], which constrain earth structure from independent seismic observations. MCMs suffer, however, in a fundamental way from lack of initial condition information. The difficulty becomes more challenging the further back in time one wants to model the evolution of mantle buoyancy forces, say over the past 10-100 million years. Lack of initial condition information is a problem shared with circulation models of the ocean and the atmosphere.

To overcome the initial condition problem one must formulate a large scale fluid dynamic inverse problem. Essentially one seeks optimal initial conditions that minimise, in a weighted least squares sense, the difference between what a mantle convection model predicts as mantle heterogeneity structure and the heterogeneity one actually infers from, say tomography. This class of problems is known in different contexts as e.g. *history matching* or *variational data-assimilation*, meaning that model parameters are inferred from a varia-

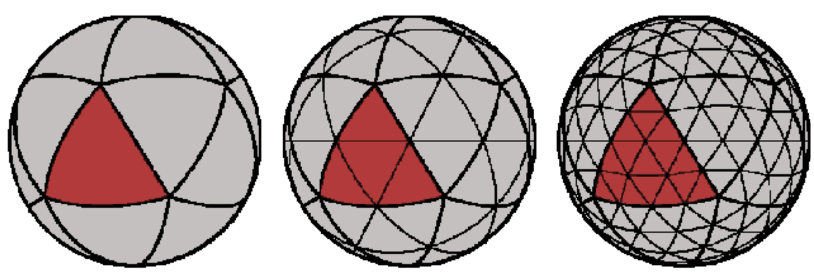


Fig. 1. Three successive mesh-refinements of the icosahedral grid

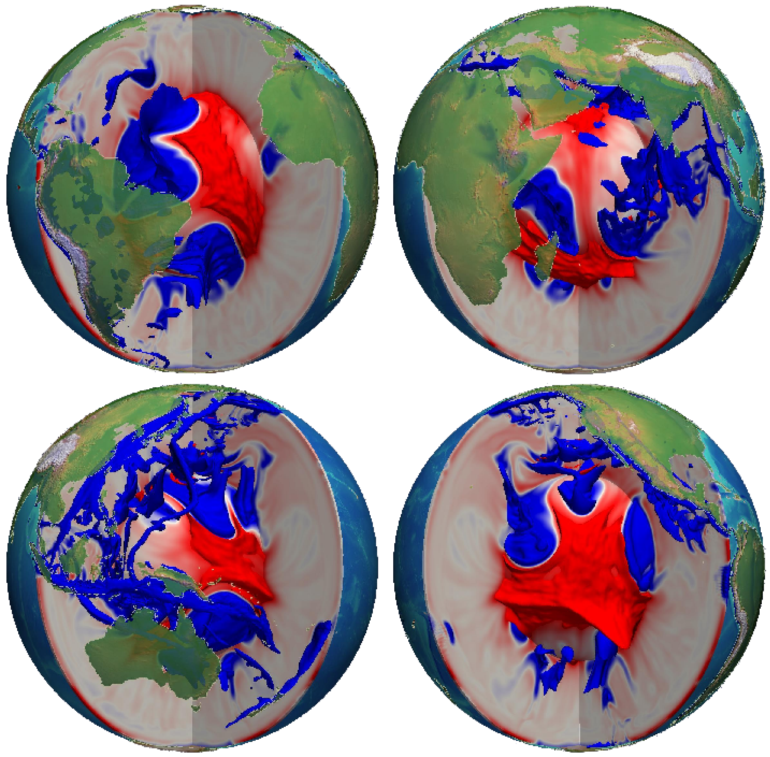
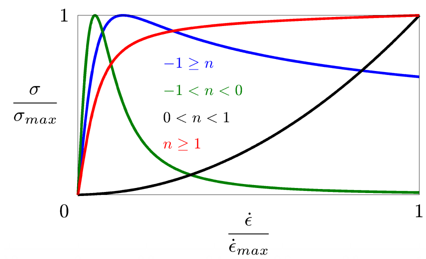


Fig. 2. 3D representation of temperature variations in a high resolution Mantle Circulation Model (MCM), see text. Shown are four cross sectional views from 35 (upper left), 125 (lower right), 215 (lower left) and 305 (upper right) degrees longitude. Continents with colour-coded topography and plate boundaries (cyan lines) are overlain for geographic reference. Iso-surfaces of temperature are taken to be at -600 and +400 Kelvin. The +400 iso-surface was clipped in the uppermost 500 kilometres in order to allow views into the mantle underneath the mid-ocean-ridge systems which span large parts of the oceanic upper mantle. The colour-scale is saturated at -400 and 400 Kelvin. About 100 million numerical grid points are used, providing a grid point spacing of at most 20 km throughout the mantle, sufficient to resolve the convective vigour of global mantle flow.

tional principle through the minimisation of a cost function F. The necessary condition for a minimum of F, that the variation $\nabla F = 0$, leads to the usual mantle convection equations coupled to a corresponding set of so-called *adjoint equations*.

The adjoint equations, which have been derived recently, [5, 23], together with large-scale simulations showing that flow can be inferred back in time for at least 100 million years, are nearly identical to the forward model except for forcing terms. Unfortunately adjoint modelling of global mantle flow at realistic convective vigour comes at a heavy computational price. Weeks to



$$\sigma(\dot{\epsilon}) = \nu(\dot{\epsilon}, T, z) \cdot \dot{\epsilon}$$
$$= A \cdot (\gamma + \dot{\epsilon}^2)^{\frac{1-n}{2n}} \cdot e^{\frac{B+Cz}{T}} \cdot \dot{\epsilon}$$

$$\sigma(\dot{\epsilon}) \propto \dot{\epsilon}^{\frac{1}{n}} \quad \text{for} \quad \dot{\epsilon} \to \infty$$
$$\sigma(\dot{\epsilon}) \propto \dot{\epsilon} \quad \text{for} \quad \dot{\epsilon} \to 0$$

Fig. 3. Generalised power law rheology, where stress σ is proportional to strain rate ϵ through a viscosity ν that depends on temperature T, strain rate and depth where A, B, C, γ and n parameterise the dependence. Note that so-called *self-lubrication* rheology arises only for a narrow and unphysical band of power law exponents ranging from -1 to 0, which is not observed for geologic materials.

months of dedicated integration time are needed to solve this class of problems even on some of the most powerful parallel machines currently in use. Such resources, however, are coming within reach of topical PC-clusters dedicated to capacity computing [29].

3 Plate Tectonics and Boundary Forces

A long persistent challenge in geophysics is the computational treatment of plate tectonics, because it is difficult to simulate shear failure along plate boundaries. One strategy, developed more than 30 years ago, models known plate structures and their influence on mantle flow by specifying regions that move in a plate-like manner, [9, 30, 14]. An alternative approach adopts highly non-linear (non-Newtonian) viscous creep, strain-rate weakening rheologies, and viscoplastic yielding, [43, 36, 31].

In [28] Moresi and Solomatov explored the effects of strongly temperature-dependent viscosity combined with a plastic yield stress: the former causes the cold upper boundary layer (lithosphere) to be strong, while the latter allows the boundary layer to fail locally in regions of high stress. The success of this *ductile* approach to plate tectonics, measured through a so-called *plateness*, is evident when one applies exotic rheologies with an extreme form of strain softening. One such rheology, where both viscosity and stress decrease with increased strain rate, is known as *self-lubrication*, see [2]. We summarise its essence in Fig. 3. Unfortunately, self-lubrication requires the use of power-law exponents ranging between -1 and 0 (see Fig. 3). These values do not agree with laboratory experiments of ductile deformation performed on olivine, which find n in the range 2 to 5, see e.g. [24].

The challenge to develop plate-like behaviour in convection models reflects the difficulty to account for brittle failure and reactivation of pre-existing faults in the uppermost cold region of the lithosphere. The high strength in the upper part of the lithosphere expresses the resistance of rocks at low temperature to break, or slide past each other when already faulted. Experimental results indicate a simple linear relationship to parameterise this behaviour, where shear stress is proportional to the effective normal pressure through a friction coefficient. Geodynamicists have introduced weak zones at the surface of mantle convection models in an attempt to account for brittle failure in the lithosphere [9]. The logical development of this approach is the inclusion of discontinuities directly into the computational grid and the representation of faults through contact-element interfaces. This has been done, for example, in the modelling work of Zhong and Gurnis [42] and the global neo-tectonic model of Kong and Bird [26].

Today the neo-tectonic models have reached a high level of maturity allowing them to account for surface topography, regional variations of lithosphere density and thickness according to either Pratt or Airy isostatic compensation, thermal regime of the lithosphere - based on heat flow measurements and crustal radioactive decay - and for realistic plate configurations [32, 3]. The models typically use finite-element formulations to solve the equations of mass and momentum conservation in the Stokes limit that we have seen before, and compute the instantaneous force balance and associated plate velocities. The use of finite elements makes it feasible to implement empirical, depth-dependent rheologies of the lithosphere to account for ductile as well as brittle deformation. We show the computational grid from the global lithosphere model of Kong and Bird [26] in Fig. 4.

A first-order result in plate tectonic modelling is the recent explanation of the plate motion change off-shore of South America (see Fig. 5). For the

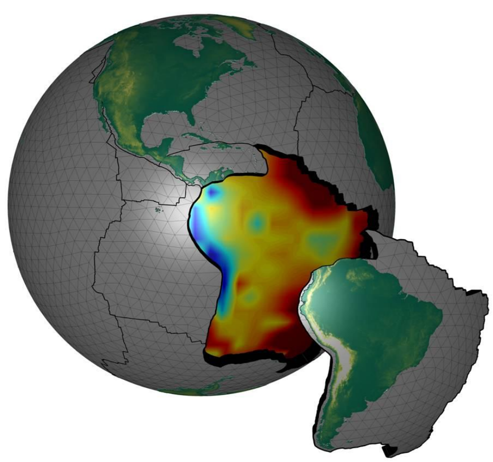


Fig. 4. Grid of global neo-tectonic SHELLS model coupled to a global mantle circulation model (see text); colours represent temperatures (red=hot, blue=cold) at a depth of 200 km below the surface.

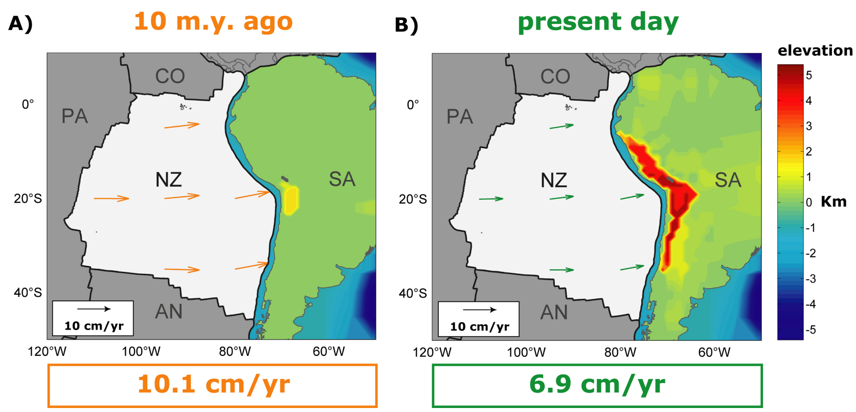


Fig. 5. Computed velocity for Nazca plate (NZ) relative to South America plate (SA) from global plate motion simulations. Topography of South America plate from numerical simulations is shown together with colourbar. Plate boundaries are in black, coastline in gray. a) For 10 Myrs ago we compute a convergence rate of 10.1 cm/yr with topography of South America plate inferred from geological indicators. b) For present day we compute a convergence rate of 6.9 cm/yr with topography of South America plate from the ETOPO5 database. 4 km of topography lifted up over the last 10 Myrs can account for the slow down of Nazca plate.

Nazca/South America plate margin a variety of data indicate a significant decline (by some 30%) in convergence velocity over the past 10 Myrs. The ability to consider past as well as present plate motions provides important constraints for our understanding of the plate tectonic force balance, because changes in plate motion are necessarily driven by changes in one or more driving or resisting forces. By explicitly coupling MCMs, which provide estimates on the mantle buoyancy field, to neo-tectonic models Iaffaldano, [20, 19], shows that the recent topographic growth of the Andes is a key factor controlling the long-term evolution of plate motion in this region.

Further supporting evidence for the dominant effect of Andean topography on plate boundary forcing along the Nazca/South America margin comes from gravity and stress field measurements, [34, 17, 44]. Heidbach, Iaffaldano and Bunge [16] show that these independent observables can also be reproduced from the coupled models.

4 Seismic Wave Propagation

In seismology there has been a gap between observations and theory for several decades in that the quality and quantity of observations far exceeds the traditional methods of seismic modelling. Although the existing tomographic images of the mantle have greatly contributed to our understanding of the planet's dynamics, the inversions of seismic observables usually involve substantially simplified forward models, namely ray theory and finite normal mode summations. Ray theory is only applicable to the arrival times of high frequency waves, therefore significantly reducing the amount of exploitable information. Conversely normal mode approximations rely on smoothly varying structure and long period waveforms, resulting in a limitation of resolution.

The fact that today's computational power is sufficient to accurately solve the wave equation in realistic earth models [22, 25] is prompting new efforts to replace the approximate ray-theory and normal mode forward models by the exact forward model of full seismic wave propagation, and to invert for seismic waveforms with shorter periods. The expectation is that the resulting increase of exploitable information will translate into an increase of resolution especially in regions poorly sampled by seismic rays.

In analogy to the efforts of using adjoint theory in geodynamics, adjoint methods are explored in seismology. The approach allows us to compute the derivative with respect to the parameters by combining the synthetic forward wavefield and an adjoint wavefield governed by a set of adjoint equations and adjoint subsidiary conditions. This concept was introduced by Tarantola [38, 39] into the field of seismology. Recently, the adjoint method was used in the context of finite-frequency traveltime kernels [40] and regional seismic models [12, 13]. It is expected that these models will yield great improvements in the imaging of earth structures.

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