High Accuracy Models for Source Terms in the Nonstandard FDTD Algorithm

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***Abstract*—The nonstandard finite difference time domain (FDTD) algorithm gives high accuracy solutions on a coarse grid to the homogeneous wave equation and the source-free Maxwell's equations. We now extend the NSFD methodology to include sources both for the scattered field and for free space sources. We demonstrate the high accuracy of this approach by comparing with analytical solutions.**

I. INTRODUCTION

For simplicity we introduce the basic concepts for the wave equation before extending them to Maxwell's equations. Let a scatterer of relative refractive index n_s be immersed in a medium of phase velocity v_0. The wave equation is

$$\left[\partial_t^2 - \frac{v_0^2}{n(\boldsymbol{x})^2}\nabla^2\right]\psi(\boldsymbol{x},t) = 0, \qquad (1.1)$$

where $\boldsymbol{x} = (x,y,z)$ and $n(\boldsymbol{x}) = n_s$ / 1 inside / outside the scatterer. The total field is $\psi = \psi_0 + \psi_s$, where ψ_0 / ψ_s is the incident / scattered field. By definition the incident field propagates as if there were no scatterer according to,

$$\left[\partial_t^2 - v_0^2\nabla^2\right]\psi_0(\boldsymbol{x},t) = 0. \qquad (1.2)$$

Subtracting (1.2) from (1.1) we obtain the wave equation for the scattered field,

$$\left[\partial_t^2 - \frac{v_0^2}{n(\boldsymbol{x})^2}\nabla^2\right]\psi_s(\boldsymbol{x},t) = s(\boldsymbol{x},t), \qquad (1.3)$$

where

$$s(\boldsymbol{x},t) = \left(\frac{n(\boldsymbol{x})^2 - 1}{n(\boldsymbol{x})^2}\right)\partial_t^2\psi_0(\boldsymbol{x},t) \qquad (1.4)$$

is the source of the scattered field.

II. STANDARD FDTD

In the conventional or standard (S) finite difference (FD) model, the derivatives of the wave equation are replaced by central finite difference (FD) approximations. Defining d_t by $d_t f(x,t) = f(x,t+\Delta t/2) - f(x,t-\Delta t/2)$ the first derivative is approximated by

$$\partial_t f(x,t) \cong d_t f(x,t)/\Delta t$$

and the second one by

$$\partial_t^2 f(x,t) \cong d_t^2 f(x,t)/\Delta t^2,$$

where $d_t^2 f(x,t) = f(x,t+\Delta t) + f(x,t-\Delta t) - 2f(x,t)$. FD operators for ∂_x, ∂_y and ∂_z are analogously defined. Forming $\boldsymbol{d}^2 = d_x^2 + d_y^2 + d_z^2$, $\nabla^2 f(\boldsymbol{x}) \cong \boldsymbol{d}^2 f(\boldsymbol{x})/h^2$, where $h = \Delta x = \Delta y = \Delta z$. Replacing the derivatives in (1.3) with FD approximations, we obtain

$$\left[d_t^2 - \frac{v_0^2\Delta t^2}{n(\boldsymbol{x})^2 h^2}\boldsymbol{d}^2\right]\psi_s(\boldsymbol{x},t) = \Delta t^2 s(\boldsymbol{x},t). \qquad (2.1)$$

Solving for $\psi_s(\boldsymbol{x},t+\Delta t)$, we find

$$\psi_s(\boldsymbol{x},t+\Delta t) = -\psi_s(\boldsymbol{x},t-\Delta t) + \left[2 + \frac{v_0^2\Delta t^2}{n(\boldsymbol{x})^2 h^2}\boldsymbol{d}^2\right]\psi_s(\boldsymbol{x},t) + \Delta t^2 s(\boldsymbol{x},t). \qquad (2.2)$$

This is the FDTD algorithm found in textbooks, such as [1]. Although simple to implement, the accuracy of standard (S) FDTD is low.

In the homogeneous case ($s = 0$) at wavelength λ, the error is $\varepsilon \sim (h/\lambda)^2$ while computational cost is $C \sim 1/h^4$ in three dimensions, because Δt must scale as h to maintain numerical stability in accord with the CFL condition [1]. Thus computational cost rises faster than the error falls. Accuracy cannot be improved by using higher order FD approximations. Mickens [2] has shown that when the order of the FD approximations in the FD model exceeds that of the derivatives in the original differential equation, numerical instability can arise and the algorithm can yield spurious solutions.

III. NONSTANDARD FDTD

For monochromatic waves the accuracy can be greatly improved by using what is called the nonstandard (NS) FDTD algorithm [3].

In one dimension (1.1) becomes

$$\left[\partial_t^2 - \frac{v_0^2}{n^2}\partial_x^2\right]\psi(x,t) = 0, \qquad (3.1)$$

and its S-FD model is

$$\left[d_t^2 - \frac{v_0^2\Delta t^2}{n^2 h^2}d_x^2\right]\psi(x,t) = 0. \qquad (3.2)$$

In each region of constant n a plane wave solution of (3.1) is

$\varphi = e^{i(nk_0 x - \omega t)}$, where $v_0 = \omega / k_0$. Substituting φ into (3.2), we find

$$\left[d_t^2 - \frac{v_0^2 \Delta t^2}{n^2 h^2} d_x^2 \right] \varphi = \varepsilon \varphi, \qquad (3.3)$$

where the S-FDTD solution error is

$$\varepsilon = 4\left[-\sin^2(\omega \Delta t/2) + \frac{v_0^2 \Delta t^2}{n^2 h^2} \sin^2(nk_0 h/2) \right]. \qquad (3.4)$$

Except for the special case $v_0^2 \Delta t^2 / n^2 h^2 = 1$, ε does not vanish because φ is not a solution of difference equation (3.2). We can, however, force ε to vanish by replacing $v_0^2 \Delta t^2 / n^2 h^2$ with $\tilde{v}_0^2 / \tilde{n}^2$ in model (3.2). The NS-FD model is

$$\left[d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} d_x^2 \right] \psi(x,t) = 0, \qquad (3.5)$$

where

$$\tilde{v}_0 = \frac{\sin(\omega_0 \Delta t/2)}{\sin(k_0 h/2)} \text{ and } \tilde{n}(x) = \frac{\sin[n(x) k_0 h/2]}{\sin[k_0 h/2]}$$ is the effective refractive index on the spatial grid. In the limits $h \to 0$ and $\Delta t \to 0$, $\tilde{v}_0 \to v_0 \Delta t$ and $\tilde{n} \to n$ as expected.

The wave equation (3.1) and the difference equation (3.5) now have the same solution. Solving (3.5) for $\psi(x, t+\Delta t)$, we obtain the NS-FDTD algorithm,

$$\psi(x,t+\Delta t) = -\psi(x,t-\Delta t) + \left[2 + \frac{\tilde{v}_0^2}{\tilde{n}^2} d_x^2 \right] \psi(x,t). \qquad (3.6)$$

This algorithm, using just second order FD approximations, is exact in each region of constant n with respect to monochromatic waves.

In two and three dimensions the S-FD model of (1.1) is

$$\left[d_t^2 - \frac{v_0^2 \Delta t^2}{n^2 h^2} \boldsymbol{d}^2 \right] \psi(\boldsymbol{x},t) = 0, \qquad (3.7)$$

and its error with respect to plane wave solutions of the form $\varphi = e^{i(n\boldsymbol{k}_0 \cdot \boldsymbol{x} - \omega_0 t)}$ (where $k_0 = |\boldsymbol{k}_0|$) is $\varepsilon_S \sim (k_0 h)^2 / 12$.

It is not possible to construct an exact NS-FDTD algorithm, but we can make a very accurate one. As shown in [4] the NS-FD model in two and three dimensions is

$$\left[d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}(\boldsymbol{x})^2} \tilde{\boldsymbol{d}}(n)^2 \right] \psi(\boldsymbol{x},t) = 0, \qquad (3.8)$$

where

$$\tilde{\boldsymbol{d}}^2 = \boldsymbol{d}^2 + \gamma_1 \left[d_x^2 d_y^2 + d_x^2 d_z^2 + d_y^2 d_z^2 \right] + \gamma_2 \left[d_x^2 d_y^2 d_z^2 \right], \qquad (3.9)$$

is a superposition of different FD operators with the superposition weights given by

$$\gamma_1(n) \cong \frac{1}{6} + \frac{(nk_0 h)^2}{180} + \frac{(nk_0 h)^4}{7698} \cdots,$$

$$\gamma_2(n) \cong \frac{1}{30} - \frac{(nk_0 h)^2}{905} - \frac{(nk_0 h)^4}{7698} - \cdots.$$

The two-dimensional form of $\tilde{\boldsymbol{d}}^2$ is given by setting $d_z = 0$ in (3.9). Note the dependence on both refractive index and free space wavenumber. With respect to plane waves it can be shown that the error of the NS-FD model is $\varepsilon_{NS} \sim (k_0 h)^6 / 24192 \ll \varepsilon_S \sim (k_0 h)^2 / 12$. In addition, ε_S is highly anisotropic with respect to the propagation direction of φ, while ε_S is very nearly isotropic.

IV. Nonstandard Model of the Scattered Field

Take the incident field to be an infinite plane wave, $\psi_0 = e^{i(\boldsymbol{k}_0 \cdot \boldsymbol{x} - \omega_0 t)}$. In free space the NS-FD model (3.8) reduces to

$$\left[d_t^2 - \tilde{v}_0^2 \tilde{\boldsymbol{d}}(1)^2 \right] \psi(\boldsymbol{x},t) = 0 \qquad (4.1)$$

Subtracting (4.1) from (3.8) we obtain the NS-FD model of the scattered field,

$$\left[d_t^2 - \frac{\tilde{v}_0^2}{\tilde{n}^2} \tilde{\boldsymbol{d}}^2(n) \right] \psi_s(\boldsymbol{x},t) = \tilde{s}(\boldsymbol{x},t), \qquad (4.2)$$

where

$$\tilde{s} = \frac{1}{\tilde{n}^2} \left[4(\tilde{n}^2 - 1) \sin^2(\omega_0 \Delta t/2) + \tilde{v}_0^2 \Delta \tilde{\boldsymbol{d}}^2(n) \right] \psi_0, \qquad (4.3)$$

and $\Delta \tilde{\boldsymbol{d}}^2(n) = \tilde{\boldsymbol{d}}^2(n) - \tilde{\boldsymbol{d}}^2(1)$. When $\boldsymbol{k}_0$ is parallel to either the *x*-, *y*- or *z*-axis it is easy to show that $\Delta \tilde{\boldsymbol{d}}^2(n) \psi_0$ vanishes. Using (1.4) and comparing with the S-FD model of (2.1), where

$$s \Delta t^2 = \Delta t^2 \omega_0^2 \left(\frac{1 - n^2}{n^2} \right) \psi_0, \qquad (4.4)$$

in the limits $h \to 0$ and $\Delta t \to 0$, we see that $s \Delta t^2 \to \tilde{s}$.

The NS-FDTD algorithm for the scattered field due to an incident monochromatic infinite plane wave is thus

$$\psi_s(\boldsymbol{x}, t+\Delta t) = -\psi_s(\boldsymbol{x}, t-\Delta t) + \left[2 + \frac{\tilde{v}_0^2}{\tilde{n}^2} \tilde{\boldsymbol{d}}^2 \right] \psi_s(\boldsymbol{x},t) + \tilde{s}(\boldsymbol{x},t). \qquad (4.5)$$

Let us now compare the performance of the S-FDTD and NS-FDTD algorithms on a scattering problem.

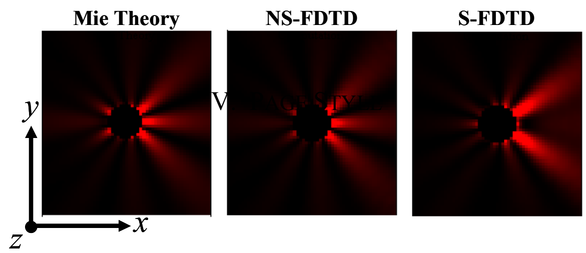

Fig. 1. Scattered intensity due to an incident electromagnetic wave with the electric field polarized along cylinder (*z*-) axis. Scattered intensity visualized in shades of red; black = zero field or cylinder interior.

A plane wave of vacuum wavelength λ_0 impinges perpendicularly to its axis upon an infinite dielectric cylinder of refractive index $n_s = 1.7$ and radius $= 0.75\lambda_0$. Computing the scattered field intensity using the S-FDTD and NS-FDTD algorithms and comparing with Mie theory [5], we find that NS-FDTD gives superior accuracy at discretization of $\lambda_0/h = 8$.

In the case an electromagnetic wave with its electric field polarized parallel to the z -axis (TE mode), it can be shown that, the scattered electric field is $\boldsymbol{E}_s = (0,0,\psi_s)$.

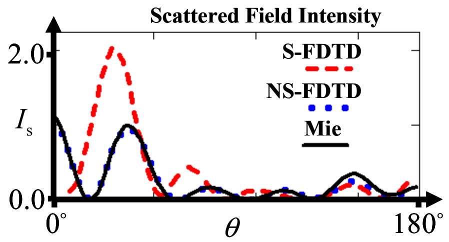

Fig. 2. Scattered intensity on a contour of outside the cylinder as a function of angle (θ) from the incident direction.

We have extended this methodology to the absorbing wave equation and to the Maxwell's equations [4] and have verified its high accuracy.

V. NS Model of a Source in Free Space

In one dimension the wave equation is with a source is

$$\left(\partial_t^2 - v^2\partial_x^2\right)\psi(x,t) = s(x,t)\,, \qquad (5.1)$$

Assuming the initial conditions

$$\psi(x,0) = 0\,, \qquad (5.2a)$$

$$\partial_t\psi(x,0) = 0\,, \qquad (5.2b)$$

let the source turn on at $t = 0$, thus

$$s(x,t) = 0 \text{ for } t \le 0\,. \qquad (5.3)$$

The Green's function, appropriate to (5.1) and (5.2) is

$$G(x-x',t-t') = \frac{1}{2v}\Theta\left(v(t-t') - |x-x'|\right), \qquad (5.4)$$

where, Θ is the step function ($\Theta(t<0)=0$, $\Theta(t \ge 0)=1$). The general solution of (5.1) is

$$\psi(x,t) = \int_{-\infty}^{\infty} dt' \int_{-\infty}^{\infty} dx' G\left(x-x',t-t'\right)s(x',t')\,. \qquad (5.5)$$

Let $s = s_0$, where $s_0(x,t) = \delta(x)\Theta(t)e^{i\omega t}$, which is a harmonic source which switches on at time =0. Carrying out the integration, the field, ψ_0, due to s_0 is

$$\psi_0(x,t) = \Theta\left(\omega t - k|x|\right)\frac{1}{2iv\omega}\left[e^{i(\omega t - k|x|)} - 1\right]. \qquad (5.6)$$

The S-FD model for $s = s_0$ is

$$\left(d_t^2 + \frac{v^2\Delta t^2}{h^2}d_x^2\right)\psi(x,t) = \frac{\Delta t^2}{h}\delta_{x,0}\,\Theta(t)\,e^{i\omega t} \qquad (5.7)$$

Inserting solution (5.6) into model (5.7) we see that it is not a solution of (5.7).

Let us now postulate a NS-FD model of (5.1) with $s = s_0$ of the form

$$\left(d_t^2 - \tilde{v}^2 d_x^2\right)\psi(x,t) = A_{\mathrm{NS}}\delta_{x,0}\,\Theta(t)\,e^{i\omega t}\,, \qquad (5.8)$$

where $\tilde{v} = \sin(\omega\Delta t/2)/\sin(kh/2)$ and A_{NS} is the NS source amplitude, which is to be determined. Inserting $\psi_0(x=0, t>\Delta x/v)$ into (5.8) and using the identities

$$d_x^2 e^{-ik|x|}\Big|_{x=0} = -4ie^{-ik\Delta x/2}\sin(k\Delta x/2)\,, \qquad (5.9a)$$

$$d_t^2 e^{i\omega t}/e^{i\omega t} = -4\sin^2(\omega\Delta t/2)\,, \qquad (5.9b)$$

the equality of (5.8) holds at both $x = 0$ and $x \ne 0$ if

$$A_{\mathrm{NS}} = \frac{2}{v\omega}\frac{\sin^2(\omega\Delta t/2)}{\tan(k\Delta x/2)}\,. \qquad (5.10)$$

In the limits $\Delta x \to 0$ and $\Delta t \to 0$, the NS-FD model reduces to the S-FD one.

It can be shown that the NS amplitude that we have derived here is valid for two and three dimensions.

VI. Conclusions

The correct treatment of source terms greatly improves the accuracy of FDTD calculations, which we have demonstrated by comparing with analytic solutions.

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