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ON EXTRAPOLATED MULTIRATE METHODS *

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Abstract. In this manuscript we construct extrapolated multirate discretization methods that allow to efficiently solve problems that have components with different dynamics. This approach is suited for the time integration of multiscale ordinary and partial differential equations and provides highly accurate discretizations. We analyze the linear stability properties of the multirate explicit and linearly implicit extrapolated methods. Numerical results with multiscale ODEs illustrate the theoretical findings.

1. Introduction. In this study we develop *multirate* time integration schemes using *extrapolation methods* for the efficient simulation of multiscale ODEs and PDEs. In multirate time integration, the timestep can vary across the solution components (e.g., spatial domain) and has to satisfy only the local stability conditions, resulting in substantially more efficient overall computations. For PDEs the method of lines (MOL) framework, where the temporal and spatial discretizations are independent, can be followed to employ the methods discussed in this paper.

The development of multirate integration is challenging due to the consistency and stability constraints that need to be satisfied by the timestepping schemes. Engstler and Lubich [1997] developed multirate schemes based on extrapolated forward Euler methods (MURX). The components with slow dynamics are inactivated at certain time levels, while the fast components are evaluated every timestep. Our work extends this strategy to extrapolated compound multirate explicit and implicit steps. In this case the extrapolation procedure operates on multirate timestepping schemes. Previous work in multirate methods includes [Rice, 1960; Gear and Wells, 1984; Günther and Rentrop, 1993; Skelboe, 1989]. The reader can also examine more recent work presented in [Günther et al., 2001; Kværnø and Rentrop, 1999; Kværnø, 2000; Bartel and Günther, 2002]. Similar concepts for conservative solutions are found in [Constantinescu and Sandu, 2007; Dawson and Kirby, 2001; Kirby, 2002; Tang and Warnecke, 2006] and for parabolic equations using a locally self-adjusting multirate timestepping [Savcenco et al., 2005, 2006].

In this paper we are concerned with solving the following initial value problem

$$\mathbf{y}'(x) = f(x, \mathbf{y}(x))\,,\ x > x_0\,,\ \mathbf{y}(x_0) = y_0\,, y \in \mathbb{R}^N \text{ with} \tag{1.1}$$
$$\mathbf{y} = [y_1\ y_2\ \dots\ y_M]^T\,,\ f(x, \mathbf{y}) = [f_1(x, \mathbf{y})\ f_2(x, \mathbf{y})\ \dots\ f_M(x, \mathbf{y})]^T \text{ and}$$
$$y_r \in \mathbb{R}^{n_r}\,,\ f_r : \mathbb{R}^{N+1} \to \mathbb{R}^{n_r}\,,\ r = 1, \dots, M\,, \text{ and } \sum_{r=1}^{M} n_r = N\,,$$

where $\mathbf{y}$ is the solution vector partitioned into components y_r, $r = 1, \dots, M$, that have their own particular time scales. Among others, these types of problems occur naturally in electric circuit simulations [Bartel and Günther, 2002] and in problems using variable grid sizes [Constantinescu et al., 2008]. We seek to apply time discretization methods with a different timestep length for each dynamic characteristic to (1.1) and consider the extrapolation methods [Deuflhard, 1985; Hairer et al., 1993a,b] with multirate explicit and implicit base schemes for time marching. When solving

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space/time-dependent PDEs in the the method of lines framework, f represents the spatial discretization.

For simplicity, but without loss of generality, we shall consider the simplified problem

$$\begin{cases} y'(t) = f\left(x, y(x), z(x)\right) \\ z'(t) = g\left(x, y(x), z(x)\right) \end{cases} \quad \left[y(x_0)\ z(x_0)\right]^T = \left[y_0\ z_0\right]^T\ ,\ x > x_0\,, \tag{1.2}$$

where y represents the slow evolving component and z the fast one.

2. Extrapolation Methods. Consider a sequence n_i of positive integers with $n_i < n_{i+1}$, $1 \le i \le E$ and define corresponding step sizes $h_1, h_2, h_3, \ldots$ by $h_i = H/n_i$. Further, define the numerical approximation of (1.1) at $x_0 + H$ using the step size h_i by

$$T_{i,1} := y_{h_i}(x_0 + H)\,,\ 1 \le i \le E\,. \tag{2.1}$$

This approximation is obtained using a *base method*. Let us assume that the local error of the p^{th} order method used to solve (2.1) has an asymptotic expansion of the form

$$y(x) - y_h(x) = e_{p+1}(x)\,h^{p+1} + \cdots + e_N(x)\,h^N + Err_h(x)\,h^{N+1}\,, \tag{2.2}$$

where $e_i(x)$ are errors that do not depend on h, and Err_h is bounded for $x_0 \le x \le x_{\text{end}}$. By using E approximations to (2.1) with different h_i's one can eliminate the error terms in the local error asymptotic expansion (2.2) by employing the same procedure as in Richardson extrapolation (see [Hairer et al., 1993a, Chap. II.9]). High order approximations of the numerical solution of (1.1-1.2) can be determined by solving a linear system with E equations. Then the k^{th} solution represents a numerical method of order $p + k - 1$ [Hairer et al., 1993a, Chap. II, Thm. 9.1]. The most economical solution to this set of linear equations is given by the Aitken-Neville formula [Aitken, 1932; Neville, 1934; Gasca and Sauer, 2000]:

$$T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{\left(n_j/n_{j-1}\right) - 1}\,,\ j = 1\ldots k. \tag{2.3a}$$

If the numerical method (2.1) is symmetric, then the Aitken-Neville formula yields

$$T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{\left(n_j/n_{j-1}\right)^2 - 1}\,,\ j = 1\ldots k. \tag{2.3b}$$

Scheme (2.1), (2.3) is called the *extrapolation method*. For illustration purposes, the $T_{j,k}$ solutions can be represented in a tableau (2.1). As it can be seen from the tableau, the method is represented by a sequence of embedded methods which can be used for step size control and variable order approaches. There are several choices for the sequences n_j; however, Deuflhard [1983] showed that the harmonic sequence $n_j = 1, 2, 3, \ldots$ is the most economical one. This sequence will be used for the rest of this study.

3. Linearly Implicit Euler. Consider the implicit Euler method applied to problem (1.1) under smoothness assumptions:

$$\begin{aligned} \mathbf{y}_{i+1} &= \mathbf{y}_i + h f\left(x_{i+1}, \mathbf{y}_{i+1}\right)\,, \\ &\approx \mathbf{y}_i + h\left(J\left(\mathbf{y}_{i+1} - \mathbf{y}_i\right) + f\left(x_{i+1}, \mathbf{y}_i\right)\right) = \mathbf{y}_i + h\left(J\left(\mathbf{y}_{i+1} - \mathbf{y}_i\right) + f\left(x_i, \mathbf{y}_i\right)\right) + O(h^2)\,, \end{aligned}$$

T_{11}				p			
T_{21}	T_{22}			p	$p+1$		
T_{31}	T_{32}	T_{33}		p	$p+1$	$p+2$	
...	...	...	...	...	...	...	...
(a) Extrapolation ($T_{j,k}$) tableau				(b) Orders for the extrapolation terms			

TABLE 2.1

Tableaux with (a) the $T_{j,k}$ solutions and (b) their corresponding orders.

where J is an approximation to $\frac{\partial f}{\partial \mathbf{y}}(x_i, \mathbf{y}_i)$. Then the *linearly implicit Euler* method is given by

$$(I - hJ)(\mathbf{y}_{i+1} - \mathbf{y}_i) = hf(x_i, \mathbf{y}_i) \,. \tag{3.1}$$

This method has been used in [Deuflhard, 1985; Deuflhard et al., 1987] as the "base method," for solving stiff ODEs of type (1.1) with the extrapolation method (2.1), (2.3).

4. Multirate Base Methods. Consider the following multirate base methods for solving (1.2) with the extrapolation algorithm (2.1), (2.3): the m−rate *multirate explicit Euler method*

$$\begin{aligned} y_{n+1} &= y_n + h\, f(y_n, z_n) \\ z_{n+\frac{i}{m}} &= z_{n+\frac{i-1}{m}} + \frac{h}{m}\, g(Y_{n+\frac{i-1}{m}}, z_{n+\frac{i-1}{m}})\,,\; i = 1, \ldots, m\,, \end{aligned} \tag{4.1a}$$

where m is a positive integer and $Y_{n+\frac{i}{m}}$ is an approximation of y at $x_{n+\frac{i}{m}}$. Forward Euler is first order accurate and hence the zeroth order interpolation can be used to approximate Y: $Y_{n+\frac{i}{m}} = y_n$ or $Y_{n+\frac{i}{m}} = y_{n+1}$; by using the former a more parallelizable implementation may be obtained. The first order interpolation can also be considered: $Y_{n+\frac{i-1}{m}} = \frac{m-i+1}{m} y_n + \frac{i-1}{m} y_{n+1}$, $i = 1, \ldots, m$. Formally we have

$$\begin{aligned} Y_{n+\frac{i-1}{m}} &= y_n\,, \\ Y_{n+\frac{i-1}{m}} &= y_{n+1}\,, \\ Y_{n+\frac{i-1}{m}} &= \frac{m-i+1}{m} y_n + \frac{i-1}{m} y_{n+1}\,. \end{aligned}$$

All three possibilities are considered in this study.

Linearly implicit Euler method (3.1) can also be considered as a candidate for the base methods used in the extrapolation procedure. The m−rate *multirate linearly implicit method* is given by

$$\begin{aligned} &\begin{bmatrix} I - hf_y(0) & -hf_z(0) \\ -\frac{h}{m} g_y(0) & I - \frac{h}{m} g_z(0) \end{bmatrix} \cdot \begin{bmatrix} y_{n+1} - y_n \\ z_{n+\frac{1}{m}} - z_n \end{bmatrix} = \begin{bmatrix} h\, f(y_n, z_n) \\ \frac{h}{m}\, g(y_n, z_n) \end{bmatrix}, \\ &\left(I - \frac{h}{m} g_z(0)\right)\left(z_{n+\frac{i}{m}} - z_{n+\frac{i-1}{m}}\right) = \frac{h}{m}\, g\left(Y_{n+\frac{i-1}{m}}, z_{n+\frac{i-1}{m}}\right),\; i = 2, \ldots, m\,, \end{aligned} \tag{4.1b}$$

where the shorthand notation $f_{\{y,z\}}(0)$ and $g_{\{y,z\}}(0)$ denotes the derivatives evaluated at x_0, the initial extrapolation time in (2.1). Methods (4.1) are first order accurate multirate schemes that are considered for the base methods of the extrapolation procedure. We next discuss the accuracy of these extrapolated multirate methods.

2					1			
2	3				1	2		
2	3	4			1	2	3	
...	...	...	...		...	...	...	...

(a) Local orders (b) Global orders

TABLE 5.1
The classical (a) local and (b) global orders for the extrapolation methods with first order base methods.

5. Accuracy of the Extrapolated Multirate Methods. In Henrici's notation [Henrici, 1962], one step methods are expressed as

$$y^{n+1} = y^n + h\,\Phi\left(x^n, y^n, h\right)\,. \tag{5.1}$$

It is easy to see that methods (4.1) can be represented in Henrici's notation. A method of order p applied to a differential equation with each term being sufficiently differentiable possesses an expansion of the *local error* of the form

$$y(x+h) - y(x) - h\,\Phi\left(x, y(x), h\right) = d_{p+1}(x)\,h^{p+1} + \cdots + d_{p+N}(x)\,h^{N+1} + O\left(h^{N+2}\right)\,. \tag{5.2}$$

Following [Gragg and Stetter, 1964; Hairer et al., 1993a] we are looking for a global error function $e_p(x)$ of the form (see [Hairer et al., 1993a, Chp. II, Thm. 3.6])

$$y(x) - y_h(x) = e_p(x)\,h^p + O(h^{p+1})\,. \tag{5.3}$$

Methods (4.1) are of this type with $p = 1$. Then we have the following result due to Gragg and Stetter [1964].

THEOREM 5.1 ([Gragg and Stetter, 1964]). *Suppose that a given method with sufficiently smooth increment function Φ satisfies the consistency condition $\Phi(x, y, 0) = f(x, y)$ and possesses an expansion (5.2) for the local error. Then the global error has an asymptotic expansion of the form*

$$y(x) - y_h(x) = e_p(x)\,h^p + \cdots + e_N(x)\,h^N + E_h(x)\,h^{N+1} \tag{5.4}$$

where $e_j(x)$, $j = p, p+1, \ldots N$, satisfies (5.3) with $e_j(x_0) = 0$ and $E_h(x)$ is bounded for $x_0 \le x \le x_{\text{end}}$ and $0 \le h \le h_0$.

Proof. See Gragg [1965] and [Hairer et al., 1993b, Chp. II, Thm. 8.1]. □

Methods (4.1) possess the local error expansion (5.2) and global error expansion (5.4) and therefore can be extrapolated using (2.1),(2.3a). It follows that the orders of accuracy of the extrapolation methods (4.1) are the ones given in Table 5.1.

Next we illustrate the theoretical accuracy results on a numerical example using the extrapolation scheme with base methods (4.1).

6. Numerical Accuracy Investigation of the Extrapolated Multirate Methods. Consider the following linear initial value problem

$$\begin{pmatrix} \widehat{y}(x) \\ \widehat{z}(x) \end{pmatrix}' = \begin{pmatrix} \Gamma & \varepsilon \\ \varepsilon & -1 \end{pmatrix} \begin{pmatrix} \widehat{y}(x) - g(x) \\ \widehat{z}(x) - g(\omega x) \end{pmatrix} + \begin{pmatrix} g(x) \\ g(\omega x) \end{pmatrix}'\,, \quad \begin{pmatrix} \widehat{y}(x_0) \\ \widehat{z}(x_0) \end{pmatrix} = \begin{pmatrix} g(x_0) \\ g(\omega x_0) \end{pmatrix},$$

where g is a known function. This problem was adapted to vector form [Bartel and Günther, 2002] from the scalar Prothero-Robinson [Hairer et al., 1993b] test problem. The exact solution is $[\widehat{y}(x)\,\widehat{z}(x)]^T = [g(x)\,g(\omega x)]^T$.

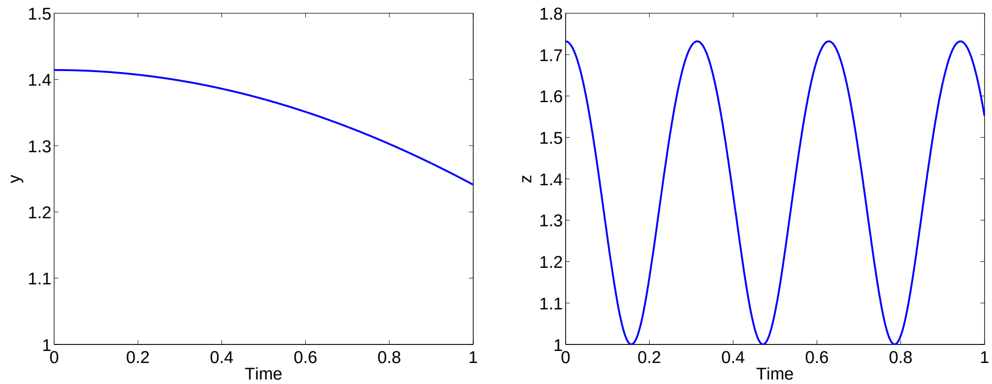

FIG. 6.1. *The exact solution of the modified nonlinear Prothero-Robinson equation (6.1) with* $\varepsilon = 0.5$, $\Gamma = -2.0$, $\omega = 20.0$.

We further consider the following change of variables:

$$\begin{pmatrix} \widehat{y}(x) \\ \widehat{z}(x) \end{pmatrix} = \begin{pmatrix} -1 + y^2(x) \\ -2 + z^2(x) \end{pmatrix}, \begin{pmatrix} \widehat{y}(x) \\ \widehat{z}(x) \end{pmatrix}' = \begin{pmatrix} 2y(x)y'(x) \\ 2z(x)z'(x) \end{pmatrix}, \begin{pmatrix} y(x_0) \\ z(x_0) \end{pmatrix} = \begin{pmatrix} \sqrt{1 + g(x_0)} \\ \sqrt{2 + g(\omega x_0)} \end{pmatrix}.$$

The problem in y and z becomes nonlinear and if $g(x) = \cos(x)$ the following problem is obtained

$$\begin{pmatrix} y(x) \\ z(x) \end{pmatrix}' = \begin{pmatrix} \Gamma & \varepsilon \\ \varepsilon & -1 \end{pmatrix} \begin{pmatrix} \left(-1 + y^2 - \cos(x)\right)/(2y) \\ \left(-2 + z^2 - \cos(\omega x)\right)/(2z) \end{pmatrix} - \begin{pmatrix} \sin(x)/(2y) \\ \omega \sin(\omega x)/(2z) \end{pmatrix}. \tag{6.1a}$$

The exact solution of (6.1a) is given by given by

$$\begin{pmatrix} y(x) \\ z(x) \end{pmatrix} = \begin{pmatrix} \sqrt{1 + \cos(x)} \\ \sqrt{2 + \cos(\omega x)} \end{pmatrix}, \tag{6.1b}$$

and represented in Figure 6.1.

We illustrate the theoretical findings using the example described by (6.1) with $\varepsilon = 0.5, \Gamma = -2.0, \omega = 20.0$ using schemes (4.1) that are implemented in Matlab® using variable precision arithmetic with 64 digits of accuracy. The experiments consist in integrating (6.1a) with successively smaller steps H using the extrapolation procedure (2.1), (2.3a) with the explicit and implicit multirate base methods (4.1) with $m = \omega = 20$.

The observed orders based on the numerical error in L_1 and L_2 norms are presented in Table 6.1 and confirm the theoretical expectations as discussed in Section 5.

7. Linear Stability Analysis of the Extrapolated Multirate Methods. Following the analysis done by Kværnø [2000], we investigate the extrapolated schemes with the base methods defined by (4.1) applied to the following generic linear test problem

$$\begin{pmatrix} \widehat{y}(x) \\ \widehat{z}(x) \end{pmatrix}' = \begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{pmatrix} \begin{pmatrix} \widehat{y}(x) \\ \widehat{z}(x) \end{pmatrix} = \begin{pmatrix} f\left(\widehat{y}(x), \widehat{z}(x)\right) \\ g\left(\widehat{y}(x), \widehat{z}(x)\right) \end{pmatrix},$$

2								
2	3							
2	3	4						
2	3	4	5					
2	3	4	5	6				
2	3	4	5	6	7			
2	3	4	5	6	7	8		
2	3	4	5	6	7	8	9	
...	...	...	...	...	...	...	...	...

TABLE 6.1
The local discretization order of the extrapolation method (2.1), (2.3a) with the multirate (two-rate ($m = \omega = 20$)) base methods.

where $\alpha_{ij} \in \mathbb{R}$. The system can be scaled to

$$\begin{pmatrix} y(x) \\ z(x) \end{pmatrix}' = \underbrace{\begin{pmatrix} -1 & \varepsilon \\ \omega & -m \end{pmatrix}}_{A} \begin{pmatrix} y(x) \\ z(x) \end{pmatrix} = \begin{pmatrix} f\left(y(x), z(x)\right) \\ g\left(y(x), z(x)\right) \end{pmatrix}. \tag{7.1}$$

In this scaling we assume for simplicity that m is an integer and thus we obtain the scale difference (m) between the slow component y and the fast one, z. The coupling between these two components is represented by ε and ω. System (7.1) is stable if the real part of the eigenvalues of A is negative, which gives $\omega\varepsilon \leq m$.

The transfer or stability function $R(\ldots hA_{ij}\ldots)$ for a numerical discretization of (7.1) is defined by the quantity that verifies

$$\begin{pmatrix} y_{n+1} \\ z_{n+1} \end{pmatrix} = R(\ldots hA_{ij}\ldots) \begin{pmatrix} y_n \\ z_n \end{pmatrix}.$$

In order for the discretization method to be stable, one needs to have the spectral radius $\rho(R(\ldots hA_{ij}\ldots)) \leq 1$. The stability functions of (4.1) can be easily calculated. The stability function of the extrapolated method is calculated from the extrapolation formula (2.3a) as [Hairer et al., 1993b, Chap. IV]:

$$R_{j,k+1}(\ldots hA_{ij}\ldots) = R_{j,k}(\ldots hA_{ij}\ldots) + \frac{R_{j,k}(\ldots hA_{ij}\ldots) - R_{j-1,k}(\ldots hA_{ij}\ldots)}{(n_j/n_{j-k}) - 1}.$$

We take a practical approach and ask the following question: How does the stability region of a multirate method with ratio m applied to (7.1) compare to the stability region of the single-rate method with the timestep length of the fastest component (i.e. H/m)? In other words we look for the degradation or appreciation in stability of the multirate method compared to the single-rate method. We note that the multirate method is more efficient in this case by taking fewer steps on the slow components.

8. Numerical Linear Stability Investigation of the Extrapolated Multirate Methods. In this section we investigate the linear stability properties of the extrapolation method (2.1), (2.3a) with the multirate base methods (4.1) applied to problem (7.1).

We consider the ratio $m = 2$ fixed and investigate the stability region ($\rho(R) \leq 1$) in the $h\omega$-$h\varepsilon$ plane.

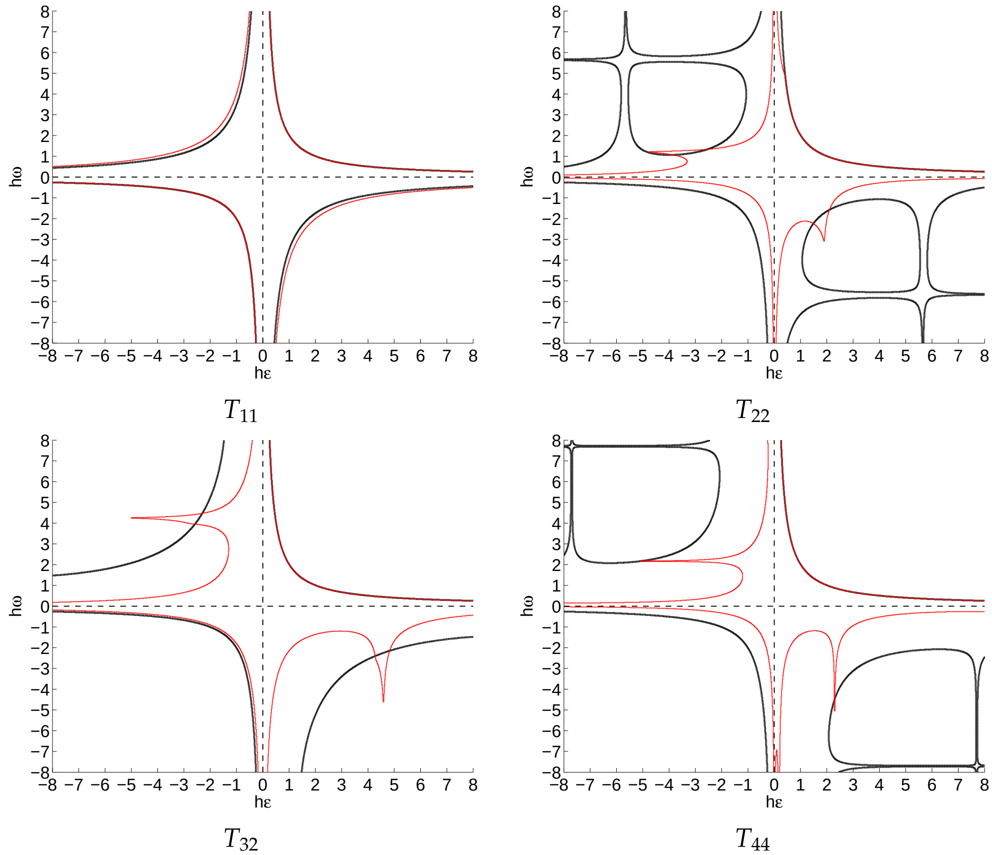

Fig. 8.1. *The stability region for problem (7.1) with the explicit multirate ($m = 2$) method (4.1a) (thin red line) and the corresponding single-rate explicit method ($m = 1$) (thick dark line) for various entries in the extrapolation tableau.*

In Figure 8.1 we show the stability regions for the extrapolated multirate explicit method (4.1a) for the extrapolation terms in positions T_{11}, T_{22}, T_{32}, and T_{44} (see Table 2.1). The stability region of the multirate method is slightly degraded; however, for practical purposes, we consider that the reduction in the stability region is acceptable.

In Figure 8.2 we show the stability regions for the extrapolated multirate implicit method (4.1b) for the extrapolation terms in positions T_{11}, T_{22}, T_{44}, and T_{55}. Experimentally, we determine that on the first column of the extrapolation tableau the multirate implicit methods preserve the "unconditional" stability of the implicit base (single-rate) method; i.e., the stability region extends to (∞, ∞) and $(-\infty, -\infty)$ in the $h\omega$-$h\varepsilon$ plane. However, when the multirate solution is extrapolated, the stability region shrinks in quadrants II and IV (of Fig. 8.2). This aspect needs to be investigated further.

9. Concluding Remarks. Multirate methods are very useful for solving multiscale problems. In this manuscript we construct extrapolated multirate implicit and explicit discretization methods that allow to efficiently solve problems that have multiple scales. We propose two extrapolation methods that are based on multirate forward and linearly implicit Euler schemes. The cost of implementing these

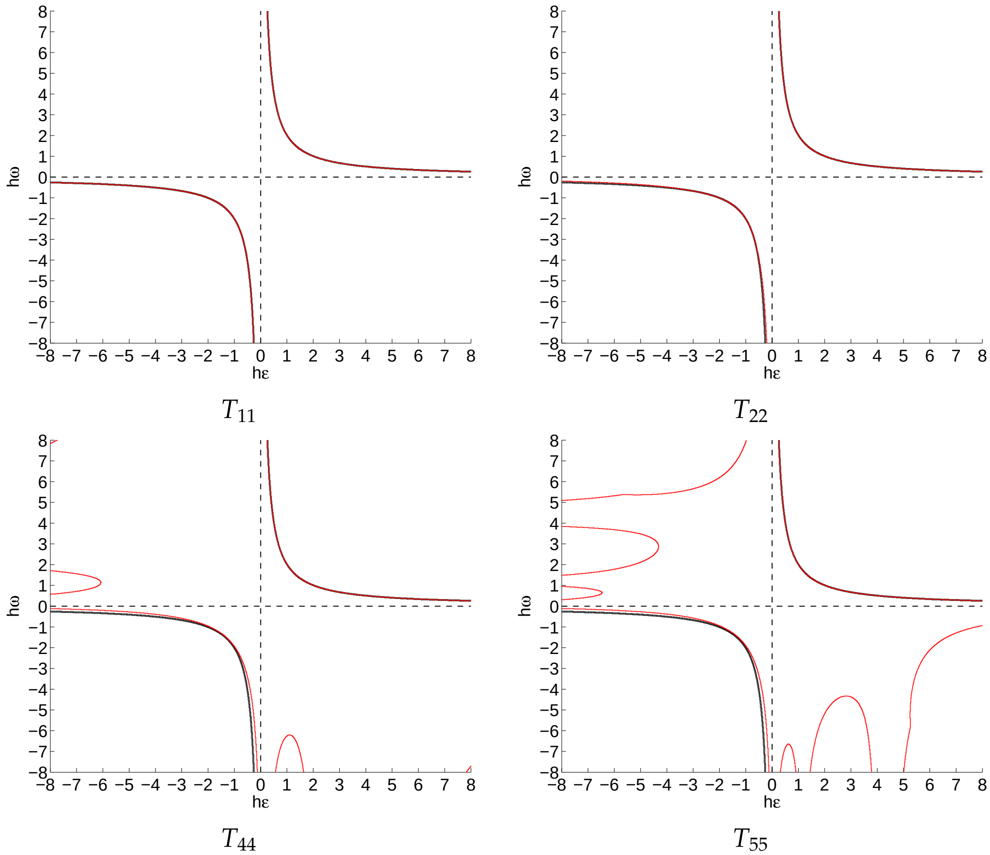

FIG. 8.2. *The stability region for problem (7.1) with the implicit multirate ($m = 2$) method (4.1b) (thin red line) and the corresponding single-rate explicit method ($m = 1$) (thick dark line) for various entries in the extrapolation tableau.*

methods is very small and can easily reach very high orders of accuracy.

The extrapolation method approach presented in this study represents a sequence of embedded methods which can be used for step size control and variable order approaches due to their trivial extension to higher orders. Extrapolation methods are less efficient than the popular Runge-Kutta or linear multistep schemes. However, the extrapolation methods can be parallelized very easily [Rauber and Rünger, 1997]. Each entry on the first extrapolation tableau column ($T_{i,1}$) can be computed independently. Moreover, the cost is linearly increasing and thus each entry can be optimally scheduled on multiprocessor/multicore machines or architectures. This could lead to more efficient overall implementations.

The extrapolated multirate forward Euler method shows only a slight degradation of the linear stability region; however, in practice we consider that the increased efficiency of the multirate method outweighs this minor drawback.

By the numerical investigation of the linear stability region we determine that extrapolated multirate linearly implicit method performs very well for nonstiff problems or for stiff problems with relaxed coupling among components. The linear stability region does not resemble the unconditional stability of the single-rate counterpart, however, the stability is probably large enough for practical applications.

This aspect needs to be further investigated.

The methods under investigation can be used in the high and very high order discretization of ODEs and PDEs using the method of lines approach. Numerical results with ODEs verify the theoretical findings.

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