Fixed angle broadband simulations in MEEP

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1 Introduction

Currently in MEEP, Bloch Periodic boundary conditions are implemented, which fix the wave vector of an incident wave [1]. As a result, the angle of an oblique incident wave becomes frequency dependent. Following the procedure detailed by B. Liang et al [2], all fields can be redefined so that the boundary conditions become periodic and the angle of the incident wave can be fixed over a broad frequency spectrum. This requires the addition of a new field. It is assumed that the reader is already familiar with the UPML formulation in MEEP [3], from which the equations will be modified.

2 Boundary conditions

The fields from section 3 of *Notes on the UPML implementation in MEEP* [3] are first redefined as:

$$\mathrm{field}'(x, y, z) = \mathrm{field}(x, y, z)e^{-i(k_x x + k_y y)}, \tag{1}$$

where k_x and k_y are the wave vector components in the x and y directions. This is for a structure which is periodic in these directions. Taking the electric field E as an example, the new boundary condition can be expressed as

$$E'(x + a, y + b, z) = E(x + a, y + b, z)e^{-i(k_x(x+a)+k_y(y+b))} \tag{2}$$

where a is the length of the unit cell in the x direction and b in the y direction. Substituting in the original Bloch periodic boundary conditions gives

$$E'(x + a, y + b, z) = E(x, y, z)e^{i(k_x a+k_y b)}e^{-i(k_x(x+a)+k_y(y+b))}. \tag{3}$$

Cancelling the a and b terms gives

$$E'(x + a, y + b, z) = E(x, y, z)e^{-i(k_x x+k_y y)} = E'(x, y, z), \tag{4}$$

and so the boundary conditions are now periodic.

3 Formulation

Equation (5) from section 3 of *Notes on the UPML implementation in MEEP* [3] is

$$\vec{K} = \nabla \times \vec{H} = -i\omega(1 + \frac{i\sigma_D}{\omega})\vec{C}, \tag{5}$$

where $\vec{H}$ is the magnetic field, σ_D the conductivity and $\vec{C}$ an auxiliary field. When the magnetic field is redefined, the curl of a product must be carried out:

$$\nabla \times \vec{H'} = \nabla \times (\vec{H}e^{-i(k_x x + k_y y)}) \tag{6}$$

so,

$$\nabla \times \vec{H'} = e^{-i(k_x x + k_y y)} \nabla \times \vec{H} + \begin{pmatrix} -ik_x \\ -ik_y \\ 0 \end{pmatrix} \times \vec{H'} \tag{7}$$

where the complex exponential in the second term has been absorbed by $\vec{H'}$. Substituting in equation (5) gives

$$\nabla \times \vec{H'} = \vec{K'} = -i\omega(1 + \frac{i\sigma_D}{\omega})\vec{C'} + \begin{pmatrix} -ik_x \\ -ik_y \\ 0 \end{pmatrix} \times \vec{H'}. \tag{8}$$

From here on in, the prime notation can be dropped since this applies to all fields. By introducing a new field $\vec{F}$, equation (8) can be written as

$$\vec{K} = -i\omega(1 + \frac{i\sigma_D}{\omega})\vec{C} - i\omega\vec{F}. \tag{9}$$

This new field satisfies the equation:

$$\vec{F} = \vec{\bar{k}} \times \vec{H}, \tag{10}$$

where

$$\vec{\bar{k}} = \frac{1}{\omega}\begin{pmatrix} k_x \\ k_y \\ 0 \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ 0 \end{pmatrix} \tag{11}$$

and so $\vec{\bar{k}}$ is the wave vector with its frequency dependence removed. θ and ϕ are the propagating direction angles and c, the speed of light is taken to be 1. Therefore by defining $\vec{F}$, the angle of the incident wave is fixed. Equation (10) can be discretized as:

$$\vec{F}^{n+1} = 2\vec{\bar{k}} \times \vec{H}^{n+0.5} - \vec{F}^{n}. \tag{12}$$

Transforming equation (5) to the time domain gives:

$$\vec{K} = \frac{\partial\vec{C}}{\partial t} + \sigma_D\vec{C} + \frac{\partial\vec{F}}{\partial t}. \tag{13}$$

This can be discretized as:

$$\vec{K}^{n+0.5} = \frac{\vec{C}^{n+1} - \vec{C}^{n}}{\Delta t} + \sigma_D \frac{\vec{C}^{n+1} + \vec{C}^{n}}{2} + \frac{\vec{F}^{n+1} - \vec{F}^{n}}{\Delta t} \tag{14}$$

and then solved to update the value of $\vec{C}$ using:

$$\vec{C}^{n+1} = (1 + \frac{\sigma_D \Delta t}{2})^{-1}[(1 - \frac{\sigma_D \Delta t}{2})\vec{C}^{n} + \Delta t \vec{K}^{n+0.5} + \vec{F}^{n} - \vec{F}^{n+1}]. \tag{15}$$

All other equations are unaffected by these changes.

A new field must be introduced because $\vec{H}$ is defined at $n + \frac{1}{2}$ timesteps whereas $\vec{C}$ is defined at n timesteps, where n is an integer. As a result, if the derivative in $\vec{F}$ in equation (14) was replaced with

$$\vec{\bar{k}} \times (\frac{\vec{H}^{n+0.5} - \vec{H}^{n-0.5}}{\Delta t}), \tag{16}$$

only first order accuracy would be achieved, since this is a backward difference scheme. To achieve second order accuracy would require $\vec{H}^{n+1.5}$ to be known.

4 Stability

As the incident angle increases, the maximum possible Δt value decreases, following the formula:

$$\frac{c\Delta t}{\Delta x} \leq \frac{(1 - sin(\theta))}{\sqrt{D}} \tag{17}$$

where D is the number of dimensions [2].

References

[1] Taflove A., Oskooi A., Johnson S.. *Advances in FDTD Computational Electrodynamics: Photonics and Nanotechnology.* Artech House, Inc.; 2013

[2] Liang B., Bai M., Ma H., Ou N., Miao J.. Wideband Analysis of Periodic Structures at Oblique Incidence by Material Independent FDTD Algorithm. *IEEE Transactions on Antennas and Propagation*, vol. 62, no. 1, pp. 354-360, Jan. 2014, doi: 10.1109/TAP.2013.2287896.

[3] Johnson S. *Notes on the UPML implementation in Meep.* Massachusetts Institute of Technology. Posted August 17, 2009; updated March 10, 2010. http://ab-initio.mit.edu/meep/pml-meep.pdf