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An adaptive implicit–explicit scheme for the DNS and LES of compressible flows on unstructured grids

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ABSTRACT

An adaptive implicit–explicit scheme for Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES) of compressible turbulent flows on unstructured grids is developed. The method uses a node-based finite-volume discretization with Summation-by-Parts (SBP) property, which, in conjunction with Simultaneous Approximation Terms (SAT) for imposing boundary conditions, leads to a linearly stable semi-discrete scheme. The solution is marched in time using an Implicit–Explicit Runge–Kutta (IMEX-RK) time-advancement scheme. A novel adaptive algorithm for splitting the system into implicit and explicit sets is developed. The method is validated using several canonical laminar and turbulent flows. Load balance for the new scheme is achieved by a dual-constraint, domain decomposition algorithm. The scalability and computational efficiency of the method is investigated, and memory savings compared with a fully implicit method is demonstrated. A notable reduction of computational costs compared to both fully implicit and fully explicit schemes is observed.

1. Introduction

Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES) are widely used to simulate compressible turbulent flows. DNS simulates all the flow scales, whereas in LES, the equations are low-pass filtered, and the small-scale turbulent eddies are modeled. Recently, there has been a growing interest in applying DNS and especially LES to practical engineering applications that typically involve high Reynolds number flows and complex geometries. An unstructured spatial discretization scheme is the preferred choice to resolve complex geometries. Both the computational grid and the flow may induce stiffness in the equations restricting the time-step size of an explicit time integrator. Typical examples include resolved boundary layers for which both the viscous and inviscid terms may be stiff. The former is due to the small grid size and the latter is due to the acoustic Courant–Friedrichs–Lewy (CFL) condition.

Several approaches have addressed stiff equations. A fully implicit approach treats every term throughout the entire computational domain implicitly. However, it requires the solution of a large non-linear system of equations. For realistic applications, the cost of solving the non-linear system may be more than marching the scheme explicitly in time. Some methods, such as relaxation-based schemes and multi-grid reduce the cost of a fully implicit approach (see [1], and for unstructured methods [2] and references therein). Furthermore, the memory required to store the Jacobian matrix and preconditioners is considerable and may prevent computations of realistic applications. The memory requirement for the Jacobian matrix can be reduced by means of a pressure-correction method [3,4] or eliminated by using a Jacobian-free Krylov subspace linear

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solver [5]. For the latter method, the sparse matrix–vector multiplication is replaced by a flux calculation, which increases the computational cost. Hence, there is considerable room for designing effective numerical schemes by avoiding fully implicit time-integration schemes.

One approach to reduce both memory and computational cost is to identify stiff parts of the Ordinary Differential Equation (ODE) system obtained from spatial discretization of the governing PDE and employ an implicit–explicit (IMEX) time-integration scheme. An IMEX scheme integrates stiff parts implicitly and the non-stiff parts explicitly in time. Such a time-advancement scheme can be constructed using linear multi-step methods [6]. Alternatively, one may use Runge–Kutta based IMEX schemes [7,8] that have better stability properties than linear multi-step methods. In any case, an IMEX method requires partitioning of the ODE system into stiff and non-stiff parts. The stiffness may originate from specific terms in the governing equations (see for instance, [9–11]) and/or from specific directions/regions in the flow (for example, the wall-normal diffusion in a boundary-layer simulation [12]). However, for the unstructured grids it is difficult to identify a stiff direction. For specially designed unstructured grids, Nompelis et al. [13] proposed a method with an implicit treatment of the wall-normal direction. Nevertheless, in many cases, the stiffness is confined to certain regions in the computational domain. A possible approach for such problems is to use a variable hybrid method that blends explicit and implicit schemes using a continuous parameter controlling the fraction of each problem [14]. Alternatively, one can decompose the computational domain into implicit and explicit regions using a measure for geometrically induced stiffness (see Kanevsky et al. [15]).

Therefore, there is potential for saving computational cost by designing an efficient algorithm that treats implicitly only those regions and/or phenomena that require it. In this paper, we propose a novel splitting algorithm that measures the stiffness and devise implicit and explicit parts, with respect to both the computational domain and the spatial directions. The splitting algorithm will be referred to as Row-Splitted IMEX (RS-IMEX) scheme. The RS-IMEX scheme operates in time allowing the decomposition to adapt at every time step. Moreover, the scheme is well-suited for large-scale computations required for the DNS/LES, as it is designed to be highly parallelizable and scalable.

In this study, we use a node-based finite-volume scheme to discretize the spatial derivatives. In [16–18], the SBP and SAT techniques for imposing boundary conditions were used to prove stability for high-order finite difference approximations of the Navier–Stokes equations. Furthermore, the SBP property was proved for node-based unstructured finite-volume schemes in [19–21]. In Section 2, we utilize these results to obtain a stable finite-volume discretization. In Section 3, we develop the RS-IMEX scheme for the advection–diffusion equation and generalize it to the Navier–Stokes equations on unstructured grids. Finally, we validate the proposed scheme and demonstrate its performance using several test cases in Section 4.

2. Governing equations and spatial discretization

The governing equations are the compressible Navier–Stokes, energy and continuity equations. Let Ω and $\partial\Omega$ be the computational domain and its boundary. By using L_r, ρ_r, u_r, T_r, and μ_r as reference length, density, velocity, temperature, and molecular viscosity, the equations can be stated as

$$\frac{\partial}{\partial t}(\underset{\sim}{\vec{U}}) + \sum_{j=1}^{3}\frac{\partial}{\partial x_j}\left(\vec{F}_j - \frac{1}{Re}\vec{G}_j\right) = 0, \tag{1}$$

where $\underset{\sim}{\vec{U}}^T = (\rho, \rho\vec{u}^T, \rho E)^T$ denotes the conservative variables and

$$\vec{F}_j = \begin{pmatrix} \rho u_j \\ \rho u_i u_j + p\delta_{ij} \\ (\rho E + p)u_j \end{pmatrix}, \quad \vec{G}_j = \begin{pmatrix} 0 \\ \tau_{ij} \\ u_i\tau_{ij} + q_j \end{pmatrix}, \quad i = 1,2,3,$$

where ρ, p, u_i, E, and $Re = \rho_r u_r L_r/\mu_r$ denote density, pressure, velocities, energy, and Reynolds number, respectively. Furthermore,

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right), \quad q_j = \frac{\mu}{(\gamma-1)PrM_r^2}\frac{\partial T}{\partial x_j},$$

where $\mu = T^n$, $n = constant$, δ_{ij} is the Kronecker's delta, $M_r = \frac{u_r}{c_r}$, c_r is the reference sound speed, and Pr is the Prandtl number. The equations are supplemented with the state equation for an ideal gas, $p = \frac{\rho T}{\gamma M_r^2}$, and a suitable boundary operator, $L_{\partial\Omega} = g(\vec{x}, t)$ on $\partial\Omega$.

The domain Ω is discretized by an unstructured grid with M grid cells $\overline{\Omega}_c$ such that $\Omega = \bigcup_{c=1}^{M}\overline{\Omega}_c$. Eq. (1) is approximated by a finite-volume method on the dual volumes, Ω_k. In 2D, the dual volumes Ω_k are constructed by connecting the edge centers (ec), to the cell centers (cc), as depicted in Fig. 1. In 3D, the dual volumes are formed by the union of several triangular faces. Each face is constructed by connecting the edge center, the cell center, and the face center of the grid cells.

A finite-volume method defined by the dual volumes is usually referred to as a node-based scheme or a cell-vertex scheme. On a fixed dual volume Ω_k with fixed boundaries $\partial\Omega_k$ and outward-facing normal $\vec{n}$, the integral form of (1) is

$$\frac{\partial}{\partial t}\int_{\Omega_k}\underset{\sim}{\vec{U}}\,dV + \int_{\partial\Omega_k}\sum_{j=1}^{3}\left(\vec{F}_j - \frac{1}{Re}\vec{G}_j\right)dn_j = 0, \tag{2}$$