Numerical Methods for Maxwell's Equations with Random Polarization

Nathan L. Gibson

Associate Professor
Department of Mathematics

Oregon State University

Conference on Computational Mathematics and Applications
UNLV

October 27, 2019

Acknowledgments

REU 2017

- Jacky Alvarez (UC Merced - Math)
- Andrew Fisher (UCLA - Physics)

Outline

Outline

Outline

Outline

Outline

Maxwell's Equations

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \text{ in } (0, T) \times \mathcal{D} \qquad \text{(Faraday)}$$

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} - \nabla \times \mathbf{H} = \mathbf{0}, \text{ in } (0, T) \times \mathcal{D} \qquad \text{(Ampere)}$$

$$\nabla \cdot \mathbf{D} = \nabla \cdot \mathbf{B} = 0, \text{ in } (0, T) \times \mathcal{D} \qquad \text{(Poisson/Gauss)}$$

$$\mathbf{E}(0, \mathbf{x}) = \mathbf{E_0}; \; \mathbf{H}(0, \mathbf{x}) = \mathbf{H_0}, \text{ in } \mathcal{D} \qquad \text{(Initial)}$$

$$\mathbf{E} \times \mathbf{n} = \mathbf{0}, \text{ on } (0, T) \times \partial\mathcal{D} \qquad \text{(Boundary)}$$

$\mathbf{E}$ = Electric field vector

$\mathbf{H}$ = Magnetic field vector

$\mathbf{J}$ = Current density

$\mathbf{D}$ = Electric flux density

$\mathbf{B}$ = Magnetic flux density

$\mathbf{n}$ = Unit outward normal to $\partial\mathcal{D}$

Constitutive Laws

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$
$$\mathbf{B} = \mu \mathbf{H} + \mathbf{M}$$
$$\mathbf{J} = \sigma \mathbf{E} + \mathbf{J}_s$$

$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

where $\epsilon = \epsilon_0 \epsilon_\infty$ and $\mu = \mu_0 \mu_r$.

Complex permittivity

The polarization is defined as the average dipole moment in a material.

- For linear materials we can define **P** in terms of a convolution with **E**

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

  where g is the dielectric response function (DRF).

Complex permittivity

The polarization is defined as the average dipole moment in a material.

- For linear materials we can define **P** in terms of a convolution with **E**

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

  where g is the dielectric response function (DRF).
- Allows for relaxation processes as well as resonance, and others.

Complex permittivity

The polarization is defined as the average dipole moment in a material.

- For linear materials we can define $\mathbf{P}$ in terms of a convolution with $\mathbf{E}$

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

  where g is the dielectric response function (DRF).
- Allows for relaxation processes as well as resonance, and others.
- In the frequency domain $\hat{\mathbf{D}} = \epsilon\hat{\mathbf{E}} + \hat{\mathbf{g}}\hat{\mathbf{E}} = \epsilon_0\epsilon(\omega)\hat{\mathbf{E}}$, where $\epsilon(\omega)$ is called the complex permittivity.

Complex permittivity

The polarization is defined as the average dipole moment in a material.

- For linear materials we can define $\mathbf{P}$ in terms of a convolution with $\mathbf{E}$

$$\mathbf{P}(t,\mathbf{x}) = g * \mathbf{E}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x};\mathbf{q})\mathbf{E}(s,\mathbf{x})ds,$$

  where g is the dielectric response function (DRF).
- Allows for relaxation processes as well as resonance, and others.
- In the frequency domain $\hat{\mathbf{D}} = \epsilon\hat{\mathbf{E}} + \hat{\mathbf{g}}\hat{\mathbf{E}} = \epsilon_0\epsilon(\omega)\hat{\mathbf{E}}$, where $\epsilon(\omega)$ is called the complex permittivity.
- We are interested in ultra-wide bandwidth electromagnetic pulse interrogation of dispersive dielectrics, therefore we want an accurate representation of $\epsilon(\omega)$ over a broad range of frequencies.

Saltwater Data

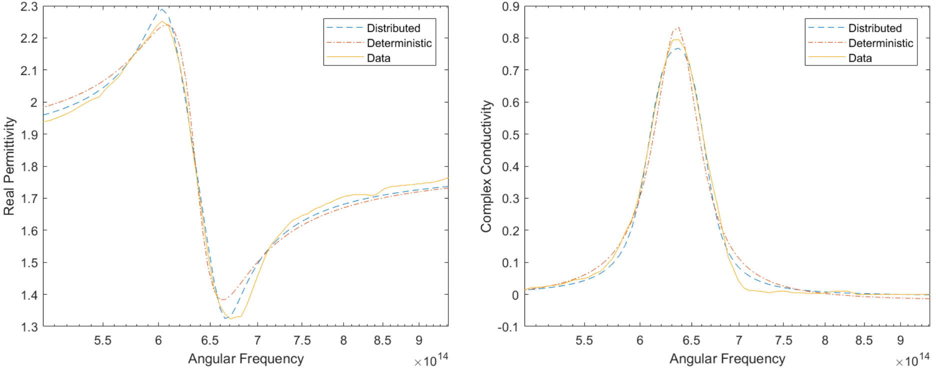

Figure: Fits for single-pole, saltwater data [Querry et al., 1972]

Distributions of Parameters

To account for the effect of distributions of parameters $\mathbf{q}$, consider the following *polydispersive* DRF

$$h(t, \mathbf{x}; F) = \int_{\mathcal{Q}} g(t, \mathbf{x}; \mathbf{q}) dF(\mathbf{q}),$$

where $\mathcal{Q}$ is some admissible set and $F \in \mathfrak{P}(\mathcal{Q})$.
Then the polarization becomes:

$$\mathbf{P}(t, \mathbf{x}; F) = \int_0^t h(t - s, \mathbf{x}; F)\mathbf{E}(s, \mathbf{x}) ds.$$

Alternatively we can define the random polarization $\mathcal{P}(t, \mathbf{x}; \mathbf{q})$ to satisfy $\mathcal{P} = g(t, \mathbf{x}; \mathbf{q}) * \mathbf{E}$ but with $\mathbf{q}$ random; the macroscopic polarization is then taken to be the expected value of the random polarization,

$$\mathbf{P}(t, \mathbf{x}; F) = \int_{\mathcal{Q}} \mathcal{P}(t, \mathbf{x}; \mathbf{q}) dF(\mathbf{q}).$$

Lorentz Model

We consider here materials modeled by the physical assumption that electrons behave as damped harmonic oscillators. This can be given in Auxiliary Differential Equation (ADE) form by the Lorentz model:

$$\ddot{\mathbf{P}} + 2\nu\dot{\mathbf{P}} + \omega_0^2\mathbf{P} = \epsilon_0\omega_p^2\mathbf{E}$$

where ω_0 is the resonant frequency, ν is a damping coefficient, and ω_p is referred to as a plasma frequency.

Random Polarization

We allow the parameter ω_0^2 be a random variable with probability distribution F on the interval (a, b). Then the random Lorentz model in ADE form is

$$\ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2\mathcal{P} = \epsilon_0\omega_p^2 E$$

The macroscopic polarization is then taken to be the expected value of the random polarization,

$$\mathbf{P}(t, \mathbf{x}) = \int_a^b \mathcal{P}(t, \mathbf{x}; \omega_0^2)\, dF(\omega_0^2).$$

Maxwell-Random Lorentz system

In a polydisperse Lorentz material, we have

$$\mu_0 \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \mathbf{E} \tag{1a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\partial \mathbf{P}}{\partial t} \tag{1b}$$

$$\ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2 \mathcal{P} = \epsilon_0 \omega_p^2 \mathbf{E} \tag{1c}$$

with

$$\mathbf{P}(t, \mathbf{x}) = \int_a^b \mathcal{P}(t, \mathbf{x}; \omega_0^2) f(\omega_0^2) d\omega_0^2.$$

2D Maxwell-Random Lorentz Transverse Electric (TE) curl equations

For simplicity in exposition and to facilitate analysis, we reduce the Maxwell-Random Lorentz model to two spatial dimensions (we make the assumption that fields do not exhibit variation in the z direction).

$$\mu_0 \frac{\partial H}{\partial t} = -\mathrm{curl}\ \mathbf{E}, \tag{2a}$$

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \mathbf{curl}\ H - \mathbf{J}, \tag{2b}$$

$$\frac{\partial \mathcal{P}}{\partial t} = \mathcal{J} \tag{2c}$$

$$\frac{\partial \mathcal{J}}{\partial t} = -2\nu \mathcal{J} - \omega_0^2 \mathcal{P} + \epsilon_0 \omega_p^2 \mathbf{E} \tag{2d}$$

where $\mathbf{E} = (E_x, E_y)^T, \mathbf{J} = (J_x, J_y)^T$, $\mathcal{J} = (\mathcal{J}_x, \mathcal{J}_y)^T, \mathcal{P} = (\mathcal{P}_x, \mathcal{P}_y)^T$ and $H = H_z$.

Note $\mathrm{curl}\ \mathbf{U} = \frac{\partial U_y}{\partial x} - \frac{\partial U_x}{\partial y}$ and $\mathbf{curl}\ V = \left(\frac{\partial V}{\partial y}, -\frac{\partial V}{\partial x}\right)^T$.

We introduce the random Hilbert space $V_F = (L^2(\Omega) \otimes L^2(\mathcal{D}))^2$ equipped with an inner product and norm as follows

$$(\mathbf{u}, \mathbf{v})_F = \mathbb{E}[(\mathbf{u}, \mathbf{v})_2],$$
$$\|\mathbf{u}\|_F^2 = \mathbb{E}[\|\mathbf{u}\|_2^2].$$

The weak formulation of the 2D Maxwell-Random Lorentz TE system is

$$\left(\mu_0 \frac{\partial H}{\partial t}, v\right)_2 = (-\mathrm{curl}\ \mathbf{E}, v)_2 \tag{3a}$$

$$\left(\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t}, \mathbf{u}\right)_2 = (\mathbf{curl}\ H, \mathbf{u})_2 - (\mathbf{J}, \mathbf{u})_2 \tag{3b}$$

$$\left(\frac{\partial \mathcal{P}}{\partial t}, \mathbf{q}\right)_F = (\mathcal{J}, \mathbf{q})_F \tag{3c}$$

$$\left(\frac{\partial \mathcal{J}}{\partial t}, \mathbf{w}\right)_F = (-2\nu \mathcal{J}, \mathbf{w})_F + \left(-\omega_0^2 \mathcal{P}, \mathbf{w}\right)_F + \left(\epsilon_0 \omega_p^2 \mathbf{E}, \mathbf{w}\right)_F. \tag{3d}$$

for $v \in L^2(\mathcal{D})$, $\mathbf{u} \in H_0(\mathrm{curl}, \mathcal{D})^2$, and $\mathbf{q}, \mathbf{w} \in V_F$.

Theorem (Stability of Maxwell-Random Lorentz)

Let $\mathcal{D} \subset \mathbb{R}^2$ and suppose that $\mathbf{E} \in C(0, T; H_0(\mathrm{curl}, \mathcal{D})) \cap C^1(0, T; (L^2(\mathcal{D}))^2)$, $\mathcal{P}, \mathcal{J} \in C^1(0, T; \left(L^2(\Omega) \otimes L^2(\mathcal{D})\right)^2)$, and $H(t) \in C^1(0, T; L^2(\mathcal{D}))$ are solutions of the weak formulation for the Maxwell-Random Lorentz system along with PEC boundary conditions. Then the system exhibits energy decay

$$\mathcal{E}(t) \leq \mathcal{E}(0) \quad \forall t \geq 0,$$

where the energy $\mathcal{E}(t)$ is defined as

$$\mathcal{E}(t)^2 = \left\|\sqrt{\mu_0}\; H(t)\right\|_2^2 + \left\|\sqrt{\epsilon_0\epsilon_\infty}\; \mathbf{E}(t)\right\|_2^2 + \left\|\sqrt{\frac{\omega_0^2}{\epsilon_0\omega_p^2}}\; \mathcal{P}(t)\right\|_F^2 + \left\|\frac{1}{\sqrt{\epsilon_0\omega_p^2}}\; \mathcal{J}(t)\right\|_F^2$$

where $\|u\|_F^2 = \mathbb{E}[\|u\|_2^2]$ and $\mathcal{J} := \frac{\partial \mathcal{P}}{\partial t}$.

Proof: (for 2D)

By choosing $v = H$, $\mathbf{u} = \mathbf{E}$, $\mathbf{q} = \mathcal{P}$ and $\mathbf{w} = \mathcal{J}$ in the weak form, and adding all equations into the time derivative of the definition of $\mathcal{E}^2$, we obtain

$$\begin{aligned}\frac{1}{2}\frac{d\mathcal{E}^2(t)}{dt} =& -\Big(\mathrm{curl}\ \mathbf{E}, H\Big)_2 + \Big(H, \mathrm{curl}\ \mathbf{E}\Big)_2 - \Big(\mathbf{J}, \mathbf{E}\Big)_2 + \left(\frac{\omega_0^2}{\epsilon_0\omega_p^2}\mathcal{J}, \mathcal{P}\right)_F \\ & - \left(\frac{2\nu}{\epsilon_0\omega_p^2}\mathcal{J}, \mathcal{J}\right)_F - \left(\frac{\omega_0^2}{\epsilon_0\omega_p^2}\mathcal{P}, \mathcal{J}\right)_F + (\mathbf{E}, \mathcal{J})_F \\ =& -\left\|\sqrt{\frac{2\nu}{\epsilon_0\omega_p^2}}\mathcal{J}\right\|_F^2\end{aligned}$$

$$\boxed{\frac{d\mathcal{E}(t)}{dt} = \frac{-1}{\mathcal{E}(t)}\left\|\sqrt{\frac{2\nu}{\epsilon_0\omega_p^2}}\mathcal{J}\right\|_F^2 \leq 0.}$$

□

Polynomial Chaos

We wish to approximate the random polarization with orthogonal polynomials of the standard random variable ξ. Let $\omega_0^2 = r\xi + m$ and $\xi \in [-1, 1]$.

Polynomial Chaos

We wish to approximate the random polarization with orthogonal polynomials of the standard random variable ξ. Let $\omega_0^2 = r\xi + m$ and $\xi \in [-1, 1]$. Suppressing the dimension of $\mathcal{P}$ and the spatial dependence, we have

$$\mathcal{P}(\xi, t) = \sum_{i=0}^{\infty} \alpha_i(t)\phi_i(\xi) \to \ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + (r\xi + m)\mathcal{P} = \epsilon_0\omega_p^2 E.$$

Utilizing the Triple Recursion Relation for orthogonal polynomials:

$$\xi\phi_n(\xi) = a_n\phi_{n+1}(\xi) + b_n\phi_n(\xi) + c_n\phi_{n-1}(\xi),$$

the differential equation becomes

$$\sum_{i=0}^{\infty} \left[\ddot{\alpha}_i(t) + 2\nu\dot{\alpha}_i(t) + m\alpha_i(t)\right]\phi_i + r\alpha_i(t)\left[a_i\phi_{i+1} + b_i\phi_i + c_i\phi_{i-1}\right] = \epsilon_0\omega_p^2 E\phi_0.$$

Galerkin Projection

We apply a Galerkin Projection onto the space of polynomials of degree at most p to get:

$$\ddot{\vec{\alpha}} + 2\nu\dot{\vec{\alpha}} + A\vec{\alpha} = \vec{f}$$

where $\vec{f} = \hat{e}_1\epsilon_0\omega_p^2 E$ and

$$A = rM + mI, \quad M = \begin{pmatrix} b_0 & c_1 & 0 & \cdots & 0 \\ a_0 & b_1 & c_2 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & a_{p-2} & b_{b-1} & c_p \\ 0 & \cdots & 0 & a_{p-1} & b_p \end{pmatrix}.$$

Or we can write as a first order system:

$$\dot{\vec{\alpha}} = \vec{\beta}$$
$$\dot{\vec{\beta}} = -A\vec{\alpha} - 2\nu\vec{\beta} + \vec{f}.$$

Finite Difference Time Domain (FDTD)

We now choose a space-time discretization of the Maxwell-PC Lorentz model. Note that any scheme can be used, independently of the spectral approach in random space employed here.

The Yee Scheme (FDTD)

- This gives an explicit second order accurate scheme in time and space.
- It is conditionally stable with the CFL condition

$$\frac{c_\infty \Delta t}{h} \leq \frac{1}{\sqrt{d}}$$

  where $c_\infty = 1/\sqrt{\mu_0 \epsilon_0 \epsilon_\infty}$ is the fastest wave speed in the medium, d is the spatial dimension, and h is the (uniform) spatial step.
- The Yee scheme can exhibit numerical dispersion and dissipation.

FDTD Discretization

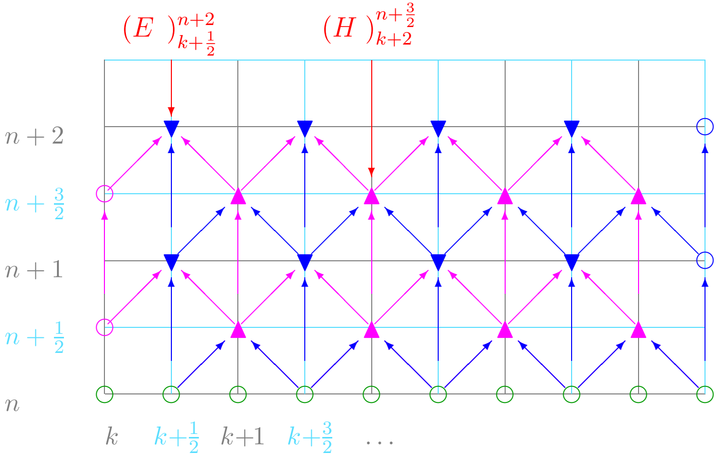

Figure: Yee Scheme

We stagger three discrete meshes in the x and y directions and two discrete meshes in time:

$$\tau_h^{E_x} := \left\{ \left(x_{\ell+\frac{1}{2}}, y_j \right) | 0 \leq \ell \leq L-1, 0 \leq j \leq J \right\}$$
$$\tau_h^{E_y} := \left\{ \left(x_{\ell}, y_{j+\frac{1}{2}} \right) | 0 \leq \ell \leq L, 0 \leq j \leq J-1 \right\}$$
$$\tau_h^{H} := \left\{ \left(x_{\ell+\frac{1}{2}}, y_{j+\frac{1}{2}} \right) | 0 \leq \ell \leq L-1, 0 \leq j \leq J-1 \right\}$$
$$\tau_t^{E} := \left\{ \left(t^n \right) | 0 \leq n \leq N \right\}$$
$$\tau_t^{H} := \left\{ \left(t^{n+\frac{1}{2}} \right) | 0 \leq n \leq N-1 \right\}.$$

Let U be one of the field variables: H, E_x, E_y, $\vec{\alpha}_x$, $\vec{\alpha}_y$, $\vec{\beta}_x$, $\vec{\beta}_y$. Let (x_i, y_j) be a node on any discrete spatial mesh, and γ be either n or $n + \frac{1}{2}$ with $\gamma \leq N$.

We define the *grid functions* or the numerical approximations

$$U_{i,j}^{\gamma} \approx U(x_i, y_j, t^{\gamma}).$$

Let U be one of the field variables: H, E_x, E_y, $\vec{\alpha}_x$, $\vec{\alpha}_y$, $\vec{\beta}_x$, $\vec{\beta}_y$. Let (x_i, y_j) be a node on any discrete spatial mesh, and γ be either n or $n + \frac{1}{2}$ with $\gamma \leq N$.

We define the *grid functions* or the numerical approximations

$$U_{i,j}^{\gamma} \approx U(x_i, y_j, t^{\gamma}).$$

We define the centered temporal difference operator and a discrete time averaging operation as

$$\delta_t U_{i,j}^{\gamma} := \frac{U_{i,j}^{\gamma+\frac{1}{2}} - U_{i,j}^{\gamma-\frac{1}{2}}}{\Delta t}, \qquad \overline{U}_{i,j}^{\gamma} := \frac{U_{i,j}^{\gamma+\frac{1}{2}} + U_{i,j}^{\gamma-\frac{1}{2}}}{2}, \tag{5}$$

Let U be one of the field variables: H, E_x, E_y, $\vec{\alpha}_x$, $\vec{\alpha}_y$, $\vec{\beta}_x$, $\vec{\beta}_y$. Let (x_i, y_j) be a node on any discrete spatial mesh, and γ be either n or $n+\frac{1}{2}$ with $\gamma \leq N$.

We define the *grid functions* or the numerical approximations

$$U_{i,j}^{\gamma} \approx U(x_i, y_j, t^{\gamma}).$$

We define the centered temporal difference operator and a discrete time averaging operation as

$$\delta_t U_{i,j}^{\gamma} := \frac{U_{i,j}^{\gamma+\frac{1}{2}} - U_{i,j}^{\gamma-\frac{1}{2}}}{\Delta t}, \qquad \overline{U}_{i,j}^{\gamma} := \frac{U_{i,j}^{\gamma+\frac{1}{2}} + U_{i,j}^{\gamma-\frac{1}{2}}}{2}, \tag{5}$$

and the centered spatial difference operators in the x and y direction, respectively as

$$\delta_x U_{i,j}^{\gamma} := \frac{U_{i+\frac{1}{2},j}^{\gamma} - U_{i-\frac{1}{2},j}^{\gamma}}{\Delta x}, \qquad \delta_y U_{i,j}^{\gamma} := \frac{U_{i,j+\frac{1}{2}}^{\gamma} - U_{i,j-\frac{1}{2}}^{\gamma}}{\Delta y}. \tag{6}$$

The Yee Scheme applied to the Maxwell-PC Lorentz yields

$$\mu_0 \delta_t H^n_{\ell+\frac{1}{2},j+\frac{1}{2}} = \left(\delta_y E^n_{x_{\ell+\frac{1}{2},j+\frac{1}{2}}} - \delta_x E^n_{y_{\ell+\frac{1}{2},j+\frac{1}{2}}}\right) \tag{7a}$$

$$\epsilon_0 \epsilon_\infty \delta_t E^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} = \delta_y H^{n+\frac{1}{2}}_{\ell+\frac{1}{2},j} - \overline{\vec{\beta}}^{n+\frac{1}{2}}_{0,x_{\ell+\frac{1}{2},j}} \tag{7b}$$

$$\epsilon_0 \epsilon_\infty \delta_t E^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} = -\delta_x H^{n+\frac{1}{2}}_{\ell,j+\frac{1}{2}} - \overline{\vec{\beta}}^{n+\frac{1}{2}}_{0,y_{\ell,j+\frac{1}{2}}} \tag{7c}$$

$$\delta_t \vec{\alpha}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} = \overline{\vec{\beta}}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} \tag{7d}$$

$$\delta_t \vec{\alpha}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} = \overline{\vec{\beta}}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} \tag{7e}$$

$$\delta_t \vec{\beta}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} = -A \overline{\vec{\alpha}}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} - 2\nu \overline{\vec{\beta}}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} + \hat{e}_1 \epsilon_0 \omega_p^2 \overline{E}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} \tag{7f}$$

$$\delta_t \vec{\beta}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} = -A \overline{\vec{\alpha}}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} - 2\nu \overline{\vec{\beta}}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} + \hat{e}_1 \epsilon_0 \omega_p^2 \overline{E}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}}. \tag{7g}$$

Staggered L^2 normed spaces

Next, we define the L^2 normed spaces

$$\mathbb{V}_E := \left\{ \mathbf{F} : \tau_h^{E_x} \times \tau_h^{E_y} \longrightarrow \mathbb{R}^2 \mid \mathbf{F} = (F_{x_{l+\frac{1}{2},j}}, F_{y_{l,j+\frac{1}{2}}})^T, \|\mathbf{F}\|_E < \infty \right\} \tag{8}$$

$$\mathbb{V}_H := \left\{ U : \tau_h^{H} \longrightarrow \mathbb{R} \mid U = (U_{l+\frac{1}{2},j+\frac{1}{2}}), \|U\|_H < \infty \right\} \tag{9}$$

with the following discrete norms and inner products

$$\|\mathbf{F}\|_E^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(|F_{x_{\ell+\frac{1}{2},j}}|^2 + |F_{y_{\ell,j+\frac{1}{2}}}|^2 \right), \forall\ \mathbf{F} \in \mathbb{V}_E \tag{10}$$

$$(\mathbf{F}, \mathbf{G})_E = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(F_{x_{\ell+\frac{1}{2},j}} G_{x_{\ell+\frac{1}{2},j}} + F_{y_{\ell,j+\frac{1}{2}}} G_{y_{\ell,j+\frac{1}{2}}} \right), \forall\ \mathbf{F}, \mathbf{G} \in \mathbb{V}_E \tag{11}$$

$$\|U\|_H^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} |U_{\ell+\frac{1}{2},j+\frac{1}{2}}|^2, \forall\ U \in \mathbb{V}_H \tag{12}$$

$$(U, V)_H = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} U_{\ell+\frac{1}{2},j+\frac{1}{2}} V_{\ell+\frac{1}{2},j+\frac{1}{2}}, \forall\ U, V \in \mathbb{V}_H. \tag{13}$$

We define a space and inner product for the random polarization in vector notation, since $\vec{\boldsymbol{\alpha}}$ and $\vec{\boldsymbol{\beta}}$ are now $2 \times p+1$ matrices:

$$\mathbb{V}_\alpha := \left\{ \vec{\boldsymbol{\alpha}} : \tau_h^{E_x} \times \tau_h^{E_y} \longrightarrow \mathbb{R}^2 \times \mathbb{R}^{p+1} \;\middle|\; \vec{\boldsymbol{\alpha}} = [\boldsymbol{\alpha}_0, \ldots, \boldsymbol{\alpha}_p], \boldsymbol{\alpha}_k \in \mathbb{V}_E, \|\vec{\boldsymbol{\alpha}}\|_\alpha < \infty \right\}$$

where the discrete L^2 grid norm and inner product are defined as

$$\|\vec{\boldsymbol{\alpha}}\|_\alpha^2 = \sum_{k=0}^{p} \|\boldsymbol{\alpha}_k\|_E^2, \quad \forall\, \vec{\boldsymbol{\alpha}} \in \mathbb{V}_\alpha$$

$$(\vec{\boldsymbol{\alpha}}, \vec{\boldsymbol{\beta}})_\alpha = \sum_{k=0}^{p} \left(\boldsymbol{\alpha}_k, \boldsymbol{\beta}_k\right)_E, \quad \forall\, \vec{\boldsymbol{\alpha}}, \vec{\boldsymbol{\beta}} \in \mathbb{V}_\alpha.$$

We choose both spatial steps to be uniform and equal ($\Delta x = \Delta y = h$), and require that the usual CFL condition for two dimensions holds:

$$\sqrt{2} c_\infty \Delta t \leq h. \tag{14}$$

Theorem (Energy Decay for Maxwell-PC Lorentz-FDTD)

If the stability condition (14) is satisfied, then the Yee scheme for the 2D TE mode Maxwell-PC Lorentz system satisfies the discrete identity

$$\delta_t \mathcal{E}_h^{n+\frac{1}{2}} = \frac{-1}{\overline{\mathcal{E}}_h^{n+\frac{1}{2}}} \left\| \sqrt{\frac{2\nu}{\epsilon_0 \omega_p^2}} \overline{\vec{\beta}}^{n+\frac{1}{2}} \right\|_\alpha^2 \tag{15}$$

for all n where

$$\mathcal{E}_h^n = \left(\mu_0 (H^{n+\frac{1}{2}}, H^{n-\frac{1}{2}})_H + \|\sqrt{\epsilon_0 \epsilon_\infty}\ \mathbf{E}^n\|_E^2 + \left\| \frac{A^{1/2}}{\sqrt{\epsilon_0 \omega_p^2}} \vec{\alpha}^n \right\|_\alpha^2 + \left\| \sqrt{\frac{1}{\epsilon_0 \omega_p^2}} \vec{\beta}^n \right\|_\alpha^2 \right)^{1/2} \tag{16}$$

defines a discrete energy.

In the above, A positive definite iff $r < m$, and assumed to have been symmetrized.

Note that $\|\vec{\alpha}\|_\alpha^2 \approx \|\mathbb{E}[\mathcal{P}]\|_2^2 + \|\mathrm{StdDev}(\mathcal{P})\|_2^2 = \mathbb{E}[\|\mathcal{P}\|_2^2] = \|\mathcal{P}\|_F^2$ so that this is a natural extension of the Maxwell-Random Lorentz energy.

Dispersion Analysis

Assuming a solution to the Maxwell-Random Lorentz system of the form $\mathbf{E} = \mathbf{E_0} exp(i(\omega t - \mathbf{k} \cdot \mathbf{x}))$, the following relation must hold.

Theorem

The dispersion relation for the Maxwell-Random Lorentz system is given by

$$\frac{\omega^2}{c^2}\epsilon(\omega) = k^2$$

where the expected complex permittivity is given by

$$\epsilon(\omega) = \epsilon_\infty + \omega_p^2 \mathbb{E}\left[\frac{1}{\omega_0^2 - \omega^2 - i2\nu\omega}\right].$$

Where $\mathbf{k} = [k_x, k_y, k_x]^T$ is the wave vector, $k = \|\mathbf{k}\|$ is the wavenumber and $c = 1/\sqrt{\mu_0 \epsilon_0}$ is the speed of light in free space.

Theorem

The discrete dispersion relation for the Maxwell-PC FDTD Lorentz scheme is given by

$$\frac{\omega_\Delta^2}{c^2}\epsilon_\Delta(\omega) = K_\Delta^2$$

Theorem

The *discrete dispersion relation* *for the Maxwell-PC FDTD Lorentz scheme is given by*

$$\frac{\omega_\Delta^2}{c^2}\epsilon_\Delta(\omega) = K_\Delta^2$$

where the *discrete expected complex permittivity* *is given by*

$$\epsilon_\Delta(\omega) := \epsilon_\infty + \omega_{p,\Delta}^2 \hat{e}_1^T \left(A_\Delta - \omega_\Delta^2 I - i2\nu_\Delta\omega_\Delta I\right)^{-1} \hat{e}_1$$

Theorem

The discrete dispersion relation *for the Maxwell-PC FDTD Lorentz scheme is given by*

$$\frac{\omega_\Delta^2}{c^2}\epsilon_\Delta(\omega) = K_\Delta^2$$

where the discrete expected complex permittivity *is given by*

$$\epsilon_\Delta(\omega) := \epsilon_\infty + \omega_{p,\Delta}^2 \hat{e}_1^T \left(A_\Delta - \omega_\Delta^2 I - i2\nu_\Delta\omega_\Delta I\right)^{-1} \hat{e}_1$$

and the discrete wavenumber *and quantity K_Δ are given by*

$$k_\Delta := \sqrt{k_{x,\Delta}^2 + k_{y,\Delta}^2}, \quad K_\Delta := \sqrt{K_{x,\Delta}^2 + K_{y,\Delta}^2},$$

with

$$K_{x,\Delta} := \frac{2}{\Delta x}\sin\left(\frac{k_{x,\Delta}\Delta x}{2}\right), \quad K_{y,\Delta} := \frac{2}{\Delta y}\sin\left(\frac{k_{y,\Delta}\Delta y}{2}\right)\ldots$$

Theorem (Continued)

and the discrete PC matrix and discrete damping are given by

$$A_\Delta := \cos^2(\omega\Delta t/2)A, \quad \nu_\Delta := cos\left(\frac{\omega\Delta t}{2}\right)\nu.$$

Similarly,

$$\omega_\Delta := \frac{2}{\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right), \quad \omega_{p,\Delta} := cos\left(\frac{\omega\Delta t}{2}\right)\omega_p.$$

Dispersion Error

The exact dispersion relation can be compared with a discrete dispersion relation to determine the amount of dispersion error.

We define the phase error Φ for a scheme applied to a model to be

$$\Phi = \left| \frac{k_{EX} - k_{\Delta}}{k_{EX}} \right|, \tag{17}$$

where the numerical wave number k_{Δ} is implicitly determined by the corresponding discrete dispersion relation and k_{EX} is the exact wave number for the given model.

Dispersion Error

The exact dispersion relation can be compared with a discrete dispersion relation to determine the amount of dispersion error.

We define the phase error Φ for a scheme applied to a model to be

$$\Phi = \left| \frac{k_{EX} - k_{\Delta}}{k_{EX}} \right|, \tag{17}$$

where the numerical wave number k_{Δ} is implicitly determined by the corresponding discrete dispersion relation and k_{EX} is the exact wave number for the given model.

- We wish to examine the phase error as a function of ω in the range around $\overline{\omega}_0$. Δt is determined by $h := \overline{\omega}_0 \Delta t/(2\pi)$, while $\Delta x = \Delta y$ are determined by the CFL condition.
- We assume a uniform distribution and the following parameters Lorentz material:

$$\epsilon_\infty = 1, \quad \epsilon_s = 2.25, \quad \nu = 2.8 \times 10^{15} \text{ 1/sec}, \quad \overline{\omega}_0 = 4 \times 10^{16} \text{ rad/sec}.$$

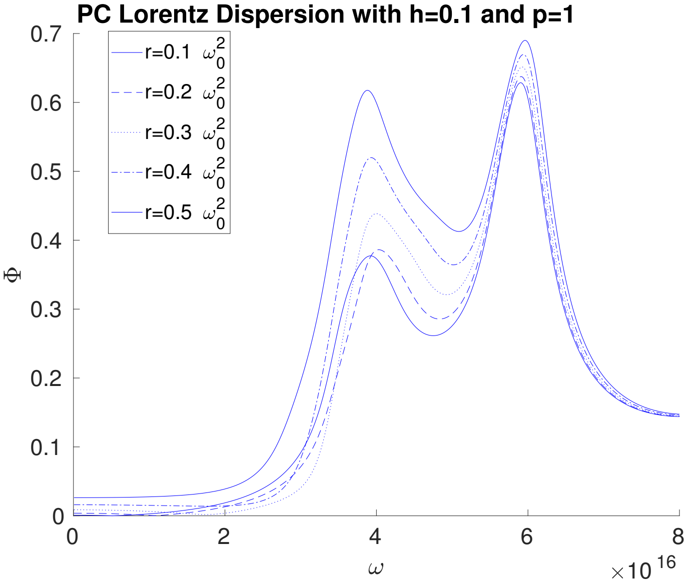

Figure: Plots of phase error at $\theta = 0$.

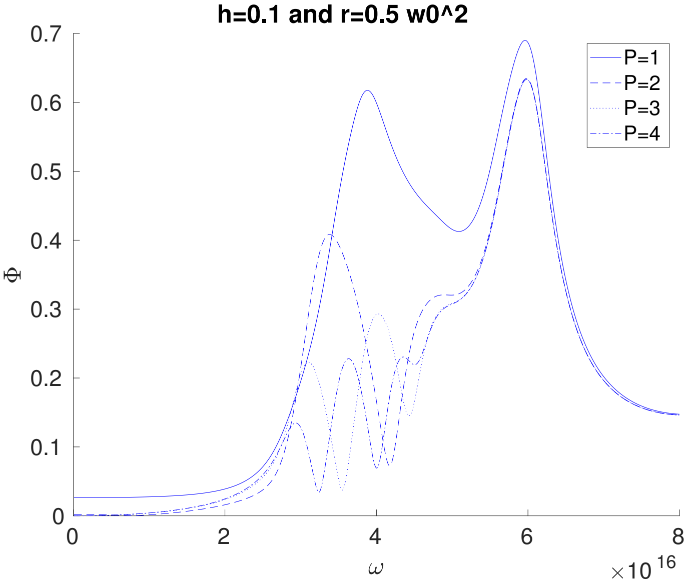

Figure: Plots of phase error at $\theta = 0$.

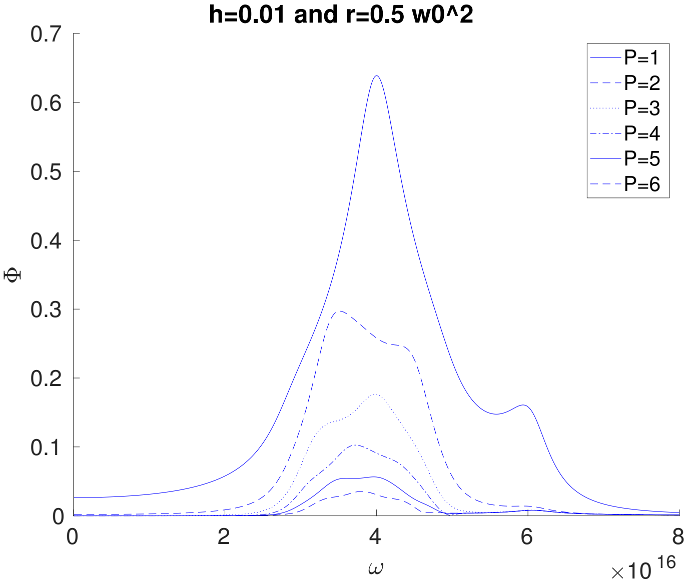

Figure: Plots of phase error at $\theta = 0$.

References

- Bokil, V. A. & Gibson, N. L. (2012), Analysis of Spatial High Order Finite Difference Methods for Maxwell's equations in dispersive media, *IMA J. Numer. Anal.* 32 (3): 926-956.
- Bokil, V. A. & Gibson, N. L. (2013), Stability and Dispersion Analysis of High Order FDTD Methods for Maxwell's Equations in Dispersive Media, *Contemporary Mathematics*, Vol. 586.
- Bokil, V. A. & Gibson, N. L. (2014), Convergence Analysis of Yee Schemes for Maxwell's Equations in Debye and Lorentz Dispersive Media, *IJNAM*, 11(4), 657-687.
- Gibson, N. L. (2015), A Polynomial Chaos Method for Dispersive Electromagnetics, *Comm. in Comp. Phys.*, vol. 18, issue 5, pp 1234-1263.
- Alvarez, Jacky & Fisher, Andrew (2017), Approximating Dispersive Materials With Parameter Distributions in the Lorentz Model, *Oregon State University Math REU.*