18.303 Problem Set 8

Due Wednesday, 23 November 2016.

Problem 1: Schrödinger discretization

Suppose that you are discretizing the 1d Schrodinger wave equation (nondimensionalized and with zero potential):

$$\frac{\partial u}{\partial t} = i\frac{\partial^2 u}{\partial x^2} + iVu,$$

where $V(x)$ is a real-valued function. Suppose that we discretize in space at intervals Δx and in time with some timestep Δt, denoting $u(m\Delta x, n\Delta t) \approx u_m^n$ as in class. We will discretize $\partial^2/\partial x^2$ with the usual center-difference approximation $\frac{u_{m+1}-2u_m+u_{m-1}}{\Delta x^2}$, and Vu by $V_m u_m$ where $V_m = V(m\Delta x)$.

(a) Come up with an *explicit* timestepping scheme with $O(\Delta t^2)$ *centered-difference* approximation for $\partial u/\partial t$, by writing $u = a + ib$ (for real a and b) and writing separately the equations for $\partial a/\partial t$ and $\partial b/\partial t$.

(b) For $V(x) = 0$, apply Von Neumann analysis to determine the stability (e.g. find conditions for stability or show unconditional stability) of your scheme. That is, consider an infinite domain, and solutions $u_m^n = \lambda^n e^{ikm}$, solve for $\lambda(k)$, and check whether $|\lambda| \le 1$ for all k.

(c) Modify the `timestep!` function from the wave-animation Julia notebook from lecture (see the web site) to implement one of your schemes, for *Dirichlet* boundary conditions $u(0) = u(L) = 0$ and $V(x) = 0$, and plot $|u(x,t)|^2$ for several representative times t given the initial condition $u(x,0) = \delta(x - L/2)$ [implement by setting u_m at one position to $1/\Delta x$ and to 0 for other m's].

Problem 2: Discretizing a 2d wave equation

Consider the scalar wave equation with constant coefficients, which can be written as in the notes as two coupled equations $\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v}$, $\frac{\partial \mathbf{v}}{\partial t} = \nabla u$. Now, let us consider this in two dimensions (for an infinite spatial domain $\Omega = \mathbb{R}^2$, don't worry about boundary conditions).

(a) Suppose that we discretize $u(x,y,t)$ as $u^n_{m_x,m_y} \approx u(m_x\Delta x, m_y\Delta y, n\Delta t)$ for integers m_x, m_y, n. Explain how (i.e. where/when) we should discretize $v_x(x,y,t)$ and $v_y(x,y,t)$ so that our equations $\frac{\partial u}{\partial t} = \nabla \cdot \mathbf{v}$ and $\frac{\partial \mathbf{v}}{\partial t} = \nabla u$ can all be implemented as explicit center differences, similar to the staggered-grid leap-frog scheme in class for the 1d case. Give the discretized equations. (Hint: v_x and v_y don't have to be discretized on the same spatial grid.)

(b) Combine your discretized equations back into a discretization of $\frac{\partial^2 u}{\partial t^2} = \nabla^2 u$, as in class, by writing:

$$\frac{\partial^2 u}{\partial t^2} \approx \frac{u^{n+1}_{m_x,m_y} - 2u^n_{m_x,m_y} + u^{n-1}_{m_x,m_y}}{\Delta t^2} = \frac{\frac{u^{n+1}_{m_x,m_y} - u^n_{m_x,m_y}}{\Delta t} - \frac{u^n_{m_x,m_y} - u^{n-1}_{m_x,m_y}}{\Delta t}}{\Delta t} = \cdots,$$

where the right-hand side is some spatial derivatives (finite differences) of u. (Do *not* re-discretize $\frac{\partial^2 u}{\partial t^2} = \nabla^2 u$ from the beginning; make sure you plug in your discretizations from the previous part.)

(c) Using the previous part (which helpfully is only in terms of u), perform a Von Neumann analysis to relate Δt to Δx and Δy: plug in $u^n_{m_x,m_y} = e^{i(k_x m_x \Delta x + k_y m_y \Delta y - \omega n \Delta t)}$ and solve for $\omega(k_x, k_y)$, and find out under what conditions (on Δt) ω is real for all possible values of k_x and k_y.