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High-order implicit time integration for unsteady turbulent flow simulations

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ABSTRACT

Higher order explicit diagonal Runge–Kutta (EDIRK) schemes are investigated for their applicability to realistic unsteady turbulent flow simulations. A second order, two new third order accurate schemes with different stage order accuracy, and a fourth order accurate scheme are tested and compared to the commonly used implicit second order backward difference (BDF2) method. All methods are implemented in a flow solver for unstructured grids where the non-linear equations from the implicit temporal discretizations are formulated as a steady state problem which is solved by standard techniques for steady flow problems. The main objective for the comparison is the accuracy and efficiency of the methods but the influence of different steady state convergence criteria is also addressed. The time integrators are evaluated on van der Pol's equations and unsteady laminar and turbulent flow cases in two and three dimensions. The design orders for all schemes are verified for all test cases except the fourth order scheme for a turbulent case which is approximately third order with increasing accuracy as the time step is refined. The second order schemes are more efficient for larger time steps. Due to lower truncation error, the second order EDIRK scheme is equally or more efficient than the BDF2 scheme although one additional implicit stage is involved per time step. The higher order ($\geqslant 3$) schemes become more competitive with smaller time steps and are often more efficient than the second order schemes.

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1. Introduction

A majority of fluid dynamics problems today in engineering applications are inherently unsteady. These flow phenomena include e.g. transition, turbulent unsteady flow separation, unsteady boundary layers and shear-flows. To accurately predict these flows, accurate and efficient time integration is required. For realistic applications the time integrator has to be implicit since the restriction on the time step from an explicit approach due to the smallest length scale on highly stretched grids is typically several orders of magnitude smaller than the temporal resolution required to resolve the time dependent flow physics. Based on our experience with various implicit and explicit schemes, we have found that the time step of an implicit scheme in a typical unsteady calculation needs to be at least about 10^2 times larger than the time step of an explicit time scheme. This is explained by the fact that implicit schemes require solutions of non-linear equations corresponding, for our methods, to a work of approximately 10^2 explicit time steps. All the cases considered in this study have time steps way above this limit.

The implicit second order backward difference method (BDF2) [1,2] is probably the most commonly used time integrator for unsteady flow problems on highly stretched grids. The scheme is A- and L-stable for arbitrary time steps and requires the solution of a non-linear problem at each time step which can be reformulated and solved as a solution to a steady state problem. To further increase the accuracy in time beyond second order it is not possible to add a third time level since the third order backward difference method is no longer A-stable which eventually can lead to instability and divergence [2]. Various alternative implicit time integrators with similar stability properties as BDF2 exist that are able to integrate beyond second order temporal accuracy. These approaches include implicit multi-stage Runge–Kutta methods such as diagonal implicit Runge–Kutta (DIRK) method and the explicit diagonal implicit Runge–Kutta (EDIRK) approach. There are also combinations of implicit multistage and multistep methods, e.g. the modified extended backward difference scheme (MEBDF) [3]. In common for these methods is that several implicit stages are involved to advance the flow solution one time step. Hence, several

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steady state problems have to be solved making these approaches more expensive than BDF2. On the other hand, more accurate schemes should allow for larger time steps that, potentially, make them computationally more efficient.

The purpose of our work is to investigate the accuracy and efficiency of higher order implicit temporal schemes for realistic turbulent unsteady flow cases on highly stretched grid and establish if they are able to compete with the BDF2 scheme. Past investigations have explored and compared different implicit integration techniques for various unsteady flow problems. Birken et al. [4] show that a third and a fourth order accurate ESDIRK (explicit singly diagonal implicit Runge–Kutta) schemes offer efficient time integration on a laminar test case at a low Reynolds number. Carpenter et al. [5,6] compare BDF, MEBDF and ESDIRK type of time integrators on both laminar and turbulent test cases. Bijl et al. make similar investigations [7]. The higher order accurate schemes for the laminar flow cases maintain design accuracy and possess superior efficiency at lower error levels where, e.g., a fourth order accurate EDIRK scheme outperforms the BDF2 scheme. Jothiprasad et al. [8] have also showed that the efficiency for a laminar case is superior with higher order temporal integration schemes. They also show that the convergence of the non-linear problems can be further enhanced by introducing different convergence acceleration techniques. The results by Carpenter et al. [5,6] are less encouraging for turbulent flow at higher Reynolds numbers where BDF2 compares about equally to the higher order schemes and where the higher order schemes obtain order reductions. The results are, however, to some extent inconclusive due to poor performance of the solution of the non-linear problems, in particular for larger time steps.

In this investigation we incorporate one second order, two third order and one fourth order accurate EDIRK schemes and compare their performances in terms of accuracy and efficiency to the results with the BDF2 scheme. The third order schemes have three implicit Runge–Kutta stages which, to our knowledge, have not been applied to flow problems in the past. These schemes differ in their stage order accuracy being first and second order accurate which is a concern for highly stiff problems [6]. We include them to investigate if this is a concern for turbulent flow calculations. The second order scheme [9] has two implicit stages, the fourth order scheme [5, 7] has 5 implicit stages. The schemes are implemented in an industrial finite volume CFD code for unstructured grids which has an efficient steady state solver that is used to solve the steady state non-linear problem in dual time. The steady state problem is not solved exactly but to some degree of accuracy which will influence the computed results. We study how the accuracy as well as the efficiency are affected by three different convergence criteria based on absolute and relative convergence levels of the residuals and by specifying a constant number of iterations.

We focus our investigation on the investigation of the accuracy and efficiency on unsteady turbulent test cases at high Reynolds numbers. We verify the design order on the algebraic van der Pol's equations and we investigate the accuracy and efficiency on a laminar flow case as well.

In the next section we describe the time integrators including their derivation and stability properties. We then describe the flow solver, its steady state solver as well as convergence criteria applied to interrupt the convergence of the steady state problem. Following that we present the numerical results including verification of the design order on the van der Pol's equations and investigations on three unsteady flow problems in two and three dimensions. Finally we summarize and conclude about the efficiency of the applied schemes and recommendations on convergence levels and criteria.

2. Time integration methods

We consider A- and L-stable implicit time integrators only since, by experience, this is a necessity when solving turbulent unsteady flow problems on highly stretched grids where the (normalized) length scales of the computational grid may vary from 10^{-6} to 10^{2} or even more. The smallest length scales exclude the use of explicit time integrators since they result in time steps that are typically 10^{2} or more smaller than the time step required to resolve the time dependent flow physics well. Furthermore, by increasing the accuracy in time there is an interest in increasing the size of the time step to make higher order methods affordable and efficient. This requires implicit methods.

The time dependent equations we are solving are the semi-discretized Navier–Stokes equations where a finite-volume discretization is applied to the space derivatives. This results in a set of ordinary differential equations (ODE's)

$$\frac{\partial q}{\partial t} = R(q) \tag{1}$$

which are to be integrated in time. q is the unknown state vector, consisting of conservative discrete flow variables, the vector $R(q)$ results from the semi-discretization of the Navier–Stokes equations involving convection, diffusion and source terms for the turbulence equations.

Eq. (1) can be solved by means of methods from the large class of general linear methods (GL), see e.g. [10,11], by

$$\begin{pmatrix} q_{\text{int}} \\ q^{n+1} \end{pmatrix} = \begin{pmatrix} A & C \\ B & D \end{pmatrix} \begin{pmatrix} \Delta t R(q_{\text{int}}) \\ q_{\text{prev}} \end{pmatrix} \tag{2}$$

where q_{int} is a $k \times 1$ vector containing k intermediate stages $q_{\text{int}} = (q^{(1)}, q^{(2)}, \ldots, q^{(k)})^T$, q^{n+1} is the solution on next global time step, q_{prev} a vector containing the solutions on m previous time steps, $q_{\text{prev}} = (q^n, q^{n-1}, \ldots, q^{n-m+1})^T$, A is a $k \times k$ matrix, B a $1 \times k$ matrix, C is an $k \times m$ matrix, D a $1 \times m$ matrix. A large number of well known methods for solving ODE:s can be embedded in Eq. (2). Among those are implicit backward difference multi step schemes (BDF) and implicit multi stage Runge–Kutta methods (IRK), which are considered in the present paper.

In order to limit the scope of the paper, combined multi step/multi stage methods like the modified extended backward difference scheme (MEBDF) have not been investigated. Another motivation for this choice is that a single level method simplifies programming; it facilitates a restart in the flow solver and is more flexible in combination with adaptive time step techniques.

2.1. Backward difference method

A general BDF method can be obtained from the GL class by choosing the matrices and vectors in Eq. (2) according to

$$\begin{aligned} &A = B = 1/a_0, \qquad C = D = (-a_1/a_0, -a_2/a_0, \ldots, -a_m/a_0) \\ &q_{\text{int}} = q^{(1)}, \qquad q_{\text{prev}} = (q^n, q^{n-1}, \ldots, q^{n-m+1})^T. \end{aligned} \tag{3}$$

The method of highest order of accuracy, which also fulfills the A- and L-stability requirements, is the second order accurate backward difference method BDF2 which reads

$$\frac{3}{2}q^{n+1} - 2q^n + \frac{1}{2}q^{n-1} = \Delta t R(q^{n+1}) \tag{4}$$

i.e. $a_0 = 3/2, a_1 = -2, a_2 = 1/2$ in Eq. (3). The BDF2 scheme requires the solution of a set of non-liner equations for each global time step

$$\widetilde{R}(q^*) = R(q^*) - \frac{3q^*}{2\Delta t} + \frac{2q^n}{\Delta t} - \frac{q^{n-1}}{2\Delta t} = 0. \tag{5}$$

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