Numerical analysis of a new time-stepping θ-scheme for incompressible flow simulations

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Dedicated to David Gottlieb on the occasion of his 60th anniversary

Abstract

In [13], we had performed numerical comparisons for different time stepping schemes for the incompressible Navier-Stokes equations. In this paper, we present the numerical analysis in the context of the Navier-Stokes equations for a new time-stepping θ-scheme which has been recently proposed by Glowinski [5]. Like the well-known classical Fractional-Step-θ-scheme which had been introduced by Glowinski [1], [4], too, and which is still one of the most popular time stepping schemes, with or without operator splitting techniques, this new scheme consists of 3 substeps with non-equidistant substepping to build one macro time step. However, in contrast to the Fractional-Step-θ-scheme, the second substep can be formulated as an extrapolation step for previously computed data only, and the two remaining substeps look like a Backward Euler step so that no expensive operator evaluations for the right hand side vector with older solutions, as for instance in the Crank-Nicolson scheme, have to be performed. This new scheme is implicit, strongly A-stable and second order accurate, too, which promises some advantageous behavior, particularly in implicit CFD simulations for the nonstationary Navier-Stokes equations. Representative numerical results, based on the software package FEATFLOW [15], are obtained for typical flow problems with benchmark character which provide a fair rating of the solution schemes, particularly in long time simulations.

1 Introduction: Aspects of discretization and solvers

We consider numerical solution techniques for the incompressible Navier-Stokes equations,

$$\mathbf{u}_t - \nu\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{f} \quad , \quad \nabla\cdot\mathbf{u} = 0 \quad , \quad \text{in } \Omega \times (0, T] \,, \tag{1}$$

for given force $\mathbf{f}$ and viscosity ν, with prescribed boundary values on the boundary $\partial\Omega$ and an initial condition at $t = 0$. Solving this problem numerically is still a considerable task in the case of long time calculations and high Reynolds numbers, particularly in 3D and also in 2D if the time dynamics is complex. In this paper we concentrate on the 2D case which is representative also for 3D problems. Examples for 2D and 3D results can be found in [7].

The common solution approach is a separate discretization in space and time. We first (semi-)discretize in time by one of the usual methods known from the treatment of ordinary differential equations, such as the Forward or Backward Euler-, the Crank-Nicolson- or Fractional-Step-θ–scheme, or others, and obtain a sequence of generalized stationary Navier-Stokes problems.

Basic θ-scheme:

Given $\mathbf{u}^n$ and the time step $k = t_{n+1} - t_n$, then solve for $\mathbf{u} = \mathbf{u}^{n+1}$ and $p = p^{n+1}$

$$\frac{\mathbf{u} - \mathbf{u}^n}{k} + \theta[-\nu\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}] + \nabla p = \mathbf{g}^{n+1} \quad , \quad \nabla\cdot\mathbf{u} = 0 \quad , \quad \text{in } \Omega \tag{2}$$

with right hand side $\mathbf{g}^{n+1} := \theta\mathbf{f}^{n+1} + (1-\theta)\mathbf{f}^n - (1-\theta)[-\nu\Delta\mathbf{u}^n + \mathbf{u}^n\cdot\nabla\mathbf{u}^n]$.

The parameter θ has to be chosen depending on the time-stepping scheme, e.g., $\theta = 1$ for the Backward Euler, or $\theta = 1/2$ for the Crank-Nicolson-scheme. The pressure term $\nabla p = \nabla p^{n+1}$ may be replaced by $\theta\nabla p^{n+1} + (1-\theta)\nabla p^n$, but, with appropriate postprocessing, both strategies lead to solutions of the same accuracy. In all cases, we end up with the task of solving, at each time step, a nonlinear saddle point problem of type (2) which has then to be discretized in space.

In the past, explicit time-stepping schemes have been commonly used in nonstationary flow calculations, but because of the severe stability problems inherent in this approach, the required small time steps prohibit the efficient treatment of long time flow simulations. Due to the high stiffness, one should prefer (semi-)implicit schemes in the choice of time-stepping methods for solving this problem. Since (semi-)implicit methods have become feasible, thanks to more efficient nonlinear and linear solvers, the schemes most frequently used are (still) either the simple first-order Backward Euler scheme (BE), with $\theta = 1$, or more preferably the second-order Crank-Nicolson scheme (CN), with $\theta = 1/2$. These two methods belong to the group of *one-step-θ-schemes*. The CN scheme occasionally suffers from numerical instabilities because of its only weak damping property (not strongly A-stable), while the BE-scheme is of first order accuracy only (however: it is a good candidate for steady-state simulations). Another method which has proven to have the potential to excel in this competition is the *Fractional-Step-θ-scheme* (FS). It uses three different values for θ and for the time step k at each time level.

For a realistic comparison of all mentioned schemes, we define a macro time step with $K = t_{n+1} - t_n$ as a sequence of 3 time steps of (possibly variable) size k. Then, in the case of the Backward Euler or the Crank-Nicolson scheme, we perform 3 substeps with the same θ ($\theta = 0.5$ or $\theta = 1$) as above and (micro) time step $k = K/3$.

Backward Euler-scheme:

$$\begin{aligned}
[I + \tfrac{K}{3}N(\mathbf{u}^{n+\frac{1}{3}})]\mathbf{u}^{n+\frac{1}{3}} + \tfrac{K}{3}\nabla p^{n+\frac{1}{3}} &= \mathbf{u}^n + \tfrac{K}{3}\mathbf{f}^{n+\frac{1}{3}} \\
\nabla\cdot\mathbf{u}^{n+\frac{1}{3}} &= 0
\end{aligned}$$

$$\begin{aligned}
[I + \tfrac{K}{3}N(\mathbf{u}^{n+\frac{2}{3}})]\mathbf{u}^{n+\frac{2}{3}} + \tfrac{K}{3}\nabla p^{n+\frac{2}{3}} &= \mathbf{u}^{n+\frac{1}{3}} + \tfrac{K}{3}\mathbf{f}^{n+\frac{2}{3}} \\
\nabla\cdot\mathbf{u}^{n+\frac{2}{3}} &= 0
\end{aligned}$$

$$\begin{aligned}
[I + \tfrac{K}{3}N(\mathbf{u}^{n+1})]\mathbf{u}^{n+1} + \tfrac{K}{3}\nabla p^{n+1} &= \mathbf{u}^{n+\frac{2}{3}} + \tfrac{K}{3}\mathbf{f}^{n+1} \\
\nabla\cdot\mathbf{u}^{n+1} &= 0
\end{aligned}$$

Crank-Nicolson-scheme:

$$[I + \tfrac{K}{6}N(\mathbf{u}^{n+\frac{1}{3}})]\mathbf{u}^{n+\frac{1}{3}} + \tfrac{K}{6}\nabla p^{n+\frac{1}{3}} = [I - \tfrac{K}{6}N(\mathbf{u}^n)]\mathbf{u}^n + \tfrac{K}{6}\mathbf{f}^{n+\frac{1}{3}} + \tfrac{K}{6}\mathbf{f}^n$$
$$\nabla\cdot\mathbf{u}^{n+\frac{1}{3}} = 0$$

$$[I + \tfrac{K}{6}N(\mathbf{u}^{n+\frac{2}{3}})]\mathbf{u}^{n+\frac{2}{3}} + \tfrac{K}{6}\nabla p^{n+\frac{2}{3}} = [I - \tfrac{K}{6}N(\mathbf{u}^{n+\frac{1}{3}})]\mathbf{u}^{n+\frac{1}{3}} + \tfrac{K}{6}\mathbf{f}^{n+\frac{2}{3}} + \tfrac{K}{6}\mathbf{f}^{n+\frac{1}{3}}$$
$$\nabla\cdot\mathbf{u}^{n+\frac{2}{3}} = 0$$

$$[I + \tfrac{K}{6}N(\mathbf{u}^{n+1})]\mathbf{u}^{n+1} + \tfrac{K}{6}\nabla p^{n+1} = [I - \tfrac{K}{6}N(\mathbf{u}^{n+\frac{2}{3}})]\mathbf{u}^{n+\frac{2}{3}} + \tfrac{K}{6}\mathbf{f}^{n+1} + \tfrac{K}{6}\mathbf{f}^{n+\frac{2}{3}}$$
$$\nabla\cdot\mathbf{u}^{n+1} = 0$$

Here and in the following, we use the more compact form for the diffusive and advective part

$$N(\mathbf{v})\mathbf{u} := -\nu\Delta\mathbf{u} + \mathbf{v}\cdot\nabla\mathbf{u}\,. \tag{3}$$

For the Fractional-Step-θ-scheme we proceed as follows. Choosing $\theta = 1 - \frac{\sqrt{2}}{2}$, $\theta' = 1 - 2\theta$, and $\alpha = \frac{1-2\theta}{1-\theta}$, $\beta = 1 - \alpha$, the macro time step $t_n \to t_{n+1} = t_n + K$ is split into the three following consecutive substeps (with $\tilde{\theta} := \alpha\theta K = \beta\theta' K$):

Fractional-Step-θ-scheme:

$$[I + \tilde{\theta}N(\mathbf{u}^{n+\theta})]\mathbf{u}^{n+\theta} + \theta K\nabla p^{n+\theta} = [I - \beta\theta K N(\mathbf{u}^n)]\mathbf{u}^n + \theta K\mathbf{f}^n$$
$$\nabla\cdot\mathbf{u}^{n+\theta} = 0$$

$$[I + \tilde{\theta}N(\mathbf{u}^{n+1-\theta})]\mathbf{u}^{n+1-\theta} + \theta' K\nabla p^{n+1-\theta} = [I - \alpha\theta' K N(\mathbf{u}^{n+\theta})]\mathbf{u}^{n+\theta} + \theta' K\mathbf{f}^{n+1-\theta}$$
$$\nabla\cdot\mathbf{u}^{n+1-\theta} = 0$$

$$[I + \tilde{\theta}N(\mathbf{u}^{n+1})]\mathbf{u}^{n+1} + \theta K\nabla p^{n+1} = [I - \beta\theta K N(\mathbf{u}^{n+1-\theta})]\mathbf{u}^{n+1-\theta} + \theta K\mathbf{f}^{n+1-\theta}$$
$$\nabla\cdot\mathbf{u}^{n+1} = 0$$

Being a strongly A-stable scheme, the FS-method possesses the full smoothing property which is important in the case of rough initial or boundary values. Further, it contains only very little numerical dissipation which is crucial in the computation of non-enforced temporal oscillations in the flow. A rigorous theoretical analysis of the FS-scheme (see [4],[8],[9]) applied to the Navier-Stokes problem establishes second order accuracy for this special choice of θ. Therefore, this scheme combines the advantages of both the classical CN-scheme (2nd order accuracy) and the BE-scheme (strongly A-stable), but with the same numerical effort.

These results have been confirmed by extensive numerical simulations which are part of our former paper [13]. While that paper examined the accuracy of the above mentioned time-stepping schemes, also the question of fully coupled vs. operator-splitting techniques as well as the treatment of the nonlinearity had been addressed. One of the main statements - see also

the results in [16] - was that the Fractional-Step-θ-scheme is our preferred method, together with a fully implicit, fully coupled approach which solves the nonlinear saddle-point problems in each time step via Newton-like techniques together with special multigrid preconditioners ('Multilevel Pressure Schur Complement' [16]). While the question of the total efficiency w.r.t. operator-splitting or fully coupled approaches is hard to answer, this fully implicit approach is definitively the most accurate and most robust - but often most expensive, too - approach which is also preferable from a purely mathematical viewpoint since finite element arguments can be used for this Galerkin approach and, hence, error control and residual based adaptivity become feasible. Therefore, we restrict the following comparisons to the Fractional-Step-θ-scheme in combination with a fully implicit, fully coupled approach in each time step. So, in each time (sub-)step we have to solve nonlinear problems of the following type:

Given $\mathbf{u}^n$, parameters $k = k(t_{n+1})$, $\theta = \theta(t_{n+1})$ and $\theta_i = \theta_i(t_{n+1}), i = 1, \ldots, 3$, then solve for $\mathbf{u} = \mathbf{u}^{n+1}$ and $p = p^{n+1}$

$$[I + \theta k N(\mathbf{u})]\mathbf{u} + k\nabla p = [I - \theta_1 k N(\mathbf{u}^n)]\mathbf{u}^n + \theta_2 k \mathbf{f}^{n+1} + \theta_3 k \mathbf{f}^n \quad , \quad \nabla \cdot \mathbf{u} = 0 \,. \tag{4}$$

For the spatial discretization, we choose a finite element approach. In setting up a finite element model of the Navier-Stokes equations, one starts with a variational formulation. On the finite mesh T_h (triangles, quadrilaterals or their analogues in 3D) covering the domain Ω with local element width h, one defines polynomial trial functions for velocity and pressure. These spaces $\mathbf{H}_h$ and L_h should lead to numerically stable approximations, as $h \to 0$, i.e., they should satisfy the *Babuska-Brezzi condition* with a mesh-independent constant γ (see [3]),

$$\min_{p_h \in L_h} \max_{\mathbf{v}_h \in \mathbf{H}_h} \frac{(p_h, \nabla \cdot \mathbf{v}_h)}{\|p_h\|_0 \|\nabla \mathbf{v}_h\|_0} \geq \gamma > 0 \,. \tag{5}$$

Many stable pairs of finite element spaces and/or stabilization techniques have been proposed in the literature (see [16]). Our favorite candidate is a nonconforming quadrilateral element (see [11]) which (in 2D) uses piecewise *rotated bilinear* shape functions for the velocities, spanned by $\langle x^2 - y^2, x, y, 1 \rangle$, and piecewise constant pressure approximations (see Figure 1).
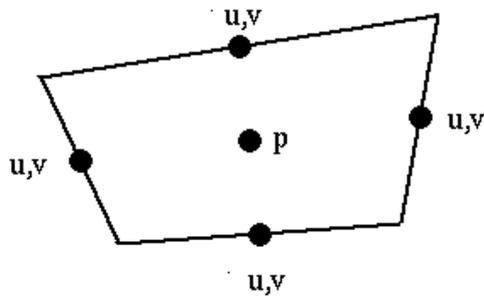

Figure 1: Nodal points of the nonconforming finite element pair

4

The nodal values are the mean values of the velocity over the element edges, and the mean values of the pressure over the elements, rendering this approach *nonconforming*. A convergence analysis is given in [11] and computational results - based on the 'Open Source' FEATFLOW package [15] - are reported in [16]. This element pair has several important features. It admits stabilization strategies for the convective terms of upwind, streamline-diffusion, internal penalty and FCT/TVD type [10]. Further, efficient multigrid solvers are available which work satisfactorily over the whole range of relevant Reynolds numbers, $1 \leq Re \leq 10^5$, and also on nonuniform meshes. In [14], we have shown by a complexity analysis that this pair of elements is one of the most efficient choices in the case of highly nonstationary flows: This can be also seen by benchmark calculations [12]. So, in combination with *discrete projection methods* [16], it works very robust and efficient in a multigrid code also on highly stretched and anisotropic grids.

Using the same symbols $\mathbf{u}$ and p also for the coefficient vectors in the nodal representation, the discrete version of problem (4) can be written as a (nonlinear) algebraic system of the form:

Given $\mathbf{u}^n$, a right hand side $\mathbf{g}$ and a time step k, then solve - in each substep - for $\mathbf{u} = \mathbf{u}^{n+1}$ and $p = p^{n+1}$

$$S\mathbf{u} + kBp = \mathbf{g} \quad , \quad B^T \mathbf{u} = 0 \tag{6}$$

with matrix S and right hand side $\mathbf{g}$ such that

$$S\mathbf{u} = [M + \theta k N(\mathbf{u})]\mathbf{u} \quad , \quad \mathbf{g} = [M - \theta_1 k N(\mathbf{u}^n)]\mathbf{u}^n + \theta_2 k \mathbf{f}^{n+1} + \theta_3 k \mathbf{f}^n \,. \tag{7}$$

Here, M is the *mass* matrix and $N(.)$ the *advection* matrix containing the diffusive and convective parts corresponding to the nonlinear form in (3). For dominant transport the advection part may include some stabilization, for instance, some upwind mechanism (see [16]). Here, B is the *gradient* matrix, and $-B^T$ the transposed *divergence* matrix. As pointed out before, we first treat the nonlinearity by an outer nonlinear iteration of fixed point or quasi–Newton type, and we obtain linear indefinite subproblems which are solved by a coupled multigrid approach ('local Multilevel Pressure Schur Complement' or 'Vanka-like'). For more details on the numerical and algorithmic components and regarding the realization in FEATFLOW, we refer to [15].

2   The new time-stepping θ-scheme

Consider an initial value problem of the form

$$\begin{cases} \dfrac{dX}{dt} &= f(X,t) \,, \quad \forall t > 0 \,, \\ &= \\ X(0) &= X_0 \,, \end{cases}$$

where $X(t) \in \mathbf{R}^d, d \geq 1$.

Then, the new θ-scheme with macro time step Δt can be written as three consecutive substeps, where $\theta = 1 - 1/\sqrt{2}$, $X^0 = X_0$, $n \geq 0$ and X^n is known:

$$
\begin{aligned}
\frac{X^{n+\theta} - X^n}{\theta \Delta t} &= f\left(X^{n+\theta}, t^{n+\theta}\right) \\
&= \\
X^{n+1-\theta} &= \tfrac{1-\theta}{\theta} X^{n+\theta} + \tfrac{2\theta-1}{\theta} X^n \\
&= \\
\frac{X^{n+1} - X^{n+1-\theta}}{\theta \Delta t} &= f\left(X^{n+1}, t^{n+1}\right)
\end{aligned}
$$

As shown in [2],[5], the most important properties of this new θ-scheme are that

- it is fully implicit;

- it is strongly A-stable;

- it is second order accurate (in fact, it is "nearly" third order accurate [5]).

These properties promise some advantageous behavior, particularly in implicit CFD simulations for nonstationary incompressible flow. Applying one step of this scheme to the Navier-Stokes equations, we obtain the following variant of the scheme:

1.
$$
\begin{cases}
\dfrac{\mathbf{u}^{n+\theta} - \mathbf{u}^n}{\theta \Delta t} + N(\mathbf{u}^{n+\theta})\mathbf{u}^{n+\theta} + \nabla p^{n+\theta} = \mathbf{f}^{n+\theta} \\[2mm]
\nabla \cdot \mathbf{u}^{n+\theta} = 0
\end{cases}
$$

2.
$$
\mathbf{u}^{n+1-\theta} = \tfrac{1-\theta}{\theta}\mathbf{u}^{n+\theta} + \tfrac{2\theta-1}{\theta}\mathbf{u}^n
$$

3.
$$
\begin{cases}
\dfrac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1-\theta}}{\theta \Delta t} + N(\mathbf{u}^{n+1})\mathbf{u}^{n+1} + \nabla \widetilde{p}^{n+1} = \mathbf{f}^{n+1} \\[2mm]
\nabla \cdot \mathbf{u}^{n+1} = 0
\end{cases}
$$

3b.
$$
p^{n+1} = (1-\theta)p^{n+\theta} + \theta \widetilde{p}^{n+1}
$$

These 3 substeps build one macro time step and have to be compared with the previous description of the Backward Euler, Crank-Nicolson and Fractional-Step-θ-scheme which all have been formulated in terms of a macro time step with 3 substeps, too. Then, the resulting accuracy and numerical cost are better comparable and the rating is fair. The main difference to the previous 'classical' schemes is that substeps 1. and 3. look like an Backward Euler step while substep 2. is an extrapolation step only for previously computed data such that no operator evaluations at previous time steps are required.

Substep 3b. can be viewed as postprocessing step for updating the new pressure which however is not a must. In fact, in our subsequent numerical tests, we omitted this substep 3b. and accepted the pressure from substep 3. as final pressure approximation, that means $p^{n+1} = \widetilde{p}^{n+1}$. Before we present the numerical results, we want to provide a (theoretical) discussion of both proposed schemes concerning their properties w.r.t. accuracy and numerical efficiency:

Accuracy of classical Fractional-Step-θ-scheme vs. new time-stepping θ-scheme

Both schemes are second order accurate such that the asymptotical behavior should be very similar. However, since the involved constants are different, the results will be different, too, for a given time step Δt. So, the question is: 'Which Δt is necessary for both schemes to provide the same accuracy?'

What about robustness for large time steps or perturbations? Can the schemes be used for special approaches - like FCT or TVD techniques for convection-dominated flows - which can lead to monotone, positivity-preserving solutions?

Numerical effort of classical Fractional-Step-θ-scheme vs. new θ-scheme

The new θ-scheme requires only 2 solution steps in each macro step, while the classical FS-scheme performs implicit and nonlinear iterations in <u>all</u> 3 substeps. The evaluation for the new θ-scheme is much easier since - due to the Backward Euler steps - no operator evaluations at previous time steps are required. Moreover, no stabilization of convective terms for such right hand side operators is required which can be critical on time dependent meshes and geometries. On the other hand, the classical FS-Scheme damps the nonlinear operator with (approximately) $\tilde{\theta} \approx 0.5$ while the new scheme, as Backward Euler step, involves no damping such that more nonlinear steps of quasi-Newton type will be necessary.

Summarizing, one may expect that the numerical effort of the new scheme for each substep is cheaper - at least for 'small' time steps (treatment of the nonlinearity) and complex right hand side evaluations (for instance, in the case of particulate flow which involves collision models for many particles as source terms and CPU dominant parts) - while the resulting accuracy is not clear. Therefore, we will analyze the actual accuracy for both schemes by examining a complex benchmark configuration, namely fully nonstationary flow through a Venturi pipe (see [6]). Incidentally, the new θ-scheme is a *Runge-Kutta* one; it has been derived in [5] as a particular case of the fractional-step-θ-scheme (see the above reference for details).

3   Numerical comparisons

In this section, we present the results of our comparisons for the FS-scheme and the new θ-scheme if applied to the flow through a Venturi pipe which is a dynamic water pump device in a sail boat (see [6] for details). Fig. 2 shows the flow configuration and several snapshots of the fully nonstationary flow features. The corresponding meshes in our multigrid calculations for this Venturi pipe range from 20 elements (coarse) to 81,920 elements (finest level).
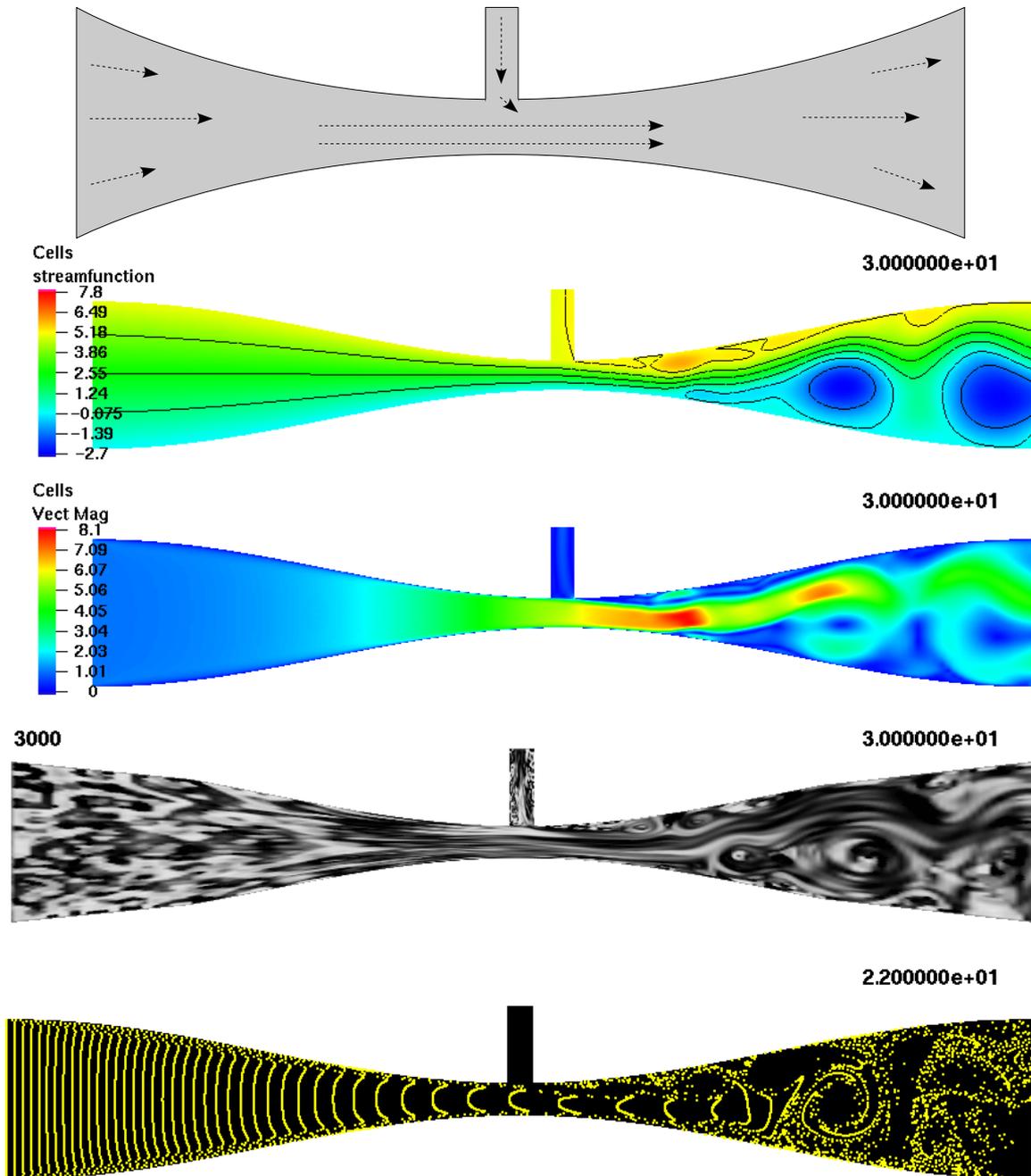
Figure 2: Snapshots (streamfunction, norm of velocity, transport of flow textures and particle tracing) for the Venturi pipe

In non-dimensional form, the total length of the Venturi pipe is $L_t = 32$, the height at the inlet is $H_t = 5$, the height in the interior is $H_i = 1$, and the width of the small upper channel is $W_i = 0.8$. At the upper small "inlet" and the right "outlet" we prescribe the zero mean pressure condition as natural boundary conditions (see [6]), while at the left inlet a parabolic velocity profile with $U_{max} = 1$ is prescribed, leading to maximum velocities of approximately 7 in the interior. At the narrowing a lower pressure is generated which enforces an incoming flux from the upper inlet, at least for the used viscosity parameter $\nu = 10^{-3}$. For this given spatial mesh, on the finest grid level, we try to reach the same accuracy - in time - for both methods proposed, by examining different time steps which are chosen by hand (remark: an implicit and adaptive time step control [16] is possible, too). This should guarantee a fair comparison of the resulting accuracy in time. In the end, we will additionally compare the total CPU cost to satisfy a prescribed accuracy criterion. We solve this problem up to the final time of 30 seconds.

The following tables present the relative error $\tilde{\mathtt{f}}$ in time (0,T] for different quantities $\mathtt{f}$ on the finest grid level with appr. 80,000 elements and 400,000 unknowns in space, always expressed in percent. Then, the relative error is defined by

$$\tilde{\mathtt{f}} = \frac{||\mathtt{f} - \mathtt{f}_{ref}||_{L_2(T)}}{||\mathtt{f}_{ref}||_{L_2(T)}}$$

where $\mathtt{f}_{ref}$ is the reference solution on the same mesh, corresponding to the classical FS-scheme with a very small time step, that is $\Delta t = 0.001$. Table 1 shows the relative error for the flux $\mathtt{fl}$ through the upper small device for different time steps ('fs 0.0033' means FS-scheme with time step 0.0033) for different final time T. Both schemes have about the same accuracy for realistic step sizes. However, it is also visible that the FS-scheme is slightly better in most cases.

T=	5 s	10 s	15 s	20 s	25 s	30 s	5 s	10 s	15 s	20 s	25 s	30 s
new 0.1	1.9	8.8	11.0	22.0	27.0	62.0	0.2	1.1	1.3	2.6	3.0	6.5
fs 0.1	0.9	2.4	8.3	14.0	29.0	42.0	0.2	0.3	1.1	1.6	3.2	4.6
new 0.033	0.4	1.2	4.2	23.0	35.0	49.0	0.08	0.1	0.5	2.9	4.1	5.5
fs 0.033	0.07	1.5	4.0	9.4	27.0	44.0	0.02	0.2	0.5	1.1	3.1	4.8
new 0.01	0.02	0.5	3.1	7.3	8.8	30.0	0.01	0.06	0.4	0.9	1.0	3.2
fs 0.01	0.006	0.1	1.1	8.0	25.0	39.0	0.003	0.02	0.2	1.0	2.9	4.4
new 0.0033	0.002	0.05	0.4	3.6	9.1	28.0	0.001	0.007	0.06	0.4	0.9	3.1
fs 0.0033	0.001	0.02	0.2	0.9	4.7	30.0	0.001	0.002	0.02	0.1	0.5	3.4

Table 1: Relative error in percent (%) for the flux $\mathtt{fl}$ and the x-component of the velocity $\mathtt{u}$ for different time steps

These results are not limited to the case of quantities (here: flux) on the boundary: The same holds also for interior points, too. Therefore, Table 1 presents also the corresponding relative error in time for the x-component of the velocity $\mathtt{u}$ at a point located in the interior of the pipe (near the center of the domain). Moreover, we discuss the resulting computational efficiency of the new scheme. Table 2 shows the CPU requirement for both schemes. As a result, the total CPU time is less for the new θ-scheme and slightly outperforms the FS-scheme.

	Δt=0.1	Δt=0.033	Δt=0.01	Δt=0.0033	Δt=0.001
new	11,325	22,471	45,922	102,187	377,222
fs	15,580	29,029	61,623	144,088	513,083

Table 2: CPU time in seconds until $T = 30$

Table 3 demonstrates the total number of nonlinear iterations that are needed for the different time steps until final time $T = 30$. And, Table 3 shows the total number of required linear multigrid iterations until the final time: This number of multigrid iterations is more or less the CPU dominant part of the performed solution algorithm and mainly determines the total CPU cost. If the time step is small enough, the ratio of required nonlinear steps for the FS-scheme vs. the new scheme approaches the expected value 1.5 since the second substep in the new scheme is a simple extrapolation step only: This behavior can be expected because the new scheme requires only 2 implicit nonlinear solution steps in each macro step, while the classical approach performs implicit and nonlinear solution steps in all 3 substeps. It will be interesting and part of a future paper to perform similar comparisons for a full Newton solver instead of the used fixed point iteration for treating the nonlinearity in each time step.

	Δt=0.1	Δt=0.033	Δt=0.01	Δt=0.0033	Δt=0.1	Δt=0.033	Δt=0.01	Δt=0.0033
new	1,760	3,130	6,645	18,000	3,681	6,908	12,921	30,142
fs	2,156	4,054	9,143	25,861	4,756	9,143	17,058	42,774
fs/new	1.22	1.29	1.37	1.44	1.29	1.32	1.32	1.41

Table 3: Total number of nonlinear iterations (left) and of linear multigrid sweeps (right)

Finally, Table 4 demonstrates the resulting averaged number of linear multigrid sweeps for each nonlinear iteration which is roughly the same for both time stepping schemes. This might be another advantage of the new time stepping scheme which shows that this new θ-scheme can lead to less nonlinear iterations, to less linear multigrid sweeps and finally to less CPU time since for long time calculations, both schemes lead to numerical solutions with no significant difference regarding the resulting accuracy.

	Δt=0.1	Δt=0.033	Δt=0.01	Δt=0.0033
new	2.09	2.21	1.94	1.67
fs	2.20	2.26	1.87	1.65

Table 4: Averaged number of linear multigrid steps per nonlinear iteration

4   Conclusion

We have presented a numerical analysis for a new time stepping θ-scheme which has been introduced and analyzed by Glowinski [5] and which has been extended for the nonstationary incompressible Navier-Stokes equations. The numerical simulations for a dynamic Venturi pipe

problem, as prototypical test case for time-dependent flow configurations with different scales in space and time, have been based on the CFD package FEATFLOW [15] which uses a FEM discretization and fast multigrid components in a fully implicit coupled framework to solve the nonlinear problems in each time step. Our tests have confirmed the theoretical results in [5], namely that the new θ-scheme implicit, strongly A-stable and second order accurate, and hence, it shows a similar advantageous behavior as the classical Fractional-Step-θ-scheme.

Looking more precisely at the resulting numerical and algorithmic behavior of this new scheme for CFD simulations, this approach even seems to excel in the "competition" with the FS scheme and analogously with the classical Crank-Nicolson method, since the total numerical effort of the new θ-scheme in each substep is cheaper: This is mainly due to the fact that only 2 nonlinear plus 1 extrapolation step compared with 3 fully nonlinear solution steps have to be performed while the resulting accuracy, which is also 2nd order in time, is comparable with both classical approaches. Since the corresponding multigrid solvers in each fixed point iteration show a similar convergence behavior, and since the nonlinear solvers behave similar, too, the total numerical cost seems to be smaller. Moreover, due to the Backward Euler character of the involved substeps, no expensive operator evaluations for solutions from former time steps are necessary. This fact might be very important for flow models which involve complex right hand side evaluations, for instance, in the case of particulate flow with expensive collision models for large numbers of particles. Since such configurations with particle numbers of 10^5 and more require implicit flow solvers for small time steps (see [5, 17]), this new θ-scheme is a quite interesting candidate for such problems and will be subject of our current research in this field.

Finally, let us remark that the Fractional-Step-θ-scheme can be rewritten, too, so that the operator evaluations in the right hand side can be saved:

Consider the following (not necessarily linear) initial value problem (IVP):

$$\frac{dX}{dt} + A(X) = f \quad , \quad X(0) = X_0$$

With the previously introduced settings for the parameters, the described Fractional-Step-θ-scheme for the solution of (IVP) can be equivalently rewritten as follows:

Given $X^0 = X_0, Z^0 = \Delta t A(X_0)$; for $n \geq 0$, X^n and Z^n being known, then compute:

$$\frac{X^{n+\theta} - X^n}{\theta \Delta t} + \alpha A(X^{n+\theta}) = f^n - (\beta/\Delta t)Z^n$$
$$Z^{n+\theta} = (\Delta t/\alpha)f^n - (\beta/\alpha)Z^n + (X^n - X^{n+\theta})/(\alpha\theta)$$

$$\frac{X^{n+1-\theta} - X^{n+\theta}}{\theta' \Delta t} + \beta A(X^{n+1-\theta}) = f^{n+1-\theta} - (\alpha/\Delta t)Z^{n+\theta}$$
$$Z^{n+1-\theta} = (\Delta t/\beta)f^{n+1-\theta} - (\alpha/\beta)Z^{n+\theta} + (X^{n+\theta} - X^{n+1-\theta})/(\beta\theta')$$

$$\frac{X^{n+1} - X^{n+1-\theta}}{\theta \Delta t} + \alpha A(X^{n+1}) = f^{n+1-\theta} - (\beta/\Delta t)Z^{n+1-\theta}$$

$$Z^{n+1} = (\Delta t/\alpha)f^{n+1-\theta} - (\beta/\alpha)Z^{n+1-\theta} + (X^{n+1-\theta} - X^{n+1})/(\alpha\theta)$$

Written this way, the FS scheme does not require operator evaluations at former time steps, too, and it might be even possible to save further operator evaluations. However, this will be part of a forthcoming paper which will analyze this modification w.r.t. numerical robustness, accuracy and, finally, computational efficiency.

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