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Higher-order accurate two-step finite difference schemes for the many-dimensional wave equation

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ABSTRACT

The accurate simulation of wave propagation is a problem of longstanding interest. In this article, the focus is on higher-order accurate finite difference schemes for the wave equation in any number of spatial dimensions. In particular, two-step schemes (which operate over three time levels) are studied. A novel approach to the construction of schemes exhibiting both isotropy and accuracy is presented using modified equation techniques, and allowing for the specification of precise stencils of operation for the scheme, and thus direct control over stencil size and thus operation counts per time step. Both implicit and explicit schemes are presented, as well as parameterised families of such schemes under conditions specifying the order of isotropy and accuracy. Such conditions are framed in terms of a set of coupled constraints which are nonlinear in general, but linear for a fixed Courant number. Depending on the particular choice of stencils, it is often possible to develop schemes for which the traditional Courant–Friedrichs–Lewy condition is exceeded. A wide variety of families of such schemes is presented in one, two and three spatial dimensions, and accompanied by illustrations of numerical dispersion as well as convergence results confirming higher-order accuracy up to eighth order.

1. Introduction

The numerical simulation of wave propagation is an important application and object of study in itself for many fields, including electromagnetics, geophysics, and acoustics. In such fields, the linear wave equation in many spatial dimensions is often used as a basic test problem for the construction of numerical methods. Solutions to the wave equation can be approximated through various numerical techniques, such as finite difference [1,2], finite element [3,4], finite volume [5], and spectral methods [6]. Of these mentioned, the finite difference method is perhaps the oldest technique to be applied to numerically solve the wave equation, going back at least as far as the seminal work of Courant [7], and still constituting a popular choice for numerical discretisation today, particularly in geophysical [8] and CFD applications [9].

An important limitation of any numerical method for the many-dimensional wave equation that operates locally in space and/or time is erroneous numerical dispersion. Spectral methods, though in theory without error in the approximation of the spatial part of a problem, can be challenging to adapt to domains of non-trivial geometry, and, furthermore, remain susceptible to time discretisation error. For this reason, finite difference schemes are often preferred, but the problem of numerical dispersion [10,11] requires grid resolution beyond the minimum two points per wavelength (on the regular Cartesian grid)—this quickly becomes infeasible in terms of computational cost for many-dimensional problems and/or large

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domains, despite the increasing availability of computing power and parallel hardware (such as Graphics Processing Units, or GPUs) [12,13]. On the other hand, high-order accurate schemes [14,2] inherently have improved numerical dispersion in the limit of low wavenumbers. High-order methods can be seen as intermediate between low-order methods and spectral methods [15], and thus offer a flexible trade-off between the ability to impose boundary conditions and the ability to accurately resolve propagating wavefronts.

The standard approach to designing high-order accurate schemes for the wave equation—which, strictly speaking, requires that both time and space operators be approximated to high orders—is to employ conventional high-order spatial differences [16,17], often over an equivalent first-order hyperbolic system, combined with high-order time integration (such as Runge–Kutta [18–20,9]). Although these techniques have shown much success, there are gains in computational efficiency to be had by working with the second-order wave equation directly (as pointed out in, e.g., [21–23]). Rather than employing high-order time integrators, which necessarily require intermediate steps and possibly additional temporary states to be stored in memory (beyond the minimum of two for a second-order system), it is possible to achieve high-order accuracy, at least for the initial value problem, using only conventional two-step leapfrog (Störmer–Verlet [24]) integration, i.e., storing only the minimal two states in memory. The manner by which this is typically accomplished is known as the *modified equation approach* [25–31,14,32–34], wherein the scheme is expanded in a Taylor series such that temporal truncation errors can be recast in terms of spatial operators and then discretised. This leads to a delicate balancing of temporal and spatial truncation errors such that they effectively cancel up to a high order.

In this paper, a novel approach to modified equation methods is applied to finite difference schemes over regular Cartesian grids in order to achieve high even-order spatiotemporal accuracy for the homogeneous constant-coefficient wave equation in d spatial dimensions. Within this approach, general parametrised constructions for the d-dimensional Laplacian are combined with constraints imposed for high-order isotropy and accuracy. Constraints for isotropy are linear in the scheme coefficients, and constraints for higher-order accuracy are dependent on the Courant number. Thus such constraints may be viewed as linear if the Courant number is specified *a priori*, and nonlinear if the Courant number is treated as a partially free additional parameter, subject to a stability condition bounding it (normally from above), but still allowed to take on values over a continuous range. In either case, parameters of high-order accurate schemes, possibly dependent on the Courant number, are obtained as solutions to a resulting linear system. Even-order schemes to any order of accuracy have previously been derived for the many-dimensional wave equation using modified equation approaches, but they tend to produce minimal "diamond"-shaped stencils [30,8] that are limited in terms of stability by the standard Courant–Friedrichs–Lewy condition. In contrast to such approaches and other applications of modified equations to leapfrog time-integrators [14,22,35], the general construction presented in this study offers more flexibility for choices of spatial discretisations that effectively cancel out temporal errors, allowing a wide variety of stencil shapes, along with the ability to impose additional high orders of isotropy (enabling, e.g., $2M$th-order accurate schemes with errors isotropic to $(2M+2)$th order, $M = 1, 2, \dots$). Schemes over diamond-shaped stencils are obtained as special cases. As shown in this paper, the resulting schemes can have Courant numbers close to unity, permitting larger time-steps for a fixed grid resolution than conventional diamond-shaped schemes [30,8]. Additionally, this general construction permits implicit two-step time integration (e.g., *theta schemes* [34]), offering high-order accuracy with smaller spatial stencils than explicit counterparts (at the cost of sparse linear system solutions at each time-step). Throughout this work, many novel schemes are derived in one, two, and three spatial dimensions, and up to eighth-order accuracy. Stability conditions are obtained through frequency-domain analyses, and the reported orders of accuracy are confirmed through convergence analyses of numerical dispersion and via numerical simulations of wave propagation.

It should be mentioned that the scope of this paper lies with the initial value problem, and as such, boundary conditions beyond periodic ones will not be addressed in this work (as in, e.g., [8]), and are left to be developed in subsequent studies. Possible avenues to deal with non-periodic boundaries are discussed in Section 6.

A brief presentation of the many-dimensional wave equation appears in Section 2. In Section 3, basic time and space difference operations over regular Cartesian grids are presented, and in particular parametrised approximations to the Laplacian operator over arbitrary symmetric stencils, as well as conditions for higher-order isotropy. A general family of implicit and explicit two-step schemes for the many-dimensional wave equation appears in Section 4, accompanied by conditions for numerical stability and accuracy to higher order in space and time. Accuracy conditions may be expressed as a set of nonlinear constraints in the free parameters and the Courant number. In Section 5, various examples of higher-order accurate schemes in 1D, 2D and 3D are given, along with numerical results illustrating the rate of convergence. Conclusions and final remarks are given in Section 6. Some additional material, with regard to various features of the designs presented here, appears in the Appendices. In Appendix A, energy-based approaches to the problem of numerical stability verification are presented, and in Appendix B, some conditions for negativity of parameterised approximations to the Laplacian are offered. Appendix C provides a brief link between the implicit family of schemes presented here and the familiar so-called theta family of schemes.

2. The wave equation

The wave equation in d spatial dimensions is defined as

$$\mathcal{L}u = 0\,, \qquad \text{where} \qquad \mathcal{L} = \partial_t^2 - \Delta\,. \tag{1}$$