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# The spectral order of accuracy: A new unified tool in the design methodology of excitation-adaptive wave equation FDTD schemes

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ABSTRACT

We define a new concept, termed the spectral order of accuracy (SOoA), which is the spectral domain analogue of the familiar order of accuracy (OoA). The SOoA is pivotal in a refined version of a recently-introduced methodology for formulating excitation-adaptive wave equation FDTD (WE-FDTD) schemes, described below. This concept is the basis for a unified classification for both existing and new schemes. Both one- and two-dimensional cases are presented for boundless, source free, homogeneous, isotropic and lossless media. The 1-D and 2-D cases are developed in detail for the $(3,2M+1)$ (temporal, spatial) and $(3,3)$ 2-D stencils, respectively. Stability analysis is built into the methodology in terms of either analytical conditions or "stability maps" defined herein. The methodology is seen as a generalization of many existing schemes that also provides a unified tool for a systematical design of WE-FDTD schemes subject to specific requirements in terms of the spectral content of the excitation. The computational efficiency for all schemes remains the same for a given stencil, since the core of the FDTD code is unchanged between schemes, the difference being only in the values of scheme coefficients.



## 1. Introduction

An inherent error source in the finite difference time domain (FDTD) method [1,2] is the existence of numerical dispersion manifested by a numerical non-linear relationship $\tilde{k}(\omega)$. Remedies to dispersion errors were originally suggested in the form of dispersion relation preserving (DRP) schemes, introduced in [3] and continued in [4]. Other error reducing methods have included finer sampling rates, higher order schemes [5–13], and non-standard FDTD (NSFDTD) schemes [14–19]. Comparison between multiresolution and higher order for dispersion reduction schemes are presented in [20]. Minimization and optimization of predefined scheme properties (e.g. broadband dispersion error, anisotropy) methods have been developed, e.g. in [21–40].

A comprehensive methodology for the formulation of wave equation FDTD (WE-FDTD) schemes with controlled order of accuracy and dispersion has been recently introduced in [38–40]. The methodology is refined in this work by fusing both the order of accuracy (OoA) and numerical dispersion into the single concept of the spectral order of accuracy (SOoA). The SOoA is defined in the context of the general dispersion equation (GDE), i.e. the spectral transform of the discretized wave with undetermined coefficients [38,39]. In the process of reducing errors, one tries to fit the GDE to the linear dispersion surface, or, in the one-dimensional case, to the curve $K=\Omega/\gamma$, where $\Omega=\omega\Delta t$ and $K=\tilde{k}\Delta x$ and $\tilde{k}$ is the numerical wavenumber. Such a fit can be realized at the origin $(\Omega,K)=(0,0)$, in which case it is seen as an optimization of the OoA only. For a one-dimensional stencil with three temporal and $2M+1$ spatial samples (denoted herein as a $(3,2M+1)$ stencil), all schemes with OoAs

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ranging from $(2,2M)$ to $(2M,2M)$ are derived from a Taylor expansion of the GDE about the origin. However, the spectral domain representation makes it possible to fit the curves or surfaces at other frequency points to a certain order, denoted the SoOA. This general definition of the SOoA enables the optimization of the schemes about any range of finite frequencies $\Omega_q$. The conventional OoA can then be traded for higher accuracy in terms of the phase or group velocities or higher order derivatives $\left(\left(\frac{\partial^n \tilde{k}}{\partial \omega^n}\right)^{-1}\right)$ at $\Omega_q$. Note that the conventional OoA is directly related to the special case of the SOoA, defined about the origin of the dispersion surface. Using the SOoA, it becomes possible to design schemes tailored to a given excitation spectrum in order to reduce the overall error. Note also, that while the OoA determines the rate by which the difference equation converges to the PDE when $\Delta t \Rightarrow 0$ and $\Delta x, y \Rightarrow 0$, for a general $\Omega_q$ convergence is achieved (e.g. for the one-dimensional case) when $\Delta t \to \Delta t_q, \Delta x \to \Delta x_q \Rightarrow \Omega \to \Omega_q = \omega_q \Delta t_q, K \to K_q = \tilde{k}_q \Delta x_q$.

The process of fitting the GDE to the linear dispersion relationship begins with the selection of a set of frequencies in accordance with the spectral content of the exciting pulse and determination of the corresponding orders of accuracy by which the GDE converges to the linear curve about these frequencies. These choices are then translated into adjustments of certain coefficients within the scheme, as detailed in Section 2. The main FDTD code that follows this computation remains unchanged for all schemes pertaining to the given stencil.

Several cases are studied in Section 3. The methodology is applied to 1-D, source free homogeneous, isotropic, lossless and boundless wave equations, using stencils sizes of (3,3), (3,5) and (3,7) for explicit, central difference discretizations of the wave equation. The entire process is carried out while assuring numerical stability by the use of the general amplification polynomial (GAP).

An example of a wideband modulated pulse, propagated over a million time steps, with a (3,5) stencil is shown in Section 4, in comparison with the standard (4,4) scheme that uses the same stencil size and hence has the same computational complexity. The notable differences are in the group delay and distortions due to numerical dispersion. The two-dimensional case is initially developed in Section 5 with a suggestion for stencil classification and detailed development for the (3,3) stencil. This methodology can be seen as a generalization of available 1-D and 2-D schemes, that also provides a tool for devising new schemes tailored to the spectrum of the excitation. As seen in the examples, this process enables FDTD simulation over long periods of time with little dispersion error effects. The computational burden remains the same for all schemes because they only differ in the pre-calculations stage of the undetermined coefficients. Conclusions to this effect are drawn in Section 7.

## 2. Generation of one-dimensional schemes with specified spectral order of accuracy

### 2.1. Convergence rate of the wave equation in the spectral domain: the spectral order of accuracy (SOoA)

The equation to be discretized is the one-dimensional wave equation (WE) in a homogeneous, lossless, boundless and source free medium:

$$\left(\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2}\right) E(x,t) = 0. \tag{1}$$

The conventional usage of a (3,3) stencil with the three point approximation of the second order derivatives in time and space leads to the following approximation of (1):

$$E_i^{n+1} - 2E_i^n + E_i^{n-1} - \gamma^2 \left(E_{i+1}^n - 2E_i^n + E_{i-1}^n\right) = 0, \quad \gamma = c\Delta t/\Delta x. \tag{2}$$

Eq. (2) can be generalized for temporal–spatial $(3,2M+1)$ stencils with symmetrical "molecules", typical of central differences:

$$\underbrace{E_i^{n+1} + E_i^{n-1}}_{\text{molecule}} + \sum_{m=0}^{M} c_m \underbrace{\left(E_{i+m}^n + E_{i-m}^n\right)}_{\text{molecule}} = 0. \tag{3}$$

Here, the molecule coefficients $c_m$ serve as degrees of freedom for formulating many schemes. The number of these degrees of freedom is seen to be $M+1$ as determined by the stencil size. Upon invoking discrete separation of variables (or using the $\mathcal{Z}$-transform) in (3), i.e.

$$E_i^n = \xi^i(\Delta x)\tau^n(\Delta t) \tag{4}$$

and using the spectral representation $(\xi, \tau) = (e^{jK}, e^{j\,\Omega})$ where $\Omega = \omega\Delta t, K = \tilde{k}\Delta x$ ($\tilde{k}$ being the numerical wave number), the *generalized dispersion equation* (GDE) emerges

$$\cos\Omega + \sum_{m=0}^{M} c_m \cos mK = 0, \tag{5}$$

whose $\cos(\cdot)$ format is again typical of central differences. Eq. (5) is also the spatial–temporal spectral transform of (3). It is our objective to generate a scheme whose GDE curve (5) approximates the linear curve