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Introduction and study of fourth order theta schemes for linear wave equations

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ABSTRACT

A new class of high order, implicit, three time step schemes for semi-discretized wave equations is introduced and studied. These schemes are constructed using the modified equation approach, generalizing the θ-scheme. Their stability properties are investigated via an energy analysis, which enables us to design super-convergent schemes and also optimal stable schemes in terms of consistency errors. Specific numerical algorithms for the fully discrete problem are tested and discussed, showing the efficiency of our approach compared to second order θ-schemes.

1. Introduction

Linear wave equations play a great role in scientific modeling and are present in many fields of physics. For instance, they arise in the Maxwell equations, the acoustic equation and the elastodynamic equation. A discrete approximation of their solutions can be found with numerical simulations. Spatial discretization of the above equations using classical finite elements methods often leads to a semi-discretized problem of the form: find $u_h \in C^2(t, \mathbb{R}^N)$ such that

$$M_h \frac{d^2}{dt^2} u_h + K_h u_h = 0, \qquad u_h(0) = u_{0,h}, \qquad \frac{du_h}{dt}(0) = u_{1,h}, \tag{1}$$

where $u_h(t)$ is a vector-unknown in $\mathbb{R}^N$, M_h a symmetric positive definite matrix and K_h a symmetric positive semi-definite matrix.

Several approaches can be adopted to tackle the time discretization of problem (1). The so called "conservative methods" (as for instance the leap frog scheme) preserve a discrete energy which is consistent with the physical energy. They can be shown to be stable as soon as some positivity properties of the discrete energy are satisfied, which generally imposes a restriction, known as the CFL condition, on the time step depending on the matrices M_h and K_h. The leap frog scheme enters a more general class of three points time step, energy preserving, implicit schemes called θ-schemes, which are parametrized by a real number θ. The over cost of these implicit schemes compared to explicit ones is balanced by the fact that stability conditions allow for a bigger time step.

For simple configurations with simple finite elements methods (such as P_1 triangular elements), explicit schemes show good performances. However they have two major drawbacks in complex configurations that have not yet been completely solved:

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- If the mesh has different scales of elements, or if the equations involve variable coefficients with strong contracts, the time step must be adapted to the worst situation (for instance the smallest element) because of the CFL condition. A natural way to avoid this restriction is to use local time stepping techniques which divide into two categories. The locally implicit technique, as developed in [1–4], is optimal in terms of CFL restriction but "only" second order accurate in time, and requires the inversion of interface matrices. The fully explicit local time stepping, as developed in [5], achieves higher order time stepping but without (up to now) a full control over the CFL condition.
- If the mass matrix is non-diagonal or non-block-diagonal, its inversion (at least one time per iteration) can lead to a dramatic over cost of the explicit schemes, whereas no over cost is observed with implicit schemes (see Remark 4.1).

The extension of conservative time discretization schemes to higher orders of accuracy is a natural question. A popular way to design explicit high order three points schemes is the modified equation approach. In this article we extend this approach to design new high order implicit schemes which are stable and present some optimal properties.

The paper is organized as follows. Section 2 recalls some well-known results concerning the leap frog and θ-schemes. In a conclusive remark we present, in the very simple case of the θ-scheme, the non-standard approach that we will choose to follow in the rest of the paper. In Section 3 we construct a family of energy preserving implicit fourth order schemes, parametrized by two real numbers (θ, φ). In Section 4 we discuss the existence of their discrete solution and some practical aspects of computation which can reduce numerical cost. Section 5 is devoted to the study of the stability of the newly introduced schemes via energy techniques. The search for "optimal" schemes is presented in Section 6, it is done by adjusting (θ, φ) to increase accuracy. Finally, numerical results compare theses schemes to classical schemes in Section 7.

In the following we will consider the semi-discretized problem

$$\frac{d^2}{dt^2}u_h + A_h u_h = 0, \qquad u_h(0) = u_{0,h}, \qquad \frac{du_h}{dt}(0) = u_{1,h}, \tag{2}$$

with A_h a symmetric positive semi-definite matrix. With no loss of generality: the analysis done below is valid if $A_h = M_h^{-1}K_h$.

Extensive use will be made of the spectral radius of the matrix A_h, defined as $\rho(A_h) = \sup_{\|v\|=1} A_h\, v \cdot v$ and coinciding with the greatest eigenvalue of A_h. Its exact expression can be given in simple cases, as for instance the 1D wave equation with constant speed c, using finite differences on a regular mesh of size h, for which $\rho(A_h) = 4c^2/h^2$. In other cases, the cost of its numerical evaluation (for example with the power iteration method) is negligible compared to the numerical resolution of the equation.

2. Classical results

In this section we recall the definitions and some properties of the classical leap frog and θ-schemes, which are widely used for the time discretization of wave equations. In the following we denote $\Delta t > 0$ as the time step of the numerical method.

2.1. Preliminary notations

The centered second order approximation of the second order derivative in time of any function $t \mapsto f(t)$ will be denoted

$$D^2_{\Delta t} f(t) = \frac{f(t+\Delta t) - 2f(t) + f(t-\Delta t)}{\Delta t^2}. \tag{3}$$

Assuming infinite smoothness on f, let us use a Taylor expansion to write the truncation error of the previous quantity:

$$D^2_{\Delta t} f(t) = \frac{d^2}{dt^2} f(t) + 2\sum_{m=1}^{\infty} \frac{\Delta t^{2m}}{(2m+2)!}\frac{d^{2m+2}}{dt^{2m+2}} f(t). \tag{4}$$

Classical θ-schemes are based upon the use of a three points centered approximation of $f(t)$ which, for $\theta \in \mathbb{R}$, is defined by

$$\{f(t)\}_\theta = \theta f(t+\Delta t) + (1-2\theta) f(t) + \theta f(t-\Delta t). \tag{5}$$

Assuming again infinite smoothness on f, we can write the truncation error of this new quantity:

$$\{f(t)\}_\theta = f(t) + 2\theta \sum_{m=1}^{\infty} \frac{\Delta t^{2m}}{(2m)!}\frac{d^{2m}}{dt^{2m}} f(t). \tag{6}$$

Both the leap frog scheme and the θ-scheme use finite differences to discretize time in order to compute an approximation of the semi-discrete solution u_h of (2). Consequently, the unknowns of those schemes stand for the values of u_h at time $t^n = n\,\Delta t : u_h^n \simeq u_h(t^n)$. The discrete versions of (3) and (5), using the same symbols, are

$$D^2_{\Delta t} u_h^n = \frac{u_h^{n+1} - 2u_h^n + u_h^{n-1}}{\Delta t^2}, \qquad \{u_h^n\}_\theta = \theta\, u_h^{n+1} + (1-2\theta) u_h^n + \theta\, u_h^{n-1}. \tag{7}$$