High-order discretizations for the wave equation based on the modified equation technique

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The accurate solution to the wave equation implies very high computational burdens, even when using high-order space discretization methods. Besides, if we use explicit time discretization methods (such as for instance the classical Leap-Frog scheme), the time step has to satisfy a CFL (Courant-Friedrichs-Lewy) condition to ensure the stability of the scheme. The smaller the space step is, the smaller the CFL condition and the higher the number of iterations will be. To improve the accuracy of the Leap-Frog scheme, we may consider the modified equation technique, which allows to obtain explicit arbitrary 2p-th order scheme in time. The price to pay is p matricial multiplications at each time step when the Leap-Frog scheme only requires one, whereas the CFL condition is multiplied by $\alpha_p \geq 1$. For p=2 (fourth-order scheme), $\alpha_2 = 1.7$, so that the additional computational cost is small, but for higher-order scheme the increase of the CFL condition is generally not sufficient to counterbalance the number of additional multiplications. Recently, a technique has been proposed to optimize the coefficients α_p, but it requires more matricial multiplications. Herein, we apply the modified equation technique in an original way, by switching the classical discretization process. Indeed, we consider first the time discretization, thanks to the modified equation technique, before addressing the question of the space one. After this time discretization, we have to deal with an additional p-laplacian operator which implies to consider C^{p-1} finite elements. In this work, we have chosen to discretize the second-order operator by the Interior Penalty Discontinuous Galerkin method and we will present how we extend this method to discretize the higher-order operators. Numerical results in 2D illustrate the performance of the 4-th order scheme.

1 Introduction

To improve the accuracy of the numerical solution of the wave equation computed with a finite element method, one must considerably reduce the space step. Obviously this will result in increasing the number of unknowns of the discrete system. Besides, the time step, which is fixing the number of needed iterations, is linked to the space step through the CFL (Courant-Friedrichs-Lewy) condition. The CFL number defines an upper bound for the time step in such a way that the smaller the space step is, the higher the number of iterations will be. In the three-dimensional case, the problem can have more than ten million unknowns, which must be evaluated at each time-iteration. However, high-order numerical methods can be used for computing accurate solutions with larger space and time steps. Recently, Joly and Gilbert [2] have optimized the Modified Equation Technique (MET), which was proposed by Shubin and Bell [4] for solving the wave equation, and it seems to be very promising given some improvements. In this work, we apply this technique in a new way. Normally, most of the study devoted to the solution of the wave equation consider first the space discretization of the system before addressing the question of the time discretization. We intend here to invert the discretization process by applying first the time discretization using the MET and then to consider the space discretization. The time discretization causes high-order operators to appear (such as p-Laplacian) and we have therefore to consider appropriate methods to discretize them. The Discontinuous Galerkin Methods are well adapted to this discretization, since they allow to consider piecewise discontinuous functions. In particular, using the Interior Penalty Discontinuous Galerkin (IPDG) method (see for instance [6, 7, 3] for the discretization of the Laplacian and [5] for the discretization of the Bilaplacian), one can enforce through the elements high-order transmission conditions, which are adapted to the high order operators to be discretized. The outline of this paper is as follows. In section 1, we describe the classical application of the MET to the semi-discretized wave equation and we recall its properties. In section 2, we obtain high-order schemes by applying this technique directly to the continuous wave equation and we present the numerical method we have chosen for the space discretization of the high order operators. In section 3, we present numerical results to compare the performances of the new technique with the ones of the classical MET.

2 The Modified Equation Technique

In this part, we briefly describe the modified equation technique applied to the acoustic wave equation in a bounded medium $\Omega \subset \mathbb{R}^d, d = 1,2,3$. For the sake of simplicity, we impose an homogeneous Neumann boundary condition on the Boundary $\Gamma := \partial\Omega$ but this study can be easily extended to Dirichlet boundary conditions. The model is then:

$$\begin{cases} \text{Find } u : \Omega \times [0,T] \mapsto \mathbb{R} \text{ such that :} \\ \dfrac{1}{\mu(x)}\dfrac{\partial^2 u}{\partial t^2} - \operatorname{div}\left(\dfrac{1}{\rho(x)}\nabla u\right) = f & \text{in } \Omega \times]0,T], \\ u(x,0) = u_0, \quad \dfrac{\partial u}{\partial t}(x,0) = u_1 & \text{in } \Omega, \\ \partial_n u = 0 & \text{on } \partial\Omega. \end{cases} \tag{1}$$

where u stands for the displacement, μ is the compressibility modulus, ρ is the density and f is the source term. We assume here that μ and ρ are piecewise polynomial. T denotes the final time, u_0 and u_1 are initial data and n is the unit outward normal vector to $\partial\Omega$.

A classical space discretization method, applied to (1) leads to the linear system,

$$M\frac{\partial^2 U}{\partial t^2} + KU = F, \tag{2}$$

where M is the mass matrix , K is the stiffness matrix, U is the vector of unknowns and F the source vector. In the following, we assume that the space discretization method is such that M is easily invertible (sparse or block-diagonal). This is the case if we consider finite differences, a spectral element method or discontinuous Galerkin methods.

Regularly, (2) is discretized by using a second-order scheme like

$$\frac{U(t+\Delta t) - 2U(t) + U(t-\Delta t)}{\Delta t^2} = \frac{\partial^2 U}{\partial t^2}(t) + O\left(\Delta t^2\right) \tag{3}$$

where Δt is the time step. Combining (2) and (3) we obtain the well-known Leap-Frog scheme,

$$\frac{U^{n+1} - 2U^n + U^{n-1}}{\Delta t^2} = -M^{-1}KU^n + M^{-1}F^n, \tag{4}$$

where U^n denotes the approximate solution of U at the instant $t^n = n\Delta t$.

Higher-order schemes can be obtained by using the modified equation technique [1, 4]. This technique relies on higher even-order Taylor expansions of the quantity $U(t+\Delta t) - 2U(t) + U(t-\Delta t)$. For instance, to obtain a fourth-order scheme requires to use a fourth-order Taylor expansion like

$$\begin{aligned} \frac{U(t+\Delta t) - 2U(t) + U(t-\Delta t)}{\Delta t^2} = & \frac{\partial^2 U}{\partial t^2}(t) \\ & + \frac{\Delta t^2}{12}\frac{\partial^4 U}{\partial t^4}(t) + O\left(\Delta t^4\right). \end{aligned} \tag{5}$$

Now (2) implies that

$$\frac{\partial^4 U}{\partial t^4} = M^{-1}KM^{-1}KU - M^{-1}KM^{-1}F + M^{-1}\frac{\partial^2 F}{\partial t^2}.$$

Consequently, we obtain the explicit fourth order modified equation scheme (MES-4)

$$\begin{aligned} \frac{U^{n+1} - 2U^n + U^{n-1}}{\Delta t^2} = & -M^{-1}KU^n \\ & + \left(M^{-1}K\right)^2 U^n + \mathcal{F}_4 \end{aligned} \tag{6}$$

where $\mathcal{F}_4$ is a modified source term defined by $M^{-1}\left(\left(I - KM^{-1}\right)F^n + \frac{\partial^2 F^n}{\partial t^2}\right)$. We can remark that applying the MES-4 involves two matricial multiplications by $M^{-1}K$ so that the computational burden of one iteration is respectively multiplied by two as compared to the Leap-Frog scheme. The stability of the Leap-Frog scheme (4) is ensured if the CFL (Courant-Friedrichs-Lewy) condition:

$$\Delta t \leq \Delta t_{LF} := \alpha h, \tag{7}$$

is satisfied. It involves the space step h and a constant α depending only on the space discretization method and on the physical coefficients.

Regarding the MES-4, the CFL condition is multiplied by $\sqrt{3}$

$$\Delta t \leq \Delta t_{MES-4} := \sqrt{3}\alpha h,$$

according to [2]. The computational cost is thus multiplied by $2/\sqrt{3} = 1.15$. It is possible to increase the CFL condition of MES-4, but according to [2], it is necessary to increase the number of multiplications by the matrix $M^{-1}K$ at each time-step.

3 The new scheme

In this section we present a new fourth-order scheme. Let us mention that higher order schemes can be obtained in the same way (see [8]).

We first perform the time discretization of (1), by applying a fourth-order Taylor expansion:

$$\begin{aligned} \frac{u(t+\Delta t) - 2u(t) + u(t-\Delta t)}{\Delta t^2} = & \frac{\partial^2 u(t)}{\partial t^2} \\ & + \frac{\Delta t^2}{12}\frac{\partial^4 u(t)}{\partial t^4} + O\left(\Delta t^4\right). \end{aligned} \tag{8}$$

Since u is solution to the wave equation (1), we can rewrite the fourth order partial derivative of u with respect to the time as

$$\begin{aligned} \frac{\partial^4 u}{\partial t^4} = & \mu\operatorname{div}\left(\frac{1}{\rho}\nabla\left[\mu\operatorname{div}\left(\frac{1}{\rho}\nabla u\right)\right]\right) \\ & + \mu\frac{\partial^2 f}{\partial t^2} + \mu\operatorname{div}\left(\frac{1}{\rho}\nabla(\mu f)\right). \end{aligned} \tag{9}$$

Finally, we obtain the semi-discretized scheme

$$\begin{aligned} \frac{1}{\mu}\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} = & \operatorname{div}\left(\frac{1}{\rho}\nabla u^n\right) \\ & + \frac{\Delta t^2}{12}\operatorname{div}\left(\frac{1}{\rho}\nabla\left[\mu\operatorname{div}\left(\frac{1}{\rho}\nabla u^n\right)\right]\right) + f_4, \end{aligned} \tag{10}$$

with $f_4 = f + \dfrac{\Delta t^2}{12}\left(\dfrac{\partial^2 f}{\partial t^2} + \operatorname{div}\left(\dfrac{1}{\rho}\nabla(\mu f)\right)\right)$.

For the space discretization, we refer to [8] where a finite element approximation has been proposed. It is based on an Interior Penalty Discontinuous Galerkin (IPDG) method [6, 7, 3] for which we have defined suitable transmission conditions. We consider a partition $\mathcal{T}_h$ of Ω composed of triangles or hexahedra K and we suppose that the functions ρ and μ are constant by element. We seek an approximation of the solution in the space:

$$V_l^h := \left\{v \in L^2(\Omega) : v_{|K} \in P_l(K), \forall K \in \mathcal{T}_h\right\}, \tag{11}$$

where $P_l(K)$ is the set of polynomials of degree $\leq l$ on K. Since we have to discretize a fourth order operator, we choose $l \geq 3$ and we consider the problem:

$$\begin{cases} \text{Find } u_h^{n+1} \in V_h \text{ such that,} \qquad \forall v \in V_h, \\ \displaystyle\sum_{K\in\mathcal{T}_h} \int_K \left(\frac{1}{\mu} \frac{u_h^{n+1} - 2u_h^n + u_h^{n-1}}{\Delta t^2} - f_4 \right) v = a_h\left(u_h^n, v\right). \end{cases} \tag{12}$$

where $a_h\left(u_h^n, v\right) = -a_{1h}\left(u_h^n, v\right) + \frac{\Delta t^2}{12} a_{2h}\left(u_h^n, v\right)$. We do not detail here the expression of the bilinear forms a_{1h}, a_{2h} corresponding respectively to the second and fourth order terms. Let us however mention that a_{1h} is obtained by the IPDG method and involves a positive penalization parameter γ_1 to ensure the coercivity of a_{1h}. We use the same technique for a_{2h} and we have to consider two positive penalization parameters $\gamma_{2,1}$ and $\gamma_{2,2}$ to ensure its stability. The discretized scheme can be rewritten as a linear system

$$\frac{U^{n+1} - 2U^n + U^{n-1}}{\Delta t^2} = M^{-1}\left[\left(K_1 + \frac{\Delta t^2}{12} K_2\right) U^n + F^n\right] \tag{13}$$

where M is the mass matrix associated to the L^2 scalar product, K_1 and K_2 are the two stiffness matrices respectively associated to a_{1h} and a_{2h} and F^n is the corresponding source vector.

4 Numerical analysis

Let us now compare the computational cost of this scheme (that we denote by Δ^2-scheme) to the one of the Leap-Frog scheme and of the MES-4. We suppose here that the matrix K in (2) has been obtained by using an IPDG method of order p, so that $(K)_{ij} = a_{1h}\left(\varphi_i, \varphi_j\right) = (K_1)_{ij}$.

In practice we compute $K^* := K_1 + \frac{\Delta t^2}{12} K_2$, so that we have only one matricial multiplication by $M^{-1}K^*$ to perform at each iteration. Moreover, it is clear that $a_{1h}\left(\varphi_i, \varphi_j\right) = a_{2h}\left(\varphi_i, \varphi_j\right) = 0$, as soon as the degrees of freedom i and j are respectively associated to two elements which do not share a common edge. This means that $M^{-1}K_1 = M^{-1}K$, $M^{-1}K_2$ and $M^{-1}K^*$ have the same number of non-zero elements and that the cost of one multiplication by $M^{-1}K^*$ is the same as the cost of one multiplication by $M^{-1}K$. It is therefore clear that the cost of one iteration of the Δ^2-scheme is the same as the cost of one iteration of the Leap-Frog scheme and is the half of the cost of one iteration of MES-4.

The global cost of these schemes is the cost of one iteration multiplied by the number of iterations, which is imposed by the CFL condition. We did not obtain an explicit CFL condition for the Δ^2-scheme, but the numerical experiments we have carried out (see section 5) show that this condition is a little bit higher than the condition of the Leap-Frog scheme, so that the global cost of the Δ^2-scheme is equivalent to the one of the Leap-Frog scheme. Moreover, since the CFL condition of MES-4 is about 1.73 times the condition of the Leap-Frog scheme, we can deduce that the global cost of the Δ^2-scheme is smaller than the one of MES-4.

5 Numerical Results

In this section, we consider the simulation of wave propagation in a 2D two-layered media $\Omega = [-1,1]^2 = \Omega_t \cap \Omega_b$ where $\Omega_t = [-1,1] \times [0,1]$ and $\Omega_b = [-1,1] \times [-1,0]$ are two homogeneous layers respectively charaterized by $\mu = 2$, $\rho = 2$ and $\mu = 8$, $\rho = 4$. We consider zero-initial conditions and a source which is a second derivative of a Gaussian in time and a point source in space:

$$f = \delta_{x_0} 2\lambda \left(\lambda \left(t - t_0\right)^2 - 1\right) e^{-\lambda (t-t_0)^2},$$

with $x_0 = (0, 0.5)$, $\lambda = \pi^2 f_0^2$, $f_0 = 5$ and $t_0 = 1/f_0$.
In this case, we discretize the wave equation (1) with the two following methods:

1. MES-4, based on a space discretization with P^3-Lagrange polynomials and a penalization parameter of $\gamma_1 = 10$. With these basis functions and this parameter, the CFL condition of the Leap-Frog scheme is (experimentally) $\Delta t_{LF_4} = 0.058h$ so that the CFL of MES-4 is $\Delta t_{MES-4} = 0.058\sqrt{3}h = 0.100h$.

2. The Δ^2-scheme, with P^3-Lagrange basis functions and with the penalization parameters $\gamma_1 = 10$, $\gamma_{2,1} = 10$ and $\gamma_{2,2} = 0$. The CFL condition of this scheme is (experimentally) $\Delta t_{opt} = 0.061h$.

Let us remark that the CFL of the Δ^2-scheme is slightly higher than the CFL of the Leap-Frog scheme Δt_{LF_4}.
To compare the performances of the different methods, we compute the solution on a receiver at point $x_1 = (0.25, 0.25)$ and we calculate the relative $L^2\left([0,T], x_1\right)$ error for different mean space steps $h = 3e-3, 1.5e-3, 7.5e-4$ and a final time approximatively equal to 2. The results are presented in Tab. 1 and we represent in Fig. 1 the relative L^2 error as a function of the mesh size for the MES-4 (red line with circles) and the Δ^2-scheme (green line with squares) in log-log scale.

h	MES-4	Δ^2-scheme
$3.0e-3$	$2.5e-2$	$2.3e-2$
$1.5e-3$	$1.2e-3$	$1.1e-3$
$7.5e-4$	$6.6e-5$	$6.5e-5$

Table 1: Relative L^2 error in time at the receiver.

We can easily verify that the two methods are fourth order approximations and give similar results. Since the CFL of the Δ^2-scheme is slightly higher than the CFL of the Leap-Frog scheme and only require one matricial multiplication at each iteration, that means that they allow for high-order accuracy with a smaller cost than the Leap-Frog scheme.

6 Conclusion

In this work, we have constructed new high-order schemes both in time and space to solve the acoustic wave equation. The numerical results we have presented illustrate the fact that the computational cost of these

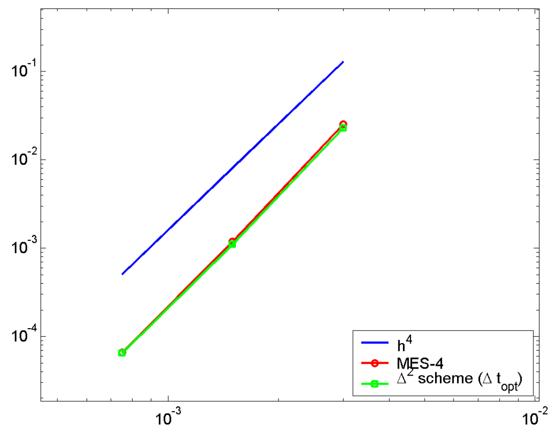

Figure 1: Convergence of the 4^{th}-order schemes in 2D

schemes is the same as the one of the Leap-Frog scheme and is therefore smaller than the one of the MES-4. However, the CFL of the new scheme are only computed numerically and we are now trying to determine them analytically. This scheme seems to be very well-adapted to p adaptivity. Indeed, if we combine the Δ^2-scheme with a mesh composed of P^1 and P^3 cells, it is clear that $a_{2h}(\phi_i, \phi_j)$ vanishes if the degrees of freedom i and j belong to a P^1-cells. Therefore, we infer that the scheme will be of second order on the P^1-cells and of fourth order on the P^3-cells. This will be the object of a forthcoming work.

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