Nonlinear Light Scattering using the FDTD Method

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Second Harmonic Generation

- Incident fields at frequency ω, if of sufficient intensity, can generate scattered fields at 2ω.
- A common example is green laser pointers
- Source term for radiation is the second-order polarization, with the dominant contribution being of the form:

$$P_i^{(2)} = \chi_{ijk}^{(2)} E_j E_k$$

Nonlinear Maxwell's Equations

$$\nabla \cdot \vec{D} = \vec{P}^{(2)} + \rho_f$$

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

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

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \frac{\partial \vec{P}^{(2)}}{\partial t} + \vec{J}$$

FDTD Method

- Basic prescription:
  - Discretize space and time
  - Express temporal and spatial derivatives in the Maxwell curl equations as finite differences
  - Split fields into scattered and incident
  - Rearrange equations to get scattered fields at time $t = (n+1)\Delta t$ in terms of earlier scattered fields and incident fields.
  - Solve for fields in solution space for each time step, alternating between evaluating E and H, and store results.
  - Handle boundary fields seperately at each time step

Advantages of FDTD

- Easy to simulate arbitrary scattering geometries (w/ staircasing error) and inhomogeneous media.
- Easy to simulate any time dependent incident field with an analytical expression (e.g. laser pulse which is Gaussian in time and/or spatial intensity)
- For multiple frequency fields, we can solve for the whole field at once, instead of superposing individual frequency solutions

Assumptions

- Medium is linearly isotropic (or diagonally anisotropic)
- Medium is nonmagnetic (i.e H = B)
- No dispersion (dielectric response is equal for all frequencies)

Example (linear case)

$$\nabla \times (\vec{H}_{inc} + \vec{H}_{scatt}) = \vec{\varepsilon}\frac{\partial}{\partial t}\left(\vec{E}_{inc} + \vec{E}_{scatt}\right) + \vec{\sigma}\left(\vec{E}_{inc} + \vec{E}_{scatt}\right)$$

$$\frac{\partial H_{z,scatt}}{\partial y} - \frac{\partial H_{y,scatt}}{\partial y} = (\varepsilon_{xx} - \varepsilon_0)\frac{\partial E_{x,inc}}{\partial t} + \varepsilon\frac{\partial E_{x,scatt}}{\partial t} + \sigma_{xx}(E_{x,inc} + E_{x,scatt})$$

$$\frac{H^{n+\frac{1}{2}}{}_{z,s}(i,j,k) - H^{n+\frac{1}{2}}{}_{z,s}(i,j-1,k)}{\Delta y} - \frac{H^{n+\frac{1}{2}}{}_{y,s}(i,j,k) - H^{n+\frac{1}{2}}{}_{y,s}(i,j,k-1)}{\Delta z}$$

$$= \varepsilon_{xx}\frac{E^{n}{}_{x,s} - E^{n-1}{}_{x,s}}{\Delta t} + (\varepsilon_{xx} - \varepsilon_o)\frac{\partial E^{n}{}_{x,inc}}{\partial t} + \sigma_{xx}(E^{n}{}_{x,inc} + E^{n}{}_{x,s})$$

Stability Issues

- Rule of thumb for spatial discretization size is $\sim\lambda/10$ for highest frequency of interest (and no bigger than $\lambda/4$)
- Need multiple samples per wavelength, also smaller grid spacing minimizes "grid dispersion"
- For time spacing, use Courant condition in 3D:

$$\Delta t = \frac{1}{c\sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2}}$$

Boundary Issues

- In real-life, the scattered fields propagate out to infinity, but we necessarily truncate our solution space
- Need to simulate boundaries that absorb the outgoing waves to minimize reflection errors
- Popular scheme is the Mur boundary condition, which estimates the fields at the boundary by interpolating past boundary fields and interior fields

Far Zone Scattering

- Approximate surface integral of tangential fields over the boundary at each time step
- Relate these to transverse radiation fields far away from the scatterer

Nonlinear Problem

- The presence of the nonlinear polarization's time derivative gives us two unknowns at time step n+1 with only one equation
- For a single incident frequency, the time derivative just becomes i2ω times the nonlinear polarization at time step n