IMPROVED DUAL TIME-STEPPING USING SECOND DERIVATIVES

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Abstract. We present an improved and modified formulation of the dual time-stepping technique which makes use of two derivatives in pseudo-time. This new technique, based on the critically damped harmonic oscillator, retains the convergence properties to the stationary solution. Furthermore, when compared with the conventional time-marching, the dual time-stepping with two derivatives reduces the stiffness of the problem and requires fewer iterations for full convergence to steady-state.

1 INTRODUCTION

The Dual Time—Stepping (DTS) technique has been first introduced in [1] for solving a large system of nonlinear equations obtained after an implicit time—discretization of the compressible Euler equations. In the original formulation, the DTS procedure consists in adding the derivative of the solution with respect to the so—called dual time and marching in time to reach the steady—state. Later, the same approach was successfully used in [2] for incompressible Euler and Navier—Stokes equations and it became commonly used in computational fluid dynamics. Other examples in which derivatives in fictitious time are introduced to solve systems of nonlinear equations include various engineering fields such as magnetohydrodynamics [3], simulations of launch environments [4] and electronics [5].

One drawback of the dual-time stepping technique is that the pseudo-time iterations must be fully converged in order to obtain an error estimate for time accuracy [6]. Moreover, if the dual time integration is carried out with an explicit scheme, the method may become unstable for pseudo-time steps exceeding the physical ones [7]. These two limitations may lead to a large number of dual-time iterations and hence to a computationally expensive method.

For these reasons, significant efforts have been made during the last decade to improve the performances of DTS. One strategy to accelerate the computations is to introduce a preconditioner multiplying the pseudo-time derivative [2, 8, 9]. Further improvements can be achieved by developing hybrid discretizations for the physical-time derivative. In [6, 10] the Alternating-Direction Implicit (ADI) scheme [11] is used in conjunction with the common BDF2. Another example is provided in [12], where the hybrid scheme is built with the Lower-Upper Symmetric-Gauss-Seidel (LU-SGS) method [13]. A further improvement of the dual time-marching is proposed in [14], where a local time-stepping approach is used.

The goal of this paper is to explore if we can accelerate the convergence of DTS by adding a second order pseudo-time derivative. The article is organized as follows: in Section 2, the DTS technique is presented and its convergence properties are shown. Section 3 describes a new class of dual time-marching procedures and introduces the second-derivative DTS. In Section 4, numerical simulations that corroborate the theoretical results are presented, while in Section 5 the main drawbacks of the scheme and alternative formulations are discussed. In Section 6 conclusions are drawn.

2 THE DUAL TIME-STEPPING TECHNIQUE

We start by illustrating how DTS is applied to a fully discretized hyperbolic problem.

2.1 The hyperbolic model problem

Consider the one-dimensional advection equation

$$u_t + au_x = 0, \quad x \in \Omega, \quad t > 0, \tag{1}$$

where a is a positive constant and Ω the spatial domain. Let $u_x \approx D\mathbf{u}$ be a general discretization of the spatial derivative, where \mathbf{u} is the vector approximating the solution on a spatial grid. By applying Euler-backward scheme in time to (1) and indicating by Δt the time-step, we get

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + aD\mathbf{u}^{n+1} = 0.$$
 (2)

Here, \mathbf{u}^{n+1} and \mathbf{u}^n represent the approximated solution at the different times $t^{n+1} = (n+1)\Delta t$ and $t^n = n\Delta t$, respectively. The calculation of \mathbf{u}^{n+1} by directly inverting the matrix

 $(I/\Delta t + aD)$ in (2) may be excessively expensive. Instead, we apply the DTS technique by renaming \mathbf{u}^{n+1} with \mathbf{w} and adding the dual-time derivative \mathbf{w}_{τ} on the left hand-side of (2) obtaining

$$\mathbf{w}_{\tau} + \frac{\mathbf{w} - \mathbf{u}^n}{\Delta t} + aD\mathbf{w} = 0, \qquad \tau > 0.$$
 (3)

If the solution w in (3) reaches steady–state, it will converge to \mathbf{u}^{n+1} in (2). The scheme (3) can be rewritten in the following compact form

$$\mathbf{w}_{\tau} + F\mathbf{w} = \mathbf{R}, \qquad \tau > 0, \tag{4}$$

where $F = I/\Delta t + aD$, $\mathbf{R} = \mathbf{u}^n/\Delta t$ and I is the identity matrix.

2.2 Nonlinear problems

Under mild restrictions, nonlinear differential problems can be related to linear formulations. As an example, consider a fully discretized problem using Euler–backward in time,

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + L\left(\mathbf{u}^{n+1}\right) = \mathbf{0}.$$
 (5)

In (5), $L(\mathbf{u})$ is a nonlinear operator, typically coming from a nonlinear space approximation. Assuming small variations of the solution in time, a linearization of L can be performed:

$$L\left(\mathbf{u}^{n+1}\right) = L\left(\mathbf{u}^{n}\right) + \frac{\partial L}{\partial \mathbf{u}} \Delta \mathbf{u} + O\left(\left\|\Delta \mathbf{u}\right\|^{2}\right),\tag{6}$$

where $\partial L/\partial \mathbf{u}$ is the Jacobian matrix of L and $\Delta \mathbf{u} := \mathbf{u}^{n+1} - \mathbf{u}^n$. By substituting (6) into (5) we obtain the linear problem

$$\left(\frac{I}{\Delta t} + \frac{\partial L}{\partial \mathbf{u}}\right) \Delta \mathbf{u} \simeq -L\left(\mathbf{u}^{n}\right),\,$$

which can be solved using the dual-time stepping technique (4) by indicating with $F = I/\Delta t + \partial L/\partial \mathbf{u}$ and $\mathbf{R} = -L(\mathbf{u}^n)$. Hence, one can relate general problems to the linear setting, as long as the Jacobian matrix $\partial L/\partial \mathbf{u}$ is well-defined. The assumption of small variations in time can be fulfilled by considering sufficiently small time steps Δt .

2.3 Convergence

A general linear time-space discretization of a differential problem has the form

$$F\mathbf{u} = \mathbf{R},\tag{7}$$

where F is a nonsingular matrix and \mathbf{R} is given and independent of \mathbf{u} . Moreover, we assume that F is diagonalizable, i.e. $F = X\Lambda X^{-1}$ where X, Λ are the matrices of the eigenvectors and eigenvalues of F, respectively.

By adding a dual–time derivative to the left hand–side of (7) we obtain (4), which converges in dual time to the solution of (7) since the following proposition holds.

Proposition 2.1. Let all the eigenvalues of the diagonalizable F have a positive real part. Then the dual–time dependent problem (4) converges to the solution of (7).

Proof. Applying the eigendecomposition of F to (4) yields

$$\mathbf{v}_{\tau} + \Lambda \mathbf{v} = X^{-1} \mathbf{R}, \qquad \tau > 0, \tag{8}$$

where ${\bf v}=X^{-1}{\bf w}.$ By multiplying (8) with $e^{\Lambda \tau}$ from the left and integrating we find

$$\mathbf{v}\left(T\right)=e^{-\Lambda T}\mathbf{v}\left(0\right)+\Lambda^{-1}\left(I-e^{-\Lambda\tau}\right)X^{-1}\mathbf{R},$$

which converges as $T \to +\infty$ if all the eigenvalues of F have positive real parts. Finally, the steady-state solution $\mathbf{w} = F^{-1}\mathbf{R}$ is recovered by multiplying \mathbf{v} with X.

Remark 2.2. Since F can be diagonalized, the eigenvalues contain all the information needed for convergence. In particular, the eigenvalue with the minimum real part determines the convergence rate in (4).

2.4 A note on preconditioning

To increase the convergence we may introduce a preconditioner Γ which multiplies the first–derivative term in (4), yielding

$$\Gamma^{-1}\mathbf{w}_{\tau} + F\mathbf{w} = \mathbf{R}.\tag{9}$$

The optimal choice of Γ in (9) depends on the specific problem, and will not be discussed in detail in this paper. We simply observe that the choice $\Gamma = cF^{-1}$, with c > 0, leads to a problem whose convergence does not depend on the eigenvalues of F, since (9) becomes

$$\mathbf{w}_{\tau} + c\mathbf{w} = cF^{-1}\mathbf{R}.\tag{10}$$

Note that, according to Proposition 2.1, this formulation is always convergent. On the other hand, even though the magnitude of c can be chosen in order to get a fast convergence of (4), the formulation (10) requires the inverse of F, which we want to avoid.

2.5 Model Problem

The proof of Proposition 2.1 indicates that rather than considering the matrix–vector problem (7) at once, one may instead study the scalar model problem

$$w_{\tau} + \lambda w = r, \qquad \tau > 0, \tag{11}$$

defined by each row in (8) separately, with the corresponding steady-state solution

$$\lambda u = r, \qquad \lambda \in \mathbb{C} \setminus \{0\}.$$
 (12)

3 THE SECOND-DERIVATIVE DTS TECHNIQUE

To possibly get an even faster decay to steady–state, we add two pseudo–time derivatives to the fully–discretized problem (7),

$$\mathbf{w}_{\tau\tau} + 2C\mathbf{w}_{\tau} + F\mathbf{w} = \mathbf{R}, \qquad \tau > 0, \tag{13}$$

where C is an arbitrary matrix to be chosen in order to improve the convergence.

Remark 3.1. A matrix parameter in front of the second derivative term in (13) would play the same role as Γ^{-1} in (9) for the classical DTS formulation, and hence we consider (13) to be the most general DTS formulation involving two derivatives in dual time.

We choose a diagonazable matrix $C = X\Theta X^{-1}$ in (13) with the same eigenvectors as F. This allows us to rewrite (13) as a system of independent ODEs of the form

$$w_{\tau\tau} + 2\theta w_{\tau} + \lambda w = r, \qquad \tau > 0, \tag{14}$$

where θ , λ are eigenvalues of C and F, respectively. Note that the steady–state solution of (14) solves the model problem (12). Thus, the convergence properties of the classical and second–derivative DTS can be compared by studying the scalar equations (11) and (14).

The second–order ordinary differential equation (14) can be written as a system of first–order equations

$$\mathbf{z}_{\tau} + A\mathbf{z} = \mathbf{b}, \quad \text{where} \quad \mathbf{z} = \begin{bmatrix} w \\ w_{\tau} \end{bmatrix}, \quad A = \begin{bmatrix} 0 & -1 \\ \lambda & 2\theta \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 0 \\ r \end{bmatrix}.$$
 (15)

By using the matrix exponential notation the solution to the system (15)

$$\mathbf{z}\left(\tau\right) = e^{-A\tau} \left(\mathbf{z}\left(0\right) - A^{-1}\mathbf{b}\right) + A^{-1}\mathbf{b} \tag{16}$$

converges to $A^{-1}\mathbf{b} = [u, 0]^T$, i.e. $w(\tau) \to u$, for any $\mathbf{z}(0)$ as $\tau \to +\infty$, if the eigenvalues of A have positive real parts.

Remark 3.2. The matrix exponential $e^{-A\tau}$ can be obtained by the Jordan form of $A = VJV^{-1}$, where V is invertible and J is a triangular matrix composed by Jordan blocks. In particular, $e^{-A\tau} = Ve^{-J\tau}V^{-1}$ and the eigenvalues of A characterize the convergence of (15). Note that for distinct eigenvalues, J and V are the matrices containing the eigenvalues and eigenvectors of A, respectively.

3.1 Initial convergence analysis

A physical interpretation of (14) is given by the damped harmonic oscillator, if the coefficients θ and λ are real. It is well–known that this system converges to steady–state if both θ and λ in (14) are positive. Furthermore, the system approaches steady–state as quickly as possible, without oscillating, when it is critically damped, i.e. when $\theta = \sqrt{\lambda}$. In this section we will use these results as guidelines for the case with complex coefficients. Hence in the rest of the section, unless stated otherwise, we consider $\theta \in \mathbb{R}$, $\lambda \in \mathbb{R} \setminus \{0\}$.

From Proposition 2.1, the classical DTS in (11) converges to the steady–state solution as $T \to +\infty$ if $\lambda > 0$. For the second–derivative DTS (14) we prove

Proposition 3.3. Let θ and λ be real coefficients. The solution to the problem (14) converges to its steady–state solution as $\tau \to +\infty$ if θ and λ are positive.

Proof. The solution (16) converges to the steady–state solution if all the eigenvalues of A have positive real parts. The characteristic polynomial of the matrix A is $\mu^2 - 2\theta\mu + \lambda = 0$ and leads to the eigenvalues

$$\mu_{1,2} = \theta \pm \sqrt{\theta^2 - \lambda}.\tag{17}$$

If θ and λ are positive, then both real parts of $\mu_{1,2}$ in (17) are positive and the solution converges.

Next, our aim is to find conditions on θ to achieve a faster convergence than the classical Dual Time–Stepping technique in (11), i.e. we need

$$Re\left(\mu_{1,2}\right) \ge Re\left(\lambda\right),$$
 (18)

where μ_1 and μ_2 are given by (17). Condition (18) gives rise to

Proposition 3.4. The solution to the unsteady problem (14) converges to the steady–state faster than the solution to (11) as $\tau \to +\infty$ if

$$0 < \lambda \le 1$$
 and $\lambda \le \theta \le \frac{1+\lambda}{2}$. (19)

Proof. By substituting (17) into (18) and observing that $\theta, \lambda \in \mathbb{R}$, we find

$$Re\left(\sqrt{\theta^2 - \lambda}\right) \ge \lambda - \theta,$$
 (20a)

$$Re\left(\sqrt{\theta^2 - \lambda}\right) \le \theta - \lambda.$$
 (20b)

In order to prove the claim, we show that the values of θ outside the interval $[\lambda, (1 + \lambda)/2]$ do not satisfy (20). If $\theta < \lambda$, then $Re\left(\sqrt{\theta^2 - \lambda}\right) > \theta - \lambda$ and consequently (20b) does not hold. Given that $\theta \ge \lambda$, the condition (20a) is always fulfilled. By squaring (20b), we get

$$\lambda \left[\lambda + (1 - 2\theta) \right] \ge 0,$$

which is satisfied for $\lambda > 0$ and $\theta \le (1 + \lambda)/2$. The remaining constraint of the claim, i.e. $\lambda \le 1$, is necessary in order to guarantee that $\lambda \le (1 + \lambda)/2$.

Proposition 3.4 provides a condition on the coefficient θ that leads to faster decay of (14) with respect to (11) for any fixed $\lambda \in \mathbb{R} \setminus \{0\}$. It is legitimate to ask if there exists an optimal choice of the free parameter θ among all the values which leads to improved convergence.

Proposition 3.5. The choice $\theta = \sqrt{\lambda}$ provides the fastest decay for the second–derivative time–stepping formulation (14).

Proof. The eigenvalue of the matrix A in (15) with the smallest real part determines the decay to the steady–state solution. According to (17), this eigenvalue has a real part given by

$$Re(\mu_1) = \begin{cases} \theta, & \text{if } \theta^2 < \lambda, \\ \theta - \sqrt{\theta^2 - \lambda}, & \text{if } \theta^2 \ge \lambda. \end{cases}$$
 (21)

Since the real part of μ_1 increases for θ less than $\sqrt{\lambda}$ and decreases for θ greater than $\sqrt{\lambda}$, we conclude that $\theta = \sqrt{\lambda}$ maximizes the real part of μ_1 .

From (17), the optimal value of θ implies that the eigenvalues of A in (15) are $\mu_1 = \mu_2 = \sqrt{\lambda}$. The new and optimal DTS formulation (14) can be rewritten as

$$w_{\tau\tau} + 2\sqrt{\lambda}w_{\tau} + \lambda w = r. \tag{22}$$

This formulation leads to convergence if $\lambda > 0$. Moreover, faster decay with respect to (11) is achieved if $0 < \lambda \le 1$, since in this case $\sqrt{\lambda} \ge \lambda$.

Next, we consider directly the formulation (22) with $\lambda \in \mathbb{C} \setminus \{0\}$ and prove

Proposition 3.6. The solution to the problem (22) converges to its steady–state solution as $\tau \to +\infty$ if, and only if, λ is not a negative real number.

Proof. The problem (22) can be written as the system of first–order equations (15) with $\theta = \sqrt{\lambda}$. The eigenvalues of A are $\mu_1 = \mu_2 = \sqrt{\lambda}$ and lead to convergence if $Re\left(\mu_{1,2}\right) > 0$. The number $\sqrt{\lambda}$, interpreted as the principal square root of λ , has always a non–negative real part. If λ is a negative real number, then $Re\left(\sqrt{\lambda}\right) = 0$ which implies non–convergence.

In conclusion, the optimal choice in (13) is $C = F^{\frac{1}{2}} = X\Lambda^{\frac{1}{2}}X^{-1}$. In $\Lambda^{\frac{1}{2}}$ only the principal square roots are considered, i.e. the square roots with non–negative real parts.

3.2 The new DTS technique

Consider the new DTS technique applied to the original problem (7)

$$\mathbf{w}_{\tau\tau} + 2F^{\frac{1}{2}}\mathbf{w}_{\tau} + F\mathbf{w} = \mathbf{R}.\tag{23}$$

We can now prove

Proposition 3.7. The decay to steady–state for the new DTS formulation (23) is determined by the square roots of the eigenvalues of F.

Proof. The pseudo-time differential problem (23) can be written as a system of first-order equations

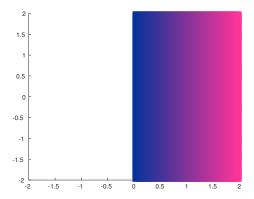
$$\begin{bmatrix} \mathbf{w} \\ \mathbf{w}_{\tau} \end{bmatrix}_{\tau} + \begin{bmatrix} I & 0 \\ F^{\frac{1}{2}} & I \end{bmatrix}^{-1} \begin{bmatrix} F^{\frac{1}{2}} & -I \\ 0 & F^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} I & 0 \\ F^{\frac{1}{2}} & I \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{w}_{\tau} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{R} \end{bmatrix}. \tag{24}$$

Clearly, the convergence of the system is determined by the eigenvalues of $F^{\frac{1}{2}}$.

The main consequence of Proposition 3.7 is that the new DTS formulation (23) converges to steady–state if the eigenvalues of F are non–zero and do not lie on the negative real axis. If the eigenvalues of F have positive real parts, then both the DTS formulations (4) and (23) are time convergent. In particular, the decay rates are determined by the eigenvalue with the smallest real part of F and $F^{\frac{1}{2}}$, respectively.

Remark 3.8. Note that the new DTS technique (23) can drive the solution to steady–state, when the classical one (4) fails to do that.

Remark 3.9. The square root of a number close to the imaginary axis has an output which is more distant from it. Similarly, if it is applied to a number with a large magnitude, the square root returns a number less distant from the origin. These two effects are illustrated in Figure 1.



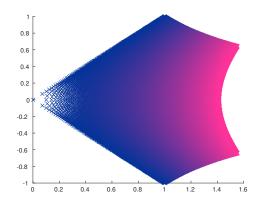


Figure 1: Complex numbers with nonnegative real parts (left figure) and their square root. Note that the distribution of points near the origin of the complex plane tends to rarefy.

As pointed out in Remark 3.9, if F has eigenvalues close to the imaginary axis, the second-derivative DTS decays faster than the classical formulation. Another effect of the square root is that it narrows the spectrum of F and enables the use of larger dual time–steps for an explicit time–integrator without causing stability issues.

4 NUMERICAL EXPERIMENTS

In this Section we perform numerical tests for both the classical (4) and the new DTS technique (23).

4.1 First-order ordinary differential equations

Consider the hyperbolic steady problem

$$u_x = f, \quad 0 < x < 1,$$

 $u(0) = g,$ (25)

where $f(x) = 10\pi \cos(10\pi x)$ and g = 1. The solution to (25) is $u(x) = \sin(10\pi x) + 1$.

To discretize (25), we use an (N+1)-point uniform grid over [0,1], where $x_j = jh$, $j = 0, \ldots, N$ and h = 1/N. Let f be a grid function such that $f_j = f(x_j)$ and u the approximate solution to (25). By applying a Summation-by-Parts (SBP) discretization to (25) for the derivative and Simultaneous-Approximation-Terms (SAT) to impose the boundary condition (see the Appendix for details and [15] for references), we get

$$P^{-1}Q\mathbf{u} = \mathbf{f} - P^{-1}\mathbf{e}_0 (u_0 - q), \qquad (26)$$

where $\mathbf{e}_0 = [1, 0, \dots, 0]^T \in \mathbb{R}^{(N+1)}$. Note that (26) has the form (7) with

$$F = P^{-1}(Q + E_0), \quad \mathbf{R} = \mathbf{f} + P^{-1}\mathbf{e}_0 g, \quad E_0 = \operatorname{diag}(1, 0, \dots, 0).$$
 (27)

The penalty term in (26) makes the classical DTS technique (4) stable in the P-norm $\|\mathbf{w}\|_P = \sqrt{\mathbf{w}^T P \mathbf{w}}$ (see Appendix B). Also, the new DTS (23) applied to (26) gives rise to a stable scheme since Proposition 3.7 holds.

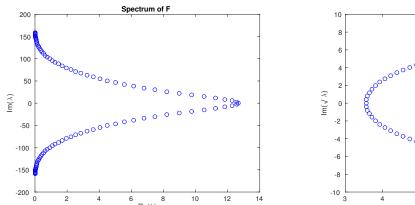
Remark 4.1. The classical pseudo-time marching technique (4) is convergent since all the eigenvalues of F have positive real parts. The new DTS formulation also converges since $F^{\frac{1}{2}}$ has only eigenvalues with positive real part, see [16] for details.

We use a spatial increment h=0.01 to represent the solution on [0,1] and the fourth order Runge-Kutta scheme as time-integrator. For both the schemes (4) and (23), we have used $\mathbf{w}=[1,\ldots,1]^T$ as the initial guess. Let \mathbf{w}^n be the solution to either (4) or (23) at the time $\tau^n=n\Delta\tau$. We consider the solution to be converged if $\|\mathbf{w}^n-\mathbf{u}\|_P<10^{-6}$, where \mathbf{u} is the solution to (26). The improved convergence can be seen directly by comparing the spectra of F and $F^{\frac{1}{2}}$. From Figure 2, it is clear that the second-derivatives DTS has better convergence properties since the eigenvalue with minimum real part is further away from the imaginary axis. The minimum number of iterations to convergence for the classical DTS is 178, corresponding to $\Delta\tau=0.0177$. Figure 3 shows that the new DTS (23) allows for the use of larger dual time-steps, since this formulation is less stiff than the classical one. The minimum number of iterations for the new DTS formulation (23) is 36, which is reached for $\Delta\tau=0.199$. We can conclude that the new DTS formulation is approximately five times more efficient than the old one, for this problem.

4.2 A model of the time-dependent compressible Navier-Stokes equations

Next, we study both DTS approaches applied to the following system

$$\mathbf{u}_{t} + A\mathbf{u}_{x} = \varepsilon B\mathbf{u}_{xx} + \mathbf{F}(x,t), \quad 0 < x < 1, \quad t > 0,
\mathbf{u}(x,0) = \mathbf{f}(x), \quad 0 < x < 1, \quad t > 0,
(u_{1} + \sqrt{2}u_{2} - \varepsilon u_{2,x})(0,t) = g_{0}(t), \quad t > 0,
(u_{1} - \sqrt{2}u_{2} - \varepsilon u_{2,x})(1,t) = g_{1}(t), \quad t > 0,$$
(28)



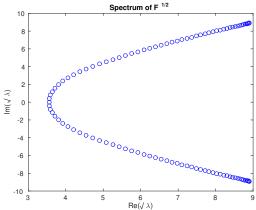
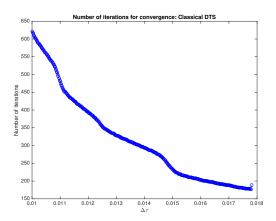


Figure 2: The spectrum of F and of its square root for the first order problem.



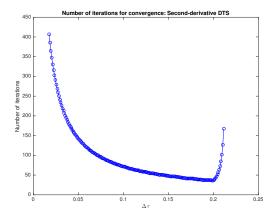


Figure 3: Number of iterations for the classical and new dual–time marching techniques. The new DTS is less stiff than the former formulation and a larger dual time–step can be chosen.

where $\mathbf{u}(x,t) = [u_1(x,t), u_2(x,t)]^T$, $\varepsilon = 10^{-2}$. The matrices A and B are real and given by

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

while $\mathbf{F}(x,t)$, $\mathbf{f}(x)$, $g_0(t)$, $g_1(t)$ are given data.

The specific boundary conditions $\left(u_1 + \sqrt{2}u_2 - \varepsilon u_{2,x}\right)(0,t) = g_0(t)$ and

 $\left(u_1 - \sqrt{2}u_2 - \varepsilon u_{2,x}\right)(1,t) = g_1(t)$ applied to the linearized Navier–Stokes like system (28) makes the problem strongly well–posed, i.e. a unique solution to (28) exists and its norm is bounded by the boundary and initial data. Moreover, the corresponding semi–discrete problem in space is strongly stable, if the SBP–SAT approach is used. These theoretical results are shown in the Appendix.

Here we limit ourselves to the study of the fully-discrete problem

$$\frac{3\mathbf{v}^{n+1} - 4\mathbf{v}^n + \mathbf{v}^{n-1}}{2\Delta t} + D \otimes A\mathbf{v}^{n+1} = \varepsilon D_2 \otimes B\mathbf{v}^{n+1} + \widetilde{\mathbf{F}}^{n+1} + \mathbf{SAT},\tag{29}$$

with $\mathbf{v}^0 = \widetilde{\mathbf{f}}$. The formulation (29) is obtained from (28) by discretizing in space with SBP–SAT and the 2nd order Backward Difference Formula (BDF2) in time. This two–step method

requires v^1 as initial data, which is recovered using the same space discretization and Euler backward in time.

We consider a grid with $x_j = jh$, j = 0, ..., N where h = 1/N is the grid spacing, and the grid functions $\tilde{\mathbf{f}}$, $\tilde{\mathbf{F}}^n \in \mathbb{R}^{2(N+1)}$ which approximate \mathbf{f} , $\mathbf{F}(t^n)$ in the continuous problem (28). With each grid point we associate the approximate solution $\mathbf{v} \in \mathbb{R}^{2(N+1)}$, such that

$$v_{2j}^n \cong u_1(x_j, t^n), \ v_{2j+1}^n \cong u_2(x_j, t^n), \quad j = 0, \dots, N.$$

In the fully–discrete problem (29), the symbol \otimes denotes the Kronecker product defined by

$$A = \{a_{ij}\} \in \mathbb{R}^{m \times n}, \ B \in \mathbb{R}^{n \times p}, \quad A \otimes B = \begin{bmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix} \in \mathbb{R}^{m \times p}.$$

Moreover, D and D_2 are SBP operators for the first and second derivatives and the vector SAT collects the penalty terms for the boundary conditions. The SAT term in (29) can be written as

$$\mathbf{SAT} = -\left(P^{-1}E_0 \otimes \Sigma\right) \left[(I_{N+1} \otimes H_0) \mathbf{v}^{n+1} - \varepsilon \left(I_{N+1} \otimes G\right) D\mathbf{v}^{n+1} - \widetilde{\mathbf{g}}_0^{n+1} \right] + \left(P^{-1}E_N \otimes \Sigma\right) \left[(I_{N+1} \otimes H_N) \mathbf{v}^{n+1} - \varepsilon \left(I_{N+1} \otimes G\right) D\mathbf{v}^{n+1} - \widetilde{\mathbf{g}}_N^{n+1} \right], \tag{30}$$

where $E_0 = \text{diag}(1, 0, \dots, 0)$, $E_N = \text{diag}(0, \dots, 0, 1)$ and I_M indicates the $M \times M$ identity matrix. Furthermore, we have used

$$\Sigma = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad H_0 = \begin{bmatrix} 1 & \sqrt{2} \\ 1 & \sqrt{2} \end{bmatrix}, \quad H_N = \begin{bmatrix} 1 & -\sqrt{2} \\ 1 & -\sqrt{2} \end{bmatrix}, \quad G = \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$$
(31)

and $\tilde{\mathbf{g}}_{0}^{n}=\left[g_{0}\left(t^{n}\right),g_{0}\left(t^{n}\right),0,\ldots,0\right]^{T},$ $\tilde{\mathbf{g}}_{N}^{n}=\left[0,\ldots,0,g_{1}\left(t^{n}\right),g_{1}\left(t^{n}\right)\right]^{T}$ are $2\left(N+1\right)$ vectors.

To solve the discrete problem (29) we can write the classical (4) and the new DTS formulation (23) by defining

$$F = \frac{3}{2\Delta t} I_{2(N+1)} + D \otimes A - \varepsilon D_2 \otimes B + (P^{-1}E_0 \otimes \Sigma) [(I_{N+1} \otimes H_0) - \varepsilon (I_{N+1} \otimes G) D] - (P^{-1}E_N \otimes \Sigma) [(I_{N+1} \otimes H_N) - \varepsilon (I_{N+1} \otimes G) D]$$
(32)

and

$$\mathbf{R} = \frac{2\mathbf{v}^n}{\Delta t} - \frac{\mathbf{v}^{n-1}}{2\Delta t} + \left(P^{-1}E_0 \otimes \Sigma_0\right)\widetilde{\mathbf{g}}_0^{n+1} - \left(P^{-1}E_N \otimes \Sigma\right)\widetilde{\mathbf{g}}_N^{n+1} + \widetilde{\mathbf{F}}^{n+1}.$$
 (33)

To obtain the computational results we have used the following manufactured solutions

$$u_1(x,t) = \cos(10\pi x - t), \qquad u_2(x,t) = \sin(10\pi x - t),$$

with a spatial increment h=0.01 and a physical time-step $\Delta t=0.1$. By choosing the fourth-order Runge-Kutta scheme as pseudo time-integrator, the optimal choice of dual time-step for the classical DTS (4) is $\Delta \tau = 0.002178$, see Figure 4.

With the stopping criterion $\|\mathbf{w}^n - \mathbf{u}\|_P < 10^{-6}$ this formulation reaches steady–state in 421 iterations. The new DTS (23) is less stiff than the classical time–marching technique (4), see Figure 5. Figure 6 shows the number of iterations needed for each dual–time step $\Delta \tau$. The optimal choice for the two–derivatives DTS is $\Delta \tau = 0.0722$ and it leads to convergence in 60 inner iterations. This implies that the new DTS is approximately seven times more efficient than the classical one.

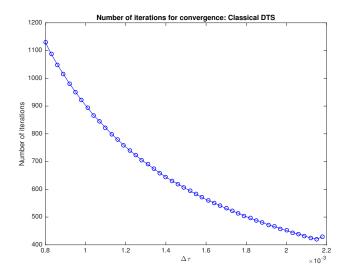


Figure 4: Number of iterations for convergence using the classical DTS.

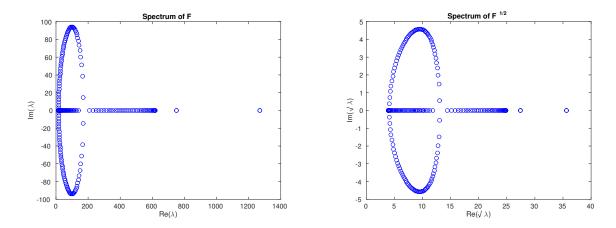


Figure 5: The spectrum of F and of its square root for the linearized Navier–Stokes equations.

5 MAIN DRAWBACKS AND OPEN QUESTIONS

The previous numerical tests show that the new DTS formulation (23) has better convergence properties compared to the conventional time-marching technique (4). However, when we rewrite (23) in first-order form as in (15) we obtain a system which has twice as the dimensions of the one in (4). Moreover, the computation of the principal square root of F may be excessively expensive to compute if the dimension of the system (7) is large. In Table 1, the computational times of both DTS techniques (4) and (23) are shown for the numerical experiment in Section 4.1. The last column provides the elapsed time for computing $F^{\frac{1}{2}}$.

Suppose that the square root of F is given. Then from Table 1 we conclude that when the number of nodes increases, the second–derivative DTS (23) provides better results with respect to the classical technique (4). However, the computation of the square root becomes expensive. Therefore, we are interested in suboptimal formulations of (13) which do not involve fractional or negative powers of F.

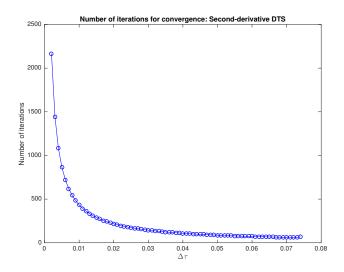


Figure 6: Number of iterations for convergence using the two-derivatives DTS.

Nodes (N)	Classical DTS (sec)	Second–derivative DTS (sec)	Square root (sec)
100	0.045337	0.107452	0.044975
1000	2.119714	1.820615	1.767909
2000	12.703043	8.927953	15.609013

Table 1: Execution times of the DTS schemes with optimal smoothing step for the hyperbolic steady problem (25). The elapsed time for the second–derivative DTS is indicated without the computation of the square root of F. The matrix $F^{\frac{1}{2}}$ is computed with the optimized routine **sqrtm** presented in [17].

5.1 Alternative formulations

Our goal is to provide provably convergent DTS schemes of the form (13), but avoid having to compute $F^{\frac{1}{2}}$. This system of second order differential equations can be written as a first-derivative formulation

$$\mathbf{z}_{\tau} + A\mathbf{z} = \mathbf{b}, \quad \text{where} \quad \mathbf{z} = \begin{bmatrix} \mathbf{w} \\ \mathbf{w}_{\tau} \end{bmatrix}, \quad A = \begin{bmatrix} 0 & -I \\ F & 2C \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} \mathbf{0} \\ \mathbf{R} \end{bmatrix}.$$

Let K = K(F) be a polynomial in F. By choosing $C = (K^{-1}F + K)/2$, we can rotate the system as

$$\begin{bmatrix} \mathbf{w} \\ \mathbf{w}_{\tau} \end{bmatrix}_{\tau} + \begin{bmatrix} I & 0 \\ K^{-1}F & I \end{bmatrix}^{-1} \begin{bmatrix} K^{-1}F & -I \\ 0 & K \end{bmatrix} \begin{bmatrix} I & 0 \\ K^{-1}F & I \end{bmatrix} \begin{bmatrix} \mathbf{w} \\ \mathbf{w}_{\tau} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{R} \end{bmatrix}. \tag{34}$$

Note that the optimal formulation with $C = K = F^{\frac{1}{2}}$ is represented in (34) and leads to (24).

There are two obvious alternatives for K. The first one is $K = \kappa I$ with $\kappa > 0$. This choice gives rise to a convergent formulation with a decay determined by κ and λ/κ , where λ is any eigenvalue of F. If κ is big, the damping of the system is dominated by the scaled eigenvalues λ/κ . However, we would have the same behavior as that of a preconditioned classical DTS (9), with $\Gamma = \kappa I$. For small values of κ , every mode of the solution to (34) converges to steady-state uniformly. The second choice is K = F, which leads to the same damping as the classical DTS (4) if all the eigenvalues have real part less than one. Otherwise, the convergence

is dominated by the spurious eigenvalues 1. Therefore, these two choices do not lead to an improved formulation with respect to the classical DTS (4).

All other alternatives for K that we have investigated lead to a matrix C which involves inverse matrices or fractional powers of F. For this reason, we conclude that the choice $C = (K^{-1}F + K)/2$ in (13) leads to either inefficient or expensive DTS schemes. The existence of alternative formulations not affected by these two effects is still matter of research.

6 CONCLUSIONS

A new two-derivative dual-time stepping technique has been proposed. The new DTS technique has been analyzed and optimized theoretically. The formulation involves a parameter in front of the first derivative in dual time which can be chosen to obtain the highest possible decay rate.

We have compared the performances of the new formulation with the ones of the classical DTS. Our technique improves the decay rate with respect to the classical time—marching technique if the eigenvalues of the operator representing the system are near the imaginary axis. Furthermore, if the spectrum is not contained within the unitary circle, the new second—derivatives technique provides a system of equations which is less stiff than the DTS formulation.

Numerical computations for a first–order ordinary differential equation and a system modelling the linearized Navier–Stokes corroborate the theoretical results. The simulations reveal that the new formulation is more efficient than the standard one as the size of the problem increase, provided that the required matrix $F^{\frac{1}{2}}$ is given. However, if the computation of $F^{\frac{1}{2}}$ is required, the new DTS formulation is less efficient than the classical dual time–stepping technique.

APPENDIX

A SBP-SAT SPACE DISCRETIZATION

For the discretization in space of the differential problems we have used the Summation–By–Parts (SBP) operators in conjunction with the Simultaneous–Approximation–Terms (SAT) for the boundary treatment. The main feature of the first is to mimic the property of integration by parts, whereas the second are penalty–like terms that enforces the boundary conditions weakly.

Definition A.1. $D = P^{-1}Q$ is a first-derivative SBP operator if P is a symmetric positive definite matrix and $Q + Q^T = H = diaq(-1, 0, ..., 0, 1)$.

These operators can be built also for the second derivative [18].

Definition A.2. $D_2 = P^{-1}(-S^TM + H)S$ is a second derivative SBP operator if M is positive semidefinite and S approximates the first derivative operator at the boundaries.

As an example, choosing $S=P^{-1}Q$ in Definition A.2 leads to the so called wide version of D_2 , i.e. $D_2=D^2$. Both first—and second—derivative SBP operators can be built for even orders 2p at the interior, while at the boundary closure their accuracy is p. For further details on the costruction of the SBP operators for the first derivative with $p \le 4$, see [19].

The SBP finite difference operators with a strong treatment of the boundary conditions only admits stability proofs for very simple problems. This result has been shown in [20], where SAT were proposed to enhance the SBP schemes. Discretizing a well–posed Initial–Boundary–Value–Problem (IBVP) in space with both SBP operators and the SAT penalty terms (SBP–SAT approach), it is possible to prove that the corresponding semidiscrete problem is stable. Further

theoretical details on the SBP–SAT discretization, well–posedness of an IBVP or the stability of its discretization are given in [15].

B STABILITY OF THE FIRST NUMERICAL TEST

In this section we verify the stability of the classical DTS (4) applied to the discretized problem (26).

For each fixed $\tau > 0$ the dual–time marching technique can be rewritten as

$$\mathbf{w}_{\tau} = \mathbf{f} - P^{-1} \left(w_0 - g \right) \mathbf{e}_0 - P^{-1} Q \mathbf{w}.$$

The P-norm of the solution \mathbf{w} is $\|\mathbf{w}\|_P = \sqrt{\mathbf{w}^T P \mathbf{w}}$. Thus

$$\frac{\mathrm{d}}{\mathrm{d}\tau} \|\mathbf{w}\|_{P}^{2} = \mathbf{w}_{\tau}^{T} P \mathbf{w} + \mathbf{w}^{T} P \mathbf{w}_{\tau} = -\mathbf{w}^{T} (Q + Q^{T}) \mathbf{w} - 2 (w_{0} - g) w_{0}$$
$$= -w_{N}^{2} - (w_{0} - g)^{2} + g^{2} \leq g^{2},$$

where w_0 and w_N are approximations for the solution at the boundaries. Since g is a given data, the P-norm of the solution \mathbf{w} is bounded in time. This implies strong stability of the classical DTS applied to the discretization (26). Equivalently, we have proven that F in (27) has only eigenvalues with non-negative real part, since the energy of the solution to (23) is bounded for any $\tau > 0$.

C WELL-POSEDNESS OF THE COMPRESSIBLE NAVIER-STOKES

Consider the model of the compressible Navier–Stokes equations (28). In Section 4.2 we claimed that the characteristic boundary conditions make the problem strongly well–posed in the Hadamard sense. To prove this statement we show that (28) admits a unique solution and that the norm of this solution is bounded by the given data $\mathbf{F}(x,t)$, $\mathbf{f}(x)$, $g_0(t)$ and $g_1(t)$.

We start by deriving the characteristic boundary conditions in (28). By premultiplying with \mathbf{u}^T and integrating over [0,1] we find

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\mathbf{u}(\cdot,t)\|^{2} + 2\varepsilon \int_{0}^{1} \mathbf{u}_{x}^{T} B \mathbf{u} \mathrm{d}x = \mathbf{u}^{T} \left(A \mathbf{u} - 2\varepsilon B \mathbf{u}_{x} \right) (0,t) - \mathbf{u}^{T} \left(A \mathbf{u} - 2\varepsilon B \mathbf{u}_{x} \right) (1,t) + \int_{0}^{1} \mathbf{u}^{T} \mathbf{F} \mathrm{d}x.$$
(35)

Furthermore, the boundary terms in (35) can be written as

$$\mathbf{u}^{T} \left(A \mathbf{u} - 2\varepsilon B \mathbf{u}_{x} \right) = \frac{1}{2\sqrt{2}} \left(u_{1} + \sqrt{2}u_{2} - \varepsilon u_{2,x} \right)^{2} - \frac{1}{2\sqrt{2}} \left(u_{1} - \sqrt{2}u_{2} - \varepsilon u_{2,x} \right)^{2}.$$

and therefore the boundary conditions

$$(u_1 + \sqrt{2}u_2 - \varepsilon u_{2,x})(0,t) = g_0(t), \quad t > 0, (u_1 - \sqrt{2}u_2 - \varepsilon u_{2,x})(1,t) = g_1(t), \quad t > 0$$
 (36)

bound the boundary terms in (35). To prove the boundedness of the solution to (28) we use the Cauchy–Schwarz and Young inequalities with a constant $\eta > 0$ for the integral with the forcing term **F** in (35). Moreover, since the matrix B is positive semidefinite,

$$\|\mathbf{u}(\cdot,T)\|^{2} \leq e^{\eta T} \left\{ \|\mathbf{f}\|^{2} + \int_{0}^{T} e^{-\eta t} \left[\frac{1}{2\sqrt{2}} \left(g_{0}(t)^{2} + g_{1}(t)^{2} \right) + \frac{1}{\eta} \|\mathbf{F}(\cdot,t)\|^{2} \right] dt \right\}$$
(37)

which proves that the solution to (28) is bounded. The estimate (37) together with the fact that we use the minimum number of boundary conditions implies both existence and uniqueness, and consequently well–posedness.

D STABILITY OF THE COMPRESSIBLE NAVIER-STOKES

In this section we will prove that the discrete energy of the solution to

$$\mathbf{w}_t + D \otimes A\mathbf{w} = \varepsilon D_2 \otimes B\mathbf{w} + \widetilde{\mathbf{F}}(\tau) + \mathbf{SAT}, \quad t > 0,$$
(38)

is bounded. Without loss of generality we consider the homogeneous problem, i.e. $\widetilde{\mathbf{F}} = \widetilde{\mathbf{g}}_0 = \widetilde{\mathbf{g}}_N = 0$ and $D_2 = D^2$. Let $\mathbb{P} = P \otimes I_2$ and $\|\mathbf{w}\|_{\mathbb{P}} = \sqrt{\mathbf{w}^T \mathbb{P} \mathbf{w}}$. Thus

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\mathbf{w}\|_{\mathbb{P}}^{2} = 2\mathbf{w}^{T} \mathbb{P} \mathbf{S} \mathbf{A} \mathbf{T} - \mathbf{w}^{T} \left(\left(Q + Q^{T} \right) \otimes A \right) \mathbf{w} + \varepsilon \left(D \mathbf{w} \right)^{T} \left(Q^{T} \otimes B \right) \mathbf{w} + \varepsilon \mathbf{w}^{T} \left(Q \otimes B \right) D \mathbf{w}.$$
(39)

Making use of the facts that $Q + Q^T = E_N - E_0$ and B is symmetric, we may write

$$\mathbf{w}^{T} (Q \otimes B) D\mathbf{w} = \mathbf{w}_{N}^{T} B (D\mathbf{w})_{N} - \mathbf{w}_{0}^{T} B (D\mathbf{w})_{0} - (D\mathbf{w})^{T} (P \otimes B) D\mathbf{w}, \tag{40}$$

$$(D\mathbf{w})^{T} (Q^{T} \otimes B) \mathbf{w} = \mathbf{w}_{N}^{T} B (D\mathbf{w})_{N} - \varepsilon \mathbf{w}_{0}^{T} B (D\mathbf{w})_{0} - (D\mathbf{w})^{T} (P \otimes B) D\mathbf{w},$$
(41)

where \mathbf{w}_0 , \mathbf{w}_N , $(D\mathbf{w})_0$, $(D\mathbf{w})_N \in \mathbb{R}^2$ are numerical approximations of the solution and its derivative to the continuous problem (28) at the boundaries, respectively. By combining (39), (40), (41) and the expression of the vector **SAT** in (30), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\mathbf{w}\|_{\mathbb{P}}^{2} = -2\varepsilon \left(D\mathbf{w}\right)^{T} \left(P \otimes B\right) D\mathbf{w} + \mathbf{w}_{0}^{T} \left[\left(A - 2\Sigma H_{0}\right) \mathbf{w}_{0} - 2\varepsilon \left(B - \Sigma G\right) \left(D\mathbf{w}\right)_{0}\right] - \mathbf{w}_{N}^{T} \left[\left(A - 2\Sigma H_{N}\right) \mathbf{w}_{N} - 2\varepsilon \left(B - \Sigma G\right) \left(D\mathbf{w}\right)_{N}\right].$$
(42)

The right hand–side of (42) can be seen as summation of three terms: the first one is non–positive, since $P \otimes B$ is positive semidefinite. The last two contributions are boundary terms, which can be expressed as

$$\begin{bmatrix} \mathbf{w}_i \\ \varepsilon (D\mathbf{w})_i \end{bmatrix}^T \begin{bmatrix} A - 2\Sigma H_i & -(B - \Sigma G) \\ -(B - \Sigma G) & 0 \end{bmatrix} \begin{bmatrix} \mathbf{w}_i \\ \varepsilon (D\mathbf{w})_i \end{bmatrix} = \mathbf{y}_i^T C_i \mathbf{y}_i, \quad i = \{0, N\}.$$
 (43)

Inserting the expression of H_0 , H_N , G and Σ in (31) into (43) leads to

Since C_0 is negative semidefinite and C_N positive semidefinite, the estimate (42) implies that the energy of the solution decreseas and proves the stability of the problem (38).

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