A low-cost time-advancing strategy for energy-preserving turbulent simulations

By F. Capuano†‡, G. Coppola‡, G. Balarac¶, H. J. Bae AND L. de Luca‡

Energy-conserving discretizations are widely regarded as a fundamental requirement for high-fidelity simulations of turbulent flows. The skew-symmetric splitting of the nonlinear term is a well-known approach to obtain semi-discrete conservation of energy in the inviscid limit. However, its computation is roughly twice as expensive as that of the divergence or advective forms alone. A novel time-advancement strategy that retains the conservation properties of skew-symmetric-based schemes at a reduced computational cost has been developed. This method is based on properly constructed Runge-Kutta schemes in which a different form (advective or divergence) for the convective term is adopted at each stage. A general framework is presented to derive schemes with prescribed accuracy on both solution and energy conservation. Simulations of homogeneous isotropic turbulence show that, on equal results, the new procedure can be considerably faster than skew-symmetric-based techniques.

1. Introduction

Demand for accurate numerical computations of turbulent flows, with both DNS and LES, has posed many challenges to the numerical community, pushing research efforts toward the construction of suitable new discretization techniques. In the context of laminar and Reynolds-Averaged Navier-Stokes equations, the classical compromise between accuracy and stability of the discretization has often been represented by upwind-like schemes. This solution, however, has been shown not to be feasible in DNS and LES (Mittal & Moin 1997), owing to the large amount of artificial numerical dissipation introduced by upwind schemes. The straightforward employment of central non-dissipative schemes, on the other hand, can pose severe stability issues, due to the nonlinear amplification of aliasing errors that occur in computing convective terms (Phillips 1959).

A possible solution to these counteracting requirements lies in the employment of nondissipative discretizations able to mimic, on a discrete level, the conservation of important invariants of the continuous equations (Koren *et al.* 2013). In the context of incompressible flows, conservation of kinetic energy in the inviscid limit can be shown to be strongly related to the preservation of some of the fundamental symmetries of the continuous operators on the discrete level (Verstappen & Veldman 2003).

In the framework of spatial discretizations of the convective term, use of the so-called skew-symmetric form has been shown to guarantee *a priori* semi-discrete conservation of energy for several high-order centered schemes, over both regular and staggered grid systems (Morinishi *et al.* 1998). The skew-symmetric form has also proved to be beneficial in terms of aliasing errors (Kravhcenko & Moin 1997). For these reasons, the

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skew-symmetric form of the nonlinear convective term is commonly adopted, and this underlying philosophy has also been employed in the context of compressible flows (Honein & Moin 2004) and for finite volume methods (Kok 2009). However, straightforward discretization of the skew-symmetric form is more expensive than classical divergence or advective forms, since evaluation of two derivatives is required for each nonlinear component of the convective term (Zang 1991). Any attempt to reduce the number of derivative evaluations in computing the convective term requires the employment of divergence or advective forms, which are not guaranteed to preserve energy, at least on non-staggered or non-uniform grids.

All these considerations refer to the problem of spatial discrete conservation. In classical analyses, the time advancement is performed in a semi-discretized approach, and the conservation properties of the numerical time integration procedure are not usually investigated in detail. Full energy conservation (i.e., in space as well as in time) can only be obtained by means of implicit methods (Sanderse 2013), but the strong demand for low-cost numerical procedures usually dictates the use of explicit time-stepping.

In this paper, a novel time-advancement strategy is presented. By weighting temporal and spatial errors, this new method is able to recover the conservation properties of skew-symmetric-based schemes just by using the more economical advective or divergence forms. It has been found that optimal energy-conservation properties can be achieved by properly constructed explicit Runge-Kutta schemes in which a different form for the convective term is adopted at each stage. The main advantage is that, on almost identical results, this method can be considerably faster than skew-symmetric-based techniques.

2. Problem formulation

In this work, the incompressible Navier-Stokes equations

$$\frac{\partial u_i}{\partial t} + \mathcal{N}_i(u) = -\frac{\partial p}{\partial x_i} + \frac{1}{\mathrm{Re}}\frac{\partial^2 u_i}{\partial x_j \partial x_j}, \tag{2.1}$$

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{2.2}$$

are considered, where $\mathcal{N}_i(u)$ is the non-linear convective term and Re is the Reynolds number. When posed on a periodic domain Ω, Eqs. (2.1)-(2.2) possess a number of invariants, most notably the momentum $m = \int_\Omega u_i dV$ and, for $\mathrm{Re} \to \infty$, the kinetic energy $e = \int_\Omega u_i^2/2\, dV$, which represent the linear and quadratic invariants, respectively. The values of momentum and kinetic energy remain fixed to their initial values during time evolution. In a continuous setting, these properties hold for any expression adopted for the non-linear term, which can be cast in several analytically equivalent forms, for instance

$$(Div.)_i \equiv \frac{\partial u_j u_i}{\partial x_j}, \tag{2.3}$$

$$(Adv.)_i \equiv u_j \frac{\partial u_i}{\partial x_j}, \tag{2.4}$$

$$(Skew.)_i \equiv \frac{1}{2}\frac{\partial u_j u_i}{\partial x_j} + \frac{1}{2} u_j \frac{\partial u_i}{\partial x_j}. \tag{2.5}$$

These are referred to as divergence, advective and skew-symmetric forms, respectively. Other forms can also be constructed (e.g., rotational), but will not be considered in this

study. When discretized, Eqs. (2.3)-(2.5) have been shown to behave differently, both in terms of conservation properties (Morinishi *et al.* 1998) and aliasing issues (Kravhcenko & Moin 1997). In the following section, the discrete conservation properties of a class of semi-discretization methods will be analyzed.

2.1. *Conservation properties of semi-discretized N-S equations*

A semi-discretized version of Eqs. (2.1)-(2.2) can be expressed as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} + \mathbf{C}(\mathbf{u})\mathbf{u} = -\mathbf{G}\mathbf{p} + \frac{1}{\mathrm{Re}}\mathbf{L}\mathbf{u}, \tag{2.6}$$

$$\mathbf{M}\mathbf{u} = \mathbf{0}, \tag{2.7}$$

where $\mathbf{u}$ is the discrete velocity vector, $\mathbf{G} \in R^{N_\mathbf{u} \times N_p}$ 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. The convective term is expressed as the product of a linear block-diagonal convective operator $\mathbf{C}(\mathbf{u})$ and $\mathbf{u}$:

$$\mathbf{C}(\mathbf{u})\mathbf{u} = \begin{bmatrix} \boldsymbol{\mathcal{C}}(\mathbf{u}) & & \\ & \boldsymbol{\mathcal{C}}(\mathbf{u}) & \\ & & \boldsymbol{\mathcal{C}}(\mathbf{u}) \end{bmatrix} \begin{bmatrix} \mathbf{u}_x \\ \mathbf{u}_y \\ \mathbf{u}_z \end{bmatrix}, \tag{2.8}$$

where the single operator $\boldsymbol{\mathcal{C}}(\mathbf{u})$ can assume one of the following forms:

$$\boldsymbol{\mathcal{C}}^{\mathrm{div}} = \mathbf{D}_x\mathbf{U}_x + \mathbf{D}_y\mathbf{U}_y + \mathbf{D}_z\mathbf{U}_z, \tag{2.9}$$

$$\boldsymbol{\mathcal{C}}^{\mathrm{adv}} = \mathbf{U}_x\mathbf{D}_x + \mathbf{U}_y\mathbf{D}_y + \mathbf{U}_z\mathbf{D}_z, \tag{2.10}$$

$$\boldsymbol{\mathcal{C}}^{\mathrm{skew}} = \frac{1}{2}\left(\boldsymbol{\mathcal{C}}^{\mathrm{div}} + \boldsymbol{\mathcal{C}}^{\mathrm{adv}}\right). \tag{2.11}$$

In Eqs. (2.9)-(2.11), the matrices $\mathbf{D}$ and $\mathbf{U}$ represent the discrete derivative operators and the diagonal matrices of the discretized velocity components along the three directions (i.e., $\mathbf{U} = \mathrm{diag}(\mathbf{u})$).

Centered finite-difference and spectral discretizations on a periodic, equally spaced grid will be considered here. The velocity components u_i and pressure p are stored at the same points. Under such hypotheses, the derivative operators satisfy a discrete summation-by-parts rule; from an algebraic point of view, this implies that the derivative matrices are all skew-symmetric, $\mathbf{D}^T = -\mathbf{D}$. As a consequence, it can easily be shown that the convective operator $\mathbf{C}^{\mathrm{skew}}$ also inherits this property for all $\mathbf{u}$, unlike the other two forms.

The discrete conservation properties can be analyzed by deriving the evolution equation of the discrete kinetic energy $E = \|\mathbf{u}\|^2/2$, which reads

$$\frac{\mathrm{d}E}{\mathrm{d}t} = -\mathbf{u}^T\mathbf{C}(\mathbf{u})\mathbf{u} - \mathbf{u}^T\mathbf{G}\mathbf{p} + \frac{1}{\mathrm{Re}}\mathbf{u}^T\mathbf{L}\mathbf{u}. \tag{2.12}$$

In Eq. (2.12), the pressure term is conservative if $\mathbf{G}^T = -\mathbf{M}$ and $\mathbf{M}\mathbf{u} = 0$. The convective and diffusive terms appear as quadratic forms with associated matrices $\mathbf{C}(\mathbf{u})$ and $\mathbf{L}$, respectively. The diffusive term is clearly not conservative (the operator $\mathbf{L}$ is a negative-definite matrix), while the convective term is conservative if the skew-symmetric operator of Eq. (2.11) is adopted. In the other two cases, the convection matrices $\mathbf{C}(\mathbf{u})$ are in general not skew-symmetric and hence conservation of energy is not guaranteed.

A more in-depth analysis reveals that errors coming from the divergence and advective forms are of opposite sign. The key observation is that, for skew-symmetric discrete

derivative operators, the following relation holds

$$\left(\mathbf{C}^{\mathrm{adv}}\right)^T = -\mathbf{C}^{\mathrm{div}}, \tag{2.13}$$

which immediately implies $-\mathbf{u}^T\mathbf{C}^{\mathrm{adv}}\mathbf{u} = \mathbf{u}^T\mathbf{C}^{\mathrm{div}}\mathbf{u}$ and hence that the energy variation due to the divergence and advective forms are equal and of opposite sign.

Adoption of the skew-symmetric form, albeit attractive for its beneficial conservation properties, turns out to be more expensive than classical advective and divergence forms. A rough estimate of the computational cost in the two cases shows that the skew-symmetric form requires twice the number of matrix-vector products. The present work aims to develop a new time-advancing strategy that is able to retain the beneficial properties of the skew-symmetric form at a reduced computational cost.

3. The alternating Runge-Kutta strategy

The rationale underlying this method stems from the fact that the global errors on energy conservation associated with discretized divergence and advective forms are of opposite sign. The basic idea is to take advantage of the time-advancement scheme to cancel the errors of these two forms up to a certain order of accuracy. By using only divergence or advective forms, the resulting scheme can be more cost-effective than a skew-symmetric-based one. In the following analysis, only inviscid flow is considered ($\mathrm{Re} \to \infty$), since interest is focused exclusively on the conservation properties of the convective term. The core of the method consists in advancing the governing equations by means of a modified explicit Runge-Kutta algorithm, which can be expressed as

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \sum_{i=1}^{s} b_i \mathbf{C}_i(\mathbf{u}_i)\mathbf{u}_i - \Delta t \mathbf{G}\mathbf{p}^{n+1}, \tag{3.1}$$

$$\mathbf{u}_i = \mathbf{u}^n - \Delta t \sum_{j=1}^{s} a_{ij} \left(\mathbf{C}_j(\mathbf{u}_j)\mathbf{u}_j - \mathbf{G}\mathbf{p}_j\right), \tag{3.2}$$

where s is the number of stages, a_{ij} and b_i are the Runge-Kutta coefficients, and pressure is to be solved from the Poisson equation, $\mathbf{p}_j = \mathbf{L}^{-1}\mathbf{M}\mathbf{C}_j(\mathbf{u}_j)\mathbf{u}_j$. Eqs. (3.1)-(3.2) differ from the standard Runge-Kutta procedure in that they can accommodate a different formulation for the non-linear term within the stages. In fact, the operator $\mathbf{C}$ is indexed by a suffix, meaning that it can be expressed in either divergence or advective form at each stage (Eqs. (2.9) and (2.10), respectively).

The overall aim of this method is to find a set of coefficients, along with a sequence of divergence and advective forms, that maximizes the formal order of accuracy on solution and energy conservation. A prescribed order of accuracy for the discrete solution $\mathbf{u}$ can be attained by imposing the classical order conditions (Butcher 2004). The resulting non-linear system is usually undetermined: the remaining degrees of freedom can be exploited to impose an additional set of equations for energy conservation. The derivation of these conditions is the central part of the novel procedure and will be described in the next section.

3.1. *Energy analysis*

The total energy error introduced over a single time-step advancement by Eqs. (3.1)-(3.2) can be obtained by taking the inner product between $\mathbf{u}^{n+1}$ and itself. By defining

$\Delta E = E^{n+1} - E^n$, Eqs. (3.1)-(3.2) can be manipulated to yield

$$\frac{\Delta E}{\Delta t} = \underbrace{-\sum_{i=1}^{s} b_i \mathbf{u}_i^T \mathbf{C}_i\left(\mathbf{u}_i\right)\mathbf{u}_i}_{I} \underbrace{-\frac{\Delta t}{2}\sum_{i,j=1}^{s}\left(b_i a_{ij} + b_j a_{ji} - b_i b_j\right)\mathbf{u}_i^T \mathbf{C}_i^T\left(\mathbf{u}_i\right)\mathbf{C}_j\left(\mathbf{u}_j\right)\mathbf{u}_j}_{II}. \tag{3.3}$$

The two terms on the right-hand side of Eq. (3.3) can be defined as

I) spatial error: $\sum_{i=1}^{s} b_i \mathbf{u}_i^T \mathbf{C}_i\left(\mathbf{u}_i\right)\mathbf{u}_i$,

II) temporal error: $\frac{\Delta t}{2}\sum_{i,j=1}^{s}\left(b_i a_{ij} + b_j a_{ji} - b_i b_j\right)\mathbf{u}_i^T \mathbf{C}_i^T\left(\mathbf{u}_i\right)\mathbf{C}_j\left(\mathbf{u}_j\right)\mathbf{u}_j$.

The first depends primarily on spatial discretization, as the s quadratic forms are identically zero if a skew-symmetric matrix $\mathbf{C}$ is adopted. The second quantity has a more complex structure, and can be nullified by so-called symplectic methods (Sanderse 2013), a special class of implicit Runge-Kutta schemes for which $b_i a_{ij} + b_j a_{ji} - b_i b_j = 0$. For standard methods ($\mathbf{C}_i \equiv \mathbf{C}$), the temporal error inherits the same order of the method and does not vanish in general, even in the case of skew-symmetric operators $\mathbf{C}$.

The use of different discretized forms inside the stages of the Runge-Kutta procedure gives rise to new possibilities for obtaining cost-effective energy-preserving algorithms. An appropriate choice of Runge-Kutta coefficients can lead to methods in which the mixed spatial and temporal errors are nullified up to a certain order of accuracy.

The starting point of the analysis is the expansion of Eq. (3.3) as a Taylor series in the time increment Δt. To this end, Eqs. (3.1)-(3.2) can be plugged into Eq. (3.3); by using the linearity of the convective operator $\mathbf{C}_i(\mathbf{u}_i)$ with respect to $\mathbf{u}_i$, after some manipulation one obtains (cf. Capuano *et al.* 2014)

$$\frac{\Delta E}{\Delta t} = \overbrace{-\mathbf{u}^T\left[\sum_i b_i \mathbf{C}_i\right]\mathbf{u}}^{1^{\text{st}}\text{ order term}} + \underbrace{\frac{\Delta t}{2}\mathbf{u}^T\left[\sum_{ij} 2 b_i a_{ij}\left(\mathbf{C}_i\mathbf{C}_j + \mathbf{C}_{ij}\right) + g_{ij}\mathbf{C}_i^T\mathbf{C}_j\right]\mathbf{u}}_{2^{\text{nd}}\text{ order term}} + O\left(\Delta t^2\right), \tag{3.4}$$

where $\mathbf{u} = \mathbf{u}^n$, $g_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j$, $\mathbf{C}_{ij} = \mathbf{C}_i\left(\mathbf{C}_j\left(\mathbf{u}^n\right)\mathbf{u}^n\right)$. In Eq. (3.4) and hereinafter, the operator $\mathbf{C}$ is assumed to be evaluated at $\mathbf{u}^n$ if not otherwise specified.

Equation (3.4) constitutes the basic relation for construction of optimized Runge-Kutta schemes. A proper choice of the coefficients b_i and a_{ij} can nullify both the first- and second-order terms appearing in Eq. (3.4), leading to schemes with optimal conservation properties. Determination of a suitable set of conditions is obtained in four steps:

(a) fix the number of stages of the method;
(b) choose a sequence of advective (A) and divergence (D) forms;
(c) group the resulting terms of Eq. (3.4) into combinations of few independent terms;
(d) impose conditions on a_{ij} and b_i to nullify the terms.

As regards step (c), it is easy to show that Eq. (2.13) allows the various products or compositions of matrices $\mathbf{C}_i$ to be transformed into groups of fewer independent terms. In particular, the linear combination appearing in the the first-order contribution can be

collected into a single term proportional to one of the forms $\mathbf{C}^{\mathrm{div}}$ or $\mathbf{C}^{\mathrm{adv}}$. By employing Eq. (2.13), and after some manipulation, it can also be shown that each of the $3s$ terms $\mathbf{C}_i\mathbf{C}_j$, $\mathbf{C}_i(\mathbf{C}_j\mathbf{u})$ and $\mathbf{C}_i^T\mathbf{C}_j$ can be recast into one of the three basic forms $\mathbf{C}^{\mathrm{adv}}\mathbf{C}^{\mathrm{adv}}$, $\mathbf{C}^{\mathrm{adv}}\mathbf{C}^{\mathrm{div}}$, and $\mathbf{C}^{\mathrm{div}}\mathbf{C}^{\mathrm{adv}}$. For a detailed description of this procedure in a one-dimensional setting the reader is referred to Capuano *et al.* (2014). The application of step (d) leads to the conclusion that one additional linear constraint on the coefficients b_i has to be added to enforce first-order conservation of energy, whereas three nonlinear equations on the coefficients b_i and a_{ij} are needed for second-order conservation. The constraints on energy can be coupled to classical order conditions to give a global system for determining new Runge-Kutta schemes.

3.2. *New Runge-Kutta schemes*

In principle, alternating Runge-Kutta schemes with an arbitrary number of stages can be derived and analyzed. However, a thorough derivation is beyond the scope of this paper. Here, attention will be focused on four-stage methods, which allow for a relatively large number of degrees of freedom and have been applied historically to numerical simulations of turbulent flows.

Four-stage methods provide $s(s+1)/2 = 10$ degrees of freedom. The third- and fourth-order conditions on solution take 4 and 8 equations, respectively, whereas the first- and second-order conditions on energy conservation for alternating schemes take 1 and 3 equations. In order to handle all possibilities, the new methods are labeled by an acronym indicating the order of accuracy on solution (S) and on energy conservation (E). A cost-coefficient proportional to the number of derivatives required per time-step is also reported in brackets, to serve as a simple cost metric for comparing the performances of the various schemes. In the case of four-stage methods, the number of matrix-vector products is $4d^2$ for advective and divergence forms and $8d^2$ for the skew-symmetric form, where d is the number of dimensions. The cost-coefficients in these two cases are 4 and 8, respectively. With this notation, two families of new schemes are expected: 4S1E(4) and 3S2E(4), which have to be compared to 4S4E(8) skew-symmetric methods.

A large number of 4S1E(4) schemes can easily be obtained by applying the first-order condition on energy to the parametrized fourth-order families provided in classical books (e.g., Butcher 2004). Perhaps the most convenient choice is to use an alternating version of the classical Runge-Kutta scheme (RK4). If one employes an ADAD or a DADA sequence inside the stages, the RK4 satisfies the first-order condition on energy conservation while retaining fourth-order accuracy on solution. The alternating RK4 will be considered as the reference 4S1E(4) scheme for the subsequent sections.

In the case of 3S2E(4) schemes, solutions exist only for the two couples of sequences DADA/ADAD and ADDA/DAAD. For the former, two families of solutions are available, each with two free parameters. The Butcher array is given by

$$
\begin{array}{c|cccc}
0 & & & \\
\frac{3\theta_1 \pm \mathcal{A}}{6\theta_1} & 0 & & \\
\frac{1}{8\theta_1} & \frac{1}{8\theta_1} & 0 & \\
-\frac{3\theta_1 - 16\theta_1\theta_2 + 4\theta_2\mathcal{B} + 4\theta_1\mathcal{B} \pm 2\mathcal{A}}{24\theta_1\theta_2} & \frac{1}{8\theta_2} & \frac{\theta_1 \pm \mathcal{A}}{6\theta_2} & 0 \\
\hline
 & \frac{1}{2} - \theta_1 & \frac{1}{2} - \theta_2 & \theta_1 \quad \theta_2
\end{array},
$$

where

$$\mathcal{A} = 3\theta_2\sqrt{-\frac{\theta_1(10\theta_1-3)}{3\theta_2(2\theta_2-1)}},\ \mathcal{B} = \theta_1 \pm \mathcal{A}.$$

The parameters θ_1 and θ_2 can be conveniently chosen to lead to a computationally efficient Runge-Kutta method. On the contrary, for the couple ADDA/DAAD it is much more difficult to obtain a solution in a closed form, even by using a symbolic tool. However, notable solutions can be obtained by adding further conditions that set some coefficients equal to zero. Two significant examples are

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{3} & 0 & & & \\ 0 & 1 & 0 & & \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & \\ \hline & \frac{1}{8} & \frac{3}{8} & \frac{1}{8} & \frac{3}{8} \end{array} \qquad \begin{array}{c|cccc} 0 & & & & \\ 1 & 0 & & & \\ 0 & \frac{1}{3} & 0 & & \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & \\ \hline & \frac{1}{8} & \frac{1}{8} & \frac{3}{8} & \frac{3}{8} \end{array},$$

3S2E(4)$_1$ 3S2E(4)$_2$

which have both third-order accuracy on the solution and second-order accuracy on energy conservation for both sequences ADDA and DAAD. The first one will be the reference 3S2E(4) scheme for the numerical tests presented in the following section.

4. Numerical results

4.1. *2D periodic inviscid flow*

Two-dimensional inviscid flow simulations are carried out on a periodic domain to confirm the theoretical results obtained in the previous sections. Following Morinishi *et al.* (1998), a square region of size $2\pi \times 2\pi$ is considered, discretized on a mesh of 16×16 mesh points. The solenoidal initial velocity field is constructed from a stream function of random numbers, normalized such that $\langle u \rangle = \langle v \rangle = 0$ and $\langle E_0 \rangle = 1.0$. A centered second-order finite-difference scheme is used for convection; for time-advancement, the various Runge-Kutta schemes developed in Section 3.2 are used.

Figure 1 (left) shows the time-step convergence of the energy error for three Runge-Kutta methods. The slopes confirm the predicted orders of accuracy for the new schemes 4S1E(4) and 3S2E(4), proving the consistency of the theoretical framework. The divergence form gives a constant error, which corresponds to the spatial contribution of Eq. (3.3); a similar behavior is found for the advective form (not shown here).

4.2. *Inviscid Homogeneous Isotropic Turbulence (HIT)*

As a second test-case, simulations of inviscid homogeneous isotropic turbulence (HIT) are performed. A standard pseudo-spectral code has been adopted, using a projection method in spectral space to enforce the divergence-free condition. Modified wavenumbers are used to emulate centered second-order finite-difference schemes (Kravhcenko & Moin 1997). The tests are performed without subgrid-scale (SGS) model and the simulations are not de-aliased. The initial condition is designed to satisfy a given energy spectrum, typical of decaying isotropic turbulence. A grid of 32^3 grid points on a domain of length 2π is used. The simulations differ only by the form of the convective term and the Runge-Kutta scheme used for time advancement.

The time evolution of the turbulence kinetic energy is shown in Figure 1 (right). The

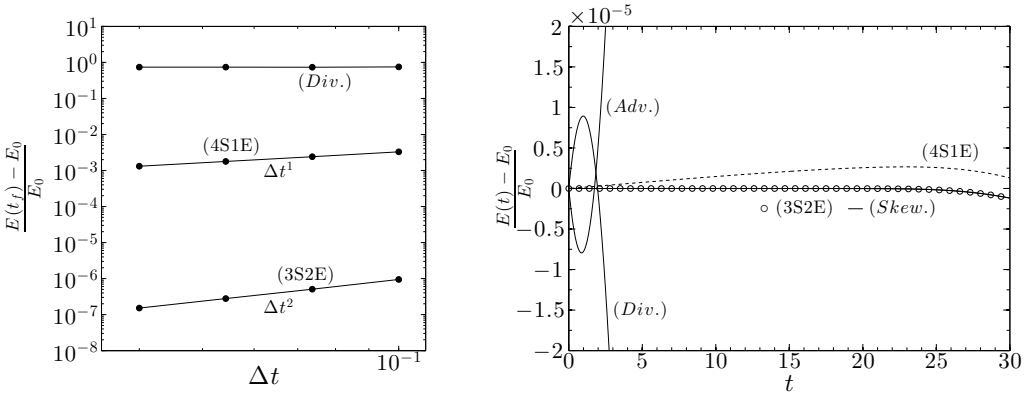

FIGURE 1. Results for periodic, inviscid flow simulations. Time-step convergence of the relative error on energy conservation for the 2D case (left panel). Time evolution of kinetic energy conservation error for inviscid HIT (right panel).

TABLE 1. Kinetic energy conservation errors at $t = 30s$ (see Figure 1) and corresponding CPU time for different Runge-Kutta methods and convective forms

Scheme	ΔE at $t = 30$	$T_{CPU}/100\Delta t$
$(Div.)$	$+\infty$	5.40 s
$(Adv.)$	$+\infty$	4.04 s
$(Skew.)$	-1.1816×10^{-6}	8.40 s
(3S2E)	-1.1896×10^{-6}	4.78 s
(4S1E)	$+1.3044 \times 10^{-6}$	4.78 s

advective and divergence forms soon diverge due to violation of kinetic energy conservation. On the other hand, the energy-preserving formulations are stable. In particular, the 3S2E(4) scheme is very close to the skew-symmetric form, while the 4S1E(4) shows a slight over-production of energy. These considerations are confirmed by the computational results shown in Table 1, in which the CPU times are also reported. In this test, the projection method does not require any iterative algorithm, hence computation of the convective term has an important impact on the global computational time. The proposed Runge-Kutta schemes allow a saving in computational time of about 43% with respect to the skew-symmetric form. Finally, it is noteworthy that for the 3S2E(4) scheme used, the error on energy is dissipative, hence the scheme is stable for long-time simulations.

4.3. *Large-eddy simulation of forced HIT*

In the last test, large-eddy simulation of forced HIT is performed and compared with direct numerical simulations. The same pseudo-spectral code of the previous test is used here, with the diffusive term being computed exactly. The forcing strategy consists of freezing the low wavenumbers ($|\vec{k}| < 3$) to avoid the introduction of randomness as in classic forcing schemes. In this test, centered second-order finite-difference schemes are mimicked by using modified wavenumbers. A dynamic Smagorinsky model is used to

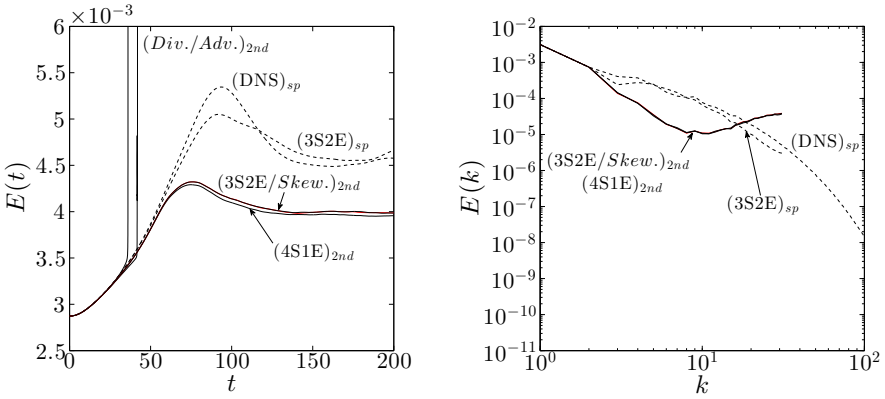

FIGURE 2. Results for forced HIT. Time evolution of kinetic energy (left panel). Three-dimensional energy spectra (right panel).

account for subgrid-scales (Germano *et al.* 1991; Lilly 1992). For the DNS the Navier-Stokes equations are discretized using 256^3 grid points on a domain of length 2π, whereas the LES are performed on 64^3 grid points. The time step is computed from the CFL condition, with a maximum CFL number of 0.5. All the results shown in this work correspond to no-dealiased simulations (but similar results are found with a dealiasing procedure). Note that for LES, the skew-symmetric form adds only 15% of additional CPU time, because the SGS model computation with the dynamic procedure has a significant impact on overall CPU time.

Figure 2 shows the kinetic energy evolution in time and the three-dimensional energy spectra for various Runge-Kutta schemes and convective forms. Two spatial schemes are considered for LES: second-order and spectral differentiation. A spectral DNS curve is also shown for comparison. In the spectral case (dashed curves) all methods coincide, both for LES and DNS. Differences emerge when a second-order modified wavenumber is used: the divergence and advective forms are unstable, while the 4S1E(4) scheme gives a slight under-prediction of energy. In both cases, the 3S2E(4) scheme is confirmed to be practically equivalent to the skew-symmetric form, its predictions being identical on plotting accuracy. Similar results can be found in wavenumber space, showing that the beneficial aliasing properties of the skew-symmetric form are also retained by the new schemes.

5. Conclusions

A novel time-advancing strategy has been developed for efficient energy-preserving simulations of incompressible turbulent flows. The method is based on a Runge-Kutta scheme in which the divergence or advective forms for convection are suitably alternated within the stages to retain the conservation properties of the skew-symmetric form up to a certain order of accuracy. A comprehensive theoretical framework has been established to derive new alternating Runge-Kutta methods with prescribed order of accuracy on both solution and energy-conservation. Direct and large-eddy simulations of homogeneous isotropic turbulence have proved that, in practical situations, these new methods provide results almost identical to those of standard skew-symmetric schemes. The maximum advantage in terms of CPU time is achieved when no subgrid-scale model is used. In this case, the time saving can reach up to 43%.

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