Richardson Extrapolation combined with the sequential splitting procedure and the $\theta$-method

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**Abstract:** Initial value problems for systems of ordinary differential equations (ODEs) are solved numerically by using a combination of (a) the $\theta$-method, (b) the sequential splitting procedure and (c) Richardson Extrapolation. Stability results for the combined numerical method are proved. It is shown, by using numerical experiments, that if the combined numerical method is stable, then it behaves as a second-order method.

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1. **Introduction**

Richardson Extrapolation is a powerful tool to increase the accuracy of any numerical method. It consists of applying the given numerical scheme with different discretization parameters (usually $h$ and $h/2$) and combining the obtained numerical solutions with properly chosen weights. Namely, if $p$ denotes the order of the selected numerical method, $w_n$ the numerical solution obtained by $h/2$ and $z_n$ that obtained by $h$, then the combined solution

$$y_n = \frac{2^p w_n - z_n}{2^p - 1},$$

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has order $p + 1$. It was first extensively used by L.F. Richardson, who called it “the deferred approach to the limit” [14]. Richardson Extrapolation is especially widely used for time integration schemes, where, as a rule, the results obtained by two different time-step sizes are combined.

Richardson Extrapolation can be implemented in two different ways when one attempts to increase the accuracy of a time integration method. The approximation improved by Richardson Extrapolation for a given time layer is not used in further computations when the passive Richardson Extrapolation is used, and it is used in the computation of the next approximation when the active Richardson Extrapolation is utilized. It is clear that if the passive device is applied and the underlying method is stable (convergent), then the combined method is also stable (convergent). However, if the active device is used, then the stability of the underlying method does not imply the stability of the combined method. Therefore, from the viewpoint of stability, the active Richardson Extrapolation requires further investigation when a given numerical method is applied. Thus in the sequel we will focus on the active version, and so Richardson Extrapolation should always be understood as active Richardson Extrapolation. In [8], the stability of the Richardson Extrapolation combined with the Backward Euler Method and the Trapezoidal Rule was studied and applied efficiently in an atmospheric chemistry model. In [20], the stability of the Richardson Extrapolation combined with the general $\theta$-method was studied in detail. In these papers Richardson Extrapolation was applied to ordinary differential equations or semi-discretized partial differential equations.

In practice, especially when large systems of PDEs are to be solved numerically (e.g., in large-scale air pollution models), it is often indispensable to apply some operator splitting method [4, 7, 9, 10, 18]. During operator splitting, the original problem is split into simpler sub-problems, which are solved successively at each time-step. Clearly, if an operator splitting method is applied to a system of PDEs and the resulting sub-systems are discretized by some numerical method, we are led to a new numerical scheme. It is natural to enhance the accuracy of the new scheme (consisting of a splitting method and a numerical method) with Richardson Extrapolation. In this paper we investigate the stability of the combined numerical method consisting of (i) sequential splitting, (ii) the general $\theta$-method and (iii) Richardson Extrapolation.

The structure of the paper is as follows. In Section 2, the combined numerical method (sequential splitting + $\theta$-method + Richardson Extrapolation) is formulated. In Section 3, the stability properties of the combined method are investigated, and, as a major result, the condition of strong A-stability of the combined method is given. In Section 4, we study the accuracy and stability of the method on a numerical example of an atmospheric chemistry model for different values of the parameter $\theta$.

## 2. Formulation of the combined numerical method

Consider the classical initial value problem for systems of ordinary differential equations (ODEs):

$$\frac{dy}{dt} = f_1(t, y) + f_2(t, y), \quad t \in [a, b], \quad b > a, \quad y \in \mathbb{R}^2, \quad f_1, f_2 \in \mathbb{R}^2, \quad s \geq 1, \quad (1)$$

with a given initial value vector $y(a) = y_0$. The two functions, $f_1(t, y)$ and $f_2(t, y)$ are also given.

Assume that $N \geq 1$ is a given positive integer and that $h = (b - a)/N$ is a given positive real constant. Consider the equidistant grid defined by $T_N = \{t_n\}_{n=0}^N$, where

$$t_0 = a, \quad t_n = t_{n-1} + h = t_0 + nh, \quad n = 1, 2, \ldots, N, \quad t_N = b.$$ 

It will also be assumed that $y_n, z_n^{(1)}, z_n^{(2)}, w_n^{(1)}$ and $w_n^{(2)}$ are some approximations of the exact solution $y(t)$ of (1) at the grid-point $t = t_n \in T_N$. Furthermore, when Richardson Extrapolation is studied together with the $\theta$-method (see more details about this method in, for example, [13]; the formula on which the $\theta$-method is based can be seen in Steps 1 and 2 below), it is appropriate to consider additionally two approximations $w^{(1)}_{n-0.5}$ and $w^{(2)}_{n-0.5}$ of $y(t)$ at the intermediate grid-point $t = t_{n-0.5} = t_n - 0.5h$. Assume that the approximation $y_{n-1}$ of $y(t_{n-1})$ has been calculated. Under these assumptions, the calculations at time $t_n$ that are related to the Richardson Extrapolation when it is combined with the sequential splitting procedure, see [19], and the $\theta$-method can be carried out in three consecutive steps.
Step 1

Use a large time-stepsize \( h \) to calculate an approximation \( z_n \) of \( y(t_n) \) by using the \( \theta \)-method and starting with the approximation \( y_{n-1} \) obtained at the previous time-step:

\[
\begin{align*}
  z_n^{(1)} &= y_{n-1} + h \left[ (1 - \theta) f_1(t_{n-1}, y_{n-1}) + \theta f_1(t_n, z_n^{(1)}) \right], \\
  z_n^{(2)} &= z_n^{(1)} + h \left[ (1 - \theta) f_2(t_{n-1}, z_n^{(1)}) + \theta f_2(t_n, z_n^{(2)}) \right], \\
  z_n &= z_n^{(2)}.
\end{align*}
\]

Step 2

Perform two small time-steps by using the \( \theta \)-method with a time-stepsize \( 0.5h \) to calculate a second approximation \( w_n \) to \( y(t_n) \), starting again with the approximation \( y_{n-1} \) obtained at the previous time-step:

\[
\begin{align*}
  w_n^{(1)} &= y_{n-0.5} + 0.5h \left[ (1 - \theta) f_1(t_{n-0.5}, y_{n-0.5}) + \theta f_1(t_n, w_n^{(1)}) \right], \\
  w_n^{(2)} &= w_n^{(1)} + 0.5h \left[ (1 - \theta) f_2(t_{n-0.5}, w_n^{(1)}) + \theta f_2(t_n, w_n^{(2)}) \right], \\
  w_n &= w_n^{(2)}.
\end{align*}
\]

Step 3

Assume that \( 0.5 \leq \theta \leq 1.0 \), and apply the formula for computing the Richardson Extrapolation with \( p = 1 \) to obtain an improved approximation \( y_n \) of \( y(t_n) \):

\[
y_n = 2w_n - z_n.
\]

Note that if \( 0.5 \leq \theta \leq 1.0 \), then the combination consisting of the \( \theta \)-method and the sequential splitting procedure is a first-order numerical method. The order of the Trapezoidal Rule, the \( \theta \)-method with \( \theta = 0.5 \), is two, but the combination of the Trapezoidal Rule and the sequential splitting is again a first-order numerical method. This justifies the application of Richardson Extrapolation with \( p = 1 \). The combination consisting of Richardson Extrapolation, the sequential splitting procedure and the \( \theta \)-method will be a second-order numerical method when \( p = 1 \) and, therefore, it should be expected that the accuracy will be improved when the stability is preserved and the time-stepsize is sufficiently small.

3. Linear stability properties of the combined method

Let us consider now the problem

\[
y' = (A_1 + A_2)y,
\]

where \( A_1 \) and \( A_2 \) are constant matrices, which are (a) diagonalizable, (b) with distinct eigenvalues and (c) the real parts of the eigenvalues are non-positive.

Use sequential splitting to obtain two systems:

\[
\begin{align*}
  \bar{y}' &= A_1 \bar{y}, \\
  \bar{y}' &= A_2 \bar{y}.
\end{align*}
\]

Assume that the approximate solution \( y_n \) of (3) at the grid-point \( t_n \) has already been calculated. Then the calculations at time-step \( n \) are carried out in the following way. Set \( \bar{y}_{n-1} = y_{n-1} \). Use any A-stable method to calculate an approximate value \( \bar{y}_n \) of (4) at the grid-point \( t_n \). Set \( \bar{y}_{n-1} = \bar{y}_n \) and calculate an approximate value \( \tilde{y}_n \) of (5) at the grid-point \( t_n \) by using the same numerical method. Set \( y_n = \tilde{y}_n \) and proceed with the calculations at the next time-step.
Assume now that an A-stable method is used in the solution of both (4) and (5). This means that the stability function $R(\mu)$ of this method (see, for example, [11–13]) satisfies the condition $R(\mu) \leq 1$ for all values of $\mu$ in $\mathbb{C}$ and it is applied twice at step $n$ (once to calculate $\tilde{y}_n$ and the second time to obtain $\hat{y}_n$). Thus, the use of the sequential procedure is in fact a numerical method with stability function $R(\mu) = R^2(\mu)$, and since $R(\mu) \leq 1$ it is clear that $\hat{R}(\mu) \leq 1$ too, which means that the A-stability of the applied method is preserved when a sequential procedure is used.

Assume now that Richardson Extrapolation is used to improve the accuracy of the approximations obtained by the sequential splitting procedure. This means that if we know $y_{n-1}$, then it is necessary to (a) calculate two approximations, $z_n$ and $w_n$, by using the sequential splitting procedure to perform one large step with a stepsize $h$ and two small steps with a stepsize $0.5h$, and (b) calculate

$$y_n = \frac{2^p w_n - z_n}{2^p - 1},$$

as stated in the introduction, where $p$ is the order of the selected numerical method. Assume now that the method is A-stable with stability function $R(\mu)$. Here $\mu = \lambda h$ and $\lambda$ is the constant in the usual Dahlquist’s test problem, which was introduced in [5] and was used in numerous papers and textbooks after that. Then the combination consisting of the numerical method, the sequential splitting procedure and Richardson Extrapolation is a numerical method with stability function

$$\hat{R}(\mu) = \frac{2^p R^4(0.5\mu) - R^2(\mu)}{2^p - 1},$$

and it is not clear whether $|\hat{R}(\mu)| \leq 1$ is satisfied or not. In the sequel our aim is to prove that this relation is true for the $\theta$-method, i.e., where $R(\mu) = [1 + (1 - \theta)\mu]/(1 - \theta\mu)$.

The three steps defined in the previous section for this stability function $R$ can be rewritten in the following way:

**Step 1A**

Use a large time-stepsize $h$ to calculate an approximation $z_n$ of $y(t_n)$, starting with the approximation $y_{n-1}$ obtained at the previous time-step:

$$z_n^{(1)} = y_{n-1} + h(1 - \theta)\lambda y_{n-1} + h\theta\lambda z_n^{(1)} \implies z_n^{(1)} = \frac{1 + h(1 - \theta)\lambda}{1 - h\theta\lambda} y_{n-1},$$

$$z_n^{(2)} = z_n^{(1)} + h(1 - \theta)\lambda z_n^{(1)} + h\theta\lambda z_n^{(2)} \implies z_n^{(2)} = \frac{1 + h(1 - \theta)\lambda}{1 - h\theta\lambda} z_n^{(1)},$$

$$z_n = z_n^{(2)} = \left[ \frac{1 + h(1 - \theta)\lambda}{1 - h\theta\lambda} \right]^2 y_{n-1}.$$

**Step 2A**

Perform two small time-steps with a time-stepsize $0.5h$ to calculate a second approximation $w_n$ to $y(t_n)$, starting again with the approximation $y_{n-1}$ obtained at the previous time-step:

$$w_n^{(1)} = y_{n-0.5} + 0.5h(1 - \theta)\lambda y_{n-0.5} + 0.5h\theta\lambda w_n^{(1)} \implies w_n^{(1)} = \frac{1 + 0.5h(1 - \theta)\lambda}{1 - 0.5h\theta\lambda} y_{n-0.5},$$

$$w_n^{(2)} = w_n^{(1)} + 0.5h(1 - \theta)\lambda w_n^{(1)} + 0.5h\theta\lambda w_n^{(2)} \implies w_n^{(2)} = \frac{1 + 0.5h(1 - \theta)\lambda}{1 - 0.5h\theta\lambda} w_n^{(1)},$$

$$w_n^{(2)} = w_n^{(2)} = \left[ \frac{1 + 0.5h(1 - \theta)\lambda}{1 - 0.5h\theta\lambda} \right]^2 y_{n-0.5},$$

$$w_n^{(3)} = w_n^{(2)} + 0.5h(1 - \theta)\lambda w_n^{(2)} + 0.5h\theta\lambda w_n^{(3)} \implies w_n^{(3)} = \frac{1 + 0.5h(1 - \theta)\lambda}{1 - 0.5h\theta\lambda} w_n^{(2)}.$$
\[ w_n^{(2)} = w_n^{(1)} + 0.5 h (1 - \theta) \lambda w_n^{(1)} + 0.5 h \theta \lambda w_n^{(2)} \Rightarrow w_n^{(2)} = \frac{1 + 0.5 h (1 - \theta) \lambda}{1 - 0.5 h \theta \lambda} w_n^{(1)} \]

\[ \Rightarrow w_n^{(2)} = \left[ \frac{1 + 0.5 h (1 - \theta) \lambda}{1 - 0.5 h \theta \lambda} \right]^4 y_{n-1}. \]

\[ w_n = w_n^{(2)} = \left[ \frac{1 + 0.5 h (1 - \theta) \lambda}{1 - 0.5 h \theta \lambda} \right]^4 y_{n-1}. \]

**Step 3A**

Apply, as in (2), the formula for computing the Richardson Extrapolation with \( p = 1 \) to compute an improved approximation \( y_n \) of \( y(t_n) \):

\[ y_n = 2w_n - z_n \Rightarrow y_n = R(\lambda, h)y_{n-1}, \]

where

\[ R(\lambda, h) = 2 \left[ \frac{1 + 0.5 h (1 - \theta) \lambda}{1 - 0.5 h \theta \lambda} \right]^4 - \left[ \frac{1 + h (1 - \theta) \lambda}{1 - h \theta \lambda} \right]^2. \]

Assume that \( \mu = h \lambda \), \( \lambda \) being a complex constant. Under this assumption we have

\[ y_n = R(\mu)y_{n-1}, \]

with

\[ R(\mu) = 2 \left[ \frac{1 + 0.5 (1 - \theta) \mu}{1 - 0.5 \theta \mu} \right]^4 - \left[ \frac{1 + (1 - \theta) \mu}{1 - \theta \mu} \right]^2. \] (6)

The last two formulae show clearly that the application of the Richardson Extrapolation, combined with the sequential splitting procedure and the \( \theta \)-method, results in a one-step numerical method for solving ODEs with stability function \( R(\mu) \) when the test-problem (3) is solved under the assumptions made above.

We are mainly interested in solving stiff systems of ODEs. Therefore, it is important to preserve the stability of the computational process. Several definitions related to the stability of numerical methods with stability function \( R(\mu) \) are proposed in the literature (see, for example, [2, 3, 11–13, 17]). The following three definitions will be used in this paper.

**Definition 3.1.**
Consider the set \( S \) containing all values of \( \mu = \alpha + i\beta \), for which \(|R(\mu)| \leq 1\). If \( S \supset \mathcal{C}^- = \{ \nu : \nu = \gamma + i\delta, \gamma \leq 0 \} \), then the method with stability function \( R(\mu) \) is called \( A \)-stable (see, for example, [11]).

**Definition 3.2.**
A numerical method with stability function \( R(\mu) \) is said to be strongly \( A \)-stable if it is \( A \)-stable and if the relationship

\[ \lim_{\mu \to \infty} |R(\mu)| \leq \xi, \] (7)

holds for some positive real constant \( \xi \) with \( 0 \leq \xi \leq 1 \), see [12].

**Definition 3.3.**
A numerical method with stability function \( R(\mu) \) is called \( L \)-stable if it is \( A \)-stable and the relationship

\[ \lim_{\mu \to \infty} R(\mu) = 0, \]

holds (this definition was originally proposed by [6], see also [11] or [12]).
It is clearly seen that the class of L-stable methods is a sub-class of the class of strongly A-stable methods. In turn, strongly A-stable methods form a class which is a sub-class of the class of A-stable methods.

The use of numerical methods which are at least A-stable is desirable when the system of ODEs is stiff. It is well-known (see, for example, [12]) that the $\theta$-method is

- only A-stable for $\theta = 0.5$,
- strongly A-stable for $\theta \in (0.5, 1.0]$, and
- L-stable for $\theta = 1.0$.

It is important to answer the question: Will the combination of Richardson Extrapolation, the sequential splitting procedure and a given numerical method for solving systems of ODEs be stable if the selected numerical method is in some sense stable?

The stability properties of the combination of Richardson Extrapolation applied together with the sequential splitting procedure and the $\theta$-method when $\theta \in [0.5, 1.0]$ will be studied in the remaining part of this paper. More precisely, the following theorem will be proved:

**Theorem 3.4.**
The numerical method consisting of a combination of Richardson Extrapolation applied together with the sequential splitting procedure and the $\theta$-method is strongly A-stable if $\theta \in [0.5, 1.0]$ with $\theta_0 \approx 0.638$.

**Proof.** A numerical method for solving systems of ODEs is A-stable if and only if

(a) it is stable on the imaginary axis (i.e., $|R(i\beta)| \leq 1$ for all real values of $\beta$), and
(b) $R(\mu)$ is analytic in $\mathbb{C}^-$.

For more details see [11].

The inequality (7) must additionally be satisfied if we require strong A-stability. Therefore, the theorem should be proved in three steps. In the first step, Step A, it will be proved that the combination of Richardson Extrapolation, the sequential splitting procedure and the $\theta$-method is stable on the imaginary axis if $\theta \in [0.5, 1.0]$ with $\theta_0 \approx 0.638$. In the second step, Step B, it will be shown that $R(\mu)$ is analytic in $\mathbb{C}^-$. Finally, it will be proved in the third step, Step C, that (7) holds.

**Step A: Stability on the imaginary axis**
The stability function $R(\mu)$ from (6) can be rewritten as a ratio of two polynomials:

$$R(\mu) = \frac{P(\mu)}{Q(\mu)},$$

where the numerator can be written as

$$P(\mu) = 2[1 + (1 - \theta)(0.5\mu)]^4(1 - \theta\mu)^2 - [1 + (1 - \theta)\mu]^2[1 - \theta(0.5\mu)]^4.$$  

The equality (9) is obviously a sixth-order polynomial with respect to $\mu$ depending on parameter $\theta$, which can be written in the form

$$P(\mu) = A\mu^6 + B\mu^5 + C\mu^4 + D\mu^3 + E\mu^2 + F\mu + 1,$$
where
\[
A = \frac{\theta^2(1 - \theta)^2(\theta^2 - 4\theta + 2)}{2^4}, \quad B = \frac{\theta(1 - \theta)[2(1 - \theta)^3 + 8\theta\theta(-\theta^2) + 4\theta^2(1 - \theta) - \theta^3]}{2^3},
\]
\[
C = \frac{2(1 - \theta)^4 - 32\theta(1 - \theta)^3 + 24\theta^2(1 - \theta)^2 + 16\theta^3(1 - \theta) - \theta^4}{2^4},
\]
\[
D = \frac{2(1 - \theta)^3 - 8\theta(1 - \theta)^2 + 2\theta^2(1 - \theta) + \theta^3}{2}, \quad E = \frac{13\theta^2 - 16\theta + 4}{2}, \quad F = 2 - 4\theta.
\]

The denominator of (8) can be written as
\[
Q(\mu) = [1 - \theta(0.5\mu)]^2(1 - \theta\mu)^2.
\]

Assume that the complex variable \(\mu\) is represented as \(\mu = \alpha + i\beta\). It is shown in [11] that the combined numerical method with stability function \(R(\mu)\) is stable on the imaginary axis if \(E(\beta) \geq 0\) for all real values of \(\beta\), where \(E(\beta)\) is defined by
\[
E(\beta) = Q(i\beta)Q(-i\beta) - P(i\beta)P(-i\beta).
\] (11)

Successful transformations of the two terms in (11) lead to the expressions
\[
Q(i\beta)Q(-i\beta) = \frac{\theta^{12}2^8\theta^{12} + 9\theta^{10}2^7\theta^{10} + 129\theta^82^6\theta^8 + 29\theta^62^5\theta^6 + 27\theta^42^3\theta^4}{2^5} + 3\theta^2\beta^2 + 1,
\] (12)
\[
P(i\beta)P(-i\beta) = A^2\theta^{12} + (B^2 - 2AC)\theta^{10} + (C^2 - 2BD + 2AE)\theta^8 + (D^2 - 2CE + 2BF - 2A)\theta^6 + (E^2 - 2DF + 2C)\theta^4 + (F^2 - 2E)\beta^2 + 1.
\] (13)

Substitute the expressions in the right-hand-sides of (12) and (13) into (11):
\[
E(\beta) = \frac{\theta^{12}2^8A^2\theta^{12} + 9\theta^{10}2^7B^2 - 2AC\theta^{10} + 129\theta^82^6C^2 - 2BD + 2AE\theta^8}{2^5} + \frac{29\theta^6 - 2(D^2 - 2CE + 2BF - 2A)\theta^6 + 27\theta^4 - 2(E^2 - 2DF + 2C)\theta^4}{2^3} + 3\theta^2\beta^2 + 1.
\]

Introduce the following notations:
\[
H_1(\theta) = \frac{\theta^{12}2^8A^2}{2^5}, \quad H_2(\theta) = \frac{9\theta^{10}2^7B^2 - 2AC}{2^5}, \quad H_3(\theta) = \frac{129\theta^82^6C^2 - 2BD + 2AE}{2^5}, \quad H_4(\theta) = \frac{29\theta^6 - 2(D^2 - 2CE + 2BF - 2A)}{2^5}, \quad H_5(\theta) = \frac{27\theta^4 - 2(E^2 - 2DF + 2C)}{2^3}.
\] (14)

It is clear that \(E(\beta)\) will be non-negative for all values of \(\beta\) and for a given \(\theta\) if all five polynomials (14) are non-negative for the selected value of \(\theta\). The curves representing the five polynomials are drawn in Fig. 1–5. The results show that the combination of Richardson Extrapolation, the sequential splitting procedure and the \(\theta\)-method is stable on the imaginary axis if \(\theta \in [\theta_0, 1.0]\) with \(\theta_0 \approx 0.638\). Thus, the first part of the theorem is proved.

**Step B: A-stability**

After the proof that the combination of Richardson Extrapolation with the \(\theta\)-method is stable on the imaginary axis if \(\theta \in [\theta_0, 1.0]\) with \(\theta_0 \approx 0.638\), it should also be proved that the function \(R(\mu)\) is analytic in \(\mathbb{C}^-\). The function \(R(\mu)\) is a ratio of two polynomials, \(P(\mu)\) and \(Q(\mu)\); see (8). It is well-known that polynomials are analytic functions and a ratio of two polynomials is analytic function in \(\mathbb{C}^-\) if the denominator \(Q(\mu)\) has no roots in \(\mathbb{C}^-\). The roots of the denominator \(Q(\mu)\) of the stability function \(R(\mu)\) are \(\mu_1 = \mu_2 = 1/\theta > 0\) and \(\mu_3 = \mu_4 = \mu_5 = \mu_6 = 2/\theta > 0\), which means that \(R(\mu)\) is analytic in \(\mathbb{C}^-\).
Richardson Extrapolation combined with the sequential splitting procedure and the $\theta$-method

Figure 1. Variation of the first polynomial in the interval $[0.5, 1.0]$. 

Figure 2. Variation of the second polynomial in the interval $[0.5, 1.0]$. 

Figure 3. Variation of the third polynomial in the interval $[0.5, 1.0]$. 

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Step C: Strong A-stability

It remains to establish for which values of \( \theta \) in the interval \([0, 1.0]\) the relationship (7) holds. Rewrite (6) as

\[
R(\mu) = 2 \left[ \frac{1}{\mu + 0.5(1 - \theta)} \right]^4 - \left[ \frac{1}{\mu + 0.5 \theta} \right]^2.
\]

It is obvious now that

\[
\lim_{\mu \to \infty} R(\mu) = 2 \left[ \frac{0.5(1 - \theta)}{0.5 \theta} \right]^4 - \left[ \frac{1 - \theta}{-\theta} \right]^2 = \frac{2(1 - \theta)^4}{\theta^4} - (1 - \theta)^2 = \frac{2 - 8\theta + 11\theta^2 - 6\theta^3 + \theta^4}{\theta^4}.
\]

Since the terms in the right-hand-side of (15) are real, the requirement of (7) reduces to \(|2 - 8\theta + 11\theta^2 - 6\theta^3 + \theta^4| \leq \theta^4\). This implies that the following relationships are satisfied:

\[
\frac{2 - 8\theta + 11\theta^2 - 6\theta^3 + \theta^4}{\theta^4} < 1 \quad \Rightarrow \quad -2 + 8\theta - 11\theta^2 + 6\theta^3 > 0, \tag{16}
\]

\[
-1 < \frac{2 - 8\theta + 11\theta^2 - 6\theta^3 + \theta^4}{\theta^4} \quad \Rightarrow \quad 2 - 8\theta + 11\theta^2 - 6\theta^3 + 2\theta^4 > 0. \tag{17}
\]
Richardson Extrapolation combined with the sequential splitting procedure and the $\theta$-method

It can easily be established that both (16) and (17) are satisfied for all values of $\theta$ in the interval $(0.5, 1.0)$, but since the method should be A-stable, we have to take the interval $(\theta_0, 1.0)$ with $\theta_0 \approx 0.638$. This completes the proof of the theorem.

**Corollary 3.5.**
If $\theta = 1.0$ (i.e., if the Backward Euler Formula is used), then the combined method is L-stable.

**Proof.** It is immediately seen that the right-hand-side of (17) is zero when $\theta = 1.0$ and, thus, the method is L-stable.

4. **Numerical experiments**

Assume that the $\theta$-method is used with three values of the parameter $\theta$: (i) $\theta = 1$ (corresponding to the Backward Euler Formula), (ii) $\theta = 0.75$ and (iii) $\theta = 0.5$ (corresponding to the Trapezoidal Rule). It will also be assumed that the sequential splitting procedure is used, either directly or in combination with Richardson Extrapolation. It will be shown that while the sequential splitting procedure behaves as a first-order numerical method, second-order accuracy can be achieved when combined with Richardson Extrapolation. A representative atmospheric chemistry scheme will be used in the experiments which will be discussed in the following sub-section.

4.1. **The atmospheric chemistry scheme**

An atmospheric chemistry scheme, in which $s = 56$ species are involved, was applied in the experimental results, which will be presented below. This scheme contains all important air pollutants (ozone, sulphur pollutants, nitrogen pollutants, ammonium-ammonia and many hydro-carbons). It is used in several well-known environmental models such as, for example, in EMEP models [15] and in UNI-DEM [18, 19]. It should be mentioned here that EMEP stands for European Monitoring and Evaluation Programme, while UNI-DEM is an abbreviation for the Unified Danish Eulerian Model. The atmospheric chemistry scheme is described mathematically as a non-linear system of ODEs of type (1). The numerical treatment of this system of ODEs is extremely difficult because (a) it is non-linear, (b) it is very badly scaled and (c) some chemical species vary very quickly during the periods of changes from daylight to night-time and from night-time to daylight. This fact is discussed and illustrated by using several plots in [8]. This atmospheric chemical scheme is also used in [20].

In this work, the atmospheric chemical scheme is split into two parts. The first part contains mainly the chemical reactions in which ozone participates. The second part contains all the other chemical reactions.

4.2. **Organization of the computations**

The atmospheric chemistry scheme, which was briefly discussed in the previous sub-section, was treated numerically on the time-interval $[a, b] = [43200, 129600]$. The value $a = 43200$ corresponds to twelve o’clock noon (measured in seconds and starting from the midnight), while $b = 129600$ corresponds to twelve o’clock noon on the next day. Thus, the length of the time-interval is 24 hours and it contains important changes from daylight to night-time and from night-time to daylight (when most of the chemical species vary very quickly).

In each experiment the first run is performed by using $N = 168$ time-steps (this means that the time-steps size is $h \approx 514.285$ seconds). After that the stepsize $h$ was halved ten times (which implies that the number of time-steps, $N$ is doubled after every successive run). The behaviour of the errors made in this sequence of 11 runs was studied. The error made in each run is measured in the following way. Denote:

$$ERR_{\theta} = \max_{k=1, \ldots, 56} \frac{|y_{n,k} - y_{\text{ref},k}|}{\max(|y_{n,k}^{\text{ref}}, 1.0)|}.$$  \hspace{1cm} (18)
where $y_{m,k}$ and $y_{m,k}^{ref}$ are the calculated value and the reference solution of the $k$th chemical species at time $t_m = t_0 + mh_0$ (where $m = 1, \ldots, 168$ and $h_0 \approx 514.285$ is the time-stepsizes that was used in the first run). The reference solution was calculated by using a three-stage fifth-order L-stable fully implicit Runge–Kutta algorithm (see [3] or [11]) with $N = 998244352$ and $h_{ref} \approx 6.130763E-05$. It is clear from the above discussion that only the values of the reference solution at the grid-points of the coarse grid (which is used in the first run) have been stored and applied in the evaluation of the error (it is, of course, also possible to store all values of the reference solution, but such an action will increase tremendously the storage requirements).

The global error made during the computations is estimated by using the following formula:

$$ ERR = \max_{n=1, \ldots, 168} ERR_n. $$ (19)

It is desirable to eliminate the influence of the rounding errors when the quantities involved in (18) and (19) are calculated. Normally, this task can successfully be accomplished when double precision arithmetic is used during the computations. Unfortunately, this is not true when the atmospheric chemistry scheme is handled. The difficulty can be explained as follows. If the problem is stiff, and the atmospheric chemistry scheme is, as mentioned above, a stiff non-linear system of ODEs, then implicit numerical methods are to be used. The application of such numerical methods leads to the solution of systems of non-linear algebraic equations, which are normally treated at each time-step by the Newton Iterative Method (see, for example, [11]). This means that long sequences of systems of linear algebraic equations are to be handled during the iterative process. As a rule, this does not cause great problems. However, the atmospheric chemistry scheme is, as mentioned in the previous sub-section, very badly scaled and the condition numbers of the involved matrices are very large. It was found, by applying a LAPACK subroutine for calculating eigenvalues and condition numbers [1], that the condition numbers of the matrices involved in the Newton Iterative Process during the numerical integration of the atmospheric chemistry scheme on the interval $[a, b]$ vary in the range $[4.56E+08, 9.27E+12]$. A simple application of error analysis arguments from [16] indicates that there is a danger that the rounding errors will affect the fourth significant digit of the approximate solution on most of the existing computers when double precision arithmetic (based on the use of REAL*8 declarations of the real numbers and leading to the use of about 16-digit arithmetic on many computers) is applied. Therefore, all computations reported in the next sub-sections were performed by selecting quadruple precision (i.e., by using REAL*16 declarations for the real numbers and, thus, about 32-digit arithmetic) in order to eliminate the influence of the rounding errors on the first 16 significant digits of the computed approximate solutions.

4.3. Runs with the Backward Euler Formula

The Backward Euler Formula (obtained when $\theta = 1$ is used) was run in combination with (a) only the sequential splitting procedure and (b) both the sequential splitting procedure and Richardson Extrapolation. Results are given in Table 1. It is clearly seen that the application of Richardson Extrapolation together with the Backward Euler Formula and the sequential splitting procedure results in a second-order numerical method and, thus, in significantly more accurate results.

4.4. Runs with the $\theta$-method with $\theta = 0.75$

The $\theta$-method with $\theta = 0.75$ was run as in the previous sub-section in combination with (a) only the sequential splitting procedure and (b) both the sequential splitting procedure and Richardson Extrapolation. Results are given in Table 2. It is again clearly seen that the application of Richardson Extrapolation together with the $\theta$-method with $\theta = 0.75$ and the sequential splitting procedure results in a second-order numerical method and, thus, in significantly more accurate results.

4.5. Runs with the Trapezoidal Rule

The Trapezoidal Rule (obtained when $\theta = 0.5$ is used) was run as in the previous two sub-sections in combination with (a) the sequential splitting procedure and (b) both the sequential splitting procedure and Richardson Extrapolation.
Richardson Extrapolation combined with the sequential splitting procedure and the $\theta$-method

<table>
<thead>
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<th>Job Number</th>
<th>Number of time-steps</th>
<th>Only sequential splitting</th>
<th>Richardson Extrapolation</th>
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<td></td>
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<td>Accuracy Rate</td>
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</table>

Table 1. Numerical results that are obtained in 11 runs when the Backward Euler Formula is used with (a) only the sequential splitting procedure and (b) both the sequential splitting procedure and Richardson Extrapolation. The errors obtained by (19) are given in the columns under “Accuracy”. The ratios of two successive errors (calculated in an attempt to measure the rate of convergence) are given in the columns under “Rate”.

<table>
<thead>
<tr>
<th>Job Number</th>
<th>Number of time-steps</th>
<th>Only sequential splitting</th>
<th>Richardson Extrapolation</th>
</tr>
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<td>Accuracy Rate</td>
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Table 2. The same as Table 1, but for the case when the $\theta$-method with $\theta = 0.75$ is used instead of the Backward Euler Formula.

Results are given in Table 3. The application of the Trapezoidal Rule only with the sequential splitting procedure results in a first-order numerical method. However the results are more accurate than the corresponding results in the previous two tables. The application of Richardson Extrapolation together with the Trapezoidal Rule and the sequential splitting procedure results in an unstable numerical method. This should be expected according to Theorem 3.4.

5. Conclusion

The stability properties for Richardson Extrapolation applied together with the $\theta$-method and the sequential splitting procedure were examined. As a main result, it was proved that the combined method is strongly A-stable if $\theta \in [\theta_0, 1.0]$ with $\theta_0 \approx 0.638$. In the particular case where $\theta = 1.0$ (i.e., if the Backward Euler Formula is used) the combined method is L-stable. Numerical results indicate that the use of Richardson Extrapolation with the $\theta$-method and the sequential splitting procedure will in general behave as a second-order numerical method.

In the future we plan to investigate the stability of higher-order splittings in combination with the $\theta$-method and Richardson Extrapolation.
Table 3. The same as Table 1, but for the case when the Trapezoidal Rule is used instead of the Backward Euler Formula; “not stable” means that the method is not stable, “n.a” means not applicable.

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The Centre for Supercomputing at the Technical University of Denmark gave us access to several powerful parallel computers for running long sequences of numerical experiments. The European Union and the European Social Fund have provided financial support to the project under the grant agreement no. TÁMOP 4.2.1/B-09/1/KMR-2010-0003.

References

Richardson Extrapolation combined with the sequential splitting procedure and the $\theta$-method