Analysis of Dual-Time-Stepping with Explicit Subiterations for Advection-Diffusion-Type Equations

G.A. Gerolymos,∗ D. Sénéchal,† and I. Vallet‡

Université Pierre-et-Marie-Curie, 75005 Paris, France

The purpose of the present paper is to study theoretically the stability and accuracy of dual-time-stepping methods for the advection-diffusion equation, in conjunction with high-order upwind-biased space-discretizations, and high-order backward-differences time-discretizations. These results are in particular analyzed for typical nondimensional time-steps encountered in the simulation of wall-bounded turbulent flows. We attempt to define optimal subiterative strategies (and dual-time-step choice), with respect to stability and accuracy requirements. Typical computational examples are presented.

1. Introduction

Most time-integration methods have been analyzed, from the point-of-view of stability and accuracy, both in general for the equation

$$\Delta t \partial_t u = Zu \quad (Z \in \mathbb{C}),$$

and in particular for the scalar advection-diffusion equation used as a mathematical model for the Navier-Stokes equations. However, little has been done for the analysis of dual-time-stepping methods used to solve, at each physical-time iteration the discrete-flow equations (obtained after discretization in space and in time).

Dual-time-stepping has shown in practice very satisfactory performance for the solution of complex flow problems. In these methods, a dual-time-derivative (pseudo-time) is added to the discrete flow equations, and subiterations are used to solve the dual-time problem, at each physical time iteration. Dual-time-stepping has been used either with explicit subiterations, eg Runge-Kutta (RK–DTS) and matrix-free (MF–DTS) approaches, or with implicit subiterations.

The purpose of the present paper is to study theoretically dual-time-stepping with explicit subiterations for the advection-diffusion equation. We examine high-order upwind-biased space-discretizations, and high-order backward-differences time-discretizations. These results are in particular analyzed for typical nondimensional time-steps encountered in the simulation of wall-bounded turbulent flows. We attempt to define optimal subiterative strategies (and dual-time-step choice), with respect to stability and accuracy requirements. Typical examples from DNS and RANS computations are presented.

2. BDFs and eDTS

2.1. Backward-Differencing (BDF)

Dual-time-stepping methods are based on backward-differencing (BDF) formulas

$$\left[ \frac{\partial u}{\partial t} \right]_{t=t_{n+1}} = \frac{1}{\Delta t_n} \sum_{\ell=-(k-1)}^{1} c_{k,\ell} u_{n+\ell} + C_{k,k} \left[ \frac{\partial u^{k+1}}{\partial t^{k+1}} \right]_{t=t_{n+1}} \Delta t_n \quad (1)$$

The coefficients $c_{k,\ell}$ can be obtained from the Taylor-expansions

$$u_{n+\ell} = u_{n+1} + \sum_{q=1}^{\infty} \frac{(t_{n+\ell} - t_{n+1})^q}{q!} \left[ \frac{\partial^q u}{\partial t^q} \right]_{t=t_{n+1}} \quad (2)$$

∗Institut d’Alembert, Case 161, 4 place Jussieu, e-mail: georges.gerolymos@upmc.fr
†Institut d’Alembert, Case 161, 4 place Jussieu, e-mail: dorothee.senechal@upmc.fr
‡Institut d’Alembert, Case 161, 4 place Jussieu, e-mail: isabelle.vallet@upmc.fr
Straightforward computation (using Maxima\cite{12} for the implicit dual-time-stepping technique, which is tabulated (Tab. 1), for the general case $r_1 < r_2 < \cdots < r_{k-1}$)

$$
\Delta t_n := t_{n+1} - t_n \\
r_{-1} \Delta t_n := t_{n+1} - t_{n-1} = \Delta t_n \Delta t_{n-1} \\
r_{-2} \Delta t_n := t_{n+1} - t_{n-2} = \Delta t_n \Delta t_{n-1} \Delta t_{n-2} \\
\vdots \\
r_{1-k} \Delta t_n := t_{n+1} - t_{n-(k-1)} = \Delta t_n \Delta t_{n-1} \cdots \Delta t_{n-(k-1)} 
$$

In the general case of varying time-step, ite where the time-step $\Delta t_n$ varies from 1 iteration to the next, let

$$
c_{k+1} = 1 + \frac{1}{r_1} + \frac{1}{r_2} + \cdots + \frac{1}{r_{1-k}} = 1 + \sum_{q=1-k}^{-1} \frac{1}{r_q} 
$$

$$
c_{k,j} = \frac{-1}{(r_1-1)(r_2-1) \cdots (r_{1-k}-1)} = \prod_{q=1-k}^{-1} \frac{r_q}{(r_q-1)} 
$$

$$
c_{k,\ell} = \prod_{q=1-k}^{-1} \frac{r_q}{r_q \ell - 1} \prod_{q=1-k}^{-1} (r_q - r_\ell) 
$$

$$
C_{k,k} = \frac{r_{-1} \cdots r_{1-k}}{(k-1)!} = \prod_{q=1-k}^{-1} \frac{r_q}{(k-1)!} 
$$

In the particular case of constant time-steps ($n^t = t_0 + n\Delta t$), where $\Delta t_n = \Delta t_{n-1} = \Delta t_{n-2} = \cdots = \Delta t_{n-k+1}$, we have simply (3) $r_1 = 2$, $r_2 = 3$, $\cdots$, $r_k = k + 1$, and (4) are simplified, to recover the standard BDF formulas\cite{13,14,15,16} The coefficients $c_{k,\ell}$, for the particular case of constant time-steps ($t_n = t_0 + n\Delta t$), were tabulated (Tab. 1), for $k \in [1, 6]$.

2.2. Dual-Time-Discretization Background

The starting point of the time-discretization used is the implicit dual-time-stepping technique, which is widely used in the solution of the Navier-Stokes equations of fluid-flow\cite{17,18,19} (the work of Jameson\cite{20} had a particular impact on the increasingly widespread use of the method), eventually augmented by additional equations for turbulence-modelling,\cite{21,22} or for chemical reactions.\cite{23,24} Denoting by $I_{t_0}$ the discretized
form of the space-operator (divergence and source-terms) the semi-discrete equation at grid-point \(n_p \in \{1, 2, \ldots, N_p\}\) gives

\[
\frac{du_{n_p}}{dt} + L_{n_p} = 0 \quad \forall \ n_p \in \{1, 2, \ldots, N_p\} \iff \frac{du}{dt} + L(u) = 0
\]

(5)

where \(u_{n_p} \in \mathbb{R}^{N_v}\) is the vector of unknowns at grid-point \(n_p\) (\(N_v\) is the number of variables in the system of PDEs), \(L_{n_p} \in \mathbb{R}^{N_v}\) is the discretized form of the space-operator (divergence and source-terms), \(u = [u^T, u^T, \ldots, u^T]^{T_T} \in \mathbb{R}^{(N_v, N_p)}\) is the global vector of the unknowns (\(N_v\) is the total number of grid-points), and \(L = [L^T, L^T, \ldots, L^T]^{T_T} \in \mathbb{R}^{(N_v, N_p)}\) is the global vector of the space-operators. If an \(O(\Delta t^k)\) backward-differences (1) scheme (BDF\(k\)) is used, in the context of an implicit time-discretization of (5), the unsteady residual between instants \(t_n\) and \(t_{n+1}\) reads

\[
R(u_{n+1}, u_n, u_{n-1}, \ldots, u_{n-(k-1)}; \Delta t_n, \Delta t_{n-1}, \ldots, \Delta t_{n-(k-1)}) := \frac{1}{\Delta t_n} \left( \sum_{k=(n-(k-1))}^{1} c_k, u_{n+k} \right) + L(u_{n+1})
\]

(6)

where \(\Delta t_n := t_{n+1} - t_n\) is the physical time-step between instants \(t_n\) and \(t_{n+1}\). The system of nonlinear equations \(R = 0\) is solved using a dual-time-stepping technique.\(^7\) Noting \(\Delta t_{n,p}\) the local dual pseudo-time-step at grid-point \(n_p\), and between instants \(t_n\) and \(t_{n+1}\), and defining the diagonal matrix

\[
\Delta t^*_n = \text{diag}[\Delta t^*_1, \Delta t^*_2, \ldots, \Delta t^*_n, \Delta t^*_N]\)

(7)

where \(I_{N_v}\) denotes the \(N_v \times N_v\) identity matrix, the dual subiteration \(m_{it} \equiv m + 1\) reads\(^7,10\)

\[
\left(\Delta t^*_{m,n+1}\right)^{-1} (u_{m+1,n+1} - u_{m,n+1}) + R(u_{n+1,n+1}, \ldots, u_{n-(k-1)}; \Delta t_n, \ldots, \Delta t_{n-(k-1)}) + c_{t,1} \left( u_{m+1,n+1} - u_{m,n+1} \right) \Delta t_n
\]

(8)

where \(\Delta t^* := I + c_{t,1} \left( \frac{\Delta t}{\Delta t_n} \right)^{-1}\) and \(\Delta t^*_{m,n+1} := \left( I + c_{t,1} \left( \frac{\Delta t^*_{m,n+1}}{\Delta t_m} \right) \right)^{-1} \Delta t^*_{m,n+1}\)

(9a)

\[
R_{m+1} := R(u_{n+1,n+1}, u_{n+1,n+1}, \ldots, u_{n-(k-1)}; \Delta t_n, \Delta t_{n-1}, \ldots, \Delta t_{n-(k-1)})
\]

(9c)

\[
R_{m+1} := R(u_{m+1,n+1}, u_{m+1,n+1}, \ldots, u_{m-(k-1)}; \Delta t_n, \Delta t_{n-1}, \ldots, \Delta t_{n-(k-1)})
\]

(9d)

where \(I \in \mathbb{R}^{(N_v, N_v)}\) is the identity-matrix, the complete algorithm can be written as

\[
do \ n_{it} = 1, N_{it}; \ n = n - n_{it} - 1; \ t_{n+1} = t_n + \Delta t_n; \ u_{0,n+1} = u_n
\]

\[
\do \ m_{it}, \text{while } [r_u \geq r_{TRO}] \equiv m \equiv m_{it} - 1; \ M_{it} = m_{it}
\]

\[
u_{m+1,n+1} \leftarrow \text{B} \left[ u_{m,n+1} - \left( I + \Delta t^*_{m,n+1} \left[ \frac{\partial L}{\partial u} \right]_{u=u_{m,n+1}} \right) \right]^{-1} \Delta t^*_{m,n+1} R_{m,n+1}
\]

end do; \(u_{n+1} = u_{M_{it},n+1}\)

(10)

where \(L'(u)\) is an approximation to the operator \(L(u)\) chosen so as to minimize implicit work,\(^9,25,26\) and the subscript \(\text{APRX}\) indicates that the matrix inversion (linear system solution) at each subiteration is approximate.\(^9,10,25,26\) The operator \(\text{B}\) is used to symbolize the explicit application of boundary-conditions, at each subiteration.\(^9,10,25,26\) If \(L'(u)\) and the solution of the linear system is exact (to a certain precision tolerance), the fully implicit DTS method is recovered. Further, setting \(\Delta t^* = \infty\) (very large), the subiterations are converted to a Newton iteration solution of the nonlinear system \(R_{n+1} = 0\).
It is possible to choose a subiterative strategy where the number of subiterations is constant for every iteration (physical time-step), i.e. \( M_{it}(n_{it}) = \text{const} \forall n_{it} \). It is, however, more efficient\(^9,25,26,28\) to adopt a dynamic increment-convergence-tolerance strategy, where the subiterative convergence of the increment \( u_{n+1} - u_n \) is required to reach a certain level of accuracy \( r_{TRG} \) (cf. eg §2.2.4). In this case the number of subiterations \( M_{it}(n_{it}) \) varies from one iteration to the next.

### 2.3. Dual-Time-Stepping with Explicit Subiterations (eDTS)

When the physical-time-step is chosen of the same order-of-magnitude as the numerical stability limit of explicit procedures, as, eg, in DNS computations,\(^{12} \) or simulations of unsteady flows requiring high time-accuracy,\(^{29,30} \) it is more efficient to use explicit subiterations (because, in that case, usually, a few explicit subiterations suffice to reach the target convergence-tolerance \( r_{TRG} \)). To do this, we simply put \( \partial_u L^i = 0 \), and obtain an explicit subiterative procedure\(^{29} \)

\[
\begin{align*}
\text{do } n_{it} = 1, N_{it}, 1; \; n \equiv n_{it} - 1; \; t_{n+1} = t_n + \Delta t_n; \; u_{0,n+1} &= u_n \\
\text{do } m_{it} \text{ while } [r_u \geq r_{TRG}]; \; m \equiv m_{it} - 1; \; M_{it} = m_{it} \\
u_{m+1,n+1} &= B \{ u_{m,n+1} - \Delta t_{m+1,n+1}^* R_{m,n+1} \} \\
\text{end do; } u_{n+1} &= u_{M_{it},n+1} \\
\text{end do; end do (11)}
\end{align*}
\]

In some instances (and also in the theoretical analysis of the method), a constant number of subiterations \( M_{it} \) is used at each iteration

\[
\begin{align*}
\text{do } n_{it} = 1, N_{it}, 1; \; n \equiv n_{it} - 1; \; t_{n+1} = t_n + \Delta t_n; \; u_{0,n+1} &= u_n \\
\text{do } m_{it} = 1, M_{it}, 1; \; m \equiv m_{it} - 1 \\
u_{m+1,n+1} &= B \{ u_{m,n+1} - \Delta t_{m,n+1}^* R_{m,n+1} \} \\
\text{end do; } u_{n+1} &= u_{M_{it},n+1} \\
\text{end do; end do (12)}
\end{align*}
\]

### 2.4. Application to the Navier-Stokes Equations for DNS Studies

The above eDTS–BDF algorithm was applied to DNS studies using the compressible Navier-Stokes equations.\(^{12} \) The number of subiterations (Eqs. 11) is adjusted dynamically, at each subiteration,\(^{10} \) to satisfy an increment \((n+1)u - n_u)\) convergence-tolerance criterion \( r_u \geq r_{TRG} \)

\[
\begin{align*}
r_u(m + 1, n + 1) &= \log_{10} \left\{ \frac{|10|e_u(m+1,n+1) - 10|e_u(m,n+1)|}{10|e_u(m,n+1)|} \right\} \\
e_u(m + 1, n + 1) &= e_u[u_n, u_{m+1,n+1} - u_n] \\
e_u[u, \Delta u] &= \log_{10} \left\{ \frac{4}{5} \left( \frac{\sum |\Delta \rho|^2}{\sum |\rho|^2} + \frac{\sum |\Delta (\rho u_i)|}{\sum |\rho u_i|^2} + \frac{\sum |\Delta (\rho e_i)|}{\sum |\rho e_i|^2} \right) \right\}
\end{align*}
\]

(13a) (13b) (13c)

where \( \sum \) implies summation over all of the grid nodes, and the summation convention for the cartesian indices \( i, j = 1, 2, 3 \) is used. The relative variation of the error \( e_u \) (Eq. 13c) is used to define the relative variation of the increment \( r_u \) between successive subiterations (Eq. 13a). The increment-convergence-tolerance \( r_{TRG} < 0 \) indicates the approximate number of digits to which the computation of the increment is converged, in the subiterative procedure.

The local dual-time-step used in the subiterative procedure (8), at grid-point \( n_p \), is based on a combined convective (Courant) and viscous (von Neumann) criterion\(^{31} \)

\[
\Delta t_{n_p}^* = \min \left\{ \text{CFL}^* \frac{\Delta t}{V + a} \bigg|_{n_p}; \text{VNN}^* \frac{\Delta t^2}{2\nu_{eq} \ell} \bigg|_{n_p} \right\} : \nu_{eq} = \max \left\{ \frac{4}{3} v, \frac{\gamma - 1}{\rho R_g} \right\}
\]

(14)

where \( \Delta \ell \) is the grid-cell-size, \( V \) is the flow velocity, \( a \) is the sound velocity, \( \nu_{eq} \) is the equivalent diffusivity,\(^{31} \) \( \nu \) is the molecular kinematic viscosity, and \( \lambda \) is the molecular heat-conductivity. The spatially homogeneous values of CFL* and VNN* are user-defined parameters.
Figure 1. Instantaneous streamwise velocity $u$ at the inflow plane and at $y^+ \in [4, 5]$ for typical supersonic (UW09–C02, $Re_{ew} = 232$, $M_{CL} = 1.50$, $\Delta y^+_w = 0.24$, $\Delta y^+_C = 5.6$, $\Delta x^+ = 24.3$, $\Delta z^+ = 12.1$, $\Delta t^+ = 16.9 \times 10^{-3}$) and subsonic (UW11–C02, $Re_{ew} = 183$, $M_{CL} = 0.35$, $\Delta y^+_w = 0.19$, $\Delta y^+_C = 4.5$, $\Delta x^+ = 19.2$, $\Delta z^+ = 9.6$, $\Delta t^+ = 5.4 \times 10^{-3}$) plane channel flow computations.\(^{12}\)

Finally, the physical time-step $\Delta t$ is chosen from physical considerations. It defines the actual CFL and VNN numbers at each grid node

$$CFL_{\text{np}} := \left. \frac{\Delta \ell}{V + a} \right|_{\text{np}} \Delta t \quad \text{;} \quad VNN_{\text{np}} := \left. \frac{\Delta \ell^2}{2 \nu_{eq}} \right|_{\text{np}} \Delta t$$ \hspace{1cm} (15)$$

The time-integration procedure is controlled by the parameters [$\Delta t$; CFL*, VNN*, $r_{\text{TRG}}$]. Discussion on the stability in the ($\text{VNN}$, CFL*)-plane should be considered with reference to the actual (VNN, CFL) numbers combinations encountered in DNS simulations of compressible turbulence, where the mesh is highly stretched near the wall. Considering typical subsonic ($Re_{ew} = 183$, $M_{CL} = 0.35$) and supersonic ($Re_{ew} = 232$, $M_{CL} = 1.50$) plane channel simulations (Fig. 1), with standard resolution,\(^{12}\) the distributions of (VNN, CFL) vs $y^+$ illustrate (Fig. 2) the high values near the wall, and their rapid decrease going toward midchannel. In the present
examples (Fig. 2) the subsonic computations correspond to CFL \(_w > \text{VNN}_w\), while the supersonic case has CFL \(_w < \text{VNN}_w\) (notice, however, that VNN \(\propto \Delta t^{-2}\) while CFL \(\propto \Delta t^{-1}\), so that further \(y\)-wise grid-refinement near the wall would tend to increase VNN with respect to CFL). The distributions of VNN/CFL vs \(y^+\) (Fig. 2), with reference to the modified viscosity (§4.3), suggest that the relative importance of the numerical viscosity induced by upwinding is substantially higher in the midchannel region compared to the near-wall region.

3. Analysis of the Method

3.1. Linear Stability Analysis in the \(Z\)-Plane

We study first the standard equation of von-Neumann stability analysis\(^{2,3,18}\)

\[
\frac{du}{dt} = \frac{u}{\Delta t} Z \quad ; \quad u, Z \in \mathbb{C} \quad ; \quad t \in \mathbb{R} \tag{16}
\]

In practice \(Z\) will depend on the order of the space-discretizations, on the CFL and VNN numbers, and on the wavenumber (§2). The dual-time-stepping discretization of (16), with constant time-steps \(\Delta t\) and \(\Delta t^*\), for subiteration \(m_{it} = m + 1\) of iteration \(n_{it} = n + 1\), reads

\[
u_{(m+1,n+1)} = u_{(m,n+1)} - \frac{\Delta t^{**}}{\Delta t} \left\{ c_{k,1} u_{(m,n+1)} + \left( \sum_{\ell=-(k-1)}^{0} c_{k,\ell} u_{n+\ell} \right) - u_{m,n+1} Z \right\} \tag{17}
\]

where (9a)

\[
\frac{\Delta t^{**}}{\Delta t} = \frac{\Delta t^*}{1 + c_{k,1} \Delta t^*} \tag{18a}
\]

\[
r^* := \frac{\Delta t}{\Delta t^*} \tag{18b}
\]

\[
\frac{\Delta t^{**}}{\Delta t} = \frac{\Delta t^*}{1 + c_{k,1} \Delta t^*} = \frac{1}{c_{k,1} + \frac{\Delta t}{\Delta t^*}} = \frac{1}{c_{k,1} + r^*} \tag{18c}
\]

and \(r^*\) (18b) is the ratio of the physical-to-dual time-steps. With (18) the dual-time-stepping subiteration (17) reads

\[
u_{m+1,n+1} = u_{m,n+1} - \frac{1}{c_{k,1} + r^*} \left\{ c_{k,1} u_{m,n+1} + \left( \sum_{\ell=-(k-1)}^{0} c_{k,\ell} u_{n+\ell} \right) - u_{m,n+1} Z \right\} \tag{19}
\]

This result (19) indicates that the stability of the edTS–BDF\(_k\) time-integration of (16) depends only on \(r^*\), and on the number of subiterations \(M_{it}\). Indeed, defining the complex amplification factors

\[
G_{m+1,n+1} := \frac{u_{m+1,n+1}}{u_{n+1}} \tag{20a}
\]

\[
G_{n+1} := \frac{u_{n+1}}{u_{n}} \tag{20b}
\]

\[
G_{n} := \frac{u_{n}}{u_{n-1}} \tag{20c}
\]

\[
G_{n+\ell+1} := \frac{u_{n+\ell+1}}{u_{n+\ell}} \tag{20d}
\]

the dual-time-stepping subiteration gives

\[
G_{m+1,n+1} = r^* + Z \frac{G_{m,n+1} - c_{k,0} \frac{G_{m,n+1}}{c_{k,1} + r^*} - \sum_{\ell=-(k-1)}^{-1} \left( \frac{c_{k,\ell}}{c_{k,1} + r^*} \prod_{q=\ell+1}^{0} \frac{1}{G_{n+q}} \right)}{c_{k,1} + r^*} \tag{21}
\]

The above relation (21) is quite general, and can be used to study (numerically) the convergence of the method, with a dynamic subiterative strategy and/or taking into account the particular choice used to start...
the method (which as all BDFs is not self-starting\textsuperscript{1}). Defining
\[
H_k(r^*, Z) := \frac{r^* + Z}{c_{k,1} + r^*} \quad (22a)
\]
\[
B_{k,n} := -\frac{c_{k,0}}{c_{k,1} + r^*} - \sum_{\ell = -(k-1)}^{-1} \left( \frac{c_{k,\ell}}{c_{k,1} + r^*} \prod_{q=\ell+1}^{0} \frac{1}{G_{n+q}} \right) \quad (22b)
\]
Equation (21) reads
\[
G_{m+1,n+1} = H_k G_{m,n+1} + B_{k,n} \quad (23)
\]
and, recursively,
\[
m + 1 = 0: \quad G_{0,n+1} = 1 \quad (24a)
\]
\[
m + 1 = 1: \quad G_{1,n+1} = H_k G_{0,n+1} + B_{k,n} = H_k + B_{k,n} \quad (24b)
\]
\[
m + 1 = 2: \quad G_{2,n+1} = H_k (G_{1,n+1} + B_{k,n}) = H_k^2 + (1 + H_k) B_{k,n} \quad (24c)
\]
\[
m + 1 = 3: \quad G_{3,n+1} = H_k (G_{2,n+1} + B_{k,n}) = H_k^3 + (1 + H_k + H_k^2) B_{k,n} \quad (24d)
\]
\[\vdots\]
\[
m + 1 = n: \quad G_{m+1,n+1} = H_k (G_{m,n+1} + B_{k,n}) = H_k^m + (1 + H_k + \cdots + H_k^m) B_{k,n} \quad (24e)
\]
and using the geometric series identity \((1 - x)(1 + x + x^2 + \cdots + x^n) = 1 - x^{n+1} \forall x \in \mathbb{C}\), the final recurrence relation is obtained
\[
G_{m+1,n+1} = H_k^m + \frac{1 - H_k^{m+1}}{1 - H_k} c_{k,0} + r^* - \sum_{\ell = -(k-1)}^{-1} \left( \frac{1 - H_k^{m+1}}{1 - H_k} \frac{c_{k,\ell}}{c_{k,1} + r^*} \prod_{q=\ell+1}^{0} \frac{1}{G_{n+q}} \right) \quad (25)
\]
\[\textbf{3.2. } M_{it}(n_{it}) = \text{const}\]
If a subiterative strategy (12) with a constant number of subiterations \(M_{it}(n_{it})\), performed at each iteration \(n_{it}\) is used, after a sufficiently large number of iterations, provided that the method is stable, we expect the amplification factors to be independent of the iteration-count \(n_{it}\) (the memory of the start-up phase is lost)
\[
M_{it}(n_{it}) = \text{const} \quad (\text{for } n_{it} \geq N) \quad G_{M_{it}, n} = G_{M_{it-1}, n-1} = \cdots = G_{M_{it-M_{it}}, n-(k-2):= G_{M_{it}}, (k, r^*, Z)} \quad (26)
\]
Substituting \(M_{it} = m + 1\) (12) in (25), the amplification factors are roots of the polynomial
\[
G_{M_{it}}^k + \left( -H_k^{M_{it}} + \frac{c_{k,0}}{r^* + c_{k,1}} \frac{1 - H_k^{m+1}}{1 - H_k} \right) G_{M_{it}}^{k-1} + \sum_{\ell = -(k-1)}^{-1} \left( \frac{c_{k,\ell}}{r^* + c_{k,1}} \frac{1 - H_k^{m+1}}{1 - H_k} \right) G_{M_{it}}^{k-\ell+1} = 0 \quad (27)
\]
The study of the roots of (Eq. 27) \(\forall Z \in \mathbb{C}\) serves to determine the stability boundaries for the generic equation \(\Delta t \partial_t u = Zu\) (16).

\[\textbf{3.3. eDTSBDF1}\]
\[\textbf{3.3.1. Stability Limit and Relation to Forward Euler}\]
The linear stability limit of the eDTSBDF1 (Fig. 3) is quite different from the stability limit of the forward Euler (FE) method, especially at the imaginary axis. For \(M_{it} \geq 3\) the limiting \((M_{it} \to \infty)\) stability boundary is reached.

\[\textbf{3.3.2. Strong Stability Preservation}\]
\[\textbf{PROPOSITION 1 (eDTSBDF1 SSP Limit): } \text{Let } u(t): \mathbb{R} \to \mathbb{R}^N \text{ and } L: \mathbb{R}^N \to \mathbb{R}^N, \text{ and assume that the forward-Euler (FE) method } u_{n+1} = u_n - \Delta t L(u_n), \text{ for the solution of } \partial_t u + L(u) = 0 \text{ is SSP for } t \leq \Delta t_{FE}. \text{ Then, the eDTSBDF1}(M_{it}, r^*) \text{ method for the solution of } \partial_t u + L(u) = 0 \text{ is SSP under the time-step limitation } \Delta t \leq r^* \Delta t_{FE} \quad (28)\]

\[7 \text{ of } 21\]

American Institute of Aeronautics and Astronautics Paper 2009–1608
\[ e^{\text{DTSBDF1}}(r^* = 1, M_t = \infty) \]
\[ e^{\text{DTSBDF1}}(r^* = 1, M_t = 3) \]
\[ e^{\text{DTSBDF1}}(r^* = 1, M_t = 5) \]
\[ e^{\text{DTSBDF1}}(r^* = 1, M_t = 10) \]
\[ e^{\text{DTSBDF1}}(r^* = 1, M_t = 15) \]

Figure 3. O\(\Delta E\) von Neumann stability analysis (stability-boundaries) for the \(O(\Delta t)\) backward-differences (BDF1) DTS scheme with explicit subiterations (eDTSBDF1), for the solution of \(\Delta t \partial_t u = Zu\) \((Z \in \mathbb{C})\), for different numbers of subiterations \(M_t\) and ratio of physical-to-pseudo-time-step \(r^* = 1\).

Proof. The eDTSBDF1 iteration reads

\[ u_{m+1,n+1} = u_{m,n+1} - \frac{1}{1 + r^*} \left( u_{m,n+1} - u_n + L(u_n) \right) \]
\[ = \frac{1}{1 + r^*} u_n + \frac{r^*}{1 + r^*} u_{m,n+1} - \frac{1}{1 + r^*} \Delta t L(u_{m,n+1}) \quad ; \quad m = 1, \ldots, M_t - 1 \] (29)

By direct comparison with the Shu\(^{32}\) RK\((\alpha, \beta)\) notation

\[ u_{0,n+1} = u_n \] (30a)
\[ u_{m+1,n+1} = \sum_{\ell=0}^{m} (\alpha_{m+1,\ell} u_{\ell,n+1} - \beta_{m+1,\ell} \Delta t L(u_{\ell,n+1})) \quad ; \quad m = 1, \ldots, M_{\text{RK}} - 1 \] (30b)

it follows that (29) is identified with (30) with

\[ \alpha_{m+1,0} = \frac{1}{1 + r^*} \] (30c)
\[ \alpha_{m+1,\ell} = 0 \quad ; \quad \ell = 1, \ldots, m - 1 \] (30d)
\[ \alpha_{m+1,m} = \frac{r^*}{1 + r^*} \] (30e)
\[ \beta_{m+1,m} = \frac{1}{1 + r^*} \] (30f)
\[ \beta_{m+1,\ell} = 0 \quad ; \quad \ell = 1, \ldots, m - 1 \] (30g)

so that the CFL-coefficient of the method is

\[ c_{\text{CFL}} = \min_{m,\ell} \frac{\alpha_{m,\ell}}{|\beta_{m,\ell}|} = r^* \] (31)

which yields (28). □

Remark 1 As can be seen in the Proof of Proposition 1 the SSP-time-step-limitation (28) is obtained without seeking the optimal Shu\(^{32}\) RK\((\alpha, \beta)\) form (which would yield the time-step above which the method is not SSP), so that (28) is sufficient but not necessary. On the other hand, in (30) \(\beta_{m,\ell} \geq 0 \forall m, \ell\), so that there is no need to compute the inverted-time operator.
3.4. eDTSBDF2

For the eDTS–BDF2 method, the 2 roots $[M_{it}, r^*] \in \mathbb{C}$ can be determined for different values of the parameters $[M_{it}, r^*] \in \mathbb{C}$, and thus define the stability boundaries in the $Z$-plane for each pair $[M_{it}, r^*]$ (Fig. 4). We studied (Fig. 4) the eDTS–BDF2 method for the cases $M_{it} = 5, 10, 15, \infty$ (in practice $\infty$ corresponds to 1000) for different values of $r^* \geq 1$ (considering that the pseudo-time-step should act as an underrelaxation parameter), in the quadrant $Re(Z) < 0$, $Im(Z) < 0$ (which is of interest for the advection-diffusion equation), and compared the corresponding stability boundaries with the standard RK4 method. In general the method has enhanced stability, compared to RK4, when $|Re(Z)|$ is large. A small number of subiterations $(M_{it} \in [5, 10])$ is in general sufficient to satisfactorily approach the limiting $(M_{it} \to \infty)$ boundary, with the exception of the immediate neighbourhood of the imaginary axis $(Re(Z) \to 0)$, where $M_{it} \in [10, 15]$ might be necessary. This behaviour, on the imaginary axis, similar to the RK2 behaviour, corresponds to a weak instability (associated for eDTS–BDF2 with the principal root), and is of no practical consequence.

3.5. eDTSBDFk

The stability limit for higher-order eDTSBDFs $(k \in \{3, \cdots, 6\})$ behaves differently on the imaginary (pure convection) or on the real (pure diffusion) axis (Fig. 5) as $k$ increases. For diffusion-dominated problems $(Im(Z) \approx 0)$, as $k$ increases, the stability limit increases (Fig. 5). On the other hand, for convection-dominated problems $(Re(Z) \approx 0)$, as $k$ increases, the stability limit decreases (Fig. 5). For $k = 3, 4$ the stability limit on the imaginary axis goes to 0 (Fig. 5), as for the FE and RK2 methods. For $k = 5, 6$, the stability limit on the imaginary axis becomes again finite (Fig. 5).
4. Theoretical Analysis for the 1-D Advection-Diffusion Equation

4.1. 1-D Advection-Diffusion Equation

We consider the 1-D linear advection-diffusion equation with periodic boundary-conditions

\[
\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}; \quad u(t, 0) = u(t, L_x) \forall t
\]

\[
; \quad 0 \leq a = \text{const}; \quad 0 \leq \nu = \text{const}
\]

Let \( u \) denote the exact solution of (Eq. 32). Because of the \( x \)-periodicity the solution can be expanded in Fourier-series

\[
u(x, t) = \Re \left\{ \sum_{\kappa} \hat{u}_{\kappa}(t) e^{i\kappa x} \right\}; \quad \kappa = \frac{2\pi n_x}{L_x}, \ n_x \in \mathbb{Z}
\]

and the equation is transformed in Fourier-space

\[
\frac{d\hat{u}_{\kappa}}{dt} + i\kappa \hat{u}_{\kappa} = -\nu \kappa^2 \hat{u}_{\kappa}; \quad \kappa = \frac{2\pi n_x}{L_x}, \ n_x \in \mathbb{Z}
\]

4.2. Space-Discretization

The advection-diffusion equation is discretized in a homogeneous \((x, t)\) grid, with \( N_j \equiv N_x \) points in space

\[
x_j = (j - 1) \Delta x; \quad \Delta x := \frac{L_x}{N_x - 1}
\]

\[
t_n = n \Delta t
\]
Figure 6. Nondimensional-modified-wavenumber$^{34}$ for the discretization of $\partial_u (\kappa_{S1}, \Delta x)$ for the UW03 to UW11 schemes (Eqs. 41), and of $\partial_x^2 u (\kappa_{S2}, \Delta x)$ using the C02 to C12 schemes (Eqs. 41) with stresses computation at the cell-interfaces and the C02(2Δx) scheme with stresses computation at the grid-nodes, compared with the the compact (hermitian) centered schemes of Lele$^{34}$ HC06 and HC10.

Table 2. Finite-difference coefficients for $\partial_u$ (upwind-biased differences).

<table>
<thead>
<tr>
<th>$r$</th>
<th>9</th>
<th>8</th>
<th>7</th>
<th>6</th>
<th>5</th>
<th>4</th>
<th>3</th>
<th>2</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\ell$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-9</td>
<td>12252240</td>
<td>1071</td>
<td>12252240</td>
<td>9792</td>
<td>377688</td>
<td>8709168</td>
<td>360360</td>
<td>360360</td>
<td>360360</td>
</tr>
<tr>
<td>-8</td>
<td>35712</td>
<td>12252240</td>
<td>35712</td>
<td>360360</td>
<td>360360</td>
<td>360360</td>
<td>360360</td>
<td>360360</td>
<td>360360</td>
</tr>
<tr>
<td>-7</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>-6</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
<tr>
<td>-5</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>-4</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
<tr>
<td>-3</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>-2</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
<tr>
<td>-1</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>0</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
<tr>
<td>1</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>2</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
<tr>
<td>3</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>4</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
<tr>
<td>5</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>6</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
<tr>
<td>7</td>
<td>2252240</td>
<td>360360</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
<td>2252240</td>
</tr>
<tr>
<td>8</td>
<td>12252240</td>
<td>360360</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
<td>12252240</td>
</tr>
</tbody>
</table>

Space discretization uses an upwind-biased scheme for $[\partial_x u]_j$, and a centered scheme for the $[\partial^2_x u]_j$

$$
[\partial u \partial x]_j \approx \frac{1}{\Delta x} \sum_{\ell=-L_1}^{L_1} (2L_1-1)! b_{1}^{(1)} u_{j+\ell} + O(\Delta x^{2L_1-1})
$$

$$
[\partial^2 u \partial x^2]_j \approx \frac{1}{\Delta x^2} \sum_{\ell=-L_2}^{L_2} (2L_2)! b_{1}^{(2)} u_{j+\ell} + O(\Delta x^{2L_2})
$$

11 of 21

American Institute of Aeronautics and Astronautics Paper 2009–1608
On this grid, because of Shannon's sampling theorem, \( \kappa \)

Notice that, in relation with upwind reconstructions

and upon introduction of the \( \partial \)

(Fig. 6).

Table 3. Finite-difference coefficients for \( \partial^2_{xx} u \) (centered differences).

<table>
<thead>
<tr>
<th>( \ell )</th>
<th>9</th>
<th>8</th>
<th>7</th>
<th>6</th>
<th>5</th>
<th>4</th>
<th>3</th>
<th>2</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( r = \pm 9 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 8 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 7 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 6 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 5 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 4 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 3 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 2 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = \pm 1 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
<tr>
<td>( r = 0 )</td>
<td>+154278224000</td>
<td>+735</td>
<td>+154278224000</td>
<td>+511120</td>
<td>+154278224000</td>
<td>+3027024000</td>
<td>+154278224000</td>
<td>+154278224000</td>
<td>+154278224000</td>
</tr>
</tbody>
</table>

Notice that, in relation with upwind reconstructions\(^30\)

\[ u_{j+1}^L - u_{j}^L = \sum_{\ell=-r}^{r-1} (2r-1) b_{\ell}^{(1)} u_{j+\ell} \]

\[ \Rightarrow \begin{cases} (2r-1) b_{\ell}^{(1)} = (2r-1) a_{\ell-1} - (2r-1) a_{\ell+1} ; \ell = -(r - 1), \ldots , (r - 2) \\ (2r-1) b_{r}^{(1)} = -(2r-1) a_{-r-1} \end{cases} \] (38)

On this grid, because of Shannon's sampling theorem,\(^35\) the maximum resolvable wavenumber is limited to \( \kappa \Delta x < \pi \)

\[ u(x, t) \approx \Re \left\{ \sum_{\kappa} \tilde{u}_{\kappa}(t) e^{i\kappa x} \right\} \; ; \; \kappa \Delta x \in (0, \pi) \] (39)

and the semi-discrete equation can be written in Fourier-space as

\[ \sum_{\kappa} \left( \frac{d\tilde{u}_{\kappa}}{dt} e^{i\kappa x} + \tilde{u}_{\kappa} \left[ \frac{\partial e^{i\kappa x}}{\partial x} - \nu \frac{\partial^2 e^{i\kappa x}}{\partial x^2} \right] \right) = 0 \] (40)

The error introduced by the space-discretization can be quantified by introducing the modified wavenumbers\(^34\) for the upwind-biased discretization of \( \partial_x e^{i\kappa x} \equiv i \kappa e^{i\kappa x} \)

\[ i\kappa_{N_1} \Delta x = \sum_{\ell=-L_1}^{L_1-1} (2L_1-1) b_{\ell}^{(1)} e^{i\ell \kappa \Delta x} \] (41)

and for the centered discretization of \( \partial^2_{xx} e^{i\kappa x} \equiv -\kappa^2 e^{i\kappa x} \)

\[ -(\kappa_{N_2} \Delta x)^2 = \sum_{\ell=-L_2}^{L_2} (2L_2+1) b_{\ell}^{(2)} e^{i\ell \kappa \Delta x} \] (42)

Since the work of Lele\(^34\) the departure of \( \kappa_{N_1} \) (Eq. 41) and of \( \kappa_{N_2} \) (Eq. 42) from the exact value of \( \kappa \) (which is only recovered by a spectral scheme\(^34\)) is used\(^33,36\) to evaluate the accuracy of the space-discretization (Fig. 6).

The following semi-discrete equation for the Fourier coefficients is obtained

\[ \frac{d\tilde{u}_{\kappa}}{dt} + \tilde{u}_{\kappa} \frac{\alpha \Delta t}{\Delta x} e^{i(\kappa_{N_1} \Delta x)} = -\tilde{u}_{\kappa} \frac{\nu \Delta t}{\Delta x^2} (\kappa_{N_2} \Delta x)^2 \] (43)

and upon introduction of the CFL (Courant-Friedrichs-Levy) and VNN (von Neumann) numbers

\[ \text{CFL} := \frac{\alpha \Delta t}{\Delta x} \] (44a)

\[ \text{VNN} := \frac{2\nu \Delta t}{\Delta x^2} \] (44b)
Defining the standard form for the von-Neumann stability analysis, where the space-discretizations and on the CFL numbers, the semi-discrete equation reads

\[ \frac{d\hat{u}_\kappa}{dt} + \frac{\hat{u}_\kappa}{\Delta t} \left\{ i\text{CFL}(\kappa_N, \Delta x) + \frac{1}{2}\text{VNN}(\kappa_N, \Delta x)^2 \right\} = 0 \quad \forall \kappa \Delta x \in (0, \pi) \] (45)

Defining

\[ \hat{Z}_\kappa(\kappa \Delta x, \text{CFL}, \text{VNN}; \kappa_N, \Delta x, \kappa_N, \Delta x) := - \left\{ i\text{CFL}(\kappa_N, \Delta x) + \frac{1}{2}\text{VNN}(\kappa_N, \Delta x)^2 \right\} \] (46)

the standard form for the von-Neumann stability analysis is obtained, with \( \hat{Z}_\kappa \) depending on the order of the space-discretizations and on the CFL and VNN numbers.

\[ \frac{d\hat{u}_\kappa}{dt} = \frac{\hat{u}_\kappa}{\Delta t} \hat{Z}_\kappa = 0 \quad \forall \kappa \Delta x \in (0, \pi) \] (47)

is obtained, with \( \hat{Z}_\kappa \) depending on the order of the space-discretizations and on the CFL and VNN numbers.

Notice that with the above definitions for CFL and VNN (Eqs. 44) the stability limit for the advection-diffusion equation, using RK2 time-integration, UW01 discretization for \( \partial_x u \), and C02 discretization for \( \partial_x^2 u \), is CFL + VNN = 1.

### 4.3. Modified Wave-Speed and Dissipation

For the upwind-biased discretizations of \( \partial_x u \) (Eqs. 37) and the centered discretizations of \( \partial_x^2 u \) (Eqs. 38), used in the present work

\[ \Im(\hat{Z}_\kappa) = -i\text{CFL}\Re(\kappa_N, \Delta x) \leq 0 \] (48a)

\[ \Re(\hat{Z}_\kappa) = - \left[ \text{CFL}\Im(-\kappa_N, \Delta x) + \frac{1}{2}\text{VNN}(\kappa_N, \Delta x)^2 \right] \leq 0 \] (48b)

Obviously \( \Im(-\hat{Z}_\kappa) \) is the representation of convection in the modified equation, and \( \Re(\hat{Z}_\kappa) \) is the representation of diffusion. Straightforward manipulation of the semi-discrete equation (Eq. 47),

\[ \frac{d\hat{u}_\kappa}{dt} + i \left( a\Re(\kappa_N) \right) \kappa \hat{u}_\kappa = - \left[ \nu \left( \frac{\kappa_N}{\kappa} \right)^2 + \frac{a\Im(-\kappa_N)}{\kappa^2} \right] \kappa^2 \hat{u}_\kappa \] (49)

and comparison with the exact equation in Fourier-space (Eq. 34) defines the modified wave-speed \( \alpha_{\kappa_m} \), and the modified viscosity \( \nu_{\kappa_m} \)

\[ \frac{\alpha_{\kappa_m}}{a} = \Re(\kappa_N) \] (50a)

\[ \frac{\nu_{\kappa_m}}{\nu} = \left( \frac{\kappa_N}{\kappa} \right)^2 + \frac{2\text{CFL}\Im(-\kappa_N)}{\text{VNN}(\kappa_N, \Delta x)} \] (50b)

The modified wave-speed has been studied by several authors, mainly within the framework of the advection equation. On the other hand the competition between the numerical dissipation added by the upwind discretization to the physical dissipation has received less attention. Obviously (Eq. 50b) the relative importance of this numerical dissipation is a function of both the particular upwind scheme used and of the ratio CFL/VNN.

### 4.4. eDTSBDF2 Time-Discretization

The equation after eDTSBDF2 time-discretization, for subiteration \( m_{it} = m + 1 \) of iteration \( n_{it} = n + 1 \), reads

\[ \Delta \hat{u}_{\kappa_{n+1}} = \frac{\Delta t^{**}}{\Delta t} \left\{ \frac{2}{m+1}\hat{u}_{\kappa_{n+1}} - \frac{2}{m}\hat{u}_{\kappa_{n+1}} + \frac{1}{m-1}\hat{u}_{\kappa_{n+1}} - \frac{m+1}{m-1}\hat{u}_{\kappa_{n+1}} \hat{Z}_{\kappa_{n+1}} \right\} \quad \forall \kappa \Delta x \in (0, \pi) \] (51)

where

\[ \frac{\Delta t^{**}}{\Delta t} = \frac{\Delta t^{**}}{\Delta t} \] (52)

\[ r^* := \frac{\Delta t^{**}}{\Delta t^{**}} = \frac{\text{CFL}}{\text{CFL}^*} = \frac{\text{VNN}}{\text{VNN}^*} \] (53)
where \( r^* \) is the physical-to-dual-time-step ratio. Defining the amplification factors

\[
\begin{align*}
G_{\kappa}^n &= \frac{n^1\hat{G}_\kappa}{n\hat{u}_\kappa} \\
G_{\kappa}^{m+1,n+1} &= \frac{m+1,n^1\hat{G}_\kappa}{n\hat{u}_\kappa} \\
G_{\kappa}^n &= \frac{n^0\hat{G}_\kappa}{n\hat{u}_\kappa}
\end{align*}
\]

the discrete equation reads

\[
m+1,n^1\hat{G}_\kappa = m,n^1\hat{G}_\kappa - \frac{2}{2} m,1,2\hat{G}_\kappa - 2 + \frac{1}{2} m,1,nG_{\kappa} - m,n^1\hat{G}_\kappa, \hat{Z}_\kappa \\
= \hat{H}_\kappa m,n^1\hat{G}_\kappa + \frac{1}{2} m,n\hat{H}_\kappa \left[ 4 - \frac{1}{M_{n^0}G_{\kappa}} \right] \quad \forall \kappa \in (0, \pi)
\]

with

\[
\hat{H}_\kappa(r^*, \hat{Z}_\kappa) := \frac{r^* + \hat{Z}_\kappa}{\frac{r^*}{2} + r^*} \quad \forall \kappa \in (0, \pi)
\]

and since \( 0,n^1\hat{G}_\kappa \equiv 1 \), the amplification factor reads (proof by induction)

\[
m+1,n^1\hat{G}_\kappa = \hat{H}_\kappa^m + \frac{1}{2} \left( 1 + \cdots + \hat{H}_\kappa^m \right) \left[ 4 - \frac{1}{M_{n^0}G_{\kappa}} \right] \quad \forall \kappa \in (0, \pi)
\]

Assuming that, for a subiterative strategy with a constant number of subiterations \( M_{it} \) at each iteration, the amplification factor \( M_{n^0}G_{\kappa} \) does not depend on the iteration counter \( n \) (for \( n \gg 1 \)), there are 2 roots for \( M_{n^0}G_{\kappa} \), the principal root \( [M_{n^0}G_{\kappa}]_1 \) approximating the solution of the equation \( e^{2\pi i} \) to the order of time-accuracy, and 1 spurious root\(^1,2 [M_{n^0}G_{\kappa}]_2 \). These roots are solutions of the quadratic equation

\[
M_{n^0}G_{\kappa}^2 = \frac{2}{2} \left( 1 + \cdots + \hat{H}_\kappa^{M_{n^0}-1} \right) \left[ 4 - \frac{1}{M_{n^0}G_{\kappa}} \right] \quad \forall \kappa \in (0, \pi)
\]

since \( m = m_{it} - 1 \) (Eq. 55). The amplification factor for each wavelength \( \text{AF}_\kappa \), and the global amplification factor \( \text{AF} \) are obviously

\[
\text{AF}_\kappa = \max \left\{ [M_{n^0}G_{\kappa}]_1, [M_{n^0}G_{\kappa}]_2 \right\} \quad \text{AF} = \max_{\kappa, \Delta x \in (0, \pi)} \left\{ \text{AF}_\kappa \right\}
\]

and a necessary condition for stability is \( \text{AF} \leq 1 \).

### 4.5. eDTSBDF2 Stability in the (VNN, CFL)-Plane

It follows, from the definition of the Fourier-symbol \( \hat{Z}_\kappa \) (Eqs. 46, 48), that for a given space-discretization which defines \( \kappa_{N_1} \) (Eq. 41) and \( \kappa_{N_2} \) (Eq. 42), the (VNN, CFL)-plane is mapped onto the \( Z \)-plane. Obviously (Eqs. 48), the inverse mapping exists \( \forall \kappa, \Delta x \in (0, \pi) \) if \( \kappa_{N_1}, \Delta x \neq 0 \neq \kappa_{N_2}, \Delta x \)

\[
\begin{align*}
\text{CFL} &= \frac{3(-\hat{Z}_\kappa)}{\Re(\kappa_{N_1}, \Delta x)} \\
\text{VNN} &= \frac{2\Re(-\hat{Z}_\kappa)(\kappa_{N_1}, \Delta x)}{\Re(\kappa_{N_1}, \Delta x)(\kappa_{N_2}, \Delta x)^2}
\end{align*}
\]

where \( \Re(\cdot) \) denotes the complex-conjugate. In that way the \( Z \)-plane stability boundaries can, as usual\(^1 \), be mapped on the (VNN, CFL)-plane. In practice, however, \( r^* \) is not fixed, but some criterion is used to define \( \Delta \tau^*_p \) (spatially varying). The particular criterion used in the present work (although not necessarily optimal) was

\[
\max(\text{CFL}^*, \text{VNN}^*) = 1 \quad \forall n_p \in [1, N_p]
\]
which, together with the physical time-step $\Delta t$ defines $c^*_n$ (Eqs. 53).

Stability-boundaries in the (VNN, CFL)-plane of eDT$S$–BDF02 with $\max((\text{VNN}^*, \text{CFL}^*)) = 1$, using UW07–C02, UW09–C02 and UW11–C02 space-discretizations, are less restrictive than the corresponding RK4 boundaries (Fig. 7). Notice also the extent of the stability region for large VNN numbers (Fig. 7). The loci of (VNN, CFL) encountered in typical wall-turbulence simulations (Figs. 1, 2) are within the eDT$S$–BDF02 stability-boundaries ($M_{lt} \to \infty$) but outside those of the RK4, for the near-wall-nodes (Fig. 7). As for the Z-plane study the $M_{lt} \to \infty$ stability-boundary is rapidly approached for $M_{lt} \in [5, 10]$ (Figs. 7–9). Considering the wall-nodes of the supersonic simulation ($Re_{lw} = 221$, $M_{lt} = 1.50$; Fig. 2), when using the UW11–C02 scheme, although the principal root is stable $\max_k |\hat{G}_k| \leq 1 \forall M_{lt} \geq 5$ (Fig. 9) the spurious root is at the limit of stability, requiring $M_{lt} \geq 15$ (Fig. 7). For the UW09–C02 scheme used in the supersonic simulations (Fig. 1) the (VNN, CFL)-loci of the grid-nodes are within the stability-boundary $\forall M_{lt} \geq 5$. For the (VNN, CFL)-values encountered away from the wall (Fig. 2), both eDT$S$–BDF02 and RK4 agree well with the exact value of the amplification factor $e^{2\pi}$ (Figs. 7–9), for which CFL $\ll 1 \gg$ VNN. For the near-wall-nodes of the subsonic computation, for which CFL $\geq$ VNN, both methods have comparable accuracy at $y^+ = 1$ (Fig. 8), but RK4 is unstable for $y = 0$. For the near-wall-nodes of supersonic computation, for which VNN $\geq$ CFL, RK4 has better spectral accuracy at $y^+ = 1$ (Fig. 9), but is again unstable at $y = 0$.

A more detailed theoretical analysis of eDT$S$ methods (which can be extended to include so-called matrix-free DT$S$ methods\cite{11}), including\cite{37,38} the determination of regions of dispersion-relation-preservation (DRP) in both the Z-plane and the (VNN, CFL)-plane, is beyond the scope of the present work. Nonetheless, the results presented here indicate that eDT$S$ may be an interesting alternative to RK for DNS computations (notice that the computational cost of 1 subiteration is exactly equivalent to the computational cost of 1 RK step, so that

$\max(\text{CFL}^*, \text{VNN}^*) = 1$

![Figure 7. Stability limits in the (VNN, CFL)-plane for the RK4 and eDT$S$–BDF02 time-integration methods, with $\max(\text{CFL}^*, \text{VNN}^*) = 1$, using the UW07–C02, UW09–C02, and UW11–C02 space-discretization schemes, and (VNN, CFL) loci for typical supersonic (UW09–C02, $Re_{lw} = 221$, $M_{lt} = 1.50$, $\Delta y_2 = 0.24$, $\Delta y_{Cl} = 5.8$, $\Delta x^+ = 24.3$, $\Delta x_{max} = 12.1$, $\Delta t^+ = 16.9 \times 10^{-3})$ and subsonic (UW11–C02, $Re_{lw} = 183$, $M_{Cl} = 0.35$, $\Delta y_{Cl} = 0.19$, $\Delta x_{max} = 4.5$, $\Delta x^+ = 19.2$, $\Delta x_{max} = 9.6$, $\Delta t^+ = 5.4 \times 10^{-3})$ plane channel flow DNS computations (Fig. 1).](image_url)
an eDTS computation with $M_{it} \in [5, 7]$ is less expensive than 2 RK4 iterations).

\[
\begin{align*}
\text{exact } (e^{\hat{Z}_{\kappa}}) & \quad \text{RDTS-BDF02: } M_{it} = 5 \\
\{\hat{G}_{\kappa}\}, \text{RDTS-BDF02: } M_{it} = 10 & \\
\{\hat{G}_{\kappa}\}, \text{RDTS-BDF02: } M_{it} = \infty & \\
\{\hat{G}_{\kappa}\}, \text{RDTS-BDF02: } M_{it} = \infty (spurious root) & \\
\text{RK4} & \\
\end{align*}
\]

\[
\begin{align*}
\text{CFL} = 1.470; \ V_{NN} = 0.600; \ \text{CFL}^* = 1; \ V_{NN}^* = 0.408; \ r^* = 1.470
\end{align*}
\]

\[
\begin{align*}
\text{CFL} = 1.170; \ V_{NN} = 0.370; \ \text{CFL}^* = 1; \ V_{NN}^* = 0.316; \ r^* = 1.170
\end{align*}
\]

\[
\begin{align*}
\text{CFL} = 0.095; \ V_{NN} = 0.001; \ \text{CFL}^* = 1; \ V_{NN}^* = 0.010; \ r^* = 0.095
\end{align*}
\]

Figure 8. Distribution of $|\hat{G}_{\kappa}|$ vs $\kappa \Delta x \in (0, \pi)$ (left) and plots of $\hat{G}_{\kappa}$ in the complex-plane (right), using the RK4 and eDTS-BDF02 time-integration methods, with UW11-C02 space discretization, for various (CFL, VNN) combinations, corresponding to values encountered in typical DNS computations of subsonic ($Re_{\tau_w} = 183$, $\bar{M}_{CL} = 0.35$) plane channel flow, viz at $y = 0$ (top), $y^+ = 1$ (middle) and $y = \delta$ (bottom).
Figure 9. Distribution of $|\hat{G}_\kappa|$ vs $\kappa \Delta x \in (0, \pi)$ (left) and plots of $\hat{G}_\kappa$ in the complex-plane (right), using the RK4 and eDTS–BDF02 time-integration methods, with $UW_{11}–C_{02}$ space discretization, for various $(CFL, VNN)$ combinations, corresponding to values encountered in typical DNS computations of supersonic ($Re_\tau = 232$, $M_{CL} = 1.50$) plane channel flow, viz at $y = 0$ (top), $y^+ = 1$ (middle) and $y = \delta$ (bottom).
4.6. eDTSBDF Stability in the (VNN, CFL)-Plane

Consideration of higher-order eDTSBDF\(k\) methods, using ieg UW17–C18 space discretization, indicates different behaviour for \(r^* = 1\) (Fig. 10) or \(\max(CFL^*, VNN^*) = 1\) (Fig. 11), the optimum being a
isothermal walls), on different grids (such as DNS relatively high time-steps, for problems where the time-step is limited by viscous stability considerations, not perform very well for convection-dominated problems. On the other hand, they will work quite well, with higher-order eDTsBDFs in both cases (Figs. 10, 11), and that the stability region, for convection-dominated flows, of these combination of these 2 choices. Notice however that the stability boundary, near the imaginary axis, is the same in both cases (Figs. 10, 11), and that the stability region, for convection-dominated flows, of these DTSBDF, from data from Kim et al.

5. Computational Examples

From the above analysis it is obvious that high-order eDTsBDF methods, although applicable, they will not perform very well for convection-dominated problems. On the other hand, they will work quite well, with relatively high time-steps, for problems where the time-step is limited by viscous stability considerations, such as DNS of wall-turbulence (Fig. 12).

<table>
<thead>
<tr>
<th>$Re_{cu}$</th>
<th>$M_{Cu}$</th>
<th>$N_x \times N_y \times N_z$</th>
<th>$L_x$</th>
<th>$L_y$</th>
<th>$L_z$</th>
<th>$\Delta x^+$</th>
<th>$\Delta y^+$</th>
<th>$\Delta z^+$</th>
<th>$N_{y^+}$</th>
<th>$N_{z^+}$</th>
<th>$c_{max}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>179</td>
<td>0.35</td>
<td>193 x 129 x 169</td>
<td>4$n\delta$</td>
<td>25</td>
<td>$\delta$</td>
<td>11.7</td>
<td>0.23</td>
<td>20</td>
<td>5.0</td>
<td>4.5</td>
<td>1086</td>
</tr>
<tr>
<td>180</td>
<td>0.35</td>
<td>129 x 129 x 129</td>
<td>4$n\delta$</td>
<td>25</td>
<td>$\delta$</td>
<td>17.7</td>
<td>0.23</td>
<td>20</td>
<td>5.0</td>
<td>3.9</td>
<td>1204</td>
</tr>
<tr>
<td>185</td>
<td>0.35</td>
<td>129 x 161 x 81</td>
<td>4$n\delta$</td>
<td>25</td>
<td>$\delta$</td>
<td>19.4</td>
<td>0.19</td>
<td>25</td>
<td>4.6</td>
<td>6.7</td>
<td>1004</td>
</tr>
<tr>
<td>179</td>
<td>0.35</td>
<td>225 x 129 x 193</td>
<td>4$n\delta$</td>
<td>25</td>
<td>$\delta$</td>
<td>10.0</td>
<td>0.23</td>
<td>20</td>
<td>5.0</td>
<td>4.9</td>
<td>1013</td>
</tr>
<tr>
<td>183</td>
<td>0.35</td>
<td>121 x 161 x 81</td>
<td>4$n\delta$</td>
<td>25</td>
<td>$\delta$</td>
<td>19.2</td>
<td>0.19</td>
<td>25</td>
<td>4.5</td>
<td>6.6</td>
<td>1011</td>
</tr>
<tr>
<td>178</td>
<td>0.00</td>
<td>128 x 129 x 128</td>
<td>4$n\delta$</td>
<td>25</td>
<td>$\delta$</td>
<td>17.7</td>
<td>0.05</td>
<td>14</td>
<td>4.4</td>
<td>5.9</td>
<td>1800</td>
</tr>
<tr>
<td>186</td>
<td>0.00</td>
<td>768 x 97 x 512</td>
<td>12$n\delta$</td>
<td>25</td>
<td>$\delta$</td>
<td>8.9</td>
<td>0.10</td>
<td>11</td>
<td>6.1</td>
<td>4.5</td>
<td>10014</td>
</tr>
</tbody>
</table>

Figure 12. Comparison of computed 1-D spectra ([E$_{uu}^{(x)}$], [E$_{ww}^{(y)}$], [E$_{ww}^{(z)}$], [E$_{uu}^{(x)}$], [E$_{ww}^{(y)}$], [E$_{ww}^{(z)}$], and [E$_{uu}^{(x)}$] at $y^+ = 5.3$ and at $y^+ = 10.4$, from eDTsBDF2 DNS computations using the UW1-C02 and UW1-C02 schemes ($Re_{cu}$ $\in [179, 185]$, $M_{CuL} = 0.35$, isothermal walls), on different grids ($225 \times 129 \times 193$, 193 x 129 x 169, 129 x 129 x 129 and 121 x 161 x 81), with incompressible DNS-data from Kim et al. (1999) and from del Alamo et al. (2004).
6. Conclusions

In the present work we studied dual-time-stepping methods with explicit subiterations, based on backward-differencing of $O(\Delta t^k)$ (eDTS–BDF$k$), for the advection-diffusion and the Navier-Stokes equations. The stability boundaries were defined, both in the generic case, and for the advection-diffusion equation, in the (\text{VNN, CFL})-plane. It was found that these methods may be of interest for the computation of diffusion-dominated problems.

Acknowledgments

The computations presented were run at the Institut pour le Développement des Ressources en Informatique Scientifique (1DRIS), where computer resources were made available by the Comité Scientifique. The authors are listed alphabetically.

References


