Assignments for

Computations in Physics

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1 FDTD

All FDTD simulations are expected to be one-dimensional.

Recommended books:

- (easy) Understanding the Finite-Difference Time-Domain Method, John B. Schneider, www.eecs.wsu.edu/~schneidj/ufdtd, 2010. (it is also available at GitHub https://github.com/john-b-schneider/uFDTD)
- (medium) Numerical electromagnetics : the FDTD method / Umran S. Inan, Robert A. Marshall. 2011
- (full) A. Taflove and S. C. Hagness, Computational Electrodynamics: The Finite-Difference Time-Domain Method, 3rd ed. Norwood, MA: Artech House, 2005.

Implementation examples: https://github.com/kostyfisik/fdtd-1d

1.1 Vanish E field in vacuum

Simulate a system with magnetic mirror boundary condition ($H = 0$) on one side and electric mirror ($E = 0$) on the other side. The source of electric field has a Gaussian profile in time, it is located exactly in the center of the simulated domain. Wave is propagating from the source to the boundaries and back. The successful presentation should provide a sequence of images as a time evolution (or animation) for electric and magnetic fields. The simulation should finish at the moment where the electric field is vanished (all energy is in the magnetic field).

Self Test:

1. Which boundary of the domain is an electric mirror and why?
2. What is the Yee cell and Yee algorithm? What is the reason to use it in space and time?
3. What is the reason for the wave to travel away from the source (from physical and numerical point of view)? In 1D simulation this means that just after the excitation wave located

left to the source goes to the left and wave located right to the source goes to the right.

4. What is the number of field components being updated every time step?
5. Why magnitude of electric field at the end of the simulation is not an exact zero? How the reminding "noise" can be increased? How it can be decreased?
6. Run a simulation using the source time-profile to be one half of the Gaussian curve. What is the reason for the flutter? How it can be fixed? Why? Hint: To provide a correct answer you should understand the origin of Courant condition, provide a Fourier image of Gaussian profile, qualitatively explain how it will change the Fourier image when the half of Gaussian profile is cropped out.
7. Is it possible to use Heaviside step function as a source? Why?
8. What changes you should put into your code to introduce a magnetic dipole source? How can you prove that it is really a magnetic dipole?

1.2 Simple ABC

Simulate a system with a simple absorbing boundary condition (ABC) as it is defined in J.B. Schneider book, section "Terminating the Grid". The source of electric field has a Gaussian profile in time; it is located exactly in the center of the simulated domain (same as in 1.1). The successful presentation should provide a sequence of images as a time evolution (or animation) for electric and magnetic fields before and after the wave hits the boundary.

Self Test:

1. Explain, why does simple ABC works as expected? Which lines in the code represent simple ABC?
2. Use the host media with the refractive index $n = 5$ for the same simulation. You should observe the increase of reflection from the boundary. Why does it happen? How it can be fixed?

1.3 Mur ABC

Same as 1.2 using Mur ABC.

Self Test:

1. Explore Mur ABC performance (amplitude ratio of incident and reflected wave from the boundary) in a wide range of refractive index values and the source parameters. Why does

Mur ABC perform better compared to simple ABC?

2. Sometimes you can observe the distortion of the Gaussian field profile propagating in the media. What is the reason? How it can be fixed?

1.4 CPML

Same as 1.2 using convolution perfectly matched layer (CPML) as a boundary condition. Compare Mur ABC with 5, 10, and 20 cell PML for few values of host media index.

Self Test:

1. Why to use CPML instead of Berenger split-field PML or uniaxial PML? What is the difference between Berenger split-field PML, uniaxial PML, complex-frequency-shifted (CFS) PML, convolution PML?
2. Why 1D simulation does not show the whole story about open boundary condition in FDTD? Can we keep it 2D or we need 3D formulation for a full characterization of such a boundary condition?
3. Why PML performance is low for 5 cell? How does it depend on total PML width and why? What it the principal difference for usage of the polynomial or geometric grading for conductivity in the PML?
4. PML is perfectly matched by impedance with free space. Why we need to use grading of conductivity in the PML to make it work? Hint: The answer is related to Yee grid.
5. What are benefits of PML compared to ABC in 2D/3D?

1.5 Fresnel equation

Compare against Fresnel equations `http://en.wikipedia.org/wiki/Fresnel_equations` , find the limits of FDTD applicability.

Self Test:

1. What is the origin of the difference between numerical (from FDTD) and analytical solution?
2. How does numerical error depend on boundary conditions? Is it possible to remove this dependence?
3. How does the numerical error depend on the refractive index of each of two materials?

1.6 Dielectric slab

Compare FDTD results against a single dielectric slab (e.g http://www.ece.rutgers.edu/ orfanidi/ewa/ch05.pdf), you should provide simulation of reflection-less cases of a quarter-wavelength and half-wavelength width slab.

Self Test:

1. In the provided task examples we use `int()` function to set the refractive index of the slab. Why do we need it? How we can avoid using `int()` function?
2. Why does the reflection from the non-reflecting slab depend on boundary conditions?
3. What is the difference between quater-wavelength and half-wavelength slab from the numerical error point of view?

2 FDFD

To read: presentation Course_FDFD.pdf at https://github.com/kostyfisik/fdfd-1d

2.1 PEC-PMC cavity

- Find the modes of the PMC-PEC cavity.
- Check how solution improves as discretization becomes finer.
- Visualize the field inside the cavity.

Hint: A good example available from 2016 year student Pavel Dmitriev https://github.com/kostyfisik/students-2017/blob/p.dmitriev/2_fdfd/Task1_PEC-PMC_Eigenmodes.ipynb

Self Test:

1. Check field visualization dependence on discretization (phase and amplitude), explain the result.

2.2 Multilayer band gap (BG) diagram

Build 1D BG diagram for a multilayer consisting of two dielectrics of ε_1 and ε_2. Assume the layers have equal thickness. See how BG opens as contrast between ε_1 and ε_2 increases.

3 FEM

To read: https://github.com/kostyfisik/fem-intro

3.1 Quadratic elements

Solve 1D Poisson's equation using FEM with quadratic elements.

Self Test:

1. Compare against analytic solution.

4 Solving PDE with finite differences

Solve the Dirichlet boundary value problem

$$\begin{cases} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, & \text{in} \quad \Omega, \\ u|_{\partial\Omega} = \phi, & \text{on} \quad \partial\Omega. \end{cases} \tag{1}$$

using finite difference method, where Ω is a rectangle with $x \in [0, a]$ and $y \in [0, b]$.

4.1 Iterative solver

Use iterative method to solve the Dirichlet boundary value problem (1) with the following boundary conditions

$$\begin{cases} \phi(x, 0) = 0, \quad \phi(x, b) = \sin(x)/\sin(a), \quad x \in [0, a] \\ \phi(0, y) = 0, \quad \phi(a, y) = \sinh(y)/\sinh(b), \quad y \in [0, b]. \end{cases} \tag{2}$$

Self Test:

1. Compare against analytic solution.

4.2 Inverse matrix method

Use the inverse matrix method to solve the corresponding linear system of algebraic equations in order to find finite difference solution to the Dirichlet boundary value problem (1) with the following boundary conditions (2).

Self Test:

1. Compare the results with ones obtained from iterative solver.

4.3 Heat transfer equation

Solve the initial-boundary problem for the heat transfer equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad u(x, 0) = \sin(\pi x), \qquad 0 \leq x \leq 1, \qquad u(0, t) = u(1, t) = 0, \qquad t \geq 0.$$

Use the generalized Crank-Nicolson finite-difference method with $\theta = 0$ (explicit scheme), $\theta = 1$ (implicit scheme), and $\theta = 1/2$ (Crank-Nicolson scheme) for a different ratio between steps in x and t. Construct the exact solution. Compare the results. Study stability.

4.4 Wave equation

Solve the initial-boundary problem for the wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \qquad u(x,0) = \sin(\pi x), \qquad u_t(x,0) = \sin(\pi x),$$

$$0 \leq x \leq 1, \qquad u(0,t) = u(1,t) = 0, \qquad t \geq 0.$$

Use the finite-difference method with explicit scheme for a different ratio between steps in x and t. Construct the exact solution. Compare the results. Study stability.