14th International ERCOFTAC symposium on engineering, turbulence, modelling and measurements (ETMM)
Barcelona, Spain, 6-8 September, 2023

On self-adaptive Runge-Kutta schemes with improved energy-conservation properties

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Keywords: CFD, Time-integration, Runge-Kutta schemes, eigenbounds, CFL, pseudo-symplectic

1 Introduction

The numerical simulation of any transport phenomenon within the Finite Volume Method (FVM) framework requires both space and time discretization of the governing equations. The incompressible Navier-Stokes equations, which models the transport of mass, momentum and energy in a fluid, are no exception. In order to deal with this, the usual methodology starts by discretizing the equations in space, yielding the semi-discrete set of equations, using the notation from [1],

$$M\mathbf{u}_s = \mathbf{0}_c, \qquad (1) \qquad\qquad \Omega\frac{d\mathbf{u}_c}{dt} + C(\mathbf{u}_s)\mathbf{u}_c - D\mathbf{u}_c + \Omega G_c\mathbf{p}_c = \mathbf{0}_c, \qquad (2)$$

where M is the face-to-cell divergence operator, Ω_c is a diagonal matrix containing the cell volumes so that $\Omega = I_3 \otimes \Omega_c$, C_c is the cell-to-cell convective operator so that $C = I_3 \otimes C_c$, D_c is the cell-to-cell diffusive operator so that $D = I_3 \otimes D_c$, G_c is the cell-to-cell gradient operator, $\mathbf{u}_s$ is the velocity field defined at the faces, and I_3 is the unit matrix of size 3.

In order to integrate in time these equations, however, multiple techniques have been used during the development of the Computational Fluid Dynamics (CFD) theory. Pioneer studies from Moin and Kim [2, 3] used different integrating schemes for both convective, a second order Adams-Bashforth (AB2); and diffusive, an implicit Crank-Nicholson; terms, while the studies that followed generally used a projection method [4] integrated completely in time using an AB2. Later studies incorporated the use of second- and third-order Runge-Kutta schemes (RK2,RK3) due to larger stability regions that provide larger time-steps [5]. More recently, Sanderse [6] explored conserving energy in time using symplectic RK schemes, yet given its implicit nature makes them unsuitable for large-scale simulations. In order to deal with that, Capuano et al. [7] developed and tested different pseudo-symplectic RK schemes in flow simulations, which are more suitable given their explicit construction.

Originally, most of the publications set time-steps according to the classical Courant-Friedrichs-Lewy (CFL) condition [8], which provides a simpler approximation to the stability region of the simulation. Nonetheless, later on Trias and Lehmkuhl [9] considered a free-parameter multi-step time integrator κ1L2 with an adaptable stability region with the free parameter and computed the time-step of the integration by enforcing the method to be in the boundary of the region, optimizing thus the time-step while keeping a stable integration.

2 Methodology and preliminary results

The methodology for self-adaptive time-step strategies was first proposed by Trias and Lehmkuhl [9] consisting on the computation of the eigenbounds by direct application of the Gershgorin circle theorem in both convection and diffusion matrices in every time-step of the computation. Nonetheless, this process required an explicit reconstruction in every time-step of both matrices and thus more efficient methodologies are seeked. In this novel approach, the construction of both diffusion and convection matrices is revisited so that eventually the computation of the eigenbounds is simplified.

For a general scalar transport equation,

$$\frac{d\boldsymbol{\phi}_c}{dt} + C_c(\mathbf{u}_s)\boldsymbol{\phi}_c - D_c(\boldsymbol{\alpha}_s)\boldsymbol{\phi}_c = \mathbf{0}_c, \tag{3}$$

where $\boldsymbol{\phi}_c$ is the transported scalar in the cells and $\boldsymbol{\alpha}_s$ is the diffusivity at the faces; this revision of the construction of the matrices has the following outcome after assuming a symmetry-preserving (SP) discretization [1, 10].

$$D_c(\boldsymbol{\alpha}_s) \equiv -T_{sc}A_s\Lambda_s\Delta_s^{-1}T_{cs} \equiv -T_{sc}\tilde{\Lambda}_s T_{cs}, \tag{4a}$$

$$C_c(\mathbf{u}_s) \equiv T_{sc}A_sU_s\Pi_{c\to s} \underbrace{\equiv}_{\text{SP}} \frac{1}{2}T_{sc}A_sU_s|T_{cs}| = \frac{1}{2}T_{sc}F_s|T_{cs}|, \tag{4b}$$

where T_{sc} is the face-to-cell incidence matrix, A_s is the face-to-face diagonal matrix containing the face surfaces, $\Lambda_s = diag(\boldsymbol{\alpha}_s)$ is the face-to-face diagonal matrix containing the face diffusivities, $\Delta_s = \Omega_s A_s^{-1}$ is the diagonal matrix containing the projected distances $\delta n_f = |\mathbf{n}_f \cdot \mathbf{c1c2}|$ between the centers c1,c2 of the two cells adjacent to face f, $T_{cs} = T_{cs}^T$ is the cell-to-face incidence matrix, $\Pi_{c\to s}$ is the interpolator from cells to faces, and $U_s = diag(\mathbf{u}_s)$ is the diagonal matrix containing the vector field at the faces. This construction will hence allow computing the bounds on the eigenvalues without the need of an explicit construction of the matrices. By doing so, a family of methods to compute the eigenvalues for both matrices arise, with the parameter α arising from the theorem that states that, for a matrix $A \in \mathbb{R}^{n\times m}$ and a matrix $B \in \mathbb{R}^{m\times n}$, the matrices $AB \in \mathbb{R}^{n\times n}$ and $A^TB^T \in \mathbb{R}^{m\times m}$ will have the same eigenvalues except for the zero-valued ones and thus, the following identity holds

$$\rho(-T_{sc}\tilde{\Lambda}T_{cs}) = \rho(-\tilde{\Lambda}^{\alpha}T_{cs}T_{cs}^T\tilde{\Lambda}^{1-\alpha}), \tag{5}$$

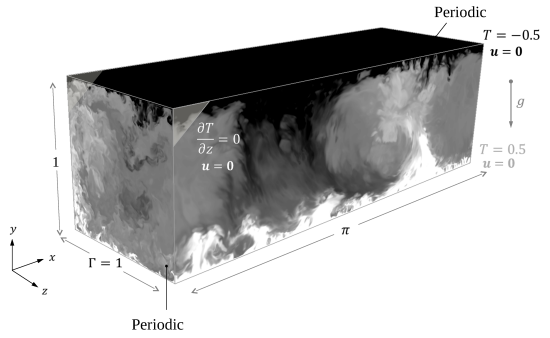
where $\rho(\xi)$ is the spectral radius of the matrix ξ. Moreover, its application to the convection operator is straightforward.

Given that the method entirely depends on the space discretization, but not on the time discretization, given a time-integrating scheme with known stability region (e.g. AB2, κ1L2, RK3) this method can be applied to obtain the optimal time-step more efficiently, compared to using the Gershgorin circle theorem, providing much more efficient time-integrations when compared to using a CFL condition.

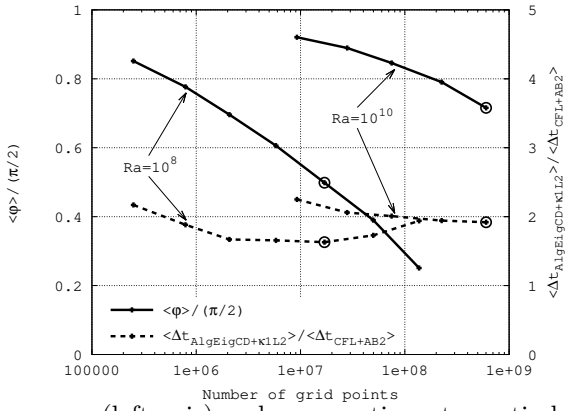
This method has already been implemented and tested in a Rayleigh-Bénard configuration (RBC) for two Rayleigh numbers (Ra), 10^8 and 10^{10} for two time-step computation and time integration combinations (Fig. 1a). First of all, used as a benchmark, AB2+CFL setup, with Courant number 0.35 and von Neumann number 0.2 was run ($\Delta t_{\text{CFL+AB2}}$). Moreover, the same tests have been run for a κ1L2+AlgEigCD ($\Delta t_{\text{AlgEigCD}+\kappa\text{1L2}}$).

It has been observed that for an increasing number of grid points the influence of the diffusive term in the magnitude of the eigenbounds has been increased, with a reduction of the average ϕ as shown in Fig. 1b. Regarding the average time-step, it has been observed that by making use of an adaptive time-step, with the improved method presented here, its ratio ranges between 1.5 and 2.2 amongst all numerical grids used for the tests.

The obtained results for the RBC in this reduced set of time-integrating schemes and time-step calculation show promising expectations for its application to Runge-Kutta schemes, given their bigger stability region when compared to standard multi-step integrators (AB2, AB3), even compared to the κ1L2 scheme, which stability region is notably larger than the standard schemes. Hence, its use for energy-conserving pseudo-symplectic explicit Runge-Kutta schemes [7] will be explored and compared to classical Runge-Kutta schemes, and the effect on the energy-preserving properties of this method, as well as the effect of skipping inter-stage pressure projections [13] in both stability and energy-conserving properties.



(a) Schema of the RBC configuration studied with an instantaneous temperature field of a $\mathrm{Ra} = 10^{10}$, $\mathrm{Pr} = 0.71$ DNS [11].



(b) Average φ (left axis) and average time-step ratio between both methods (right axis) for the RBC from Fig. 1a for both $\mathrm{Ra} = 10^8$ and $\mathrm{Ra} = 10^{10}$. Circled dots: Previous DNS results [11, 12].

Figure 1: Schema of the test case (a) and current results obtained for a κ1L2 scheme with the AlgEigCD time-step setup, compared to the classical framework (b).

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