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Nonstandard Fourier Pseudospectral Time Domain (PSTD) Schemes for Partial Differential Equations

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Abstract. A class of nonstandard pseudospectral time domain (PSTD) schemes for solving time-dependent hyperbolic and parabolic partial differential equations (PDEs) is introduced. These schemes use the Fourier collocation spectral method to compute spatial gradients and a nonstandard finite difference scheme to integrate forwards in time. The modified denominator function that makes the finite difference time scheme exact is transformed into the spatial frequency domain or k-space using the dispersion relation for the governing PDE. This allows the correction factor to be applied in the spatial frequency domain as part of the spatial gradient calculation. The derived schemes can be formulated to be unconditionally stable, and apply to PDEs in any space dimension. Examples of the resulting nonstandard PSTD schemes for several PDEs are given, including the wave equation, diffusion equation, and convection-diffusion equation.

AMS subject classifications: 65M70, 65M06, 65M80

Key words: Nonstandard finite difference, pseudospectral time domain, PSTD, Fourier collocation spectral method, wave equation, diffusion.

1 Introduction

Over the last decade, nonstandard finite difference methods have been used for the numerical solution of a wide range of differential equations [8, 11]. These schemes are constructed by modifying the denominator of conventional finite difference formulae such that the phase error introduced by the discretisation is eliminated [10]. This is particularly useful in the context of large-scale problems, as it alleviates the need to use dense spatial and temporal grids to avoid the accumulation of numerical dispersion. However, while the idea behind nonstandard finite difference methods is very appealing, many of

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the existing schemes have only been derived in one space dimension, and are not easily generalisable to higher dimensions [9]. Moreover, for solving time dependent partial differential equations (PDEs), the denominator functions typically depend on the Fourier representation of the independent variables (e.g., the spatial or temporal frequency). To evaluate the resulting numerical scheme in the time and space domain, a single value for these variables must be chosen, which means the schemes are only exact for the chosen Fourier component [2].

Recently, modified pseudospectral time domain (PSTD) schemes for solving time dependent PDEs in acoustics and electromagnetics have also been proposed [5, 7, 14, 15]. These schemes use the Fourier pseudospectral (or collocation) method to compute spatial derivatives, and a corrected finite difference scheme to integrate forwards in time. In contrast to nonstandard finite difference schemes, the correction to the finite difference time scheme is applied in the *spatial* frequency domain (often referred to as *k*-space) as part of the spectral calculation of spatial derivatives. The appropriate correction factor is derived by considering the Green's function solution for the governing PDE [3, 7], and eliminates the phase error introduced by the finite difference time step. For linear problems, these methods have the advantage of being exact for all spatial and temporal frequencies up to the Nyquist limit, and can be applied in any space dimension.

Here, the idea of nonstandard PSTD schemes is generalised to a broader class of hyperbolic and parabolic PDEs, and the derivation of these schemes from nonstandard finite difference methods is shown. The schemes are based on the Fourier pseudospectral method for discretising spatial gradients, and a nonstandard finite difference scheme for time integration. The modified denominator function for the nonstandard finite difference time scheme is transformed into the spatial frequency domain (or *k*-space) using the dispersion relation for the governing PDE. This allows the correction term to be applied in the spatial frequency domain as part of the spatial gradient calculation. The general formulation of the nonstandard PSTD schemes for constant coefficient PDEs is given in Section 2, with several examples given in Section 3. Application to the case of non-constant coefficient PDEs is discussed in Section 4. Discussion and summary are then provided in Section 5.

2 Formulation of nonstandard PSTD schemes for constant-coefficient PDEs

2.1 Problem formulation

We are interested in deriving exact explicit schemes for numerically solving inhomogeneous linear hyperbolic and parabolic PDEs in an unbounded domain, where the PDEs are in the form

$$\frac{\partial^a}{\partial t^a} u(\mathbf{x},t) = \mathrm{L} u(\mathbf{x},t) + S(\mathbf{x},t). \tag{2.1}$$