Approximation of acoustic waves by explicit Newmark’s schemes and spectral element methods

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Abstract

A numerical approximation of the acoustic wave equation is presented. The spatial discretization is based on conforming spectral elements, whereas we use finite difference Newmark’s explicit integration schemes for the temporal discretization. A rigorous stability analysis is developed for the discretized problem providing an upper bound for the time step $\Delta t$. We present several numerical results concerning stability and convergence properties of the proposed numerical methods.

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1. Introduction

The numerical approximation of propagation problems is an interesting issue in geophysics and seismic engineering. An increasing number of applications of the wave equation requires methods characterized by high accuracy. High-order methods have been studied extensively in the last decades. We recall the $p$ and $h–p$ version finite element and spectral element methods, originated and initially developed in computational structural mechanics and fluid dynamics. While earlier works on spectral methods focused...
on a single region (e.g., [6,5]), these methods were then extended to many subregions (or elements) partitioning the given computational domain. We note that the $p$ and $h-p$ version finite elements differ from spectral elements in the choice of basis functions and quadrature formulas used in evaluating the integrals of the Galerkin formulation. See [2,3,16,28,29] for the $p$ and $h-p$ version finite element method; [12,9,20] for spectral elements.

Classic simulations of acoustic wave propagation are based on finite difference (e.g., [1,21,4]), or on finite element space discretizations (e.g., [11,17]). Fewer works have studied spectral elements for wave propagation problems. We recall here the papers on monodomain spectral methods for acoustic waves by [23], and for elastic waves by [34] and [25]; the paper on explicit spectral elements by [10], where the focus is on the numerical validation on realistic tests in geophysics rather than on the theoretical discussion; the paper by Casadei et al. [7] for elastodynamics problems in complex geometries. A review of previous works on spectral methods for hyperbolic problems can be found in [15].

In this paper, we study the numerical approximation of the acoustic wave equation using the spectral element method based on Gauss–Lobatto–Legendre (GLL) quadrature formulas and finite difference first- and second-order Newmark’s explicit time advancing scheme. The novelty of this paper is the generalization to the whole Newmark’s explicit family of our recent work [33] considering only the Leap–Frog scheme, which is an explicit second-order accurate method with respect to the time discretization parameter $\Delta t$. The allowed choices of the parameters in the family of Newmark’s schemes provide methods having different order of accuracy with respect to $\Delta t$ and different stability and dissipation properties. The optimization of Newmark’s parameters with respect to accuracy, stability and dissipation is beyond the scope of this paper; for a detailed discussion in the finite element case we refer, e.g., to [31] and [17]. The main result of the paper is a rigorous analysis of the stability and numerical validation of the spectral element method combined with Newmark’s explicit schemes in time, providing an upper bound for the time step $\Delta t$ depending on the parameters of both the spectral element discretization and the Newmark’s time advancing scheme. For simplicity of exposition we consider the model problem with classic Dirichlet boundary conditions. Nevertheless typical applications require the simulation of wave propagation in unbounded domains. In obtaining a numerical solution the infinite domain is then necessarily truncated onto a finite region with artificial boundaries, where suitable absorbing boundary conditions have to be set. The generalization of our study to the more realistic case of unbounded domains will be dealt within a future work.

In order to state precisely the numerical approximation of the acoustic wave problem, we first consider the discretization of the space variable which is based on the conforming spectral element method. The basic idea behind this approach consists in partitioning the original domain into nonoverlapping quadrilateral elements (subdomains) of characteristic size $H$, each of them being mapped into a reference square. Within each quadrilateral element the solution is approximated by an algebraic polynomial of degree $p$ in each variable and these local polynomials are matched continuously at the interface between elements. Then, the bilinear form, inner products and norms turn out to be sums over all quadrilateral elements of local GLL numerical bilinear form, inner products and norms using, for each time instant, the values of the spectral element solution at GLL collocation points of each element. The semidiscrete continuous-in-time spectral element approximation leads to a system of second-order ordinary differential equations with initial conditions on the pressure and velocity vectors. For the approximation of time derivatives, we introduce the family of Newmark’s explicit finite difference schemes. In general, each step of an explicit scheme involves the resolution of a diagonal system and one matrix-by-vector product, whereas each step of a general implicit scheme requires the numerical resolution of a globally assembled...
spectral element system. Note also that for explicit methods, the time step $\Delta t$ is subject to a stability condition, while implicit methods are unconditionally stable and the time step $\Delta t$ is dictated by accuracy considerations.

An outline of the paper is as follows. In Section 2, we recall the governing equations of the model problem and fundamental results of its mathematical analysis. In Section 3, we introduce the numerical approximation based on spectral elements and finite difference Newmark’s schemes. In Section 4, we develop a detailed theoretical analysis of the stability of the proposed scheme, providing an upper bound for the time step $\Delta t$ with respect to the parameters of the discretization. Finally in Section 5, we present the results of several numerical experiments in order to both validate the stability estimates obtained in Section 4 and to study the convergence of our numerical methods with respect to the discretization parameter: namely, the local degree $p$ of the basis functions, the size $H$ of each element of the triangulation, and the time step $\Delta t$.

2. The model problem and mathematical analysis

We consider a bounded open domain $\Omega$ of $\mathbb{R}^2$ with boundary $\partial \Omega \equiv \Gamma$. Any point of $\Omega$ is denoted by $x = (x_1, x_2)$, while $t$ represents the time. The problem of interest here is the two-dimensional acoustic wave problem (e.g., [19,18])

$$\frac{\partial^2 u(x, t)}{\partial t^2} - \Delta u = f(x, t) \quad \text{in } \Omega \times (0, T)$$

with Dirichlet boundary conditions

$$u(x, t) = \Phi(x, t) \quad \text{on } \Gamma \times (0, T)$$

and initial conditions

$$u(x, 0) = u_0(x), \quad \frac{\partial u}{\partial t}(x, 0) = u_1(x) \quad \text{in } \Omega.$$

In the above equations $f$ is the source term, $\Phi$ is a given boundary data, $u_0$ and $u_1$ are the initial pressure and velocity, respectively, and $u$ is the unknown pressure. The case of mixed Dirichlet–Neumann boundary conditions is presented in [33], whereas the generalization to absorbing boundary conditions will be dealt with in a future work.

Assuming that, for each $t \in (0, T)$, $f \in L^2(\Omega \times (0, T))$ and $\Phi \in H^{1/2}(\partial \Omega)$ (for the definition of the latter boundary spaces we refer, e.g., to [22, vol. I]), $u_0 \in H^1(\Omega)$ and $u_1 \in L^2(\Omega)$, the weak formulation of problem (1)–(3) reads as follows. Find $u : (0, T) \to H^1(\Omega)$, such that $\forall t \in (0, T), \; u(t) = \Phi(t)$ on $\Gamma$ and

$$\left( \frac{\partial^2 u}{\partial t^2}, v \right) + a(u, v) = (f, v) \quad \forall v \in V,$$

where

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx_1 \, dx_2, \quad (f, v) = \int_{\Omega} f v \, dx_1 \, dx_2.$$
and \( V = H^1_0(\Omega) \). We remind that the bilinear form \( a(\cdot, \cdot) \) is symmetric, \( V \)-elliptic and continuous; these conditions imply that problem (4) admits a unique solution \( u \). Furthermore, the solution \( u \) satisfies a stability estimate (see, e.g., [27,22]).

3. Spectral elements and explicit Newmark’s schemes

In this Section, we introduce the numerical approximation of the variational formulation (4). The discretization of the space variable \( \mathbf{x} = (x_1, x_2) \) is based on the conforming spectral element method (SE for brevity), whereas the time discretization is based on Newmark’s explicit time advancing schemes.

3.1. Spectral element discretizations

The basic idea of the SE approach consists in partitioning the original domain into nonoverlapping quadrilateral elements. Each element is mapped into a reference square, inside which the local solution \( u(t) \) is approximated by an algebraic polynomial \( u_{p,i}(t) \) of degree \( p \) in each variable. These local polynomials are then matched continuously at the interface between elements. Then the bilinear form \( a(\cdot, \cdot) \), the inner product \( (\cdot, \cdot) \) and corresponding norm turn out to be sums over all quadrilateral elements of local Gauss–Lobatto–Legendre (GLL for brevity) numerical bilinear forms, inner products and norms, for each \( t \), the values of the local solution \( u_{p,i} \) at GLL collocation points of \( \Omega \) (e.g., [26,5]).

The computational domain \( \Omega \) is here the unit reference square \( \Omega_{\text{ref}} = (-1, 1)^2 \). Given a positive integer \( M \), we consider a uniform partition \( T_H \) of \( \Omega \) into nonoverlapping quadrilateral elements \( \Omega_i, \quad i = 1, \ldots, N_e \), with side \( 2H = 2/M \) and \( N_e = M \times M \). More general affine elements can be considered. Then

\[
\Omega = \bigcup_{i=1}^{N_e} \Omega_i
\]

is a conforming partition of \( \Omega \), i.e., if the intersection \( \Omega_i \cap \Omega_j \) between two distinct elements of \( T_H \) is not empty, then \( \Omega_i \cap \Omega_j \) is a common vertex or side of \( \Omega_i \) and \( \Omega_j \). Furthermore, given a positive integer \( p \) and being \( P_p \) the \( p \)th Legendre polynomial in \( \mathbb{I}_{\text{ref}} = [-1, 1] \), we introduce the polynomial

\[
(1 - z^2) \frac{\partial P_p(z)}{\partial z}
\]

which has \((p+1)\) zeros in \([−1, 1]\). Then we consider the tensor product of the \((p+1)\) 1-dimensional nodes in \( \mathbb{I}_{\text{ref}} \) in order to define the 2-dimensional set of \((p+1)^2\) GLL nodes in \( \Omega_{\text{ref}} \) and denote by

\[
C^i = \{x^i_{km} = (x^i_{1,k}, x^i_{2,m}), \quad 0 \leq k, m \leq p\}
\]

the set of GLL nodes in \( \Omega_i \) which are the images of the GLL nodes in \( \Omega_{\text{ref}} \), through the linear transformation that maps \( \Omega_i \) into \( \Omega_{\text{ref}} \). We partition \( C_i \) into two subsets associated with \( \Omega \) and \( \partial \Omega \), respectively:

\[
C^i = C^i,\Omega \cup C^i,\Gamma,
\]

where

\[
C^i,\Omega = C^i \cap \Omega_i, \quad C^i,\Gamma = C^i \cap \Gamma.
\]
We define the local GLL discrete inner products and bilinear forms that approximate those in (4):

\[(u, v)_{p,i} = \sum_{k,m=0}^{p} (uv)(x_{km}^i)\omega_k\omega_m, \quad (6)\]

\[a_{p,i}(u, v) = \left( \frac{\partial u}{\partial x_1}, \frac{\partial v}{\partial x_1} \right)_{p,i} + \left( \frac{\partial u}{\partial x_2}, \frac{\partial v}{\partial x_2} \right)_{p,i}, \quad (7)\]

where the \(\omega_j\)'s are the images on \(\Omega_i\) of the GLL weights \(\rho_j\)'s associated with the GLL nodes \(x_j\)'s of \(I_{\text{ref}}\).

Precisely,

\[\omega_j = H\rho_j, \quad j = 0, \ldots, p. \quad (8)\]

Let \(Q_p(\Omega_i)\) be the space of functions that are defined on \(\Omega_i\) and that are algebraic polynomials of degree \(\leq p\) in each variable, and \(Q_p^1(\Omega_i) = Q_p(\Omega_i) \cap V\). Owing to the exactness of the GLL quadrature formula, we have:

\[(u, v)_{p,i} = \int_{\Omega_i} uv \, dx_1 \, dx_2, \quad \forall uv \in Q_{2p-1}(\Omega_i). \quad (9)\]

Then we set

\[V_H = \{ w_H \in C^0(\overline{\Omega}) : w_H|_{\Omega_i} \in Q_p(\Omega_i), \quad \forall \Omega_i \in T_H \}\]

and \(w_{p,i} = w_H|_{\Omega_i}\). Error estimates for spectral element interpolation, quadrature and convergence estimates can be found in [5] in the monodomain case and in [14,13] in the spectral element case.

Stemming from the variational formulation (4) of the acoustic problem, we can formulate the semidiscrete continuous-in-time SE approximation: for each \(t \in (0, T)\), find \(u_H \in V_H\) such that \(u_H = \Phi\) at all nodes of \(\partial \Omega\) and

\[\left( \frac{\partial^2 u_H}{\partial t^2}, v \right)_H + a_H(u_H, v) = (f, v)_H, \quad \forall v \in V_H, \quad (10)\]

where

\[ (\cdot, \cdot)_H \equiv \sum_{i=1}^{N_e} (\cdot, \cdot)_{p,i}, \quad a_H(\cdot, \cdot) \equiv \sum_{i=1}^{N_e} a_{p,i}(\cdot, \cdot) \quad (11)\]

are built using the local GLL discrete inner products and bilinear forms defined in (6) and (7). We denote by \(\| \cdot \|_H\) the discrete norm associated with the inner product \((\cdot, \cdot)_H\).

Let us consider now the algebraic form of problem (10). To this aim, we recall that a Lagrangian-nodal basis for \(Q_p(\Omega_i)\) is built by tensor product as

\[L_{km}^i(x_1, x_2) = L_k^i(x_1)L_m^i(x_2), \quad (12)\]

where \([L_j^i(z), j = 0, \ldots, p]\) are the Lagrangian basis polynomials associated with the GLL nodes of \(\Omega_i\) with respect to the \(z\)-variable, i.e., \(L_j^i(x, n) = \delta_{jn}\), for \(0 \leq j, n \leq p, \forall i = 1, \ldots, N_e\).
In particular, denoting by \( r = r(i, k, m) \) the global index numbering the nodes of \( T_H, \ i = 1, \ldots, N_e, \ 0 \leq k, m \leq p \), then \( 1 \leq r \leq N_{p,M} \), where \( N_{p,M} \equiv (pM + 1)^2 \) is the total number of degrees of freedom of the SE problem. We also set:

\[
L^r(x) \equiv L_{km}^i(x_1, x_2)
\]

and

\[
x^r \equiv (x^i_{1,k}, x^i_{2,m}).
\]

According to the above global numbering and notations, every piecewise polynomial can be written as

\[
w_H(x) = \sum_{r=1}^{N_{p,M}} w^r_H(x^r) L^r(x).
\]

If we choose \( v = L_{km}^i \) in (10) and apply a standard technique (e.g., [5,32]) consisting of using integration by parts and exactness of GLL quadrature formula, it can be easily seen that (10) is equivalent to a system of second-order ordinary differential equations:

\[
B \ddot{u}_p(t) + K u_p(t) = \Theta(t) + F(t)
\]

with initial conditions:

\[
u_p(0) = u_0, \quad \dot{u}_p(0) = u_1.
\]

In the above system \( K \) and \( B \) are the assembled stiffness and mass SE matrices, respectively, and, \( \forall t \in (0, T) \), \( u_p(t) \) is the vector of nodal values of \( u_H \). Finally, \( \Theta(t) \) and \( F(t) \) are known vectors accounting for the contribution of \( \Phi \) and \( f \). Precisely,

\[
u_p(t) = \{u_H(x^r), \ 1 \leq r \leq N_{p,M}\},
\]

\[
K = \{a_H(L^{r1}, L^{r2}), \ 1 \leq r_1, r_2 \leq N_{p,M}\}
\]

and

\[
B = \{(L^{r1}, L^{r2})_H, \ 1 \leq r_1, r_2 \leq N_{p,M}\}.
\]

Moreover, the vector \( \Theta(t) \) accounts for the contribution of the known values of the solution \( u_p(t) \) at the boundary expressed by the Dirichlet boundary condition (2), i.e.,

\[
\Theta(t) = -B \ddot{\Phi}_p(t) - K \Phi_p(t),
\]

where \( \Phi_p(t) \) is the vector of nodal values of the boundary data \( \Phi \) at time \( t \). Finally,

\[
F(t) = \{(f, L^r)_H, \ 1 \leq r \leq N_{p,M}\}.
\]

We note that \( K \) and \( B \) are \( N_{p,M} \times N_{p,M} \) symmetric, positive definite matrices and \( B \) is diagonal. Precisely,

\[
B_{rr} = \beta \omega_{ki} \omega_{mi}, \quad r = r(i, k_i, m_i),
\]

where \( \beta \) denotes the number of elements which meet at node \( (x_{1,k}, x_{2,m}) \) of \( \Omega_i \). Then \( \beta = 1 \) or \( 2 \) or \( 4 \).
3.2. Newmark’s explicit time discretization

Let us now introduce a family of explicit finite difference schemes for the approximation of time derivatives. We can represent (12) in compact form

$$B\ddot{u}_p(t) = G(t),$$

where

$$G(t) = \Theta(t) + F(t) - K u_p(t).$$

The temporal interval \((0, T)\) is subdivided into subintervals \([t_s, t_{s+1}]\), with \(t_0 = 0, t_S = T, t_{s+1} = t_s + \Delta t, s = 0, \ldots, (S - 1)\). We recall here the general Newmark’s method [24],

$$B \frac{u_{s+1} - 2u_s + u_{s-1}}{\Delta t^2} = \left[ \gamma G_{s+1} + \left( \frac{1}{2} - 2\gamma + \delta \right) G_s + \left( \frac{1}{2} + \gamma - \delta \right) G_{s-1} \right],$$

where \(\gamma\) and \(\delta\) are positive real numbers. By using Taylor expansions it can be shown that the Newmark’s method is first-order accurate with respect to \(\Delta t\) if \(\delta \neq \frac{1}{2}\), whereas it is second order if \(\delta = \frac{1}{2}, \forall \gamma\). Moreover, the scheme at hand is explicit if \(\gamma = 0\) and reads:

$$B \frac{u_{s+1} - 2u_s + u_{s-1}}{\Delta t^2} = \left[ \left( \frac{1}{2} + \delta \right) G_s + \left( \frac{1}{2} - \delta \right) G_{s-1} \right].$$

Finally, it coincides with the Leap–Frog scheme when \(\gamma = 0\) and \(\delta = \frac{1}{2}\), which in particular is explicit and second-order accurate with respect to \(\Delta t\).

We also recall that each step of an explicit scheme involves the resolution of a diagonal system and one matrix-by-vector product. On the other hand, each step of a general implicit scheme, requires the numerical resolution of a linear SE system, possibly involving preconditioning techniques. Note also that for explicit methods the time step \(\Delta t\) is subject to a stability condition (see Section 4), whereas implicit methods turn out to be unconditionally stable regardless of the time step \(\Delta t\). The analysis of implicit methods and SE when applied to acoustic wave problems will be dealt with in a future work.

A review of the Newmark’s method, which was introduced in [24], can be found, e.g., in [31], where the convergence and stability analysis and its necessary mathematical background are developed in the framework of the finite element method. We recall also the papers on explicit and implicit time advancing schemes for monodomain spectral methods for the approximation of acoustic waves by [23], and of elastic waves by [34] and [25]. The paper on explicit spectral elements by [10], focuses instead on the numerical validation on realistic tests in geophysics rather than on the theoretical analysis. The application of the second order explicit Newmark’s scheme (the Leap–Frog scheme) to the spectral element method for acoustic wave problems has been recently discussed in [33], where the theory of stability and convergence, as well as several numerical examples, are reported.
4. Stability inequalities

In this section we generalize the analysis that has been carried out in [33] for the Leap–Frog scheme.

**Proposition 1.** The solution $u_H$ of the semidiscrete SE continuous-in-time problem (10) satisfies the following stability estimate:

$$|||u_H|||^2_{H(T)} \lesssim \exp(T) \left[ |||u_H|||^2_{H(0)} + \int_0^T \|f\|^2_H(s) \exp(-s) \, ds \right],$$

where

$$|||u_H|||^2_H \equiv \left\| \frac{\partial u}{\partial t} \right\|^2_H + a_H(u, u).$$

**Proof.** The estimate is obtained by following a standard approach (e.g., [27]), consisting in choosing as test function in (10) $v = \frac{\partial u}{\partial t}$ and integrating in time from $t = 0$ to $T$. Then the estimate follows using the Cauchy–Schwarz inequality and the Gronwall’s lemma. See [33] for details. □

Let us consider now the stability of the fully discrete (14). We can obtain a stability upper bound for $\Delta t$ by standard arguments, following the guidelines of [8] and [27]. For the sake of simplicity the analysis is limited to the case of homogeneous data, i.e., $f = 0, \Phi = 0$. An explicit Newmark’s method reads:

$$B \frac{u_{s+1} - 2u_s + u_{s-1}}{\Delta t^2} + K \left[ \left( \frac{1}{2} + \delta \right) u_s + \left( \frac{1}{2} - \delta \right) u_{s-1} \right] = 0. \tag{15}$$

We recall that $B$ is diagonal with positive entries and $K$ is symmetric positive definite.

**Proposition 2.** The symmetric definite pencil $(K - \lambda B)$ has $N_{p,M}$ real positive eigenvalues $\lambda_j$ and $N_{p,M}$ linear independent eigenvector $\varphi_j$ verifying:

$$\lambda_j B \varphi_j = K \varphi_j, \quad j = 1, \ldots, N_{p,M}. \tag{16}$$


The above proposition implies that each vector $u_s$ can be written as

$$u_s = \sum_{j=1}^{N_{p,M}} \xi_j^s \varphi_j, \tag{17}$$

according to which the system (15) reads

$$\frac{1}{\Delta t^2} B \sum_{j=1}^{N_{p,M}} (\xi_j^{s+1} - 2\xi_j^s + \xi_j^{s-1}) \varphi_j + K \sum_{j=1}^{N_{p,M}} \left[ \left( \frac{1}{2} + \delta \right) \xi_j^s + \left( \frac{1}{2} - \delta \right) \xi_j^{s-1} \right] \varphi_j = 0. \tag{18}$$
Using relation (16) we obtain

\[
\frac{1}{\Delta t^2} B \sum_{j=1}^{N_{p,M}} (\xi^{s+1}_j - 2\xi^s_j + \xi^{s-1}_j) \varphi_j + B \sum_{j=1}^{N_{p,M}} \left[ \left( \frac{1}{2} + \delta \right) \xi^s_j + \left( \frac{1}{2} - \delta \right) \xi^{s-1}_j \right] \lambda_j \varphi_j = 0.
\]

As \( B \) is nonsingular and the \( \varphi_j \)'s are linear independent vectors, it follows that the analysis of stability for (15), or equivalently for (18), is reduced to that of \( N_{p,M} \) scalar equations:

\[
\frac{1}{\Delta t^2} (\xi^{s+1}_j - 2\xi^s_j + \xi^{s-1}_j) + \lambda_j \left[ \left( \frac{1}{2} + \delta \right) \xi^s_j + \left( \frac{1}{2} - \delta \right) \xi^{s-1}_j \right] = 0, \quad j = 1, \ldots, N_{p,M},
\]

(19)

that are, respectively, explicit finite difference discretizations of the ordinary differential equations

\( \ddot{\xi} + \lambda_j \xi = 0 \)

with suitable initial conditions.

Proposition 3. If \( \delta \geq \frac{1}{2} \), scheme (19) is stable under the assumption

\[
\sqrt{\lambda_j} \Delta t < \sqrt{\frac{2}{\delta}}.
\]

(20)

Proof. Scheme (19) can be written in matrix form as

\[
\begin{bmatrix}
\xi^s_j \\
\xi^{s+1}_j
\end{bmatrix}
= A
\begin{bmatrix}
\xi^s_j \\
\xi^{s-1}_j
\end{bmatrix}, \quad \text{with } A = \begin{bmatrix}
0 & \left[ 1 + \alpha_j^2 \left( \frac{1}{2} - \delta \right) \right] & 2 - \alpha_j^2 \left( \frac{1}{2} + \delta \right)
\end{bmatrix},
\]

where we have set \( \alpha_j \equiv \sqrt{\lambda_j} \Delta t \). The eigenvalues \( \mu \) of \( A \) are the roots of the characteristic equation

\[
\mu^2 - \mu \left[ 2 - \alpha_j^2 \left( \frac{1}{2} + \delta \right) \right] + 1 + \alpha_j^2 \left( \frac{1}{2} - \delta \right) = 0
\]

with discriminant

\[
D = \left[ 2 - \alpha_j^2 \left( \frac{1}{2} + \delta \right) \right]^2 - 4 \left[ 1 + \alpha_j^2 \left( \frac{1}{2} - \delta \right) \right] = \alpha_j^2 \left[ \alpha_j^2 \left( \frac{1}{2} + \delta \right)^2 - 4 \right].
\]

It is well-known from the literature of difference equations that a necessary condition for the (19) to be stable is that the spectral radius of \( A \) is less than or equal to 1. We note that the product of the roots \( \mu_1 \mu_2 \) is equal to \( 1 + \alpha_j^2 \left( \frac{1}{2} - \delta \right) \). Then, a necessary condition to have

\[
|\mu_1| \leq 1 \quad \text{and} \quad |\mu_2| \leq 1
\]

is

\[
|\mu_1 \mu_2| \leq 1 \implies \frac{1}{2} - \delta \leq 0 \implies \delta \geq \frac{1}{2}.
\]

(21)

Under condition (21) we can now discuss the stability of the scheme (19) according to the sign of \( D \).

(C1) If \( D < 0 \), i.e.,

\[
\alpha_j^2 \left( \frac{1}{2} + \delta \right)^2 < 4,
\]

(22)
then the roots are complex with \( \mu_1 = \bar{\mu}_2 \) and \( |\mu_1| = |\mu_2| \leq 1 \). Precisely, \( |\mu_1| = |\mu_2| = 1 \) if \( \delta = \frac{1}{2} \); \( |\mu_1| = |\mu_2| < 1 \) if \( \delta > \frac{1}{2} \).

(C2) If \( D > 0 \), i.e.,
\[
x_j^2 \left( \frac{1}{2} + \delta \right)^2 > 4,
\]
then the roots \( \mu_1 \) and \( \mu_2 \) are real with:
\[
\mu_1 = \frac{2 - x_j^2 \left( \frac{1}{2} + \delta \right) - \sqrt{D}}{2} < \mu_2 = \frac{2 - x_j^2 \left( \frac{1}{2} + \delta \right) + \sqrt{D}}{2}.
\]
It can be easily proved that \( \mu_2 < 1 \), whereas the inequality \( \mu_1 \geq -1 \) is satisfied if
\[
x_j^2 \leq \frac{2}{\delta}.
\]

(C3) If \( D = 0 \), i.e.,
\[
x_j^2 \left( \frac{1}{2} + \delta \right)^2 = 4 \implies x_j^2 = \frac{4}{(\frac{1}{2} + \delta)^2},
\]
then
\[
\mu_1 = \mu_2 = 1 - 2(\frac{1}{2} + \delta)^{-1}
\]
with \( |\mu_1| = |\mu_2| < 1 \) if \( \delta > \frac{1}{2} \); \( \mu_1 = \mu_2 = -1 \) if \( \delta = \frac{1}{2} \).

We can conclude that the (19) is stable under the constraint
\[
x_j^2 < \frac{2}{\delta} \implies \lambda_j \Delta t < \sqrt{\frac{2}{\delta}}.
\]
We also observe that when \( \delta = \frac{1}{2} \) and \( x_j^2 = 4 \), the scheme is \textit{weakly unstable} since \( \|A^4\| = O(s) \) (see, e.g., [8]).

\textbf{Proposition 4.} The maximum eigenvalue of the generalized eigenvalue problem (16) is bounded by
\[
\max_{1 \leq j \leq N_{p,M}} \lambda_j \leq \tilde{C} p^4 \frac{H^2}{\delta},
\]
where \( \tilde{C} > 0 \) is a positive constant which is independent of \( H \) and \( p \).

See [33] for proof.

\textbf{Proposition 5.} The Newmark’s schemes (15) are stable under the assumption
\[
\Delta t < \tilde{C} H p^{-2} \delta^{-1/2}.
\]

\textbf{Proof.} The result easily follows from (20) and (25).
We now turn to the convergence analysis of the fully discrete problem, where again we assume homogeneous data for simplicity.

For regular problems such that \( u \in C^2(0, T; H^l(\Omega)) \cap C^3(0, T; L^2(\Omega)) \), or, if \( \delta = \frac{1}{2} \), \( u \in C^2(0, T; H^l(\Omega)) \cap C^4(0, T; L^2(\Omega)) \) and under the stability conditions on \( \Delta t \) above, the following convergence estimate

\[
\forall t_s > 0, \quad \| u(t_s) - u_s \|_{L^2(\Omega)} \leq \begin{cases} 
O(H^{-l + \delta} \Delta t) & \text{if } \delta \neq 1/2 \\
O(H^{-l} \Delta t^2) & \text{if } \delta = 1/2
\end{cases},
\]

is proved in [33], with an optimal order in \( p \) but a non-optimal order in \( H \), because of the power \( \min(p, l) \) instead of \( \min(p + 1, l) \) in the right-hand side of (27). As a matter of fact, classic convergence estimates for the \( h \)-version of the finite element method are satisfied with the power \( p + 1 \) (see, e.g., [27]).

For regular problem such that \( \min(p, l) = p \), the dependence of the error on \( H^{p+1} \) is also confirmed by numerical results reported in Section 5. In particular, the estimate is optimal for monodomain spectral methods, where partitions consist of one domain only, i.e., \( H = 1 \). Finally, we remark that when \( u(t) \) is analytical for all \( t \), then the error decays faster than algebraically in \( 1/p \) and the scheme is commonly said to be spectrally accurate (in space).

5. Numerical validation

We present now some numerical experiments concerning the stability and convergence of our approximation schemes with respect to the discretization parameters \( H, \Delta t, p \) and \( \delta \). The model problem is the acoustic wave equation (1) in \( \Omega = \Omega_{\text{ref}} \) with Dirichlet boundary conditions. We remark that the numerical features of the scheme remain unchanged when Neumann boundary conditions are prescribed, i.e., \( \Gamma_N \neq \emptyset \).

The right-hand side \( f \), the given pressure \( \Phi \) and the initial data \( u_0 \) and \( u_1 \) are assigned in such a way that the exact solution of the problem (1)–(3) is given by

\[
u(x, t) = \sin \pi x_1 \sin \pi x_2 (x_1^2 - 1)(x_2^2 - 1) \exp(-t^2).
\]

For each time step \( t_s > 0 \) we compare the above exact solution \( u(x, t) \) with the SE one \( u_s \) at the nodes of the discretization. To this aim, we compute the euclidean norm in \( \mathbb{R}^{N_{p,M}} \) of the difference between the two vectors. Precisely, we introduce the error

\[
e(t_s, p, H, \Delta t) = \left( \sum_{r=1}^{N_{p,M}} [u(x^r, t_s) - (u_s)_r]^2 \right)^{1/2},
\]

where \( u_s \) is the vector of nodal values of the numerical solution corresponding to the discretization parameters \( p, H, \Delta t \) at time \( t_s \). We recall that \( r = r(i, k, m) \) is the index, ranging from 1 to \( N_{p,M} \), corresponding to the global numbering of GLL nodes.
An alternative choice would be to use the norm induced by the GLL discrete scalar product introduced in (11), providing a new formula for the evaluation of the error, that reads:

$$E(t_s, p, H, \Delta t) = \left( \sum_{i=1}^{N_e} \sum_{k,m=0}^{p} [u((x_{km}^i), t_s) - (u_s)_{r(i,k,m)}] \omega_k \omega_m \right)^{1/2},$$

(29)

where the nodes $x_{km}^i$ and the weights $\omega_k \omega_m$ have been defined in (5) and (8), respectively. We observe that numerical results reported in tables below show that the differences between the two choices are not significant.

From now on, all computed errors reported in the figures and tables below refer to $t_s = 1$.

In Fig. 1 we show the spectral behaviour of the error $e(t_s, p, H, \Delta t)$ as a function of the degree of the polynomials $p$, for two fixed values of $\Delta t$ ($\Delta t = 0.01, 0.001$) and $H = 1$. Precisely, we plot $e(1, p, 1, 0.01)$ and $e(1, p, 1, 0.001)$. Here $\delta = \frac{1}{2}$ in the Newmark’s scheme, corresponding to the second-order accurate Leap–Frog method. We have used a logarithmic scale for the vertical axis. Results show the second order of accuracy of the Leap–Frog method with respect to $\Delta t$, as well as the spectral behaviour of the error until the influence of $\Delta t$ becomes predominant.

The order of accuracy with respect to the time step $\Delta t$ is emphasized in Fig. 2 where we report the quantity $e(1, 16, 1, \Delta t)$ for $\Delta t$ ranging from 0.001 to 0.01, and different values of the Newmark’s parameter $\delta$. We have used logarithmic scales for both axes. Results show the first (resp. second) order of accuracy of the Newmark’s scheme with respect to $\Delta t$ for $\delta > \frac{1}{2}$ (resp. $\delta = \frac{1}{2}$). Furthermore, there is numerical evidence that the error increases for growing values of the parameter $\delta$. 

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**Fig. 1.** Spectral accuracy of the Leap–Frog scheme until the influence of $\Delta t$ becomes predominant. The error $e(1, p, H, \Delta t)$ is plotted as a function of $p$, for $H = 1$, $\Delta t = 0.01, 0.001$. 

---

**Fig. 2.** Order of accuracy with respect to the time step $\Delta t$. The error $e(1, 16, 1, \Delta t)$ is plotted for $\Delta t$ ranging from 0.001 to 0.01, and different values of the Newmark’s parameter $\delta$. Results show the first (resp. second) order of accuracy of the Newmark’s scheme with respect to $\Delta t$ for $\delta > \frac{1}{2}$ (resp. $\delta = \frac{1}{2}$). Furthermore, there is numerical evidence that the error increases for growing values of the parameter $\delta$. 

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**Acknowledgments.**

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While the main emphasis in the mathematics literature is on the order of accuracy of a numerical solution, in practice there are other considerations regarding, for instance, the stability conditions for long time integrations as well as dissipation and dispersion properties of the numerical method. The study of an optimal choice of Newmark’s parameters with respect to these properties is beyond the scope of this paper; for a detailed discussion on the choice of the parameters $\delta$ in the finite element case, we refer, e.g., to [31] and [17].

We consider now the dependence of the error on the size $H$ of the SE partition $T_H$, fixed $\delta = \frac{1}{2}$. We compare the two proposed formulas for the computation of the error (28) and (29). In Table 1 we report the detailed values of the errors $e(1, 2, H, 0.01)$ and $e(1, 2, H, 0.02)$ as well as $E(1, 2, H, 0.01)$ and $E(1, 2, H, 0.02)$ as a function of the size $H$ of each element. Then in Table 2 we report $e(1, 4, H, \Delta t)$ for $\Delta t = 0.01, 0.005, 0.001$, whereas in Table 3 we report $E(1, 4, H, \Delta t)$ for $\Delta t = 0.01, 0.005, 0.001$.

We also study experimentally the asymptotic behaviour of the exponent of $H$ in (27). Precisely, fixed $p$, $\Delta t$ and $\delta$, the expected trend of the error is $O(H^\varphi)$ with $\varphi = p + 1$. Therefore, for all $H < 0.5$, we compare $e(1, p, H, \Delta t)$ (resp. $E(1, p, H, \Delta t)$) with $e(1, p, 0.5, \Delta t)$ (resp. $E(1, p, 0.5, \Delta t)$), and compute the quantities

$$
\varphi = \frac{\log(e(1, p, H, \Delta t)/e(1, p, 0.5, \Delta t))}{\log(H/0.5)}, \quad \text{or} \quad \varphi = \frac{\log(E(1, p, H, \Delta t)/E(1, p, 0.5, \Delta t))}{\log(H/0.5)}.
$$

(30)
Asymptotic behaviour of the error $e(1,2,H,\Delta t)$ and $E(1,2,H,\Delta t)$ as a function of $H$, for $\Delta t = 0.01$, 0.02

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Table 2
Asymptotic behaviour of the error $e(1,4,H,\Delta t)$ as a function of $H$, for $\Delta t = 0.01$, 0.005, 0.001

<table>
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<tr>
<th>1/H</th>
<th>$e(1,4,0.01)$</th>
<th>$\varphi$</th>
<th>$e(1,4,0.005)$</th>
<th>$\varphi$</th>
<th>$e(1,4,0.001)$</th>
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<td>1.52e-04</td>
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<td>7.25e-05</td>
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<td>7.32e-05</td>
<td>4.97</td>
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<tr>
<td>7</td>
<td>6.75e-05</td>
<td>4.41</td>
<td>4.49e-05</td>
<td>4.74</td>
<td>4.00e-05</td>
<td>4.83</td>
</tr>
</tbody>
</table>

Table 3
Asymptotic behaviour of the error $E(1,4,H,\Delta t)$ as a function of $H$, for $\Delta t = 0.01$, 0.005, 0.001

<table>
<thead>
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<th>1/H</th>
<th>$E(1,4,0.01)$</th>
<th>$\varphi$</th>
<th>$E(1,4,0.005)$</th>
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<td>2.61e-04</td>
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</table>

Numerical results show that $\varphi \to 3$ when $p = 2$, whereas $\varphi \to 5$ when $p = 4$. Therefore we can conclude that there is numerical evidence that the error behaves as $H^{p+1}$ until the term depending on $(\Delta t)^2$ becomes predominant.

We consider now the problem of numerical stability to the Newmark’s schemes. From the theoretical analysis carried out in Section 4 the scheme is conditionally stable. Precisely, Proposition 4.5 states that the maximum allowable time step $\Delta t$—in order for the scheme to be stable—is proportional to $H$ (fixed $p$ and $\delta$), and to $1/p^2$, (fixed $H$ and $\delta$). Finally, it is proportional to $1/\sqrt{\delta}$, fixed $p$ and $H$. 


Fig. 3. Stability constraint for the Leap–Frog scheme. The error $e(1, p, H, \Delta t)$ is plotted as a function of $\Delta t$, for $H = 1$ and varying $p$.

Fig. 4. Stability constraint for the Leap–Frog scheme. The error $e(1, p, H, \Delta t)$ is plotted as a function of $\Delta t$, for $p = 2$ and varying $H$. 

In Fig. 3 we report the error $e(1, p, 1, \Delta t)$ as a function of $\Delta t$ for different choices of $p$ ($p = 16, 20, 24$). In Fig. 4 we report the error $e(1, 2, H, \Delta t)$ as a function of $\Delta t$ for different choices of $H$ ($H = \frac{1}{6}, \frac{1}{8}, \frac{1}{10}$). In both cases $\delta = \frac{1}{2}$. We have used logarithmic scale for both axes.

Finally, in Fig. 5 we report the maximum allowable time step $\Delta t$—in order for the scheme to be stable—as a function of the parameter $\delta$. Such values have been computed experimentally, through successive tests with increasing values of the time step $\Delta t$ until instability is observed. In the first case $H = \frac{1}{2}$ and $p = 8$, whereas in the second case we have chosen $H = \frac{1}{4}$ and $p = 4$. We note that the two sets of data yield the same number of degrees of freedom $N_{p,M}$. Therefore, fixing the global number of unknowns $N_{p,M}$, if we increase the degree of the polynomial $p$ within each element and decrease the number of quadrilateral elements $N_e$ we obtain a better accuracy but the stability constraint is more severe. On the contrary, if we decrease the degree $p$ and refine the triangulation the error grows slightly but we can choose a higher time step $\Delta t$.

6. Conclusions

We have considered the numerical approximation of the acoustic wave equation by the spectral element method based on Gauss–Lobatto–Legendre quadrature formulas, and finite difference Newmark’s explicit time advancing schemes. A detailed theoretical analysis of the stability of the numerical approximation is presented, providing an upper bound for the time step $\Delta t$ with respect to the parameters of the spectral element discretization and of the Newmark’s scheme. Several numerical experiments have been presented in order to validate the stability constraints. The approach described in this paper is a generalization of
a recent work on an explicit second-order spectral element method for acoustic waves and of previous works in the monodomain case, and represents a first step towards the study of implicit time advancing schemes and more general problems involving also absorbing boundary conditions.

References