Modeling Dispersive Materials with Parameter Distributions in the Lorentz Model

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Background

Maxwell's Equations:

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \times \mathbf{H}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

Constitutive Relations:

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$

$$\mathbf{B} = \mu \mathbf{H} + \mathbf{M}$$

$$\mathbf{J} = \sigma \mathbf{E} + \mathbf{J}_s$$

Boundary Conditions:

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

Initial Conditions:

$$\mathbf{E}(0, \mathbf{x}) = 0, \quad \mathbf{H}(0, \mathbf{x}) = 0, \text{ in } \mathcal{D}.$$

Lorentz Model

We employ the physical assumption that electrons behave as damped harmonic oscillators,

$$m\ddot{x} + 2m\nu\dot{x} + m\omega_0^2 x = F_{driving}.$$

The polarization is then defined as electron dipole moment density:

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

where ω_0 is the resonant frequency, ν is a damping coefficient, and ω_p is referred to as a plasma frequency defined by $\omega_p^2 = (\epsilon_s - \epsilon_\infty)\omega_0^2$.
Taking a Fourier transform and inserting the polarization differential equation into constitutive equation, we get $\hat{D}(\omega) = \epsilon_0\epsilon(\omega)\hat{E}(\omega)$ where

$$\epsilon(\omega) = \epsilon_\infty + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i2\nu\omega}.$$

For multiple Lorentz poles, the permittivity merely includes a summation:

$$\epsilon(\omega) = \epsilon_\infty + \sum_{i=1}^{\infty} \frac{\omega_{p,i}^2}{\omega_{0,i}^2 - \omega^2 - i2\nu_i\omega}.$$

Random Polarization

We define random polarization where η is a random variable. We now express the random Lorentz model:

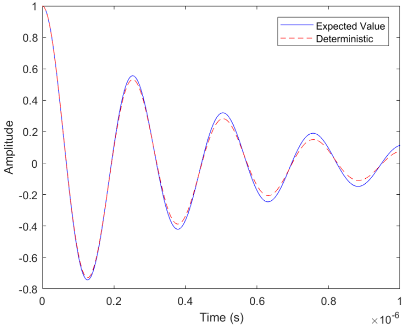
$$\ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2\mathcal{P} = \epsilon_0\omega_p^2 E$$

$$\epsilon(\omega) = \epsilon_\infty + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i2\nu\omega}.$$

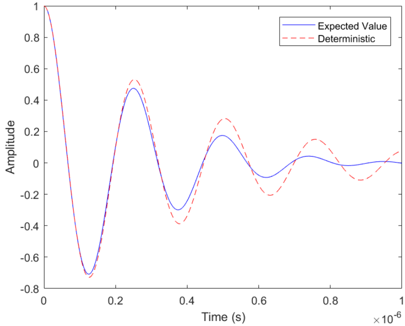
Three parameters potentially random: ν, ω_0^2, and ω_p^2 The macroscopic polarization is identified as the expected value of the random polarization,

$$P(t,z) = \int_a^b \mathcal{P}(t,z;\eta)\, dF(\eta).$$

Random Polarization



(a) ν Distribution: $\mathcal{U}(0.5\nu, 1.5\nu)$



(b) ω_0^2 Distribution: $\mathcal{U}(0.75\omega_0^2, 1.25\omega_0^2)$

Figure 1: Solutions for Unforced Differential Equation

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Complex Permittivity with random ω_0^2

Separate complex permittivity into real and imaginary parts ($\epsilon = \epsilon_r + i\epsilon_i$):

$$\epsilon_r = \epsilon_\infty + \frac{\omega_p^2(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + 4\nu^2\omega^2}$$

$$\epsilon_i = \frac{2\omega_p^2\nu\omega}{(\omega_0^2 - \omega^2)^2 + 4\nu^2\omega^2}.$$

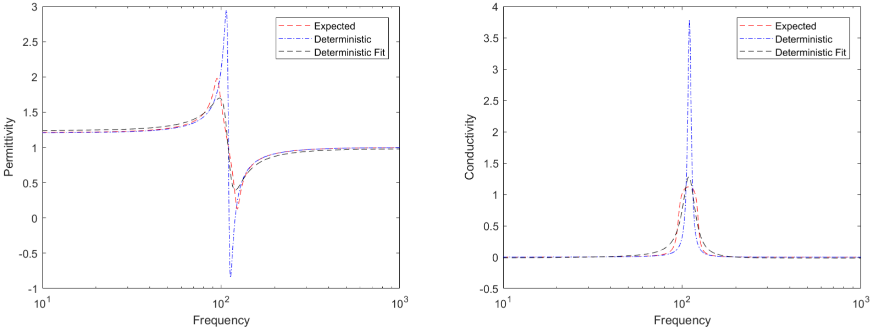
Analytic integration is possible for uniform distribution:

$$\mathbb{E}[\epsilon_r] = \frac{1}{b-a}\int_a^b \epsilon_r d\omega_0^2 = \epsilon_\infty + \frac{\omega_p^2}{2(b-a)}\left(\ln((\omega_0^2)^2 - 2\omega_0^2\omega^2 + \omega^4 + 4\nu^2\omega^2\right)\Big|_a^b$$

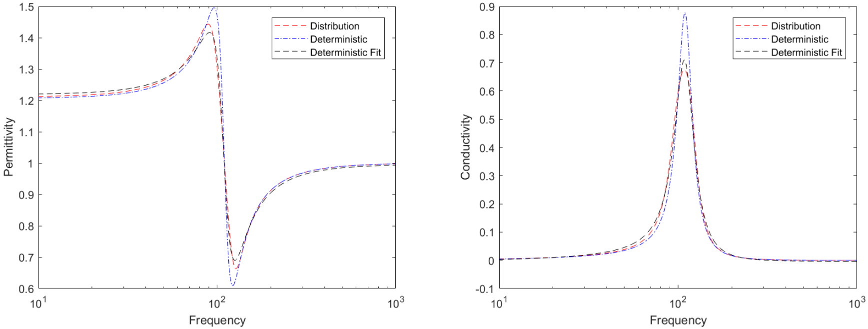
$$\mathbb{E}[\epsilon_i] = \frac{1}{b-a}\int_a^b \epsilon_i d\omega_0^2 = \frac{\omega_p^2}{(b-a)}\arctan\left(\frac{\omega^2 - \omega_0^2}{2\nu\omega}\right)\Big|_a^b$$

For the general Jacobi polynomials and Beta distribution, one must use Monte Carlo sampling or numerical integration.

Frequency Domain Fit ($\nu = 3$)



Frequency Domain Fit ($\nu = 10$)



Saltwater Data

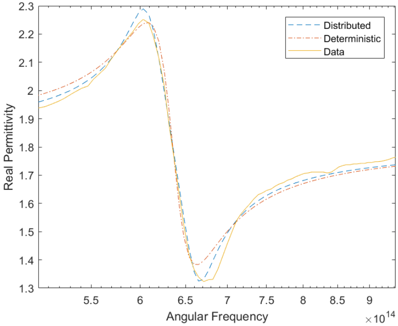


Figure 4: Fits for single-pole, saltwater data [Querry et. al., 1972]

Outline

Maxwell-Random Lorentz system

In a polydisperse Lorentz material, we have

$$\epsilon_0\epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\partial \mathbf{P}}{\partial t} \tag{5a}$$

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0}\nabla \times \mathbf{E} \tag{5b}$$

$$\ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2\mathcal{P} = \epsilon_0\omega_p^2\mathbf{E} \tag{5c}$$

with

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

Theorem (Stability of Maxwell-Random Lorentz)

Let $\mathcal{D} \subset \mathbb{R}^2$ and suppose that $\mathbf{E} \in C(0, T; H_0(\mathrm{curl}, \mathcal{D})) \cap C^1(0, T; (L^2(\mathcal{D}))^2)$, $\mathcal{P} \in C^1(0, T; \left(L^2(\Omega) \otimes L^2(\mathcal{D})\right)^2)$, *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

$$\mathcal{E}(t) = \left(\left\| \sqrt{\mu_0}\, H(t) \right\|_2^2 + \left\| \sqrt{\epsilon_0 \epsilon_\infty}\, \mathbf{E}(t) \right\|_2^2 + \left\| \frac{\omega_0}{\omega_p \sqrt{\epsilon_0}}\, \mathcal{P}(t) \right\|_F^2 + \left\| \frac{1}{\omega_p \sqrt{\epsilon_0}}\, \mathcal{J}(t) \right\|_F^2 \right)^{\frac{1}{2}} \tag{6}$$

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

Proof involves showing that

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

Polynomial Chaos

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

$$\mathcal{P}(\xi, t) = \sum_{i=0}^{\infty} \alpha_i(t)\phi_i(\xi) \to \ddot{\mathcal{P}} + 2\nu\dot{\mathcal{P}} + \omega_0^2\mathcal{P} = \epsilon_0\omega_p^2 E.$$

Utilizing Triple Recurrence 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

$$\sum_{i=0}^{\infty} \left[\ddot{\alpha}_i(t) + 2\nu\dot{\alpha}_i(t) + m\alpha_i(t)\right]\phi_i(\xi)$$

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

Galerkin Projection

Apply Galerkin Projection onto the space of polynomials of degree at most p:

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

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

Or we can write as a first order system:

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

where $\vec{f} = \hat{e}_1\epsilon_0\overline{\omega_p}^2 E$ with $\overline{\omega_p}$ meaning expected value.

Maxwell-PC Lorentz

The polynomial chaos system coupled with 1D Maxwell's equations become

$$\begin{aligned}\epsilon_\infty \epsilon_0 \frac{\partial E}{\partial t} &= -\frac{\partial H}{\partial z} - \beta_0 \\ \frac{\partial H}{\partial t} &= -\frac{1}{\mu_0}\frac{\partial E}{\partial z} \\ \dot{\vec{\alpha}} &= \vec{\beta} \\ \dot{\vec{\beta}} &= -A\vec{\alpha} - 2\nu I \vec{\beta} + \vec{f}\end{aligned}$$

Initial Conditions:

$$E(0,z) = H(0,z) = \vec{\alpha}(0,z) = \vec{\beta}(0,z) = 0$$

Boundary Conditions:

$$E(t,0) = E_L(t) \text{ and } E(t,z_0) = 0$$

FDTD Discretization

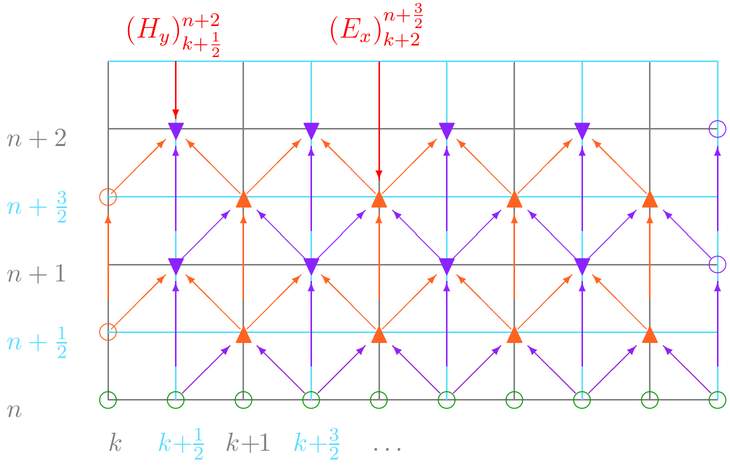


Figure 5: Yee Scheme

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

$$\tau_h^{E_x} := \left\{ \left(x_{\ell+\frac{1}{2}}, y_j \right) | 0 \leq \ell \leq L-1, 0 \leq j \leq J \right\} \quad (9)$$

$$\tau_h^{E_y} := \left\{ \left(x_{\ell}, y_{j+\frac{1}{2}} \right) | 0 \leq \ell \leq L, 0 \leq j \leq J-1 \right\} \quad (10)$$

$$\tau_h^{H} := \left\{ \left(x_{\ell+\frac{1}{2}}, y_{j+\frac{1}{2}} \right) | 0 \leq \ell \leq L-1, 0 \leq j \leq J-1 \right\} \quad (11)$$

$$\tau_t^{E} := \left\{ \left(t^n \right) | 0 \leq n \leq N \right\} \quad (12)$$

$$\tau_t^{H} := \left\{ \left(t^{n+\frac{1}{2}} \right) | 0 \leq n \leq N-1 \right\}. \quad (13)$$

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

$$\delta_t U_{i,j}^{\gamma} := \frac{U_{i,j}^{\gamma+\frac{1}{2}} - U_{i,j}^{\gamma-\frac{1}{2}}}{\Delta t}, \tag{14}$$

$$\overline{U}_{i,j}^{\gamma} := \frac{U_{i,j}^{\gamma+\frac{1}{2}} + U_{i,j}^{\gamma-\frac{1}{2}}}{2}, \tag{15}$$

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

$$\delta_x U_{i,j}^{\gamma} := \frac{U_{i+\frac{1}{2},j}^{\gamma} - U_{i-\frac{1}{2},j}^{\gamma}}{\Delta x}, \tag{16}$$

$$\delta_y U_{i,j}^{\gamma} := \frac{U_{i,j+\frac{1}{2}}^{\gamma} - U_{i,j-\frac{1}{2}}^{\gamma}}{\Delta y}. \tag{17}$$

Maxwell-PC Lorentz-FDTD

The Yee Scheme applied to the Maxwell-PC Lorentz yields

$$\delta_t H^n_{\ell+\frac{1}{2},j+\frac{1}{2}} = \frac{1}{\mu_0}\left(\delta_y E^n_{x_{\ell+\frac{1}{2},j+\frac{1}{2}}} - \delta_x E^n_{y_{\ell+\frac{1}{2},j+\frac{1}{2}}}\right) \tag{18a}$$

$$\epsilon_0\epsilon_\infty \delta_t E^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} = \delta_y H^{n+\frac{1}{2}}_{\ell+\frac{1}{2},j} - \overline{\vec{\beta}}^{n+\frac{1}{2}}_{0,x_{\ell+\frac{1}{2},j}} \tag{18b}$$

$$\epsilon_0\epsilon_\infty \delta_t E^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} = -\delta_x H^{n+\frac{1}{2}}_{\ell,j+\frac{1}{2}} - \overline{\vec{\beta}}^{n+\frac{1}{2}}_{0,y_{\ell,j+\frac{1}{2}}} \tag{18c}$$

$$\delta_t \vec{\alpha}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} = \overline{\vec{\beta}}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} \tag{18d}$$

$$\delta_t \vec{\alpha}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} = \overline{\vec{\beta}}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} \tag{18e}$$

$$\delta_t \vec{\beta}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} = -A\overline{\vec{\alpha}}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} - 2\nu\overline{\vec{\beta}}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} + \hat{e}_1\epsilon_0\omega_p^2\overline{E}^{n+\frac{1}{2}}_{x_{\ell+\frac{1}{2},j}} \tag{18f}$$

$$\delta_t \vec{\beta}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} = -A\overline{\vec{\alpha}}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} - 2\nu\overline{\vec{\beta}}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}} + \hat{e}_1\epsilon_0\omega_p^2\overline{E}^{n+\frac{1}{2}}_{y_{\ell,j+\frac{1}{2}}}. \tag{18g}$$

Staggered L^2 normed spaces

Next, we define the L^2 normed spaces

$$\mathbb{V}_E := \left\{ \mathbf{F} : \tau_h^{E_x} \times \tau_h^{E_y} \longrightarrow \mathbb{R}^2 \mid \mathbf{F} = (F_{x_{l+\frac{1}{2},j}}, F_{y_{l,j+\frac{1}{2}}})^T, \|\mathbf{F}\|_E < \infty \right\} \tag{19}$$

$$\mathbb{V}_H := \left\{ U : \tau_h^{H} \longrightarrow \mathbb{R} \mid U = (U_{l+\frac{1}{2},j+\frac{1}{2}}), \|U\|_H < \infty \right\} \tag{20}$$

with the following discrete norms and inner products

$$\|\mathbf{F}\|_E^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(|F_{x_{\ell+\frac{1}{2},j}}|^2 + |F_{y_{\ell,j+\frac{1}{2}}}|^2 \right), \forall\ \mathbf{F} \in \mathbb{V}_E \tag{21}$$

$$(\mathbf{F}, \mathbf{G})_E = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} \left(F_{x_{\ell+\frac{1}{2},j}} G_{x_{\ell+\frac{1}{2},j}} + F_{y_{\ell,j+\frac{1}{2}}} G_{y_{\ell,j+\frac{1}{2}}} \right), \forall\ \mathbf{F}, \mathbf{G} \in \mathbb{V}_E \tag{22}$$

$$\|U\|_H^2 = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} |U_{\ell+\frac{1}{2},j+\frac{1}{2}}|^2, \forall\ U \in \mathbb{V}_H \tag{23}$$

$$(U, V)_H = \Delta x \Delta y \sum_{\ell=0}^{L-1} \sum_{j=0}^{J-1} U_{\ell+\frac{1}{2},j+\frac{1}{2}} V_{\ell+\frac{1}{2},j+\frac{1}{2}}, \forall\ U, V \in \mathbb{V}_H. \tag{24}$$

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

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

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

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

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

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:

$$\sqrt{2} c_\infty \Delta t \leq h. \tag{25}$$

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

If the stability condition (25) *is satisfied, then the Yee scheme for the 2D TE mode Maxwell-PC Lorentz system given in* (18) *satisfies the discrete identity*

$$\delta_t \mathcal{E}_h^{n+\frac{1}{2}} = \frac{-1}{\overline{\mathcal{E}}_h^{n+\frac{1}{2}}} \left\| \sqrt{\frac{2\nu}{\epsilon_0 \omega_p^2}} \overline{\vec{\beta}}_h^{n+\frac{1}{2}} \right\|_A^2 \tag{26}$$

for all n where

$$\mathcal{E}_h^n = \left(\mu_0 (H^{n+\frac{1}{2}}, H^{n-\frac{1}{2}})_H + \|\sqrt{\epsilon_0 \epsilon_\infty}\ \mathbf{E}^n\|_E^2 + \left\| \sqrt{\frac{\omega_0^2}{\epsilon_0 \omega_p^2}} \vec{\alpha}^n \right\|_\alpha^2 + \left\| \sqrt{\frac{1}{\epsilon_0 \omega_p^2}} \vec{\beta}^n \right\|_\alpha^2 \right)^{1/2} \tag{27}$$

defines a discrete energy.

In the above $\|\vec{\boldsymbol{\alpha}}\|_A^2 := (A\vec{\boldsymbol{\alpha}}, \vec{\boldsymbol{\alpha}})_\alpha$ given A positive definite, which is true iff $r < m$. Note that $\|\vec{\boldsymbol{\alpha}}\|_\alpha^2 \approx \|\mathbb{E}[\mathcal{P}]\|_2^2 + \|\text{StdDev}(\mathcal{P})\|_2^2 = \mathbb{E}[\|\mathcal{P}\|_2^2] = \|\mathcal{P}\|_F^2$ so that this is a natural extension of the Maxwell-Random Debye energy (6).

Outline

Current/Future Work

Current Work:

- Analyze the dispersion error of the model

Future Work:

- Explore the Jacobi polynomials and beta distributions
- Analyze multiple poles in time domain

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