Modeling and Simulation of Microwaves in Biological Tissue

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Graduate Student Seminar
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Acknowledgements

Collaborators

- H. T. Banks (NCSU)
- V. A. Bokil (OSU)
- W. P. Winfree (NASA)

Students

- Karen Barrese and Neel Chugh (REU 2008)
- Anne Marie Milne and Danielle Wedde (REU 2009)
- Erin Bela and Erik Hortsch (REU 2010)
- Megan Armentrout (MS 2011)
- Brian McKenzie (MS 2011)

Outline

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1. **Preliminaries**
   - PDEs
2. **Dispersive Media**
   - Maxwell's Equations
   - Polarization Models
   - Distribution of Parameters

Outline

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Scientific Computing

- The scientific community now recognizes simulation (computational modeling) as the essential "third leg" of research alongside theory and experimentation.
- Some experiments are too expensive, time consuming, dangerous, impossible
- Numerical computation allows for "artificial experiments"

Numerical Analysis

- Numerical methods are algorithms for approximating solutions to equations, including
  - Matrix equations
  - Differential equations
  - Integral equations
- Numerical analysis seeks to understand the error in the approximation, usually as a function of the work required
- It is the mathematical branch of scientific computing and involves
  - Analytical solutions
  - Linear algebra
  - Functional analysis

A General First Order Linear PDE System

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where u is called a state variable, $\mathcal{A}$ is a linear operator depending on a set of parameters q, and f is a source term.

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Examples

- $\mathcal{A} = c\frac{\partial}{\partial x}$ yields a one-way wave equation.
- $u = [H, E]^T$ and
$$\mathcal{A} = \begin{bmatrix} 0 & \frac{1}{\mu}\frac{\partial}{\partial x} \\ \frac{1}{\epsilon}\frac{\partial}{\partial x} & 0 \end{bmatrix}$$
yields 1D Maxwell's equations in a dielectric, equivalent to the wave equation with speed $c = \sqrt(1/\epsilon\mu)$.

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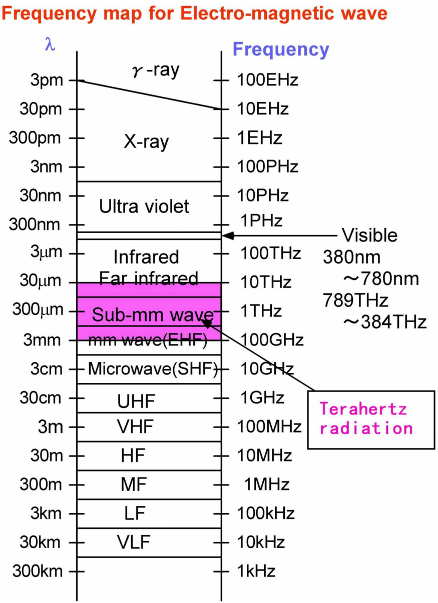
- $u = [\mathbf{H}, \mathbf{E}]^T$

  $$\mathcal{A} = \begin{bmatrix} 0 & \frac{1}{\mu}\nabla\times \\ \frac{1}{\epsilon}\nabla\times & \frac{\sigma}{\epsilon} \end{bmatrix}$$

  yields 3D Maxwell curl equations in a conductive dielectric.

Electromagnetic Applications

- Computers
- Cell Phones
- Aging Aircraft
- Biomedical
- Astronomy
- Resources Exploration
- GPS
- Gas Milage



Outline

Maxwell's Equations

$$
\begin{aligned}
\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} &= \nabla \times \mathbf{H} && \text{(Ampere)} \\
\frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \mathbf{E} && \text{(Faraday)} \\
\nabla \cdot \mathbf{D} &= \rho && \text{(Poisson)} \\
\nabla \cdot \mathbf{B} &= 0 && \text{(Gauss)}
\end{aligned}
$$

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

With appropriate initial conditions and boundary conditions.

Constitutive Laws

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

$$\boxed{\begin{aligned} \mathbf{D} &= \epsilon \mathbf{E} + \mathbf{P} \\ \mathbf{B} &= \mu \mathbf{H} + \mathbf{M} \\ \mathbf{J} &= \sigma \mathbf{E} + \mathbf{J}_s \end{aligned}}$$

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

Complex permittivity

- We can define **P** in terms of a convolution

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

  where g is the dielectric response function (DRF).
- In the frequency domain $\hat{\mathbf{D}} = \epsilon_0\epsilon(\omega)\hat{\mathbf{E}}$, where $\epsilon(\omega)$ is called the complex permittivity.
- $\epsilon(\omega)$ described by the polarization model
- 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.

Dry skin data

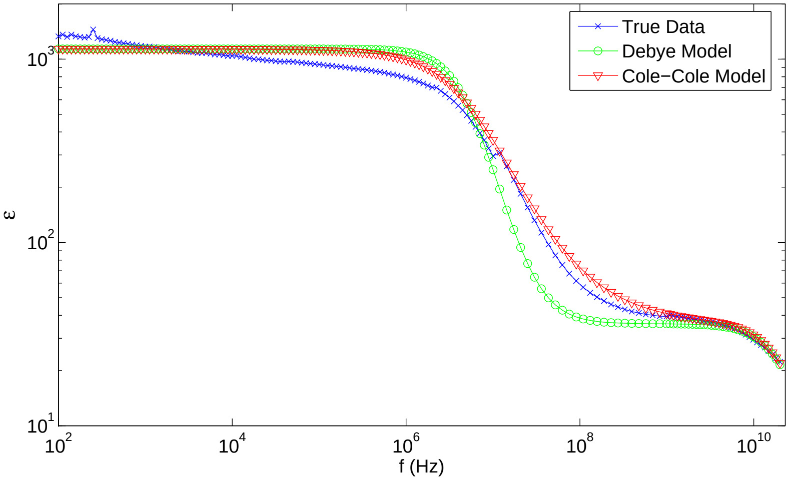


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [GLG96].

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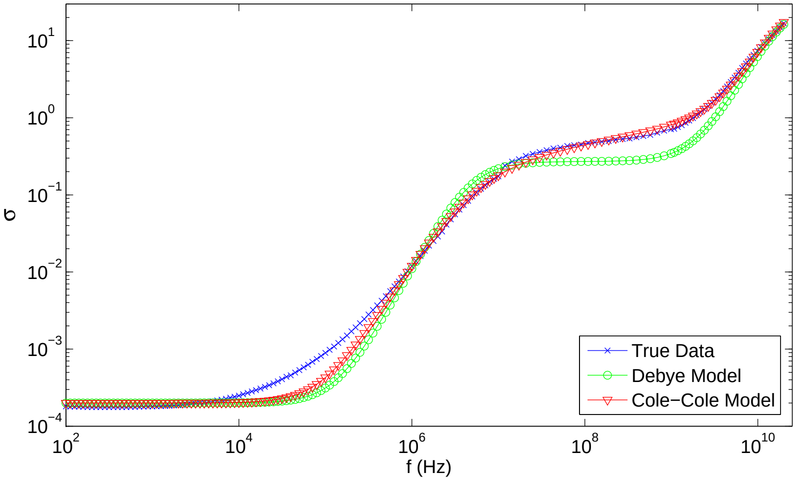

Figure: Imaginary part of $\epsilon(\omega)$, σ, or the conductivity.

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- Debye model [1929] $\mathbf{q} = [\epsilon_d, \tau]$

$$g(t,\mathbf{x}) = \epsilon_0\epsilon_d/\tau \quad e^{-t/\tau}$$

$$\text{or} \quad \tau\dot{\mathbf{P}} + \mathbf{P} = \epsilon_0\epsilon_d\mathbf{E}$$

$$\text{or} \quad \epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1+i\omega\tau}$$

with $\epsilon_d := \epsilon_s - \epsilon_\infty$.

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  with $\epsilon_d := \epsilon_s - \epsilon_\infty$.

- Cole-Cole model [1936] (heuristic generalization) $\mathbf{q} = [\epsilon_d, \tau, \alpha]$

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_d}{1+(i\omega\tau)^{1-\alpha}}$$

  The DRF for the Cole-Cole is

$$g(t,\mathbf{x}) = \frac{1}{2\pi i}\int_{\zeta-i\infty}^{\zeta+i\infty} \frac{\epsilon_0(\epsilon_s-\epsilon_\infty)}{1+(s\tau)^{1-\alpha}} e^{st} ds.$$

Dispersive Dielectrics

Debye Material

Input is five cycles (periods) of a sine curve.

Dispersive Media

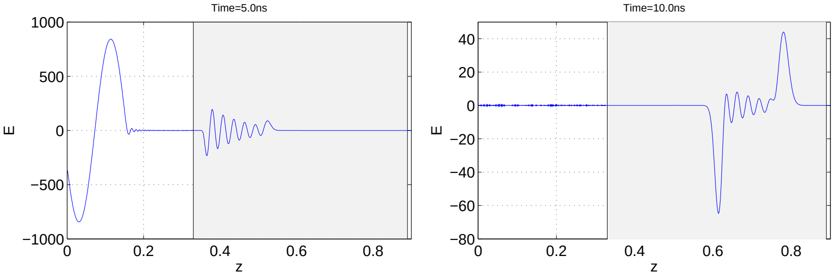

Figure: Debye model simulations.

Motivation

- The Cole-Cole model corresponds to a fractional order ODE in the time-domain and is difficult to simulate
- Debye is efficient to simulate, but does not represent permittivity well
- Better fits to data are obtained by taking linear combinations of Debye models (discrete distributions), idea comes from the known existence of multiple physical mechanisms: multi-pole debye (like stair-step approximation)
- An alternative approach is to consider the Debye model but with a (continuous) distribution of relaxation times [von Schweidler1907]
- Empirical measurements suggest a log-normal distribution [Wagner1913], but uniform is easier
- Using Mellin transforms, can show Cole-Cole corresponds to a distribution

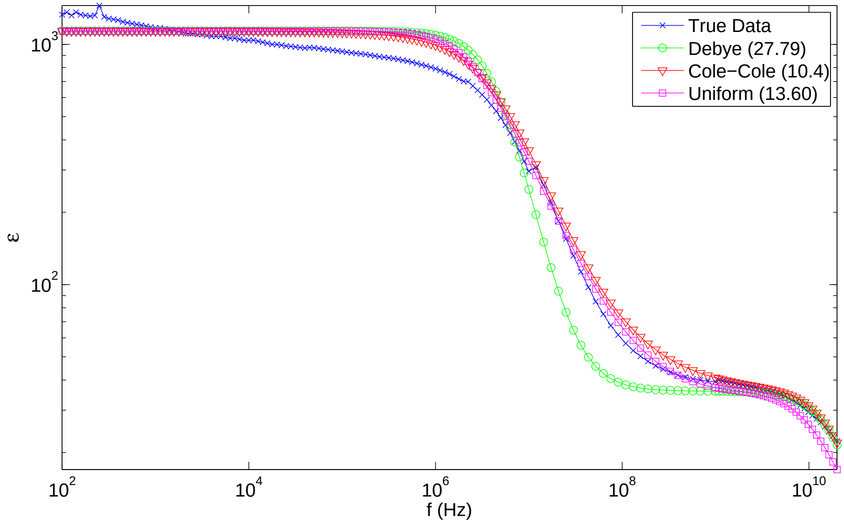

Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity [REU2008].

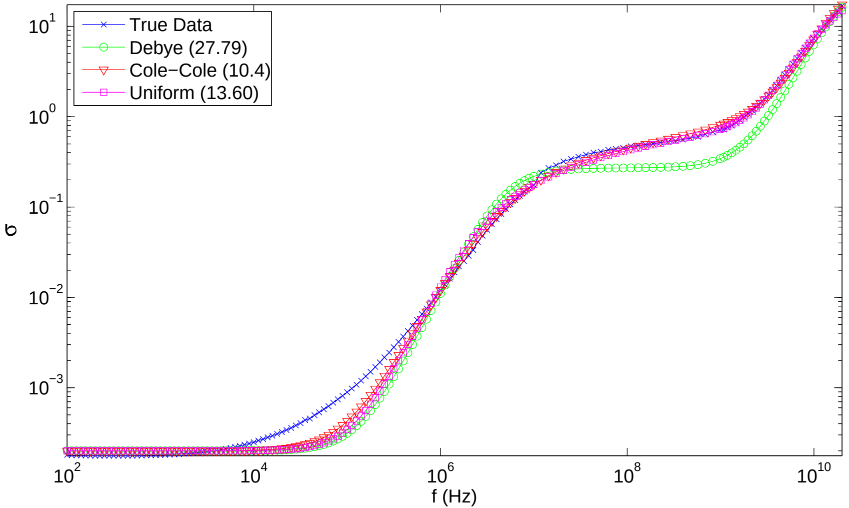

Figure: Imaginary part of $\epsilon(\omega)/\omega$, σ, or the conductivity [REU2008].

Distributions of Parameters

To account for the effect of possible multiple parameter sets $\mathbf{q}$, consider

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

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

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

Alternatively we can define the random polarization $\mathcal{P}(t, \mathbf{x}; \tau)$ to be the solution to

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0\epsilon_d\mathbf{E}$$

where τ is a random variable with PDF $f(\tau)$, for example,

$$f(\tau) = \frac{1}{\tau_b - \tau_a}$$

for a uniform distribution.
The electric field depends on the macroscopic polarization, which we take to be the expected value of the random polarization at each point $(t, \mathbf{x})$

$$\mathbf{P}(t, \mathbf{x}) = \int_{\tau_a}^{\tau_b} \mathcal{P}(t, \mathbf{x}; \tau) f(\tau) d\tau.$$

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We say the "forward problem" is to find the solution to the system for some given value of the parameter set q (and everything else is known).

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$$u(x_i, t_j) \approx U_{i,j}.$$

An example of a numerical method is to replace $\frac{\partial u}{\partial x}$ at (t_j, x_i) with

$$\frac{U_{i,j} - U_{i-1,j}}{\Delta x} \quad \text{or} \quad \frac{U_{i+1,j} - U_{i-1,j}}{2\Delta x}$$

for some fixed $\Delta x = x_i - x_{i-1}$. These are called finite differences. Errors are $\mathcal{O}(\Delta x)$ and $\mathcal{O}(\Delta x^2)$, respectively.

Inverse Problems

Definition

An inverse problem estimates quantities *indirectly* by using measurements of other quantities.

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For example, a parameter estimation inverse problem attempts to determine values of a parameter set q given (discrete) observations of (some) state variables.
Examples:

- distance of an object using echo-location (easily invertible)
- amount of oil/water/cave in the ground using RADAR backscatter
- geometry or composition of a defect using measurements of EM fields (CT, MRI, etc.)

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- Mathematically, find

$$\min_{q \in Q_{ad}} \left\| error \left(E(q), \hat{E} \right) \right\| .$$

For example, with data measured at fixed x and discrete times t_j

$$\min_{q \in Q_{ad}} \frac{1}{N} \sum_{j=1}^{N} \left(E(t_j; q) - \hat{E}_j \right)^2$$

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  is called the nonlinear least squares method.
- Need to develop a fast and accurate method for simulating E. Consider improvements to models and numerical methods.

Random Polarization

Apply Polynomial Chaos method to approximate the random polarization

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E, \quad \tau = \tau(\xi) = r\xi + m$$

resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0(\epsilon_s - \epsilon_\infty)E\vec{e_1}$$

or

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{g}.$$

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The macroscopic polarization, the expected value of the random polarization at each point (t, x), is simply

$$P(t, x; F) = \alpha_0(t, x).$$

Inverse Problem for F

- Given data $\{\hat{E}\}_j$ we seek to determine a probability distribution F^*, such that
$$F^* = \min_{F \in \mathfrak{P}(\mathcal{Q})} \mathcal{J}(F),$$
where, for example,
$$\mathcal{J}(F) = \sum_j \left(E(t_j; F) - \hat{E}_j \right)^2 .$$
- Given a trial distribution F_k we compute $E(t_j; F_k)$ and test $\mathcal{J}(F_k)$, then update F_{k+1} as necessary to find a minimum.
- Need either a parametrization or a discretization of F_k to have a finite dimensional problem.
- Need a fast and accurate method for simulating $E(x, t; F)$.

Stability (Well-Posedness) of Inverse Problem

- Existence and uniqueness of solutions to weak formulation of the forward problem follows as a special case of work in [BBL00]
- Continuous dependence of $(E, \dot{E})$ on F in the Prohorov metric shown in [BG05]

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- Continuous dependence of $(E, \dot{E})$ on F in the Prohorov metric shown in [BG05]
- Continuity of $F \to (E, \dot{E}) \implies$ continuity of $F \to \mathcal{J}(F)$, for a continuous objective function J
- Compactness of $\mathcal{Q} \implies$ compactness of $\mathfrak{P}(\mathcal{Q})$ with respect to the Prohorov metric
- Therefore, a minimum of $\mathcal{J}(F)$ over $\mathfrak{P}(\mathcal{Q})$ exists [BG05]

Outline

Finite Difference Methods

The Yee Scheme

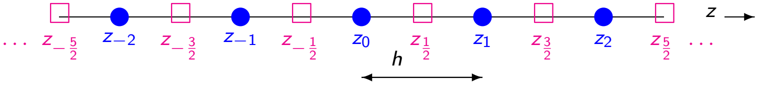
- In 1966 Kane Yee originated a set of finite-difference equations for the time dependent Maxwell's curl equations.
- The finite difference time domain (FDTD) or Yee algorithm solves for both the electric and magnetic fields in time and space using the coupled Maxwell's curl equations rather than solving for the electric field alone (or the magnetic field alone) with a wave equation.

Yee Scheme in One Space Dimension

- **Staggered Grids**: First order derivatives are much more accurately evaluated on staggered grids, such that if a variable is located on the integer grid, its first derivative is best evaluated on the half-grid and vice-versa.
- Staggered Grids of $\mathbb{R}$ with space step size $\Delta z = h$

$$\text{Primary Grid } G_p = \{z_\ell = \ell h \mid \ell \in \mathbb{Z}\},$$

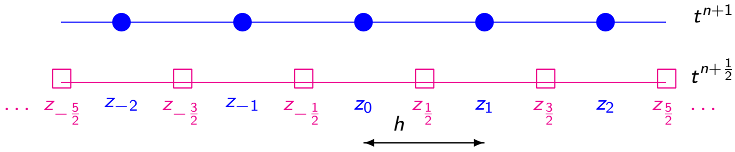
$$\text{Dual Grid } G_d = \left\{z_{\ell+\frac{1}{2}} = \left(\ell + \frac{1}{2}\right) h \mid \ell \in \mathbb{Z}\right\}.$$



Yee Scheme in One Space Dimension

- **Staggered Grids**: The electric field/flux is evaluated on the primary grid in both space and time and the magnetic field/flux is evaluated on the dual grid in space and time.
- The Yee scheme is

$$
\boxed{
\begin{aligned}
\frac{H|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H|_{\ell+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} &= -\frac{1}{\mu}\,\frac{E|_{\ell+1}^{n} - E|_{\ell}^{n}}{\Delta z} \\
\frac{E|_{\ell}^{n+1} - E|_{\ell}^{n}}{\Delta t} &= -\frac{1}{\epsilon}\,\frac{H|_{\ell+\frac{1}{2}}^{n+\frac{1}{2}} - H|_{\ell-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z}
\end{aligned}
}
$$



Yee Scheme in One Space Dimension

- This gives an explicit second order accurate scheme in both time and space.

Yee Scheme in One Space Dimension

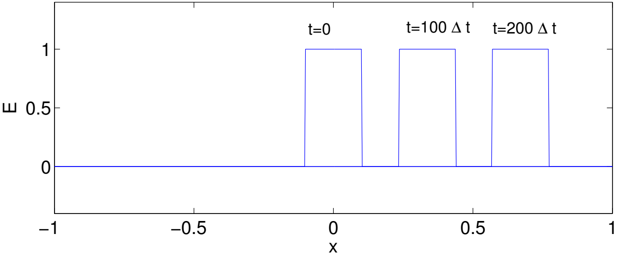
- This gives an explicit second order accurate scheme in both time and space.
- It is conditionally stable with the CFL condition

$$\nu = \frac{c\Delta t}{\Delta z} \leq 1$$

where ν is called the Courant number and $c = 1/\sqrt{\epsilon\mu}$.

Numerical Stability: A Square Wave

- Case $c\Delta t = \Delta z$



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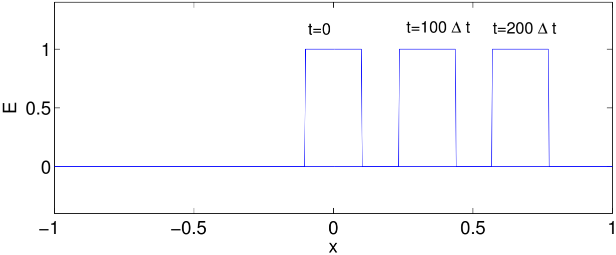
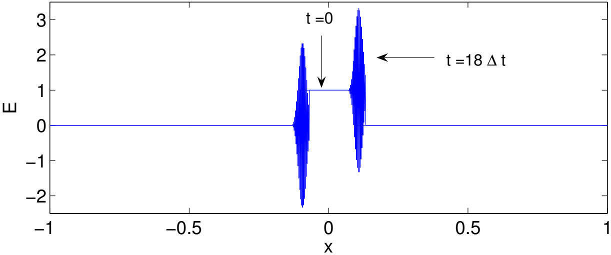


- Case $c\Delta t > \Delta z$



Numerical Dispersion: A Square Wave

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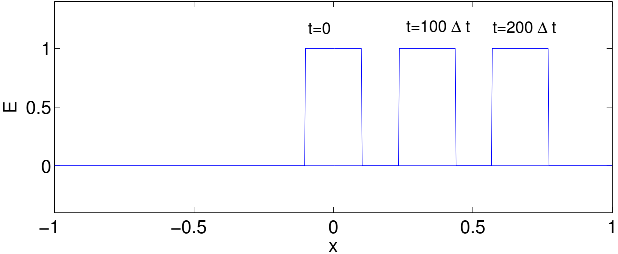

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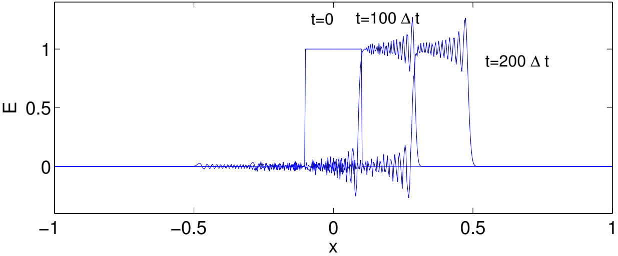

The Need for Higher Order

- The Yee scheme can exhibit numerical dispersion
- Dispersion error can be reduced more cheaply by requiring higher order accuracy than by simply reducing mesh sizes
- In 3D a large mesh size is desireable, yet one cannot sacrifice accuracy.
- We will consider here $(2, 2M)$ order accurate methods, with second order accuracy in time and $2M$, $M \in \mathbb{N}$ order accuracy in space.
- The Yee scheme is second order accurate, i.e., a $(2, 2)$ scheme.

Discrete Approximations of Order $2M$ to $\partial/\partial z$ on Staggered Grids

Staggered Grids of $\mathbb{R}$ with space step size h

$$\text{Primary Grid } G_p = \{z_\ell = \ell h \mid \ell \in \mathbb{Z}\},$$

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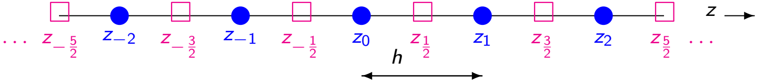


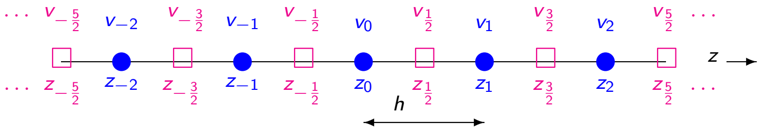
Discrete Approximations of order $2M$ to $\partial/\partial z$ on Staggered Grids

Staggered ℓ^2 Normed Spaces

For any function v, $v_\ell = v(\ell h)$, $v_{\ell+\frac{1}{2}} = v((\ell + \frac{1}{2})h)$.

$$V_0^1 = \{(v_\ell),\ \ell \in \mathbb{Z} |\ ||v||_0^2 = h \sum_{\ell \in \mathbb{Z}} |v_\ell|^2 \leq \infty\}$$

$$V_{\frac{1}{2}}^1 = \{(v_{\ell+\frac{1}{2}}),\ \ell \in \mathbb{Z} |\ ||v||_{\frac{1}{2}}^2 = h \sum_{\ell \in \mathbb{Z}} |v_{\ell+\frac{1}{2}}|^2 \leq \infty\}$$



Discrete Approximations of order $2M$ to $\partial/\partial z$ on Staggered Grids

- Finite difference approximations of order $2M$ of the first derivative operator $\partial/\partial z$ will be denoted as
  - $\mathcal{D}_{1,h}^{(2M)} : V_0^1 \rightarrow V_{\frac{1}{2}}^1$ on primary grid, and
  - $\tilde{\mathcal{D}}_{1,h}^{(2M)} : V_{\frac{1}{2}}^1 \rightarrow V_0^1$ on dual grid.

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- These operators can be considered from two different points of view:
  - **(V1)** As linear combinations of second order approximations to $\partial/\partial z$ computed with different space steps, and
  - **(V2)** As a result of the truncation of an appropriate series expansion of the symbol of the operator $\partial/\partial z$.

First Point of View: Discrete Second Order Accurate Operators

- Define Discrete Operators
  - $\mathcal{D}^{(2)}_{p,h} : V^1_0 \to V^1_{\frac{1}{2}}$ defined by $\left(\mathcal{D}^{(2)}_{p,h} u\right)_{\ell+\frac{1}{2}} = \dfrac{u_{\ell+p} - u_{\ell-p+1}}{(2p-1)h}$

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  - $\tilde{\mathcal{D}}^{(2)}_{p,h} : V^1_{\frac{1}{2}} \to V^1_0$ defined by $\left(\tilde{\mathcal{D}}^{(2)}_{p,h} u\right)_{\ell} = \dfrac{u_{\ell+p-\frac{1}{2}} - u_{l-p+\frac{1}{2}}}{(2p-1)h}$

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- If $u \in C^{2M+1}(\mathbf{R})$, with $M \in \mathbb{N}$, and $m \geq 1$, using the Taylor expansions at z_ℓ

$$\left(\tilde{\mathcal{D}}^{(2)}_{p,h} u\right)_{\ell} = \partial_z u_\ell + \sum_{i=1}^{M-1} \left(\frac{(2p-1)h}{2}\right)^{2i} \frac{1}{(2i+1)} \frac{\partial^{2i+1} u_\ell}{\partial z^{2i+1}} + \mathcal{O}\left(h^{2M}\right)$$

First Point of View: Discrete Second Order Accurate Operators

- Consider the linear combination

$$\tilde{\mathcal{D}}_{1,h}^{(2M)} = \sum_{p=1}^{M} \lambda_{2p-1}^{2M} \tilde{\mathcal{D}}_{p,h}^{(2)}$$

- To approximate $\partial u_\ell / \partial z$ with error $\mathcal{O}(h^{2M})$ leads to the Vandermonde system

$$\begin{pmatrix} 1^0 & 3^0 & 5^0 & \dots & (2M-1)^0 \\ 1^2 & 3^2 & 5^2 & \dots & (2M-1)^2 \\ 1^4 & 3^4 & 5^4 & \dots & (2M-1)^4 \\ \vdots & & & & \\ 1^{2M-2} & 3^{2M-2} & 5^{2M-2} & \dots & (2M-1)^{2M-2} \end{pmatrix} \begin{pmatrix} \lambda_1^{2M} \\ \lambda_3^{2M} \\ \lambda_5^{2M} \\ \vdots \\ \lambda_{2M-1}^{2M} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

First Point of View: Discrete Second Order Accurate Operators

Theorem

For any $M \in \mathbf{N}$, the coefficients λ_{2p-1}^{2M} are given by the explicit formula

$$\lambda_{2p-1}^{2M} = \frac{2(-1)^{p-1}[(2M-1)!!]^2}{(2M+2p-2)!!(2M-2p)!!(2p-1)},$$

where $1 \leq p \leq M, \forall p.$

and the double factorial is defined as

$$n!! := \begin{cases} n \cdot (n-2) \cdot (n-4) \ldots 5 \cdot 3 \cdot 1 & n > 0, \text{ odd} \\ n \cdot (n-2) \cdot (n-4) \ldots 6 \cdot 4 \cdot 2 & n > 0, \text{ even} \\ 1, & n = -1, 0 \end{cases}$$

Table of Coefficients: (V1)

Table: Coefficients λ_{2p-1}^{2M}

2M	λ_1	λ_3	λ_5	λ_7
2	1			
4	$\frac{9}{8}$	$\frac{-1}{8}$		
6	$\frac{75}{64}$	$\frac{-25}{128}$	$\frac{3}{128}$	
8	$\frac{1225}{1024}$	$\frac{-245}{1024}$	$\frac{49}{1024}$	$\frac{-5}{1024}$

Second Point of View: Symbols of Differential and Discrete Operators

- If $v(z) = \mathrm{e}^{ikz}$ then $\dfrac{\partial v}{\partial z} = ikv(z)$, and the Symbol of $\dfrac{\partial}{\partial z}$ is defined to be

$$\mathcal{F}\left(\partial/\partial z\right) := ik,$$

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- We can show that the Symbol of $\tilde{\mathcal{D}}_{1,h}^{(2M)}$ is

$$\mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = \frac{2i}{h}\sum_{p=1}^{M}\frac{\lambda_{2p-1}^{2M}}{2p-1}\sin(kh(2p-1)/2)$$

Second Point of View: Symbols of Differential and Discrete Operators

Theorem (Bokil-Gibson2011)

The symbol of the operator $\tilde{\mathcal{D}}_{1,h}^{(2M)}$ *can be rewritten in the form*

$$\mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = \frac{2i}{h}\sum_{p=1}^{M}\gamma_{2p-1}\sin^{2p-1}(kh/2),$$

where the coefficients γ_{2p-1} *are strictly positive, independent of* M*, and are given by the explicit formula*

$$\gamma_{2p-1} = \frac{[(2p-3)!!]^2}{(2p-1)!}.$$

Table of Coefficients: (V2)

Table: Coefficients γ_{2p-1}

γ_1	γ_3	γ_5	γ_7
1	$\frac{1}{6}$	$\frac{3}{40}$	$\frac{5}{112}$

$$M = 1;\ \mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2)}\right) = \frac{2i}{h}\sin(K)$$

$$M = 2;\ \mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(4)}\right) = \frac{2i}{h}\left(\sin(K) + \frac{1}{6}\sin^3(K)\right)$$

$$M = 3;\ \mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(6)}\right) = \frac{2i}{h}\left(\sin(K) + \frac{1}{6}\sin^3(K) + \frac{3}{40}\sin^5(K)\right)$$

Second Point of View: Symbols of Differential Operators

Theorem

$\forall M \in \mathbb{N}$, M finite we have

$$\mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = \frac{2i}{h}\sum_{p=1}^{M}\frac{\lambda_{2p-1}^{2M}}{2p-1}\sin\left((2p-1)K\right) = \frac{2i}{h}\sum_{p=1}^{M}\gamma_{2p-1}\sin^{2p-1}(K),$$

where $K = kh/2$.

Second Point of View: Symbols of Differential Operators

Proof.

Let $K := kh/2$.

1. Since $\tilde{\mathcal{D}}_{1,h}^{(2M)}$ is of order $2M$ the difference in the symbols of $\partial/\partial z$ and the symbol of $\tilde{\mathcal{D}}_{1,h}^{(2M)}$ must be of $\mathcal{O}\left(K^{2M+1}\right)$ for small K.
2. Thus, we have

$$\mathcal{F}\left(\partial_z\right) = ik = \frac{2iK}{h} = \frac{2i}{h}\left(\sum_{p=1}^{M} \gamma_{2p-1} \sin^{2p-1} K\right) + \mathcal{O}\left(K^{2M+1}\right).$$

This implies that the γ_{2p-1} are the first M coefficients of a series expansion of K in terms of $\sin K$.

Second Point of View: Symbols of Differential Operators

Set $x = \sin K$ for $|K| < \pi/2$. Then, $K = \sin^{-1} x$, $x \in (-1, 1)$ with

$$\sin^{-1} x = \sum_{p=1}^{M} \gamma_{2p-1} x^{2p-1} + \mathcal{O}\left(x^{2M+1}\right).$$

Requiring this to be true $\forall M \in \mathbb{N}$ implies that if a solution exists for $\{\gamma_{2p-1}\}_{p=1}^{M}$, then it is unique. We note that the function $Y(x) = \sin^{-1} x$ obeys the differential equation

$$(1 - x^2) Y'' - x Y' = 0, \ x \in (-1, 1)$$

with the conditions

$$Y(0) = 0, \ Y'(0) = 1.$$

Second Point of View: Symbols of Differential Operators

- Substituting, formally, the series expansion $Y(x) = \sum_{p=1}^{\infty} \gamma_{2p-1} x^{2p-1}$ into the ODE we obtain the equation

$$(6\gamma_3 - \gamma_1) + \sum_{p=2}^{\infty} \beta_{2p-1} x^{2p-1} = 0$$

where

$$\beta_{2p-1} = (2p+1)(2p)\gamma_{2p+1} - (2p-1)^2 \gamma_{2p-1}.$$

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- This implies that $\gamma_3 = \dfrac{1}{6}\gamma_1$, and

$$\gamma_{2p+1} = \frac{(2p-1)^2}{(2p)(2p+1)} \gamma_{2p-1},$$

which gives us the formula $\gamma_{2p-1} = \dfrac{[(2p-3)!!]^2}{(2p-1)!} \gamma_1$.

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which gives us the formula $\gamma_{2p-1} = \dfrac{[(2p-3)!!]^2}{(2p-1)!}\gamma_1$.

- From the initial conditions we see that $\gamma_1 = 1$.

Second Point of View: Symbols of Differential Operators

- To show direct equivalence, for integers $1 \leq j \leq M$,

$$\sin\left((2j-1)K\right) = (-1)^{j-1} T_{2j-1}\left(\sin\left(K\right)\right),$$

T_{2j-1} (Chebyshev polynomials of degree $2j-1$) :

$$\sin\left((2j-1)K\right) = \sum_{p=1}^{j} \alpha_p^j \sin^{2p-1}(K),$$

for $1 \leq p \leq j$,

$$\alpha_p^j = (-1)^{2j-p-1} \left(\frac{2j-1}{j+p-1}\right) \left(\frac{(j+p-1)!}{(j-p)!}\right) \frac{2^{2p-2}}{(2p-1)!}.$$

Second Point of View: Symbols of Differential Operators

- Rearranging terms,

$$\mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = \frac{2i}{h}\sum_{j=1}^{M}\frac{\lambda_{2j-1}^{2M}}{2j-1}\sin\left((2j-1)K\right)$$

$$= \frac{2i}{h}\sum_{j=1}^{M}\frac{\lambda_{2j-1}^{2M}}{2j-1}\sum_{p=1}^{j}\alpha_p^j \sin^{2p-1}(K).$$

- This gives

$$\mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = \frac{2i}{h}\sum_{p=1}^{M}\left(\sum_{j=p}^{M}\frac{\lambda_{2j-1}^{2M}}{2j-1}\alpha_p^j\right)\sin^{2p-1}(K).$$

Second Point of View: Symbols of Differential Operators

- Putting things together,

$$\sum_{j=p}^{M} \frac{\lambda_{2j-1}^{2M}}{2j-1} \alpha_p^j = \sum_{j=p}^{M} \frac{(-1)^{3j-p-2}(j+p-2)![(2M-1)!!]^2 2^{2p-1}}{(2p-1)!(j-p)!(2j-1)(2M-2j)!!(2M+2j-2)!!}.$$

Second Point of View: Symbols of Differential Operators

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- Then a miracle occurs!

$$\sum_{j=p}^{M} \frac{\lambda_{2j-1}^{2M}}{2j-1}\alpha_p^j = \frac{[(2M-1)!!]^2 2^{2p}}{2^{2M}(2p-1)!} \frac{\left[\Gamma(p-\frac{1}{2})\right]^2}{4\left[\Gamma(M+\frac{1}{2})\right]^2}$$

$$= \frac{[(2p-3)!!]^2}{(2p-1)!} = \gamma_{2p-1}.$$

Series Convergence

Lemma

The series $\sum_{p=1}^{\infty} \gamma_{2p-1}$ is convergent and its sum is $\pi/2$.

Proof.

The values γ_{2p-1} are simply the Taylor coefficients of $\sin^{-1}(x)$.

Maxwell's Equations in a Debye Media

Maxwell's equations in a Debye medium can be written using the electric flux density $D = \epsilon_\infty E + P$

$$\frac{\partial B}{\partial t} = \frac{\partial E}{\partial z},$$

$$\frac{\partial D}{\partial t} = \frac{1}{\mu_0}\frac{\partial B}{\partial z},$$

$$\frac{\partial D}{\partial t} + \frac{1}{\tau}D = \epsilon_\infty \frac{\partial E}{\partial t} + \frac{\epsilon_s}{\tau}E$$

$2-2M$ Order Methods for Debye Media

- Second order in time and $2M$th order in space schemes that are staggered in both space and time. (Here $h = \Delta z$)

$$\frac{B_{j+\frac{1}{2}}^{n+\frac{1}{2}} - B_{j+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = \sum_{p=1}^{M} \frac{\lambda_{2p-1}^{2M}}{(2p-1)\Delta z} \left(E_{j+p}^{n} - E_{j-p+1}^{n}\right),$$

$$\frac{D_j^{n+1} - D_j^n}{\Delta t} = \frac{1}{\mu_0} \sum_{p=1}^{M} \frac{\lambda_{2p-1}^{2M}}{(2p-1)\Delta z} \left(B_{j+p-1/2}^{n+\frac{1}{2}} - B_{j-p+1/2}^{n+\frac{1}{2}}\right),$$

$$\frac{D_j^{n+1} - D_j^n}{\Delta t} + \frac{1}{\tau} \frac{D_j^{n+1} + D_j^n}{2} = \epsilon_\infty \frac{E_j^{n+1} - E_j^n}{\Delta t} + \frac{\epsilon_s}{\tau} \left(\frac{E_j^{n+1} + E_j^n}{2}\right)$$

Stability Analysis: von Neumann Analysis

1. Linear models.
2. Analyze the models in the frequency domain.
3. Look for plane wave solution numerically evaluated at the discrete space-time point (t^n, z_j), or $(t^{n+1/2}, z_{j+1/2})$.
4. Assume a spatial dependence of the form

$$
\begin{aligned}
B_{j+\frac{1}{2}}^{n+\frac{1}{2}} &= \hat{B}^{n+\frac{1}{2}}(k)\mathrm{e}^{\mathrm{i}kz_{j+\frac{1}{2}}}, \\
E_j^n &= \hat{E}^n(k)\mathrm{e}^{\mathrm{i}kz_j}, \\
D_j^n &= \hat{D}^n(k)\mathrm{e}^{\mathrm{i}kz_j},
\end{aligned}
$$

- k: wavenumber

Stability Analysis

1. Define the vector $\mathbf{U}^n = [\hat{B}^{n-\frac{1}{2}}, \hat{E}^n, \frac{1}{\epsilon_0\epsilon_\infty}\hat{D}^n]^T$.
2. We obtain the system $\mathbf{U}^{n+1} = \mathcal{A}\mathbf{U}^n$, where the amplification matrix $\mathcal{A}$ is

$$\mathcal{A} = \begin{bmatrix} 1 & -\sigma & 0 \\ \left(\frac{2+h_\tau}{2+h_\tau\eta_s}\right)\sigma^* & \left(\frac{2(1-q)-h_\tau(\eta_s+q)}{2+h_\tau\eta_s}\right) & \left(\frac{2h_\tau}{2+h_\tau\eta_s}\right) \\ \sigma^* & -q & 1 \end{bmatrix},$$

3.

$$\sigma := -\eta_\infty \Delta z \mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = -2\mathrm{i}\nu_\infty \sum_{p=1}^{M} \gamma_{2p-1} \sin^{2p-1}\left(\frac{k\Delta z}{2}\right),$$

$$q := \sigma\sigma^* = |\sigma|^2.$$

$2-2M$ Order Methods for Debye Media

The parameters $c_\infty, \nu_\infty, h_\tau$ and η_s are defined as

$$\begin{aligned} c_\infty^2 &:= 1/(\epsilon_0 \mu_0 \epsilon_\infty) = c_0^2/\epsilon_\infty, \\ \nu_\infty &:= (c_\infty \Delta t)/\Delta z, \\ h_\tau &:= \Delta t/\tau, \\ \eta_s &:= \epsilon_s/\epsilon_\infty, \end{aligned}$$

- c_0: Speed of light in vacuum
- c_∞: speed of light in the Debye medium.
- ν_∞: Courant (stability) number.
- $\epsilon_s > \epsilon_\infty$ and $\tau > 0$.

Stability Conditions

1. A scheme is stable $\iff$ the sequence $(\mathbf{U}^n)_{n\in\mathbb{N}}$ is bounded.
2. Since $\mathcal{A}$ does not depend on time, then $\mathbf{U}^n = \mathcal{A}^n\mathbf{U}^0$, and stability is also the boundedness of $(\mathcal{A}^n)_{n\in\mathbb{N}}$.
3. If the eigenvalues of $\mathcal{A}$, i.e., the roots of the Characteristic Polynomial $P^D_{(2,2M)}$, lie outside the unit circle, then $\mathcal{A}^n$ grows exponentially and the scheme is unstable
4. If the eigenvalues of $\mathcal{A}$, lie inside the unit circle, then $\lim_{n\to\infty}\mathcal{A}^n = 0$ and the sequence is bounded.
5. The intermediate case may lead to different situations.

Characteristic Polynomial

The characteristic polynomial of the system $\mathbf{U}^{n+1} = \mathcal{A}\mathbf{U}^n$ is

$$\begin{aligned} P^{D}_{(2,2M)}(X) =& X^3 + \left(\frac{q\epsilon_\infty(2+h_\tau) - (6\epsilon_\infty + h_\tau\epsilon_s)}{2\epsilon_\infty + h_\tau\epsilon_s} \right) X^2 \\ & + \left(\frac{q\epsilon_\infty(h_\tau - 2) + (6\epsilon_\infty - h_\tau\epsilon_s)}{2\epsilon_\infty + h_\tau\epsilon_s} \right) X \\ & - \left(\frac{2\epsilon_\infty - h_\tau\epsilon_s}{2\epsilon_\infty + h_\tau\epsilon_s} \right). \end{aligned}$$

Stability Conditions

Theorem (Bokil-Gibson2011)

A necessary and sufficient stability condition for the $(2, 2M)$ scheme for Debye is that $q \in (0, 4)$, for all wavenumbers, k, i.e.,

$$4\nu_\infty^2 \left(\sum_{p=1}^{M} \gamma_{2p-1} \sin^{2p-1}\left(\frac{k\Delta z}{2} \right) \right)^2 < 4, \ \forall k,$$

which implies that

$$\nu_\infty \left(\sum_{p=1}^{M} \gamma_{2p-1} \right) < 1 \Longleftrightarrow \nu_\infty \left(\sum_{p=1}^{M} \frac{[(2p-3)!!]^2}{(2p-1)!} \right) < 1.$$

Stability Bounds

For different values of M we obtain the following stability conditions

$$M = 1,\ \nu_\infty < 1 \Longleftrightarrow \Delta t < \frac{\Delta z}{\mathrm{c}_\infty},$$

$$M = 2,\ \nu_\infty \left(1 + \frac{1}{6}\right) < 1 \Longleftrightarrow \Delta t < \frac{6\Delta z}{7c_\infty},$$

$$M = 3,\ \nu_\infty \left(1 + \frac{1}{6} + \frac{3}{40}\right) < 1 \Longleftrightarrow \Delta t < \frac{120\Delta z}{149\mathrm{c}_\infty},$$

$$\vdots$$

$$M = M,\ \nu_\infty \left(\sum_{p=1}^{M} \gamma_{2p-1}\right) < 1 \Longleftrightarrow \Delta t < \frac{\Delta z}{\left(\sum_{p=1}^{M} \frac{[(2p-3)!!]^2}{(2p-1)!}\right) \mathrm{c}_\infty}.$$

Stability Bounds

1. In the limiting case (as $M \to \infty$), we may evaluate the infinite series using the convergence Lemma
2. Therefore,

$$M = \infty,\ \nu_{\infty}\left(\frac{\pi}{2}\right) < 1 \Longleftrightarrow \Delta t < \frac{2\Delta z}{\pi\ c_{\infty}}.$$

3. The positivity of the coefficients γ_{2p-1} gives that the constraint on Δt is a lower bound on all constraints for any M. Therefore this constraint guarantees stability for all orders.

Other Details

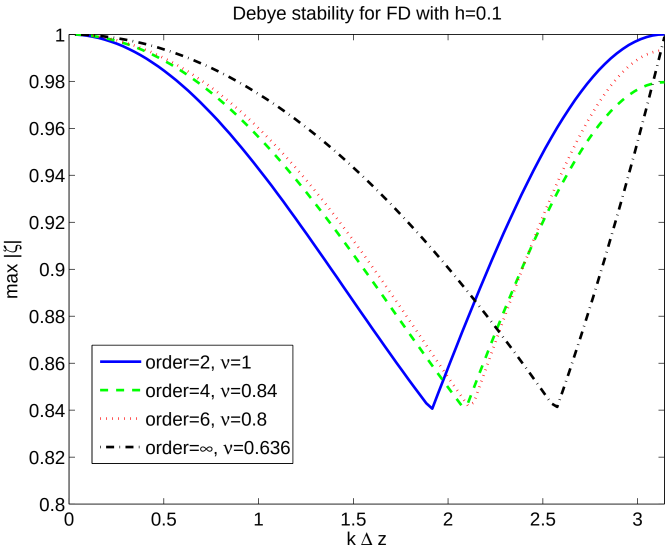
1. This type of stability analysis can be applied to different polarization models written as ODEs augmented to the Maxwell system, e.g., Lorentz, Drude, multipole Debye, Lorentz media.
2. The second point of view also helps in obtaining closed from numerical dispersion relations for all $(2, 2M)$ order schemes. See [Bokil-Gibson2011].

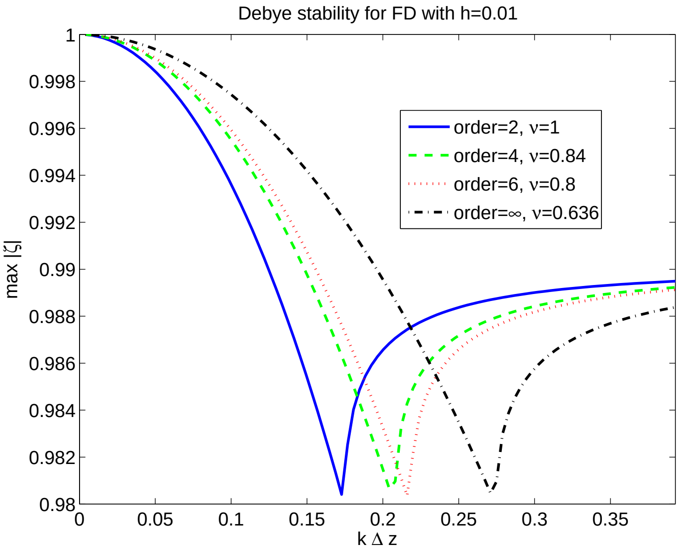
We plot the maximum complex-time eigenvalue for the schemes. For the continuous model, this value should be one, thus the any difference is due to numerical dissipation error.

Physical parameters:

$$\begin{aligned} \epsilon_\infty &= 1 \\ \epsilon_s &= 78.2 \\ \tau &= 8.1 \times 10^{-12} \text{ sec.} \end{aligned}$$

These are appropriate constants for modeling water and are representative of a large class of Debye type materials.


Debye stability for FD with h=0.1
max |ζ|
k Δ z
1
0.98
0.96
0.94
0.92
0.9
0.88
0.86
0.84
0.82
0.8
0
0.5
1
1.5
2
2.5
3
order=2, ν=1
order=4, ν=0.84
order=6, ν=0.8
order=∞, ν=0.636


Debye stability for FD with h=0.01
max |ζ|
k Δ z
1
0.998
0.996
0.994
0.992
0.99
0.988
0.986
0.984
0.982
0.98
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
order=2, ν=1
order=4, ν=0.84
order=6, ν=0.8
order=∞, ν=0.636