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High-order linearly implicit two-step peer schemes for the discontinuous Galerkin solution of the incompressible Navier–Stokes equations

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ABSTRACT

In this work the use of high-order linearly implicit Rosenbrock-type two-step peer schemes has been investigated to integrate in time the high-order discontinuous Galerkin space discretization of the incompressible Navier–Stokes equations.

The aim of the present paper is (i) to describe the implementation of the schemes in the DG code MIGALE with focus on the computation of the set of the coefficients and the starting procedure, (ii) to describe the coupling of the scheme with an adaptive time-step strategy in order to investigate its effect on the robustness and computational efficiency of the simulations, and (iii) to provide some practical informations regarding the choice of the "optimal" time integration for LES and DNS on the basis of the requested accuracy. Peer schemes, up to sixth order, have been considered and compared with traditional one-step linearly implicit Rosenbrock, up to fifth order, and ESDIRK, up to fourth order, schemes available in literature in terms of accuracy and computational efficiency. For the sake of completeness, the sets of coefficients of the schemes here considered have been reported in an appendix.

The reliability, robustness and accuracy of the proposed implementation have been assessed by computing the Prothero–Robinson example, the laminar travelling waves solution on a doubly periodic unit square domain and the laminar flow around a circular cylinder for a Reynolds number $Re = 100$. Travelling waves and cylinder testcases have been also modified to investigate the behaviour of the schemes with time-dependent boundary conditions. In the former case replacing periodic boundary conditions with given boundary condition based on the analytical solution, while in the latter case considering a rotating cylinder.

1. Introduction

In recent years the potential of high-order methods has been deeply investigated to perform turbulent unsteady simulations based on RANS equations, DNS, and LES. In this context DG methods, due to their favourable dispersion and dissipation properties, proved to be very well suited for DNS [1–3], LES [4,5], and hybrid RANS-LES approaches [6]. Consequently, renewed attention has been paid to the analysis and development of time integration schemes to couple the high-order discretization both in space and time, and of space-time DG methods [7,8].

Some features of the DG methods, *e.g.* compactness and flexibility, can be advantageous both for explicit and implicit time integration approaches. Explicit schemes can achieve a very high accuracy [9–11] but are limited by time-step restriction. Otherwise, implicit schemes, although memory consuming due to the need of the Jacobian matrix, can be *A*-stable and *L*-stable even for high order of accuracy. Several implicit high-order time integration schemes, relying on multistage and multistep schemes, have been developed and succesfully coupled with the DG spatial discretization, such as linearly implicit Rosenbrock-type Runge–Kutta schemes (*A*-stable up to order five) [12], Explicit Singly Diagonally Implicit Runge-Kutta (ESDIRK) schemes (*A*-stable up to order five) [13], Modified Extended BDF (MEBDF) schemes (*A*-stable up to order four) [14], and Two Implicit Advanced Step-point (TIAS) schemes (*A*-stable up to order six) [15]. The higher order versions of the Rosenbrock

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schemes, as shown in [13], turned out to be the more efficient, requiring to solve only linear systems in the stages within each time-step, *i.e.* the Jacobian matrix needs to be assembled and factored only once per time-step. The other schemes at each time-step require to solve several non linear systems of equations, a task that can be efficiently performed, for example, by means of the quasi-Newton method.

However, Rosenbrock methods may suffer from order reduction for very stiff problems [16,17]. To overcome this limitation, recently, a new type of linearly implicit Rosenbrock-type time integration schemes called peer schemes has been proposed in literature [16]. Such methods take a linear combination of stage values to approximate the exact solution at intermediate points. All stage values have the same order of accuracy and the same stability properties, which is the reason for calling the methods "peer", and this is in contrast to one-step schemes, where intermediate stages solutions have lower order than the final solution. Peer schemes up to order eight are available and are characterized by good stability properties, strong damping properties at infinity without further restrictions and robustness with respect to step-size changes. Furthermore, due to their linearly implicit structure, only linear systems have to be solved in each time-step. Since all stage solutions have the same accuracy and stability properties, a continuous high-order output is also available with no extra-cost. As all multi-step schemes, peer schemes are non self-starting and, thus, they need a starting procedure in order to obtain required initial solutions.

The aim of the present paper is (i) to describe the implementation of high-order linearly implicit Rosenbrock-type two-step peer schemes in the DG code MIGALE [6,18] for the time integration of the incompressible Navier–Stokes (INS) equations, (ii) to describe the coupling of the schemes with an adaptive time-step strategy in order to investigate its effect on the robustness and computational efficiency of the simulations, and (iii) to provide some practical informations regarding the choice of the "optimal" time integration scheme for LES and DNS on the basis of the requested accuracy. Furthermore peer schemes have been compared with traditional one-step Rosenbrock and ESDIRK schemes: the fourth order/six stages (ESDIRK46) [19], the third order/three stages (ROS3PL) [20], the fourth order/six stages (RODASP) [21] and the fifth order/eight stages (ROD5_5) [22] linearly implicit Rosenbrock schemes [23] available in literature in terms of accuracy and computational efficiency.

The reliability, robustness and accuracy of the proposed implementation have been assessed by computing the Prothero–Robinson example, the laminar travelling waves solution on a doubly periodic unit square domain, and the laminar flow around a circular cylinder for a Reynolds number $Re = 100$. Travelling waves and cylinder testcases have been also modified to investigate the behaviour of the schemes with time-dependent boundary conditions. In the former case replacing periodic boundary conditions with given boundary condition based on the analytical solution, while in the latter case considering a rotating cylinder.

The paper is organized as follow: Section 2, after a brief introduction on the traditional one-step time integration schemes used for comparison, describes peer schemes with focus on the computation of the set of the coefficients and the starting procedure. Furthermore, this section describes the adaptive time-step strategy considered in this work. Numerical results are described in Section 3, while conclusions in Section 4. Finally Appendix A reports the set of the coefficients of the traditional one-step schemes.

2. Time discretization

The discrete problem corresponding to the DG discretization of the incompressible Navier–Stokes equations can be written as:

$$\widehat{\mathbf{M}}\frac{d\mathbf{Q}}{dt} + \mathbf{R}(\mathbf{Q}) = \mathbf{0}, \tag{1}$$

where $\mathbf{Q}$ is the global vector of unknown degrees of freedom, $\mathbf{R}$ the residuals vector, and $\widehat{\mathbf{M}}$ the global block diagonal mass matrix with the block corresponding to the pressure degree of freedom null. Eq. (1) defines a system of non-linear Differential Algebraic Equations (DAEs).

2.1. ESDIRK schemes

This class of Runge-Kutta schemes can be constructed to be $A-$ and $L-$stable for any temporal order of accuracy. A $s-$stage ESDIRK scheme, applied to Eq. (1), can be written as

$$\begin{aligned} \widehat{\mathbf{M}}\mathbf{Q}^i &= \widehat{\mathbf{M}}\mathbf{Q}^n - \Delta t \sum_{j=1}^{i} a_{ij}\mathbf{R}\left(\mathbf{Q}^j\right) \qquad i = 1, \ldots, s, \\ \mathbf{Q}^{n+1} &= \mathbf{Q}^s, \end{aligned} \tag{2}$$

where a_{ij} are the Butcher coefficients of the scheme, β_i the fraction of the time-step corresponding to each stage i, and $\hat{b}_i$ the coefficients to obtain the embedded solution. Table 11 summarizes the coefficients of fourth order/six stages ESDIRK46 scheme and its embedded method. The first stage is explicit ($a_{11} = 0$) and the last stage defines the solution for the next time-step [19]. The solution $\hat{\mathbf{Q}}^{n+1}$ of the embedded method is obtained from Eq. (2) replacing a_{si} with $\hat{b}_i$. The scheme corresponding to Eq. (2) for non autonomous problems, *i.e.* problems with time-dependent boundary conditions, is obtained replacing $\mathbf{R}\left(\mathbf{Q}^j\right)$ by $\mathbf{R}\left(t^j, \mathbf{Q}^j\right)$ with $t^j = t^n + \beta_j \Delta t^n$. Each non-linear stage of the ESDIRK schemes is solved by means of an iterative Newton–Krylov method. The kth Newton–Krylov iteration entails the solution of the following linear system:

$$\begin{aligned} \left(\frac{\widehat{\mathbf{M}}}{a_{ii}\Delta t} + \mathbf{J}_k\right)\left(\mathbf{Q}^i_{k+1} - \mathbf{Q}^i_k\right) = &- \frac{\widehat{\mathbf{M}}}{a_{ii}\Delta t}\left(\mathbf{Q}^i_k - \mathbf{Q}^n\right) \\ &- \sum_{j=1}^{i-1} \frac{a_{ij}}{a_{ii}}\mathbf{R}\left(\mathbf{Q}^j\right) - \mathbf{R}\left(\mathbf{Q}^i_k\right) \quad i = 1, \ldots, s. \end{aligned} \tag{3}$$

The analytical Jacobian matrix $\mathbf{J}$ is here computed at the beginning of the simulation and recomputed only if the convergence rate of the quasi-Newton method between iteration k and $k+1$ decreases below a given tolerance or after 10 time-steps since the last evaluation, *i.e.*

$$\frac{\|\Delta\mathbf{Q}_{k+1}\|_2}{\|\Delta\mathbf{Q}_k\|_2} > tol_J \qquad \text{or} \qquad n_{\Delta t} = 10,$$

where tol_J is a tolerance which is set to 0.2, $n_{\Delta t}$ the number of time steps after the last Jacobian computation and $\|\Delta\mathbf{Q}_k\|_2$ the L^2 norm of the solution increment at the $k-th$ Newton iteration. Due to the peculiar treatment of the convective numerical flux [24], $\mathbf{J}_k$ has non null entries for pressure degrees of freedom. It follows that, despite the singularity of matrix $\widehat{\mathbf{M}}$, linear systems can be solved with standard algorithms. The linear system arising at each Newton step is solved using the GMRES algorithm preconditioned with the block Jacobi method as available in the PETSc library [25]. In this work the GMRES relative tolerance is set to $tol_{GMRES} = 10^{-2}$ for ESDIRK46 scheme.

2.2. Linearly implicit Rosenbrock-type Runge–Kutta schemes

The linearly implicit Rosenbrock-type Runge–Kutta schemes entail the solution of a sequence of linear systems. This class of