Assignments for

Computations in Physics

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Important! For all problems students have to investigate the result (additionally to "Self Test" subsections), e.g. check a numerical solution against an analytic one, check the dependence of the resulting error against the mesh, the domain size, the positions of source and monitor points (if any), etc. "Self Test" subsections are just hints for possible directions of research.

There are four modules (PDE with FD, FDTD, FDFD, and FEM), problems in each module should be solved in sequence.

1 Solving PDE with finite differences

Recommended book: "Finite Difference Computing with PDEs" by Hans Petter Langtangen and Svein Linge https://link.springer.com/book/10.1007%2F978-3-319-55456-3

Solve a 2D 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 the finite difference method, where Ω is a rectangle with $x \in [0, a]$ and $y \in [0, b]$.

1.1 Iterative solver

Use the iterative method (an explicit scheme with finite differences) to solve 2D 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 an analytic solution.

(a) Check the convergence dependence on the mesh size (on each direction) and the number of Jacobi iterations.

(b) How to set the simulation so that some elements of the matrix has 100% relative error? What is the location of these elements.

(c) Plot a color map with numerical and analytic solutions, and the difference (error).

(d) Plot $r.m.s. = \sqrt{\sum_N (u_{numerical} - u_{exact})^2/N}$ a root-mean-square of the error weighted by number of points vs mesh step as you decrease mesh step along x- and y-axis and extract the convergence rate.

2. Increase a ten-fold, keep b the same. Run simulation, explain the result.
3. (Optional) Change the boundary condition to become discontinuous. Run simulation, explain the result.
4. (Optional) Check the evaluation time dependence on mesh size and number of iterations.
5. (Optional) Check the evaluation speed difference when using nested cycles, sections of NumPy arrays, and Numba JIT compilation in your Python implementation.

1.2 Inverse matrix method

Write down 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). Use a central difference 5-point stencil for Laplace operator. Solve the linear system by matrix inverse. See https://github.com/kostyfisik/FD-Zalipaev/blob/master/lec7.pdf, sec. 2 for additional reference

Self Test:

1. Compare the results with ones obtained from Jacobi iterative solver. What are the benifits and drawbacks?
2. Prove the order of accuracy for the numerical scheme. What is the order of accuracy for numerical scheme? Hint: you need to plot wieghted r.m.s.
3. (Optional) Compare the evaluation time and memory consumption with an iterative solver depending on mesh size. Try several matrix solvers (e.g. inverting the full matrix, using sparse matrix generalized minimal residual iteration solver, etc.).

1.3 Heat transfer equation

Solve the initial-boundary problem for the heat transfer equation

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

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.

Self Test:

1. What is the difference between implicit, explicit, and Crank-Nicolson schemes? What is tht convergence order in time and space for each scheme?
2. Compare against the exact solution for all schemes. Check the stability and accuracy of a normalized solution depending on Courant number (e.g. use values of 0.2, 0.5-ε, 0.5+ε, and 1.0) and mesh size for long enough simulations.
3. Check the solution accuracy behavior depending on discretization parameters for all schemes. Which scheme provides the best result? Hint: The answer depends on the parameters.

1.4 Wave equation

Solve the initial-boundary problem for the wave equation

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

$$0 \le x \le 1, \qquad u(0,t) = u(1,t) = 0, \qquad t \ge 0.$$

Use the finite-difference method with explicit scheme for a different ratio between steps in x and t.

Self Test:

1. Compare against the exact solution. Check the stability and accuracy depending on Courant number (e.g. use values of 0.2, 1.0-ε, 1.0+ε, and 1.2) and mesh size for long enough simulations. What is the optimal value of Courant number?

2 FDTD

All FDTD simulations are expected to be one-dimensional. For plotting multiply the magnetic field to the impedance of free space.

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

2.1 Vanish electric 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 the 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 vanishes (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 difference between them? What is the reason to use it in space and time? What is the convergence order of the scheme?
3. What is the reason for the wave to travel away from the source (from a physical and numerical point of view)? In a 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 (with an abrupt change of the amplitude). What is the reason for the flutter? How it can be fixed? Why? What will happen if we increase the mesh density? Hint: To provide a

correct answer you should understand the origin of Courant condition, provide a Fourier image of a Gaussian profile, qualitatively explain how it will change the Fourier image when the half of Gaussian profile is cropped out.

7. What will happen if you use a Heaviside step function as a source? Why?
8. What you should put into your code to introduce a magnetic dipole source? How can you prove that it is really a magnetic dipole?

2.2 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 the electric field has a Gaussian profile in time; it is located exactly in the center of the simulated domain (same as in 2.1). The successful presentation should provide a sequence of images as a time evolution (preferred) or animation (with an ability to skip initial part of the simulation and to pause at any given moment for visual investigation of result) 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 $n = 2$ for the same simulation. You should observe the increase of reflection from the boundary. Why does it happen? How it can be fixed? (provide at least two approaches, one works only for integer n, another works for any n)
3. What and why will happen if you mess the order of lines in main loop (update equations and boundary condition)?
4. How you can turn simple ABC on the e-field ending edge of the domain into PMC boundary condition? Why does it work so?

2.3 Mur ABC

Same as 2.2 using Mur ABC.

Self Test:

1. Explore Mur ABC performance (amplitude ratio of the incident and the 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 (short pulses on coarse mesh). Why this simulation conditions lead to distortion?
3. Name few other types of ABC.

2.4 CPML

Same as 2.2 using convolution perfectly matched layer (CPML) as a boundary condition.

Self Test:

1. Compare Mur ABC against 5, 10, and 20 cells of PML for few values of host media index.
2. What is the difference of CPML compared to Berenger PML, UPML, CFS-PML, etc? Which one you should select depending on the model under consideration?
3. Find out in the literature the benefits of PML over ABC (including 2D and 3D cases). Hint: Consider evanescent waves, discursive and non-linear media, etc.
4. 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?
5. 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.
6. What is the optimal power of polynomial grading? Check the cases of 10 and 100 PML cells, explain the difference. Hint: consider reflection and attenuation within each layer of PML.

2.5 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 analytic solution?
2. How does numerical error depend on boundary conditions? Is it possible to remove this dependence?
3. Check the dependence of error on the position of monitor point (including points very

close to the boundary and the interface).

4. How does the numerical error depend on the refractive index of each of two materials? How the numerical error can be reduced? Hint: consider the influence of Courant number.

2.6 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 depends on boundary conditions?
3. What is the difference between quater-wavelength and half-wavelength slab from the numerical error point of view?
4. (optional) Plot a transmission spectra from a single simulation run. Hint: Use a short pulse to cover the spectral range of interest and discrete Fourie transform

$$F(f) = \Delta t \sum_{m=1}^{M} \left(e^{-j2\pi f \Delta t}\right)^m f(m),$$

where $f(m)$ field values at given time-step. Perform the summation via the main loop (so, no need to store field time-profile). Compare the performance, when expression in round brackets is evaluated inside of loop or computed in advance.

3 FDFD

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

3.1 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 is available from 2016 year student Pavel Dmitriev https://github.com/kostyfisik/students-2018/blob/p.dmitriev/2_fdfd/Task1_PEC-PMC_Eigenmodes.ipynb

Self Test:

1. Check field dependence on discretization (phase and amplitude), explain the result. Why does amplitude depends on discretization? Why the phase can be occasionally shifted by π?
2. How the boundary condition is applied? Point corresponding elements in forward and backward difference matrices.
3. (Optional) Check memory consumption and performance when using sparse and full matrix representation of the problem depending on the mesh size.

3.2 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 the contrast between ε_1 and ε_2 increases.

Self Test:

1. Check the light line in free space. Why it looks to be folded?
2. How does the boundary condition works?
3. What are the parameters of `eigs()` function? How does the solution depends on it?

4 FEM

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

4.1 Quadratic elements

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

Self Test:

1. Compare against the analytic solution, change the number of elements (start from one element). Include values from inside of the elements to the comparison.
2. Plot on the same figure shape functions multiplied by wight the solution for each element. In spite of using quadratic functions sometimes you can observe straight lines, why so?
3. What is the main idea of the Galerkin method?

4.2 (optional) Scattering on infinite cylinder

Evaluate electric field for the scattering on TM^z plane wave on PEC infinite cylinder using Fenics Project FEM library https://fenicsproject.org/. Hint: After getting acquainted with Fenics tutorial https://fenicsproject.org/tutorial/ use the mathematical statement of the problem from Anastasis C. Polycarpou book "Introduction to the Finite Element Method in Electromagnetics" sec. 2.10.2 to solve the problem in Python.

Self Test:

1. Compare against the analytic solution, change the number of elements and the order of approximation.