PERFORMANCE AND ERROR ANALYSIS OF STRUCTURE-PRESERVING TIME-INTEGRATION PROCEDURES FOR INCOMPRESSIBLE-FLOW SIMULATIONS

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Abstract

The effects of kinetic-energy preservation errors due to Runge-Kutta (RK) temporal integrators have been analyzed for the case of large-eddy simulations of incompressible turbulent channel flow. Simulations have been run using the open-source solver Xcompact3D with an implicit spectral vanishing viscosity model and a variety of temporal Runge-Kutta integrators. Explicit *pseudo-symplectic* schemes, with improved energy preservation properties, have been compared to standard RK methods. The results show a marked decrease in the temporal error for higher-order pseudo-symplectic methods, and suggest that these schemes could be used to attain results comparable to traditional methods at a reduced computational cost.

1 Introduction

Guaranteeing the conservation of linear and quadratic invariants of the Navier-Stokes equations at a discrete level is considered to be of great importance for both direct and large-eddy simulations (LES) of turbulent flows (Coppola et al. (2019b)). For incompressible flows, the lack of kinetic energy preservation, either due to spatial or to temporal schemes, can lead to contamination of the energy cascade mechanism with artificial dissipation.

This work focuses on analyzing and quantifying the dissipative errors by the temporal integrator for large-eddy simulations (LES) of a turbulent channel flow. Research on the time-integration errors in numerical simulations of turbulent flows is relatively scarce in the existing literature. Choi and Moin (1994) investigated the effect of large time steps for the turbulent channel flow, determining that they might be responsible for unphysical behaviour on the turbulent structures or the laminarization of the flow. A systematic study about time-integration errors in LES of Taylor-Green-Vortex has been carried out by Capuano et al. (2019), emphasizing the benefits and efficiency of Runge-Kutta methods with improved energy conservation properties, such as the pseudo-symplectic schemes.

The aim of this work is to investigate the time-integration errors (particularly the dissipative component) of standard and pseudo-symplectic RK schemes for turbulent wall-bounded flows, at time steps close to the ones dictated by the linear stability limit.

The high-order finite-difference flow solver Xcompact3D (Bartholomew et al. (2020)) has been employed to run the simulations: the implicit LES (iLES) model is adopted through the use of a spectral vanishing viscosity operator, so that the extra-dissipation is enforced directly in the second derivative scheme of the diffusive term of the Navier-Stokes equations (Lamballais et al. (2011)).

Classical and innovative Runge-Kutta (RK) time integrators have been implemented in addition to the ones already present in the code.

2 Mathematical formulations

Classical RK schemes of s stages are usually constructed to maximize the temporal order of accuracy p. For these schemes, p also coincides with the pseudo-symplectic order q, defined so that the discrete evolution of the global kinetic energy for $Re \to \infty$ is

$$\frac{\Delta E}{\Delta t} = O(\Delta t^q). \tag{1}$$

A pseudo-symplectic method is one for which $q > p$ (Capuano et al. (2017)). The schemes investigated in this analysis are 3p5q(4), 3p6q(5), 4p7q(6); the naming convention npmq(s) indicates a method with $p = n$ temporal order of accuracy, $q = m$ pseudo-symplectic order, and s stages.

The dissipative effects of the temporal error can be efficiently investigated introducing the effective Reynolds number Re_{eff} (Capuano et al. (2017)), that can be defined, starting from the discrete evolution of the global kinetic energy, as

$$\frac{\Delta E}{\Delta t} = \frac{1}{Re}\Phi + \varepsilon_{\text{RK}} = \frac{1}{Re_{\text{eff}}}\Phi \tag{2}$$

where the term $\frac{1}{Re}\Phi$ represents the physical dissipation rate, whereas ε_{RK} is the temporal numerical dissipation. The second term indeed represents a source of error, due to the lack of the summation by parts rule of

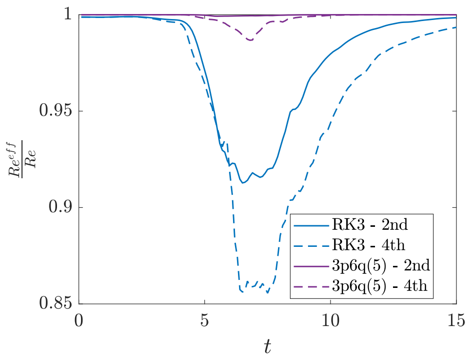


Figure 1: Comparison of the effective Reynolds number for the Taylor-Green-Vortex at $Re = 3000$, $N = 65^3$, for different temporal and spatial schemes, at CFL $= 1$.

the RK integrator (Capuano and Vallefuoco (2018)). By deriving the fully discrete evolution energy equation for a general RK scheme, one can obtain an expression for the discrete counterpart of the physical dissipation rate, and for the RK temporal error for kinetic energy, which read respectively

$$\varepsilon_\nu = \frac{1}{Re}\sum_{i=1}^{s} b_j \boldsymbol{u}_j^T \boldsymbol{L}\boldsymbol{u}_j \qquad (3)$$

$$\varepsilon_{RK} = -\frac{\Delta t}{2}\sum_{i,j=1}^{s}(b_i a_{ij} + b_j a_{ji} + -b_j b_i)\, \boldsymbol{u_i}^T \tilde{\boldsymbol{F}}_{\boldsymbol{i}}^T \tilde{\boldsymbol{F}}_{\boldsymbol{j}} \boldsymbol{u_j} \qquad (4)$$

where $\boldsymbol{u}_j$ represents the j-th intermediate velocity field inside the s inner stages of the RK procedure, $\boldsymbol{F_j} = -\boldsymbol{C}(\boldsymbol{u_j}) + \nu\boldsymbol{L} = \boldsymbol{F}(u_j)$, $\tilde{\boldsymbol{F}}(u_i) = \boldsymbol{PF}(\boldsymbol{u_i})$ and $\boldsymbol{P} = \boldsymbol{I} - \boldsymbol{GL}^{-1}\boldsymbol{M}$, with $\boldsymbol{M}$, $\boldsymbol{C}$, $\boldsymbol{L}$ and $\boldsymbol{G}$ being the discretization of the divergence, convective, diffusion and gradient operators, respectively.

3 Results

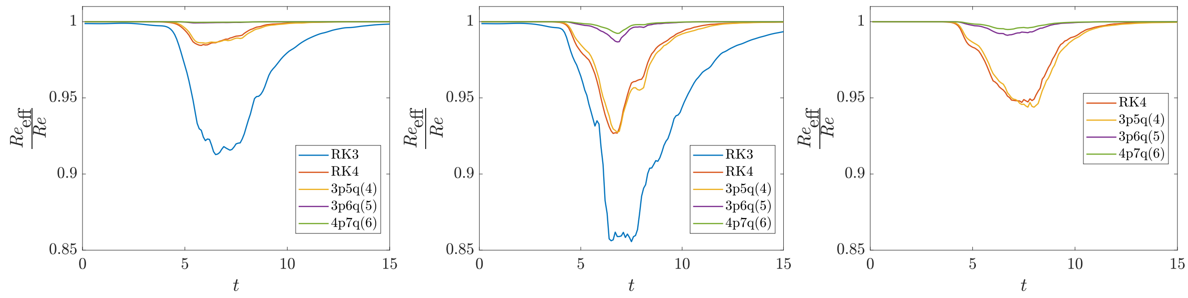
The numerical results presented in this section have all been performed with the open-source solver Xcompact3D. A skew-symmetric form of the convective term is employed, therefore the spatial discretization globally preserves kinetic energy (Coppola et al. (2019a)). As a first step, to determine the influence of the spatial schemes on the effective Reynolds number (which is indicative of the temporal kinetic-energy preservation error), the numerical simulation of the Taylor-Green-Vortex at $Re = 3000$ and CFL $= 1$ has been performed in a triperiodic square domain of side length $L = 2\pi$, discretized using $N = 65^3$ nodes. In particular, the temporal error of classical and innovative RK schemes have been compared by employing different spatial schemes: central 2nd order, compact 4th and 6th order Padé schemes.

In Figure 1 the evolution in time of the effective Reynolds number $Re_{\text{eff}}/Re = \frac{\varepsilon_\nu}{\varepsilon_{\text{RK}}+\varepsilon_\nu}$ is reported, in which $\varepsilon_\nu = \Phi/Re$ is the physical dissipation rate.

For both RK3 and 3p6q(5), the use of the higher order spatial schemes leads to a higher production of artificial dissipation than the central second order spatial scheme. The origin of this behaviour has been investigated by studying the physical dissipation rate ε_ν and temporal error ε_{RK} independently. The influence of the spatial discretization order on ε_ν is much smaller than the effect on ε_{RK}, so it is the last one that is responsible for the noticeable change in the effective Reynolds number. The same behaviour has been found to hold also for the other temporal integrators tested, with higher order spatial schemes leading to a higher artificial viscosity. This particular behaviour may be explained by considering that higher order spatial schemes resolve smaller scales more accurately and that leads to a higher dissipation. Indeed, the range of scales that are well-represented for the compact schemes are wider, capturing thoroughly the smallest length scales, i.e. the highest wavenumbers (Lele (1992)), up to the dissipative scales, because of the spectral-like accuracy of the compact schemes. In Figure 2 the effective Reynolds number for the central-second order, compact fourth order and sixth order are reported.

Numerical Results for the Channel Flow

The channel flow configuration has been investigated for $Re_\tau = 180$, 395, and 590. Several implicit large-eddy simulations have been performed in a domain of size $4\pi \times 2 \times \frac{4}{3}\pi$ for $Re_\tau = 180$ and in a domain of size $2\pi \times 2 \times \pi$ for the other cases. The iLES has been carried out using a spectral vanishing viscosity operator (Lamballais et al. (2011)), by means of 6th order compact Padé scheme, hence no explicit subgrid model has been used. In addition to the pseudo-symplectic schemes, the third-order Runge-Kutta-Wray (RK3) and classical fourth-order RK (RK4) schemes have been used to compare the results. The numerical grid is uniform in the homogeneous directions (x and z), while the grid in the wall normal direction is nonuniform and gradually stretched with the particular use of a tangent hyperbolic function. Therefore, the bilinear forms of the ε_ν and ε_{RK} have been modified according to the use of a mapping metric term, to take into account the non-uniform grid in the wall direction (Capuano and Vallefuoco (2018)). Note that the discrete global kinetic energy equation, Eq. (2), has been written for sake of simplicity in the absence of forcing terms. Obviously, in this case, a forcing is added to drive the flow through the channel (particularly, a constant pressure gradient is used). The main parameters for each simulations are summarized and reported in Table 1. In Figures 3a, 3b and 3c the ratio of the effective Reynolds number with respect to the nominal Reynolds number for $Re_\tau = 180$, 395 and 590 are shown as a function of time. The second drop corresponds to the starting point of the transition to turbulence, until it reaches a condition where the ratio



(a) Central second order (b) Compact fourth order (c) Compact sixth order

Figure 2: Ratio of effective to nominal Reynolds number at CFL $= 1$ for the Taylor-Green-Vortex at $Re = 3000$, $N = 65^3$ with different spatial schemes.

Re_τ	L_x	L_z	$Nx \times Ny \times Nz$	Δt	CFL
180	$4\pi\delta$	$\pi\delta$	$50 \times 33 \times 34$	0.17	0.8
395	$2\pi\delta$	$\pi\delta$	$54 \times 55 \times 54$	0.058	0.7
590	$2\pi\delta$	$\pi\delta$	$84 \times 129 \times 94$	0.0262	0.5

Table 1: Main parameters and numerical setup for the simulation of the turbulent channel flow.

Scheme	Relative max error		
	$Re_\tau = 180$	$Re_\tau = 395$	$Re_\tau = 590$
RK3	14.2%	16%	8.6%
RK4	4.9%	4%	0.7%
3p5q(4)	6.4%	4%	0.7%
3p6q(5)	0.9%	0.1%	0.2%
4p7q(6)	0.7%	0.07%	0.1%

Table 2: Maximum error of the effective Reynolds number compared to nominal Reynolds number, for various temporal schemes and $Re_\tau = 180$, 395 and 590.

can be considered to be stationary; hence the channel flow has reached the condition of being fully developed. The figures do not show noticeable differences between the pseudo-symplectic schemes of higher order, i.e., 4p7q(6) and 3p6q(5), while on the other hand RK3, RK4 and 3p5q(4) schemes vary significantly, reaching a deviation from the nominal Reynolds number up to 16% for the RK3 and up to 4% for the four-stage RK schemes at $Re_\tau = 395$.

In Table 2 the maximum deviation of the effective Reynolds number from the nominal value for different temporal schemes are reported. The pseudo-symplectic schemes of higher-order are able to keep the lowest level of production of artificial dissipation, with a maximum error below 1%.

Performance Analysis

A more meaningful comparison can be achieved by means of a cost analysis, where the minimum of the ratio of effective to nominal Reynolds number is reported with respect to a cost function, which is defined as the number of the right-hand side evaluations required to reach the fully developed channel flow with different time steps. As it is shown in Figures 4, 5 and 6, the analysis shows that higher order methods, in particular 3p6q(5) and 4p7q(6), are the most cost-effective and efficient among the temporal schemes investigated, as they require the minimum cost for a given value of the error. However, the 3p6q(5) performs slightly better than the more accurate pseudo-symplectic scheme of higher-order 4p7q(6), as already shown for different boundary and initial conditions and numerical setup by Capuano et al. (2019), which is confirmed within the range of Re_τ investigated.

4 Conclusions

The temporal error of standard and pseudo-symplectic RK methods has been investigated for incompressible flows. Firstly, the influence of the spatial schemes upon the time-integration error of the temporal schemes has been studied. The results show that high-order spatial schemes lead to a significant increase in the production of artificial dissipation. Indeed, low order spatial schemes, such as the central second order finite difference method does not resolve well a wide range of length scales, while on the other hand the set of the well-resolved waves for compact schemes stay close to the exact differentiation over a wider range of wavenumbers, up to the smallest scales, which are the most active in the dissipative spectrum. The improved energy-conservation properties of pseudo-symplectic schemes have been assessed also for a turbulent channel flow, being able to keep the error on the preservation of global kinetic energy below 1%, and minimizing the temporal error. Furthermore, a performance analysis for the channel flow results shows that high-order pseudo-symplectic schemes, such as the 3p6q(5) method, are the most efficient and cost-effective ones among other pseudo-symplectic schemes and standard RK methods.

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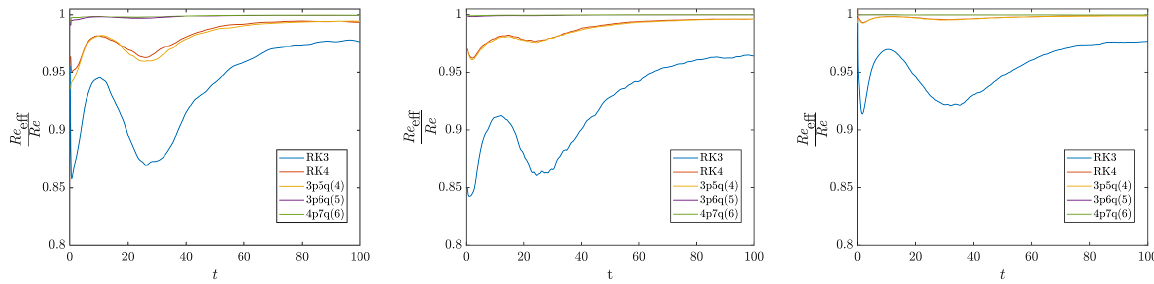

(a) CFL = 0.8, $Re_\tau = 180$. (b) CFL = 0.7, $Re_\tau = 395$. (c) CFL = 0.5, $Re_\tau = 590$.

Figure 3: Ratio of effective to nominal Reynolds number for the numerical simulation of the turbulent channel flow.

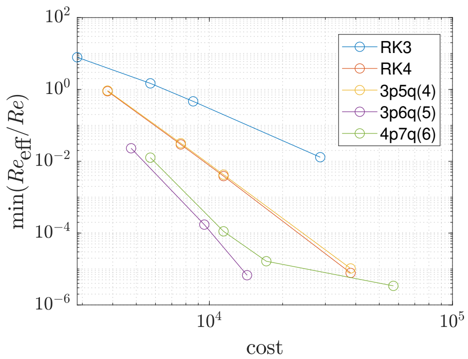

Figure 4: Minimum of the ratio of effective to nominal Reynolds number for the LES as a function of number of right-hand side evaluations for $Re_\tau = 180$ and CFL varying from 0.08 to 0.8.

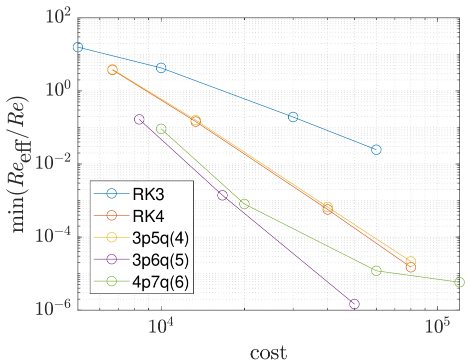

Figure 5: Minimum of the ratio of effective to nominal Reynolds number for the LES as a function of number of right-hand side evaluations for $Re_\tau = 395$ and CFL varying from 0.06 to 0.7.

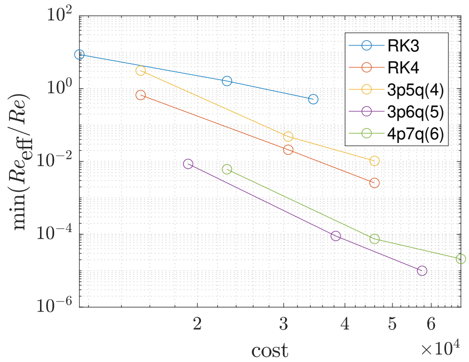

Figure 6: Minimum of the ratio of effective to nominal Reynolds number for the LES as a function of number of right-hand side evaluations for $Re_\tau = 590$ and CFL varying from 0.16 to 0.5.

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