Spectral element modelling of three-dimensional wave propagation in a self-gravitating Earth with an arbitrarily stratified outer core

Emmanuel Chaljub$^1$ and Bernard Valette$^2$

$^1$LGIT, CNRS, BP 53, 38041 Grenoble Cedex 9, France
$^2$LGIT, IRD, Université de Savoie, 73376 Le Bourget-du-Lac Cedex, France. E-mail: Emmanuel.Chaljub@obs.ujf-grenoble.fr

SUMMARY

This paper deals with the spectral element modelling of seismic wave propagation on a global scale. Two aspects relevant to low-frequency studies are particularly emphasized. First, the method is generalized beyond the Cowling approximation in order to fully account for the effects of self-gravitation. In particular, the perturbation of the gravity field outside the Earth is handled by a projection of the spectral element solution onto the basis of spherical harmonics. Second, we propose a new formulation inside the fluid which allows us to account for an arbitrary density stratification. It is based upon a decomposition of the displacement into two scalar potentials, and results in a fully explicit fluid–solid coupling strategy. The implementation of the method is carefully detailed and its accuracy is demonstrated through a series of benchmark tests.

Key words: Brunt–Väisälä frequency, elastodynamics, global seismology, numerical modelling, self-gravitation, spectral element method, synthetic seismograms.

1 INTRODUCTION

It has been recently established by several authors (Chaljub 2000; Komatitsch & Tromp 2002a,b; Capdeville et al. 2003; Chaljub et al. 2003) that the spectral element method (SEM) provides an efficient solution to the issue of computing synthetic seismograms in three-dimensional (3-D) models of the Earth. Whereas most of current spectral element studies aim to push calculations toward high frequencies, where the methods traditionally used on a global scale reach their limits, this paper focuses on some physical effects that are critical for the lower part of the seismic frequency band: (i) the full treatment of self-gravitation and (ii) the ability to take into account any density stratification in the fluid regions of the Earth.

The first novelty of this paper stands in the incorporation of self-gravitation, the effect of which is important for seismic and gravimetric observations with periods larger than 100 s. All the previously mentioned studies based upon the SEM accounted for the effects of gravity within the Cowling approximation (Cowling 1941), i.e. by neglecting the perturbation of the gravity field by seismic waves. The main reason for making this assumption lies in the intrinsic difficulty of the problem. Considering the full effects of self-gravitation requires solving Poisson’s equation for the perturbed gravitational potential which is defined over the whole space. Unlike spherical harmonics approaches, the use of a grid-based method such as the SEM does not provide a natural framework for the resolution of the exterior problem. Grid-based approximations in unbounded domains proceed first by restricting the computational domain, then by imposing an appropriate condition on the truncating boundary. Different methods arise depending on whether the artificial boundary condition (ABC) is local or not. Methods based upon a local ABC have the advantage of being computationally inexpensive and valid for arbitrary geometries. An example is the infinite-element method (e.g. Bettess 1992; Gerdes & Demkowicz 1996), in which the behaviour of the exterior solution is enforced in the radial direction. Methods of the second class, based upon a non-local ABC, are not as general since they usually require the knowledge of an analytical, or semi-analytical, solution to the exterior problem. They usually have very attractive properties with regard to their accuracy, while being restricted to simple (usually spherical) geometries. The non-local ABC can be implemented into the finite-element method within the rigorous framework of a Dirichlet-to-Neumann (DtN) operator (e.g. Givoli 1992). This is the approach that we retain here. The DtN operator that suits our problem relies on the spherical harmonic decomposition of the solution of the Laplace equation outside the Earth. Unlike the one introduced by Capdeville et al. (2003) to couple a time-dependent spectral element calculation to a modal solution in the frequency domain, our DtN operator is much simpler to derive because it is applied to a static problem. The spectral element discretization of the Poisson–Laplace equation yields a symmetric algebraic system which has to be inverted at each time step to obtain the perturbation of the gravitational potential. In practice, this is done by iterating a conjugate gradient method, the preconditioning of which is critical for carrying out routine calculations.
The other aspect we consider in detail is the treatment of the fluid part of the Earth’s core. A parameter which is of particular importance with regard to core dynamics is the squared Brunt–Väisälä frequency $N^2$ that characterizes the local response of the fluid to perturbations in density. To first order, the core can be considered as neutrally stratified, i.e. $N^2 = 0$, because a neutral buoyancy is expected in the bulk of a region subject to vigorous convection. However, there is seismological evidence for a negative $N^2$ at the top of the core and a positive $N^2$ in its bulk (Masters 1979). For the sake of generality, our description of the core’s structure will make no assumption about the profile of the buoyancy frequency. To this end, we introduce a two-potential formulation of the wave equation in the fluid that generalizes the neutral buoyancy formulation of Komatitsch & Tromp (2002b) and Chaljub et al. (2003). Contrary to these studies, which considered the velocity potential in the fluid, our decomposition is applied to the displacement field in order to obtain natural solid–fluid boundary conditions for the perturbed gravitational potential. An attractive consequence of this choice is to yield a fully explicit solid–fluid coupling strategy, as opposed to the studies mentioned above. Note finally that our formulation is close to the two-potential description proposed by Wu & Rochester (1990) in the context of core dynamics studies, which is optimal with respect to the number of unknowns in the fluid regions.

The remainder of the paper is organized as follows: in Section 2, we recall the equations of motion in a self-gravitating Earth in their strong and weak form. We introduce the two-potential decomposition of the displacement field in the fluid regions and we define the $DtN$ operator that permits us to handle the equations within a finite domain. In Section 3, we recall the principles of the spectral element approximation in space and we make a detailed presentation of our explicit time-marching algorithm. Finally, numerical results are shown in Section 4 for a set of spherically symmetric models that validate the implementation of the method.

## 2 Wave Equation in a Self-Gravitating Earth

In this section we recall the strong and weak forms of the wave equation, which is obtained through a first-order Lagrangian perturbation around a non-rotating, hydrostatically pre-stressed, state of equilibrium. The reader is referred to Komatitsch & Tromp (2002b) for the extension to the rotating case. Throughout the paper, the Earth is denoted by $\oplus$ and its outer boundary by $\partial_0$. The solid (resp. fluid) parts of $\oplus$ are referred to as $\oplus_2$ (resp. $\oplus_f$), and the set of all solid–fluid interfaces is denoted $\Sigma_2$. Whenever topography or ellipticity is considered on $\partial_0$, $B$ will denote a ball of radius $b$ that contains the aspherical Earth (i.e. $\oplus \subset B$) and $S$ will stand for its spherical boundary ($S = \partial B$).

### 2.1 Strong form

Solving the wave equation within the previous assumptions consists in finding the Lagrangian perturbation of the displacement, $u$, such that:

$$\ddot{u} + A(u) = -\rho \dot{f},$$

(1)

$$\rho A(u) = -\nabla \cdot T(u) - \nabla (\rho u \cdot g) + [\nabla \cdot (\rho u)] g + \rho \nabla \psi,$$

(2)

where $A$ is the elastic-gravitational operator, $T(u)$ is the Lagrangian incremental stress tensor, $\rho$ is density, $g$ is the acceleration due to gravity, $\psi$ is the Eulerian perturbation of the gravitational potential, also known as the mass redistribution potential (MRP), and $f$ is the forcing term.

As usual, a dot over a symbol implies time derivation and $\nabla \tau$ (resp. $\nabla \cdot \tau$) stands for the gradient (resp. the divergence) of a given tensor field $\tau$.

In the (inviscid) fluid regions the stress tensor takes the form:

$$T(u) = \rho c^2 \nabla \cdot u \ I,$$

(3)

where $c$ is the speed of sound and $I$ denotes the second-order identity tensor. Neglecting any source term in the fluid, the wave equation can then be rewritten as:

$$\ddot{u} = -A(u) = \nabla [c^2 \nabla \cdot u + u \cdot g - \psi] + c^2 \nabla \cdot u \ s,$$

(4)

where $s$ is defined by:

$$s = \frac{\nabla \rho}{\rho} - \frac{g}{c^2},$$

(5)

and can be shown to be proportional to the gradient of specific entropy. Another parameter of interest in the fluid is the square of the Brunt–Väisälä frequency $N^2$, which is related to $s$ by:

$$N^2 = s \cdot g = \frac{1}{\rho} \left( \nabla \rho - \frac{\rho}{c^2} g \right) \cdot g.$$

(6)

The Brunt–Väisälä frequency arises naturally when analysing the local stability of the fluid since it provides a simple way of formulating the Schwarzschild criterion (Schwarzschild 1906). An inspection of the expression of the energy indeed reveals that the local convective stability of the fluid is determined by the sign of $N^2$ (e.g., Friedman & Schutz 1978; Valette 1986). Actually, $N^2$ controls the non-seismic part of the spectrum of the elastic-gravitational operator, $\sigma_s(A)$:

$$\sigma_s(A) = \left[ \min \left( 0, N_{\text{crit}}^2 \right), \max \left( 0, N_{\text{sup}}^2 \right) \right],$$

(7)
where $N^2_{\text{inf}}$ and $N^2_{\text{sup}}$ stand for the extrema of $N^2$ over $\mathbb{S}^2$ (Valette 1989). This implies that the corresponding squared eigenfrequencies range in the latter interval. In the Earth, these eigenfrequencies merely exceed $50 \mu$Hz, a value which is well below that of the gravest seismic oscillation $o_{S2}$.

In this paper, we only intend to compute the seismic part of the fluid outer core’s response, which is also affected by the variations of $N^2$. Taking into account a fluid region within the framework of the finite element method is known to be a difficult problem, due to the possible splitting of the zero eigenfrequency induced by the numerical discretization of the elastic operator (Hamdi et al. 1978). A key issue to produce a numerical solution free of spurious modes is the correct representation of the null space of the elastic-gravitational operator, $\mathcal{N}(A)$ (Bermúdez & Rodríguez 1994). An alternative to the discretization of $\mathcal{N}(A)$ is to solve the wave equation in the range of the operator, $\mathcal{R}(A)$. To proceed, we note from eq. (4) that an acceptable form for any displacement field in $\mathcal{R}(A)$ is:

$$u = \nabla \chi + \xi s,$$

(8)

where $\chi$ and $\xi$ denote two arbitrary scalar fields. Differentiating twice in time and identifying each term with the right-hand side of eq. (4), we obtain two scalar wave equations, one for each potential:

$$\ddot{\xi} = c^2 \nabla \cdot (\nabla \chi + \xi s),$$

(9)

$$\ddot{\chi} = \ddot{\xi} + \nabla \chi \cdot g + N^2 \xi - \psi.$$  

(10)

Eventually, the MRP $\psi$ appearing in eqs (2) and (10) is obtained by solving the Poisson–Laplace equation over the entire space. This is written as:

$$\nabla^2 \psi = \begin{cases} -4\pi G \nabla \cdot (\rho u) & \text{in } \mathbb{S}^2, \\ -4\pi G \nabla \cdot (\rho \nabla \chi + \rho \xi s) & \text{in } \mathbb{F}^2, \\ 0 & \text{outside } \mathbb{F}, \end{cases}$$

(11)

where $G$ is the gravitational constant.

### 2.2 Boundary conditions

The complete set of boundary conditions for displacement, traction and MRP can be found in Dahlen & Tromp (1998, p. 104). Here we recall these boundary conditions that concern the MRP or involve a solid–fluid interface.

Let $\Sigma$ be a given interface in the medium. The condition that the MRP must be continuous across $\Sigma$ reads:

$$[\psi]_\Sigma = 0,$$

(12)

where $[\ ]_\Sigma$ stands for the jump operator across $\Sigma$, defined in accordance with the unit normal vector $\hat{n}$: $[\psi]_\Sigma = \psi^+ - \psi^-$ and $\hat{n}$ points from the $-$ to the $+$ side. The normal derivative of $\psi$ can have a jump which is controlled by:

$$[\nabla \psi \cdot \hat{n}]_\Sigma = -4\pi G [\rho u \cdot \hat{n}]_\Sigma.$$  

(13)

The condition that both traction and normal displacement must be continuous across the solid–fluid boundaries can be written as a set of equalities on $\Sigma_{\text{SF}}$:

$$u \cdot \hat{n} = (\nabla \chi + \xi s) \cdot \hat{n},$$

(14)

$$T(u) \cdot \hat{n} = \rho \ddot{\xi} \hat{n}.$$  

(15)

Note that to obtain eq. (15) we have used eqs (3), (8) and (9).

### 2.3 Weak form

The weak form of the wave equation in the solid regions is obtained after multiplying each side of eq. (1) by an admissible displacement field $w$, then integrating over $\mathbb{S}^2$. This is written as:

$$(\ddot{u} + A(u); \rho w)_{\mathbb{S}^2} = (f; w)_{\mathbb{S}^2},$$

(16)

where $\langle ; \rangle_{\mathbb{S}^2}$ stands for the $L^2$ scalar product on $\mathbb{S}^2$. For example, integrating by parts the divergence of the stress tensor in eq. (2) yields:

$$-(\nabla \cdot T(u); w)_{\mathbb{S}^2} = \int_{\mathbb{S}^2} T(u) \cdot \nabla w \, dV - \int_{\Sigma_{\text{SF}}} T(u) \cdot \hat{n} \cdot w \, dS,$$

(17)

where $\hat{n}$ stands for the unit vector normal to $\Sigma_{\text{SF}}$ pointing away from $\mathbb{S}^2$. Note that the condition of free traction at the surface of the Earth $\partial_{\mathbb{S}}$ is naturally satisfied in eq. (17) as we have set the corresponding integral to zero. On the contrary, the continuity of traction (15) across the
solid–fluid boundaries has to be enforced. To proceed, we simply replace the traction vector in the surface integral of eq. (17) with its fluid counterpart:

$$-\nabla \cdot T(u); w)_{\partial B} = \int_{\partial B} T(u) \cdot \nabla w \, dS - \int_{\partial B} \rho \hat{n} \cdot w \, dS.$$ (18)

The weak form of the wave equation in the fluid regions is obtained similarly after dotting each side of eqs (9) and (10) with admissible potentials \( \xi \) and \( \hat{\chi} \), integrating (possibly by parts) over \( \partial B \), then forcing the continuity of the normal displacement (14) across the fluid–solid interfaces. One gets:

$$\int_{\partial B} 1 \, \xi \, dV = \int_{\partial B} (\nabla \chi + \xi s) \cdot \nabla \xi \, dV + \int_{\partial B} u \cdot \hat{n} \, \xi \, dS,$$

and

$$\int_{\partial B} 1 \, \hat{\chi} \, dV = \int_{
\partial B} 1 \, (\xi + \nabla \chi \cdot g + N^2 \xi - \psi) \, \hat{\chi} \, dV.$$ (19)

In eq. (19), \( \hat{n} \) denotes the unit vector normal to \( \Sigma_{SF} \) that points outward from the fluid. Note that the scaling factor \( c^{-2} \) has been included in eq. (20) in order to get the same left-hand side as in eq. (19). This will make the description of the time-marching algorithm easier in Section 3.

Now, in order to establish the weak form of eq. (11), it is convenient to first consider Poisson’s equation within the finite (spherical) volume \( B \). Multiplying by an admissible potential \( \tilde{\psi} \) defined over \( B \), then integrating by parts the Laplacian and the divergence we get:

$$\int_{\partial B} \nabla \tilde{\psi} \cdot \nabla \tilde{\psi} \, dV - \int_{\partial B} \nabla \tilde{\psi} \cdot \hat{n} \tilde{\psi} \, dS = -4\pi G \int_{\partial B} \rho u \cdot \nabla \tilde{\psi} \, dV$$

\[- \int_{\partial B} \rho u \cdot \hat{n} \tilde{\psi} \, dS + \int_{\partial B} \rho (\nabla \chi + \xi s) \cdot \nabla \tilde{\psi} \, dV\},$$

with the boundary term involving the normal displacement being null, except in the absence of topography (i.e. when \( S = \partial B \)). It is important to note that the jump condition (13) across the fluid–solid interfaces is naturally taken into account in (21). This property, which stems from the potential decomposition (8), is a key argument that guided our choice to work with the displacement field (and not velocity) in the fluid.

2.4 DtN operator

The harmonic behaviour of \( \psi \) outside \( B \) has not been considered yet. In order to proceed, let \( \psi_{\text{int}} \) denote the MRP interior to \( B \). At the (spherical) surface \( S \), consider the expansion of \( \psi_{\text{int}} \) onto the orthonormal basis of real spherical harmonics \( Y_{lm} \) (see Dahlen & Tromp 1998, p. 851):

$$\psi_{\text{int}}(b, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \psi_{\text{int}}^{lm}(b) Y_{lm}(\theta, \phi).$$ (22)

where \((\theta, \phi)\) are the spherical coordinates and where \( \psi_{\text{int}}^{lm}(b) = \int_{S} \psi_{\text{int}} Y_{lm} \, dS \). It is straightforward to extend \( \psi_{\text{int}} \) continuously to a potential \( \psi_{\text{ext}} \) that satisfies Laplace’s equation outside \( B \) and vanishes at infinity:

$$\psi_{\text{ext}}(r, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \psi_{\text{ext}}^{lm}(b) \left( \frac{b}{r} \right)^{l+1} Y_{lm}(\theta, \phi), \quad r \geq b.$$ (23)

The normal derivative of \( \psi_{\text{ext}} \) on \( S \) is readily obtained by differentiating with respect to \( r \):

$$\nabla \psi_{\text{ext}}, \hat{n}(b, \theta, \phi) = -\frac{1}{B} \sum_{l=0}^{\infty} (l+1) \sum_{m=-l}^{l} \psi_{\text{ext}}^{lm}(b) Y_{lm}(\theta, \phi).$$ (24)

Eq. (24) which relates the normal derivative of the potential to the potential itself is called a Dirichlet-to-Neumann (DtN) operator on the spherical boundary \( S \). Its action, which is non-local, is rather simple to express in the spherical harmonics basis: it consists in multiplying each coefficient by \((-1-l)/b\). Recall that the condition that the normal derivative of a given field is proportional to the field at the surface is referred to as a Robin boundary condition. Applying the DtN operator is therefore equivalent to imposing a Robin boundary condition on each component of the spherical harmonics expansion of the original potential, and this yields a well-posed problem.

Taking into account the jump condition (13) across \( S \), we can write the final weak form of the Poisson–Laplace equation as:

$$-\int_{B} \nabla \psi \cdot \nabla \psi \, dV + \int_{S} \nabla \psi_{\text{int}}, \hat{n} \psi \, dS = 4\pi G \int_{\partial B} \rho u \cdot \nabla \psi \, dV + \int_{\partial B} \rho (\nabla \chi + \xi s) \cdot \nabla \psi \, dV\},$$

with:

$$\int_{S} \nabla \psi_{\text{int}}, \hat{n} \psi \, dS = -\frac{1}{B} \sum_{l=0}^{\infty} (l+1) \sum_{m=-l}^{l} \psi_{\text{int}}^{lm}(b) \psi_{\text{ext}}^{lm}(b).$$ (25)

In practice, the infinite sum present in eq. (26) will be limited to angular orders \( l < l_{\text{max}} \). Note that the effect of the truncation is to apply a Neumann boundary condition to the high wavenumber content of the MRP, which according to eq. (23) is asymptotically consistent with the behaviour of the MRP outside \( B \).

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3 NUMERICAL APPROXIMATION

This section deals with the numerical approximation of the wave equation in a self-gravitating Earth, which we achieve in two steps. First, the SEM is applied to the weak form of the equations in the space domain. Then a finite-difference scheme is used to advance the system in time.

For the sake of conciseness, details of the method are avoided as much as possible. The reader is referred to Komatitsch & Vilotte (1998) and to Komatitsch & Tromp (1999) for a general description of the SEM applied to the elastic wave equation, and to Chaljub (2000), Komatitsch & Tromp (2002a,b) and Chaljub et al. (2003) for its extension to global seismology, including its parallel implementation on modern computers with distributed memory.

3.1 Spatial discretization

3.1.1 Hexahedral mesh

The first discretization step consists of decomposing the spherical Earth into a collection of non-overlapping hexahedral elements. This process is detailed in Chaljub et al. (2003), where non-conforming interfaces are introduced to avoid an excessive refinement of the grid with depth. Such a strategy allows the refinement (or coarsening) of the mesh to be spatially localized, the complexity being related to the continuity requirements between elements that do not match across the interfaces. For the sake of simplicity, this paper is restricted to the case of a spherical, geometrically conforming mesh such as the one represented in Fig. 6. Note that taking into account the elliptical figure of the Earth or accounting for surface topography would require in the self-gravitating case to extend the mesh outside the artificial boundary \( S \).

3.1.2 Spectral element method

Based upon the 3-D paving of the sphere, the MRP (\( \psi \)) as well as the displacement in the solid (\( u \)) and the potentials in the fluid (\( \chi \) and \( \xi \)) are approximated using continuous tensorized polynomials. Note that the continuity of the normal displacement within the fluid regions is naturally satisfied in the weak forms (19) and (20).

The basis polynomials used on each spectral element are defined as the shape functions of the collocation points. One of the particularity of the SEM is that the collocation points are the so-called Gauss–Lobatto–Legendre points, i.e. the same points that are used to evaluate the integrals present in the weak form of the equations. One consequence of this choice is that the matrix representation of the \( L^2 \) scalar product is diagonal, a property that allows us to design explicit time schemes (see e.g. Komatitsch & Vilotte 1998; Komatitsch & Tromp 1999).

3.2 Time evolution

The different steps of the spatial discretization yield a system of ordinary differential equations in time:

\[
\begin{align*}
\mathbf{M}_S \dot{d}(t) + \mathbf{K}_S d(t) + \mathbf{G} \psi(t) + \mathbf{C}_{SS} \dot{\xi}(t) &= \mathbf{F}(t) \\
\mathbf{M}_F \dot{\xi}(t) + \mathbf{K}_F (\xi, \chi)(t) + \mathbf{C}_{SF} \dot{d}(t) &= 0 \\
\mathbf{M}_F \ddot{\chi}(t) + \mathbf{B}_F (\ddot{\xi}, \chi, \psi)(t) &= 0 \\
\mathbf{P} \dot{\psi}(t) &= \mathbf{D}(d, \xi, \chi)(t)
\end{align*}
\]

In these equations, \( d \) stands for the displacement vector in the solid regions, \( \mathbf{F} \) is the approximation of the source term and \( \psi, \chi, \xi \) respectively denote the nodal values of the MRP and of the displacement potentials in the fluid. \( \mathbf{M}_S \) is the mass matrix in the solid regions, i.e. the matrix representation of the \( L^2 \) scalar product weighted by density. Similarly, \( \mathbf{M}_F \) is the matrix representation of the scalar product in the fluid regions weighted by the quantity \( c^{-2} \). As outlined before, both matrices are diagonal. \( \mathbf{K}_S \) and \( \mathbf{K}_F \) are the stiffness matrices which arise from the approximation of the volume integrals in eqs (18) and (19). The discretization of the surface integrals in the latter equations yields the solid–fluid coupling matrices \( \mathbf{C}_{SF} \) and \( \mathbf{C}_{SS} \). \( \mathbf{B}_F \) arises from the discretization of the right-hand side of eq. (20) and only involves a pointwise operation on \( \ddot{\xi}, \dot{\xi}, V \chi \) and \( \psi \). Finally, \( \mathbf{G}, \mathbf{D} \) and \( \mathbf{P} \) are the matrix representations of the gradient, divergence and Poisson–Laplace operator respectively. Note that \( \mathbf{D} \) contains the factor \( 4 \pi G \rho \) and that \( \mathbf{P} \) is symmetric according to eqs (25) and (26).

To advance the equations forward in time we use the explicit, second-order accurate, Newmark scheme (e.g. Hugues 1987). Let for example \( X_n \) denote the snapshot at time \( t_n \) of one of the unknown vectors \( d, \chi \) or \( \xi \) involved in eqs (27)–(29). The values of \( X \) and its time derivative at the next time step are extrapolated as follows:

\[
\begin{align*}
X_{n+1} &= X_n + \Delta \dot{X}_n + \frac{\Delta t^2}{2} \ddot{X}_n \\
\dot{X}_{n+1} &= \dot{X}_n + \frac{\Delta t}{2} (\ddot{X}_n + \ddot{X}_{n+1}).
\end{align*}
\]
As is readily seen from the previous equations, the algorithm is fully explicit in terms of $\mathbf{X}$ and consists in a simple centred finite-difference scheme in $\mathbf{X}$. The process of updating the time derivatives of $\mathbf{X}$ is achieved in two steps: first $\dot{\mathbf{X}}_{n+1}$ is computed from the discrete version of the wave eqs (27)–(29) by inverting a diagonal mass matrix ($\mathbf{M}_S$ or $\mathbf{M}_P$), then $\mathbf{X}_{n+1}$ can be updated using (32). Note that the wave equation has to be solved in the fluid regions first, since the coupling operator $\mathbf{C}_{np}$ in eq. (27) acts on $\dot{\mathbf{X}}_{n+1}$, which is not known at time $t_n$.

Let us stress that the coupling between the fluid and the solid regions does not require iterations of eqs (31) and (32) as would be the case if a velocity potential formulation were used (e.g. Komatitsch et al. 1990; Chaljub et al. 2003). This attractive property stems from the potential decomposition (8) applied to the displacement, which is the explicit variable in the Newmark scheme.

The previous remark remains valid when the full effects of self-gravitation are taken into account. The computation of the MRP from the displacement field is indeed explicit in the sense that it does not involve any time derivative $\mathbf{X}$ or $\dot{\mathbf{X}}$. Needless to say, this task is expensive as it requires formal inversion of the symmetric, ill-conditioned matrix $\mathbf{P}$ (e.g. Deville et al. 2002). In practice, we solve eq. (29) for the MRP with a conjugate gradient (CG) method with iterations stopped once the residual has decreased by a factor $\epsilon$ to be chosen. The issue of building an efficient preconditioner for the Poisson–Laplace solver is not addressed in this paper, but it is certainly critical in order to avoid a performance bottleneck.

4 NUMERICAL RESULTS

In this section, we demonstrate the validity of our approach through a couple of examples for which a reference, semi-analytical, solution can be derived. First, the two-potential formulation is tested within the Cowling approximation, i.e. without computing the MRP, for models having a constant Brunt–Väisälä frequency. Second, the effects of mass redistribution are included within the PREM model (Dziewonski & Anderson 1981).

4.1 Validation of the two-potential formulation

In order to define some benchmarks to test our formulation, we consider the oceanless version of the PREM model shown in Fig. 1. This reference model is further constrained to fit a given profile of the squared Brunt–Väisälä frequency in the fluid outer core. To proceed, we simply vary the $P$ velocity, $c$, in eq. (6), keeping the density, its gradient and the gravitational acceleration unchanged. Note that a realistic way of adjusting the Brunt–Väisälä frequency would be to modify density rather than $P$ velocity (see e.g. Wu & Rochester 1993) because the latter is much better constrained in the Earth. However, acting on the $P$-velocity profile is straightforward and still fully acceptable for numerical validation purposes.

Fig. 2 shows three models that were built following the above procedure. The ‘N’ label refers to a neutrally stratified outer core (i.e. with $N^2 = 0$), whereas the models labelled ‘S’ and ‘U’ correspond to a stable and unstable stratification, respectively. For the sake of simplicity, we chose the value of the squared Brunt–Väisälä frequency to be constant throughout models ‘S’ and ‘U’, respectively equal to $N^2 = 10^{-7}$ rad$^2$ s$^{-2}$ and $N^2 = -5 \times 10^{-8}$ rad$^2$ s$^{-2}$. These values correspond to the extrema that are expected from the inversion of seismic free oscillations of the Earth. Note that the values of $N^2$ within PREM are about one order of magnitude smaller, as illustrated by the similarity of the PREM $P$-velocities to those of a neutrally stratified profile.
Modelling wave propagation in a self-gravitating Earth

Figure 2. Different profiles of $P$ velocity used to test the two-potential formulation in the fluid outer core. The dashed curve represents the variation of the sound speed within the model detailed in Fig. 1. Each solid curve corresponds to a modification of that profile such that the square of the Brunt–Väisälä frequency is constant throughout the fluid. The label ‘$N$’ corresponds to a neutrally stratified outer core, whereas ‘$S$’ (resp. ‘$U$’) stands for a stable (resp. unstable) stratification for which $N^2 = 10^{-7}$ rad$^2$ s$^{-2}$ (resp. $N^2 = -5 \times 10^{-8}$ rad$^2$ s$^{-2}$).

Figure 3. Time window of the longitudinal surface displacement recorded at 90° in the models labelled ‘$N$’, ‘$S$’ and ‘$U$’ in Fig. 2. The large waveform differences stem from the sensitivity of the seismic modes to the variation of the $P$ velocity within the three models.

All three models are excited by a shallow explosive point source, the time dependence of which is a Ricker wavelet (i.e. the second derivative of a Gaussian function) with dominant frequency $f_0 = 1$ mHz. The source is located on the Equator at depth $d_s \simeq 61$ km, and the receivers are placed along the Equator. Fig. 3 shows the longitudinal displacement recorded at an epicentral distance of 90° in the three models. The traces are computed within the Cowling approximation using a summation of the eigenmodes of each model. The waveform differences illustrate the sensitivity of the seismic waves to the stratification of the fluid core and suggest that models ‘$U$’ and ‘$S$’ constitute a suited benchmark for the two-potential formulation. In Figs 4 and 5, the spectral element results obtained with those two models are compared to the modal solutions for a couple of epicentral distances. The two solutions are in very close agreement, with the largest relative differences being as small as a few per mil over the time interval considered.

The spectral element grid used to carry out the calculations is shown in Fig. 6. It consists of 1024 elements in which the polynomial degree varies from 2 (in the crust) to 10 (in the outer core) in the radial direction and is kept constant, equal to 8, in the tangential direction. The total number of gridpoints is 443 232 corresponding to a number of points per wavelength much greater than 5, which is the empirical minimal ratio to get an accurate solution (e.g. Komatitsch & Vilotte 1998). This explains the match between the spectral element calculations and the reference solutions.

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Figure 4. Radial (left panel) and longitudinal (right panel) components of the surface displacement recorded at 45° (top) and 90° (bottom) in the model labelled ‘S’ in Fig. 2. In each plot, the spectral element solution (dashed line) is compared with the normal-mode reference (solid thin line) and the residual (solid thick line) is amplified by a factor of 10.

4.2 Validation of the whole formulation

As a last example, we consider the computation of the elastic-gravitational response of the Earth model of Fig. 1. This test contains all the difficulties mentioned in this paper: The stratification of the fluid core is arbitrary and the physical description includes the full effects of self-gravitation.

The parameters of the simulations are slightly different from above, since the source dominant frequency is set to a lower value $f_0 = 0.5\,\text{mHz}$ to maximize the effects of mass redistribution. The spectral element grid is consequently adapted, and roughly coarsened by a factor of 2 in each direction compared with that of Fig. 6.

In order to check that the test is demanding enough with regard to the implementation of self-gravitation, we compare in Fig. 7 the surface longitudinal displacement recorded with or without including the perturbation of the gravitational potential. Both traces are computed by normal-mode summation and recorded at an epicentral distance of 90° for about 10 hr. The differences in phase and amplitude illustrate that the Cowling approximation is not valid in the frequency range of the experiment.

Finally, the results obtained with the SEM are compared with the reference solution in Fig. 8. Two cases are considered that correspond to a different accuracy of the spectral element solution regarding the CG resolution of the discrete Poisson–Laplace eq. (29). In the first case the CG iterations are stopped once the residual has decreased by three orders of magnitude, which means that $\epsilon = 10^{-3}$. The resulting spectral element solution is clearly not accurate enough and contains a secular term that seems to break the conservation of energy at the discrete level. To correct this behaviour, we consider a second test where the stopping criterion is set to $\epsilon = 10^{-5}$. In that case, the calculation is stable upon the time interval considered and the accuracy of the spectral element solution is acceptable, its relative difference from the reference solution being less than a few per mil.

In each of the previous cases, the angular order truncation in eq. (26) was set to $l_{\text{max}} = 20$, based on the a priori knowledge of the dispersion relation in PREM. In any realistic application $l_{\text{max}}$ will always be much smaller than 100, since the effects of mass redistribution are negligible for periods shorter than 100 s. The effect of underestimating the truncation order is to add characteristic oscillations to the spectral element solution (not shown in this paper). It is interesting to note that the two possible sources of numerical errors ($\epsilon$ too big or $l_{\text{max}}$ too small) lead to a different signature. This provides two different diagnostics that permit us to build a spectral element solution with arbitrary accuracy.
Figure 5. Radial (left panel) and longitudinal (right panel) components of the surface displacement recorded at 45° (top) and 90° (bottom) in the model labelled ‘U’ in Fig. 2. In each plot, the spectral element solution (dashed line) is compared with the normal-mode reference (solid thin line) and the residual (solid thick line) is amplified by a factor of 10.

Figure 6. Spectral element mesh used to compute the results shown in Figs 4 and 5. Two blocks of the 3-D mesh have been removed to allow a view inside the volume. The mesh is composed of 1024 spectral elements with varying polynomial order, for a total number of gridpoints equal to 443,232. The process of building the mesh is detailed in Chaljub et al. (2003).

5 CONCLUSIONS

We have shown how the SEM can be adapted to account for two effects relevant to global seismology: the full treatment of self-gravitation and the ability to consider any density stratification in the fluid outer core. The accuracy of the method has been illustrated through a series
**Figure 7.** Longitudinal component of the surface displacement recorded at 90° in the Earth model of Fig. 1. The trace computed with the full treatment of self-gravitation (solid thin line) is compared with the one computed within the Cowling approximation (dashed thick line). The waveform differences illustrate that the effect of the MRP cannot be neglected at the frequencies considered in this experiment.

\[ \epsilon = 10^{-3} \]

![Image](image1.png)

**Figure 8.** Longitudinal surface displacements recorded at 90° in the Earth model of Fig. 1. The left (resp. right) plot corresponds to a low- (resp. high-) accuracy test in which the CG iterations used to compute the MRP are stopped once the residual has decreased by three (resp. five) orders of magnitude. In each plot, the spectral element solution (dashed line) is compared with the normal-mode reference (solid thin line) and the residual (solid thick line) is amplified by a factor of 10.

of numerical tests conducted in spherically symmetric models. With the incorporation of the two aforementioned effects, we believe that numerical simulations based on the SEM will provide new estimates of the elastic-gravitational response of 3-D models of the Earth.

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**REFERENCES**


Modelling wave propagation in a self-gravitating Earth


