Computational Physics

Finite difference time-domain: stability and accuracy

Once again: FDTD method for 1d wave equation

Last week, we derived the classic FDTD method

$$
\begin{aligned}
v_i^{(j+1)} =& v_i^{(j)} + h^{-1}\Delta t[w_{i+1/2}^{(j)} - w_{i-1/2}^{(j)}],\\
w_{i+1/2}^{(j+1)} =& w_{i+1/2}^{(j)} + h^{-1}\Delta t[v_{i+1}^{(j+1)} - v_i^{(j+1)}],
\end{aligned}
$$

for the 1d wave equation

$$[\partial_t^2 - \partial_x^2]p(x,t) = 0.$$

We found that it sometimes explodes and that it can produce artifacts like ringing on the trailing end of a pulse.

Today we analyze this behavior.

Semi-discrete forms of a PDE

PDEs for time-domain problems can be written in the form

$$[\hat{A} + \hat{B}\partial_t + \hat{C}\partial_t^2 + \ldots]\mathbf{u}(\mathbf{r}; t) = 0,$$

where $\hat{A}, \hat{B}, \hat{C}, \ldots$ are differential operators in space.

One way to tackle such equations is to first discretize space. We introduce a set of basis functions $\phi_i(\mathbf{r})$ and test functions $\psi_i(\mathbf{r})$. Usually $\psi_i(\mathbf{r}) = \phi_i(\mathbf{r})$.

We expand $\mathbf{u}$ and project the operators to obtain a vector-valued ODE:

$$\begin{aligned}
\mathbf{u}(\mathbf{r}; t) = \sum_i \mathbf{u}_i(t)\phi_i(\mathbf{r}); \\
A_{ij} = \langle \psi_i | \hat{A} | \phi_j \rangle, \quad B_{ij} = \langle \psi_i | \hat{B} | \phi_j \rangle, \quad C_{ij} = \langle \psi_i | \hat{C} | \phi_j \rangle; \\
\sum_j [A_{ij} + B_{ij}\partial_t + C_{ij}\partial_t^2 + \ldots]\mathbf{u}_j(t) = 0.
\end{aligned}$$

This known as a **semi-discrete** form of the PDE.

Stability of a semi-discrete PDE solver

Example 1d wave equation with finite-difference discretization:

$$[\partial_t^2 - \underbrace{\partial_x^2}_{=\hat{A}}]u(x,t) = 0, \qquad \Rightarrow \qquad A = \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & \ddots \\ 0 & \ddots & \ddots \end{pmatrix}$$

A semi-discrete form is just a large ODE. If linear, it can be brought to first order form

$\partial_t v_i = \sum_j M_{ij} v_j$

and solved with any ODE integrator.

We remember that the these integrators are stable if all eigenvalues of the system matrix lie inside the **stability contours**.

The stability of a time-domain method based on a semi-discrete form is given by the spectrum of M, i.e. on the **type** and the **number** of basis functions $\phi(\mathbf{r})$.

Classroom exercise: Spectrum of the finite-difference operator

Set up a matrix A that performs the second derivative on a state vector:

$$\mathbf{y} = A\mathbf{x} \quad \text{such that} \quad y_i = h^{-2}(x_{i+1} - 2x_i + x_{i-1}).$$

Find the eigenvalues λ_i of A.

The semidiscrete wave equation is $(\partial_t^2 - A)u = 0$, so the eigenfrequencies are given as the square roots of the eigenvalues:

$$\omega_i = \pm\sqrt{\lambda_i}.$$

Where do the eigenfrequencies lie in the complex plane? What does this mean?

Stability of FDTD

The stability of FDTD is given by the spectrum of the finite-difference operator and the stability contour of the leapfrog integrator.

This binds the time step Δt to the spatial grid spacing h.

We introduce the Courant-Friedrichs-Lewy (CFL) number

$$c = \frac{v\Delta t}{h},$$

where v is the propagation velocity of the wave and FDTD is guaranteed to be stable if $c < 1$ everywhere in the simulations domain.

The classic CFL number is restricted to FDTD, but similar expressions exist for most time-domain methods based on a semi-discrete form.

Errors and convergence of a semi-discrete PDE solver

There are two independent sources of errors:

- Errors accumulated during time-evolution (discussed earlier)
- Errors introduced by the spatial discretization

Spatial discretization errors can be classified in two categories:

- Local errors stem from the fundamental inability of the basis to reproduce features of the solution. Further away the solution and physical observables can be fine.
- Phase errors stem from incorrect eigenvalues of the discretized operator. This means that fields oscillate with a slightly incorrect frequency. This effect reduces as the spatial discretization converges when refining the grid.

In semi-discrete PDE-solvers, convergence is an issue with respect to the time step and the spatial grid spacing.
They are usually bounded via the CFL-criterion.

A well-designed method will balance them, e.g. by matching the convergence order of the time-integrator to that of the spatial discretization.

Example: Numerical dispersion in FDTD

The phase error of FDTD can be understood by studying the equation:

$$\partial_t^2 u(x,t) = \partial_x^2 u(x,t) \approx h^{-2}[u(x-h,t) - 2u(x,t) + u(x+h,t)].$$

We know that plan waves are solutions to the 1d wave equation, so we make the ansatz

$$u(x,t) = \exp(\mathrm{i}kx - \mathrm{i}\omega t).$$

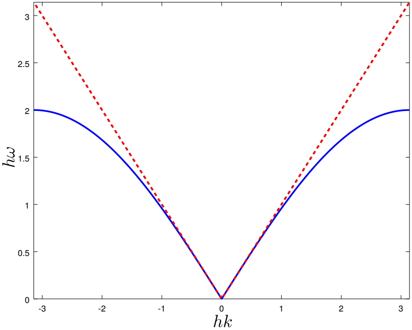
We find:

$$\begin{aligned} \partial_t^2 u = &- \omega^2 u = h^{-1}[\exp(\mathrm{i}kh) - 2 + \exp(-\mathrm{i}kh)]u \\ \Rightarrow \quad h\omega = &\sqrt{2(1-\cos kh)}. \end{aligned}$$

This is not the mathematically correct dispersion relation $\omega = \pm k$.

Example: Numerical dispersion in FDTD (cont'd)

Comparison of mathematically correct (red dashed) and numerical FDTD (blue solid) dispersion relation:



FDTD reproduces the the correct dispersion relation for $kh \approx 0$.
A rule of thumb for acceptable performance is $hk \approx 0.1$.
The minimum discretization is determined by the fastest spatial Fourier component that will appear during the simulation.

Homework

Implement a 2d finite difference simulator (see problem sheet).

Literature:
A. Taflove, S.C. Hagness,
"Computational Electrodynamics – The Finite-Difference Time-Domain Method"
Artech House Publishing