Computers and Fluids 138 (2016) 9–25

Contents lists available at ScienceDirect

Computers and Fluids

journal homepage: www.elsevier.com/locate/compfluid

Improving the boundary efficiency of a compact finite difference scheme through optimising its composite template

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ARTICLE INFO

Article history:
Received 19 December 2015
Revised 20 May 2016
Accepted 12 August 2016
Available online 13 August 2016

Keywords:
Compact finite difference
Boundary closure
Optimization
Genetic algorithm
Composite template

ABSTRACT

This paper presents efforts to improve the boundary efficiency and accuracy of a compact finite difference scheme, based on its composite template. Unlike precursory attempts the current methodology is unique in its quantification of dispersion and dissipation errors, which are only evaluated after the matrix system of equations has been rearranged for the derivative. This results in a more accurate prediction of the boundary performance, since the analysis is directly based on how the derivative is represented in simulations. A genetic algorithm acts as a comprehensive method for the optimisation of the boundary coefficients, incorporating an eigenvalue constraint for the linear stability of the matrix system of equations. The performance of the optimised composite template is tested on one-dimensional linear wave convection and two-dimensional inviscid vortex convection problems, with uniform and curvilinear grids. In all cases, it yields substantial accuracy and efficiency improvements while maintaining stable solutions and fourth-order accuracy.

1. Introduction

Compact finite differences are numerical schemes used to accurately calculate derivatives. They are implicit in nature, based upon a banded Hermitian matrix system of equations. Although inverting such a system requires a higher computational cost, they can offer vastly superior resolution for a given stencil size compared to their explicit counterparts. This quality has made them increasingly popular in the fields of computational aeroacoustics (CAA) [1,2], large eddy simulation (LES) [3–5], and direct numerical simulation (DNS) [6–8], particularly when high resolution is a necessity in order to properly resolve the relevant physical scales.

Typically, central differences are used to construct compact schemes for use at interior nodes. However, such schemes are not always applicable at domain boundaries, and therefore in order to properly close the matrix system of equations non-central differences are often a necessity. This unfortunately will have a detrimental effect on accuracy; introducing additional dissipation as well as dispersion, if the boundary schemes are not sufficiently optimised. Consequently, to ensure that the same level of accuracy is achieved throughout the entire domain, grid refinements are regularly made to the boundary regions. This will inevitably reduce computational efficiency due to the decreased time step required by the smaller grid cells. The objective of this paper is to build upon past attempts to maximise boundary scheme performance, and thereby minimise efficiency losses, while also ensuring the combination of interior and boundary schemes meets requirements for linear stability.

As well as changes in formal order of accuracy, enhancements to compact schemes can also be achieved through coefficient optimisation based on resolution characteristics. A previous attempt at this was undertaken by Kim [1]. Kim introduced a highly optimised fourth-order pentadiagonal compact scheme and set of boundary closures particularly for CAA applications. Optimisations were based on an integral error measure between the exact and modified wavenumber solutions (similar to Kim and Lee [9]). Very low resolution errors were obtained with this method, in particular for the interior scheme, which remains below 0.1% over the grid spaced scaled wavenumber range $0 \le \omega \le 0.839\pi$. The boundary schemes were designed to maintain the same stencil size and order of accuracy as the interior schemes, which was accomplished by employing extrapolation functions based on both polynomial and trigonometric series for solutions outside of the domain. After some algebraic manipulation, these were then converted into a set of non-central differences for use at the domain boundaries. The resultant boundary schemes were optimised by means of control variables left open in the trigonometric series of each extrapolation function. As in Carpenter et al. [10] the linear stability of

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http://dx.doi.org/10.1016/j.compfluid.2016.08.007

the matrix system was investigated using eigenvalue analysis. Kim [1] found that with a coarse grid the schemes contained some slightly positive eigenvalue components. Although, after some grid refinement it was demonstrated that these will tend towards zero, hence implying neutral stability.

Liu et al. [11] expanded on the optimisation strategy of Kim [1] by introducing a sequential quadratic programming technique (SQP). This iteratively increased the upper limit of the optimisation range (r), establishing optimal values for both interior and boundary schemes. Furthermore, they showed that scheme stability is heavily dependent on the chosen error tolerances, as well as the formal order of accuracy, implying that the optimisation process can often be detrimental to the numerical stability. To compensate for this, Liu et al. [11] reduced the order of accuracy of their first and third boundary schemes by one stage. Such stability issues were also recognised by Carpenter et al. [10], who suggested that a scheme's numerical stability and its spectral resolution do not always coincide.

Jordan [12] introduced an alternative approach for analysing spectral resolution properties through composite templates. Unlike the more traditional decoupled Fourier approach where the resolution of each differencing stencil is studied separately, this consists of Fourier analysis of the whole matrix system of equations, consisting of both the interior and boundary stencils. The result is a set of pseudo-wavenumber curves for each point in the grid, dependent on the number of grid points used in the analysis. Jordan applied this analysis to tridiagonal systems, employing a least squares optimisation strategy to minimise the total resolution error across the whole template. In a later paper Jordan [13] applied the same technique to pentadiagonal systems producing a set of boundary closure schemes to be used alongside the interior scheme of Kim [1]. Although the modified wavenumber curves produced by this technique are dependent on the number of grid points used in the analysis, they appear to be much more representative of the performance we achieve once schemes are applied to actual simulations. Despite this, it is still unclear how to best optimise the resolution properties of a given composite template, making it far from a trivial task. For instance one could prioritise minimising the relative resolution error between neighbouring points in the composite template, or perhaps the aggregate resolution error of the whole template with respect to the exact wavenumber.

This paper aims to extend the composite template strategy of Jordan [12] by redefining how the composite template modified wavenumber is evaluated. Unlike the original approach, Fourier analysis will not be conducted until the matrix system of equations has already been rearranged for the derivative. This should lead to better predictions of the resolution properties attained in simulations because this is a closer depiction of how the derivative is represented numerically. The chosen optimisation method is a Genetic Algorithm (GA) containing both an objective function for the composite template's resolution characteristics, and a nonlinear constraint for eigenvalue stability. In this paper, the optimisation procedure is applied to the pentadiagonal finite-difference system outlined by Kim [1], although a similar approach would be applicable to other systems if desired. The newly optimised boundary closure coefficients are successful in producing large accuracy improvements while maintaining stable solutions in all test problems. In addition to the primary optimisation which focuses on the aggregate resolution error of the composite template, further accuracy enhancements are attempted by introducing pseudo-boundary schemes. Essentially these are tuned central schemes applied as intermediate steps between the boundary and interior regions, with the aim of reducing the relative resolution error between consecutive points. They are successful in achieving further accuracy improvements, albeit with some penalty to numerical stability.

The paper is organised as follows. Section 2 introduces the compact finite-difference system, and outlines the new composite template modified wavenumber analysis. Section 3 provides details of the boundary closure scheme coefficient optimisation procedure. This includes the optimisation platform, objective function and stability constraints. Section 4 presents the optimisation results, including the resultant wavenumber characteristics and eigenvalue distribution. In Section 5 the performance of the newly optimised finite-difference system is tested in three benchmark problems, designed to analyse their performance in a variety of scenarios. In Section 6 pseudo-boundary schemes are introduced and their performance analysed. Finally concluding remarks are given in Section 7.

2. Compact finite difference schemes and composite template modified wavenumber analysis

We consider the following general compact finite difference template, based on a pentadiagonal Hermitian matrix. It is constructed from one central interior and three non-central boundary closure schemes, each in conservative form and utilising a seven-point stencil [1].

$$\mathbf{P}\bar{\mathbf{f}}' = \frac{1}{h}\mathbf{Q}\mathbf{f} \tag{1}$$

where $\mathbf{P}$ and $\mathbf{Q}$ are the following $(N+1)\times(N+1)$ matrices

$$\boldsymbol{P} = \begin{pmatrix} 1 & \gamma_{01} & \gamma_{02} & 0 & \cdots & 0 & 0 & 0 & 0 \\ \gamma_{10} & 1 & \gamma_{12} & \gamma_{13} & 0 & \cdots & 0 & 0 & 0 \\ \gamma_{20} & \gamma_{21} & 1 & \gamma_{23} & \gamma_{24} & 0 & \cdots & 0 & 0 \\ 0 & \beta & \alpha & 1 & \alpha & \beta & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \beta & \alpha & 1 & \alpha & \beta & 0 \\ 0 & 0 & \cdots & 0 & \gamma_{24} & \gamma_{23} & 1 & \gamma_{21} & \gamma_{20} \\ 0 & 0 & 0 & \cdots & 0 & \gamma_{13} & \gamma_{12} & 1 & \gamma_{10} \\ 0 & 0 & 0 & 0 & \cdots & 0 & \gamma_{02} & \gamma_{01} & 1 \end{pmatrix}$$

$$\mathbf{Q} = \begin{pmatrix} b_{00} & b_{01} & b_{02} & b_{03} & b_{04} & b_{05} & b_{06} & 0 & 0 & \cdots & 0 \\ b_{10} & b_{11} & b_{12} & b_{13} & b_{14} & b_{15} & b_{16} & 0 & 0 & \cdots & 0 \\ b_{20} & b_{21} & b_{22} & b_{23} & b_{24} & b_{25} & b_{26} & 0 & 0 & \cdots & 0 \\ -a_3 & -a_2 & -a_1 & 0 & a_1 & a_2 & a_3 & 0 & 0 & \cdots & 0 \\ 0 & -a_3 & -a_2 & -a_1 & 0 & a_1 & a_2 & a_3 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -a_3 & -a_2 & -a_1 & 0 & a_1 & a_2 & a_3 & 0 \\ 0 & \cdots & 0 & 0 & -a_3 & -a_2 & -a_1 & 0 & a_1 & a_2 & a_3 \\ 0 & \cdots & 0 & 0 & -b_{26} & -b_{25} & -b_{24} & -b_{23} & -b_{22} & -b_{21} & -b_{20} \\ 0 & \cdots & 0 & 0 & -b_{16} & -b_{15} & -b_{14} & -b_{13} & -b_{12} & -b_{11} & -b_{10} \\ 0 & \cdots & 0 & 0 & -b_{06} & -b_{05} & -b_{04} & -b_{03} & -b_{02} & -b_{01} & -b_{00} \end{pmatrix}$$

and

$$\bar{\mathbf{f}}' = (\bar{f}'_0, \bar{f}'_1, \bar{f}'_2, \ldots, \bar{f}'_N)^T, \quad \mathbf{f} = (f_0, f_1, f_2, \ldots, f_N)^T$$

where $\bar{f}'_i$ is a finite difference approximation to the exact spatial derivative f'_i at a nodal point i and $b_{ii} = -\sum_{j=0,\neq i}^{6} b_{ij}$. The three boundary closure schemes are applied at the $i = \{0, N\}$, $\{1, N-1\}$ and $\{2, N-2\}$ nodes. They comprise of 27 unique coefficients:

$$\begin{aligned} &\gamma_{ij} \quad \text{for} \quad i \quad = \quad \{0,1,2\} \quad j = \{0, \ldots, i+2\}, \neq i \\ &b_{ij} \quad \text{for} \quad i \quad = \quad \{0,1,2\} \quad j = \{0, \cdots, 6\}, \neq i. \end{aligned} \tag{2}$$

The central interior scheme consists of five coefficients (α, β, a_1, $a2$, $a3$), and is applied throughout the remainder of the domain ($3 \le i \le N-3$). The template we will consider in the current paper is fourth-order accurate in the interior and at the boundaries. For the interior nodes we implement the optimised fourth-order coefficients suggested by Kim [1]. (Full details of the interior scheme performance, including its modified wavenumber characteristics can be found in [1].)