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A MINIMUM-DISSIPATION TIME-INTEGRATION STRATEGY FOR LARGE-EDDY SIMULATION OF INCOMPRESSIBLE TURBULENT FLOWS

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Abstract. *Adaptive time stepping can significantly enhance the accuracy and the efficiency of computational methods. In this work, a time-integration strategy with adaptive time step control is proposed for large-eddy simulation of turbulent flows. The algorithm is based on Runge-Kutta methods and consists in adjusting the time-step size dynamically to ensure that the numerical dissipation rate due to the temporal scheme is smaller than the molecular and subgrid-scale ones within a desired tolerance. The effectiveness of the method, as compared to standard CFL-like criteria, is assessed by large-eddy simulations of the three-dimensional Taylor-Green Vortex.*

1 INTRODUCTION

Large-eddy simulations (LES) of turbulent flows are typically carried out on spatially coarse grids and by using correspondingly large time steps. This poses severe challenges to the numerical method, both in terms of accuracy and stability. From the point of view of spatial discretization, typical remedies are energy-conserving and/or high-resolution schemes, which are capable of suppressing nonlinear instabilities while allowing accurate results with only a few points per wavelength [1]. On the other hand, less care is generally taken to control the time-integration error. Indeed, simulations are usually time-advanced by means of standard explicit or semi-implicit methods (e.g., multistep or Runge-Kutta schemes for convection and Crank-Nicolson for diffusion) and the time step is loosely chosen to satisfy the linear stability constraint [2]. The choice of the time-integration strategy is regarded as to be more important for the overall efficiency of the LES solution than for the accuracy [3], and recent trends tend to maximize the time step by dynamically analyzing the eigenvalues of the semi-discretized system [4].

The concepts of adaptive time stepping and error control in the framework of time integration of the Navier-Stokes equations have been explored only a few times in literature, despite the great potential benefits in terms of both accuracy and efficiency. John and Rang [5] compared different classes of time-integration schemes for the 2D laminar flow around a circular cylinder, using embedded methods to adjust the time step. They obtained good efficiency but also reported high sensitivity of the results with respect to the chosen tolerance. Kay *et al.* [6] proposed an implicit trapezoidal rule in conjunction with an explicit Adams-Bashforth method for error control, and concluded that adaptive time stepping is essential for unsteady flows with multiple time scales. Using an embedded error control method, Colomes and Badia [7] gained a 42.8% reduction of CPU time with respect to a fixed time step integration, again for the case of laminar flow around a circular cylinder case. To the authors' knowledge, adaptive time-integration methods have not been analyzed thoroughly for turbulent flow simulations.

The scope of this work is to propose an adaptive time-stepping strategy aimed to control the temporal error, with the goal of creating an efficient minimum-dissipation time-integration method for LES of turbulent flows. The proposed strategy is based on Runge-Kutta methods and relies on the analysis of the global discrete energy balance induced by the spatial and temporal discretizations. The time-step size is then adjusted dynamically to ensure that the numerical dissipation rate due to the temporal error is smaller than the molecular and subfilter-scale model ones within a desired tolerance. The method is independent of the spatial mesh, and can be implemented with minimum additional computational cost into structured and unstructured energy-preserving codes.

The paper is organized as follows. Section 2 presents the theoretical framework and the discretization of the Navier-Stokes equations. The new adaptive time-stepping

strategy is outlined in Section 3. In Section 4, the effectiveness of the proposed approach is assessed by large-eddy simulations of the Taylor-Green Vortex. Concluding remarks are given in Section 5.

2 FULLY DISCRETE NAVIER-STOKES EQUATIONS

In this work, the filtered incompressible Navier-Stokes equations are considered,

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

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0 \ , \tag{2}$$

where $\mathcal{N}_i(u)$ is the nonlinear convective term, $\mathcal{R}_i = \overline{\mathcal{N}_i(u)} - \mathcal{N}_i(\overline{u})$ is the subfilter scale term and the overbar denotes a properly defined filtering operator which provides scale separation. The use of a subfilter-scale model yields $\mathcal{R}_i\left(u, \overline{u}\right) \rightarrow \mathcal{R}_i\left(\overline{u}\right)$.

In the framework of finite-difference or finite-volume methods, a semi-discrete version of Eqs. (1)-(2) can be expressed as

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

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

where $\overline{\mathbf{u}}$ is the filtered discrete velocity vector containing the three components on the three-dimensional mesh, and the matrices $\mathbf{G}$, $\mathbf{M}$, $\mathbf{L}$ are proper spatial discretizations of the gradient, divergence and Laplacian operators respectively. The convective term is expressed as the product of a linear convective operator $\mathbf{C}(\overline{\mathbf{u}})$ and $\overline{\mathbf{u}}$, while $\mathbf{r}\left(\overline{\mathbf{u}}\right)$ is the spatially discretized subfilter-scale model. For the sake of simplicity, equally spaced Cartesian grids will be considered in this work, but this does not come at a loss of generality. It will also be assumed that the differential operators are discretized consistently, e.g. $\mathbf{G}^T = -\mathbf{M}$. Note that Eqs. (3)-(4) constitute an index-2 Differential Algebraic Equation (DAE) system. Upon enforcing the incompressibility constraint via the solution of the pressure Poisson equation [8], one obtains the ODE system

$$\frac{\mathrm{d}\overline{\mathbf{u}}}{\mathrm{d}t} = \mathbf{P}\mathbf{f}\left(\overline{\mathbf{u}}\right) \equiv \widetilde{\mathbf{f}}\left(\overline{\mathbf{u}}\right) \ , \tag{5}$$

where $\mathbf{f} = -\mathbf{C}(\overline{\mathbf{u}})\overline{\mathbf{u}} + \frac{1}{\mathrm{Re}}\mathbf{L}\overline{\mathbf{u}} - \mathbf{r}\left(\overline{\mathbf{u}}\right)$ and $\mathbf{P} = \mathbf{I} - \mathbf{G}\boldsymbol{\mathcal{L}}^{-1}\mathbf{M}$, with $\boldsymbol{\mathcal{L}} = \mathbf{M}\mathbf{G}$, is the projection operator.

Time advancement of the ODE Eq. (5) is now straightforward and can be accomplished by means of any ODE integrator. In this work, Runge-Kutta (RK) methods are

considered, which can be formulated as

$$\overline{\mathbf{u}}^{n+1} = \overline{\mathbf{u}}^{n} + \Delta t \sum_{i=1}^{s} b_i \widetilde{\mathbf{f}}(\overline{\mathbf{u}}_i) \ , \tag{6}$$

$$\overline{\mathbf{u}}_i = \overline{\mathbf{u}}^{n} + \Delta t \sum_{j=1}^{s} a_{ij} \widetilde{\mathbf{f}}(\overline{\mathbf{u}}_j) \ , \tag{7}$$

where a_{ij} and b_i are the RK coefficients, and s is the number of stages.

Since the pioneering works from the Stanford group [9], Runge-Kutta methods have become very popular in the turbulence community due to their favorable properties, such as their self-starting capability and relatively large stability limit. The overwhelming majority of turbulence simulations are nowadays performed by using three-stage (particularly the low-storage Wray's scheme [10]) or four-stage (the classical RK4) methods in conjunction with fractional-step procedures.

3 ADAPTIVE TIME-STEPPING STRATEGY

The scope of this work is to propose an accurate and efficient dynamic selection of the time step size Δt in Eqs. (6)-(7). In numerical simulations of turbulent flows, the time step selection is generally guided by two criteria: i) *accuracy* constraints, i.e. adequate representation of the smallest time scale of motion τ_η, and ii) *stability* constraints due to convective and diffusive terms (for explicit or semi-implicit schemes). These stability constraints read, respectively

$$\frac{U_{\text{max}} \Delta t}{\Delta x} \leq \sigma^c \ , \tag{8}$$

$$\frac{\nu \Delta t}{(\Delta x)^2} \leq \sigma^d \ , \tag{9}$$

where Δt and Δx are the time- and grid-spacing, ν is the kinematic viscosity, U_{max} the maximum velocity over the computational domain, and σ^c and σ^d are two constants that depend on the particular combination of the temporal and spatial schemes employed. In practical computations, explicit schemes are often preferred due to ease of implementation, lower cost per time step, and efficient parallelization (although this depends on the stiffness of the problem). The majority of turbulence computations are indeed performed using explicit time-advancement schemes, and the time step is selected according to the stability constraint. This choice can be also justified on the basis of simple scaling arguments: the stability conditions (8) and (9) can be expressed, in a

proper nondimensional form, as

$$\frac{\Delta t}{\tau_\eta} < \frac{U}{U_{\max}} \mathrm{Re}^{-1/4} \frac{\Delta x}{\eta} \,, \tag{10}$$

$$\frac{\Delta t}{\tau_\eta} < \left(\frac{\Delta x}{\eta} \right)^2 , \tag{11}$$

where $\Delta x/\eta$ is the ratio between the grid spacing and the Kolmogorov size, and U is the characteristic velocity of large eddies. In a wide operative range of these parameters, and especially for LES, in which $\Delta x/\eta$ is typically large, the time step is limited by Eq. (10), thus justifying the use of fully explicit schemes [4]. Furthermore, the resolution requirement (i), i.e. $\Delta t < \tau_\eta$, is often automatically satisfied [2].

The application of criteria (i) and (ii) is in many cases satisfactory, although the actual time-integration error is not being controlled. This can lead to inaccurate and/or inefficient simulations, in which the time step is either under- or over-estimated with respect to the accuracy requirement.

In this regard, adaptive time step size selection is a popular remedy in the numerical community to increase the efficiency of the time-advancement strategy, i.e., to obtain the same accuracy with fewer steps or better accuracy with the same number of steps [11]. Adaptive time stepping techinques are mainly based on the idea of computing a proper (error) controller, and to adjust the step size dynamically and automatically to ensure that the error is kept within the desired values. In most situations, the controller is the local truncation error T^{n+1}, and the updating formula for the time step size to keep it within the desired tolerance δ^u reads

$$\Delta t^{n+1} = \Delta t^n \left| \frac{\delta^u}{T^{n+1}} \right|^{1/(p+1)} , \tag{12}$$

where p is the order of the method. In general, the local trucation error is computed by comparing two numerical solutions, with one being more accurate than the other. This usually leads to non-negligible increase in computational cost, as for the case of the Taylor-series method or the Richardson extrapolation [11]. Of particular interest are methods with built-in error estimates, such as the so-called *embedded* Runge-Kutta schemes, which are able to provide two numerical solutions of different accuracy with little additional computational cost [12]. Embedded methods will be addressed in more detail in future work.

3.1 Minimum-dissipation criterion

The adaptive time-stepping strategy proposed in this paper is inspired by the principle of physics-compatible discretizations [13]. A significant amount of research carried out

in the last two decades has indicated that for convection-dominated, multi-scale problems, it is fundamental for the numerical discretization to preserve the symmetries and the invariants of the continuous system. Particularly for the Navier-Stokes equations, it is now consolidated that kinetic energy, which is an inviscid quadratic invariant of the NS system, should be preserved also on a discrete level. Besides providing a nonlinear stability bound to the computed solution, the occurrence of discrete energy conservation contributes to increase the physical realism of a simulation, by ensuring that the turbulence cascade and/or the subfilter-scale model are not artificially contaminated [14].

A relevant discrete global kinetic energy is defined as $E = \overline{\mathbf{u}}^T\overline{\mathbf{u}}/2$, representing the energy of the filtered velocity field. A fully discrete evolution equation for E can be obtained by manipulating Eqs. (6)-(7), to yield

$$\frac{\Delta E}{\Delta t} = \underbrace{\frac{1}{\mathrm{Re}}\sum_{i=1}^{s} b_i \overline{\mathbf{u}}_i^T \mathbf{L}\overline{\mathbf{u}}_i}_{\varepsilon^{\nu}} - \underbrace{\sum_{i=1}^{s} b_i \overline{\mathbf{u}}_i^T \mathbf{r}\left(\overline{\mathbf{u}}_i\right)}_{\varepsilon^{\mathrm{SGS}}} - \underbrace{\frac{\Delta t}{2}\sum_{i,j=1}^{s}\left(b_i a_{ij} + b_j a_{ji} - b_i b_j\right)\widetilde{\mathbf{f}}_i^T\widetilde{\mathbf{f}}_j}_{\varepsilon^{\mathrm{RK}}} , \quad (13)$$

where $\Delta E = E^{n+1} - E^n$ and $\widetilde{\mathbf{f}}_i = \widetilde{\mathbf{f}}(\mathbf{u}_i)$. The terms in the right-hand side of Eq. (13) are, in order, the viscous (physical) dissipation rate ε^{ν}, the subfilter-scale contribution $\varepsilon^{\mathrm{SGS}}$, and the temporal error $\varepsilon^{\mathrm{RK}}$. It is worth to note that neither the pressure gradient nor the convective term contributions appear in Eq. (13). The former vanishes for staggered arrangements of flow variables [15], while the latter vanishes as a consequence of the skew-symmetry of the convective operator [1]. In practice, this requirement is usually achieved by either discretizing the so-called *skew-symmetric form* of convection [14], or by employing the classical second-order staggered method originally proposed by Harlow and Welch [16]. The resulting discrete spatial conservation of kinetic energy is beneficial for stable and accurate computation of turbulent flows.

In a LES simulation, it would be desirable to have the filtered energy balance be modified only by the viscous dissipation and the modeling terms. For standard explicit methods of order p, the temporal energy error $\varepsilon^{\mathrm{RK}}$ typically decreases with order $q = p$; also, it usually has a dissipative character. The dissipative effects of the temporal error can be more effectively perceived upon definition of an *effective* Reynolds number [17], which in the case of no subgrid-scale model reads

$$\mathrm{Re}^{\mathrm{eff}} \equiv \frac{\sum_i b_i \mathbf{u}_i^T \mathbf{L}\mathbf{u}_i}{\Delta E/\Delta t} . \quad (14)$$

In [17], it has been demonstrated that without proper remedies, the standard explicit schemes commonly used in the turbulence community can lead to deviations in the effective Reynolds number up to 10% with respect to the nominal Reynolds number. It is thus desirable to keep the temporal error $\varepsilon^{\mathrm{RK}}$ bounded as compared to the physical and SGS model terms ε^{ν} and $\varepsilon^{\mathrm{SGS}}$. The above considerations suggest to introduce a

minimum-dissipation criterion, based on ε^{RK}, stating that

$$\chi = \left| \frac{\varepsilon^{\text{RK}}}{\varepsilon^{\nu} + \varepsilon^{\text{SGS}}} \right| < \delta^{E}. \tag{15}$$

To ensure that Eq. (15) is satisfied at each time step, one can apply Eq. (12) and take χ as the error estimate, yielding the updating formula

$$\Delta t^{n+1} = \Delta t^{n} \left| \frac{\delta^{E}}{\chi^{n+1}} \right|^{1/q}, \tag{16}$$

where δ^{E} is the chosen tolerance for χ. Preliminary tests and physical intuition suggest to take $\delta^{E} = 0.01$, i.e., the temporal dissipation rate should not overcome the sum of physical and modeling terms by more than 1%; of course, lower values for δ^{E} can be selected depending on the required accuracy of the problem under study.

Note that the practical implementation of Eq. (16) requires the computation of ε^{RK}, ε^{ν} and ε^{SGS}. The last two terms can be easily computed and are commonly stored in a computer code as useful diagnostic parameters regardless. For what concerns ε^{RK}, it can be obtained by subtraction upon calculation of the global energy, which is another parameter of interest in numerical simulations. Therefore, the adaptive time stepping method based on minimum dissipation can be easily implemented in an existing spatially energy-conserving code with minimum additional cost. It is also worth to note that the method is independent of the spatial discretization method and the underlying mesh (either structured or unstructured). The minimum-dissipation criterion will be hereafter referred to also as the δ^{E} criterion.

3.2 Symplectic and pseudo-symplectic methods

As mentioned in the previous section, standard Runge-Kutta methods of order p lead to temporal energy errors which are, in general, of the same order p. However, special RK schemes exist which are able to eliminate or reduce the magnitude of the temporal error, on equal time step, as outlined in the following.

So-called *symplectic* methods satisfy the condition $b_i a_{ij} + b_j a_{ji} - b_i b_j = 0$, thus leading to exact energy conservation in the inviscid limit, see Eq. (13). A notable example of this class of methods is the one-stage, second-order Gauss scheme, also known as implicit midpoint. Higher-order, fully implicit methods are also available. Symplectic methods are popular in the context of Hamiltonian systems but have been applied to the Navier-Stokes equations only recently [18]. The major drawback of symplectic schemes is their implicit nature, which can lead to unaffordable computational cost for large-scale turbulent simulations.

Alternatively, the energy-conservation property can be satisfied approximately up to an order of accuracy $q > p$, as in the case of *pseudo-symplectic* methods, which are

Method	s	p	q	σ^c	Symbol
RK3	3	3	3	$\sqrt{3}$	$\times$
RK4	4	4	4	2.85	$\circ$
3p6q	5	3	6	2.85	$\square$
4p7q	6	4	7	3.71	$+$

Table 1: Summary of Runge-Kutta methods used in numerical tests.

fully explicit. Pseudo-symplectic methods can be derived by coupling the classical order conditions to additional nonlinear equations in the coefficients b_i and a_{ij} [19]. Pseudo-symplectic methods have been recently analyzed in the context of incompressible flow simulations, showing that they are able to keep very low numerical dissipation levels, on equal time step, in comparison to standard Runge-Kutta schemes [17].

While in case of symplectic methods there is clearly no advantage in using the minimum-dissipation criterion, the pseudo-symplectic schemes will benefit from an adaptive step size selection.

4 NUMERICAL RESULTS

The selected test case is the canonical Taylor-Green Vortex (TGV) flow, which is a challenging benchmark involving creation of small scales, transition to turbulence, and turbulent decay. Being a transient problem, the TGV flow is well suited to analyze adaptive time-stepping techniques. The initial conditions prescribed in a tri-periodic box of side 2π are given as follows [20]

$$u(x,y,z,0) = U_0 \frac{2}{\sqrt{3}} \sin(\theta + \frac{2}{3}\pi) \sin(x)\cos(y)\cos(z) \,, \tag{17}$$

$$v(x,y,z,0) = U_0 \frac{2}{\sqrt{3}} \sin(\theta - \frac{2}{3}\pi) \cos(x)\sin(y)\cos(z) \,, \tag{18}$$

$$w(x,y,z,0) = U_0 \frac{2}{\sqrt{3}} \sin(\theta) \cos(x)\cos(y)\sin(z) \,, \tag{19}$$

with $\theta = 0$. The spatial discretization employed in the following sections is based on a second-order energy-conserving method mentioned earlier. The domain is divided into 64^3 mesh points, and the selected Reynolds number is 1600. This combination corresponds to a typical large-eddy simulation resolution [21].

4.1 Standard and pseudo-symplectic methods

In this section, standard and pseudo-symplectic methods are tested in conjunction with the minimum-dissipation adaptive time-stepping method outlined in Section 3. The analyzed Runge-Kutta methods are reported in Table 1, along with their number of stages s, the order of accuracy on solution p and on energy conservation q, and the

value of σ^c to be used in Eq. (8). The scheme denoted as RK3 is the low-storage third-order scheme of Wray [10], while RK4 is the standard fourth-order RK scheme. The schemes 3p6q and 4p7q are two pseudo-symplectic schemes (see [17] for details).

Figure 1 shows the evolution of Δt for the schemes in Table 1, prescribed by

- the convective stability constraint (CFL), Eq. (8);
- the minimum-dissipation criterion (δ^E), Eq. (16);
- the Kolmogorov time scale τ_η, which is supposed to be constant in time.

The Kolmogorov time scale is computed by classical relations [22]. The black curves correspond to no-model LES, while the red ones to computations with the standard dynamic Smagorinsky model [22]. The Δt selected at each time step is chosen to be the minimum among the ones prescribed by the three criteria. The behaviour is very different for the various schemes, proving that the step size selection is not trivial. For the RK3, the Δt is initially dictated by stability, but starting from $t^* \approx 5$ the minimum-dissipation criterion prevails. This change in behaviour can be attributed to the fact that the initial energy is cascading to smaller scales, reaching the maximum wavenumber of the grid at approximately $t^* = 5$ and thus enhancing the numerical dissipation, which is active mostly at the smallest resolved scales. The δ^E criterion provides time steps that are approximately one-half of the one imposed by stability, indicating that the CFL criterion alone would lead to significant temporal dissipation. These observations are confirmed in the cases with the dynamic Smagorinsky model, with the Δt provided by the δ^E and CFL criteria being generally higher than the corresponding ones in the no-model case. The higher time steps are attributed to the additional dissipation of the SGS model, which smoothes the velocity field (thus reducing U_{max} in the CFL criterion) and reduces the impact of the temporal dissipation in the global energy budget. For the higher-order methods, the time step is initially constrained by the Kolmogorov time scale. However, while for the RK4 the δ^E criterion is still prevailing after $t^* = 5$, the pseudo-symplectic methods show comparable time-step sizes and the stability limit is eventually the determinant one. This is due to the inherent reduction of temporal dissipation error of these schemes. It is also worth noting that the time step based on δ^E leads to larger step sizes as the accuracy of the RK method is increased.

Figure 2 shows the time evolution of the error controller χ. The adaptive step size selection based on the minimum-dissipation criterion starts to operate from $t^* \approx 5$ and is able to bound the error to the selected tolerance, $\delta^E = 0.01$. Note that for simplicity, Eq. (16) has been implemented in an explicit fashion, i.e., using the value χ^n; this leads to few time steps in which $\chi > \delta^E$. Refined approaches in which Eq. (16) is properly iterated within one time step will be considered in future work.

Interestingly, in the performed simulations the four schemes of Table 1 provided similar efficiency, namely the r.h.s. evaluations needed to integrate until $t^* = 12$ were

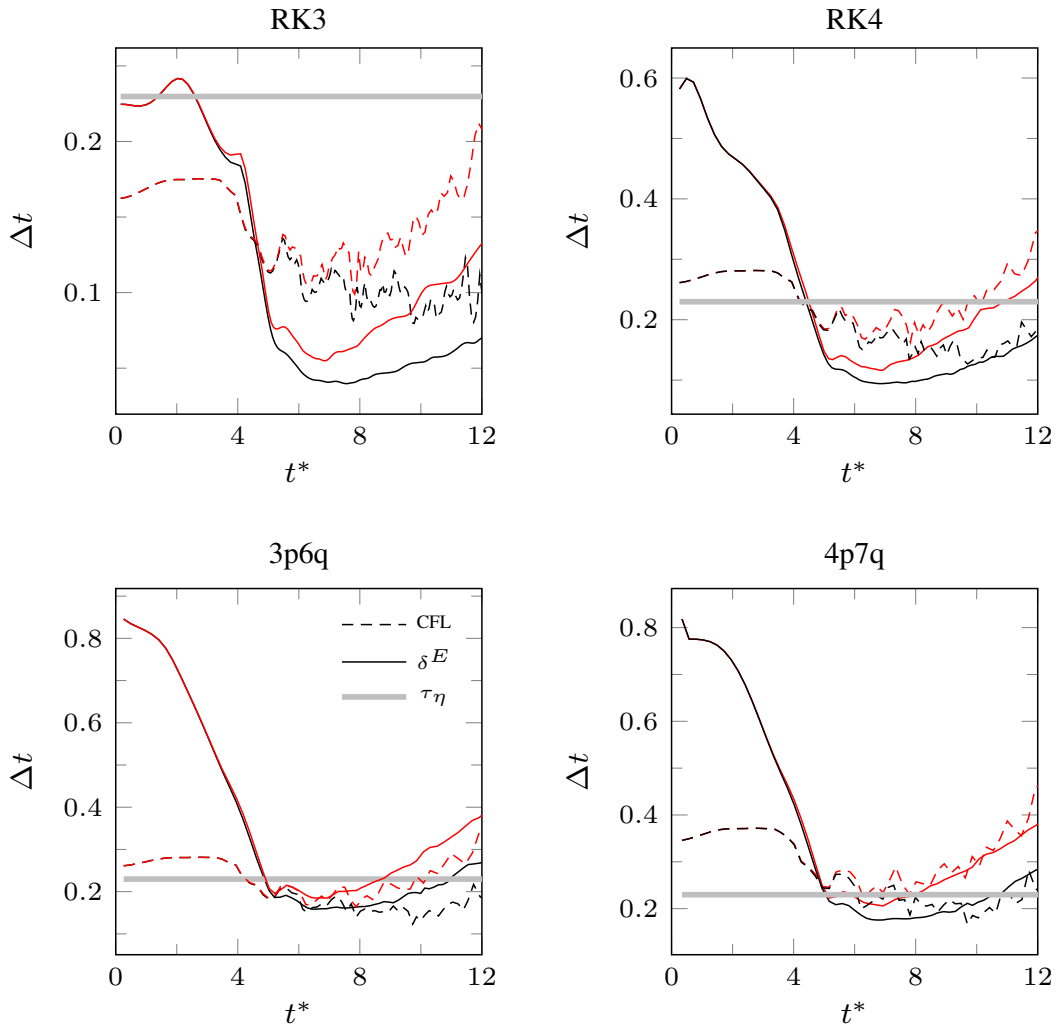

Figure 1: Time-step size dictated by the CFL criterion, the δ^E criterion, and the Kolmogorov time scale. Black: no model simulations; red: simulations with dynamic Smagorinsky model.

roughly the same. The higher order pseudo-symplectic schemes in combination with error estimation and control are therefore the preferred methods for performing this type of turbulence simulations.

It is worth to mention that other simulations (not shown here) performed at higher spatial resolutions provided similar results.

5 CONCLUSIONS

A new adaptive time-stepping strategy for large-eddy simulations of turbulent flows has been developed. The method is based on the analysis of the discrete global energy

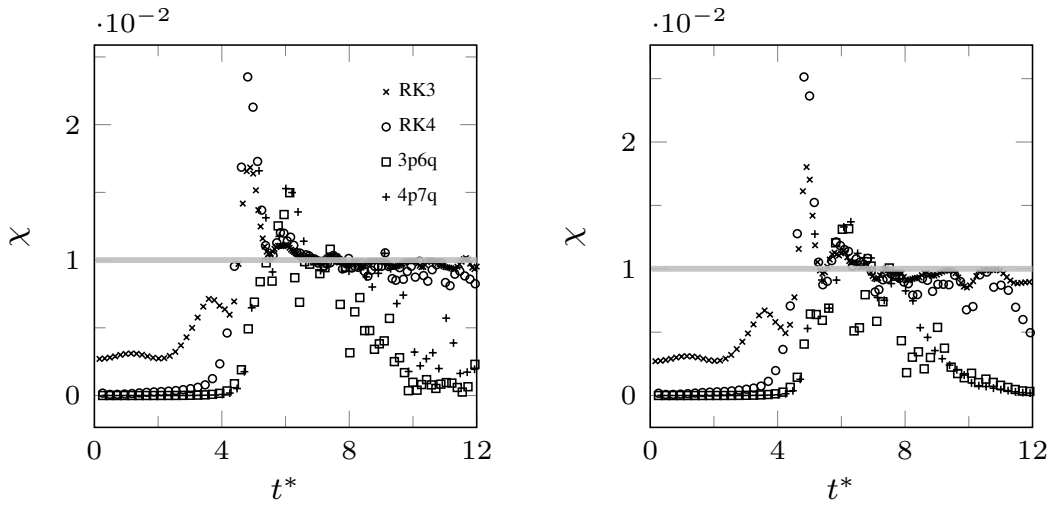

Figure 2: Time evolution of the error controller χ for no-model case (left) and dynamic Smagorinsky simulations (right). Also shown in gray is the selected tolerance δ^E.

equation, and consists in adjusting the time-step size dynamically to ensure that the temporal dissipation does not overcome the sum of the physical and SGS model terms by more than a desired tolerance. This minimum-dissipation time-advancement method can be easily implemented in an existing spatially energy-conserving code with negligible additional cost, provides a simple mean to control the time-integration error and can significantly increase the efficiency of time integration.

The adaptive time-stepping strategy has been preliminarily tested on a canonical Taylor-Green vortex case, in conjunction with both standard RK schemes and recently developed pseudo-symplectic methods. The new adaptive step size selection has been compared to more standard criteria based on a CFL-like condition, or on the Kolmogorov time scale. In all cases, the time step selection criterion changed during the time evolution. The new strategy proved to reduce the temporal dissipation below the desired tolerance; also, for standard third-order and fourth-order RK schemes, the time step sizes dictated by the minimum-dissipation criterion turned out to be lower than the ones imposed by the stability constraint, showing that standard criteria can lead to a significant amount of temporal dissipation.

Future work includes the application of the minimum-dissipation time-stepping strategy to more complex test cases, as well as the simultaneous control of the local truncation error of the velocity field by means of embedded Runge-Kutta methods.

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