Stability and accuracy of time-extrapolated ADI-FDTD methods for solving wave equations

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Abstract

Some recent work on the ADI-FDTD method for solving Maxwell's equations in 3-D have brought out the importance of extrapolation methods for the time stepping of wave equations. Such extrapolation methods have previously been used for the solution of ODEs. The present context (of wave equations) brings up two main questions which have not been addressed previously: (1) when will extrapolation in time of an unconditionally stable scheme for a wave equation again feature unconditional stability, and (2) how will the accuracy and computational efficiency depend on how frequently in time the extrapolations are carried out. We analyze these issues here.

Key words: Wave equations, Maxwell's equations, GBS method, extrapolation methods, stability domains, ADI-FDTD.
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1 Introduction

There are a variety of approaches available for numerical solution of ODEs, including linear multistep (LM), Runge Kutta (RK), Taylor, and extrapolation methods. For Method-of-lines (MOL) solution of PDEs [5], [23], [24], LM and RK methods have in the past been dominant. However, in the context that motivates the present study – fast solution of the 3-D Maxwell's equations in the presence of detailed geometries – extrapolation methods appear to be the most promising approach for reaching high temporal accuracies [11], [16]. This study therefore focuses on improving the understanding of extrapolation methods for wave equations.

Almost all the difficulties that arise in the numerical solution of Maxwell's equations are due to material interfaces or boundaries. When the features of these are much smaller in size than a typical wave length, one would like to use small space steps (which are needed to resolve these features) together with long time steps (which are sufficient to follow the wave's time evolution). Such a combination – small space steps and long time steps – will violate the classical CFL stability condition for explicit methods, often by several orders of magnitude.

The first time stepping method which overcomes this CFL limitation and combines a very low cost per time step with unconditional stability was a generalized alternating direction implicit (ADI) method, introduced in 1999 [29], [30]. A split step (SS) procedure that was introduced shortly afterwards [15] also achieves unconditional stability for the 3-D Maxwell's equations. Since higher order methods generally turn out to be more economical than lower order ones, this raised the issue whether the naturally second order ADI approach could be brought to higher order in time with preserved unconditional stability, as studied in [16].

In the present study, we explore two enhancement procedures introduced in [16]: Richardson extrapolation and 're-starts'. In Section 2, we describe the ADI method, as applied to Maxwell's equations, followed by the ADI-FDTD test problem, and then review relevant findings from [16]. It transpires that most convergence/divergence features that are seen for the ADI-FDTD method can be reproduced even with the very simple ODE

$$y' = \lambda\, y\ . \tag{1.1}$$

In Section 3, we review two ODE solvers (TR and GBS) and compare their stability domains in Section 4. We then analyze how stability depends on the order of extrapolation, and on how often in time the extrapolations are performed (i.e. how many re-starts are done). In the concluding Section 6, we summarize the main results that have been reached - all supporting the viability of Richardson extrapolation as a very valuable enhancement to the ADI-FDTD procedure.

2 The ADI scheme for the 3-D Maxwell's equations

2.1 Maxwell's equations and Alternating direction implicit (ADI) method

In 1873, James Clark Maxwell first formulated what is now known as the Maxwell's equations [18]. For a medium with permittivity ε and permeability μ, and assuming no free charges or currents, the 3-D Maxwell's equations can be written as a system of six first-order PDEs:

$$\left\{\begin{array}{rcl}
\frac{\partial E_x}{\partial t} & = & \frac{1}{\varepsilon}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right)\\
\frac{\partial E_y}{\partial t} & = & \frac{1}{\varepsilon}\left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}\right)\\
\frac{\partial E_z}{\partial t} & = & \frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right)\\
\frac{\partial H_x}{\partial t} & = & -\frac{1}{\mu}\left(\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z}\right)\\
\frac{\partial H_y}{\partial t} & = & -\frac{1}{\mu}\left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x}\right)\\
\frac{\partial H_z}{\partial t} & = & -\frac{1}{\mu}\left(\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y}\right)
\end{array}\right. \tag{2.1}$$

Here E_x, E_y, E_z and H_x, H_y, H_z denote the components of the electric and magnetic fields, respectively. The arguably most straightforward numerical scheme possible - using centered finite differences for all the derivatives in space and time - leads, when combined with a suitable staggering of the data in space and time, to the well-known Yee scheme [27] (proposed in 1966). Besides its low accuracy (second order), the biggest drawback is that it, like other fully explicit schemes, is subject to the CFL stability condition, severely restricting the time steps that can be used in cases where an irregular geometry forces the use of particularly small space steps. Later improvements of the Yee scheme includes an interesting way to enhance the accuracy for specific frequency ranges by means of a 'non-standard finite difference enhancement' [4]. The first practical way to largely bypass the CFL limitation for Maxwell's equations is the ADI method, which is described next.

The ADI approach has proven to be very successful for parabolic and elliptic PDEs for the last 50 years. Seminal papers in the area include [9] and [21]. Various similar 3-stage dimensional splittings for the 3-D Maxwell's equations have been tried, but have invariably fallen short of the goal of unconditional time stability. However, a 2-stage splitting introduced in 1999 by Zheng et al. [29], [30] does achieve the goal. The original way to state this scheme introduces a half-way time level $n+1/2$ between the adjacent time levels n and $n+1$. We advance our six variables as follows:

Stage 1:

$$\left\{\begin{array}{lcl}
\frac{E_x\,|_{i,j,k}^{n+1/2} - E_x\,|_{i,j,k}^{n}}{\Delta t/2} & = \frac{1}{\varepsilon} & \left(\frac{H_z\,|_{i,j+1,k}^{n+1/2} - H_z\,|_{i,j-1,k}^{n+1/2}}{2\Delta y} - \frac{H_y\,|_{i,j,k+1}^{n} - H_y\,|_{i,j,k-1}^{n}}{2\Delta z} \right) \\
\frac{E_y\,|_{i,j,k}^{n+1/2} - E_y\,|_{i,j,k}^{n}}{\Delta t/2} & = \frac{1}{\varepsilon} & \left(\frac{H_x\,|_{i,j,k+1}^{n+1/2} - H_x\,|_{i,j,k-1}^{n+1/2}}{2\Delta z} - \frac{H_z\,|_{i+1,j,k}^{n} - H_z\,|_{i-1,j,k}^{n}}{2\Delta x} \right) \\
\frac{E_z\,|_{i,j,k}^{n+1/2} - E_z\,|_{i,j,k}^{n}}{\Delta t/2} & = \frac{1}{\varepsilon} & \left(\frac{H_y\,|_{i+1,j,k}^{n+1/2} - H_y\,|_{i-1,j,k}^{n+1/2}}{2\Delta x} - \frac{H_x\,|_{i,j+1,k}^{n} - H_x\,|_{i,j-1,k}^{n}}{2\Delta y} \right) \\
\frac{H_x\,|_{i,j,k}^{n+1/2} - H_x\,|_{i,j,k}^{n}}{\Delta t/2} & = \frac{1}{\mu} & \left(\frac{E_y\,|_{i,j,k+1}^{n+1/2} - E_y\,|_{i,j,k-1}^{n+1/2}}{2\Delta z} - \frac{E_z\,|_{i,j+1,k}^{n} - E_z\,|_{i,j-1,k}^{n}}{2\Delta y} \right) \\
\frac{H_y\,|_{i,j,k}^{n+1/2} - H_y\,|_{i,j,k}^{n}}{\Delta t/2} & = \frac{1}{\mu} & \left(\frac{E_z\,|_{i+1,j,k}^{n+1/2} - E_z\,|_{i-1,j,k}^{n+1/2}}{2\Delta x} - \frac{E_x\,|_{i,j,k+1}^{n} - E_x\,|_{i,j,k-1}^{n}}{2\Delta z} \right) \\
\frac{H_z\,|_{i,j,k}^{n+1/2} - H_z\,|_{i,j,k}^{n}}{\Delta t/2} & = \frac{1}{\mu} & \left(\frac{E_x\,|_{i,j+1,k}^{n+1/2} - E_x\,|_{i,j-1,k}^{n+1/2}}{2\Delta y} - \frac{E_y\,|_{i+1,j,k}^{n} - E_y\,|_{i-1,j,k}^{n}}{2\Delta x} \right)
\end{array}\right. \tag{2.2}$$

Stage 2:

$$\left\{\begin{array}{lcl}
\frac{E_x\,|_{i,j,k}^{n+1} - E_x\,|_{i,j,k}^{n+1/2}}{\Delta t/2} & = \frac{1}{\varepsilon} & \left(\frac{H_z\,|_{i,j+1,k}^{n+1/2} - H_z\,|_{i,j-1,k}^{n+1/2}}{2\Delta y} - \frac{H_y\,|_{i,j,k+1}^{n+1} - H_y\,|_{i,j,k-1}^{n+1}}{2\Delta z} \right) \\
\frac{E_y\,|_{i,j,k}^{n+1} - E_y\,|_{i,j,k}^{n+1/2}}{\Delta t/2} & = \frac{1}{\varepsilon} & \left(\frac{H_x\,|_{i,j,k+1}^{n+1/2} - H_x\,|_{i,j,k-1}^{n+1/2}}{2\Delta z} - \frac{H_z\,|_{i+1,j,k}^{n+1} - H_z\,|_{i-1,j,k}^{n+1}}{2\Delta x} \right) \\
\frac{E_z\,|_{i,j,k}^{n+1} - E_z\,|_{i,j,k}^{n+1/2}}{\Delta t/2} & = \frac{1}{\varepsilon} & \left(\frac{H_y\,|_{i+1,j,k}^{n+1/2} - H_y\,|_{i-1,j,k}^{n+1/2}}{2\Delta x} - \frac{H_x\,|_{i,j+1,k}^{n+1} - H_x\,|_{i,j-1,k}^{n+1}}{2\Delta y} \right) \\
\frac{H_x\,|_{i,j,k}^{n+1} - H_x\,|_{i,j,k}^{n+1/2}}{\Delta t/2} & = \frac{1}{\mu} & \left(\frac{E_y\,|_{i,j,k+1}^{n+1/2} - E_y\,|_{i,j,k-1}^{n+1/2}}{2\Delta z} - \frac{E_z\,|_{i,j+1,k}^{n+1} - E_z\,|_{i,j-1,k}^{n+1}}{2\Delta y} \right) \\
\frac{H_y\,|_{i,j,k}^{n+1} - H_y\,|_{i,j,k}^{n+1/2}}{\Delta t/2} & = \frac{1}{\mu} & \left(\frac{E_z\,|_{i+1,j,k}^{n+1/2} - E_z\,|_{i-1,j,k}^{n+1/2}}{2\Delta x} - \frac{E_x\,|_{i,j,k+1}^{n+1} - E_x\,|_{i,j,k-1}^{n+1}}{2\Delta z} \right) \\
\frac{H_z\,|_{i,j,k}^{n+1} - H_z\,|_{i,j,k}^{n+1/2}}{\Delta t/2} & = \frac{1}{\mu} & \left(\frac{E_x\,|_{i,j+1,k}^{n+1/2} - E_x\,|_{i,j-1,k}^{n+1/2}}{2\Delta y} - \frac{E_y\,|_{i+1,j,k}^{n+1} - E_y\,|_{i-1,j,k}^{n+1}}{2\Delta x} \right)
\end{array}\right. \tag{2.3}$$

For comments on interpretations and implementations of these equations, see [11]. For overviews of the recent ADI-FDTD literature, see for ex. [2], [7], [12], [17], [20], [25], [26], [28].

The ADI-FDTD method is mainly of interest in cases when intricate spatial geometry forces the use of very small space steps. Therefore, there is not very much need for increasing the spatial order of accuracy in (2.2) and (2.3). Compared to the size of the wave length, the spatial resolution is already very high. The situation in time is entirely different. In that direction, the domain is simply an interval. We want to increase the order of accuracy so that we

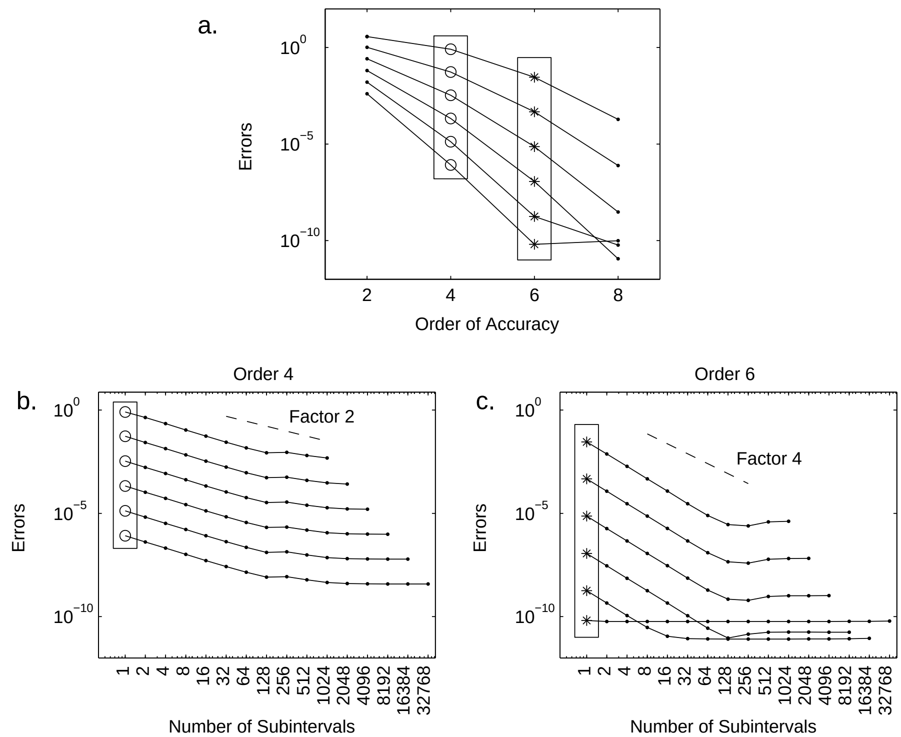

Fig. 1. A test case of 3-D Maxwell's equations using Richardson extrapolation in time, as described in [16]. Here, the pseudospectral method is employed for spatial discretization, and we display the combined least square error for the six fields at final time $T = 32$. The curves, from top to bottom, correspond to different time step sizes $k = \Delta t = T/N,\ \ N = 2048 \cdot 2^{j-1},\ \ j = 1, \ldots, 8$. (a) Errors for different time step sizes at final time $T = 32$ when Richardson extrapolated to higher orders of accuracy. (b) Accuracies in the case of 4th order, with increasing numbers of re-starts. (c) Accuracies in the case of 6th order, with increasing numbers of re-starts.

can use longer (and thereby more economical) time steps.

2.2 Review and motivation

In [16] it was discovered that Richardson extrapolation in time could achieve the goal just mentioned: increasing temporal order of accuracy while preserving the unconditional stability, and thereby significantly reducing the computational cost. Richardson extrapolation is very much in the style of the extrapolation methods, which have been well-known since the middle of the last century for accurate solution of ODEs. The additional idea of re-starts was considered in [16], and found to further improve the accuracy at no increase in cost. However, the stability situation in the case of re-starts remained unclear.

Figure 1 summarizes the result of a test case of 3-D Maxwell's equations using Richardson extrapolation in time. Clearly, large increases in computational efficiency can be achieved through Richardson extrapolation. The main purpose of this present study is to add more theoretical understanding to the idea of re-starts and, in particular, to their stability (or lack thereof). The slopes that are marked by dashed lines in subplots b and c will be confirmed by our analysis in Section 5.2.1. As noted in the Introduction, most convergence/divergence features for the ADI-FDTD method (applied to the 3-D Maxwell's equations) can be reproduced with the very simple ODE (1.1).

For the present context of wave equations, we need to analyze somewhat different features of ODE solvers than what are usually considered. Of particular interest will be the extent of the stability domains along the imaginary axis (the stability ordinate), how this depends on the order of extrapolation, and on how often in time the extrapolations are performed (i.e. how many re-starts are done). A second main goal of the present study is to contrast unconditionally stable methods - such as the trapezoidal rule (TR) - with conditionally stable ones, represented for ex. by the Gragg-Bulirsch-Stoer (GBS) scheme.

2.3 Description of ADI-FDTD test problem

The fields

$$\begin{aligned}
E_x &= \cos(2\pi(x+y+z) - 2\sqrt{3}\pi t) & H_x &= \sqrt{3}E_x \\
E_y &= -2E_x & H_y &= 0 \\
E_z &= E_x & H_z &= -\sqrt{3}E_x
\end{aligned}$$

with $\varepsilon = \mu = 1$ satisfy (2.1) over a periodic unit cube, and correspond to waves propagating along the main diagonal of the computational lattice. Since the ADI-FDTD method is mainly of interest in cases when the geometry forces the use of very small space steps, spatial errors in resolving a wave will contribute little to the overall error. In this case we employed the pseudospectral method in space in order to see most clearly how Richardson extrapolations in time, described in [16], improves the temporal accuracy. In the computations from $t = 0$ to $t = T = 32$ shown in Figure 1, the leftmost point markers (order of accuracy = 2) in part (a) show how the final error (measured in the ℓ^2-norm, over all the six fields) decreases when the time step in (2.2), (2.3) is successively decreased by factors of two - from $1/2^5$ to $1/2^{10}$. Each time the time step is halved, the computational cost doubles. In contrast, each Richardson extrapolation (moving to next column in Figure 1a) only increases computational cost by 50%. Not only is this much less costly than refining the time step, the gain in accuracy is seen to be much larger. The leftmost columns in Figures 1b and c correspond to the fourth and sixth order methods, as shown in part a of the figure. The re-starts (as described in [16] and here in Section 5.2) decrease time errors by some additional orders of magnitude, without any further increases in cost. As noted in the introduction, one of the main purpose of the present study is to clarify the stability situation when extrapolation is used in this way at the end of each computational temporal subinterval.

3 Two second order ODE solvers

An extrapolation method typically starts with a scheme which is second order accurate in time, and for which the error expansion contains only even powers of the time step k. In the case of solving

$$y' = f(t, y) \quad , \tag{3.1}$$

two such schemes are described next. Based on the insights we gain from these two cases, we will be able to address the corresponding issue for the extrapolated ADI method for Maxwell's equations.

3.1 Trapezoidal rule

To advance (3.1) with initial condition (IC) $y(t_0) = y_0$ forward N time steps to reach time t_N, the trapezoidal rule (TR) amounts to repeating

$$\frac{y_{n+1} - y_n}{k} = \frac{1}{2}(f(t_{n+1}, y_{n+1}) + f(t_n, y_n)), \qquad n = 0, 1, 2, \ldots, N-1. \tag{3.2}$$

Comparing the computed solution y_N to the exact value Y_N at time t_N, we obtain

$$y_N - Y_N = \sum_{j=1}^{\infty} c_j k^{2j} \quad , \tag{3.3}$$

containing only even powers of k [14]. Extrapolation in time for this scheme is discussed in Section 5.1.1. The procedure is seldom used for this scheme, but is nevertheless instructive for our subsequent analysis. This scheme is conceptually very similar to the ADI-FDTD scheme in being unconditionally stable and unchanged under time reversal.

3.2 *Gragg-Bulirsch-Stoer*

Since extrapolation methods for ODEs are most commonly based on the GBS scheme [13], we included it here for the purpose of comparison. The basic second order (un-extrapolated) version of GBS consists of the steps

$$\begin{cases} \dfrac{y_1 - y_0}{k} = f(t_0, y_0) & \text{Forward Euler} \\[2em] \dfrac{y_{n+1} - y_{n-1}}{2k} = f(t_n, y_n) & \text{Leap-frog, } n = 1, 2, \ldots, N \\[2em] y_N^* = \frac{1}{4}(y_{N-1} + 2y_N + y_{N+1}) & \text{Averaging} \end{cases} \tag{3.4}$$

where y_N^* is the approximation that is accepted at time t_N. We rename y_N^* as y_N. If N is even, it transpires that we get again an error expansion of the form (3.3) in even powers only [3], [13], [14]. Many other second order ODE solvers feature error expansions with all powers of k present, and they are therefore not equally well suited for subsequent extrapolation [13] (gaining only one rather than two orders of accuracy for each extrapolation). Time extrapolations for GBS are discussed in Section 5.1.2.

4 Stability domains

These domains are essential in determining when an ODE solver can be used for MOL solution of a PDE. They are obtained by considering the numerical scheme applied to the simple linear ODE (1.1). For the ODE itself, solutions will not grow when Re $\lambda \leq 0$. For each ODE solver applied to (1.1), we similarly obtain a certain domain in a complex $\xi = \lambda k$ plane for which solutions will not grow. Figure 2 shows these stability domains for Forward Euler (FE), Leap-frog (LF), and p-stage explicit Runge-Kutta methods of order p (RK$_p$), $p = 1,\ 2,\ 3,\ 4$. More details on these well-known stability domains can, for example, be found in [1] (p.407), [10] (Appendix G), and [19] (p.69). The fact that the domains for FE, RK$_1$ and RK$_2$ do not include any interval along the imaginary axis tells that an MOL solution based on them will be unconditionally unstable for wave equations. For LF, RK$_3$ and RK$_4$, the stability ordinates are 1, $\sqrt{3}$ and $2\sqrt{2}$ respectively (cf. Figure 2).

The stability condition on k/h (time step divided by space step for a wave equation) will be proportional to this stability ordinate (and will also depend on the space operator; see for ex. Example 5, Section 4.5 in [10]).

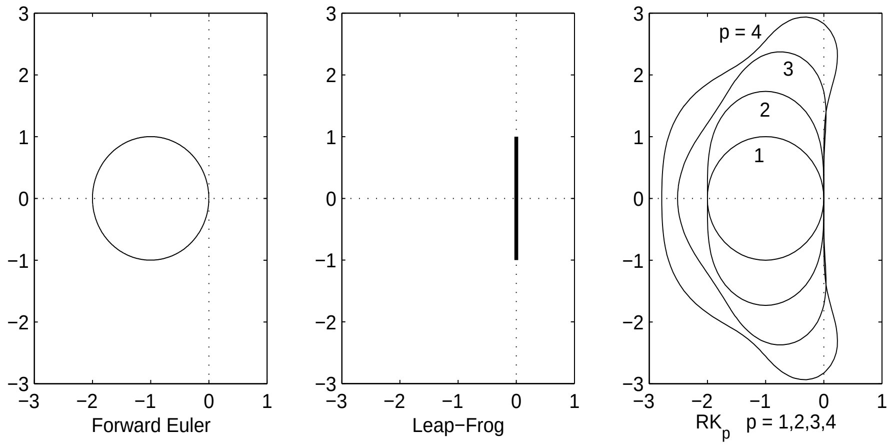

Fig. 2. Some examples of stability domains in a complex $\xi = \lambda k$ plane.

4.1 Stability domain for the trapezoidal rule

The TR scheme applied to (1.1) becomes

$$\frac{y_{n+1} - y_n}{k} = \frac{\lambda}{2}\left(y_{n+1} + y_n\right) \ ,$$

i.e.

$$y_{n+1} = \frac{1+\frac{\xi}{2}}{1-\frac{\xi}{2}} y_n \ , \tag{4.1}$$

with non-growing solutions if and only if $\mathrm{Re}\,\xi \leq 0$. The stability domain is therefore precisely the left half plane, just as is the domain of no-growth for the ODE itself.

4.2 Stability domain for second order GBS

The analysis for the GBS scheme is more complicated, partly since it also depends on N (the number of time steps that are taken before the averaging is performed).

Applying (3.4) to (1.1) with $y_0 = 1$ gives

$$\begin{aligned}
y_1 &= 1 + \lambda k &&= 1 + \xi \\
y_2 &= y_0 + 2k\lambda y_1 &&= 1 + 2\xi + 2\xi^2 \\
y_3 &= y_1 + 2k\lambda y_2 &&= 1 + 3\xi + 4\xi^2 + 4\xi^3 \\
y_4 &= y_2 + 2k\lambda y_3 &&= 1 + 4\xi + 8\xi^2 + 8\xi^3 + 8\xi^4 \\
y_5 &= y_3 + 2k\lambda y_4 &&= 1 + 5\xi + 12\xi^2 + 20\xi^3 + 16\xi^4 + 16\xi^5 \\
&\dots
\end{aligned}$$

For even values of N, we form $y_N^* = \frac{1}{4}(y_{N-1} + 2y_N + y_{N+1})$, i.e.

$$\begin{aligned}
y_2^* &= 1 + 2\xi + 2\xi^2 + \xi^3 \\
y_4^* &= 1 + 4\xi + 8\xi^2 + 10\xi^3 + 8\xi^4 + 4\xi^5 \\
y_6^* &= 1 + 6\xi + 18\xi^2 + 35\xi^3 + 48\xi^4 + 48\xi^5 + 32\xi^6 + 16\xi^7 \\
&\dots
\end{aligned} \tag{4.2}$$

From these expressions, we can plot the corresponding stability domains, as will later be done in Section 5.1.2.

In the context of wave equations, the key question is whether or not any interval along the imaginary axis around the origin is included in the stability domain. This can be settled by series expansions for fixed N (even) and small ξ, as follows:

$$\begin{aligned}
y_N^* = 1 &+ N\xi + \tfrac{1}{2}N^2\xi^2 + \tfrac{1}{6}N(N^2-1)\xi^3 + \tfrac{1}{24}N^2(N^2-4)\xi^4 + \\
&+ \tfrac{1}{120}N(N^2-4)(N^2-6)\xi^5 + \tfrac{1}{720}N^2(N^2-4)(N^2-16)\xi^6 + \\
&+ \tfrac{1}{5040}N(N^2-4)(N^2-15)(N^2-16)\xi^7 + \dots
\end{aligned}$$

The multiplication factor per time step thus becomes

$$\begin{aligned}
\sigma_N = &\ \sqrt[N]{y_N^*} \\
&= 1 + \xi + \tfrac{1}{2}\xi^2 - \tfrac{1}{8}\xi^4 + \tfrac{1}{8}\xi^5 - \tfrac{1}{16}(2N-3)\xi^6 + \tfrac{1}{24}(N-2)(2N+1)\xi^7 + \dots
\end{aligned}$$

and we can further compute

$$\rho_N = \ln\ \sigma_N = \xi - \tfrac{1}{6}\xi^3 + \tfrac{1}{5}\xi^5 - \tfrac{1}{8}N\ \xi^6 + \tfrac{1}{84}(7N^2-16)\ \xi^7 + \dots\ . \tag{4.3}$$

For an exact ODE solver, this last quantity should satisfy $\rho_N = \xi$. The fact that next term is of the form $c \cdot \xi^3$ signifies that the scheme is of second order accuracy.

The stability domain consists of ξ-values such that $|\sigma_N| \le 1$. Because of the general formula for z complex: $\ln z = \ln|z| + i \ \arg z$, this domain is also described by $\operatorname{Re}\rho_N \le 0$. Letting ξ vary along the imaginary axis near the origin, the first three terms in (4.3) tell that the edge of the stability domain, to leading orders, also follows the imaginary axis. However, the fourth term $-\frac{1}{8}N\,\xi^6$ tells that $\operatorname{Re}\rho_N > 0$ when ξ is small and purely imaginary. Thus, all these methods ($N = 2,\ 4,\ 6,\ \ldots$) lack imaginary axis coverage near the origin, and they will therefore become unconditionally unstable in case of MOL time stepping of wave equations. Illustrations of the second order GBS stability domains in cases of $N = 2, 4, 8, 16$ appear later in this paper as the leftmost column in Figure 4.

For comparison, we can note that for TR, the counterpart to (4.3) will not feature any N-dependence. From (4.1) follows

$$\rho = \ln \frac{1+\frac{\xi}{2}}{1-\frac{\xi}{2}} = \sum_{n=1}^{\infty} \frac{\xi^{2n-1}}{(2n-1)\,4^{n-1}} \quad , \tag{4.4}$$

containing only odd powers in ξ. This is consistent with the fact that the stability domain boundary for TR does not deviate in either direction from the imaginary axis.

5 Extrapolations to higher orders

Richardson extrapolation [22] has often been used when numerical calculations feature error expansions of the form (3.3), e.g. Romberg's method for quadrature [6], and extrapolation methods for ODEs [8], [13]. In the context of solving ODEs, frequent extrapolations/re-starts are usually advantageous. In our present context of MOL solution of wave-type PDEs, the issue is more complicated since we also need to take into account if the resulting stability domains cover part of the imaginary axis. To our knowledge, this has not been studied previously.

The two main options when extrapolating are whether to perform it every N time steps (i.e. increasingly many times as the grid is refined) or a fixed number M of times (i.e. progressively more rarely under mesh refinement). We will see in Section 5.1 that the former option never works for TR, but that it can give conditional stability in some cases for extrapolated GBS schemes. However, since our interest lies in unconditional stability, we turn in Section 5.2 to the case of extrapolating only a fixed number M times (even as the time step is refined). This was the case considered in [16]. We can here both confirm and interpret (in the case of TR) the favorable convergence and stability situation that was previously observed (for ADI-FDTD).

5.1 Extrapolation every N time steps

We need to analyze this separately for the TR and the GBS schemes, as follows.

5.1.1 Stability analysis for TR

If we advance TR N steps forward with a time step inversely proportional to N, the solution gets multiplied by $\left(\frac{1+\frac{1}{2}\frac{\xi}{N}}{1-\frac{1}{2}\frac{\xi}{N}}\right)^N$. We can then build up the Romberg table

$$\begin{array}{lllll}
y_1^{(2)} = \frac{1+\frac{1}{2}\frac{\xi}{1}}{1-\frac{1}{2}\frac{\xi}{1}} & & & & \\
y_2^{(2)} = \left(\frac{1+\frac{1}{2}\frac{\xi}{2}}{1-\frac{1}{2}\frac{\xi}{2}}\right)^2 & y_2^{(4)} & & & \\
y_4^{(2)} = \left(\frac{1+\frac{1}{2}\frac{\xi}{4}}{1-\frac{1}{2}\frac{\xi}{4}}\right)^4 & y_4^{(4)} & y_4^{(6)} & & \\
y_8^{(2)} = \left(\frac{1+\frac{1}{2}\frac{\xi}{8}}{1-\frac{1}{2}\frac{\xi}{8}}\right)^8 & y_8^{(4)} & y_8^{(6)} & y_8^{(8)} & \\
\quad\vdots & \vdots & \vdots & \vdots & \ddots
\end{array} \tag{5.1}$$

where the superscripts (p) denote the order of accuracy and – as before – subscripts denote N. The elements in successive columns are computed recursively by

$$y_{2^i}^{(p)} = \frac{2^{p-2}y_{2^i}^{(p-2)} - y_{2^{i-1}}^{(p-2)}}{2^{p-2}-1} \quad .$$

For example, in the special case of extrapolating from second to fourth order ($p = 4$), we have

$$y_{2^i}^{(4)} = \frac{4}{3}\, y_{2^i}^{(2)} - \frac{1}{3}\, y_{2^{i-1}}^{(2)} \quad . \tag{5.2}$$

In the same way as how we obtained the stability domains and equation (4.3) for the 2^{nd} order GBS scheme, we can now compute the corresponding data for the extrapolated methods. However, it is hard to read off from Figure 3 whether there is any imaginary axis coverage or not. Inspection of the corresponding ρ_N- functions (shown in the left part of Table 1) settles that issue.

The orders of accuracy are seen to increase as expected by two for each level of extrapolation. The signs in front of the first even power (negative for orders 4, 8, 12, ... and positive for orders 6, 10, ...) show that, in contrast to the perfect stability situation for un-extrapolated TR, the extrapolated TR methods never offer any imaginary axis coverage near the origin. In our context of MOL solution of wave equations, these methods will therefore all feature unconditional instability.

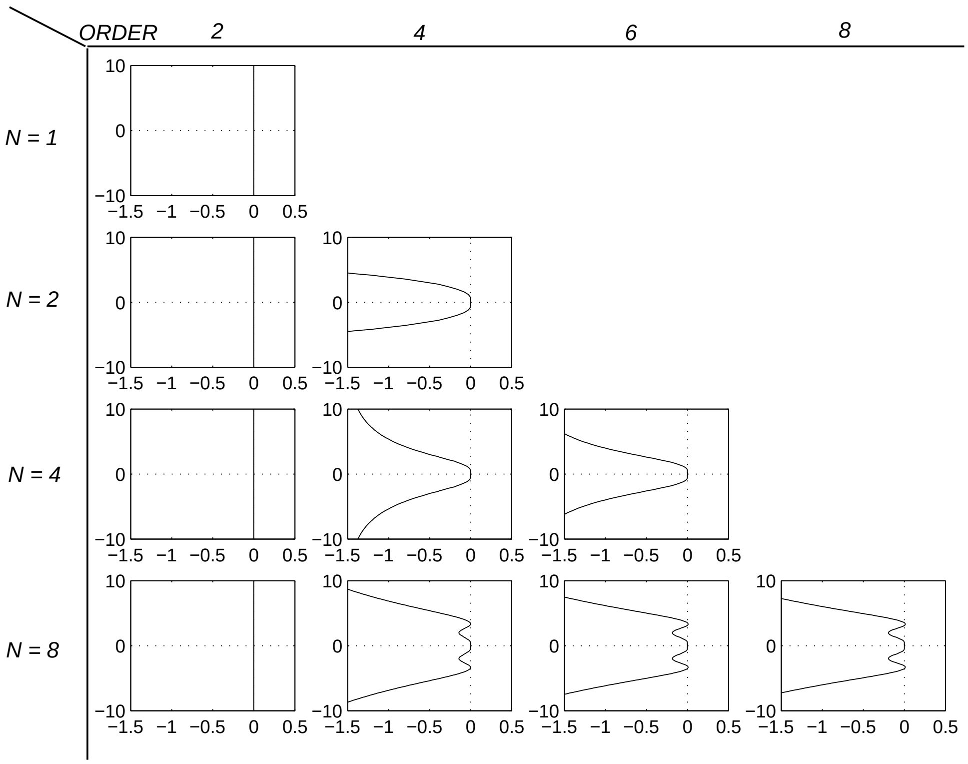

Fig. 3. Stability domains for TR methods (including extrapolations to different orders).

Table 1
Stability domains for TR and GBS; Expansions around origin

Order	$\rho_N(\xi)$ for TR	$\rho_N(\xi)$ for GBS
2	$\xi + \frac{1}{12}\xi^3 + \{\text{odd powers of } \xi \text{ only} \quad \}$	$\xi - \frac{1}{6}\xi^3 + \frac{1}{5}\xi^5 - \frac{1}{8}N\,\xi^6 + \ldots$
4	$\xi - \frac{1}{20}\xi^5 - \frac{1}{72}N\,\xi^6 + \ldots$	$\xi - \frac{2^2}{5}\xi^5 + \frac{2^2}{9}N\,\xi^6 + \ldots$
6	$\xi + \frac{1}{7}\xi^7 + \frac{1}{15}N\,\xi^8 + \ldots$	$\xi - \frac{2^8}{21}\xi^7 + \frac{2^7}{15}N\,\xi^8 + \ldots$
8	$\xi - \frac{2^4}{9}\xi^9 - \frac{2^3 \cdot 71}{525}N\,\xi^{10} + \ldots$	$\xi - \frac{2^{15}}{45}\xi^9 + \frac{2^{19}}{175}N\,\xi^{10} + \ldots$
10	$\xi + \frac{2^{10}}{11}\xi^{11} + \frac{2^{11} \cdot 31}{945}N\,\xi^{12} + \ldots$	$\xi - \frac{2^{26}}{385}\xi^{11} + \frac{2^{32} \cdot 31}{945}N\,\xi^{12} + \ldots$
12	$\xi - \frac{2^{18}}{13}\xi^{13} - \frac{2^{17} \cdot 3043}{24255}N\,\xi^{14} + \ldots$	$\xi - \frac{2^{37}}{819}\xi^{13} + \frac{2^{37}}{4851}N\,\xi^{14} + \ldots$
...	...	...

5.1.2 Stability analysis for GBS

The algebra becomes very similar to the TR case, with the exception that the entries from the closed form expressions for $\sigma_N = \sqrt[N]{y_N^*}$ (cf. (4.2)) need to be used in place of the explicit ratios in the left-most column in (5.1). Figure 4 displays the resulting stability domains, and the series expansions for ρ_N are shown in the right column of Table 1. The top entry corresponds to (4.3).

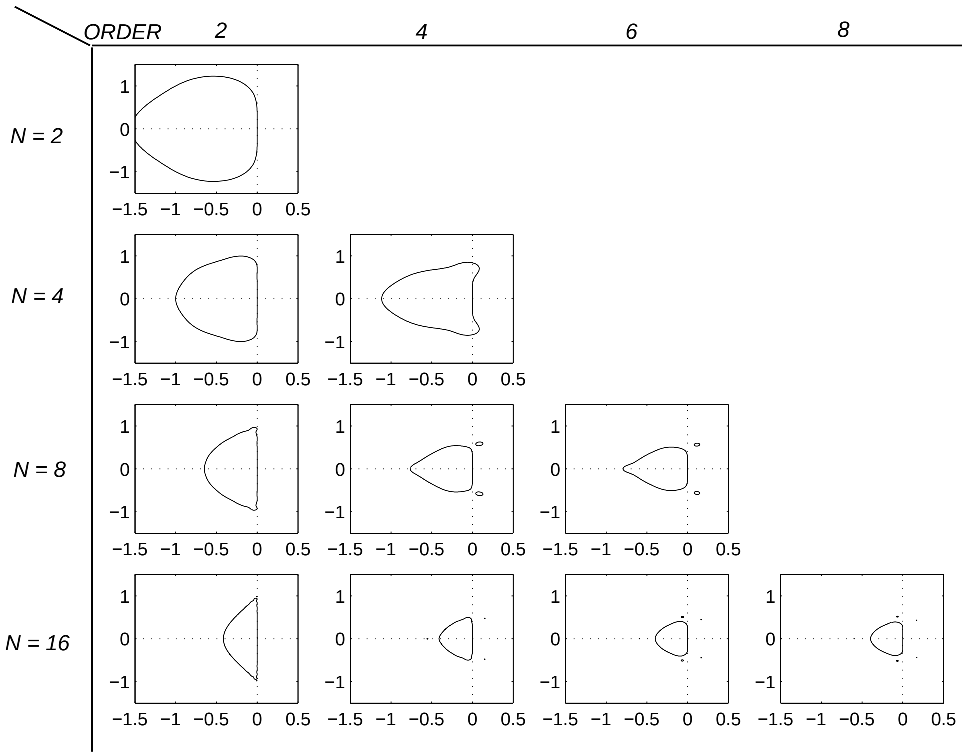

Fig. 4. Stability domains for GBS methods (including extrapolations to different orders).

Table 2
Stability Ordinates for GBS methods of orders $p = 4, 8, 12, ...$

	4	8	12	...
$N = 4$	0.84090			
8	0.28008			
16	0.14187	0.25390		
32	0.07115	0.06680		
64	0.03560	0.03355	0.05881	
128	0.01780	0.01614	0.01636	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Although the stability situation in the un-extrapolated GBS case is much more restrictive than for the un-extrapolated TR (which featured A -stability), we now obtain some imaginary axis coverage near the origin for orders $p = 4,\ 8,\ 12,\ \ldots$ Table 2 gives numerical values of the stability ordinate in these cases.

In the context of MOL solution of wave equations, we will in these cases obtain *conditional* stability (of the form $k/h <$ constant) - however never the unconditional stability that made the ADI-FDTD scheme so attractive.

5.2 Extrapolation M times during a time integration

5.2.1 Accuracy

In this case, stability will always be preserved (when the time step is decreased), since a fixed linear combination of bounded results will again become bounded. The approach is therefore 'safe', and it allows the accuracy to be increased to any order. This was exploited in [16], where it was furthermore empirically noted - as we recalled in the introduction of the present paper - that the accuracy improves roughly by a factor of two each time M is doubled in case of extrapolating ADI from order 2 to 4, and by a factor of 4 when extrapolating from order 4 to 6, etc. We will see next that (i) a gain of two orders of accuracy for each Richardson extrapolation corresponds to $\rho(\xi)$ being an odd function, (ii) the gains in accuracy due to re-starts occur only if $\lambda\tau$ is large, where τ is the time over which the ODE is solved, (iii) we can theoretically reproduce these observed improvement factors for re-starts, and (iv) the error (for very large values of λ) can grow with a factor of $5/3$ for each re-start (i.e. by a factor of $(5/3)^M$ in case of M re-starts, severely restricting the number of subintervals/re-starts that can be used in practice).

The numerical solution of (1.1) at time $\tau = T/M$, starting with $y(0) = 1$ and using a time step k, becomes

$$y(\tau) = \sigma(\xi)^{\frac{\tau}{k}} = e^{\frac{\tau}{k}\ln\sigma(\xi)} = e^{\frac{\tau}{k}\rho(\xi)} = e^{\frac{\tau}{k}\rho(\lambda k)}.$$

The error

$$y(\tau) - Y(\tau) = e^{\frac{\tau}{k}\rho(\lambda k)} - e^{\lambda\tau}$$

becomes an even function of k if and only if $\rho(\xi)$ is an odd function. It can therefore be expanded as $\rho(\xi) = \xi + c_3\xi^3 + c_5\xi^5 + c_7\xi^7 + \ldots$ (We can note that there is no contradiction between this and the presence of even powers of ξ in (4.3) since there $N = \frac{\tau}{k} = \frac{\lambda\tau}{\xi}$). Expanding $y(\tau) = e^{\frac{\tau}{k}\rho(\lambda k)}$ gives

$$\begin{aligned} y(\tau) &= e^{\lambda\tau}\cdot e^{c_3\lambda^3\tau\, k^2 + c_5\lambda^5\tau\, k^4 + c_7\lambda^7\tau\, k^6 + \ldots} \\ &= e^{\lambda\tau} + e^{\lambda\tau}c_3\lambda^3\tau\, k^2 + \tfrac{1}{2}e^{\lambda\tau}\lambda^5\tau(2c_5 + c_3^2\lambda\tau)k^4 + \\ &+ \tfrac{1}{6}e^{\lambda\tau}\lambda^7\tau(6c_7 + 6c_3c_5\lambda\tau + c_3^3\lambda^{2\tau 2})k^6 + \ldots \end{aligned} \tag{5.3}$$

Richardson extrapolation to 4th order, combining the above with a calculation using time step $2k$, gives

$$y(\tau) = e^{\lambda\tau} - e^{\lambda\tau}\lambda^5\tau(4c_5 + 2c_3^2\lambda\tau)k^4 - \tfrac{10}{3}e^{\lambda\tau}\lambda^7\tau(6c_7 + 6c_3c_5\lambda\tau + c_3^3\lambda^2\tau^2)k^6 + \ldots \tag{5.4}$$

If we want to reach the time $T = M\,\tau$ (by repeating the procedure M times), the result becomes

$$y(T) = y(\tau)^M = e^{\lambda T}\left[1 + 2T\lambda^5\left(2c_5 + \frac{c_3^2 \lambda T}{M}\right) k^4 + O(k^6)\right]. \tag{5.5}$$

Assuming that k is small enough that the $O(k^4)$-term dominates the $O(k^6)$-term, and that λT is large compared to M, the error has therefore gone down by a factor of M. In particular, it goes down by a factor of two each time M is doubled, as noted in [16].

Similarly, we can Richardson extrapolate (5.4) to also eliminate the k^4-term and, in place of (5.4), obtain

$$y(\tau) = e^{\lambda\tau} + \tfrac{32}{3} e^{\lambda\tau}\lambda^7\tau(6c_7 + 6c_3c_5\lambda\tau + c_3^3\lambda^2\tau^2)k^6 + \ldots$$

The solution at time $T = M\,\tau$ becomes

$$y(T) = y(\tau)^M = e^{\lambda T}\ \left[1 + 32\ T\ \lambda^7(2c_7 + 2c_3c_5\frac{\lambda T}{M} + \frac{1}{3}c_3^3\frac{\lambda^2 T^2}{M^2})k^6 + O(k^8)\right] \tag{5.6}$$

This time, the error similarly goes down with a factor of M^2, i.e. by a factor of four each time M is doubled. For extrapolation from 6th to 8th order, the corresponding factor becomes M^3, etc. The factor 'M' in (5.5) and 'M^2' in (5.6) imply that a doubling of M will reduce the error by factors of 2 and 4 respectively, giving slopes as shown with labels 'Factor 2' and 'Factor 4' in Figures 1 and 5.

5.2.2 Stability

Next we want to understand the stability situation when using repeated restarts in the context of wave equations. In this case, λ is purely imaginary and increases in size proportionally to $1/h$, where h is the spatial step size. Smaller h means larger λ, and the restriction on k in the previous analysis (section 5.2.1) gets more severe. When it is violated, we can still estimate a worst-case error growth as follows. When each Richardson extrapolation is performed (going from second to fourth order), we combine, with the weights $\frac{4}{3}$ and $-\frac{1}{3}$ (as in (5.2)), two results that have preserved their magnitude but whose phases might be entirely wrong. This can, at worst, increase the magnitude of the approximate solution by a factor of $\frac{5}{3}$. This growth is feasible at *each* of the M extrapolations. However, the amplitudes of these highest modes should initially be vanishingly small (we need to recall that the grid is fine only to accommodate an intricate geometry – we assumed the wave length to be large). Increasing the amplitudes of these high modes by a factor of up to $\frac{5}{3}$ a total of M times is therefore acceptable if M is not very large. The overall error (all modes included) will decrease initially when M is increased (since we improve

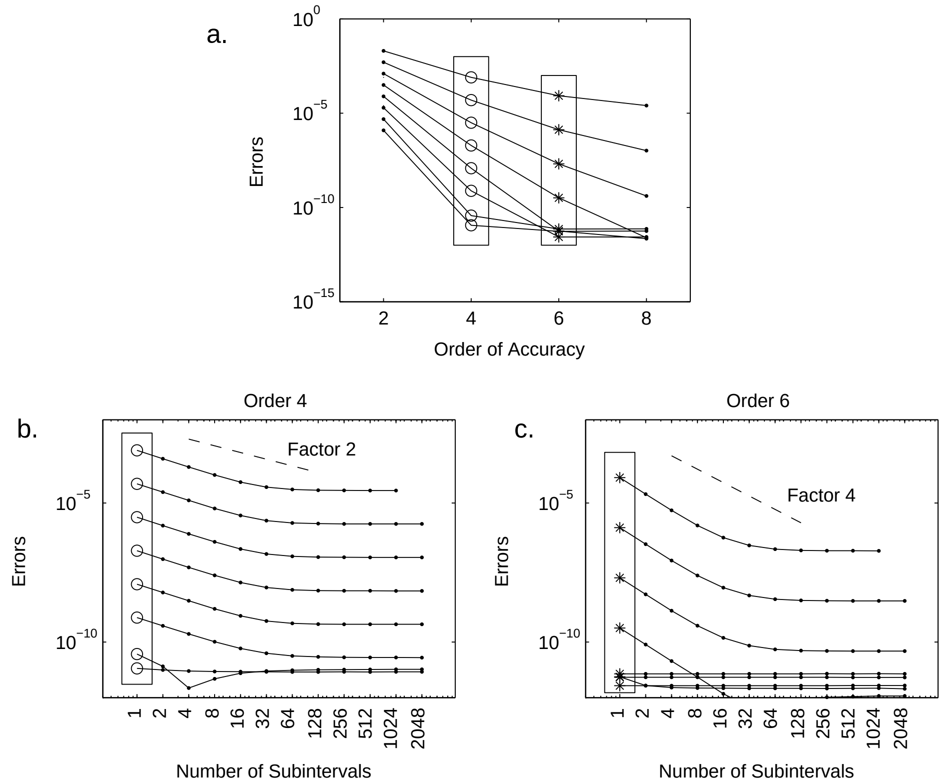

Fig. 5. Trapezoidal rule solutions to $y' = i\ y$: the curves, from top to bottom, represent errors at time steps $k = \Delta t = T/N,\ N = 2048 \cdot 2^{j-1},\ j = 1, \ldots, 8$. (a) Errors when solution at final time $T = 100$ is Richardson extrapolated to higher orders of accuracy. (b) Accuracies in the case of 4th order, with increasing numbers of re-starts. (c) Accuracies in the case of 6th order, with increasing numbers of re-starts.

the accuracy in dominant low modes), but it will grow eventually (since high modes – initially with negligible energy – can diverge exponentially with M). The break point between these two trends will depend on the initial data, and is most certainly best determined numerically, by checking at what point the highest modes in the computed wave solution start to exceed the desired accuracy level.

5.3 Numerical test of re-starts for TR

To compare how the accuracy improvements due to re-starts compare with the theoretical predictions we have just obtained, we implemented TR for (1.1) in the case of $\lambda = i$.

Figure 5a shows major accuracy gains by Richardson extrapolation, and parts b and c show that the accuracy with re-starts improve just as predicted. We also see - again as predicted - that the benefits of re-starts taper off as they are

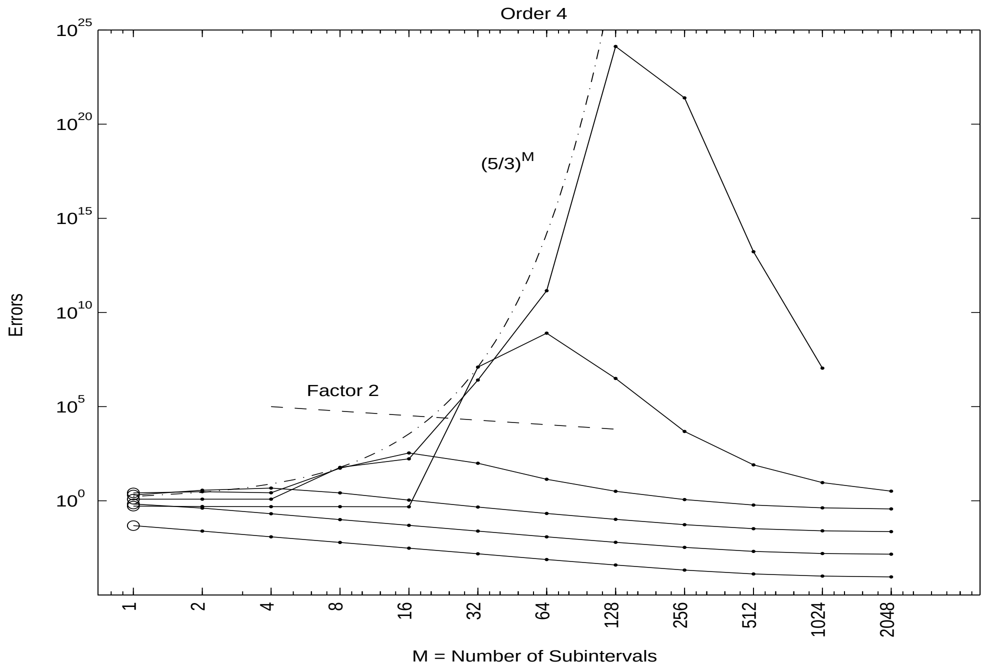

Fig. 6. Errors at final time $T = 100$ when TR is extrapolated to fourth order. The only difference from Figure 5b is that the equation now is $y' = 20iy$ instead of $y' = iy$.

performed increasingly often. We can gain close to two orders of magnitude in accuracy when applying it at order 4, and close to three orders of magnitude at order 6.

The general character of Figure 5 is qualitatively identical to that of Figure 1, leaving little doubt that we have indeed, in our ODE-based analysis for the small k case, caught the mechanisms controlling the convergence rates of the extrapolated ADI-FDTD scheme.

Repeating the same computation with $\lambda = 20i$ gives, in place of Figure 5b, the result shown in Figure 6. For the largest values of k, we get precisely the $(5/3)^M$ growth just discussed (cf. the dot-dashed curve). This growth by $(5/3)^M$ is independent of the integration length in time, and affects only modes that are so high that the time integration fails to resolve them. We conclude that using only a few subintervals (low values of M) is always acceptable, improving the lowest modes (which contain the physical energy), and cause only a moderate growth in the higher modes (which should contain no energy). If one, contrary to our recommendation, would wish to use many subintervals (high values of M), this still ought to be possible if combined with some sort of filter which takes out the (physically meaningless) highest modes.

6 Conclusions

The unconditionally stable ADI-FDTD scheme for the 3-D Maxwell's equations features only second order accuracy in time. It was observed in [16] that it could be beneficial to enhance it with Richardson extrapolation in time. In this study, we have:

- Explained why the Richardson extrapolation procedure to higher orders of accuracy preserves the ADI-FDTD schemes unconditional stability,
- By analysis of a model problem, clarified why use of increasingly frequent re-starts give precisely the type of accuracy enhancements that were earlier observed empirically,
- Demonstrated that only a limited number of re-starts are beneficial in view of the growth that otherwise can occur in high (unphysical) modes, and proposed a practical approach to deciding on how many re-starts to use,
- Contrasted the behavior of unconditionally stable schemes, such as ADI-FDTD and trapezoidal rule with that of the GBS approach (the main starting point in extrapolation methods for ODEs). In contrast to the unconditional instability of the former (ADI schemes with re-starts performed so often that only a fixed number of time steps are performed between each extrapolation), GBS-type schemes can give conditional stability also in this case. However, this is of limited interest in our present context of exploring schemes with unconditional stability.

Based on the observations above, we (again) recommend the ADI-FDTD scheme - together with Richardson extrapolation - in cases when we want to use a time step which is much larger than what the CFL condition would permit in the case of fully explicit schemes.

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