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Analysis of a multirate theta-method for stiff ODEs

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Dedicated to Prof. K. Strehmel for his numerous contributions on the numerical integration of differential equations

Abstract

This paper contains a study of a simple multirate scheme, consisting of the θ-method with one level of temporal local refinement. Issues of interest are local accuracy, propagation of interpolation errors and stability. The theoretical results are illustrated by numerical experiments, including results for more levels of refinement with automatic partitioning.

JEL classification: 65L05; 65L06; 65L50; 65M06; 65M20

Keywords: Multirate time stepping; Local time stepping; Stiff differential equations

1. Introduction

For large, stiff systems of ordinary differential equations (ODEs), some components may show a more active behaviour than others. To solve such problems multirate time stepping schemes can be efficient. With such schemes different solution components can be integrated with different time steps. A multirate procedure with automatic partitioning and step size control was introduced and tested in [12]. In the present paper some theoretical issues are studied for a simplified situation. For this purpose we will consider the θ-method with one level of temporal refinement.

The systems of ODEs with given initial values in $\mathbb{R}^m$ are written as

$$w'(t) = F\big(t, w(t)\big), \qquad w(0) = w_0. \tag{1.1}$$

The numerical approximations to the exact ODE solution at the global time levels $t_n = n\tau$ will be denoted by w_n. For the step from t_{n-1} to t_n, we first compute a tentative approximation at the new time level. For those components for which an error estimator indicates that smaller steps would be needed, the computation is redone with halved step size $\frac{1}{2}\tau$. The result with the coarser time step will furnish data for this refined step by interpolation at the intermediate time level $t_{n-1/2} = \frac{1}{2}(t_{n-1} + t_n)$. This procedure then can be continued recursively with further refinements, but for the analysis here only the most simple case with one level of refinement will be considered.

We study this case to obtain a better understanding of more general multirate schemes. Particular attention will be given to the build-up of local errors which will be composed of discretization errors of the θ-method and interpolation

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errors. For simplicity we consider the θ-method with a fixed global time step τ. The component set where the (halved) local time steps are taken is given by a diagonal projection J, with diagonal entries zero or one, where an entry one indicates that the component will be refined. Such J could be determined by some error estimator as in [12]; it then will vary from step to step, so in general $J = J_n$.

Summarizing, the scheme reads as follows: first we take the tentative global step

$$\overline{w}_n = w_{n-1} + (1-\theta)\tau F(t_{n-1}, w_{n-1}) + \theta\tau F(t_n, \overline{w}_n), \tag{1.2a}$$

from which we also obtain an approximation $\overline{w}_{n-1/2}$ at the intermediate time level $t_{n-1/2}$ by interpolation. Then we compute the local updates

$$w_{n-\frac{1}{2}} = J_n\left(w_{n-1} + \frac{1}{2}(1-\theta)\tau F(t_{n-1}, w_{n-1}) + \frac{1}{2}\theta\tau F(t_{n-\frac{1}{2}}, w_{n-\frac{1}{2}})\right) + (I - J_n)\overline{w}_{n-\frac{1}{2}}, \tag{1.2b}$$

$$w_n = J_n\left(w_{n-\frac{1}{2}} + \frac{1}{2}(1-\theta)\tau F(t_{n-\frac{1}{2}}, w_{n-\frac{1}{2}}) + \frac{1}{2}\theta\tau F(t_n, w_n)\right) + (I - J_n)\overline{w}_n. \tag{1.2c}$$

The θ-method is considered here as basic method since it represents the most simple Runge–Kutta method (and also linear multistep method). For stiff systems the cases $\theta = \frac{1}{2}$ (trapezoidal rule) and $\theta = 1$ (backward Euler) are of practical interest; for non-stiff systems we can also consider $\theta = 0$ (forward Euler). It is assumed in the following that $0 \leqslant \theta \leqslant 1$. For the interpolation we shall primarily consider linear interpolation

$$(I - J_n)\overline{w}_{n-\frac{1}{2}} = (I - J_n)\left(\frac{1}{2}w_{n-1} + \frac{1}{2}\overline{w}_n\right). \tag{1.3}$$

However, we will see that this may affect the accuracy in case $\theta = \frac{1}{2}$, and therefore the quadratic interpolation formula

$$(I - J_n)\overline{w}_{n-\frac{1}{2}} = (I - J_n)\left(\frac{3}{4}w_{n-1} + \frac{1}{4}\overline{w}_n + \frac{1}{4}\tau F(t_{n-1}, w_{n-1})\right) \tag{1.4}$$

will be considered as well.

For this simple multirate scheme a detailed description of the error propagations will be derived for linear systems that may be stiff. Compared to the non-stiff case, it is not only stability that needs careful consideration, but also local discretization errors can be affected by stiffness. For example, it will be seen that for stiff systems the linear interpolation may give an $\mathcal{O}(\tau^2)$ contribution to the local error, whereas this contribution will always be $\mathcal{O}(\tau^3)$ for non-stiff systems.

Even though the multirate scheme considered in this paper is quite simple, the stability analysis will turn out to be complicated. Some pertinent properties for general linear systems can be derived, but to obtain detailed results we will also have to study linear test problems in $\mathbb{R}^2$.

Related stability results can be found in [4,8,13,15] for multirate schemes with a so-called compound step, where approximations $(I - J)w_n$ and $Jw_{n-1/2}$ are computed simultaneously. The above multirate approach (but then with more levels of refinement and with a two-stage Rosenbrock method as basic integrator) was considered in [12]. In this approach there is some overhead, because $J\overline{w}_n$ will not be directly used anymore. However, by computing the whole approximation $\overline{w}_n$, the structure of the implicit relations remains the same as for the corresponding single-rate scheme. Moreover, by using an embedded method, it is then relatively easy to make an automatic partitioning J_n based on local error estimations. For a detailed discussion and implementation issues we refer to [12]; some additional test results are presented in Section 5 of the present paper.

The contents of this paper is as follows. In Section 2 error recursions are derived that show how the global discretization errors for the multirate scheme are build up. Bounds for the local discretization errors are obtained in Section 3. Stability and contractivity properties of the multirate scheme are discussed in Section 4. In Section 5 some numerical test results are presented, both for the dual-rate scheme (1.2) used for the theoretical investigation and for an automatic multirate scheme, based on the trapezoidal rule, with local error estimation and variable time steps. Finally, Section 6 contains conclusions.

2. Error propagations

2.1. Preliminaries

For the analysis it will be assumed that the problem (1.1) is linear with constant coefficients,

$$w'(t) = Aw(t) + g(t) \tag{2.1}$$

with an $m \times m$ matrix $A = (a_{ij})$. In fact, to study the local truncation errors, the restriction to the linear constant-coefficient case is not necessary, but it gives a convenient compact notation. On the other hand, to obtain stability results we will also consider even more simple problems where $m = 2$.

For multirate schemes the aim is to have errors in active components of the same size as in components with larger timescales and less activity. Therefore the maximum norm is a natural norm to consider for analysis purposes. Stability of the multirate scheme will be considered under the assumption

$$a_{ii} + \sum_{j \neq i} |a_{ij}| \leqslant 0 \quad \text{for } i = 1, \ldots, m. \tag{2.2}$$

In terms of logarithmic matrix norms this means $\mu_\infty(A) \leqslant 0$. It is well known, see [5,7] for instance, that we then have $\|\exp(tA)\|_\infty \leqslant 1$ for all $t \geqslant 0$, showing that initial perturbations are not amplified in the ODE system (2.1) itself.

Let in the following $Z = \tau A$. Furthermore, we denote the stability function of the θ-method by $R(z) = (1 + (1 - \theta)z)/(1 - \theta z)$. The corresponding matrix function is given by

$$R(Z) = (I - \theta Z)^{-1}\bigl(I + (1 - \theta)Z\bigr) \tag{2.3}$$

where I is the identity matrix.

Let $e_n = w(t_n) - w_n$ be the global discretization error at time t_n. These global errors will satisfy a recursion of the form

$$e_n = S_n e_{n-1} + d_n. \tag{2.4}$$

This error recursion describes the amplification of existing errors, through S_n, and the appearance of new errors d_n during the step from t_{n-1} to t_n. These d_n are called the local discretization errors. The scheme is called consistent of order p if $\|d_n\| \leqslant C\tau^{p+1}$. To have convergence of order p, that is, $\|e_n\| \leqslant C\tau^p$ for all n, we will also need suitable bounds on the norms of (products of) the matrices S_n.

2.2. Error recursions

In this section recursions are derived for the global discretization errors e_n. The errors of the intermediate approximations are denoted in the same way as $\bar{e}_n = w(t_n) - \overline{w}_n$ and $e_{n+1/2} = w(t_{n+1/2}) - w_{n+1/2}$. The linear and quadratic interpolation formulas are covered by

$$(I - J_n)\overline{w}_{n-\frac{1}{2}} = (I - J_n)\left(\frac{1}{2}w_{n-1} + \frac{1}{2}\overline{w}_n + \frac{1}{4}\gamma\bigl(w_{n-1} - \overline{w}_n + \tau F(t_{n-1}, w_{n-1})\bigr)\right) \tag{2.5}$$

with $\gamma = 0$ for linear interpolation and $\gamma = 1$ for the quadratic case.

Inserting exact solution values into the scheme (1.2) gives residual errors in the various stages of the scheme, which are easily found by Taylor expansion. Subtraction of (1.2) then leads to the following error relations

$$\bar{e}_n = e_{n-1} + (1 - \theta)Ze_{n-1} + \theta Z\bar{e}_n + \rho_{0,n}, \tag{2.6a}$$

$$\begin{aligned} e_{n-\frac{1}{2}} = {} & J_n\left(e_{n-1} + \frac{1}{2}(1 - \theta)Ze_{n-1} + \frac{1}{2}\theta Ze_{n-\frac{1}{2}} + \rho_{1,n}\right) \\ & + (I - J_n)\left(\frac{1}{2}e_{n-1} + \frac{1}{2}\bar{e}_n + \frac{1}{4}\gamma(e_{n-1} - \bar{e}_n + Ze_{n-1}) + \sigma_n\right), \end{aligned} \tag{2.6b}$$

$$e_n = J_n\left(e_{n-\frac{1}{2}} + \frac{1}{2}(1 - \theta)Ze_{n-\frac{1}{2}} + \frac{1}{2}\theta Ze_n + \rho_{2,n}\right) + (I - J_n)\bar{e}_n, \tag{2.6c}$$

where the $\rho_{j,n}$ are local, residual errors caused by the underlying θ-method,

$$\rho_{0,n} = \left(\frac{1}{2}-\theta\right)\tau^2 w''(t_{n-\frac{1}{2}}) - \frac{1}{12}\tau^3 w'''(t_{n-\frac{1}{2}}) + \mathcal{O}(\tau^4), \tag{2.7a}$$

$$\rho_{1,n} = \frac{1}{4}\left(\frac{1}{2}-\theta\right)\tau^2 w''(t_{n-\frac{1}{2}}) - \frac{1}{16}\left(\frac{2}{3}-\theta\right)\tau^3 w'''(t_{n-\frac{1}{2}}) + \mathcal{O}(\tau^4), \tag{2.7b}$$

$$\rho_{2,n} = \frac{1}{4}\left(\frac{1}{2}-\theta\right)\tau^2 w''(t_{n-\frac{1}{2}}) + \frac{1}{16}\left(\frac{1}{3}-\theta\right)\tau^3 w'''(t_{n-\frac{1}{2}}) + \mathcal{O}(\tau^4), \tag{2.7c}$$

and

$$\sigma_n = \frac{1}{8}(\gamma-1)\tau^2 w''(t_{n-\frac{1}{2}}) - \frac{1}{48}\gamma\tau^3 w'''(t_{n-\frac{1}{2}}) + \mathcal{O}(\tau^4) \tag{2.8}$$

is a residual error due to interpolation.

In the first stage of the scheme, with global step size τ, we thus obtain

$$\bar{e}_n = R(Z)e_{n-1} + (I-\theta Z)^{-1}\rho_{0,n}. \tag{2.9}$$

At the first refined time level it follows that

$$\begin{aligned} e_{n-\frac{1}{2}} = {} & \left(I - \frac{1}{2}\theta J_n Z\right)^{-1}\left(J_n\left(I + \frac{1}{2}(1-\theta)Z\right) + (I-J_n)Q\right)e_{n-1} \\ & + \left(I - \frac{1}{2}\theta J_n Z\right)^{-1}\left(J_n\rho_{1,n} + (I-J_n)\left(\sigma_n + \left(\frac{1}{2}-\frac{1}{4}\gamma\right)(I-\theta Z)^{-1}\rho_{0,n}\right)\right) \end{aligned} \tag{2.10}$$

with interpolation matrix

$$Q = \frac{1}{2}I + \frac{1}{2}R(Z) + \frac{1}{4}\gamma\big(I + Z - R(Z)\big). \tag{2.11}$$

For the global discretization errors of the total scheme this finally leads to the error recursion (2.4) with amplification matrix

$$\begin{aligned} S_n = {} & \left(I - \frac{1}{2}\theta J_n Z\right)^{-1}\left(J_n R\left(\frac{1}{2}J_n Z\right)J_n\left(I + \frac{1}{2}(1-\theta)Z\right)\right. \\ & \left. + J_n R\left(\frac{1}{2}J_n Z\right)(I-J_n)Q + (I-J_n)R(Z)\right), \end{aligned} \tag{2.12}$$

and local discretization error

$$\begin{aligned} d_n = {} & \left(I - \frac{1}{2}\theta J_n Z\right)^{-1}\left(J_n R\left(\frac{1}{2}J_n Z\right)\big(J_n\rho_{1,n} + (I-J_n)\sigma_n\big) + J_n\rho_{2,n}\right. \\ & \left. + \left(I + \left(\frac{1}{2}-\frac{1}{4}\gamma\right)J_n R\left(\frac{1}{2}J_n Z\right)\right)(I-J_n)(I-\theta Z)^{-1}\rho_{0,n}\right). \end{aligned} \tag{2.13}$$

3. Local discretization errors

It is clear from (2.7), (2.8) that $\sigma_n = \mathcal{O}(\tau^3)$ if $\gamma = 1$ and $\rho_{j,n} = \mathcal{O}(\tau^3)$ if $\theta = \frac{1}{2}$. In other cases we only have $\mathcal{O}(\tau^2)$ bounds. Here the constants in the $\mathcal{O}(\tau^q)$ estimates are not affected by stiffness; they only depend on the smoothness of the solution. To derive similar bounds for the local discretization errors it will be assumed that

$$\big\|R(\tau A)\big\|_\infty \leqslant C, \qquad \left\|\left(I - \frac{1}{2}\tau\theta J_n A\right)^{-1}\right\|_\infty \leqslant C, \tag{3.1}$$

with $C \geqslant 1$ a fixed constant. These assumptions are taken such that both cases $\theta = 0$ and $\theta > 0$ are covered. In fact, if $\theta > 0$ then (3.1) will be a consequence of (2.2), with C independent of τ, but for $\theta = 0$ it will impose a restriction on the step size.

Theorem 3.1. *Let* $0 \leqslant \theta \leqslant 1$ *and assume* (3.1) *holds. If* $\theta = \frac{1}{2}$ *and* $\gamma = 1$*, then* $\|d_n\|_\infty = \mathcal{O}(\tau^3)$*. Otherwise, we have* $\|d_n\|_\infty = \mathcal{O}(\tau^2)$.

Proof. For $\theta > 0$ assumption (3.1) implies

$$\left\|R\left(\frac{1}{2}J_n Z\right)\right\|_\infty \leqslant \theta^{-1}(1-\theta) + \theta^{-1}\left\|\left(I - \frac{1}{2}\theta J_n Z\right)^{-1}\right\|_\infty \leqslant \theta^{-1}(1-\theta+C),$$
$$\left\|(I-\theta Z)^{-1}\right\|_\infty = \left\|(1-\theta)I + \theta R(Z)\right\|_\infty \leqslant 1-\theta+\theta C,$$

whereas for $\theta = 0$, that is, $R(z) = 1+z$, we will have

$$\left\|R\left(\frac{1}{2}J_n Z\right)\right\|_\infty = \left\|\left(I - \frac{1}{2}J_n\right) + \frac{1}{2}J_n(I+Z)\right\|_\infty \leqslant 1 + \frac{1}{2}C.$$

Since $\|\rho_{j,n}\|_\infty = |\theta - \frac{1}{2}|\mathcal{O}(\tau^2) + \mathcal{O}(\tau^3)$ and $\|\sigma_n\|_\infty = |\gamma - 1|\mathcal{O}(\tau^2) + \mathcal{O}(\tau^3)$, the required bounds thus follow from the local error expression (2.13). □

If $\theta \neq \frac{1}{2}$ this result cannot be improved in general, since the θ-method itself is then first-order consistent. The interesting question is whether we can have consistency of order two for $\theta = \frac{1}{2}$ with linear interpolation ($\gamma = 0$). The next result shows that will be valid if the coupling from the slow towards the more active components is bounded,

$$\left\|J_n A(I - J_n)\right\|_\infty \leqslant K \tag{3.2}$$

with a moderate constant K. This will hold in particular for non-stiff problems.

Theorem 3.2. *Let* $\theta = \frac{1}{2}$, $\gamma = 0$*, and suppose that* (3.1), (3.2) *hold. Then we have the local error bound* $\|d_n\|_\infty = \mathcal{O}(\tau^3)$.

Proof. Since

$$J_n R\left(\frac{1}{2}J_n Z\right)(I - J_n) = J_n\left(I + \left(I - \frac{1}{2}\theta J_n Z\right)^{-1}\frac{1}{2}J_n Z\right)(I - J_n),$$

it follows that

$$\left\|J_n R\left(\frac{1}{2}J_n Z\right)(I - J_n)\right\|_\infty \leqslant \frac{1}{2}\left\|J_n\left(I - \frac{1}{2}\theta J_n Z\right)^{-1}\right\|_\infty \left\|J_n Z(I - J_n)\right\|_\infty \leqslant \frac{1}{2}CK\tau.$$

Expression (2.13) thus leads directly to the proof. □

In case $\theta = \frac{1}{2}$ and $\gamma = 0$, but (3.2) is not satisfied with a moderate constant K, then the order of consistency will be less than two in general. For stiff systems, the order of convergence can be larger than the order of consistency, due to damping and cancellation effects (similar to [7, Lemma I.2.3] for Runge–Kutta methods), but we will see in Section 5 that for a simple example (semi-discrete heat equation) the scheme will not converge with order two.

4. Stability and contractivity

4.1. Contractivity with linear interpolation

Consider one step of (1.2) with $J_n = \mathrm{diag}(J_{ii})$. We denote by $\mathcal{I}_1 = \{i\colon\ J_{ii} = 0\}$ the index set where the step is not refined, and likewise $\mathcal{I}_2 = \{i\colon\ J_{ii} = 1\}$ stands for the index set where we do refine the step. For the multirate scheme we consider the time step restrictions

$$\begin{cases} |(1-\theta)\tau a_{ii}| \leqslant 1 & \text{for } i \in \mathcal{I}_1, \\ |(1-\theta)\tau a_{ii}| \leqslant 2 & \text{for } i \in \mathcal{I}_2. \end{cases} \tag{4.1}$$

Theorem 4.1. *Consider* (2.12) *with* $0 \leqslant \theta \leqslant 1$ *and* $\gamma = 0$*. Assume* (2.2) *and* (4.1) *are valid. Then* $\|S_n\|_\infty \leqslant 1$.

Proof. From assumption (2.2) and the unconditional contractivity of the backward Euler method, see [6,7] for instance, it follows that

$$\left\|(I-\theta Z)^{-1}\right\|_\infty \leqslant 1, \qquad \left\|\left(I-\frac{1}{2}\theta J_n Z\right)^{-1}\right\|_\infty \leqslant 1. \tag{4.2}$$

Moreover, the time step restriction (4.1) implies

$$\left\|(I-J_n)\big(I+(1-\theta)Z\big)\right\|_\infty \leqslant 1, \qquad \left\|J_n\left(I+\frac{1}{2}(1-\theta)Z\right)\right\|_\infty \leqslant 1.$$

We can write S_n as

$$S_n=\left(I-\frac{1}{2}\theta J_n Z\right)^{-1}\left(J_n\left(I+\frac{1}{2}(1-\theta)Z\right)T_n+(I-J_n)R(Z)\right),$$
$$T_n=\left(I-\frac{1}{2}\theta J_n Z\right)^{-1}\left(J_n\left(I+\frac{1}{2}(1-\theta)Z\right)+(I-J_n)Q\right),$$

where $Q=\frac{1}{2}(I+R(Z))$ for linear interpolation, see (2.10)–(2.12).

First consider the term

$$(I-J_n)R(Z)=(I-J_n)(I-\theta Z)^{-1}\big(I+(1-\theta)Z\big).$$

Because $(I-\theta Z)^{-1}$ and $(I+(1-\theta)Z)$ commute we have

$$\left\|(I-J_n)R(Z)\right\|_\infty \leqslant \left\|(I-J_n)\big(I+(1-\theta)Z\big)\right\|_\infty \left\|(I-\theta Z)^{-1}\right\|_\infty \leqslant 1,$$

and consequently also

$$\left\|(I-J_n)Q\right\|_\infty \leqslant 1.$$

Using the fact that $\|J_nU+(I-J_n)V\|_\infty \leqslant 1$ for any two matrices $U, V \in \mathbb{R}^{m\times m}$ with $\|U\|_\infty \leqslant 1$, $\|V\|_\infty \leqslant 1$, it now easily follows that $\|T_n\|_\infty \leqslant 1$ and subsequently $\|S_n\|_\infty \leqslant 1$. □

The above conditions (4.1) for having $\|S_n\|_\infty \leqslant 1$ are sharp, as is seen from the following simple 3×3 example.

Example 4.2. Consider

$$A=\begin{pmatrix}-2 & -2 & 0\\ 0 & -1 & -1\\ 0 & 0 & 0\end{pmatrix}, \qquad J=\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

Then both restrictions in (4.1) reduce to

$$(1-\theta)\tau \leqslant 1.$$

With $e=(1,1,1)^T$, it follows by some calculations that the second component of Se is given by

$$(Se)_2=-1+2\frac{1-(1-\theta)\tau}{1+\theta\tau}.$$

It is now easily seen that $\|S\|_\infty > 1$ whenever (4.1) is not satisfied.

So for the backward Euler case, $\theta=1$, we will have unconditional contractivity; see [11] for a related (nonlinear) result for a backward Euler scheme with a compound step. Also for $\theta=0$ (forward Euler) the result of Theorem 4.1 is entirely satisfactory; in fact, necessity of (4.1) is then already clear for diagonal matrices A. However, for $\theta=\frac{1}{2}$ (trapezoidal rule), the time step conditions in (4.1) are very strict. After all, the trapezoidal rule itself is A-stable.

The strict time steps for the trapezoidal rule are to some extent due to the insistence on contractivity, $\|S_n\| \leqslant 1$, rather than stability, where it is merely required that the error growth is moderate. From a practical point of view, having

$$\|S_nS_{n-1}\cdots S_2S_1\|_\infty \leqslant M \quad \text{for all } n \geqslant 1 \tag{4.3}$$

with some moderate constant M would be a sufficient stability condition. However, we will see below that for a standard linear example, arising from the heat equation, this will not be satisfied for the trapezoidal rule with linear interpolation if the step size τ is too large. This is due to the multirate procedure. The trapezoidal rule itself is stable in the maximum norm for this example (see e.g. [2]), and in the discrete L_2-norm it will even be contractive (see e.g. [5,7]). The same heat equation example will also show that with quadratic interpolation stability can even be lost for $\theta = 1$.

4.2. Stability for fixed partitioning and non-stiff couplings

Consider $J_n = J$ fixed. Since the time step is also assumed to be constant, the amplification matrix S will then no longer depend on n either, so the stability condition (4.3) becomes the power boundedness condition $\|S^n\|_\infty \leqslant M$. In the following we mostly restrict our attention to $\theta > 0$ and linear interpolation, $\gamma = 0$. Some remarks on quadratic interpolation are given near the end of this section.

For fixed J it can be assumed without loss of generality that

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \qquad J = \begin{pmatrix} O & \\ & I \end{pmatrix}. \tag{4.4}$$

This block partitioning can always be achieved by an index permutation. The same partitioning will be used for

$$Z = [Z_{ij}] = [\tau A_{ij}], \quad R(Z) = \big[R(Z)_{ij}\big], \quad Q = [Q_{ij}], \quad S = [S_{ij}].$$

Further we denote $U_{22} = (I - \frac{1}{2}\theta Z_{22})^{-1}$ for brevity. Then it is found by some calculations that the blocks of S are given by

$$\begin{cases} S_{11} = R(Z)_{11}, \quad S_{12} = R(Z)_{12}, \\ S_{21} = \dfrac{1}{2}(1-\theta)U_{22}R\left(\dfrac{1}{2}Z_{22}\right)Z_{21} + \dfrac{1}{2}U_{22}^2 Z_{21}Q_{11} + \dfrac{1}{2}\theta U_{22}Z_{21}R(Z)_{11}, \\ S_{22} = R\left(\dfrac{1}{2}Z_{22}\right)^2 + \dfrac{1}{2}U_{22}^2 Z_{21}Q_{12} + \dfrac{1}{2}\theta U_{22}Z_{21}R(Z)_{12}. \end{cases} \tag{4.5}$$

The actual form of the blocks $R(Z)_{ij}$ is somewhat complicated for general non-commuting A_{ij}, but if A is upper or lower block-triangular we obtain more simple expressions. Stability for those cases is considered under the following assumption on the diagonal blocks:

$$\big\|R(\tau A_{11})^n\big\|_\infty \leqslant K_1 r_1^n, \qquad \left\|R\left(\frac{1}{2}\tau A_{22}\right)^{2n}\right\|_\infty \leqslant K_2 r_2^n \quad \text{for } n \geqslant 1, \tag{4.6}$$

with $K_1, K_2 > 0$ and $0 \leqslant r_1, r_2 \leqslant 1$.

Theorem 4.3. *Assume $\theta > 0$, $\gamma = 0$, (2.2), (4.6), and let $r = \min(r_1, r_2)$. Furthermore, assume that either $A_{21} = 0$ or $A_{12} = 0$. Then there is a $K > 0$ such that*

$$\|S^n\|_\infty \leqslant K \sum_{j=0}^{n} r^j \quad \textit{for } n \geqslant 1.$$

Proof. We present the proof for the lower block-diagonal case $A_{12} = 0$. The proof for $A_{21} = 0$ is easier because most of the terms in (4.5) then cancel.

If $A_{12} = 0$, we find that $R(Z)_{12} = Q_{12} = 0$ and $R(Z)_{11} = R(Z_{11})$, which gives

$$S_{12} = 0, \quad S_{11} = R(Z_{11}), \quad S_{22} = R\left(\frac{1}{2}Z_{22}\right)^2.$$

Moreover, from $S_{12} = 0$, it follows that

$$S^n = \begin{pmatrix} S_{11}^n & O \\ \sum_{j=1}^{n} S_{22}^{n-j} S_{21} S_{11}^{j-1} & S_{22}^n \end{pmatrix},$$

and hence

$$\|S^n\|_\infty \leqslant \|S_{11}^n\|_\infty + \|S_{21}\|_\infty \sum_{j=1}^{n} \|S_{22}^{n-j}\|_\infty \|S_{11}^{j-1}\|_\infty + \|S_{22}^n\|_\infty.$$

It remains to show that $\|S_{21}\|_\infty$ is bounded. Let $U = [U_{ij}] = (I - \frac{1}{2}\theta JZ)^{-1}$. Then U_{22} is as above and $U_{21} = \frac{1}{2}\theta U_{22}Z_{21}$ in this lower block-diagonal case. Moreover, as seen in (4.2), assumption (2.2) implies $\|U\|_\infty \leqslant 1$, and consequently also $\|U_{21}\|_\infty \leqslant 1$, $\|U_{22}\|_\infty \leqslant 1$. It thus follows that

$$U_{22}R\left(\frac{1}{2}Z_{22}\right)Z_{21} = \frac{\theta-1}{\theta}U_{22}Z_{21} + \frac{1}{\theta}U_{22}^2 Z_{21}$$

can be bounded as well for $\theta > 0$. The same applies for the other terms in the expression (4.5) for S_{21}, where we note that $Q_{11} = \frac{1}{2}(I + R(Z_{11}))$ because of the linear interpolation. □

If $r < 1$ the theorem provides a stability result with $\|S^n\|_\infty \leqslant K/(1-r)$ for all $n \geqslant 1$. If $r = 1$ it merely demonstrates weak stability $\|S^n\|_\infty \leqslant Kn$ where a linear error growth is possible.

The above result for lower or upper block triangular matrices can be extended to non-stiff couplings by a perturbation argument, where we assume that A is not too far from a simpler matrix $\tilde{A}$ for which stability with the corresponding amplification matrix $\tilde{S}$ is known,

$$\|A - \tilde{A}\|_\infty \leqslant L, \quad \|\tilde{S}^n\|_\infty \leqslant M \quad \text{for all } n \geqslant 1. \tag{4.7}$$

Then stability of the scheme with the original amplification matrix S can be concluded on finite time intervals $0 \leqslant t_n \leqslant T$.

Theorem 4.4. *Suppose $\theta > 0$, $\gamma = 0$. Further assume that $\mu_\infty(\tilde{A}) \leqslant 0$ and (4.7). Then there exist $C > 0$ and $\tau_* > 0$ (depending only on γ, L, M) such that*

$$\|S^n\|_\infty \leqslant M\exp(CMt_n) \quad \textit{whenever } \tau \leqslant \tau_*.$$

Proof. It is to be shown that $\|S - \tilde{S}\|_\infty \leqslant C\tau$. Then the result follows from a standard perturbation argument; see for example [9, p. 58]. The estimate on $S - \tilde{S}$ requires some care.

We can decompose S as

$$S = VJ\left(I + \frac{1}{2}(1-\theta)Z\right) + V(I-J)Q + W, \tag{4.8}$$

where

$$V = \left(I - \frac{1}{2}\theta JZ\right)^{-1} JR\left(\frac{1}{2}JZ\right), \qquad W = \left(I - \frac{1}{2}\theta JZ\right)^{-1}(I-J)R(Z). \tag{4.9}$$

For $\tilde{S}$ we consider the same form based on $\tilde{Z}$. Then

$$\begin{aligned} S - \tilde{S} = {} & [V - \tilde{V}]J + \frac{1}{2}(1-\theta)[V-\tilde{V}]JZ + \frac{1}{2}(1-\theta)\tilde{V}J[Z - \tilde{Z}] \\ & + [V - \tilde{V}](I-J)Q + \tilde{V}(I-J)[Q - \tilde{Q}] + [W - \tilde{W}]. \end{aligned} \tag{4.10}$$

Let us first consider $R(Z) - R(\tilde{Z})$. We have

$$R(Z) - R(\tilde{Z}) = (I - \theta Z)^{-1}(Z - \tilde{Z})(I - \theta\tilde{Z})^{-1},$$
$$(I - \theta Z)^{-1} = \left(I - \theta(I - \theta\tilde{Z})^{-1}(Z - \tilde{Z})\right)^{-1}(I - \theta\tilde{Z})^{-1}.$$

Since $\mu_\infty(\tilde{A}) \leqslant 0$ we know that $\|(I - \theta\tilde{Z})^{-1}\|_\infty \leqslant 1$. This leads to[2]

$$\|(I - \theta Z)^{-1}\|_\infty \leqslant \frac{1}{1 - \theta L\tau}, \qquad \|R(Z) - R(\tilde{Z})\|_\infty \leqslant \frac{L\tau}{1 - \theta L\tau} \leqslant 2L\tau$$

[2] Note that $\|X\| \leqslant 1$ implies that $\|(I - XY)^{-1}\| \leqslant (1 - \|Y\|)^{-1}$.

provided that $\tau < 1/(2\theta L)$. The same applies to the perturbations for $R(\frac{1}{2}JZ)$. If we take $\tau_* = 1/(4\theta L)$ then these bounds are valid uniformly for $\tau \in (0, \tau_*]$.

The most difficult term to estimate in (4.10) is $[V - \tilde{V}]JZ$, because Z is not bounded by the assumptions. Denoting as before $U = (I - \frac{1}{2}\theta JZ)^{-1}$, we have

$$V - \tilde{V} = [U - \tilde{U}]JR\left(\frac{1}{2}JZ\right) + \tilde{U}J\left[R\left(\frac{1}{2}JZ\right) - R\left(\frac{1}{2}J\tilde{Z}\right)\right],$$

and hence

$$[V - \tilde{V}]JZ = \frac{1}{2}\theta\tilde{U}J[Z - \tilde{Z}]UJR\left(\frac{1}{2}JZ\right)JZ + \frac{1}{2}\tilde{U}J\tilde{U}J[Z - \tilde{Z}]UJZ.$$

Now, by noticing that

$$UJR\left(\frac{1}{2}JZ\right)JZ = \frac{\theta - 1}{\theta}UJZ + \frac{1}{\theta}U^2JZ$$

and using the bounds for $\|U\|_\infty$ and $\|UJZ\|_\infty$ for $\tau \leqslant \tau_*$, it follows that $\|[\tilde{V} - V]JZ\|_\infty$ can be bounded by $C\tau$. Estimation of the remaining terms in (4.10) proceeds in a similar way using the above estimates. □

The above perturbation result can be combined with Theorem 4.4 to obtain a stability result for non-stiff couplings, where either $\|A_{21}\|_\infty$ or $\|A_{12}\|_\infty$ is bounded by a moderate constant.

Remark 4.5. For $\theta = 0$ similar results can be derived if the assumptions $\mu_\infty(Z) \leqslant 0$ or $\mu_\infty(\tilde{Z}) \leqslant 0$ are replaced by appropriate boundedness assumptions. Results for $\theta > 0$ with quadratic interpolation require additional assumptions that are not satisfied in general for stiff systems. For example, in the proof of Theorem 4.3, an explicit Z_{11} terms then appears in Q_{11} in which case additional assumptions are needed to bound the term $U_{22}^2 Z_{21} Z_{11}$. For Theorem 4.4 it is similar. We will see in the next section that the stability properties of the multirate scheme are very poor indeed if quadratic interpolation is used, even if $\theta = 1$.

4.3. *Asymptotic stability for* 2×2 *test equations*

In this section we present some detailed results on stability of the scheme (1.2) for the linear test equation (2.1) with real 2×2 matrices

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \qquad J = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.11}$$

We denote

$$\kappa = \frac{a_{11}}{a_{22}}, \qquad \beta = \frac{a_{12}a_{21}}{a_{11}a_{22}}. \tag{4.12}$$

By assumption (2.2) we have $\kappa \geqslant 0$ and $|\beta| \leqslant 1$. We can regard κ as a measure for the stiffness of the system, and β gives the amount of coupling between the fast and slow part of the equation. For this two-dimensional test equation we will consider asymptotic stability whereby it is required that the eigenvalues of the amplification matrix S are bounded by one in modulus. Similar stability considerations for 2×2 systems are found in [3,4,8,10,13–15] for multirate schemes with a compound step.

The elements of the 2×2 amplification matrix S will depend on the four parameters $z_{ij} = \tau a_{ij}$, $1 \leqslant i, j \leqslant 2$. However, the eigenvalues of S, which depend only on the determinant and trace of S, can be written as functions of three parameters: κ, β and z_{22}. This can be seen by elaborating (4.5) for this 2×2 case. Instead of $z_{22} \leqslant 0$ we will use the quantity

$$\alpha = \frac{1 + \frac{1}{2}(1 - \theta)z_{22}}{1 - \frac{1}{2}\theta z_{22}}, \tag{4.13}$$

which is bounded for $z_{22} \leqslant 0$ and $\theta \geqslant \frac{1}{2}$.

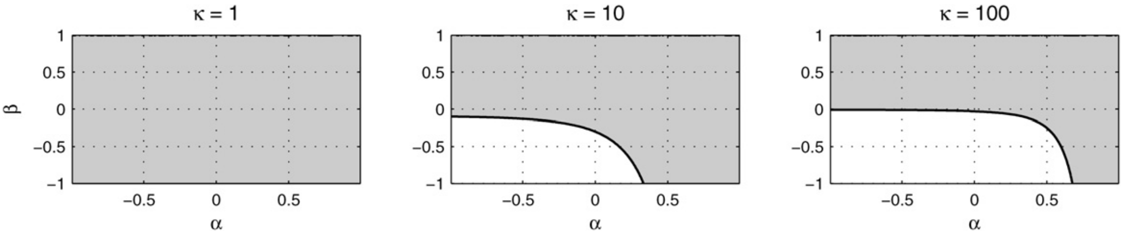

Fig. 1. Asymptotic stability domains (gray areas) for the trapezoidal rule with linear interpolation, $\kappa = 1, 10, 100$.

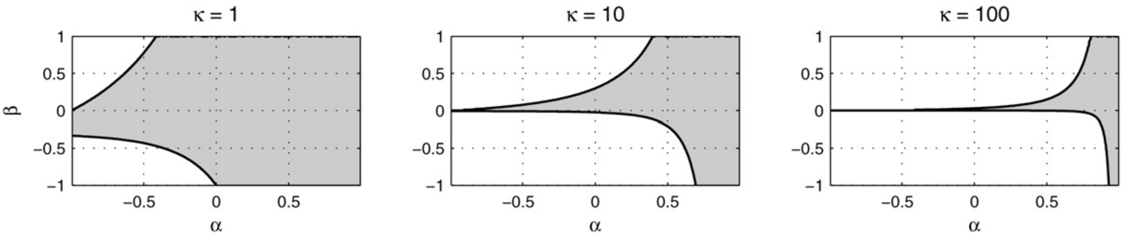

Fig. 2. Asymptotic stability domains (gray areas) for the trapezoidal rule with quadratic interpolation, $\kappa = 1, 10, 100$.

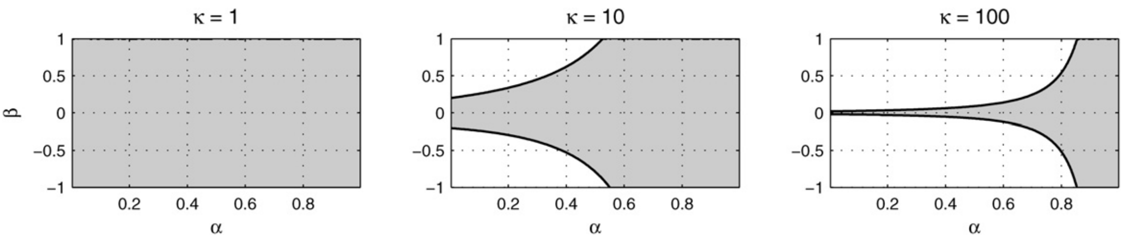

Fig. 3. Asymptotic stability domains (gray areas) for backward Euler with quadratic interpolation, $\kappa = 1, 10, 100$.

The domains of asymptotic stability, where the spectral radius of S is bounded by one, are shown in Figs. 1–3 for $\theta = \frac{1}{2}, 1$ and linear or quadratic interpolation. We present these domains in the (α, β)-plane for three values of $\kappa = 10^j,\ j = 0, 1, 2$. Notice that $\alpha \in [-1, 1]$ if $\theta = \frac{1}{2}$ and $\alpha \in [0, 1]$ if $\theta = 1$. Generally the asymptotic stability domains are decreasing when κ is increased.

From Fig. 1 it is seen that the combination of the trapezoidal rule and linear interpolation will be stable if $\beta \geqslant 0$, whereas for $\beta < 0$ the domain of instability increases when κ gets large. For the trapezoidal rule with quadratic interpolation, the scheme becomes unstable for large κ, unless $\beta = 0$. For both quadratic and linear interpolation, the limit case $\kappa \to 0$, with α, β fixed, gives stability of the scheme because then both z_{22} and z_{21} tend to zero as well.

As we already saw in Theorem 4.1, using the backward Euler method as underlying time integration method, the scheme will be stable with linear interpolation. However, as seen in Fig. 3, the combination of backward Euler and quadratic interpolation is no longer stable when κ becomes large. Of course, in terms of accuracy it is for the backward Euler method not necessary to use quadratic interpolation, but the observed instability is of interest anyway.

Remark 4.6. Stability conditions based on eigenvalues of S are rather weak. If we have spectral radius $\rho(S) < 1$, then it is known that $S^n \to 0$ as $n \to \infty$, but this does not guarantee that $\max_{n \geqslant 0} \|S^n\|_\infty$ is bounded by a moderate number because the bound may depend on τ and A. If $\rho(S) = 1$ is allowed, then even polynomial growth may occur. In our opinion, (4.11) is primarily a useful test equation for showing *instability* of certain schemes, such as the schemes with quadratic interpolation in this paper. Demonstrating stability for (4.11) in some suitable norm is somewhat less relevant, because for an m-dimensional system with partitioning (4.4), the blocks A_{ij} may have complex eigenvalues, and, moreover, they will not commute in general.

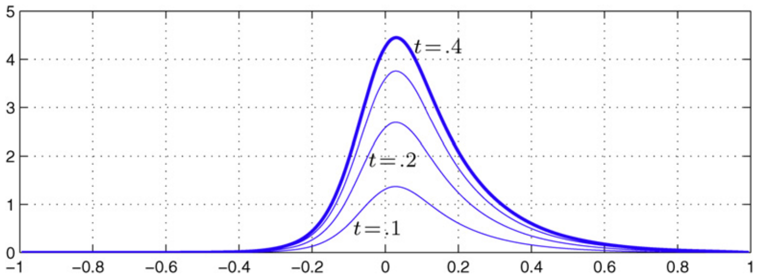

Fig. 4. Solution for the parabolic test problem (5.1) at intermediate times $t = 0.1, 0.2, 0.3$ and the final time $t = T = 0.4$ (thick line).

Table 1
Relative L_2-errors at $t = T$ versus N for the parabolic test problem. Results for the non-refined θ-method, $\theta = 1, \frac{1}{2}$, and for the scheme with one level of refinement and linear interpolation on the spatial region $-0.2 \leqslant x_j \leqslant 0.2$

N	10	20	40	80	160
$\theta = 1$, non-ref.	1.57×10^{-3}	7.96×10^{-4}	4.00×10^{-4}	2.00×10^{-4}	1.00×10^{-4}
$\theta = 1, \gamma = 0$	1.21×10^{-3}	5.93×10^{-4}	2.86×10^{-4}	1.37×10^{-4}	6.55×10^{-5}
$\theta = \frac{1}{2}$, non-ref.	1.81×10^{-4}	3.76×10^{-6}	8.12×10^{-7}	2.03×10^{-7}	5.07×10^{-8}
$\theta = \frac{1}{2}, \gamma = 0$	4.17×10^{-4}	4.74×10^{-5}	1.49×10^{-5}	4.85×10^{-6}	1.58×10^{-6}

5. Numerical experiments

5.1. A linear parabolic example

As a test model we consider the parabolic equation

$$u_t + au_x = du_{xx} - cu + g(x,t), \tag{5.1a}$$

for $0 < t < T = 0.4$, $-1 < x < 1$, with initial- and boundary conditions

$$u(x,0) = 0, \quad u(-1,t) = 0, \quad u(1,t) = 0. \tag{5.1b}$$

The constants and source term are taken as

$$a = 10, \quad d = 1, \quad c = 10^2, \quad g(x,t) = 10^3 \cos\left(\frac{1}{2}\pi x\right)^{100} \sin(\pi t). \tag{5.1c}$$

The solution at the end time $T = 0.4$ is illustrated in Fig. 4.

Semi-discretization with second-order differences on a uniform spatial grid with m points and mesh width $h = 2/(m+1)$, leads to an ODE system of the form (2.1). We use for this test $m = 400$, and the temporal refinements are taken for the components corresponding to spatial grid points $x_j \in [-0.2, 0.2]$. (Spatial grid refinements are not considered here; we use the semi-discrete system just as an ODE example.)

Table 1 shows the discrete L_2-errors (scaled Euclidean norm) at $t = T$ with respect to a time-accurate ODE solution; the maximum errors were quite similar. The results are given for linear interpolation with the backward Euler method ($\theta = 1$) and the implicit trapezoidal rule ($\theta = \frac{1}{2}$), both with uniform, non-refined time steps $\tau = T/N$ and with locally refined steps $\tau/2$ on part of the spatial domain.

The refinement region $-0.2 \leqslant x_j \leqslant 0.2$ was only chosen for test purposes; it is clear from Fig. 4 that it is not a very good choice. Considering this fact, the results for $\theta = 1$ are satisfactory. However, for $\theta = \frac{1}{2}$ the errors with the local refinements are much larger than those for the non-refined scheme. This loss of accuracy is due to the linear interpolation, which lowers the order of consistency in this example.

Quadratic interpolation did give very large errors due to instabilities in this test, both for $\theta = 1$ (with errors in the range 10^2–10^{16}) and $\theta = \frac{1}{2}$ (errors in the range 10^7–10^{91}). In view of the unfavourable results that were found already for the 2×2 example in the previous section, this is not surprising anymore.

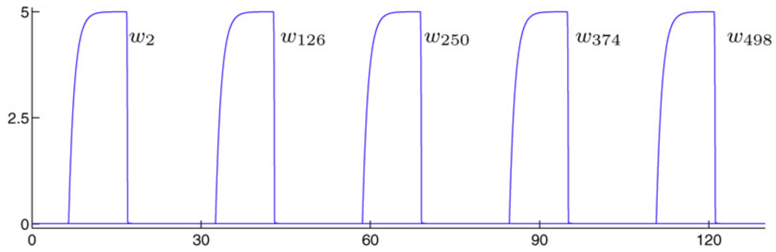

Fig. 5. Solution components $w_j(t)$, $j = 2, 126, 250, 374, 498$, for the inverter chain test problem (5.2).

5.2. The inverter chain problem

As a second test example we consider the inverter chain problem from [1]. The model for m inverters consists of the equations

$$\begin{cases} w_1'(t) = U_{\text{op}} - w_1(t) - \Upsilon g\big(u_{\text{in}}(t), w_1(t)\big), \\ w_j'(t) = U_{\text{op}} - w_j(t) - \Upsilon g\big(w_{j-1}(t), w_j(t)\big), \quad j = 2, \ldots, m, \end{cases} \tag{5.2a}$$

where

$$g(u, v) = \big(\max(u - U_{\text{thres}}, 0)\big)^2 - \big(\max(u - v - U_{\text{thres}}, 0)\big)^2. \tag{5.2b}$$

The coefficient Υ serves as stiffness parameter. We solve the problem for a chain of $m = 500$ inverters with $\Upsilon = 100$, $U_{\text{thres}} = 1$ and $U_{\text{op}} = 5$, over the time interval $[0, T]$, $T = 130$. The initial condition is

$$w_j(0) = 6.247 \times 10^{-3} \quad \text{for } j \text{ even}, \qquad w_j(0) = 5 \quad \text{for } j \text{ odd}. \tag{5.2c}$$

The input signal is given by

$$u_{\text{in}}(t) = \begin{cases} t - 5 & \text{for } 5 \leqslant t \leqslant 10, \\ 5 & \text{for } 10 \leqslant t \leqslant 15, \\ \frac{5}{2}(17 - t) & \text{for } 15 \leqslant t \leqslant 17, \\ 0 & \text{otherwise}. \end{cases} \tag{5.2d}$$

An illustration for some even components of the solution is given in Fig. 5.

This problem is solved using the self-adjusting multirate time stepping strategy introduced in [12]. Given a global time step $\Delta t_n = t_n - t_{n-1}$, we compute a first, tentative approximation at the new time level for all components. For those components for which the error estimator indicates that smaller steps are needed, the computation is redone with $\frac{1}{2}\Delta t_n$. The refinement is continued recursively with local steps $2^{-l}\Delta t_n$, until the error estimator is below a prescribed tolerance for all components. For details on the selection of the time step and number of refinement levels we refer to [12].

As the basic time integration method we use a linearized version of the trapezoidal rule,

$$w_n = w_{n-1} + \frac{1}{2}\tau\big(F(t_{n-1}, w_{n-1}) + F(t_n, w_{n-1}) + A(w_n - w_{n-1})\big) \tag{5.3}$$

where $A = \frac{\partial}{\partial w}F(t_n, w_{n-1})$. With this linearized trapezoidal rule non-linear algebraic systems are avoided. To estimate the error of a step we compare the result with a step using the forward Euler method. It should be noted that the t_n argument is retained in the linearization (5.3). This done because the solution of this inverter chain problem has very steep temporal gradients, which are induced by earlier changes in the input function u_{in}. Further linearization, replacing $F(t_n, w_{n-1})$ in (5.3) by $F(t_{n-1}, w_{n-1}) + \tau\frac{\partial}{\partial t}F(t_{n-1}, w_{n-1})$, would give larger errors in this problem, because the forward Euler method also only uses information from time level t_{n-1}, so changes over the interval $[t_{n-1}, t_n]$ are then felt too late by the error estimator.

In Table 2 the maximal errors over all components and all times t_n (measured with respect to an accurate reference solution) are presented for several tolerances with the single-rate scheme (without local temporal refinements) and the multirate strategy. The results are given for linear interpolation at the coupling interface; quadratic interpolation

Table 2
Absolute maximal errors, work amount and CPU times with different tolerances for the inverter chain problem

	Single-rate			Multirate		
tol	error	work	CPU	error	work	CPU
5×10^{-4}	1.55×10^{-1}	32 089 000	20.12	2.10×10^{-1}	4 266 674	4.06
1×10^{-4}	2.93×10^{-2}	70 156 000	44.06	3.52×10^{-2}	7 294 108	7.52
5×10^{-5}	1.32×10^{-2}	98 750 000	61.97	6.67×10^{-3}	9 410 734	9.94
1×10^{-5}	1.74×10^{-3}	219 320 500	137.76	2.27×10^{-3}	26 586 200	23.14

gave similar results, without instabilities, in this example. As a measure for the amount of work we consider the total number of components at which solutions are computed over the complete integration interval $[0, T]$; this is proportional to the number of scalar function evaluations (5.2b). In addition, the CPU times are given.

It is seen from the table that for the prescribed tolerances we get roughly a factor 10 of improvement in work with the multirate scheme, compared to the standard single-rate method, whereas for each given tolerance the errors of the multirate scheme are of similar size as those of the single-rate scheme. In terms of CPU times we get a speed-up factor 6 approximately.

So for this test problem the multirate scheme with the (linearized) trapezoidal rule works well. There is no instability when using quadratic interpolation and there is no reduction in accuracy due to linear interpolation. It should be noted that this example is only mildly stiff, in contrast to the semi-discrete parabolic system in the first example.

Finally we note that the results in Table 2 are similar to those in [12] for a two-stage Rosenbrock method of order two. For practical problems that method seems preferable over the linearized trapezoidal rule (5.3), because the order of accuracy remains two if inexact Jacobians are used in the two-stage method. Moreover, the two-stage method allows an embedded (one-stage) method for error estimation with the same stability properties.

6. Conclusions

To obtain a better understanding of general multirate schemes, a simple scheme was studied in this paper, with the θ-method as basic time integration method and with one level of refinement.

As seen from the local error bounds for the trapezoidal rule with linear interpolation ($\theta = \frac{1}{2}$, $\gamma = 0$), stiffness may lead to an order reduction where we obtain a lower order of consistency than for non-stiff problems.

A proper stability analysis is very difficult in general, even for the simple multirate scheme studied here. Detailed (numerical) results for very simple 2×2 cases are helpful to better understand possible instabilities for the schemes.

In spite of the lack of definitive theoretical results, multirate schemes can be efficient for problems with different levels of activities in the various components. The automatic partitioning strategy derived and tested in [12] (used in this paper for the inverter chain test problem with a linearized trapezoidal rule) provides in many cases of practical interest a significant speed-up compared to the corresponding single-rate scheme.

Finally we note that for higher-order Runge–Kutta or Rosenbrock schemes the class of possible interpolation formulas is larger than for the simple θ-method considered in this paper, because then also internal stage values are available. For example, for the two-stage Rosenbrock method used in [12] preliminary tests have shown that there are interpolations of second-order consistency which are stable for the stiff test problems that were considered in this paper. Extensions to methods of order larger than two are currently under investigation.

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