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Short note

Explicit Runge–Kutta schemes for incompressible flow with improved energy-conservation properties

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ABSTRACT

The application of *pseudo-symplectic* Runge–Kutta methods to the incompressible Navier–Stokes equations is discussed in this work. In contrast to fully energy-conserving, implicit methods, these are explicit schemes of order p that preserve kinetic energy to order q, with $q > p$. Use of explicit methods with improved energy-conservation properties is appealing for convection-dominated problems, especially in case of direct and large-eddy simulation of turbulent flows. A number of pseudo-symplectic methods are constructed for application to the incompressible Navier–Stokes equations and compared in terms of accuracy and efficiency by means of numerical simulations.

1. Introduction

Discrete conservation of kinetic energy is an important requirement in the numerical solution of the incompressible Navier–Stokes equations. In the inviscid limit, the global kinetic energy $e = \int_\Omega u_i^2/2\,\mathrm{d}V$ (i.e. the kinetic energy integrated over the domain Ω) is an invariant of the continuous equations when periodic or homogeneous boundary conditions are applied [1]. The reproduction of this property on a discrete level is especially important when dealing with turbulent flow simulations, in the framework of either Direct (DNS) or Large-Eddy Simulation (LES) techniques. Enforcing discrete conservation of kinetic energy can lead to a number of desirable features, such as zero or negligible artificial dissipation, a well represented energy transfer mechanism as well as a nonlinear stability bound to the numerical solution [2–4].

The Navier–Stokes equations are usually tackled numerically by means of a semi-discrete approach, in which the various terms are first discretized in space and then integrated in time. In general, both the space discretization and time advancement algorithms contribute to violation of the discrete conservation of kinetic energy in the inviscid limit [5]. While various methods are available to accomplish spatial conservation, only a limited class of numerical algorithms can provide this property for the time-advancement step. These methods are necessarily implicit [6], and the application of fully implicit schemes to the Navier–Stokes equations presents several drawbacks. It is computationally expensive, especially when managing very large systems, and it is difficult to be carried out efficiently for massively parallel architectures. Explicit methods with optimal energy-preserving properties are thus warranted.

In this short note, the use of *pseudo-symplectic* Runge–Kutta (RK) schemes for time-integration of the Navier–Stokes equations is investigated. These are explicit methods that preserve quadratic invariants approximately up to a certain order

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of accuracy, and were introduced in the context of Hamiltonian systems [7,8]. The application of such schemes to the fluid flow equations is appealing and appears to have never been pursued in the available literature. Existing as well as newly derived pseudo-symplectic methods are constructed and optimized for application to the Navier–Stokes equations.

The short note is organized as follows. Details about the spatial and temporal discretization are briefly recalled in Section 2. Newly derived as well as existing pseudo-symplectic schemes are presented in Section 3. The performances of three selected methods are discussed in Section 4 by means of numerical tests. Concluding remarks are given in Section 5.

2. Spatial and temporal discretizations

The incompressible Navier–Stokes equations in Cartesian coordinates read:

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \tag{1}$$

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{2}$$

where summation over repeated indices is assumed. In the framework of finite-difference or finite-volume methods, a semi-discrete version of Eqs. (1–2) can be expressed as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} + \mathbf{C}(\mathbf{u})\mathbf{u} = -\mathbf{G}\mathbf{p} + \frac{1}{\mathrm{Re}}\mathbf{L}\mathbf{u}, \tag{3}$$

$$\mathbf{M}\mathbf{u} = \mathbf{0}, \tag{4}$$

where $\mathbf{u}$ is the discrete velocity vector containing the three components on the three-dimensional mesh, $\mathbf{u} = \left[\mathbf{u}_x\, \mathbf{u}_y\, \mathbf{u}_z\right]^T$, the matrices $\mathbf{G} \in R^{N_\mathbf{u} \times N_p}$ and $\mathbf{M} \in R^{N_p \times N_\mathbf{u}}$ are the discrete gradient and divergence operators, respectively, while $\mathbf{L} \in R^{N_\mathbf{u} \times N_\mathbf{u}}$ is the block-diagonal Laplacian operator. The convective term is expressed as the product of a linear convective operator $\mathbf{C}(\mathbf{u})$ and $\mathbf{u}$. The specific forms of the operators $\mathbf{C}$, $\mathbf{L}$, $\mathbf{G}$ and $\mathbf{M}$ depend upon the details of the discretization scheme. For the sake of simplicity, equally spaced Cartesian grids will be considered in the following. This hypothesis does not prevent the generality and can be easily extended by considering a relevant inner product. It will also be assumed that the differential operators are discretized consistently, e.g. $\mathbf{G}^T = -\mathbf{M}$. Note that the index-2 Differential Algebraic Equation (DAE) system of Eqs. (3–4) can be recast concisely by enforcing the incompressibility constraint through the solution of the pressure Poisson equation [9]. Substitution of the constraint leads to the ODE system

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{P}\mathbf{F}(\mathbf{u})\,\mathbf{u}, \tag{5}$$

where $\mathbf{F} = -\mathbf{C}(\mathbf{u}) + \frac{1}{\mathrm{Re}}\mathbf{L}$ and the projection operator $\mathbf{P} = \mathbf{I} - \mathbf{G}\mathcal{L}^{-1}\mathbf{M}$, with $\mathcal{L} = \mathbf{M}\mathbf{G}$, has been introduced.

This work is focused on the evolution of discrete kinetic energy. A global kinetic energy is defined as $E = \mathbf{u}^T\mathbf{u}/2$, and its semi-discrete evolution equation reads

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\mathbf{u}^T\mathbf{C}(\mathbf{u})\mathbf{u} - \mathbf{u}^T\mathbf{G}\mathbf{p} + \frac{1}{\mathrm{Re}}\mathbf{u}^T\mathbf{L}\mathbf{u}. \tag{6}$$

In Eq. (6), the only physical contribution is due to the diffusive term, that correctly dissipates energy since $\mathbf{L}$ is a negative-definite matrix. The pressure gradient contribution vanishes if $\mathbf{G}^T = -\mathbf{M}$ and $\mathbf{M}\mathbf{u} = 0$. It is useful to recall that this is true for *regular* or *staggered* arrangements of flow variables (using the terminology given in [10]), whereas pressure can contribute to the kinetic energy balance in *collocated* layouts as an error of order $\mathcal{O}(\Delta t^2 \Delta x^2)$ [11]. The convective term preserves energy if a skew-symmetric operator is adopted [12]. This property can be achieved in various ways; most notably, one can either discretize the so-called *skew-symmetric form* of convection [13], or adopt a proper staggered arrangement for the flow variables, with the convective term discretized in conservative formulation [14,10]. In the latter case, simultaneous enforcement of discrete mass conservation is required. In this work, discretely energy-conserving spatial schemes will be employed. In such cases, Eq. (5) forms a system of ODE possessing global kinetic energy as a quadratic invariant, for $\mathrm{Re} \to \infty$.

This short note is focused on numerical methods that are capable of preserving energy also for the time-advancement step. In general, time integration schemes do not preserve the quadratic invariants of the continuous system of ODE. While all RK and linear multistep methods preserve linear invariants [15], multistep schemes do not preserve quadratic invariants, while this is possible for some special implicit Runge–Kutta methods.

A general s-stage Runge–Kutta method applied to Eq. (5) can be expressed as

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \sum_{i=1}^{s} b_i \widetilde{\mathbf{F}}(\mathbf{u}_i)\mathbf{u}_i \tag{7}$$

$$\mathbf{u}_i = \mathbf{u}^n + \Delta t \sum_{j=1}^{s} a_{ij} \widetilde{\mathbf{F}}(\mathbf{u}_j)\mathbf{u}_j, \tag{8}$$