18.303 Problem Set 7

Due Wednesday, 21 November 2012.

Problem 1: Crank-Nicolson

Suppose we are discretizing a wave equation $\frac{\partial \mathbf{w}}{\partial t} = \hat{D}\mathbf{w}$ for an anti-Hermitian $\hat{D}$. We discretize space to obtain an anti-Hermitian matrix D. Show that the Crank-Nicolson time discretization

$$\frac{\mathbf{w}^{n+1} - \mathbf{w}^n}{\Delta t} = D\frac{\mathbf{w}^{n+1} + \mathbf{w}^n}{2}$$

is unconditionally stable.

Problem 1: Schrödinger

Suppose that you are discretizing the 1d Schrödinger wave equation (nondimensionalized and with a real potential $V(x)$):

$$\frac{\partial u}{\partial t} = i\left[\frac{\partial^2 u}{\partial x^2} + V(x)u\right].$$

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 discretized $\partial^2/\partial x^2$ with the usual center-difference approximation $\frac{u_{m+1} - 2u_m + u_{m-1}}{\Delta x^2}$.

(a) Describe a second-order accurate (in space and time) explicit timestepping scheme, constructed by using center differences in both space *and* time. [Hint: write $u = a + bi$ in terms of its real part $a(x,t)$ and its imaginary part $b(x,t)$, and discretize a and b at different times (offset by $\Delta t/2$); you should be able to write two coupled *real* PDEs for a and b.]

(b) Anayze the stability of your scheme using Von Neumann analysis, assuming $V(x) = 0$. (Hint: similar to how we analyzed the wave equation in class, take an additional time derivative, or the discrete analogue thereof, to obtain an equation just in a or just in b, and then plug in e.g. $a_m^n = e^{i(k\Delta x \cdot m - \omega\Delta t \cdot n)}$ and solve for Δt, if any, such that ω is real for all k.)

(c) Plot the dispersion relation $\omega(k)$ from the previous part for $V_0 = 0$, using some Δt such that the scheme is stable, and compare to the $\omega(k) = k^2$ from the exact wave equation. What does this tell you about how, qualitatively, the wave solutions should differ in the discrete vs. exact case, from what we know about group velocity and dispersion?