

Runge-Kutta Methods with Time Step Control and Adaptive Grid Refinement for Maxwell's Equations

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Abstract

The purpose of the present paper is to present a time-space adaptive finite difference scheme for the solution of the bidimensional TE_z mode Maxwell's equations. Using multiresolution techniques of interpolating wavelets, the method leads to sparse grids that adapt to the local smoothness of the fields and track their evolution over time, while controlling the level of accuracy of the finite difference scheme of the regular grid. The time integration is performed by embedded Runge-Kutta 2(3) scheme that allow a controlled time stepping procedure, where the time step is automatically adjusted during the time evolution. A good agreement of the solutions computed with the adaptive and uniform grids schemes is obtained. Stable simulations are produced by the controlled time stepping, even with a CFL input outside the constant CFL stability limit of the RK 2(3) scheme.

1 Introduction

Multiresolution techniques have been successfully used in the definition of adaptive strategies in combination with different forms of discretizations of partial differential equations. In the present paper, the Sparse Point Representation (SPR) method [1], which falls into this category,

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is employed for adaptive discretizations of Maxwell's equations. The principle is to represent the fields in the physical domain by non uniform samples chosen from uniform meshes, which are dynamically updated as time evolves. For the organization of the discrete fields information, interpolating wavelets are used to indicate where a fine spatial resolution is needed, by choosing those points where significant wavelet coefficients occur. The computation of partial derivatives of a function from the information of its SPR representation is performed in two steps. The first one is a refinement procedure to extend the SPR representation by the inclusion of new interpolated point values in a security zone. Then, for points in the refined grid, such derivatives are approximated by uniform finite differences, using step size proportional to each point local scale. Eventually, required neighboring stencils are not present in the grid. In such case, the corresponding missing point values are approximated from coarser scales. As indicated by the simulation results of previous papers [1, 4, 3], the method leads to sparse grids that adapt to the local smoothness of the fields and track their evolution over time, with substantial gain in computational resources, while controlling the level of accuracy of the finite difference scheme of the regular grid.

In the present paper, we apply the SPR method for the solution of the bidimensional TE_z mode Maxwell's equations, where a fourth order finite difference model in non-staggered grids is used for the discretization of spatial derivatives. However, instead of a low order discretization in time used in our previous work [3], the purpose of the present paper is to improve the performance of the SPR method when applied to the simulation of this kind of problems by considering higher order Runge-Kutta (RK) type schemes. Furthermore, we introduce in the SPR method a controlled time stepping (CTS) procedure to make integration more safe and efficient. The idea is to allow variable time steps, depending on the magnitude of local truncation errors, a usual practice in the ODE community. For the estimation of local truncation errors, we adopt the application of two embedded RK solvers of different orders, in the spirit of the methodology used in [5].

The sections of the paper is organized as follows. Section 2 is dedicated to a brief overview about the SPR method. In Section 3, we present the high order finite difference models, which are adopted in the operational part of the SPR method for our applications of interest. The CTS procedure is described in Section 4. In Section 5, we present some results of numerical simulations. We analyze the effects of the different parameters involved, and discuss the performance improvements of the adaptive strategies. Our concluding remarks are included in Section 6.

2 The SPR Method

The SPR method is an adaptive finite difference strategy for numerical solution of evolution partial differential equations

$$v_t(x, t) = Lv(x, t), \quad t > 0, \quad x \in \Omega \subset \mathbb{R}^d,$$

augmented with initial and boundary conditions. The method combines the simplicity and accuracy of traditional finite difference schemes with the ability of wavelet coefficients in the characterization of local regularity of functions. The method has two basic parts: the operational part, and the representation part. In the operational part, the background context is of an accurate and stable finite difference scheme where the solutions are represented by vectors $V^n = V^{n,j}$ containing approximated node values at points ν in a uniform grid X^j , and time $t^n = n\Delta t$. Namely, $V_\nu^n \approx v(\nu, n\Delta t)$, $\nu \in X^j$. At the next time step, V^{n+1} is obtained by the application of a discrete evolution operator, $V^{n+1} = \mathcal{L}V^n$. The action of $\mathcal{L} = \mathcal{L}^{j,\Delta t}$ includes the discretization of the spatial differential operator L by a difference scheme, the discretization in time by means of some ODE solver, and the enforcement of boundary conditions.

In the representation part, the data is organized by levels of resolution $0 \leq \ell \leq j$, j being the finest scale level. In such multilevel context, the key role is played by interpolating subdivision schemes, which are the basis for the definition of reconstruction operators, wavelet coefficients being precisely the interpolation errors at the new points occurring when going from one level of discretization to the next finer one. At each level l , the wavelet coefficients d^l are defined in terms of local interpolation errors at the new points of the current level of discretization. In the construction of the adapted grids, the idea is to use the wavelet coefficients as indicators of local smoothness of the solution. This is the main ingredient in the definition of the thresholding operator $\mathcal{T}_\varepsilon$: only those points corresponding to wavelet coefficients of magnitude greater than ε should be kept in the adapted grid $\Gamma_\varepsilon \subset X^j$.

In the adaptive SPR method, the goal consists of performing the finite difference model in a more economic fashion, by taking into account local regularity information about the numerical solution. The first step in this direction is the representation of the numerical solution $U_a^n = U_a^{j,n}$ in a sparse grid $\Gamma^n = \Gamma^{j,n}$. Γ^n is expected to be coarse where the solution is smooth, and refined in regions of sharp variations. For the solution to evolve from V_a^n into V_a^{n+1} , three basic steps are undertaken.

1. **Refinement:** $V_a^{n+} \leftarrow \mathcal{E}V_a^n$
2. **Evolution:** $\bar{V}_a^{n+1} \leftarrow \mathcal{L}_a V_a^{n+}$
3. **Coarsening:** $V_a^{n+1} \leftarrow \mathcal{T}_\varepsilon \bar{V}_a^{n+1}$

Refinement is a preemptive processes to prevent possible movement or steepness of the solution between time steps. Since the regions of smoothness or irregularities of the solution may change with time, Γ^n may not be convenient anymore at the next time step $t = t^{n+1}$. Therefore, before

doing the time evolution, the representation of the solution should be extended to a grid Γ^{n+} , which is expected to contain Γ^n and Γ^{n+1} as well. Then, a time evolution operator $\mathcal{L}_a$ is applied. The spatial derivatives at points $\mu \in \Gamma^{n+}$ are performed by means of uniform finite differences, using step size that can be made proportional to the point local scale. Finally, a thresholding operation $\mathcal{T}_\epsilon$ (coarsening) is applied, in order to eliminate from Γ^{n+} those points that are unnecessary for an accurate representation of V_a^{n+1} .

Therefore, in the SPR method the numerical solution is represented in sparse grids dynamically adapted to the solution. The grid updating is performed by two operators: refinement and coarsening. In both cases, the interpolating subdivision scheme plays a crucial role. In the coarsening, it is the basic tool for the definition of the wavelet coefficients which are used as local regularity indicators. In the refinement, it is used to predict the solution at new points added to the grid. It is also used in the computations of the adapted finite differences, when some required stencil points are not in Γ^{n+} . For details of such procedures we refer to [1, 4, 3].

3 High Order Finite Difference Model for Maxwell's Equations

We consider the TE_z mode system in the free space

$$\begin{aligned}\mu \frac{\partial H^z}{\partial t} &= \frac{\partial E^x}{\partial y} - \frac{\partial E^y}{\partial x}, \\ \epsilon \frac{\partial E^x}{\partial t} &= \frac{\partial H^z}{\partial y}, \\ \epsilon \frac{\partial E^y}{\partial t} &= -\frac{\partial H^z}{\partial x},\end{aligned}$$

where $\mathbf{E} = (E^x, E^y, 0)$ and $\mathbf{H} = (0, 0, H^z)$ are the electrical and magnetic fields, ϵ is the electrical permittivity and μ is the magnetic permeability. Both fields are sampled at the same uniform grid $H_{k,l}^z(t) = H^z(k\Delta x, l\Delta y, t)$, $E_{k,l}^x(t) = E^x(k\Delta x, l\Delta y, t)$ and $E_{k,l}^y(t) = E^y(k\Delta x, l\Delta y, t)$. Discretizing in space we obtain the set of ordinary differential equations

$$\frac{d}{dt}H_{k,l}^z = \frac{1}{\mu}(\partial^y E^x)_{k,l} - \frac{1}{\mu}(\partial^x E^y)_{k,l}, \quad (1)$$

$$\frac{d}{dt}E_{k,l}^x = \frac{1}{\epsilon}(\partial^y H^z)_{k,l}, \quad (2)$$

$$\frac{d}{dt}E_{k,l}^y = E_{k,l}^y - \frac{1}{\epsilon}(\partial^x H^z)_{k,l}, \quad (3)$$

where we introduce the finite difference operators

$$(\partial^x v)_{k,l} = \frac{1}{\Delta x} \sum_{k'} v_{k',l} \beta(k - k') \quad (\partial^y u)_{k,l} = \frac{1}{\Delta y} \sum_{l'} u_{k,l'} \beta(l - l'),$$

We consider the fourth order scheme where the non vanishing values for $\beta(k)$, $k > 0$ are $\beta(1) = -\frac{2}{3}$, $\beta(2) = \frac{1}{2}$. For $k < 0$ we have $\beta(k) = -\beta(-k)$, and $\beta(0) = 0$.

3.1 RK2 time integration

Given the vector of the fields samples $H^{z,n} = (H_{k,l}^z(n\Delta t))$, $E^{x,n} = (E_{k,l}^x(n\Delta t))$, and $E^{y,n} = (E_{k,l}^y(n\Delta t))$ at $t = n\Delta t$, we introduce the following two-stage RK formula for the integration of the ODE system (1-3):

1. First stage:

$$H^{z,(1)} = H^{z,n} + \frac{\Delta t}{\mu} (\partial^y E^{x,n}) - \frac{\Delta t}{\mu} (\partial^x E^{y,n}), \quad (4)$$

$$E^{x,(1)} = E^{x,n} + \frac{\Delta t}{\epsilon} (\partial^y H^{z,(1)}), \quad (5)$$

$$E^{y,(1)} = E^{y,n} - \frac{\Delta t}{\epsilon} (\partial^x H^{z,(1)}). \quad (6)$$

2. Second stage

$$H^{z,n+1} = \frac{1}{2} [H^{z,n} + H^{z,(1)} + \frac{\Delta t}{\mu} (\partial^y E^{x,(1)}) - \frac{\Delta t}{\mu} (\partial^x E^{y,(1)})], \quad (7)$$

$$E^{x,n+1} = \frac{1}{2} [E^{x,n} + E^{x,(1)} + \frac{\Delta t}{\epsilon} (\partial^y H^{z,n+1})], \quad (8)$$

$$E^{y,n+1} = \frac{1}{2} [E^{y,n} + E^{y,(1)} - \frac{\Delta t}{\epsilon} (\partial^x H^{z,n+1})]. \quad (9)$$

3.2 Embedded RK2(3) time integration

We also consider the third order embedded RK2(3) scheme where the first stage is the one given by the RK2 scheme and the second and third stages are

Second stage

$$H^{z,(2)} = \frac{1}{4} [3H^{z,n} + H^{z,(1)} + \frac{\Delta t}{\mu} (\partial^y E^{x,(1)}) - \frac{\Delta t}{\mu} (\partial^x E^{y,(1)})], \quad (10)$$

$$E^{x,(2)} = \frac{1}{4} [3E^{x,n} + E^{x,(1)} + \frac{\Delta t}{\epsilon} (\partial^y H^{z,(2)})], \quad (11)$$

$$E^{y,(2)} = \frac{1}{4} [3E^{y,n} + E^{y,(1)} - \frac{\Delta t}{\epsilon} (\partial^x H^{z,(2)})], \quad (12)$$

Third stage

$$H^{z,n+1} = \frac{1}{3}[H^{z,n} + 2(H^{z,(2)} + \frac{\Delta t}{\mu}(\partial^y E^{x,(2)}) - \frac{\Delta t}{\mu}(\partial^x E^{y,(2)}))], \quad (13)$$

$$E^{x,n+1} = \frac{1}{3}[E^{x,n} + 2(E^{x,(2)} + \frac{\Delta t}{\epsilon}(\partial^y H^{z,n+1}))], \quad (14)$$

$$E^{y,n+1} = \frac{1}{3}[E^{y,n} + 2(E^{y,(2)} - \frac{\Delta t}{\epsilon}(\partial^x H^{z,n+1}))], \quad (15)$$

It should be noted that these two schemes are not expressed in the standard formulations for the explicit RK2 and RK2(3) schemes. In fact, at each stage, the components of the electrical field are computed using of the spatial derivatives of the currently updated component of the magnetic field.

Introducing the matrices

$$L = \begin{bmatrix} 0 & 0 & 0 \\ -\frac{\Delta t}{\epsilon}\partial^y & 0 & 0 \\ \frac{\Delta t}{\epsilon}\partial^x & 0 & 0 \end{bmatrix}, \quad U = \begin{bmatrix} 0 & \frac{\Delta t}{\mu}\partial^y & -\frac{\Delta t}{\mu}\partial^x \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and denoting by $V = [H^z, E^x, E^y]^T$, then the RK2 and RK2(3) schemes can be expressed in matrix form by

RK2:

$$\begin{aligned} (I + L)V^{(1)} &= V^n + UV^n \\ (I + \frac{1}{2}L)V_{RK2}^{n+1} &= \frac{1}{2}[V^n + (I + U)V^{(1)}] \end{aligned}$$

RK2(3):

$$\begin{aligned} (I + L)V^{(1)} &= V^n + UV^n \\ (I + \frac{1}{4}L)V^{(2)} &= \frac{1}{4}[3V^n + (I + U)V^{(1)}] \\ (I + \frac{2}{3}L)V_{RK2(3)}^{n+1} &= \frac{1}{3}[V^n + 2(I + U)V^{(2)}] \end{aligned}$$

4 Controlled Time Stepping

For the integration of ODE systems, it is desirable to have a code that automatically adjusts the time step size Δt , which must be chosen sufficiently small to have a required precision $\delta_{desired}$

of the computed results, but it must be sufficiently large to avoid unnecessary computational work. To make such kind of algorithm as efficient as possible, the concept of embedded pairs of Runge-Kutta formulae is helpful. For instance, this is the case of explicit RK2 and RK 2(3) schemes, as described in the previous section. Suppose that we are in possession of the solution $V^n = V(t^n)$ and let V_{RK2}^{n+1} and $V_{RK2(3)}^{n+1}$ be the numerical results of one step of size Δt using the two ODE solvers of order 2 and 3, respectively. The local truncation errors of the two schemes may be expressed in the form

$$V(t^n + \Delta t) - V_{RK2}^{n+1} = \alpha_1 \Delta t^3 + O(\Delta t^4) \quad (16)$$

$$V(t^n + \Delta t) - V_{RK2(3)}^{n+1} = \alpha_2 \Delta t^4 + O(\Delta t^5) \quad (17)$$

Then, for sufficiently small Δt ,

$$V_{RK2(3)}^{n+1} - V_{RK2}^{n+1} \approx C \Delta t^3.$$

This gives the a posteriori estimate

$$|C| \approx \frac{\|V_{RK2(3)}^{n+1} - V_{RK2}^{n+1}\|}{\Delta t^3},$$

and hence the new stepsize required to make the local truncation error of about magnitude $\delta_{desired}$ is $\Delta t_{new} = \Delta t \xi$, where

$$\xi = \left[\frac{\delta_{desired}}{\|V_{RK2(3)}^{n+1} - V_{RK2}^{n+1}\|} \right]^{1/3}.$$

One advantage of using embedded RK schemes is that part of the computation of the higher order solution is already done in the computation of the low order solution. Furthermore, it is never necessary to calculate the low order solution V_{RK2}^{n+1} explicitly. In fact, since $4(I + \frac{1}{4}L)V^{(2)} - 3V^n = (I + U)V^{(1)}$, we can express the RK2 solution as

$$\begin{aligned} V_{RK2}^{n+1} &= \frac{1}{2}(I + \frac{1}{2}L)^{-1}[V^n + (I + U)V^{(1)}] \\ &= (I + \frac{1}{2}L)^{-1}[2(I + \frac{1}{4}L)V^{(2)} - V^n]. \end{aligned}$$

This means that to obtain the solution $V_{RK2(3)}^{n+1}$ at t^{n+1} and to perform the CTS analysis we only need the solution at t^n and result of the second stage $V^{(2)}$. Consequently, during one RK2(3) step we only need to store the solution at t^n and the result at the current stage.

In typical CTS implementations, and depending on the size of Δt_{new} , the computed solution is

accepted or rejected. As proposed in [5], we never reject the current solution, and the estimated Δt_{new} is used to perform the next time stepping. To increase the likelihood that, in fact, this strategy produces an error less than $\delta_{desired}$ after few iterations, and that this level of accuracy is preserved for the remaining time interval, we impose the limitation of the step variation

$$-\frac{\mathcal{S}}{2} \leq \frac{\Delta t_{new} - \Delta t}{\Delta t} \leq \frac{\mathcal{S}}{2},$$

where $\mathcal{S}$ is a given safety factor. As shown in the numerical tests of the next section, the choice of $\mathcal{S}$ is an important issue.

5 Numerical Results

In the present section we analyze the performance of the SPR method for the numerical solution of the TE mode system of Maxwell's equations. In the operational part, we shall use the finite difference scheme described in Section 3, namely, the fourth order finite difference scheme in non-staggered grids combined with high order time integrations by RK2 or RK2(3). Our purpose is to analyse the effect of increasing the time integration order, when compared with the low order scheme presente in [3], and to illustrate the accuracy and efficiency of the space adaptivity by means of the SPR scheme when combined with a control of the time stepping.

We consider an example where the fields at $t = 0$ are assumed to be $E^x(x, y) = E^y(x, y) = 0$ and $H^z(x, y) = e^{-3500(x-\frac{1}{2})^2} e^{-3500(y-\frac{1}{2})^2}$. We restrict the problem to the computational domain $R = [0, 1] \times [0, 1]$, and we assume PEC+PML boundary conditions. We assume that the uniform grids X^j have the same spacing in both directions $\Delta^j x = \Delta^j y = \Delta = 2^{-j}$.

In the SPR simulations, the coarsest grid is X^3 , having 9×9 points. If ε_H is the threshold for the magnetic field, then the threshold for the electrical fields is $\varepsilon_E = 100 \times \varepsilon_H$. Since the time evolution of the electrical fields requires the partial derivatives of the magnetic field, and vice versa, the time stepping in the SPR scheme is performed on a nonuniform sparse grid formed by the union of the extended SPR grids of the three fields.

For the CTS schemes, an input CFL parameter $CFL(0)$ is provided by the user, and $CFL(t)$ evolves according to the new Δt obtained by the time step control. Since the electric fields are about two orders of magnitude larger than the magnetic field, we only monitor the error in the E^x field.

5.1 Calibration of the Parameters

To analyse the effect of the parameters involved in the reference scheme, we perform the tests in a uniform grid X^7 , and time interval $0 \leq t \leq 1$.

CFL stability limits with constant time step

For this problem, the simulations of the reference finite difference scheme in the time interval $[0, 5.0]$ (ns), with constant time step, we found stable results for $CFL \leq 0.84$, with the RK2 scheme and $CFL \leq 1.05$ with RK2(3) scheme, where

$$CFL = \frac{\Delta t}{\sqrt{\mu\epsilon}\Delta}.$$

For the corresponding lower order scheme (explicit Euler scheme) present in [4], the Von Neumann stability analysis gives the stability limit $CFL \leq 1.0306$.

Effects of the Safety Factor $\mathcal{S}$, initial $CFL(0)$ and desired accuracy $\delta_{desired}$

To analyze the effect of safety factor parameter, we considered $\mathcal{S} = 0.025$ and 0.05 in the CTS scheme, and we observed the behavior of the $CFL(t)$ evolution for different values of initial input $CFL(0)$, under, close and above the constant time step stability limit, and different levels of desired accuracy levels. We concluded from these results that allowing only 0.25% of time step variation, and if we start with large CFL, then the CTS scheme can not control the error in the early stages. If $CFL(0)$ is chosen outside the stability limit of the RK2(3) scheme, then the problem becomes even worst, since instabilities may occur before the error can be controlled. Increasing the safety factor, allowing 0.5% of step variation, helps to alleviate these problems. However, it is clear that using a constant safety factor is not the best option in such kind of CTS strategy. The proposal in [5] is to use a large safety factor $\mathcal{S}_0$ at the early stages, to get the desired accuracy as fast as possible. Then, the time step variation is forced to decrease exponentially to a lower level $\mathcal{S}_{min}$ that is able to guarantee a safe time evolution.

For the results shown in Figure 1 the choice is $\mathcal{S}_0 = 0.5$ and $\mathcal{S}_{min} = 0.05$. To illustrate the effect of the parameters $CFL(0)$ and $\delta_{desired}$, for the plots show the evolution of the CFL parameter given the inputs $CFL(0) = 0.4$ (top), 0.8 (middle) and 1.2 (bottom), for $\delta_{desired} = 0.1, 0.01$ and 0.001 . On the right side of Figure 1 the plots indicate the the truncation error for these tests. In all the cases we can observe that there is an early stage when the CFL is decreased to a minimum level in order to get the desired accuracy. After that, the truncation error is kept controlled while $CFL(t)$ is allowed to increase. Close to the final time, when the fields are damped, the tendency is of decreasing error magnitude, and the CFL may reach values outside the constant CFL stability limit, without unstabilizing the computations.

For the results in Figure 2 we reduce the safety factor variation to $0.01 \leq \mathcal{S} \leq 0.1$, with exponential decay. For $\delta_{desired} = 0.05$, the plots show the evolution of CFL parameter and truncation errors given the inputs $CFL(0) = 0.4, 0.8$ and 1.2 . Due to the reduced safety factor, the scheme takes more iterations to put the truncation error under the desired accuracy level.

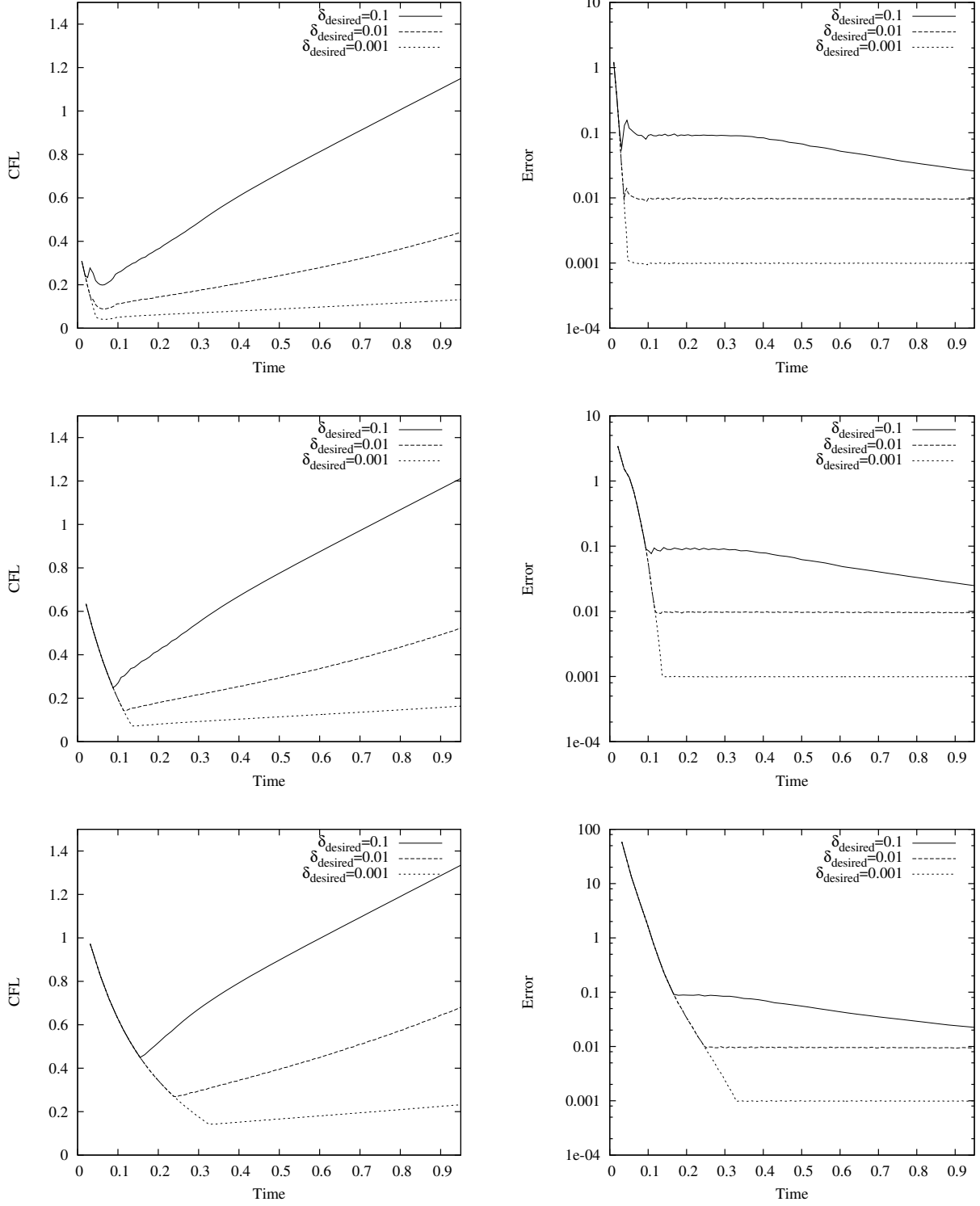


Figure 1: The effect of $CFL(0)$ and δ_{desired} using variable safety factor $0.05 \leq \mathcal{S} \leq 0.5$, with exponential decay.

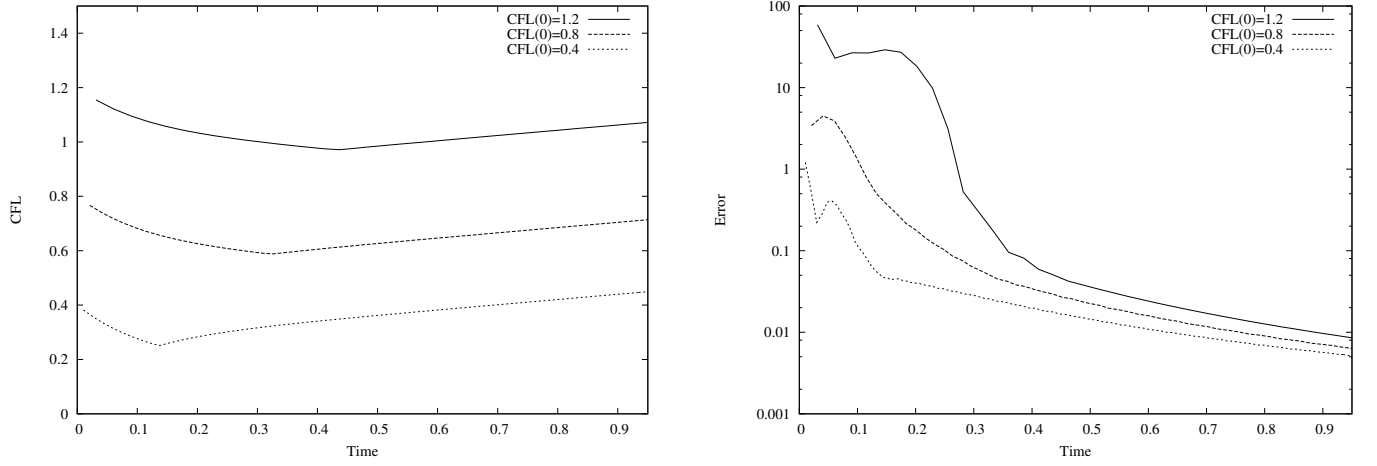


Figure 2: CFL and truncation error evolutions for $\delta_{desired} = 0.05$ and variable safety factor $0.01 \leq \mathcal{S} \leq 0.1$, with exponential decay.

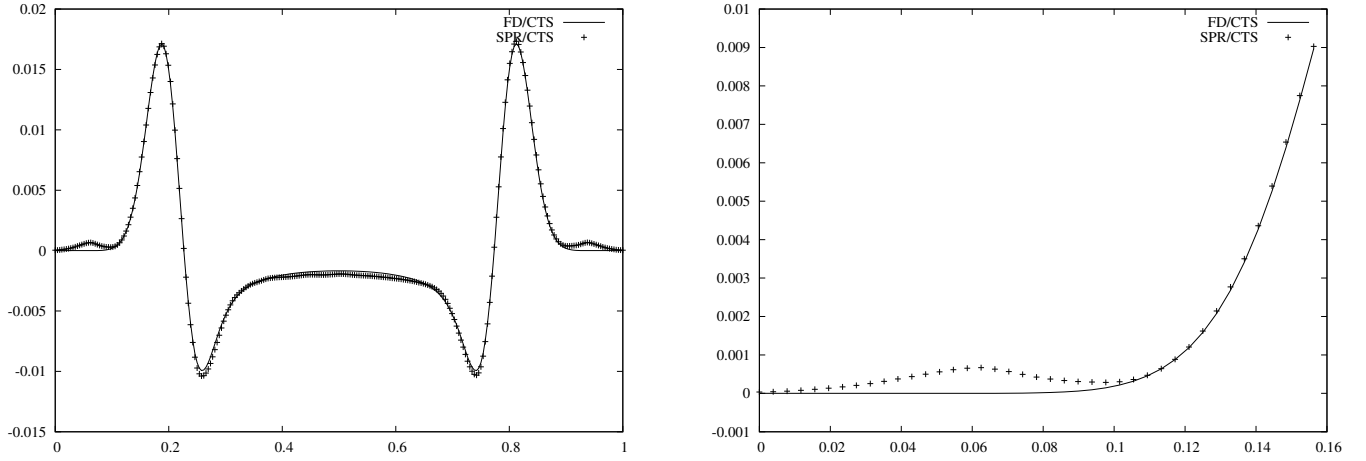


Figure 3: Contours for the magnetic field (left) on the line $y = 0.5$ for $t = 1.0ns$, $j = 8$, $\varepsilon_H = 10^{-4}$, $\delta_{desired} = 0.05$. Corresponding zoom of the left PML layer.

After that, the error is kept controlled for the remaining time, but the CFL is maintained almost constant.

5.2 The Combined SPR/CTS Scheme

The plots in Figure 3 correspond to cuts at the line $y = 0.5$ of the magnetic fields at the final time $t = 1.0ns$ computed with the FD/CTS and SPR/CTS methods with $j = 8$. The CTS parameters are $\delta_{desired} = 0.05$, $CFL(0) = 0.8$ and $0.01 \leq \mathcal{S} \leq 0.1$, and the SPR threshold parameter is $\varepsilon_H = 0.0001$. We find good agreement between both CTS schemes in regular and adaptive grids. The zoom in of the left PML layer reveals a small perturbation in the SPR solution.

6 Concluding Remarks

In the present paper, we apply the SPR method for the solution of the bidimensional TE_z mode Maxwell's equations. A fourth order finite difference model in non-staggered grids is used for the SPR discretization of spatial derivatives. The time integration is performed by embedded Runge-Kutta 2(3) scheme that allow a controlled time stepping (CTS) procedure, where the time step is automatically adjusted during the time evolution. A good agreement of the solutions computed with regular and adaptive CTS schemes is obtained. Stable simulations are produced by the CTS scheme, even with a CFL input outside the constant CFL stability limit of the RK2(3) scheme.

In future work we plan perform more tests to better calibrate the parameters involved. For instance, we believe that the safety factor deserves a more detailed analysis, other embedded schemes may be considered, and the error control may be improved by allowing step rejections.

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