Harnessing the cloud to understand light: A whitepaper detailing the MaxwellFDS core solver

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Introduction

MaxwellFDS is a cloud-powered electromagnetic solver, tailored specifically to the field of nanophotonics. MaxwellFDS stands for Frequency-Domain Solver.

1 Motivation: why another electromagnetic solver?

Although many electromagnetic simulation packages are currently available, we found it necessary, for our own purposes, to create our own. Specifically, we desired a simulator which

- operates in the frequency-domain, as opposed to the time-domain.
- scales to multiple high-resolution three-dimensional domains,
- is readily accessible via Matlab.

1.1 The advantages of frequency-domain solutions

The advantages of solving Maxwell's equations in the *frequency*-domain as opposed to simulating them in the *time*-domain include

- clean excitation of input modes,
- precise characterization of material dispersion,
- calculation of figure of merits outside of the simulation,
- explicit measurement of simulation error, and
- explicit calculation of eigenmodes.

1.1.1 Input: clean excitation of modes

1.1.2 Dispersion: precise characterization of frequency-dispersion

1.1.3 Output: complete description of device performance

1.1.4 Error: explicit measurement of simulation error

1.1.5 Eigenmodes: explicit calculation of eigenmodes

1.2 The advantages of simulating in the cloud

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2 Harnessing the cloud to understand light

2.1 Accessing

3 Solving the electromagnetic wave equation using MaxwellFDS

3.1 Analytic derivation of the electromagnetic wave equation

The electromagnetic wave equation can be derived from the differential form of Maxwell's equations, that is,

$$\nabla \times E = -\mu \frac{\partial H}{\partial t} \tag{1a}$$

$$\nabla \times H = J + \epsilon \frac{\partial E}{\partial t}, \tag{1b}$$

where E, H, and J are the electric, magnetic and electric current vector fields, respectively, ϵ is the permittivity and μ is the permeability.

Assuming the time dependence $\exp(-i\omega t)$, where ω is the angular frequency, these become

$$\nabla \times E = -i\mu\omega H \tag{2a}$$
$$\nabla \times H = J + i\epsilon\omega E, \tag{2b}$$

which we can combine to form the time-harmonic wave equation for E,

$$\nabla \times \mu^{-1}\nabla \times E - \epsilon\omega^2 E = -i\omega J, \tag{3}$$

which MaxwellFDS solves

Note that the alternative wave equation for H, where we consider the magnetic current source M instead of J,

$$\nabla \times \epsilon^{-1}\nabla \times H - \mu\omega^2 H = -i\omega M, \tag{4}$$

can also be solved using MaxwellFDS .

3.2 Numerical discretization of the wave equation

3.2.1 Use of the Yee cell

To solve (3) we discretize our vector fields based on a primitive Yee cell, as shown in figure 1. Similarly to the finite-difference time-domain simulation technique, the use of the Yee cell allows the $\nabla\times$ operators to be well-defined.

In this configuration, the E, J, and ϵ vector fields are positioned on the $E_{x,y,z}$ locations while the H, M (in the case of (4)) , and μ vector fields are placed on the $H_{x,y,z}$ locations.

To define the distances between adjacent field components, MaxwellFDS uses the following convention:

- d_w^{prim} denotes the distance in the direction i between E_w components for $w = x, y, z$, and
- d_w^{dual} denotes the distance in the direction i between H_w components for $w = x, y, z$.

This definition allows us to precisely define the numerical derivatives found in the $\nabla\times$ operators.

3.2.2 Use of a periodic "wrap-around" grid

MaxwellFDS features periodic "wrap-around" boundary conditions in the definition of the $\nabla\times$ operators in (3). For example, this means that the operation $\frac{\partial}{\partial x}H_y$ is still well-defined at the $x = 0$ boundary as $(H_y|^{x=0} - H_y|^{x=x_{\max}})/d_x^{\text{prim}}$.

More specifically, MaxwellFDS calls the elements in the Yee cell at (i, j, k) as $E_x(i, j, k)$, $E_y(i, j, k)$, ... and then denotes

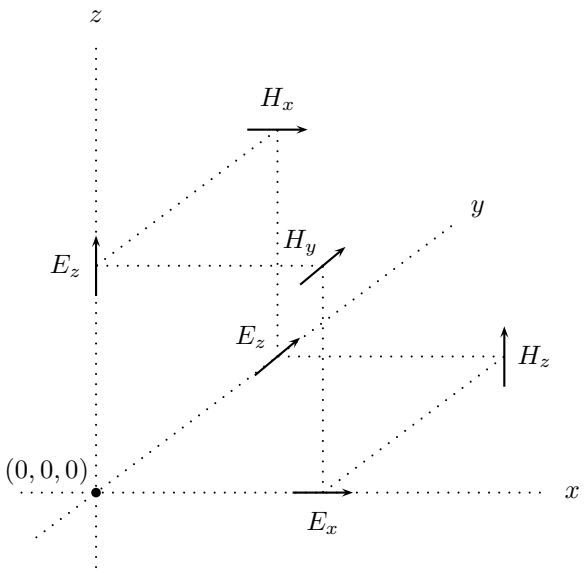

Figure 1: The primitive Yee cell. The computational grid is formed by tiling this pattern in three dimensions such that no two field components of E or H are co-located. The grid used in MaxwellFDS has periodic "wrap-around" boundary conditions, and the relevant distances between adjacent field components are denoted by $d^{\text{prim}}_{x,y,z}$ and $d^{\text{dual}}_{x,y,z}$.

- $d_x^{\text{prim}}(0)$ as the distance between $E_x(x_{\max}, j, k)$ and $E_x(0, j, k)$,
- $d_y^{\text{prim}}(0)$ as the distance between $E_y(i, y_{\max}, k)$ and $E_y(i, 0, k)$,
- $d_z^{\text{prim}}(0)$ as the distance between $E_z(i, j, z_{\max})$ and $E_y(i, j, 0)$,
- $d_x^{\text{dual}}(x_{\max})$ as the distance between $H_x(x_{\max}, j, k)$ and $H_x(0, j, k)$,
- $d_y^{\text{dual}}(y_{\max})$ as the distance between $H_y(i, y_{\max}, k)$ and $H_y(i, 0, k)$, and
- $d_z^{\text{dual}}(z_{\max})$ as the distance between $H_z(i, j, z_{\max})$ and $H_y(i, j, 0)$.

It should be noted that MaxwellFDS 's strictly periodic grid still allows the use of Bloch periodic, mirror and perfectly-matched layer boundary conditions. This is accomplished by setting the $d^{\text{prim,dual}}$ values to the appropriate complex values or even ∞, both of which MaxwellFDS is able to understand.

3.2.3 The wave equation in terms of matrices and vectors

With these definitions we now can see how MaxwellFDS formulates the wave equation in the language of linear algebra. Specifically, MaxwellFDS formulates (3) as

$$(A_1 \mathrm{diag}(\mu^{-1}) A_2 - \omega^2 \mathrm{diag}(\epsilon))x = b, \tag{5}$$

where

- A_1 and A_2 represent the first and second $\nabla\times$ operators respectively,
- $x \rightarrow E$, and
- $b \rightarrow -i\omega J$.

The vector fields E is converted into vector x as

$$x = \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} \tag{6}$$

where

$$e_w = \begin{bmatrix} E_w(0,0,0) \\ E_w(1,0,0) \\ \vdots \\ E_w(x_{\max}, y_{\max}, z_{\max}) \end{bmatrix}, \tag{7}$$

and so on for all vector fields.