Computational Physics II 5640   Spring 2018

Project Assignment 4

Due: Wednesday April 25

1. Finite-difference method for advection equation. Consider the one-dimensional advection equation:

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = 0. \tag{1}$$

Write a code to implement the Lax finite difference scheme (here $u_j^n = u(x_j, t_n)$):

$$u_j^{n+1} = \frac{1}{2}(u_{j+1}^n + u_{j-1}^n) - \frac{v\Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n), \tag{2}$$

and use it to study the evolution of the wave form $u(x,t)$. More explicitly, set $v = 1$ and $\Delta x = 0.1$ and consider an initial Gaussian wave form $u(x,0) = \exp(-x^2/w^2)$ with width $w = 5$. Run the Lax simulation using time step $\Delta t = 0.06$, 0.1, and 0.14 and compare the results; see Fig. 1. Show that the total "energy" $E \equiv \int_{-\infty}^{\infty} u^2(x,t)dx$ is conserved in Eq. (1). Plot E vs t using different time steps Δt (see Fig. 1).

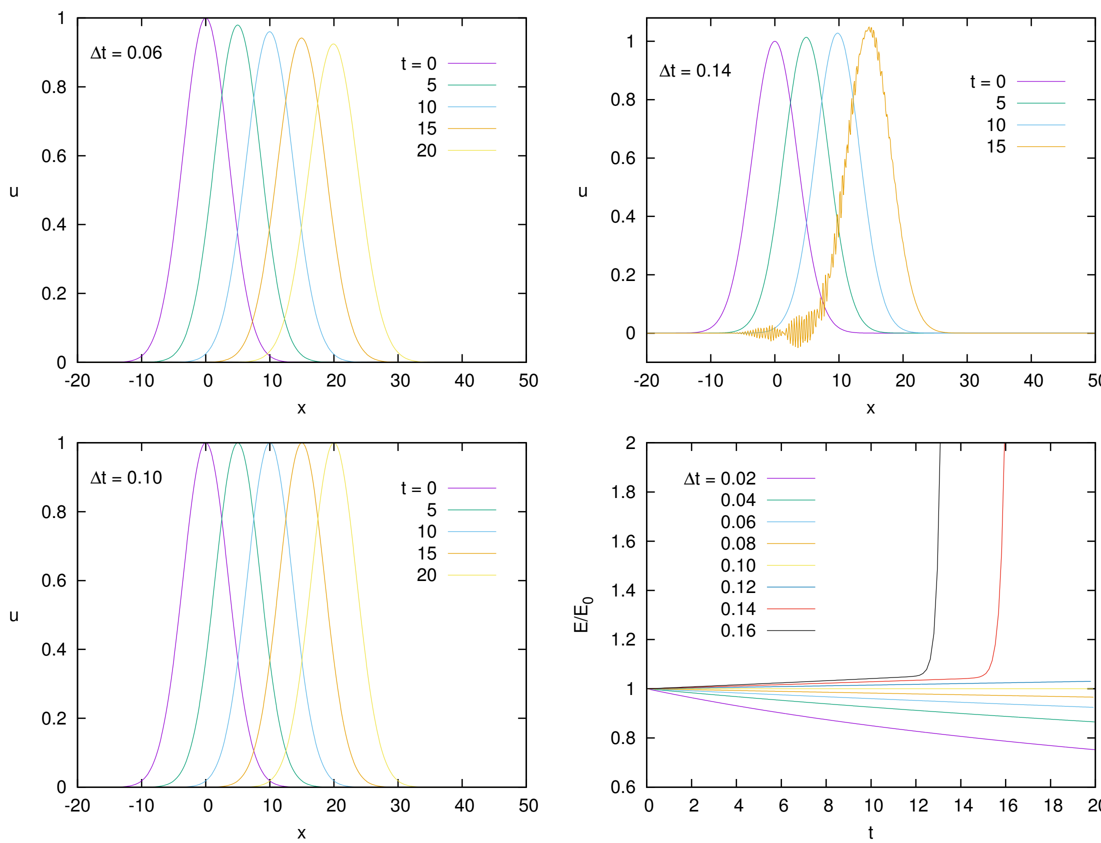

Figure 1: The temporal development of wave form $u(x)$ obtained using different time steps Δt. The right lower panel shows the time dependence of total energy E for varying Δt.

However, this energy does *not* always remain constant in numerical simulations due to finite-difference errors. Calculate analytically the amplification factor ξ_k of the Lax method for the advection equation. Compare it to the exact amplification factor (derive it) and explain why the total 'energy' is not conserved in the first two top panels of Fig. 1, when $\Delta t < \Delta x/v$ and $\Delta t > \Delta x/v$ (which is also unstable).

(Bonus) Repeat the above analysis using the implicit Crank-Nicholson method and particularly examine the effect of different time step Δt on the energy conservation.

2. Crank-Nicholson method for diffusion equation. Next we consider the diffusion equation, which is the canonical example of parabolic PDE:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}. \tag{3}$$

Write a code to implement the Crank-Nicholson finite difference scheme:

$$u_j^{n+1} = u_j^n + \frac{D\Delta t}{2\Delta x^2}\Big[(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + (u_{j+1}^n - 2u_j^n + u_{j-1}^n)\Big], \tag{4}$$

and use it to simulate the evolution of an initial Gaussian wave form $u(x,0) = \exp(-x^2/w^2)$; see Fig. 2. The diffusion equation (3) with an initial Gaussian distribution can also be solved exactly using the Fourier transform method. Show that the exact solution is given by

$$u(x,t) = \frac{1}{\sqrt{1+4Dt/w^2}}\,\exp\left(-\frac{x^2}{w^2+4Dt}\right). \tag{5}$$

Compare the numerical results with the analytical solution for $u(x=0,t)$, i.e. the peak value. The Crank-Nicholson method is unconditionally stable and very accurate. For, e.g. $D = 0.5$ and $\Delta x = 0.1$ (with an initial width $w \approx 10$), the discrepancy between numerical and analytical solutions for $\Delta t < 1$ is of the order of 10^{-6}. Compare the error for larger time step Δt; see the right panel of Fig. 2, and see whether you can verify the Δt^2 scaling for the numerical error (bonus).

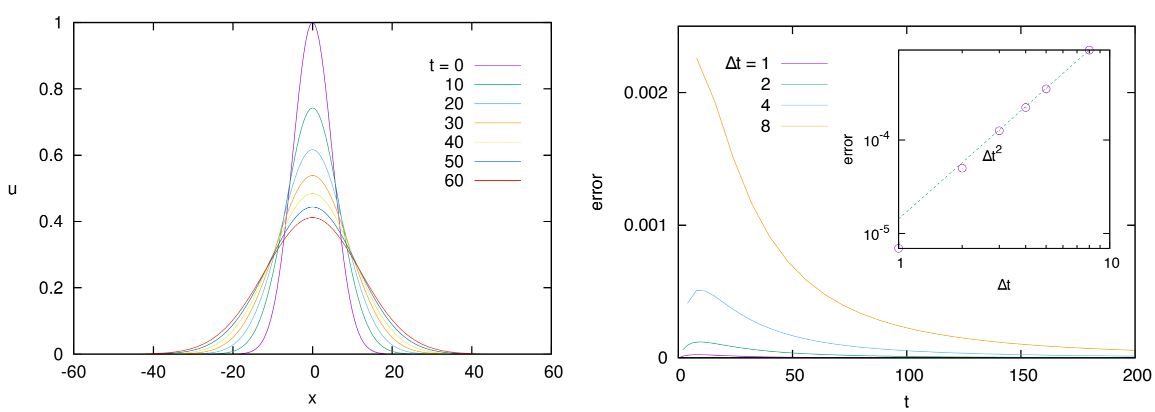

Figure 2: Diffusion of an initial Gaussion wave form obtained using Crank-Nicholson finite-difference scheme. The right panel shows the discrepancy between numerical and analytical results for the peak value $u(x=0,t)$ as a function of time for increasing time step Δt; the inset there shows the Δt^2 scaling of the numerical error.

3. Korteweg – de Vries equation. One of the most extensively studied nonlinear partial differential equation is the so-called KdV equation:

$$\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} + \delta^2\,\frac{\partial^3 u}{\partial x^3} = 0, \tag{6}$$

here δ is a parameter characterizing the dispersion effect. Write a code to implement the explicit leapfrog method for the KdV equation [1]:

$$u_j^{n+1} = u_j^{n-1} - \frac{\Delta t}{3\Delta x}(u_{j+1}^n + u_j^n + u_{j-1}^n)(u_{j+1}^n - u_{j-1}^n) - \frac{\delta^2 \Delta t}{\Delta x^3}(u_{j+2}^n - 2u_{j+1}^n + 2u_{j-1}^n - u_{j-2}^n). \tag{7}$$

This method is the one employed in the original work of Zabusky and Kruskal (Ref. [1]). Perform a simulation to study the formation of solitons (here we mainly repeat the work of Ref. [1]). Use a dispersion parameter $\delta = 0.022$. Following Ref. [1], we restrict the spatial domain to be $0 \le x < 2$ with **periodic boundary conditions**. Start the simulation with a cosine wave form $u(x, t = 0) = \cos(\pi x)$ and study the evolution of $u(x)$; see Fig. 3. An important time scale is the breakdown time $t_B = 1/\pi$. This is the time scale for the formation of singularity where $\partial u/\partial x$ diverges and its breakdown into soliton trains. For example, at $t = 3t_B$ the wave is broken into 8 solitons in Fig. 3. The trajectories of solitons can be obtained from the contour plot of $u(x,t)$ (or you can trace the maxima of $u(x)$ or invent your methods); see the right panel of Fig. 3. These solitons behave as particle-like objects. Verify these results with your code.

[1] N. J. Zabusky and M. D. Kruskal, Physical Review Letters **15**, p.240 (1965).

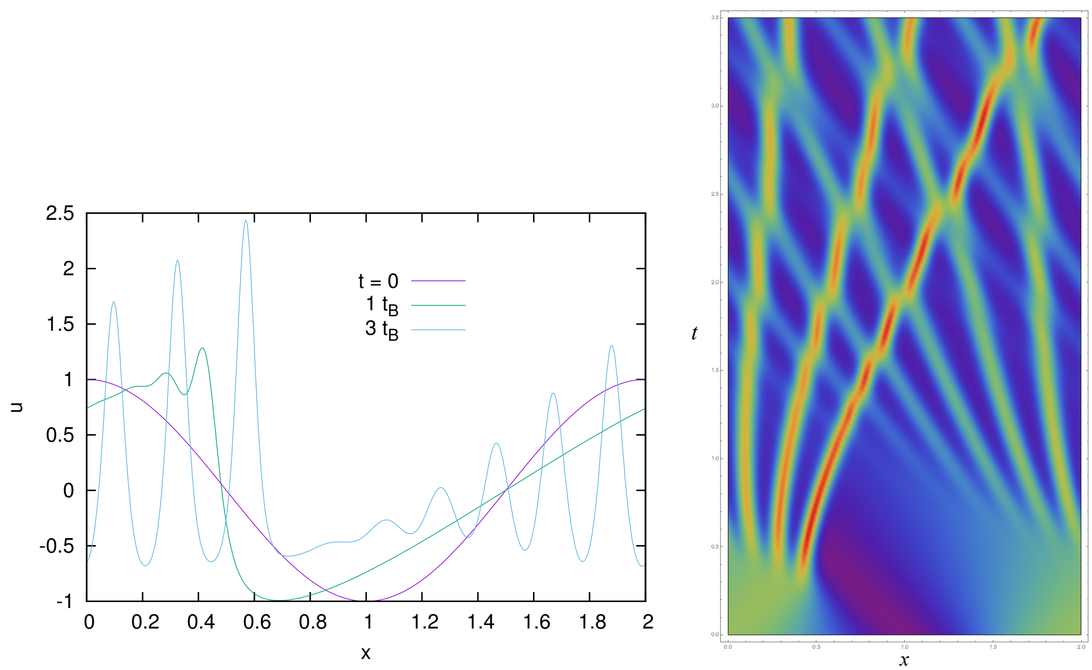

Figure 3: (Left) Temporal development of the wave form in KdV equation with an initial condition $u(x, 0) = \cos(\pi x)$. Here the breakdown time scale $t_B = 1/\pi$. The contour plot of $u(t, x)$ in the right panel shows particle-like trajectories of the KdV solitons.