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New optimized fourth-order compact finite difference schemes for wave propagation phenomena

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ABSTRACT

Two optimized fourth-order compact centered finite difference schemes are presented in this paper. By minimizing, over a range of the wave numbers domain, the variations of the phase speed with the wave number, an optimization least-squares problem is formulated. Hence, solving a linear algebraic system, obtained by incorporating the relations between the coefficients for the fourth-order three-parameter family schemes, the corresponding well-resolved wave number domains, and the related optimized coefficients, for two levels of accuracy, are analytically evaluated. Several dispersion comparisons, including the asymptotic behavior between the proposed and other existing optimized pentadiagonal fourth-order schemes, are presented and discussed. The schemes applicable directly on the interior nodes, are associated with a set of fourth-order boundary closure expressions. By adopting a fourth-order six-stage optimized Runge–Kutta algorithm for time marching, the stability bounds, the global errors, and the computational efficiency, for the fully discrete schemes, are examined. The performances of the presented schemes are tested on benchmark problems that involve both the one-dimensional linear convection and the one-dimensional nonlinear shallow water equations. Finally, the one-dimensional schemes are extended to two dimensions and, using the two dimensional shallow water equations, classical applications are presented. The results allow us to propose, as the ideal candidate for simulating wave propagation problems, the scheme which corresponds to the strict level of accuracy with the maximum resolution over a narrow wave number space.

1. Introduction

For providing accurate solutions for wave propagation phenomenon in several fields, including acoustic, electromagnetic, and water waves, high-order compact or implicit finite difference (FD) spatial schemes, coupled with optimized time advancement Runge–Kutta (RK) algorithm, are widely used. Many of these schemes are analyzed and compared, among others, in [7,9,18,27,32,52].

In compact FD schemes, for its implicit nature, the derivatives are unknowns at several mesh points instead of at one point such as in the traditional explicit schemes. Therefore, for their computation, a solution of a linear system of equations is required. However, these systems can be stored in a banded matrix, normally tridiagonal or pentadiagonal, which can be efficiently solved. Again, compact FD schemes for the same stencil width are more accurate than the explicit schemes. Otherwise compact schemes use smaller stencil than the corresponding explicit schemes of the same order. Therefore, *implicitness* and *compactness* are the two essential features that make the general compact schemes more advantageous.

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Historically, these methods have their origin in the first years of the last century (see [14] for references). Later on, their interest was renewed with Hirsh [17], and Adam [1] who, following an idea of Kreiss and Oliger [26], developed and applied a fourth-order tridiagonal scheme. But, compact schemes have become popular only in the last two decades, thanks to the elucidated paper of Lele [30]. For instance, we recall that compact FD methods are also called by different names (i.e., Operator Compact Implicit, Padé, Hermitian or *Mehrstellen*) by different authors, as listed in [16,38].

Starting from Lele's paper, compact centered, i.e. nondissipative, FD schemes are considered in the present work. From these, we confine the attention to the fourth-order three-parameter optimized pentadiagonal formulations. For compact upwind schemes, the reader is directed to the papers of Sengupta et al. [42], and of De and Eswaran [8]. Lele examined and compared in terms of resolution, i.e. accuracy in Fourier space, a variety ranging from second- to tenth-order compact centered schemes. So, from the fourth-order pentadiagonal three-parameter family, on the seven-point stencil, fitting at three high wave numbers, for which 'no attempt was made to optimize the choice,' the modified wave number corresponding to the exact wave number, Lele [30] obtains an optimized, so called 'spectral-like' resolution, scheme. This scheme, from comparisons carried out by Lele, provided a better resolution than the tenth-order scheme having the same support.

In order to improve the spatial resolution characteristics, a few years after Lele's paper, a variety of fourth-order pentadiagonal optimized schemes have been proposed. Combining the Dispersion–Relation–Preserving (DRP) idea of Tam and Webb [44] with compact centered formulations, a class ranging from second- to eighth-order optimized schemes has been obtained by Kim and Lee [23]. In order to make the integrand error, defined following the DRP method by the differences between the modified and the exact wave numbers, analytically integrable, an appropriate weighting function is introduced in [23]. Moreover, in order to emphasize the high wave numbers, a revised form of its weighting function is adopted by the authors. A better resolution than Lele's spectral-like scheme, is presented by optimized second- to sixth-order pentadiagonal schemes. The fourth-order pentadiagonal optimized Kim and Lee's scheme, considered in the following, is denoted here KL4.

Using the spectral method approach (see [10] for details), good wave resolution, especially for the high wave numbers, is obtained with the second-order tridiagonal and the fourth-order pentadiagonal schemes proposed by Lee and Seo [29], and called by the authors CSS-2, and -4, respectively. On the basis of the measure of the integral errors between the modified and the exact wave numbers, over the whole wave numbers spectrum, CSS-4 scheme shows a greater wave resolution capability than the KL4 scheme. However, it is well known (e.g. [10] §2.4), that in the spectral methods, the good resolution in the high wave number region, is accomplished, by an appreciable overshoot, i.e. the largest deviation from the exact differentiation in the optimization range. Then, the so-called Gibb's phenomenon in the numerical solution, can be produced (see [41] §11.16).

Following Lele's strategy, other choices, however arbitrary of the three wave numbers where the modified wave number is forced equal to the exact value, are proposed by Tyler [48]. Unfortunately, the corresponding schemes are not adequately discussed in order to understanding the different choices of the wave numbers.

Compared with Lele's 'spectral-like' scheme, high resolution is shown by the optimized fourth-order Kim's [22] scheme. This scheme presents good spectral performance also with respect to KL4 scheme that is obtained using a five times more generous tolerance. However, in the integrand error, formulated, as in DRP method, three adjustable parameters are introduced by the author. Therefore, in order to find the set of optimized coefficients, a trial and error procedure is required.

Lastly, in the paper of Liu et al. [34] the sequential quadratic programming method is employed to find the minimum of the integrand error, formulated again as in DRP approach. A fourth-order pentadiagonal optimized scheme, referred to as high accuracy and maximum resolution (HAMR) by the authors, is obtained. Compared to Kim's scheme, HAMR scheme presents less dispersive behavior in the well-resolved wave numbers domain, that ranges from 0 to about 0.8π, but is more dispersive for the high wave numbers, up to the Nyquist limit, where it fails as do as all other centered schemes.

At this point, accordingly to [29], the following question is raised: 'Is it better for a scheme to have the modified wavenumber approximating exact wavenumber over a *wide* region of wavenumbers within a relatively *large* error bound than it is to have a good approximation in a *narrow* region with a *small* error?' In order to avoid a response to the above crucial issue for wave propagation phenomena, the aim of the present work is to propose two FD compact fourth-order pentadiagonal schemes, one with small and the other with less restrictive tolerance errors, to obtain the maximum resolution over a narrow, and a wide wave numbers domain, respectively.

Since in the exact solution of the original wave equation, all waves travel with the same constant phase speed, which is identical to the group speed, while in the discrete solution the phase speed, different from the group speed, is wave number dependent, an optimization procedure is achieved by minimizing the variations of the phase speed with respect to the wave number. This approach, for the connection between the group speed with the phase speed, is very attractive, since also the group speed is controlled. Thus, incorporating the relations between the coefficients for the fourth-order three-parameter family schemes into a least-squares problem, a system of linear algebraic equations is obtained. In order to solve this system analytically, an appropriate weighting function in the integrand error is introduced. Hence, the optimization domain, and the complete set of the optimized coefficients are determined for two very different levels of accuracy.

So as, to faithfully represent the physics of the wave propagation problems, a clear understanding of the dispersion errors associated with the semi-discretization numerical schemes, is necessary. Therefore, several comparisons, over the entire range of wave numbers, i.e. accuracy-in-the-large [51], are presented between the schemes presented in this paper and those currently known by the author. In addition, the phase and the group speed, obtained from Fourier analysis, are used to investigate the asymptotic behavior, or rate of convergence, as the particle spacing goes to zero, i.e. accuracy-in-the-small [51].