A Dispersion Optimized Mimetic Finite Difference Method for Maxwells Equations in Linear Dispersive Media

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Maxwell's Equations

- Let $\Omega \subset \mathbb{R}^d$ be a bounded domain, $d = 2, 3$. Let $T > 0$. On $\Omega \times (0, T]$

$$\begin{aligned}
\mathbf{D}_t &= \mathbf{curl\ H} && \text{(Amperé's Law)} \\
\mathbf{B}_t &= -\mathbf{curl\ E} && \text{(Faraday's Law)} \\
\nabla \cdot \mathbf{D} &= 0 && \text{(Poisson/Gauss Law)} \\
\nabla \cdot \mathbf{B} &= 0 && \text{(Gauss Law)}
\end{aligned}$$

$\mathbf{E} =$	Electric field vector	$\mathbf{D} =$	Electric flux density
$\mathbf{H} =$	Magnetic field vector	$\mathbf{B} =$	Magnetic flux density

- On $\partial\Omega \times [0, T]$

$$\mathbf{E} \times \mathbf{n} = \mathbf{0}, \quad \text{(Perfect Electric Conducting Condition)}$$

with $\mathbf{n}$ the unit outward normal vector to $\partial\Omega$.

- Appropriate initial conditions.

Linear Dispersive Materials: Polarization Laws

- Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.
- Linear Dispersive Material: Characterized by physical dispersion: frequency dependent speed of propagation. Modeled by the macroscopic polarization **P**.

$$\mathbf{D} = \epsilon_0 \epsilon_r \mathbf{E} + \mathbf{P}$$
$$\mathbf{B} = \mu_0 \mathbf{H}$$

$\mathbf{P} =$	Polarization	$\epsilon_0 =$	vacuum electric permittivity
$\epsilon_r =$	Relative permittivity	$\mu_0 =$	vacuum magnetic permeability

Linear Dispersive Materials: Complex permittivity

- We can define $\mathbf{P}$ in terms of a convolution [Taflove & Hagness 2000]

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

where g is the dielectric response function (DRF).

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- For most materials of interest, we can replace the convolution by a system of ODEs describing the evolution of the polarization forced by the electric field (Auxiliary Differential Equation (ADE)).
- The model for EM wave propagation in the material is given by Maxwell's equations along with ODEs for the dynamic evolution of **P**.
- To obtain a numerical method for simulating wave propagation in these materials we have to simultaneously discretize the hybrid PDE-ODE system.

1. Maxwells Equations in Cold Plasma: 2D Formulation

Cold Plasma (CP) model – special case of the *Lorentz model* for partially ionized gases without magnetization effects.

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Cold Plasma (CP) model – special case of the *Lorentz model* for partially ionized gases without magnetization effects.

- Define $\mathbf{J} = \mathbf{P}_t$.
- First order formulation on $\Omega \subset \mathbb{R}^2$. Eliminate $\mathbf{D}$.

$$\begin{cases} \mathbf{E}_t &= -\epsilon_0^{-1}\mathbf{J} + c_0^2 \ \mathbf{curl} \ B \\ B_t &= -\operatorname{curl} \ \mathbf{E} \\ \mathbf{J}_t &= \epsilon_0 \omega_{\mathrm{p}}^2 \mathbf{E} - \omega_{\mathrm{icf}} \mathbf{J} \end{cases} \qquad \text{in} \quad \Omega \times (0, T]$$

$$\mathbf{E} \times \mathbf{n} = 0 \qquad \text{on} \quad \partial\Omega \times (0, T]$$

$\mathbf{J}$ – polarization current density;
c_0 – the speed of light;
ω_{icf} – ion collision frequency;
ω_{p} – plasma frequency;

Subject to appropriate initial conditions.

2. Maxwells Equations in Cold Plasma

Second order formulation (eliminating **B**)

$$\begin{cases} \mathbf{E}_{tt} + \epsilon_0^{-1}\mathbf{J}_t = -c_0^2 \,\mathbf{curl}\, \mathrm{curl}\, \mathbf{E} \\ \mathbf{J}_t = -\omega_{\mathrm{icf}}\mathbf{J} + \epsilon_0 \omega_{\mathrm{p}}^2 \mathbf{E} \end{cases} \quad \text{in} \quad \Omega \times (0, T]$$

$$\mathbf{E} \times \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega \times (0, T]$$

E – electric field intensity; **J** – polarization current density;

c_0 – the speed of light; ϵ_0 – the electric permittivity of free space;
ω_{icf} – ion collision frequency; ω_{p} – plasma frequency;
n – unit outward normal to the boundary $\Omega \subset \mathbb{R}^2$.

Subject to appropriate initial conditions.

MFD discretization will be based on this formulation.

FDTD/FEM for Linear Dispersive Media

- [Kane Yee-1966]: Yee or FDTD method for time domain ME. Second order accurate method in space/time. Non-dissipative, but dispersive.

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- Nédélec 1980: Mixed FEM for ME. ([Peter Monk], [Jichun Li])
- Mimetic Finite Differences: Generalization of Yee scheme to polygonal, polyhedral meshes. ([Hyman & Shashkov], [Beirao da Veiga, Lipnikov and Manzini]).

Goal and Outline of Talk

Goal: Construct a mimetic finite difference method (MFD) for the cold plasma model that has better dispersion properties than the Yee/FDTD method using the MFD methodology.

1. Build Mimetic Finite Difference (MFD) discretization in space – parameterized family of methods
2. Exponential time difference discretization
3. Compute Dispersion relation (in general form) for parameterized family.
4. M-adaptation: Pick the member of parameterized family with lowest numerical dispersion error.
5. Numerical tests.

1. MFD discretization in Space

Weak formulation: *find* $\mathbf{E}, \mathbf{J} \in \mathcal{E} := H_0(\mathrm{curl}, \Omega)$ *s.t. for any* $\phi, \psi \in \mathcal{E}$

$$\begin{cases} [\mathbf{E}_{tt}, \phi]_{\mathcal{E}} + c_0^2 \, [\mathrm{curl}\, \mathbf{E}, \mathrm{curl}\, \phi]_{\mathcal{F}} + \epsilon_0^{-1} \, [\mathbf{J}_t, \phi]_{\mathcal{E}} & = 0, \\ [\mathbf{J}_t, \psi]_{\mathcal{E}} + \omega_{\mathsf{icf}} \, [\mathbf{J}_t, \psi]_{\mathcal{E}} - \epsilon_0 \omega_{\mathsf{p}}^2 \, [\mathbf{J}_t, \psi]_{\mathcal{E}} & = 0, \end{cases}$$

where

$$[\mathbf{J}, \mathbf{E}]_{\mathcal{E}} := \int_{\Omega} \mathbf{J} \cdot \mathbf{E} \; d\Omega \qquad [J, E]_{\mathcal{F}} := \int_{\Omega} J \; E \; d\Omega.$$

1. MFD discretization in Space

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<u>**Semi-discrete formulation**</u>, Finite Element viewpoint on MFD:

$$\begin{cases} \left[\mathbf{E}_{tt}^h, \phi^h\right]_{\mathcal{E}_h} + c_0^2\left[\mathrm{curl}^h\,\mathbf{E}^h, \mathrm{curl}^h\,\phi^h\right]_{\mathcal{F}_h} + \epsilon_0^{-1}\left[\mathbf{J}_t^h, \phi^h\right]_{\mathcal{E}_h} & = 0, \\ \left[\mathbf{J}_t^h, \psi^h\right]_{\mathcal{E}_h} + \omega_{\mathrm{icf}}\left[\mathbf{J}_t^h, \psi^h\right]_{\mathcal{E}_h} - \epsilon_0 \omega_{\mathrm{p}}^2\left[\mathbf{J}_t^h, \psi^h\right]_{\mathcal{E}_h} & = 0. \end{cases}$$

1. MFD discretization in Space

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Need to define:

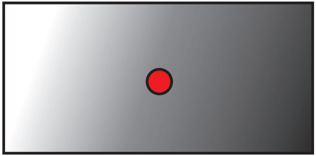
- $\mathcal{F}_h$ with $[\cdot, \cdot]_{\mathcal{F}_h}$,
- $\mathcal{E}_h$ with $[\cdot, \cdot]_{\mathcal{E}_h}$ and
- $\mathrm{curl}_h : \mathcal{E}_h \to \mathcal{F}_h$.

1. Face/Cell based Approximation Space $\mathcal{F}_h$ with $[\cdot,\cdot]_{\mathcal{F}_h}$

- Standard assembly of $\mathcal{F}_h$ with $[\cdot,\cdot]_{\mathcal{F}_h}$ from the local $\mathcal{F}_E$ with $[\cdot,\cdot]_{\mathcal{F}_E}$ on each element E.

- Interpolation operator $\mathcal{I}^{\mathcal{F}_E}$
  Degrees of Freedom:

$$\mathcal{I}^{\mathcal{F}_E}[p] = \frac{1}{|E|}\int_E p \; dE \qquad \text{– constant on } E.$$



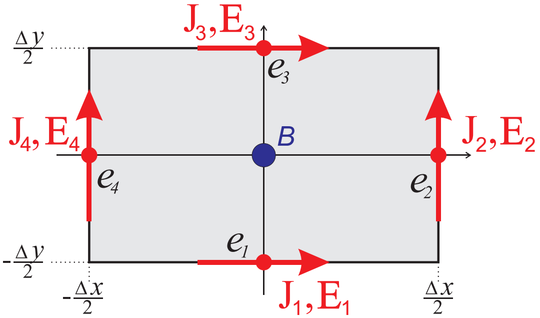
- **Inner product**: $\left[\mathcal{I}^{\mathcal{F}_E}[p], \mathcal{I}^{\mathcal{F}_E}[q]\right]_{\mathcal{F}_E} = |E|\,\mathcal{I}^{\mathcal{F}_E}[p]\mathcal{I}^{\mathcal{F}_E}[q].$

1. Edge-based approximation space $\mathcal{E}_h$

- Interpolation operator $\mathcal{I}^{\mathcal{E}_h}$
- **Degrees of Freedom**:

$$\mathcal{I}^{\mathcal{E}_e}[\mathbf{p}] = \frac{1}{|e|}\int_e \mathbf{p}\cdot\tau_e \, de \quad \text{– constant on } e.$$

τ_e – unit tangent to e.



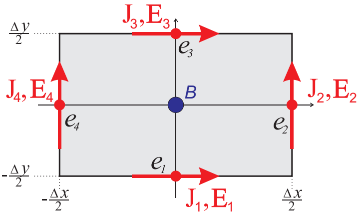
1. Inner product $[\cdot,\cdot]_{\mathcal{E}_h}$

- MFD Construction is non-unique and leads to parameterized family of methods with equivalent properties such as base convergence rate. We obtain a matrix with 3 free parameters $\omega_1, \omega_2, \omega_3$.
- Non-standard Mass Lumping: Instead of computing $\mathbb{M}_{\mathcal{E}_E}$ associated with the inner product $[\cdot,\cdot]_{\mathcal{E}_E}$ we will compute its inverse $\mathbb{W}_{\mathcal{E}_E} \approx \mathbb{M}_{\mathcal{E}_E}^{-1}$

$$\mathbb{W}_{\mathcal{E}_E} = \frac{1}{4\triangle x\,\triangle y}\begin{bmatrix} 1+4\omega_1 & 4\omega_2 & 1-4\omega_1 & -4\omega_2 \\ 4\omega_2 & 1+4\omega_3 & -4\omega_2 & 1-4\omega_3 \\ 1-4\omega_1 & -4\omega_2 & 1+4\omega_1 & 4\omega_2 \\ -4\omega_2 & 1-4\omega_3 & 4\omega_2 & 1+4\omega_3 \end{bmatrix}.$$

- E.g. $\omega_1 = \omega_3 = \frac{1}{4}$, $\omega_2 = 0$ gives the Yee-FDTD scheme.
- M-adaptation – optimize the choice of free parameters $\omega_1, \omega_2, \omega_3$ for selected criteria – reduction of numerical dispersion.

1. $\text{curl}_E : \mathcal{E}_E \to \mathcal{F}_E$



$$\int_E \text{curl}\,\mathbf{J}\; dE = \int_{\partial E} \mathbf{J}\cdot\tau\; de.$$

$$\left(\frac{1}{|E|}\int_E \text{curl}\,\mathbf{J}\; dE\right) = \frac{1}{|E|}\sum_{e\in\partial E}|e|\left(\frac{1}{|e|}\int_e \mathbf{J}\cdot\tau\; de\right).$$

- $\text{curl}_E : \mathcal{E}_E \to \mathcal{F}_E$

$$\text{curl}_E = \frac{1}{\triangle x\,\triangle y}\left[\;\triangle x \quad \triangle y \quad -\triangle x \quad -\triangle y\;\right].$$

2. Time discretization

- Dispersion reduction will be achieved by cancelling temporal and spatial errors at the leading orders (by a proper choice of the MFD parameters).
- Standard leapfrog discretization DOES NOT allow for dispersion reduction beyond second order for linear dispersive media. However, for non-dispersive materials it does.
- Thus, the correct choice of time discretization is crucial for M-adaptation. We use Exponential time differences (ETD as our time discretization.

2. Exponential time differencing (ETD)

- Integrating factor e^{-ct}:

$$\left(e^{-ct}u\right)_t = e^{-ct}\left(u_t - cu\right).$$

- For a first-order **scalar ODE**:

$$\dot{u} = cu + F(u,t)$$

the exponential time difference scheme yields

$$u^{n+1} = e^{ct}u^n + c^{-1}(e^{c\triangle t} - 1)F^{n+1/2}.$$

- For a **vector ODE** with invertible $\mathbb{X}$

$$\dot{\mathbf{u}} = \mathbb{X}\mathbf{u} + \mathbf{F}(\mathbf{u},t)$$

the exponential time difference scheme yields

$$\mathbf{u}^{n+1} = e^{\mathbb{X}\triangle t}\mathbf{u}^n + \mathbb{Y}\mathbf{F}^{n+1/2}, \qquad \mathbb{Y} := \mathbb{X}^{-1}\left(e^{\mathbb{X}\triangle t} - \mathbb{I}\right).$$

2. Semi-discrete formulation: ETD

- Original first-order formulation:

$$\begin{cases} \mathbf{E}_t = -\epsilon_0^{-1}\mathbf{J} + c_0^2 \,\mathbf{curl}\; B \\ \mathbf{J}_t = \epsilon_0 \omega_{\mathrm{p}}^2 \mathbf{E} - \omega_{\mathrm{icf}} \mathbf{J} \\ B_t = -\,\mathrm{curl}\,\mathbf{E} \end{cases} \quad \text{in} \quad \Omega \times (0, T]$$

- **Matrix form**:

$$\begin{cases} \mathbf{u}_t = \mathbb{X}\mathbf{u} + \mathbf{F} \\ B_t = -\,\mathrm{curl}\;\mathbf{E} \end{cases} \quad \text{in} \quad \Omega \times (0, T]$$

$$\mathbf{u} = \begin{bmatrix} \mathbf{E} \\ \mathbf{J} \end{bmatrix} \qquad \mathbb{X} = \begin{bmatrix} 0 & -\epsilon_0^{-1} \\ \epsilon_0 \omega_{\mathrm{p}}^2 & -\omega_{\mathrm{icf}} \end{bmatrix} \qquad \mathbf{F} = \begin{bmatrix} c_0^2 \mathbf{curl} B \\ 0 \end{bmatrix}$$

- Time discretization:

$$\begin{cases} \mathbf{u}^{n+1} = e^{\mathbb{X}\triangle t}\mathbf{u}^n + \mathbb{Y}\mathbf{F}^{n+1/2} \\ B^{n+1/2} = B^{n-1/2} - \triangle t \,\mathrm{curl}\,\mathbf{E}^n \end{cases}$$

2. Semi-discrete formulation: ETD

- Eliminate B by considering $\mathbf{u}^{n+1} - \mathbf{u}^n$:

$$\begin{cases} (\mathbf{u}^{n+1} - \mathbf{u}^n) & = & e^{\mathbb{X}\triangle t}(\mathbf{u}^n - \mathbf{u}^{n-1}) + \mathbb{Y}(\mathbf{F}^{n+\frac{1}{2}} - \mathbf{F}^{n-\frac{1}{2}}) \\ B^{n+1/2} - B^{n-1/2} & = & -\triangle t \,\mathrm{curl}\, \mathbf{E}^n \end{cases}$$

$$\mathbf{F}^{n+\frac{1}{2}} - \mathbf{F}^{n-\frac{1}{2}} = \left[\begin{array}{c} c_0^2 \mathbf{curl}(B^{n+\frac{1}{2}} - B^{n-\frac{1}{2}}) \\ 0 \end{array} \right] = \left[\begin{array}{c} c_0^2 \triangle t \mathbf{curl}\, \mathrm{curl}\, \mathbf{E}^n \\ 0 \end{array} \right].$$

- Second order formulation:

$$\frac{1}{\triangle t}\mathbb{Y}^{-1}\left(\left[\begin{array}{c} \mathbf{E}^{n+1} \\ \mathbf{J}^{n+1} \end{array} \right] - (\mathbb{I} + e^{\mathbb{X}\triangle t}) \left[\begin{array}{c} \mathbf{E}^{n} \\ \mathbf{J}^{n} \end{array} \right] + e^{\mathbb{X}\triangle t} \left[\begin{array}{c} \mathbf{E}^{n-1} \\ \mathbf{J}^{n-1} \end{array} \right] \right) =$$

$$= - c_0^2 \left[\begin{array}{c} \mathbf{curl}\, \mathrm{curl}\, \mathbf{E}^n \\ 0 \end{array} \right].$$

$$\mathbb{Y} := \mathbb{X}^{-1}\left(e^{\mathbb{X}\triangle t} - \mathbb{I}\right).$$

3. Dispersion Relations

- *Dispersion relation* – relation between the wave frequency ω and the wave number $\mathbf{k}$ for a plane wave

$$e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\mathbf{u}_0 = e^{i\mathbf{k}\cdot\left(\mathbf{x}-\frac{\mathbf{k}}{k}\frac{\omega}{k}t\right)}\mathbf{u}_0, \qquad k = |\mathbf{k}|.$$

  Wave speed $c := \frac{\omega}{k}$.
- *Symbols* – generalized eigenvalues of the temporal and the spatial operators for a plane wave eigenfunction $e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}\mathbf{u}_0$.
  Continuous symbols: $\mathcal{T}(\omega)$ and $\mathcal{S}(\mathbf{k})$.
  Discrete symbols: $\mathcal{T}_{\triangle t}(\omega)$ and $\mathcal{S}_h(\mathbf{k})$.
- Dispersion relations using symbols:

$$\begin{aligned}
\mathcal{T}(\omega) &= \mathcal{S}(\mathbf{k}) && \text{- fully continuous,}\\
\mathcal{T}(\omega) &= \mathcal{S}_h(\mathbf{k}) && \text{- continuous in time, discrete in space,}\\
\mathcal{T}_{\triangle t}(\omega) &= \mathcal{S}(\mathbf{k}) && \text{- discrete in time, continuous in space,}\\
\mathcal{T}_{\triangle t}(\omega) &= \mathcal{S}_h(\mathbf{k}) && \text{- fully discrete,}
\end{aligned}$$

3. Discrete symbols

- **Discrete temporal symbol** for ETD formulation:

$$\mathcal{T}_{\triangle t}(\omega) = \frac{1}{\triangle t}\mathbb{Y}^{-1}\left(e^{i\triangle t\omega}\mathbb{I} - (\mathbb{I} + e^{\triangle t\mathbb{X}}) + e^{-i\triangle t\omega}e^{\triangle t\mathbb{X}}\right) =$$

$$= (-\omega^2\mathbb{I} + i\omega\mathbb{X}) + \frac{\triangle t^2}{12}(-\omega^2\mathbb{I} + i\omega\mathbb{X})^2 + \mathcal{O}(\triangle t^4).$$

- **Discrete spatial symbol**:

$$\begin{aligned}\mathcal{S}_h(\mathbf{k}) = &- c_0^2\,\mathrm{trace}(\overline{\mathbb{W}}_{\mathcal{E}}\overline{\mathbb{A}}_h) = \\ = &- \frac{4c_0^2}{\triangle x^2}\sin^2\left(\frac{k_x\triangle x}{2}\right)\left(1 + (1-4\omega_3)\sin^2\left(\frac{k_x\triangle x}{2}\right)\right) - \\ &- \frac{32c_0^2}{\triangle x\triangle y}\omega_2\sin^2\left(\frac{k_x\triangle x}{2}\right)\sin^2\left(\frac{k_y\triangle y}{2}\right) - \\ &- \frac{4c_0^2}{\triangle y^2}\sin^2\left(\frac{k_y\triangle y}{2}\right)\left(1 + (1-4\omega_1)\sin^2\left(\frac{k_y\triangle y}{2}\right)\right).\end{aligned}$$

3. Discrete spatial symbol (continued)

- Taylor expansion in $h = dx$, $(\gamma \triangle y/dx)$:

$$\mathcal{S}_h(\mathbf{k}) = -(c_0 k)^2 \Big\{ 1 + \\ + \Big(\tfrac{3\omega_3 - 1}{3} \cos^4(\theta) + 2\gamma\omega_2 \cos^2(\theta)\sin^2(\theta) + \tfrac{\gamma^2(3\omega_1 - 1)}{3} \sin^4(\theta) \Big) k^2 h^2 + \\ + \mathcal{O}(h^4) \Big\}.$$

- Eliminate angular dependence through parameter choice:

$$\tfrac{3\omega_3 - 1}{3} = \gamma\omega_2 = \tfrac{\gamma^2(3\omega_1 - 1)}{3} \quad \Rightarrow \quad \begin{cases} \omega_1 = \frac{3\omega_2\gamma^{-1} + 1}{3} \\ \omega_3 = \frac{3\omega_2\gamma \quad + 1}{3} \end{cases}$$

- Result:

$$\mathcal{S}_h(\mathbf{k}) = -(c_0 k)^2 \Big\{ 1 + \gamma\omega_2 k^2 h^2 + \mathcal{O}(h^4) \Big\}.$$

4. Final step: M-adaptation

- Combining temporal and spatial symbols:

$$(\mathcal{T}_{\triangle t}(\omega) - \mathcal{S}_h(\mathbf{k})\mathbb{P}_1) \begin{bmatrix} E_0 \\ J_0 \end{bmatrix} = \frac{h^2}{12c_0}(\nu^2 + 12\gamma\omega_2)c_0^4 k^4 \mathbb{P}_1 + \mathcal{O}(h^4).$$

- Last parameter:

$$\omega_2 = -\frac{\nu^2}{12\gamma} \quad \Rightarrow \quad (\nu^2 + 12\gamma\omega_2) = 0 \quad \Rightarrow$$

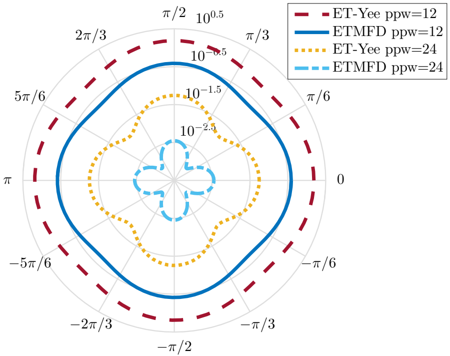
$$(\mathcal{T}_{\triangle t}(\omega) - \mathcal{S}_h(\mathbf{k})\mathbb{P}_1) \begin{bmatrix} E_0 \\ J_0 \end{bmatrix} = \mathcal{O}(h^4).$$

5. Numerical results: Experiment 1

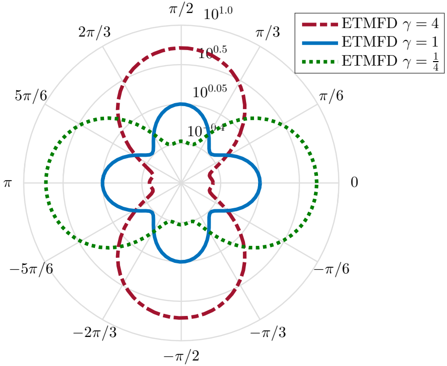
Cold isotropic plasma with $\omega_\mathrm{p} = 1$ and ω_icf.

Relative dispersion error:

$\gamma = 1$, $\nu = \frac{1}{2}$.



$\gamma = 4, 1, 4^{-1}$, $\nu = \frac{1}{2}$, $\triangle x \triangle y$-const.



5. Numerical results: Experiment 2

Exact solution:

$$\mathbf{E}(x,y,t) = e^{at}\cos(bt)\begin{bmatrix} -k_y\cos(k_x x)\sin(k_y y) \\ k_x\sin(k_x x)\cos(k_y y)\end{bmatrix}$$

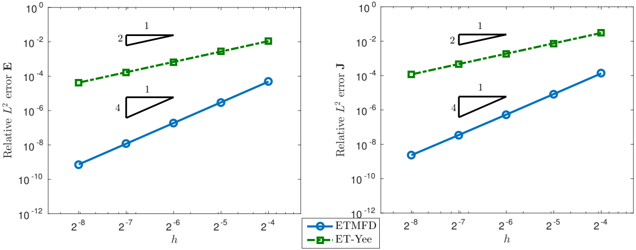
$$\mathbf{J}(x,y,t) = \epsilon_0\omega_{\mathrm{p}}^2\frac{(a+\omega_{\mathrm{icf}})\cos(bt)+b\sin(bt)}{b^2+(a+\omega_{\mathrm{icf}})^2}\mathbf{E}(x,y,t)$$

$a + ib = \omega$ – complex root of the disp. relation.

ϵ_0 – the electric permittivity of free space;

ω_{icf} – ion collision frequency; ω_{p} – plasma frequency;

Relative L^2 errors for ETMFD vs ET Yee:



Conclusions

- MFD discretization of Maxwell's equation in cold plasma.
- Generalized mass lumping for efficiency of time integration on rectangular meshes.
- Using standard leapfrog time discretization does not allow to reduce the numerical dispersion.
- Exponential time differencing (integration factor) allows to perform m-adaptation. Numerical dispersion reduced from 2nd to 4th order.
- The choice of the parameters in the MFD mass matrix is the same as in the vacuum $\Rightarrow$ generalization.
- FUTURE: Analyze divergence-free condition.

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