Energy Stable Discontinuous Galerkin Methods for Maxwell's Equations in Nonlinear Optical Media

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"Computational Aspects of Time Dependent Electromagnetic Wave Problems in Complex Materials", ICERM, June 2018

Joint work with Vrushali Bokil, Fengyan Li, Yan Jiang

Outline

1. Introduction
2. Numerical methods
   - Temporal discretizations
   - Spatial discretizations
3. Numerical results
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Nonlinear optics

- Nonlinear optics is the study of the behavior of light propagating in optical media where the material response depends on the fields nonlinearly. Nonlinearity is particularly relevant when the intensity of the light is very high (e.g. laser).
- Examples of nonlinear behavior
  - The refractive index, and consequently the speed of light in a nonlinear optical medium, depends on light intensity.
  - The frequency of light is altered as it passes through a nonlinear optical medium. For example, the light can change from red to blue.
- Applications: laser frequency conversion, second/third-harmonic generation (frequency-mixing), self-phase modulation.

References: *Bloembergen (96), Boyd (03), New (11).*

Numerical simulations

- Common approach: simulate **approximate models**, such as nonlinear Schrödinger equation (NLS) equation, beam propagation method (BPM) for wavepackets.
- More costly approach: simulate nonlinear Maxwell models directly. This approach is more robust because it avoids the simplifying assumptions that lead to conventional asymptotic and paraxial propagation analyses, and can treat interacting waves at different frequencies directly.

The model under consideration

Maxwell's equations in a non-magnetic nonlinear optical medium

$$\partial_t \mathbf{B} + \nabla \times \mathbf{E} = 0, \text{ in } (0, T) \times \Omega, \tag{1a}$$

$$\partial_t \mathbf{D} + \mathbf{J_s} - \nabla \times \mathbf{H} = 0, \text{ in } (0, T) \times \Omega, \tag{1b}$$

$$\nabla \cdot \mathbf{B} = 0, \ \nabla \cdot \mathbf{D} = \rho, \text{ in } (0, T) \times \Omega, \tag{1c}$$

where $\mathbf{E}, \mathbf{D}, \mathbf{H}, \mathbf{B}$ are the electric field, electric flux density, magnetic field, magnetic induction, $\rho, \mathbf{J_s}$ are the charge and source current density.

Constitutive relations

$$\mathbf{D} = \epsilon_0(\epsilon_\infty \mathbf{E} + \mathbf{P}^{\mathrm{L}}_{\mathrm{delay}} + a(1-\theta)\mathbf{E}|\mathbf{E}|^2 + a\theta Q\mathbf{E}), \quad \mathbf{B} = \mu_0 \mathbf{H}, \tag{2}$$

which takes into account the following effects.

The model

- linear instantaneous response $\epsilon_0\epsilon_\infty \mathbf{E}$.
- linear Lorentz response, where

$$\frac{\partial^2 \mathbf{P}^{\mathrm{L}}_{\mathrm{delay}}}{\partial t^2} + \frac{1}{\tau}\frac{\partial \mathbf{P}^{\mathrm{L}}_{\mathrm{delay}}}{\partial t} + \omega_0^2 \mathbf{P}^{\mathrm{L}}_{\mathrm{delay}} = \omega_p^2 \mathbf{E}. \tag{3}$$

  Here ω_0, ω_p are the resonance and plasma frequencies of the medium. τ^{-1} is a damping constant.
- nonlinear response.

$$\mathbf{P}^{\mathrm{NL}} = \mathbf{P}^{\mathrm{NL}}_{\mathrm{Kerr}} + \mathbf{P}^{\mathrm{NL}}_{\mathrm{delay}} = \underbrace{a(1-\theta)\mathbf{E}|\mathbf{E}|^2}_{\mathrm{Kerr}} + \underbrace{a\theta Q\mathbf{E}}_{\mathrm{Raman}}.$$

  Here a, θ are constants. Q describes the natural molecular vibrations within the dielectric material that has frequency many orders of magnitude less than the optical wave frequency, where

$$\frac{\partial^2 Q}{\partial t^2} + \frac{1}{\tau_v}\frac{\partial Q}{\partial t} + \omega_v^2 Q = \omega_v^2 |\mathbf{E}|^2, \tag{4}$$

  where ω_v is the resonance frequency of the vibration, and τ_v^{-1} a damping constant.

Previous work for nonlinear Maxwell model with Kerr/Raman effects

Relatively fewer papers compared with linear media.

- FDTD approach: Hile, Kath (96), Sorenson et al (05), Giles et al. (00)
- Pseudospectral method: Tyrrell et al (05)
- FVM approach for Kerr media: De La Bourdonnaye (00), Aregba-Driollet (15)
- DG for Kerr media: Fezoui (15)

Simplified 1D model

In 1D, by using the ADE approach, we have

$$\mu_0 \partial_t H = \partial_x E, \tag{5a}$$

$$\partial_t D = \partial_x H, \tag{5b}$$

$$\partial_t P = J, \tag{5c}$$

$$\partial_t J = -\frac{1}{\tau} J - \omega_0^2 P + \omega_p^2 E, \tag{5d}$$

$$\partial_t Q = \sigma, \tag{5e}$$

$$\partial_t \sigma = -\frac{1}{\tau_v} \sigma - \omega_v^2 Q + \omega_v^2 E^2, \tag{5f}$$

with the constitutive law

$$D = \epsilon_0 (\epsilon_\infty E + P + a(1-\theta) E^3 + a\theta Q E), \tag{6}$$

Energy relations

We consider the model in 1D, and under the assumption of periodic boundary conditions, the energy

$$\mathcal{E} = \int_\Omega \Big(\frac{\mu_0}{2}H^2 + \frac{\epsilon_0\epsilon_\infty}{2}E^2 + \frac{\epsilon_0}{2\omega_p^2}J^2 + \frac{\epsilon_0\omega_0^2}{2\omega_p^2}P^2 + \frac{\epsilon_0 a\theta}{4\omega_v^2}\sigma^2 + \frac{\epsilon_0 a\theta}{2}QE^2 + \frac{3\epsilon_0 a(1-\theta)}{4}E^4 + \frac{\epsilon_0 a\theta}{4}Q^2\Big)dx,$$

satisfies the following relation,

$$\frac{d}{dt}\mathcal{E} = -\frac{\epsilon_0}{\omega_p^2\tau}\int_\Omega J^2 dx - \frac{\epsilon_0 a\theta}{2\omega_v^2\tau_v}\int_\Omega \sigma^2 dx \le 0.$$

Note that $\mathcal{E}(t)$ is guaranteed non-negative only when $\theta \in [0, \frac{3}{4}]$.
Objective of this work: develop nonlinear Maxwell solver with provable energy stability.

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Temporal discretizations

Scheme1: Leap-frog staggered in time for the PDE part, and implicit in ODE part

$$\mu_0 \frac{H^{n+1/2} - H^n}{\Delta t/2} = \frac{\partial E^n}{\partial x}, \quad \frac{D^{n+1} - D^n}{\Delta t} = \frac{\partial H^{n+1/2}}{\partial x}, \tag{8a}$$

$$D^{n+1} = \epsilon_0(\epsilon_\infty E^{n+1} + P^{n+1} + a(1-\theta) Y^{n+1} + a\theta Q^{n+1} E^{N+1}), \tag{8b}$$

$$Y^{n+1} = Y^n + \frac{3}{2}((E^{n+1})^2 + (E^n)^2)(E^{n+1} - E^n), \tag{8c}$$

$$\frac{P^{n+1} - P^n}{\Delta t} = \frac{1}{2}\left(J^n + J^{n+1}\right), \quad \frac{Q^{n+1} - Q^n}{\Delta t} = \frac{1}{2}\left(\sigma^n + \sigma^{n+1}\right), \tag{8d}$$

$$\frac{J^{n+1} - J^n}{\Delta t} = -\frac{1}{2}\left(\frac{1}{\tau}\left(J^n + J^{n+1}\right) + \omega_0^2\left(P^n + P^{n+1}\right) - \omega_p^2\left(E^n + E^{n+1}\right)\right), \tag{8e}$$

$$\frac{\sigma^{n+1} - \sigma^n}{\Delta t} = -\frac{1}{2}\left(\frac{1}{\tau_v}\left(\sigma^n + \sigma^{n+1}\right) + \omega_v^2\left(Q^n + Q^{n+1}\right) - 2\omega_v^2 E^n E^{n+1}\right), \tag{8f}$$

$$\mu_0 \frac{H^{n+1} - H^{n+1/2}}{\Delta t/2} = \frac{\partial E^{n+1}}{\partial x}. \tag{8g}$$

Scheme2: Implicit trapezoidal, replace (8a), (8g) by

$$\mu_0 \frac{H^{n+1} - H^n}{\Delta t} = \frac{1}{2}\left(\frac{\partial E^n}{\partial x} + \frac{\partial E^{n+1}}{\partial x}\right), \quad \frac{D^{n+1} - D^n}{\Delta t} = \frac{1}{2}\left(\frac{\partial H^n}{\partial x} + \frac{\partial H^{n+1}}{\partial x}\right)$$

Discrete energy relation

With periodic boundary condition, then we have

$$\mathcal{E}^{n+1} - \mathcal{E}^n = -\frac{\epsilon_0 \Delta t}{4\omega_p^2 \tau} \int_\Omega (J^{n+1} + J^n)^2 dx - \frac{\epsilon_0 a\theta \Delta t}{8\omega_v^2 \tau_v} \int_\Omega (\sigma^{n+1} + \sigma^n)^2 dx \leq 0, \quad (9)$$

where the discrete energy for scheme1 is

$$\begin{aligned} \mathcal{E}^n \;=\; & \int_\Omega \frac{\mu_0}{2} H^{n+1/2} H^{n-1/2} + \frac{\epsilon_0 \epsilon_\infty}{2} (E^n)^2 + \frac{\epsilon_0}{2\omega_p^2} (J^n)^2 + \frac{\epsilon_0 \omega_0^2}{2\omega_p^2} (P^n)^2 \qquad (10) \\ & + \frac{\epsilon_0 a\theta}{4\omega_v^2} (\sigma^n)^2 + \frac{\epsilon_0 a\theta}{2} Q^n (E^n)^2 + \frac{3\epsilon_0 a(1-\theta)}{4} (E^n)^4 + \frac{\epsilon_0 a\theta}{4} (Q^n)^2 dx \end{aligned}$$

the discrete energy for scheme2 is

$$\begin{aligned} \mathcal{E}^n \;=\; & \int_\Omega \frac{\mu_0}{2} (H^n)^2 + \frac{\epsilon_0 \epsilon_\infty}{2} (E^n)^2 + \frac{\epsilon_0}{2\omega_p^2} (J^n)^2 + \frac{\epsilon_0 \omega_0^2}{2\omega_p^2} (P^n)^2 \qquad (11) \\ & + \frac{\epsilon_0 a\theta}{4\omega_v^2} (\sigma^n)^2 + \frac{\epsilon_0 a\theta}{2} Q^n (E^n)^2 + \frac{3\epsilon_0 a(1-\theta)}{4} (E^n)^4 + \frac{\epsilon_0 a\theta}{4} (Q^n)^2 dx. \end{aligned}$$

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Spatial discretizations

- We use discontinuous Galerkin (DG) discretizations for the unknowns. We consider central/upwind/alternating type of fluxes.
- Optimal error estimates are obtained for alternating/upwind fluxes, and suboptimal error estimates are obtained for central flux with assumptions on the smallness of nonlinearity.
- We have similar type of energy relations as the semi-discrete case (with additional damping from upwind flux). The proof can be done by using same test functions. The trapezoidal schemes are unconditionally stable, while the leap frog scheme has cfl restriction resulted from the positivity requirement of the energy.
- We have also extend the work to arbitrary even order FDTD methods in a subsequent work.

Spatial discretizations: DG scheme

DG methods.

- Invented by Reed and Hill (73) for neutron transport.
- First analysis by Lesaint and Raviart (74).
- Runge-Kutta discontinuous Galerkin (RKDG) method by Cockburn and Shu (89, 90,...) for general conservation laws.
- Many works on DG methods of various kinds for wave equations, Maxwell's equations.

Semi-discrete DG formulation

Let $\Omega = [x_L, x_R]$ be the computational domain, with mesh $x_L = x_{1/2} < x_{3/2} < \cdots < x_{N+1/2} = x_R$, is introduced. Let $I_j = [x_{j-1/2}, x_{j+1/2}]$ $h_j = x_{j+\frac{1}{2}} - x_{j-\frac{1}{2}}$ as its length, and $h = \max_{1 \le j \le N} h_j$ as the largest meshsize. We now define a finite dimensional discrete space,

$$V_h^k = \{v : v|_{I_j} \in P^k(I_j), j = 1, 2, \cdots, N\}. \tag{12}$$

Semi-discrete DG formulation

We find $H_h(t,\cdot)$, $D_h(t,\cdot)$, $E_h(t,\cdot)$, $P_h(t,\cdot)$, $J_h(t,\cdot)$, $Q_h(t,\cdot)$, $\sigma_h(t,\cdot) \in V_h^k$, such that $\forall j$,

$$
\begin{aligned}
&\mu_0 \int_{I_j} \partial_t H_h \phi dx + \int_{I_j} E_h \partial_x \phi dx - (\widehat{E_h}\phi^-)_{j+1/2} + (\widehat{E_h}\phi^+)_{j-1/2} = 0, \quad \forall \phi \in V_h^k, \\
&\int_{I_j} \partial_t D_h \phi dx + \int_{I_j} H_h \partial_x \phi dx - (\widetilde{H_h}\phi^-)_{j+1/2} + (\widetilde{H_h}\phi^+)_{j-1/2} = 0, \quad \forall \phi \in V_h^k, \\
&\partial_t P_h = J_h, \\
&\partial_t J_h = -\left(\frac{1}{\tau} J_h + \omega_0^2 P_h - \omega_p^2 E_h\right), \\
&\partial_t Q_h = \sigma_h, \\
&\int_{I_j} \partial_t \sigma_h \phi dx = -\int_{I_j} \left(\frac{1}{\tau_v}\sigma_h + \omega_v^2 Q_h - \omega_v^2 E_h^2\right) \phi dx, \quad \forall \phi \in V_h^k.
\end{aligned}
$$

The constitutive law is imposed via the L^2 projection, namely,

$$
\int_{I_j} D_h \phi dx = \int_{I_j} \epsilon_0 \left(\epsilon_\infty E_h + a(1-\theta)E_h^3 + P_h + a\theta Q_h E_h\right) \phi dx, \quad \forall \phi \in V_h^k. \tag{14}
$$

Semi-discrete DG formulation

As for numerical fluxes, we take either central fluxes,

$$\widehat{E_h} = \{E_h\}, \quad \widetilde{H_h} = \{H_h\}, \tag{15}$$

one of the following alternating flux pair

$$\widehat{E_h} = E_h^-, \ \ \widetilde{H_h} = H_h^+; \qquad \widehat{E_h} = E_h^+, \ \ \widetilde{H_h} = H_h^-, \tag{16}$$

or the dissipative flux inspired by the upwind flux for the Maxwell system without Kerr, linear Lorentz and Raman effects,

$$\widehat{E_h} = \{E_h\} + \frac{1}{2}\sqrt{\frac{\mu_0}{\epsilon_0\epsilon_\infty}}[H_h], \quad \widetilde{H_h} = \{H_h\} + \frac{1}{2}\sqrt{\frac{\epsilon_0\epsilon_\infty}{\mu_0}}[E_h]. \tag{17}$$

Semi-discrete stability

Theorem (Semi-discrete stability)

Under the assumption of periodic boundary conditions, the semi-discrete DG scheme with central and alternating fluxes satisfies

$$\frac{d}{dt}\mathcal{E}_h = -\frac{\epsilon_0}{\omega_p^2\tau}\int_\Omega J_h^2 dx - \frac{\epsilon_0 a\theta}{2\omega_v^2\tau_v}\int_\Omega \sigma_h^2 dx \le 0,$$

and the DG scheme with the upwind flux satisfies

$$\frac{d}{dt}\mathcal{E}_h = -\frac{\epsilon_0}{\omega_p^2\tau}\int_\Omega J_h^2 dx - \frac{\epsilon_0 a\theta}{2\omega_v^2\tau_v}\int_\Omega \sigma_h^2 dx - \frac{1}{2}\sqrt{\frac{\mu_0}{\epsilon_0\epsilon_\infty}}\sum_{j=1}^N [H_h]_{j+1/2}^2 - \frac{1}{2}\sqrt{\frac{\epsilon_0\epsilon_\infty}{\mu_0}}\sum_{j=1}^N [E_h]_{j+1/2}^2 \le 0,$$

where

$$\mathcal{E}_h = \int_\Omega \left(\frac{\mu_0}{2}H_h^2 + \frac{\epsilon_0\epsilon_\infty}{2}E_h^2 + \frac{\epsilon_0}{2\omega_p^2}J_h^2 + \frac{\epsilon_0\omega_0^2}{2\omega_p^2}P_h^2 + \frac{\epsilon_0 a\theta}{4\omega_v^2}\sigma_h^2 + \frac{\epsilon_0 a\theta}{2}Q_h E_h^2 + \frac{3\epsilon_0 a(1-\theta)}{4}E_h^4 + \frac{\epsilon_0 a\theta}{4}Q_h^2\right) dx \tag{18}$$

is the discrete energy. Moreover, $\mathcal{E}_h \ge 0$ when $\theta \in [0, \frac{3}{4}]$.

Semi-discrete error estimates

Theorem (Error estimates of semi-discrete scheme)

Let $\kappa_{err} \in (0,1)$ and $\rho_{err} \in (0,1)$ be two arbitrary parameters. Assume the periodic boundary condition and

$$E, H, P, Q, J, \sigma \in W^{1,\infty}([0,T], H^{k+1}(\Omega)),$$

and

$$E \in W^{1,\infty}([0,T], W^{1,\infty}(\Omega)), \quad Q \in W^{1,\infty}([0,T], L^{\infty}(\Omega)).$$

Then

$$\|u - u_h\| \leq C C_{model} C(\kappa_{err}, \rho_{err}) h^r, \qquad u = E, H, P, Q, J, \sigma,$$

where

$$r = \begin{cases} k & \text{for central flux (15)}, \\ k+1 & \text{for alternating flux (16) and upwind flux (17)}, \end{cases}$$

under the conditions on θ

$$\theta \in [0, \frac{1}{3(1-\rho_{err})^{-2}+1}],$$

and on the strength of nonlinearity,

$$a\theta C_k \|Q\|_\infty \leq \epsilon_\infty (1-\kappa_{err}),$$
$$a\left(\frac{3-\theta}{\rho_{err}} C_k^2 \|\partial_t E\|_\infty^2 + 3(1-\theta) C_k^2 \|\partial_t E\|_\infty \|E\|_\infty + \frac{\theta}{2} C_k \|\partial_t Q\|_\infty\right) \leq \frac{\epsilon_\infty \kappa_{err}}{4}.$$

Fully discrete stability: leap-frog-DG

Assuming the periodic boundary condition, then the fully discrete scheme with central and alternating fluxes, satisfies

$$\mathcal{E}_h^{n+1} - \mathcal{E}_h^n = -\frac{\epsilon_0 \Delta t}{4\omega_p^2 \tau} \int_\Omega (J_h^{n+1} + J_h^n)^2 dx - \frac{\epsilon_0 a\theta \Delta t}{8\omega_v^2 \tau_v} \int_\Omega (\sigma_h^{n+1} + \sigma_h^n)^2 dx \le 0, \tag{19}$$

$$\begin{aligned} \mathcal{E}_h^n \quad = \quad & \int_\Omega \frac{\mu_0}{2} H_h^{n+1/2} H_h^{n-1/2} + \frac{\epsilon_0 \epsilon_\infty}{2} (E_h^n)^2 + \frac{\epsilon_0}{2\omega_p^2} (J_h^n)^2 + \frac{\epsilon_0 \omega_0^2}{2\omega_p^2} (P_h^n)^2 \\ & + \frac{\epsilon_0 a\theta}{4\omega_v^2} (\sigma_h^n)^2 + \frac{\epsilon_0 a\theta}{2} Q_h^n (E_h^n)^2 + \frac{3\epsilon_0 a(1-\theta)}{4} (E_h^n)^4 + \frac{\epsilon_0 a\theta}{4} (Q_h^n)^2 dx \end{aligned} \tag{20}$$

is the discrete energy. In addition, $\mathcal{E}_h \ge 0$ if $\theta \in [0, \frac{3}{4}]$ and the CFL condition $\frac{\Delta t}{h} \le C_\star \sqrt{\mu_0 \epsilon_0 \epsilon_\infty}$ is satisfied.
The fully discrete scheme with the upwind flux satisfies

$$\begin{aligned} \mathcal{E}_h^{n+1} - \mathcal{E}_h^n = & -\frac{\epsilon_0 \Delta t}{4\omega_p^2 \tau} \int_\Omega (J_h^{n+1} + J_h^n)^2 dx - \frac{\epsilon_0 a\theta \Delta t}{8\omega_v^2 \tau_v} \int_\Omega (\sigma_h^{n+1} + \sigma_h^n)^2 dx \\ & - \frac{\Delta t}{8} \sqrt{\frac{\mu_0}{\epsilon_0 \epsilon_\infty}} \sum_{j=1}^N [H_h^{n-1/2} + H_h^{n+1/2}]_{j+1/2}^2 - \frac{\Delta t}{8} \sqrt{\frac{\epsilon_0 \epsilon_\infty}{\mu_0}} \sum_{j=1}^N [E_h^n + E_h^{n+1}]_{j+1/2}^2 \le 0, \end{aligned} \tag{21}$$

$$\begin{aligned} \mathcal{E}_h^n \quad = \quad & \int_\Omega \frac{\mu_0}{2} H_h^{n+1/2} H_h^{n-1/2} + \frac{\epsilon_0 \epsilon_\infty}{2} (E_h^n)^2 + \frac{\epsilon_0}{2\omega_p^2} (J_h^n)^2 + \frac{\epsilon_0 \omega_0^2}{2\omega_p^2} (P_h^n)^2 + \frac{\epsilon_0 a\theta}{4\omega_v^2} (\sigma_h^n)^2 \\ & + \frac{\epsilon_0 a\theta}{2} Q_h^n (E_h^n)^2 + \frac{3\epsilon_0 a(1-\theta)}{4} (E_h^n)^4 + \frac{\epsilon_0 a\theta}{4} (Q_h^n)^2 dx + \frac{\Delta t}{8} \sqrt{\frac{\mu_0}{\epsilon_0 \epsilon_\infty}} \sum_{j=1}^N ([H_h^{n-1/2}][H_h^{n-1/2} + H_h^{n+1/2}])_{j+1/2} \end{aligned} \tag{22}$$

is the discrete energy. In addition, $\mathcal{E}_h \ge 0$ if $\theta \in [0, \frac{3}{4}]$ and the CFL condition $\frac{\Delta t}{h} \le \frac{C_\star \mu_0 \min(1, \sqrt{\frac{\epsilon_0 \epsilon_\infty}{\mu_0}})}{(\sqrt{2} + \min(1, \sqrt{\frac{\epsilon_0 \epsilon_\infty}{\mu_0}}))}$ is satisfied.

Fully discrete stability: trapezoidal-DG

The schemes are unconditionally stable. In particular, with central and alternating fluxes satisfies

$$\mathcal{E}_h^{n+1} - \mathcal{E}_h^n = -\frac{\epsilon_0 \Delta t}{4\omega_p^2 \tau} \int_\Omega (J_h^{n+1} + J_h^n)^2 dx - \frac{\epsilon_0 a\theta \Delta t}{8\omega_v^2 \tau_v} \int_\Omega (\sigma_h^{n+1} + \sigma_h^n)^2 dx \leq 0, \tag{23}$$

and that with the upwind flux satisfies

$$\begin{aligned} \mathcal{E}_h^{n+1} - \mathcal{E}_h^n = & -\frac{\epsilon_0 \Delta t}{4\omega_p^2 \tau} \int_\Omega (J_h^{n+1} + J_h^n)^2 dx - \frac{\epsilon_0 a\theta \Delta t}{8\omega_v^2 \tau_v} \int_\Omega (\sigma_h^{n+1} + \sigma_h^n)^2 dx \\ & - \frac{\Delta t}{8} \sqrt{\frac{\mu_0}{\epsilon_0 \epsilon_\infty}} \sum_{j=1}^N [H_h^n + H_h^{n+1}]_{j+1/2}^2 - \frac{\Delta t}{8} \sqrt{\frac{\epsilon_0 \epsilon_\infty}{\mu_0}} \sum_{j=1}^N [E_h^n + E_h^{n+1}]_{j+1/2}^2 \leq 0, \end{aligned} \tag{24}$$

where

$$\begin{aligned} \mathcal{E}_h^n \quad = \quad & \int_\Omega \frac{\mu_0}{2} (H_h^n)^2 + \frac{\epsilon_0 \epsilon_\infty}{2} (E_h^n)^2 + \frac{\epsilon_0}{2\omega_p^2} (J_h^n)^2 + \frac{\epsilon_0 \omega_0^2}{2\omega_p^2} (P_h^n)^2 \\ & + \frac{\epsilon_0 a\theta}{4\omega_v^2} (\sigma_h^n)^2 + \frac{\epsilon_0 a\theta}{2} Q_h^n (E_h^n)^2 + \frac{3\epsilon_0 a(1-\theta)}{4} (E_h^n)^4 + \frac{\epsilon_0 a\theta}{4} (Q_h^n)^2 dx. \end{aligned} \tag{25}$$

It is non-negative when $\theta \in [0, \frac{3}{4}]$.

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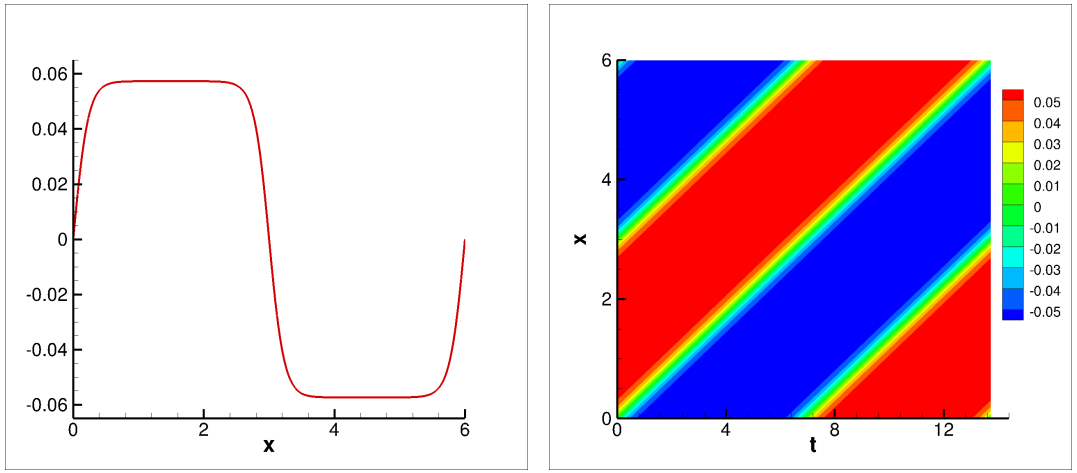
Kink shaped solution

We consider kink shaped solutions (*Sorensen et al. 05*), where a traveling wave solution was constructed for the instantaneous intensity-dependent Kerr response neglecting the influence of damping, i.e., $\theta = 0$, $\tau = \infty$.

$$\begin{aligned}
&\epsilon_\infty = 2.25, \quad \epsilon_s = 5.25, \quad \beta_1 = \epsilon_s - \epsilon_\infty, \\
&\omega_0 = 93.627179982222216, \quad \omega_p = \omega_0\sqrt{\beta_1}, \\
&a = \epsilon_\infty/3, \quad v = 0.6545/\sqrt{\epsilon_\infty}, \\
&E(0) = 0, \quad \Phi(0) = 0.24919666777865812.
\end{aligned}$$

Solutions are of the form $u(x,t) = u_0(x - vt)$. We compute until $T = 6/v$, when the solutions recover its initial state.

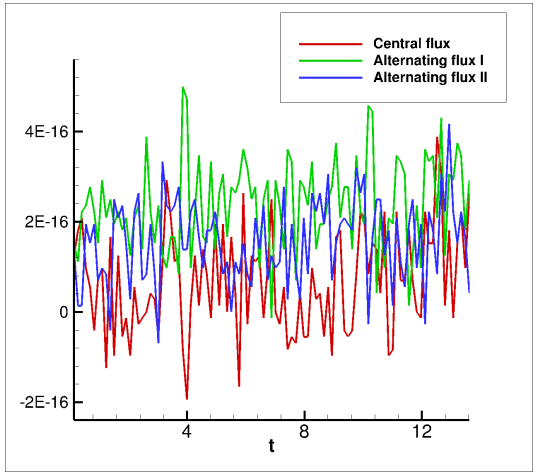


(a) Initial condition $E(x,0)$.

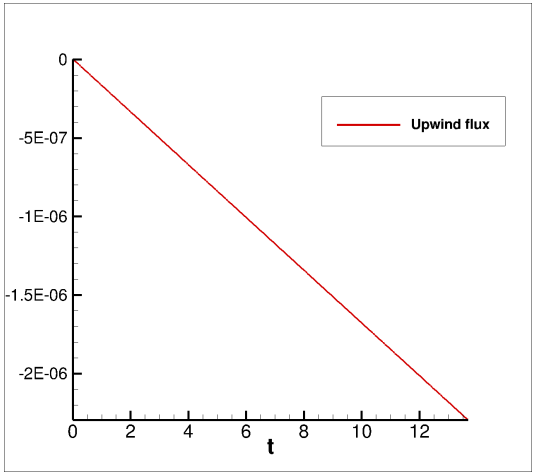
(b) Reference solution $E(x,t)$.

Figure: *A traveling kink and antikink wave: the electric field.*

Energy conservation



(a) Leap-frog scheme. $k = 1$.



(b) Leap-frog scheme. $k = 1$.

Figure: *A traveling kink and antikink wave: the time evolution of the relative deviation in energy. $N = 400$ grid points.*

Table: *A traveling kink and antikink wave: errors and orders of accuracy of E. $k = 1$.*

	N	Leap-frog scheme				Fully implicit scheme			
		L_2 errors	order	L_∞ error	order	L_2 errors	order	L_∞ error	order
upwind flux	100	4.48E-04	–	1.80E-03	–	9.24E-03	–	2.38E-02	–
	200	7.68E-05	2.55	3.46E-04	2.38	3.75E-03	1.30	1.16E-02	1.04
	400	1.32E-05	2.54	5.92E-05	2.55	1.15E-03	1.71	4.20E-03	1.46
	800	2.75E-06	2.26	1.17E-05	2.33	3.01E-04	1.93	1.20E-03	1.80
	1600	6.57E-07	2.06	3.10E-06	1.92	7.59E-05	1.99	3.11E-04	1.95
central flux	100	1.07E-03	–	4.53E-03	–	9.13E-03	–	2.36E-02	–
	200	2.77E-04	1.94	1.31E-03	1.79	3.64E-03	1.33	1.18E-02	1.12
	400	7.12E-05	1.96	3.59E-04	1.87	1.10E-03	1.72	4.20E-03	1.49
	800	1.97E-05	1.85	1.05E-04	1.78	2.90E-04	1.93	1.23E-03	1.77
	1600	6.91E-06	1.51	3.51E-05	1.57	7.32E-05	1.98	3.24E-04	1.93
alternating flux I	100	1.15E-04	–	5.22E-03	–	9.38E-03	–	2.41E-02	–
	200	2.96E-05	1.96	1.13E-04	2.21	3.77E-03	1.31	1.16E-02	1.06
	400	8.91E-06	1.73	3.45E-05	1.71	1.15E-03	1.71	4.21E-03	1.46
	800	2.01E-06	2.15	9.48E-06	1.86	3.01E-04	1.93	1.21E-03	1.80
	1600	4.62E-07	2.12	2.03E-06	2.22	7.59E-05	1.99	3.11E-04	1.95
alternating flux II	100	9.41E-05	–	4.79E-04	–	9.39E-03	–	2.41E-02	–
	200	3.04E-05	1.63	1.49E-04	1.69	3.78E-03	1.31	1.16E-02	1.05
	400	8.36E-06	1.86	3.61E-05	2.04	1.15E-03	1.71	4.20E-03	1.47
	800	1.87E-06	2.16	8.79E-06	2.04	3.01E-04	1.93	1.21E-03	1.80
	1600	5.40E-07	1.79	2.65E-06	1.73	7.59E-05	1.99	3.11E-04	1.95

Table: *A traveling kink and antikink wave: errors and orders of accuracy of E. $k = 2$.*

	N	Leap-frog scheme				Fully implicit scheme			
		L_2 errors	order	L_∞ error	order	L_2 errors	order	L_∞ error	order
upwind flux	100	2.49E-05	–	1.50E-04	–	3.66E-03	–	1.13E-02	–
	200	3.04E-06	3.04	1.88E-05	3.00	5.71E-04	2.68	2.21E-03	2.35
	400	3.69E-07	3.04	2.28E-06	3.04	7.29E-05	2.97	2.99E-04	2.89
	800	4.72E-08	2.96	3.04E-07	2.91	9.13E-06	3.00	3.77E-05	2.99
central flux	100	2.32E-05	–	1.05E-04	–	3.66E-03	–	1.13E-02	–
	200	2.97E-06	2.96	1.38E-05	2.92	5.72E-04	2.68	2.21E-03	2.35
	400	3.71E-07	3.00	1.75E-06	2.99	7.29E-05	2.97	2.99E-04	2.89
	800	4.62E-08	3.00	2.19E-07	2.99	9.13E-06	3.00	3.77E-05	2.99
alternating flux I	100	2.38E-05	–	1.04E-04	–	3.66E-03	–	1.13E-02	–
	200	2.98E-06	3.00	1.33E-05	2.96	5.71E-04	2.68	2.21E-03	2.35
	400	3.72E-07	3.00	1.70E-06	2.96	7.29E-05	2.97	2.99E-04	2.89
	800	4.62E-08	3.01	2.08E-07	3.04	9.13E-06	3.00	3.77E-05	2.99
alternating flux II	100	2.41E-05	–	1.25E-04	–	3.66E-03	–	1.13E-02	–
	200	3.03E-06	2.99	1.67E-05	2.91	5.72E-04	2.68	2.21E-03	2.35
	400	3.73E-07	3.02	1.98E-06	3.07	7.29E-05	2.97	2.99E-04	2.89
	800	4.66E-08	3.00	2.67E-07	2.89	9.13E-06	3.00	3.77E-05	2.99

Soliton propagation (Giles et al, 00) - Third harmonic generation

$$\epsilon_\infty = 2.25, \quad \epsilon_s = 5.25, \quad \beta_1 = \epsilon_s - \epsilon_\infty,$$
$$1/\tau = 1.168 \times 10^{-5}, \quad 1/\tau_v = 29.2/32,$$
$$a = 0.07, \quad \theta = 0.3, \quad \Omega_0 = 12.57,$$
$$\omega_0 = 5.84, \quad \omega_v = 1.28, \quad \omega_p = \omega_0\sqrt{\beta_1}.$$

Initially, all fields are zero.

The left boundary is injected with an incoming solitary wave, for which the electric field is prescribed as

$$E(x = 0, t) = f(t)\cos(\Omega_0 t), \tag{26}$$

where $f(t) = M\,\mathrm{sech}(t - 20)$. The boundary condition of H can be approximated from the linearized dispersion relation. Right boundary: absorbing wall.

We simulate the transient fundamental ($M = 1$) and second-order ($M = 2$) temporal soliton evolutions.

Boundary treatment: left boundary

The boundary condition of H can be approximated from the linearized dispersion relation. Assuming a space-time harmonic variation $e^{i(\omega t - kx)}$ of all fields, the exact dispersion relation associated with the linear parts of the system is

$$\epsilon_\infty \omega^4 - i\frac{\epsilon_\infty}{\tau}\omega^3 - (\epsilon_\infty \omega_0^2 + \omega_p^2 + k^2)\omega^2 + i\frac{1}{\tau}k^2\omega + k^2\omega_0^2 = 0. \tag{27}$$

The solution corresponding to the wave propagating to the right is

$$k = \omega\sqrt{\epsilon_\infty}\sqrt{1 - \frac{\omega_p^2/\epsilon_\infty}{\omega^2 - i\omega/\tau - \omega_0^2}}. \tag{28}$$

Then we take the approximate value of H as

$$\begin{aligned} H(x=0,t) &= \int_{-\infty}^{\infty} \hat{H}(\omega) e^{i\omega t} d\omega \\ &\simeq \frac{1}{2}\Big[\sum_{m=0}^{8} \frac{(-i)^m}{m!}\big(\frac{1}{Z}\big)^{(m)}|_{\omega=\Omega_0} f^{(m)}(t)\Big] e^{i\Omega_0 t} + c.c., \end{aligned} \tag{29}$$

where $c.c.$ denotes the complex conjugate of the first term, $f^{(m)}(t)$ is the m-th derivative of $f(t)$, and $(\frac{1}{Z})^{(m)}$ is the m-th derivative of $Z = -\omega/k$ with respect to ω.

Boundary treatment: right boundary

We treat the right boundary as an absorbing wall corresponding to the linearized system, similar to the procedure performed in Hile et al. (96). Neglecting the nonlinear effects and the delayed response, we have

$$\partial_t(H+\sqrt{\epsilon_\infty}E) = \frac{1}{\sqrt{\epsilon_\infty}}\partial_x(H+\sqrt{\epsilon_\infty}E)$$
$$\partial_t(H-\sqrt{\epsilon_\infty}E) = -\frac{1}{\sqrt{\epsilon_\infty}}\partial_x(H-\sqrt{\epsilon_\infty}E).$$

Because only waves that propagate to the right are allowed, the left going characteristic variable $H+\sqrt{\epsilon_\infty}E$ is set to be zero at the right boundary $x_R = x_{N+1/2}$. Therefore, for semi-discrete scheme, we require

$$(H_h+\sqrt{\epsilon_\infty}E_h)^+_{N+1/2} = 0,$$
$$(H_h-\sqrt{\epsilon_\infty}E_h)^+_{N+1/2} = (H_h-\sqrt{\epsilon_\infty}E_h)^-_{N+1/2}.$$

This corresponds to rewriting the central flux (and also the alternating fluxes) as

$$\widehat{E_h}|_{N+1/2} = \frac{3}{4}E_h|^-_{N+1/2} - \frac{1}{4\sqrt{\epsilon_\infty}}H_h|^-_{N+1/2}, \quad \widetilde{H_h}|_{N+1/2} = \frac{3}{4}H_h|^-_{N+1/2} - \frac{\sqrt{\epsilon_\infty}}{4}E_h|^-_{N+1/2}, \quad (30)$$

and rewriting the upwind flux as

$$\widehat{E_h}|_{N+1/2} = \frac{1}{2}E_h|^-_{N+1/2} - \frac{1}{2\sqrt{\epsilon_\infty}}H_h|^-_{N+1/2}, \quad \widetilde{H_h}|_{N+1/2} = \frac{1}{2}H_h|^-_{N+1/2} - \frac{\sqrt{\epsilon_\infty}}{2}E_h|^-_{N+1/2}. \quad (31)$$

Energy analysis with boundary effects has been conducted.

Simulation results

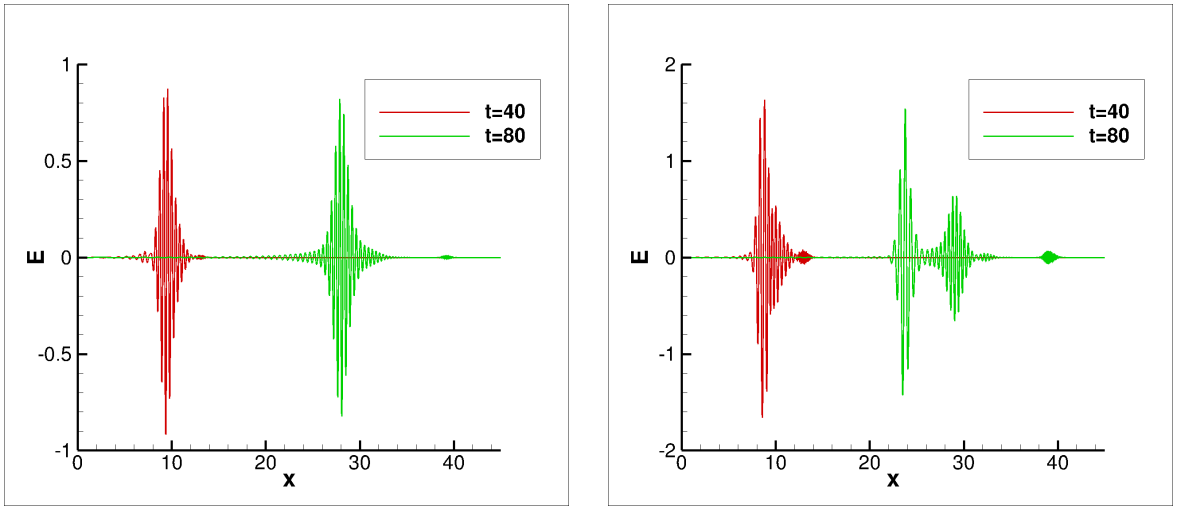


Figure: *leap-frog scheme.* $N = 6400$ *grid points.* $k = 3$, *alternating flux I. Left:*$M = 1$, *right:* $M = 2$.

Results agree with literature. (For upwind flux with $k = 1$, the daughter pulse is not evident due to numerical dissipation.)

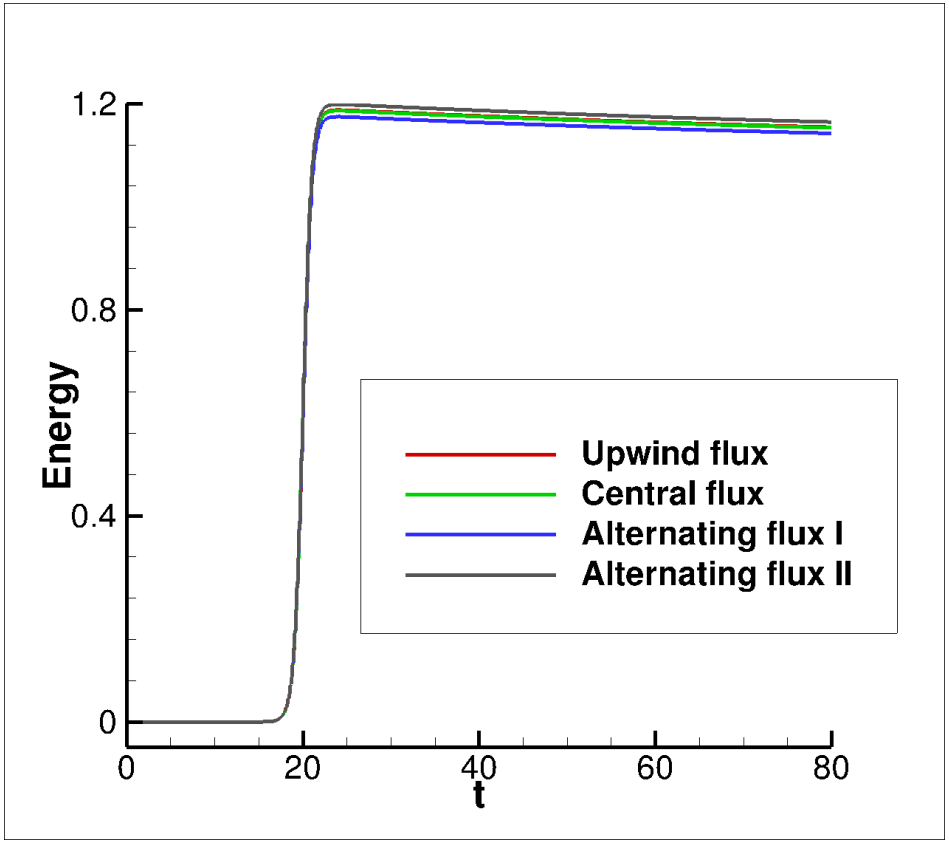


Figure: *leap-frog scheme.* $N = 6400$ *grid points.* $k = 3$, *alternating flux I.* $M = 1$. *Energy relation.*

Outline

1. Introduction
2. Numerical methods
   - Temporal discretizations
   - Spatial discretizations
3. Numerical results
4. Conclusion

Conclusion

- We developed energy-stable DG methods for nonlinear Maxwell equations with Lorentz, Kerr and Raman effects in 1D.
- Main ingredients: second order time discretizations with special treatment of nonlinear terms, DG spatial discretizations.
- Overall, the alternating fluxes show the best performance.
- The scheme has been extended to arbitrary order FDTD method on staggered mesh. Study of numerical dispersion for the linearized Lorentz model is on-going.
- Future work :
  - higher order, higher dimensions
  - other nonlinear models.

Reference

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The END!

Thank You!