An Improved Parallel Compact Scheme for Domain-Decoupled Simulation of Turbulence

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Abstract: An improved interface-coupling compact scheme for first and second spatial derivatives is proposed for domain-decomposition-based parallel computational fluid dynamics. The method improves the accuracy of previously developed decoupled schemes and preserves the accuracy and bandwidth properties of fully-coupled compact schemes, even for a very large degree of parallelism, and enables the Navier-Stokes equations to be solved independently on each processor. The scheme is analysed using Fourier analysis and error analysis, and tested on one-dimensional wave-packet propagation, a two-dimensional vortex convection problem, and in the direct numerical simulation of the 3-D Taylor-Green vortex problem and turbulent channel flow. Our results demonstrate the scheme's effectiveness in performing direct numerical simulation of turbulence in terms of accuracy and scalability.

Keywords: High-order compact scheme; Finite difference method; Domain-decomposition; Large-scale parallel computation; Direct numerical simulation

1 Introduction

Compact or Padé-type schemes have been developed and studied for over 6 decades. In 1955, Kopal [1] presented a successive extrapolation method to solve differential equations, in which the conception of compact schemes was adopted to approximate first and second derivatives. Kopal mentioned that it represented the most accurate recursion formula employing three successive ordinates. In the 1970s, compact schemes for the finite difference method were further developed by Kreiss and Oliger [2,3], Adam [4,5] and Hirsh [6], among whom Hirsh [6] may be the first person to use a compact scheme for computational fluid dynamics (CFD) problems. They all have proved compact schemes are

efficient and accurate in solving ordinary differential and partial differential equations. Lele [7] then presented a detailed analysis of compact schemes upto fourth derivatives, including their boundary closures. The small stencil and spectral-like resolution of compact schemes are highly desirable in CFD methods with structured meshes [8], especially for direct numerical [9,10,11,12]/large-eddy simulation [13,14] (DNS/LES) of turbulence and computational aeroacoustics (CAA) [15,16,17,18], in which small-scale flow structures need to be resolved. Compact schemes have advantages regarding high accuracy, small truncation error, low dissipation, and a compact stencil. The penalty is the implicit nature of compact schemes, which means the solution of a linear narrow-banded system (e.g. a tridiagonal or pentadiagonal linear system) of equations for unknown derivative values is required. In a serial environment, a version of Gaussian elimination known as the Thomas algorithm can be used to solve a linear system having N unknowns with $O(N)$ operations, but difficulties arise in a domain-decomposition-based parallel environment. In both forward and backward sweeps of the Thomas algorithm, the solution is recursive, and a local node depends on solutions from its neighbouring nodes.

Significant effort has been devoted to the parallelisation of compact schemes. In general, there are two categories of methods for dealing with a parallel compact scheme. The first group focuses on the method of solving a linear system in parallel, using either pipeline methods [19,20], alternating direction methods [21], parallel diagonal dominant algorithms [22,23], or line-relaxation methods [24]. The second group essentially decouples compact schemes to enable them to be solved independently on each processor. Consequently, the computational field can be partitioned with classic domain decomposition methods [25] and each subdomain is solved independently on a processor, in common with most CFD solvers using explicit schemes. The term, decoupled, here means the operation of numerical differentiation inside a subdomain or processor is independent of other parts of the domain at a particular computational step. Physically, all parts of the domain are still coupled dependent on the problem being solved. The decoupled approach has shown superior parallel performance as demonstrated by Sengupta *et al.* [26], Chao *et al.* [27], Kim and Sandberg [28], and Kim [29]. The decoupling methods inevitably introduce interdomain interfaces, on which a boundary method is required to close the compact scheme inside of each subdomain. From this point of view, the decoupled scheme is similar to the concept of hybrid methods, where different schemes are applied in different regions of the domain, such as hybrid compact-WENO schemes [27, 30, 31] and hybrid compact-TVD schemes [32]. The interdomain interface problem is also involved in multi-block solvers, in which the focus is mainly on the stability and conservation properties of the interface treatment methods [33, 34, 35, 36]. Carpenter *et al.* [33] derived stable and conservative interface

conditions for high-order schemes for the scalar advection-diffusion equation on multiple domains. Nordström *et al.* [34, 35] further developed the method for the Navier-Stokes equations. Gao [37] proposed an interface flux-reconstruction method based on a Riemann solver, where a 4th-order decoupled compact scheme is used for a multi-block solver.

Different boundary methods for interdomain interfaces have been developed. A straightforward way is to use an explicit scheme at an interface to provide a boundary value to two adjacent subdomains. Chao *et al.* [27] first introduced the idea in developing a 5th-order hybrid compact-WENO scheme. For the convective fluxes, an explicit 5th-order upwind scheme was used at the interface to decouple a 5th-order compact upwind scheme, hybridising with a WENO scheme to capture shock-waves. For the computation of the diffusive fluxes, a 6th-order explicit central scheme was used at the block interface to decouple the 6th-order compact central scheme. Their decoupling method has shown good stability and scalability [27]. The same strategy was also adopted by Fico *et al.* [32]. Chao's method has a clear advantage that two adjacent subdomains are assigned the same interface value and no extra data exchange is needed, which helps to ensure good parallel efficiency. The drawback is that the benefits of the compact scheme, in terms of accuracy and error, might be lost at an interface. As noted by Chao *et al.* [27], the global resolution property is affected by the degree of parallelism.

Sengupta *et al.* [26] proposed a different approach for interdomain interfaces. They adopted biased boundary schemes and large node-overlapping to close and decouple the compact scheme in each subdomain. High-frequency spurious wave packets were observed due to the asymmetry of the biased boundary scheme propagating downstream. It was proposed that spurious wave packets could be removed by larger overlapping, or applying a compact low-pass filter, and the scheme was successfully applied in DNS of compressible flows.

Kim [38] proposed an optimised boundary compact scheme, in which a particular spline function was devised to extrapolate the objective function and its first derivative beyond boundaries. Kim and Sandberg [28] then developed the idea to decouple the compact scheme for parallel computations. They extended Kim's boundary formulation to halo nodes from the adjacent subdomains and the approximation of the derivatives at nodes close to the interface are then obtained to close the pentadiagonal matrix system within each subdomain. Furthermore, Kim and Sandberg [28] proposed a decoupled 6th-order compact filter with a prediction-correction procedure. They proved the developed compact scheme and compact filter provide linear stability and 4th-order accuracy throughout the domain. However, the scheme of Kim and Sandberg [28] presents non-uniformity in resolution characteristics across subdomain interfaces, and numerical dissipation arises accordingly.

This drawback was then largely reduced by Kim [29] by implementing a linear-algebraic transformation technique to obtain quasi-disjoint pentadiagonal matrix systems. Kim's scheme was then successfully applied in simulations of acoustics problems [39, 40, 41].

Keller and Kloker [42, 43] adopted an 8th-order explicit scheme on halo nodes to decouple the 6th-order compact scheme, and it is shown that the decoupled compact scheme has good robustness and accuracy. A linear speedup has been shown up to 4800 cores, and the computing time was less than the fully explicit scheme due to cache effects. They also discussed the effect of the number of ghost nodes, and eventually adopted one level of ghost nodes in DNS of boundary layer flows [44,45,46]. Recently, a similar approach was adopted by Capuano et al. [47] in developing a parallel compact finite-volume scheme, who used a 4th-order explicit scheme and cell overlapping to decouple the compact scheme. Conservation is enforced by another application of the compact formula around interdomain interfaces. Their result has shown the conservation property of the finite-volume method is retained, and the accuracy is also well preserved within an acceptable tolerance.

Inspired by Sengupta *et al.* [26], Chao *et al.* [27], Kim [28], Keller and Kloker [42,43], and Capuano et al. [47], this paper presents a modified class of decoupled finite difference compact schemes for both 1st- and 2nd-derivatives aiming to improve the accuracy of the decoupled compact scheme. An explicit scheme, with the same order of accuracy as the corresponding compact scheme, is employed on the halo nodes to close the tridiagonal system within each subdomain, and a correction step is then introduced to further improve the accuracy of the scheme. The analysis and tests demonstrate that the proposed scheme has bandwidth properties and truncation errors close to the fully coupled scheme. Scalability is ensured because the scheme is decoupled at the interface of each subdomain. The scheme is assessed for the one-dimensional (1-D) linear equation for the wave-packet propagation problem and the two-dimensional (2-D) Euler equations for the vortex convection problem. It is then used to solve the three-dimensional (3-D) Navier-Stokes equations for DNS of the Taylor-Green Vortex problem and turbulent channel flow demonstrating its effectiveness in DNS of turbulent flows as well as its good scalability.

2 Development of a domain-decoupled compact scheme

In this section, the principle of the proposed decoupled compact (DCOM) scheme for both 1st- and 2nd-derivatives is introduced in a general form, and the formulas of 6th-order DCOM central schemes are also given in detail.

2.1 First-derivative

For a general continuously differentiable function, ϕ , discretised on a uniform 1-D mesh

$x_i = i\Delta, i = 0, 1, \dots, N$, in which Δ is the distance between two consecutive mesh nodes. The derivative, ϕ' , at the i -th mesh node (internal node) is approximated using the following general compact central scheme,

$$\alpha \tilde{\phi}'_{i-1} + \tilde{\phi}'_i + \alpha \tilde{\phi}'_{i+1} = \frac{1}{\Delta} \sum_{m=1}^S a_m (\phi_{i+m} - \phi_{i-m}), \quad (1)$$

where $\tilde{\phi}'_i$ is the approximation of ϕ' at x_i , and α and a_m are coefficients defining a specific scheme with a $2S$ wide stencil. For nodes close to a physical boundary, modified schemes are needed to ensure the scheme's stencil does not go beyond the boundary, whose general formulas are given as [8, 48],

$$\tilde{\phi}'_0 + \alpha_0 \tilde{\phi}'_1 = \frac{1}{\Delta} \sum_{m=0}^{S_0} b_m \phi_m, \quad (2)$$

and

$$\alpha_1 \tilde{\phi}'_0 + \tilde{\phi}'_1 + \alpha_1 \tilde{\phi}'_2 = \frac{1}{\Delta} \sum_{m=0}^{S_1} c_m \phi_m, \quad (3)$$

for the node on the boundary ($i = 0$) and the first node away from the boundary ($i = 1$), respectively, and the coefficients, α_0 , b_m , α_1 and c_m , define specific schemes. The widths of the stencils are given by S_0 and S_1 , respectively. Symmetric operations can be employed for the $i = N$ and $i = N - 1$ nodes.

Although compact schemes have the advantage of a smaller stencil, higher bandwidth resolution, and smaller truncation errors over an explicit scheme of the same order, the drawback is the implicit solution of Eq. (1-3). The following linear algebra system needs to be solved to obtain $\tilde{\phi}'_i$,

$$\begin{bmatrix} 1 & \alpha_0 & & & & \\ \alpha_1 & 1 & \alpha_1 & & & \\ & \alpha & 1 & \alpha & & \\ & & \ddots & \ddots & \ddots & \\ & & & \alpha & 1 & \alpha \\ & & & & \alpha_1 & 1 & \alpha_1 \\ & & & & & \alpha_0 & 1 \end{bmatrix} \begin{bmatrix} \tilde{\phi}'_0 \\ \tilde{\phi}'_1 \\ \tilde{\phi}'_2 \\ \vdots \\ \tilde{\phi}'_{N-2} \\ \tilde{\phi}'_{N-1} \\ \tilde{\phi}'_N \end{bmatrix} = \mathbf{RHS}, \quad (4)$$

where **RHS** is the vector of known terms defined on the right-hand-side of Eqs. (1-3). Equation (2) can be solved efficiently using the classic Thomas algorithm in a serial environment, but well-known difficulties arise in parallel.

In our approach to the domain-decomposition-based parallel environment, we assume that a 1-D domain discretised with N nodes is decomposed into M subdomains. Figure 1 shows the distribution of the nodes around the interface between subdomains k and $k+1$, with $\phi_i, i = -4, -3, \dots, N_k + 4$ defined on subdomain k . Four halo nodes at each side of the subdomain are used to exchange data from neighboring subdomains, targeting a 6th-order

central scheme. More halo nodes could also be defined for higher-order schemes.

Figure 1: Schematic representation of the overlap region between two subdomains.

To decouple the compact scheme between subdomains k and $k+1$, an explicit central scheme (ECS) with the same order of accuracy as the compact scheme is implemented for $i = -1$ and $N_k + 1$ halo nodes to close the tridiagonal matrix. The procedure is shown in following Figure 2,

Figure 2: Procedure for the implementation of the DCOM scheme.

Its implementation is detailed as follows,

- a) At the first layer of halo nodes, $i = -1$ and $N_k + 1$, the ECS of the same order as the compact scheme is used to compute $\tilde{\phi}'_{-1}$ and $\tilde{\phi}'_{N_k+1}$ as,

$$\tilde{\phi}'_{-1} = \frac{1}{\Delta} \sum_{m=1}^{S^*} d_m (\phi_{-1+m} - \phi_{-1-m}), \quad (5)$$

and

$$\tilde{\phi}'_{N_k+1} = \frac{1}{\Delta} \sum_{m=1}^{S^*} d_m (\phi_{N_k+1+m} - \phi_{N_k+1-m}), \quad (6)$$

respectively, where c_m is the coefficient defining an explicit central scheme, and S^* is the half width of the stencil of the ECS scheme.

- b) At the interface nodes, $i = 0$ and N_k , Eq. (1) is reduced to,

$$\tilde{\phi}'_0 + \alpha \tilde{\phi}'_1 = \frac{1}{\Delta} \sum_{m=1}^S a_m (\phi_m - \phi_{-m}) - \alpha \tilde{\phi}'_{-1}, \quad (7)$$

and

$$\tilde{\phi}'_{N_k} + \alpha \tilde{\phi}'_{N_k+1} = \frac{1}{\Delta} \sum_{m=1}^S a_m (\phi_{N_k+m} - \phi_{N_k-m}) - \alpha \tilde{\phi}'_{N_k+1}. \quad (8)$$

c) The tridiagonal matrix in subdomain k is, therefore, closed as,

$$\mathbf{A}_k = \begin{bmatrix} 1 & \alpha & & & & \\ \alpha & 1 & \alpha & & & \\ & \alpha & 1 & \alpha & & \\ & & \ddots & \ddots & \ddots & \\ & & & \alpha & 1 & \alpha \\ & & & & \alpha & 1 & \alpha \\ & & & & & \alpha & 1 \end{bmatrix}. \quad (9)$$

It can be solved independently with the classic Thomas algorithm within the subdomain.

d) Correction Step:

d1. Update $\tilde{\phi}'_{-1}$ and $\tilde{\phi}'_{N_k+1}$ by swapping data with neighboring nodes, e.g.

exchanging $\tilde{\phi}'_{N_k+1}$ in subdomain k with $\tilde{\phi}'_1$ in subdomain $k + 1$.

d2. Repeat steps b) and c) to re-calculate the tridiagonal matrix and update $\tilde{\phi}'_i$.

e) The final interface value is obtained by averaging $\tilde{\phi}'_{N_k}$ from subdomain k and $\tilde{\phi}'_0$ from subdomain $k + 1$.

In the above procedure, the correction steps (d) can be avoided or run many times, depending on the accuracy required and computing time available.

Unlike the scheme proposed by Sengupta *et al.* [26], no asymmetric schemes or operations near interdomain interfaces are introduced. Therefore, the spurious wave packets due to the asymmetry of the scheme can be avoided by the DCOM scheme.

Chao *et al.* [27] also adopted an ECS approach to decouple the corresponding compact scheme. They implement ECS on the interface nodes, i.e. $i = 0$ and $i = N_k$ in Figure 1. Therefore, the benefit of the compact scheme is lost for interface nodes. The DCOM scheme implements the ECS approach on the halo nodes, i.e. $i = -1$ and $i = N_k + 1$ and the scheme remains compact for all physical nodes. A comparison of the two schemes will be given in Section 3.

The implementation of a 6th-order DCOM scheme (DCOM6) is detailed as follows:

$\tilde{\phi}'_{-1}$ and $\tilde{\phi}'_{N_k+1}$ are first calculated with a 6th-order explicit central scheme (ECS6):

$$\tilde{\phi}'_{-1} = \frac{\phi_2 - \phi_{-4}}{60\Delta} - 3 \frac{\phi_1 - \phi_{-3}}{20\Delta} + 3 \frac{\phi_0 - \phi_{-2}}{4\Delta}, \quad (10)$$

and

$$\tilde{\phi}'_{N_k+1} = \frac{\phi_{N_k+4} - \phi_{N_k-2}}{60\Delta} - 3 \frac{\phi_{N_k+3} - \phi_{N_k-1}}{20\Delta} + 3 \frac{\phi_{N_k+2} - \phi_{N_k}}{4\Delta}. \quad (11)$$

At $i = 0$ and $i = N_k$, the scheme reduces to,

$$\tilde{\phi}'_0 + \frac{1}{3}\tilde{\phi}'_1 = \frac{1}{36\Delta}(\phi_2 - \phi_{-2}) + \frac{7}{9\Delta}(\phi_1 - \phi_{-1}) - \frac{1}{3}\tilde{\phi}'_{-1}, \quad (12)$$

and

$$\frac{1}{3}\tilde{\phi}'_{N_k-1} + \tilde{\phi}'_{N_k} = \frac{1}{36\Delta}(\phi_{N_k+2} - \phi_{N_k-2}) + \frac{7}{9\Delta}(\phi_{N_k+1} - \phi_{N_k-1}) - \frac{1}{3}\tilde{\phi}'_{N_k+1}. \quad (13)$$

For internal nodes ($i = 1, 2, \dots, N_k-1$) in the subdomain, the classic 6th-order compact central scheme (COM6) [7] is implemented,

$$\frac{1}{3}\tilde{\phi}'_{i-1} + \tilde{\phi}'_i + \frac{1}{3}\tilde{\phi}'_{i+1} = \frac{1}{36\Delta}(\phi_{i+2} - \phi_{i-2}) + \frac{7}{9\Delta}(\phi_{i+1} - \phi_{i-1}). \quad (14)$$

Eqs. (12-14) is then solved independently in each subdomain using the Thomas algorithm against a closed tridiagonal matrix Eq. (9). At the correction step, $\tilde{\phi}'_{-1}$ and $\tilde{\phi}'_{N_k+1}$ are updated with values from the neighboring subdomain, and Eqs. (12-14) are recalculated using the updated $\tilde{\phi}'_{-1}$ and $\tilde{\phi}'_{N_k+1}$. The final interface value is acquired by averaging $\tilde{\phi}'_{N_k}$ from subdomain k and $\tilde{\phi}'_0$ from subdomain $k+1$.

2.2 Second derivative

For the approximation of the 2nd derivative, $\tilde{\phi}''$, the same principle as the 1st derivative is applied to decouple the compact scheme. For brevity, we only give the formulas of the 6th-order DCOM scheme. The 6th-order compact and explicit schemes are respectively given as,

$$\frac{2}{11}\tilde{\phi}''_{i-1} + \tilde{\phi}''_i + \frac{2}{11}\tilde{\phi}''_{i+1} = 3\frac{\phi_{i+2} - 2\phi_i + \phi_{i-2}}{44\Delta^2} + 12\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{11\Delta^2}, \quad (15)$$

and

$$\tilde{\phi}''_i = \frac{\phi_{i+3} - 2\phi_i + \phi_{i-3}}{90\Delta^2} - 3\frac{\phi_{i+2} - 2\phi_i + \phi_{i-2}}{20\Delta^2} + 3\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{2\Delta^2}. \quad (16)$$

The same idea is applied to decouple Eq. (15) at the interface $i = 0$ as,

$$\tilde{\phi}''_0 + \frac{2}{11}\tilde{\phi}''_1 = 3\frac{\phi_{i+2} - 2\phi_i + \phi_{i-2}}{44\Delta^2} + 12\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{11\Delta^2} - \frac{2}{11}\tilde{\phi}''_{-1}, \quad (17)$$

and $\tilde{\phi}''_{-1}$ is calculated with the explicit scheme given by Eq. (16). A symmetric operation is implemented for $i = N_k$ and $i = N_k + 1$. At the last step, the interface values from two neighbouring subdomains are averaged as the final interface values.

3 Analysis of numerical schemes

3.1 Fourier analysis

The spectral properties of the proposed schemes can be investigated using Fourier analysis. For a pure harmonic function,

$$\phi(x) = e^{i\omega x}, \quad (18)$$

where $i = \sqrt{-1}$ is the imaginary unit, and ω is the wavenumber. The 1st and 2nd derivatives

of $\phi(x)$ are respectively expressed as,

$$\phi'(x) = i\omega e^{i\omega x} = i\omega\phi(x), \quad (19)$$

and

$$\phi''(x) = -\omega^2 e^{i\omega x} = -\omega^2\phi(x). \quad (20)$$

The approximation of $\phi'(x)$ and $\phi''(x)$ by a finite difference scheme can be expressed in the modified wavenumber as,

$$\tilde{\phi}' = i\hat{\omega}\phi, \quad (21)$$

and

$$\tilde{\phi}'' = -\omega''\phi. \quad (22)$$

The relationship between $\hat{\omega}$ and ω'' with ω can therefore be reduced to,

$$\hat{\omega} = -i\tilde{\phi}'/\phi, \quad (23)$$

and

$$\omega'' = -\tilde{\phi}''/\phi, \quad (24)$$

for the 1st and 2nd derivatives, respectively.

The implementation of the DCOM scheme is related to the number of nodes in the subdomain, data swapping and averaging between neighbouring subdomains, and analytical expressions for $\hat{\omega}$ and ω'' are therefore hard to obtain. To analyse its spectral property, the numerical approximations of the 1st and 2nd derivatives of $\phi(x)$ (i.e. $\tilde{\phi}'$ and $\tilde{\phi}''$), with ω ranging from 0 to π , are calculated by specific schemes in a 1-D domain $x \in [0, 2\pi]$ discretised with N nodes. These nodes are distributed in M subdomains, and $\hat{\omega}$ and ω'' are calculated by using Eqs. (23) and (24), respectively. The analysis of mean values for $\hat{\omega}$ and ω'' , averaged on all nodes, and the values of $\hat{\omega}$ and ω'' on the interface node are conducted. It is necessary to clarify that the Fourier analysis here is only for inner nodes, and the influence of boundary constrains, which has been well discussed previously [7,49,50], is not taken into account.

The real part of the modified wavenumber, $\hat{\omega}$, for the 1st derivatives with $N=64$ are shown in Figure 3 (a). It considers subdomain number M equal to 4 and 16, corresponding to $N_k = 16$ and 4 ($N_k = N/M$). As expected, the compact schemes show higher resolution at large wavenumbers than the explicit scheme of the same order. Chao's scheme, shown in Figure 3, refers to the 6th-order decoupled compact scheme (see Chao *et al.* [27]). It falls between those of ECS6 and COM6, and approaches that of COM6 as N_k is increased. The DCOM6 scheme proposed in the present paper shows a better spectral performance than Chao's scheme. Its spectral property is closer to that of the COM6 scheme and is less sensitive to the number of subdomains. Tests with $N_k = 4$ show that the implementation of the

correction step can be used to effectively improve the accuracy of the DCOM scheme. The imaginary parts of $\hat{\omega}$ for all tested schemes are zero (not shown here), indicating their non-dissipative nature due to the symmetric form of the schemes. This is important in DNS/LES of turbulence, because the numerical dissipation has a critical effect on the prediction of kinetic energy of turbulent eddies. [51,52,53,54]

The spectral properties of the schemes at the interface node are presented in Figure 3 (b). At the interface node, Chao's scheme degrades to the ECS approach, since the ECS scheme is used to acquire $\tilde{\phi}'$ at the interface. For the DCOM6 scheme without a correction step, a clear improvement over Chao's scheme is observed, and the DCOM6 scheme with the correction step shows an almost identical result to the fully coupled COM6 scheme.

Figure 3: Mean (a) and Interface (b) values of $\hat{\omega}$ (real part) of 6th-order central schemes for the 1st derivative.

The error in the 2nd derivative approximation is measured as $|\omega'' - \omega^2|$ [7] and presented in Figure 4. Similar to the observation of the 1st derivatives, the mean value of $|\omega'' - \omega^2|$ of the DCOM6 scheme is very close to that of the COM6 scheme, even for the case with $N_k = 4$, and without any correction step. At the interface node, Chao's scheme collapses again onto the curve of the EXP6 scheme, and the curve of the DCOM6 scheme without the correction step is close to the COM6 scheme. The inclusion of the correction step further improves the result towards the COM6 scheme.

Figure 4: Mean (a) and Interface (b) values of $|\omega'' - \omega^2|$ of 6th-order central schemes for the 2nd derivative.

It can be seen that the proposed DCOM6 scheme possesses superior characteristics in wavenumber space compared to Chao's scheme, and its performance is close to the fully-coupled compact scheme.

3.2 Error analysis

The numerical error of a scheme can be evaluated by calculating the 1st and 2nd derivatives of the following test function:

$$f(x) = \sin(4x), \quad x \in [0, 2\pi], \quad (25)$$

and the l_2 -errors against the exact solution. The l_2 -errors is defined as $\sqrt{\frac{1}{N} \sum_{i=1}^N (\hat{f}'_i - f')^2}$, where $\hat{f}'_i$ is the approximation of f' at node i , and N is the number of nodes.

The l_2 -errors of the approximation of the 1st derivative against both the number of nodes and the number of subdomains are presented in Figure 5. It can be seen in Figure 5(a) that all schemes can ensure an N^{-6} slope, indicating a 6th-order of accuracy being preserved for all schemes. The l_2 -error of the DCOM6 scheme with one correction step overlaps that of the COM6 scheme. The DCOM6 scheme without any correction step contains larger errors than with the correction step but smaller errors than Chao's scheme. According to Figure 5(b), the level of errors for all tested decoupled schemes has shown a trend of approaching the COM6 scheme as the number of nodes in each subdomain increases (*i.e.* the degree of parallelism decreases). Once again, the DCOM6 scheme with the correction step has shown similar performance to the COM6 scheme, and the DCOM6 scheme without a correction step gives smaller errors than Chao's scheme.

Figure 5: l_2 -errors of the approximation of the 1st derivative using 6th-order schemes. (a) is based on the number of subdomains $M=32$ and (b) is based on the total number of nodes $N=512$.

Figure 6 plots the l_2 -errors of the approximation of the 2nd derivative using 6th-order schemes. All schemes tested achieve 6th-order accuracy, although errors increase after their values are reduced to 10^{-10} , due to machine round-off error. Note that the DCOM6 schemes with and without the correction step produce almost the same error as that of the COM6 scheme. In Figure 6 (b), with the increase of N_k , l_2 -errors of both DCOM6 and Chao's schemes fall to the value of the COM6 scheme, although Chao's scheme generates larger errors than the DCOM6 scheme at small N_k .

Figure 6: l_2 -error of the approximation of the 2nd derivative using 6th-order schemes. (a) is based on the number of subdomains $M=32$ and (b) is based on the total number of nodes $N=512$.

4 Numerical tests

In this section, the DCOM6 schemes are tested in canonical cases.

4.1 1-D wave-packet propagation

The performance of the DCOM6 schemes is now tested for a 1-D wave-packet propagation problem, and compared with the ECS6, COM6 and Chao's schemes. The 1-D linear convection equation is solved as,

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0, \quad (26)$$

where u is a time-spatial variable, and t and x are the time and spatial coordinates, respectively.

The equation describes the propagation of the initial wave-packet with a constant speed, c , and it has been widely used to study the dispersion property of numerical schemes [26, 55]. By referencing the numerical test done by Sengupta *et al.* [26], the convection speed is set as $c = 0.5$, and the initial wave-packet is given as,

$$u(x, 0) = e^{-A(x-x_0)^2} \sin(\omega_0 x), \quad (27)$$

in which $A = 50$, $x_0 = 1.5$, and $\omega_0 = 0.838242/\Delta x$, Δx is the size of the mesh. The computational domain is $x \in [0, 10]$ with periodic conditions applied at both ends. A 1-D uniform mesh with 664 nodes is used to solve Eq. (26). A four-step Runge–Kutta scheme [56] is implemented as the time integration strategy because of its good numerical stability and dispersion relation preservation property. The time step is set as $\Delta t = 0.0006$.

The profiles of u at $t=0, 3, 6, 9, 12$, and 15 by the ESC6 scheme are shown in Figure 7 (a). The spurious wiggles (i.e. the so-called q-waves) on the left-hand side of the wave-packet are produced by the dispersive error of the numerical method [57], and they grow and spread upstream with time. By comparing the results of different schemes at $t=15$ in Figure 7 (b), we can see that the spurious wiggles are effectively removed by using compact schemes, including both Chao's scheme and the DCOM6 scheme, due to their higher resolution and smaller dispersive errors at high wavenumbers, as presented in Figure 3. The results of compact schemes lie on top of the exact solution in Figure 7 (b). A detailed analysis will be presented later.

Figure 7: Capture of wave-packet from $t=0$ to $t=15$ by ECS6 scheme, and the comparison of results from different scheme. For the tests of parallel schemes, the computational domain is split into 4 even subdomains, and each subdomain has 166 nodes.

The temporal evolution of the results from Chao's scheme with the largest degree of parallelism permitted is presented in Figure 8 (a), in which the computational domain is split into 166 subdomains and each subdomain contains only 4 nodes. It can be observed that with a large degree of the parallelism, the results from Chao's scheme have deteriorated, and strong wiggles are generated on the left-hand side of the wave-packet, similar to the result of the ECS6 scheme shown in Figure 7(a). Moreover, weak wiggles appear across the whole domain for the result at $t=15$. By comparing the results of Chao's and the DCOM schemes at $t=15$ in Figure 8 (a), it can be confirmed that the DCOM6 scheme shows much improved results, and the scheme, even without the correction step, shows only very weak wiggles at $t=15$, and the correction step removes the wiggles very effectively.

Figure 8: The propagation of the wave-packet by Chao's scheme (a), and comparison to the results from the decoupled schemes (b). The computational domain is split into 166 even subdomains.

By examining the details of the left-hand side of the wave-packet at $t=15$ in Figure 9, weak wiggles generated by Chao's scheme are observed for the case with 4 subdomains, and the wiggles are amplified with an increase in the number of subdomains. The DCOM6 scheme shows a more stable performance, and the correction step can further recover the result to that of the COM6 scheme.

The l_2 -errors, $\sqrt{\frac{1}{N} \sum_{i=1}^N (u_i - u_{exact})^2}$, for the solution at $t=20$ against the number of nodes per subdomains are presented in Figure 10, in which $u_{exact}(x, 20) = u(x, 0)$. For this test, the total number of nodes is set to 512 so that the nodes can be evenly distributed. It can be confirmed that the DCOM6 scheme has smaller errors than Chao's scheme and the correction step can restore the DCOM6 scheme to the accuracy of the fully-coupled compact scheme. It is interesting to note that the DCOM6 scheme, without any correction step, can

produce even smaller errors than the COM6 scheme, and the errors decrease with the decrease of the number of nodes per subdomain. By examining the distribution of errors, defined as $|u_i - u_{exact}|$ at $t=20$ for the case with 8 nodes per subdomain, in Figure 11, we can see the DCOM6 scheme without a correction step produces smaller errors within the wave-packet centred at $x=1.5$ which makes the l_2 -errors being smallest among all tested schemes, although wiggles can be observed on the profile away from the wave-packet. Since the value of u is close to zero away from the wave-packet, the ratio of the errors to the local value of u is much bigger than the COM6 scheme. From Figure 11 we can see similar results between the DCOM6 scheme with the correction step and the fully-coupled COM scheme, since the profiles from these two schemes lie on top of each other.

Figure 9: Detailed comparison of the wave-packets at $t=15$. The computational domain is split into 4 and 166 subdomains in (a) and (b) respectively.

Figure 10: l_2 -norm errors of results of different schemes at $t=20$.

Figure 11: Distributions of errors of results at $t=20$ for the case with 64 subdomains.

4.2 2-D vorticity wave convection problem

The DCOM6 scheme is further tested on a 2-D vorticity wave convection in a subsonic freestream by solving the 2-D Euler equations,

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0, \\ \frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j + p \delta_{ij})}{\partial x_j} &= 0, \\ \frac{\partial \rho e}{\partial t} + \frac{\partial (\rho e + p) u_j}{\partial x_j} &= 0, \end{aligned} \quad (28)$$

in which the primary variables are the density ρ , the pressure p , the velocity component u_i , and the total energy per unit mass e , defined as, $e = \frac{p}{(\gamma-1)\rho} + \frac{1}{2}u_i u_i$, with the ratio of specific heats $\gamma = 1.4$. The standard Einstein summation notation is used and notations x_i and u_i , $i = 1, 2$ are adopted to represent (x, y) and (u, v) , respectively. The Euler equations are non-dimensionalised with the freestream density, ρ_0 , velocity, u_0 , temperature, T_0 , and the reference length, L .

The convective terms are solved in the skew-symmetric form to reduce the aliased errors arising from nonlinear terms [58,59,60,61,62]. The time integration is conducted using the classic 3-step 3rd-order TVD Runge-Kutta scheme [63]. A 2-D domain with size $L_x \times L_y = [0, 20] \times [0, 10]$ is discretised with a 64×32 uniform mesh, and periodic boundary conditions are applied at all boundaries. The initial conditions are,

$$\begin{aligned}
\rho &= 1 \\
u &= 1 - C_{vs} \frac{y - y_c}{R_{vs}^2} e^{-r^2/2}, \\
v &= C_{vs} \frac{x - x_c}{R_{vs}^2} e^{-r^2/2}, \\
p &= p_0 - 0.5 \frac{C_{vs}^2}{R_{vs}^2} e^{-r^2},
\end{aligned} \tag{29}$$

with $x_c = 10$ and $y_c = 5$ as the initial location of the vortical core, the freestream pressure is given as, $p_0 = 1/\gamma Ma^2$, and the size and strength of the initial vortex is specified with $R_{vs} = 1$ and $C_{vs} = 0.01 u_0 R_{vs}$. The freestream Mach number is, $Ma = u_0/\sqrt{\gamma RT_0} = 0.1$, with the gas constant $R = 287.1 \text{ J/(K}\cdot\text{kg)}$. This case has been widely adopted to test numerical schemes with respect to vortex preservation [8,38,64,65,66]. The exact solution of the equations at time t can be obtained by shifting the initial solution by $u_0 t$ in the x -direction [38].

The computational domain was split into 16×8 subdomains for parallel computations, as shown in Figure 12, and each subdomain contains 4×4 nodes. The vorticity field, given by $\omega = \partial v / \partial x - \partial u / \partial y$, at $t=20$, obtained from the DCOM scheme with the corrector is shown in Figure 12, from which we can see that the vortex is well resolved. The temporal evolution of l_2 -errors are presented in Figure 13 where the l_2 -error here is defined as $\frac{1}{\omega_{max}} \sqrt{\frac{1}{N_i N_j} \sum_{j=1}^{N_j} \sum_{i=1}^{N_i} (\omega_{i,j} - \omega_{exact})^2}$, in which $\omega_{i,j}$ is the vorticity on the node (i, j) , ω_{exact} is the exact solution of the vorticity, ω_{max} is the maximum of the initial vorticity, and N_i and N_j are the nodes' numbers in the x and y -directions, respectively.

The proposed DCOM6 scheme produces smaller errors than Chao's scheme, as expected. For Chao's scheme, errors increase with an increase in the degree of parallelism, and the DCOM6 scheme gives a relatively stable performance, especially with the correction step. Once again, the decrease of numerical errors with an increase in subdomain number for the DCOM6 scheme, without any correction step, is observed. By examining the distribution of errors, $|\omega_{i,j} - \omega_{exact}|$, in Figure 14, we can confirm that the errors of the ECS6 scheme is the highest, and Chao's scheme induces errors across the entire domain. The DCOM6 scheme without a correction step gets the smallest errors around the vortex but it generates ripples outside of the vortex. The implementation of the correction step causes higher errors within the vortex, but it gives a clean result in the rest of the domain. Therefore, the quality of the result of the DCOM6 scheme with the correction step is regarded as the best.

Figure 12: Vorticity field at $t=20.0$ by the DCOM6 with correction step. The mesh lines mark the interdomain interfaces.

Figure 13: Temporal evolution of l_2 -norm errors. (a): 4 subdomains; (b): 128 subdomains.

Figure 14: Distribution of errors at $t=20$ with 128 subdomains. (a): ECS6 scheme; (b): Chao's scheme; (c): DCOM6 scheme without correction step; (d): DCOM scheme with the correction step.

5 Application of the DCOM6 scheme to turbulence simulations

In this section, the DCOM6 scheme is applied to solve the 3-D Navier-Stokes (N-S) equations with an in-house finite-difference solver, ASTR, for two classic problems: the 3-D Taylor-Green vortex problem and planar turbulent channel flow to show its capability in DNS of turbulent flows. The 3-D N-S equations are given in non-dimensional form as,

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0, \\ \frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j + p \delta_{ij})}{\partial x_j} &= \frac{\partial \sigma_{ij}}{\partial x_j} + s_i, \\ \frac{\partial \rho e}{\partial t} + \frac{\partial (\rho e + p) u_j}{\partial x_j} &= \frac{\partial (\sigma_{ij} u_i - q_j)}{\partial x_j} + s_e,\end{aligned}\tag{30}$$

The stress tensor and the heat flux vector are expressed as,

$$\sigma_{ij} = \frac{\mu}{\text{Re}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right),\tag{31}$$

and

$$q_i = - \frac{\mu}{\text{PrRe}(\gamma - 1) Ma^2} \frac{\partial T}{\partial x_i},\tag{32}$$

The non-dimensional parameters which appear on the stress and the heat flux are the Reynolds number and Prandtl number, $\text{Re} = \rho_0 u_0 L / \mu_0$ and $\text{Pr} = \mu C_p / \vartheta = 0.72$, where $C_p = \gamma R / (\gamma - 1)$ is the specific heat capacity of the gas at constant pressure, and ϑ is thermal conductivity coefficient. The dynamic viscosity coefficient, μ , is calculated via Sutherland's law,

$$\mu = T^{1.5} \frac{T_s / T_0 + 1}{T + T_s / T_0}.\tag{33}$$

According to the analysis in Section 2, the DCOM scheme with one correction step gives the best result, and the DCOM scheme without any correction is considered as the second best. However, the computing time using the DCOM scheme with one correction step is about twice the DCOM without any correction step. Therefore, for the trade-off between accuracy and computing time, the correction step is not implemented for simulations of 3D turbulent flows in the present paper.

The convective terms and time integration are solved in the same way as the Euler equations Eq. (28). The diffusive terms are solved in the Laplacian form [67] to improve the stability of the solver. The 2nd derivatives in the diffusion terms, i.e. $\partial^2 u_i / \partial x_j^2$ and $\partial^2 T / \partial x_j^2$, are also calculated by using the DCOM6 scheme for 2nd derivatives Eq. (15-17).

5.1 3-D Taylor-Green vortex problem

The DCOM6 scheme is implemented for the 3-D Taylor-Green Vortex (TGV) problem [68] by solving the N-S equations in a 2π cubic domain. A 256^3 uniform mesh is used to discretise the domain and the computational domain is split into 768 ($12 \times 8 \times 8$) subdomains.

The initial condition is set as [69, 70],

$$\begin{aligned}\rho &= 1, \\ u &= \sin(x)\cos(y)\cos(z), \\ v &= -\cos(x)\sin(y)\cos(z), \\ w &= 0, \\ p &= 1/\gamma M^2 + \frac{1}{16} [\cos(2x) + \cos(2y)][\cos(2z) + 2].\end{aligned}\tag{34}$$

The reference Mach number is $Ma = 0.1$ and the reference Reynolds number is 1600.

The evolution of the spatially averaged kinetic energy and enstrophy obtained with the DCOM6 schemes is compared to that obtained with a pseudo-spectral method [71] on a 512^3 mesh, shown in Figure 15. Both the kinetic energy and enstrophy profiles agree well with the data from the pseudo-spectral code, although a slight underprediction of the enstrophy peak value by the DCOM6 schemes can be observed. The 3-D fields of enstrophy and coherent structures visualised with iso-surfaces of λ_{ci} at $t=0, 10$, and 20 are shown in Figure 16 and Figure 17, respectively. The imaginary part of the complex eigenvalue of the velocity gradient tensor λ_{ci} was first proposed by Zhou *et al.* [72] to visualise turbulent coherent structures, and it was then known as swirling strength [10], and widely adopted as a vortex identification scheme [73,74]. It can be seen that the flow structures evolve into smaller vortical structures with higher vorticity from $t=0$ to $t=10$, and from $t=10$ to $t=20$, the vortical structures become more chaotic, occupying a greater space, although the maximum strength of the enstrophy is reduced, indicating a dissipation and diffusion process. At $t=0, 10$, and 20 , the symmetry of the flow field is well preserved.

Figure 15: Temporal evolution of kinetic energy (a) and enstrophy (b)

Figure 16: Enstrophy field at t=0 (a), t=10 (b), and t=20 (c)

Figure 17: Vortical structures visualised with iso-surfaces of λ_{ci} equaling to 1% of its maximum and coloured with enstrophy. (a): t=0, (b): t=10, (c): t=20

5.2 Turbulent channel Flow

The performance of the DCOM6 scheme in DNS of wall-bounded flow and its stability in long-time integration are assessed in a turbulent channel flow, in which periodic conditions are applied to the x - and z -boundaries, and isothermal no-slip conditions are applied to the walls, as sketched in Figure 19. To drive the flow, an unsteady uniform body force is applied to the x -momentum and energy equations in Eq. (30) as,

$$\begin{aligned} s_1 &= f_x, \\ s_e &= f_x u_b, \end{aligned} \tag{35}$$

in which f_x is the body force and u_b is the bulk velocity. The body force is calculated based on its previous value, the wall friction and the mass flux at the current step to ensure a constant mass flux, following the procedure given by Lenormand *et al.* [75]. The size of the domain is $L_x \times L_y \times L_z = [0, 2\pi] \times [0, 2] \times [0, 4/3\pi]$, matching the setting of Moser *et al.* [76]

Figure 18: Sketch of open turbulent channel flow

The initial condition is a laminar profile with superimposed random fluctuations up to 30% of the mean velocity,

$$\begin{aligned} u &= 1.5(1 - (y - 1)^2)(1 + 0.3\epsilon), \\ v &= w = 0, \\ T &= 1 + \frac{y - 1}{3} \text{Pr} \cdot M^2 1.5(1 - (y - 1)^4), \end{aligned} \quad (36)$$

where ϵ is a random number within the range $[-1, 1]$.

At the mesh node on the wall and the first node away from the wall, the stencil of the scheme has to be shortened to fit the boundary. Therefore, 2nd- and 4th-order boundary schemes are used at the wall and at the first node away from the wall, respectively [7, 8, 48],

$$\begin{aligned} \tilde{\phi}'_0 + \tilde{\phi}'_1 &= \frac{2}{\Delta}(\phi_1 - \phi_0), \\ \frac{1}{4}\tilde{\phi}'_0 + \tilde{\phi}'_1 + \frac{1}{4}\tilde{\phi}'_2 &= \frac{3}{4\Delta}(\phi_2 - \phi_0), \end{aligned} \quad (37)$$

for the first derivative terms and

$$\begin{aligned} \tilde{\phi}''_0 &= \frac{1}{\Delta^2}(2\phi_0 - 5\phi_1 + 4\phi_2 - \phi_3), \\ \frac{1}{10}\tilde{\phi}''_0 + \tilde{\phi}''_1 + \frac{1}{10}\tilde{\phi}''_2 &= \frac{6}{5\Delta^2}(\phi_2 - 2\phi_1 + \phi_0), \end{aligned} \quad (38)$$

for the 2nd derivative terms.

The Reynolds number based on the bulk velocity, bulk density, the half-height of the channel and the viscosity at the wall is $Re = 2,897.5$, corresponding to a friction Reynolds number $Re_\tau = 183.2$. The Mach number based on the bulk velocity and the speed of sound at the wall is $Ma = 0.5$. A mesh with 6,291,456 ($256 \times 192 \times 128$) nodes is used to discretise the domain. These nodes are evenly distributed in the x - and z -directions, and concentrated towards the walls in the y -direction. The detailed information of the mesh

resolution is presented in Table 1, in which the superscript '+' stands for variables in wall units.

Table 1. Domain and mesh information of the DNS of turbulent channel flow

L_x	L_y	L_z	N_x	N_y	N_z
4π	2	$4/3\pi$	256	192	128
Δx	$\Delta y_1 \sim \Delta y_m^*$	Δz	Δx^+	$\Delta y_1^+ \sim \Delta y_m^+$	Δz^+
0.0491	0.00326~0.0171	0.0327	8.99	0.598~3.128	5.99

* Δy_1 and Δy_m are the mesh size of the first node away from the wall and the node in the middle of the channel.

The simulation is run in parallel using 768 processors and the domain is split into 16, 8 and 6 subdomains in the x -, y - and z -directions, respectively. The non-dimensional time step of the simulation is 1.25×10^{-3} . The temporal evolution of spatially averaged skin friction is shown in Figure 19, from which we can see the flow goes through a laminar-turbulent transition in the early stage of the simulation and reaches a statistically steady state around $t=100$. For further discussions on the division of stages in late transition, see Ref. [77]. The data collection begins at $t=193.8$, and 3400 samples are used to calculate the statistics.

The instantaneous turbulent structures in the fully developed channel are illustrated in Figure 20. The classic hairpin counter-rotating vortices [72] and streamwise elongated low-speed streaks are well captured.

Figure 19: Temporal profiles of spatially averaged skin friction coefficient.

Figure 20: Instantaneous turbulent coherent structures in the lower half of the channel visualised with iso-surfaces of λ_{ci} equaling to 1.25% of its maximum and colored with streamwise vorticity (a) and velocity streaks at $y^+=10$ (b).

The mean velocity profile, root-mean square (RMS) velocity fluctuations and Reynolds shear stress in wall units are presented in Figure 21. The incompressible DNS data of

channel flow at a similar Reynolds number obtained by Moser *et al.* [76] are plotted as a reference. Good agreement between the present DNS using the DCOM6 scheme and the incompressible DNS data of Moser *et al.* [76] is achieved. Therefore, the applicability of the proposed DCOM6 scheme for DNS of wall-bounded turbulence and long-time integration is validated.

Figure 21: (a): Mean velocity profile and (b): RMS velocity fluctuations and Reynolds shear stress. All variables are normalised with friction velocity, density and viscosity at the wall

5.3 Scalability

The scalability of the DCOM6 schemes in the TGV problem with a 512^3 mesh is evaluated using ASTR on the HAZEL HEN machine [78], with up to 12288 cores. The wall time consumption per time step (this is obtained by averaging the wall time consumed for 100 steps) with different numbers of processors are listed in Table 2, and the data are plotted in Figure 22. A clear linear acceleration with a 0.9 slope is obtained, indicating that the proposed schemes are well adapted to domain-decomposition-based parallel computation.

Table 2. Scalability of the DCOM6 scheme based on ASTR code and HAZEL HEN machine

HPC Nodes	Cores	Time per step (s)	Speedup	Ideal Speedup
4	96	25.63	1.0	1.00
8	192	12.94	1.98	2.00
16	384	6.62	3.87	4.00
32	768	3.54	7.24	8.00
64	1536	1.86	13.81	16.00
128	3072	0.96	26.78	32.00
256	6144	0.53	48.44	64.00
512	12288	0.29	87.65	128.00

Figure 22: CPU time per time step (a) and speedup (b)

6 Summary and Conclusions

A class of domain-decoupled compact schemes for 1st and 2nd derivatives is proposed for domain-decomposition-based parallel computational fluid dynamics. The compact scheme is decoupled at the interdomain interface, and the tridiagonal matrix system is closed using an explicit scheme of the same order on halo nodes. The accuracy of the scheme can be further improved with the implementation of a correction step with an increased cost of computing resources. The proposed scheme can also be applied for multi-block structured solvers using compact schemes.

The analysis of the 6th-order DCOM scheme shows that the proposed scheme has a higher spectral resolution, smaller truncation error, and produces weaker wiggles than Chao's scheme of the same order and the non-dissipative property of a central scheme is well preserved. A correction step can further improve the accuracy of the DCOM scheme in all aspects and restore the scheme towards results obtained by a fully-coupled compact scheme, although it requires additional computational time. The DCOM6 scheme was tested for the 1-D wave-packet propagation and 2-D vortex convection problems, showing improved performance against Chao's scheme in terms of accuracy and independence on the degree of parallelism. The application of the DCOM6 scheme without any correction step in DNS of the Taylor-Green vortex problem and turbulent channel flow demonstrates its suitability in domain-decomposition-based parallel solution for DNS of turbulent flows. In addition, the scalability of the proposed scheme is evaluated on the HAZEL HEN machine with up to 12288 cores, showing that a linear speed-up can be achieved.

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