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Efficient parallel computing with a compact finite difference scheme

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ABSTRACT

This paper proposes an efficient parallel computing approach based on a high-order accurate compact finite difference scheme in conjunction with a conventional domain decomposition method and MPI libraries. The proposed parallel computing approach consists of two major features: (a) a newly developed compact finite difference scheme with extended stencils containing halo points around subdomain boundaries, and (b) a predictor–corrector type implementation of a compact filter that effectively suppresses spurious errors from the subdomain boundaries. The current work employs three halo cells for the inter-node communication, based on which the coefficients of the new compact scheme at the subdomain boundaries are optimized to achieve as high level of resolution and accuracy as the interior compact scheme provides. Also, an optimal set of cut-off wavenumbers of the compact filter that minimizes spurious errors is suggested. It is shown that the level of errors from the proposed parallel calculations lies within the same order of magnitude of that from the single-domain serial calculations. The overall accuracy and linear stability of the new parallel compact differencing-filtering system are confirmed by grid convergence tests and eigenvalue analyses. The proposed approach shows a substantial improvement with respect to existing methods available.

1. Introduction

Over the last decade, compact finite difference schemes have become widespread in direct numerical simulation (DNS), large eddy simulation (LES) and computational aeroacoustics (CAA) because they provide both high-order accuracy and high-resolution characteristics via optimization of the coefficients [1–5]. Currently, almost every research activity in the area of CAA/LES/DNS makes extensive use of parallel computing techniques owing to the rapid growth of modern supercomputing capabilities. However, the use of the compact finite difference schemes in a parallel computing environment is not straightforward, particularly when domain decomposition with MPI (message passing interface) libraries is concerned. This is mainly due to their implicit nature associated with the solution of banded Hermitian matrix systems. Common approaches for parallelizing such systems include: reduced parallel diagonal dominant algorithm [6]; alternating-direction line-relaxation method [7]; pipelined implementation of Thomas algorithm [8]; and using a large area of overlap between two neighboring subdomains [9]. These approaches, currently available for tridiagonal matrix systems, are significantly more expensive in terms of inter-node communication than parallelizing standard finite difference schemes, which undermines the genuine advantage of using compact schemes.

Recently, Sengupta et al. [9], after reviewing the current state-of-the-art of parallel computing strategies for compact schemes, suggested that the implementation of compact schemes in an overlapped fashion with inclusion of filters might be used as an efficient alternative to earlier more computationally expensive parallelization strategies. They developed a new tridiagonal compact scheme for this purpose incorporating six-point overlap between two adjacent subdomains. However, their benchmark tests on vortex convection showed a controversial behavior of their scheme resulting in higher error on a finer grid [9]. Also, some of the unaddressed issues in their approach include: whether the parallelized system achieves the desired grid convergence rate, and how much improvement could be made with different filters or cut-off wavenumbers. These are important questions that need to be answered. This paper takes all these issues into account and aims to deliver a more reliable and efficient strategy of parallelizing compact schemes based on a halo-cell approach instead of the overlapping method that demands more operations and memory.

In the current work the main platform is based on a pentadiagonal compact scheme contrary to the other above mentioned works that are currently limited to tridiagonal schemes. The new platform employs one of the latest pentadiagonal compact schemes with fourth-order accuracy proposed by Kim [5] and extends his boundary formulations to accommodate wider stencils that contain three halo cells from the adjacent subdomains.

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Although the new compact scheme across the subdomain boundaries does not precisely reproduce the interior resolution, the loss of accuracy can be minimized. The new platform also includes a pentadiagonal compact filter with sixth-order accuracy [10] to remove spurious errors, and introduces a predictor–corrector type of execution in order to achieve almost identical error levels to those from single-domain serial calculations. The compact filter has a variable cut-off wavenumber that may change locally across the subdomain boundaries, and this helps improve the filter performance. Eigenvalue analyses and grid convergence tests confirm that the entire differencing-filtering system provides linear stability and fourth-order accuracy throughout the domain. The proposed parallel computing approach is rigorously tested through a variety of one-, two- and three-dimensional test cases using fully nonlinear compressible Euler and Navier–Stokes equations in both Cartesian and generalized coordinates.

The paper is organized as follows. Section 2 shows the development of the new compact finite difference scheme with halo points. Section 3 describes the implementation of a compact filter based on predictor–corrector steps. Section 4 performs grid convergence tests and linear stability analysis of the proposed compact differencing-filtering system. Section 5 briefly introduces the governing equations solved for the numerical tests. The results of Euler and direct numerical simulations are presented and discussed in Sections 6 and 7. Performance and efficiency of the proposed parallel computing approach is demonstrated in Section 8. Finally concluding remarks are made in Section 9.

2. New compact finite difference scheme with halo points

This section presents a new compact finite difference scheme developed for parallel computing based on domain decomposition and MPI (message passing interface) libraries. It consists of a central interior scheme and non-central boundary schemes that involve three halo cells from the adjacent subdomain. Fourth-order accuracy is maintained throughout the domain. The new boundary schemes are specifically designed to construct a closed pentadiagonal matrix system within each subdomain. They are optimized to achieve similar resolution characteristics to those of the interior scheme.

2.1. Interior compact finite difference scheme

The present work employs a fourth-order central compact scheme [5] for interior points, which is based on a pentadiagonal platform and a seven-point stencil. It may be expressed as

$$\beta\bar{f}'_{i-2}+\alpha\bar{f}'_{i-1}+\bar{f}'_i+\alpha\bar{f}'_{i+1}+\beta\bar{f}'_{i+2} = \frac{1}{\Delta x}\sum_{m=1}^{3}a_m(f_{i+m}-f_{i-m}) \quad \text{for } 2\leqslant i\leqslant N-2 \tag{2.1}$$

where f_i and f'_i represent an objective function $f(x)$ and its spatial derivative $\partial f(x)/\partial x$ respectively at a location of interest x_i. The bar "–" is used in order to distinguish numerical derivative ($\bar{f}'$) from the exact derivative (f'). The spatial interval $\Delta x = x_{i+1} - x_i$ is a constant independent of the index i in the computational domain where all the grid points are equally spaced. The coefficients α, β, a_1, a_2 and a_3 optimized in [5] are listed in Table 1. The index runs through $0\leqslant i\leqslant N$ within a subdomain, where $i=0$ and $i=N$ represent the subdomain boundaries. Accordingly, $i\leqslant -1$ or $i\geqslant N+1$ indicate halo points from the adjacent subdomains. Eq. (2.1) being used at $i=2$ or $i=N-2$ involves one of the halo points (f_{-1} or f_{N+1}) on the right-hand-side.

With Eq. (2.1) used for the interior points ($i\geqslant 2$), two additional schemes are required for the boundary points ($i=0$ and 1) in order to close the pentadiagonal matrix and enable independent inversion of the matrix in each subdomain. This approach demands less inter-node communication than the earlier approaches mentioned in Section 1. The formulation of the two additional schemes obtained by using an extrapolation technique and optimization procedure is described in the following.

2.2. Formulation of boundary schemes with halo points

It is obvious that Eq. (2.1) applies directly on the interior points. To be able to keep applying it at the boundary points ($i=0$ and 1), an extrapolation may be used to approximate the unknown derivatives $f'(x)$ in the halo area and substitute them with interior (or known) terms. The following is a spline function from the boundary ($x=x_0$) and its first derivative that may be used for the extrapolation [5]:

$$g(x^*)=\sum_{m=0}^{N_A}p_m x^{*m}+\sum_{m=1}^{N_B}[q_m\cos(\phi_m x^*)+r_m\sin(\phi_m x^*)] \tag{2.2}$$

$$g'(x^*)=\frac{dg(x^*)}{dx} =\frac{1}{\Delta x}\left\{\sum_{m=1}^{N_A}mp_m x^{*m-1}-\sum_{m=1}^{N_B}\phi_m[q_m\sin(\phi_m x^*)-r_m\cos(\phi_m x^*)]\right\} \tag{2.3}$$

where $x^*=(x-x_0)/\Delta x$ is the non-dimensional coordinate from the boundary. The extrapolation function is a linear combination of polynomials and trigonometric series. The constants N_A and N_B represent the orders of each series. In this paper, $N_A=4$ is selected to maintain the fourth-order accuracy and $N_B=3$ to match the number of coefficients and available constraints. The coefficients p_m ($m=0,\ldots,N_A$), q_m and r_m ($m=1,\ldots,N_B$) should be determined by matching constraints as described below. The control variables ϕ_m ($m=1,\ldots,N_B$) are introduced to optimize the resulting schemes for the best resolution characteristics.

Eleven matching constraints are necessary since the number of coefficients to be determined is $1+N_A+2N_B=11$, and they are as follows:

$$g(m)=f_m \quad \text{for} \quad m=-3,-2,-1(\text{halo points}) \text{ and } 0,\ldots,4, \tag{2.4}$$

$$g'(m)=\bar{f}'_m \quad \text{for } m=0,1,2. \tag{2.5}$$

Solving Eqs. (2.4) and (2.5) leads to the coefficients p_m ($m=0,\ldots,4$), q_m and r_m ($m=1,2,3$) being replaced by linear combinations of the known function values ($f_{-3},\ldots,f_4$) and the interior derivatives ($\bar{f}'_0,\bar{f}'_1,\bar{f}'_2$). However, the final coefficients are yet to be determined once the control variables ϕ_1, ϕ_2 and ϕ_3 have been fixed, which is shown later. Once all the coefficients are determined,

Table 1
Coefficients for Eq. (2.1).

α	β	a_1	a_2	a_3
0.5862704032801503	0.9549533555017055e−1	0.6431406736919156	0.2586011023495066	0.7140953479797375e−2