PHY 604: Computational Methods in Physics and Astrophysics II

Homework #5

Due: Nov. 11, 2021

Programs can be written in any language, In addition to the program, you should have a writeup that contains the plots requested in the homework questions, answers to any analytical or explanation questions, and a short description of your code and how to run it. This can be done via, e.g., LaTeX, markdown, jupyter notebooks, etc.

Code and writeup should be submitted using `git` *via github in the repo that was created from the* github classroom *link.*

1. *Relaxation methods for the Poisson equation* (based on Garcia)

(**a**) Write a program that solves the two-dimensional Poisson equation in a square geometry with the Dirichlet boundary conditions $\Phi = 0$ at the boundaries using one of the relaxation methods discussed in class (i.e., Jacobi, Gauss-Seidel, or SOR). Map the potential for a single charge at the center of the system. Compare with the potential for a charge in free space (recall that a point charge in 2D is equivalent to a line charge in 3D).

(**b**) Modify your program to use periodic boundary conditions. Compare the result to part (a).

2. *Stability analysis* (based on Garcia) In class we discussed two methods for assessing the stability of PDEs, *von Neumann stability analysis* and *matrix stability analysis*. In this problem, we will explore these approaches on a variety of explicit/implicit schemes. Note: Several parts of this problem do not require writing any programs.

(**a**) Consider the leapfrog scheme for solving the advection equation introduced in question 3(b) of Homework 4:

$$\frac{a_i^{n+1} - a_i^{n-1}}{2\tau} = -c\frac{a_{i+1}^n - a_{i-1}^n}{2h}. \tag{1}$$

Use the von Neumann stability analysis to show that the method is stable only if $\tau \leq h/|c|$.

(**b**) Consider the Richardson scheme for solving the diffusion equation introduced in question 2(a) of Homework 4:

$$\frac{T_i^{n+1} - T_i^{n-1}}{2\tau} = \kappa\frac{T_{i+1}^n + T_{i-1}^n - 2T_i^n}{h^2}. \tag{2}$$

Use the von Neumann stability analysis to show that this scheme is unconditionally unstable.

(**c**) The Lax scheme for the advection equation with periodic boundary conditions may be written as

$$\mathbf{a}^{n+1} = \left(\frac{1}{2}\mathbf{C} - \frac{c\tau}{2h}\mathbf{B}\right)\mathbf{a}^n \equiv \mathbf{A}\mathbf{a}^n \tag{3}$$

where

$$\mathbf{a}^n = \begin{bmatrix} a_0^n \\ a_1^n \\ a_2^n \\ \vdots \\ a_{N-1}^n \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 & 1 \\ 1 & 0 & 1 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \dots & 1 & 0 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 & -1 \\ -1 & 0 & 1 & \dots & 0 & 0 \\ 0 & -1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & \dots & -1 & 0 \end{bmatrix}. \tag{4}$$

Demonstrate that the matrix stability analysis gives by $\tau \leq h/|c|$ by plotting the spectral radius versus time step of $\mathbf{A}$.

(**d**) A stricter condition for matrix stability is that the *norm* of $\mathbf{A}$ is less than or equal to unity. There are a variety of ways to compute the norm. The easiest is the so-called 1-norm:

$$||\mathbf{A}||_1 = \max_{j=0,\ldots,N-1} \left\{ \sum_{i=0}^{N-1} |A_{ij}| \right\} \tag{5}$$

which is simply the maximum absolute column sum of the matrix, and the ∞-norm:

$$||\mathbf{A}||_\infty = \max_{i=0,\ldots,N-1} \left\{ \sum_{j=0}^{N-1} |A_{ij}| \right\} \tag{6}$$

which is the maximum absolute row sum of the matrix. Do the same matrix analysis as you did in part (c), but plotting these matrix norms instead of the spectral radius.

(**e**) Recall the diffusion equation

$$\frac{\partial}{\partial t} T(x,t) = \kappa \frac{\partial^2}{\partial x^2} T(x,t), \tag{7}$$

Use von Neumann and matrix analysis to demonstrate that the Crank-Nicolson is unconditionally stable for this equation (with periodic boundary conditions).

3. *Schrödinger equation with the spectral method* (Based on Newman exercise 9.9) Consider the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2}. \tag{8}$$

In this problem, we will solve for $\psi(x,t)$ of a particle in a box of length L using spectral methods similar to those discussed in class for the Poisson equation. Take as basis functions

$$\psi_k(x,t) = \sin\left(\frac{\pi k x}{L}\right) e^{iEt/\hbar} \tag{9}$$

where

$$E = \frac{\pi^2 \hbar^2 k^2}{2mL^2}. \tag{10}$$

Thus we will seek solutions of the form:

$$\psi(x_n,t) = \frac{1}{N} \sum_{k=1}^{N-1} b_k \sin\left(\frac{\pi k n}{L}\right) \exp\left(i \frac{\pi^2 \hbar k^2}{2mL^2} t\right) \tag{11}$$

where b_k are a set of complex coefficients. Our initial form of the wave function will be the wave packet discussed in class:

$$\psi(x, t=0) = \frac{1}{\sqrt{\sigma_0 \sqrt{\pi}}} \exp\left(ik_0 x\right) \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right] \tag{12}$$

Use natural units ($\hbar = m = 1$), $L = 100$ Bohr, $N = 1000$, $x_0 = L/2$, $\sigma_0 = L/10$, and $k_0 = 0.5$.

(**a**) First write a program that obtains the coefficient b_k via a discrete sine transformation of $\psi(x, t = 0)$. Do the transformation separately for the real and imaginary part of $\psi(x, t = 0)$, obtaining two sets of coefficients a_k and η_k such that $b_k = a_k + i\eta_k$.

(**b**) Obtain the real part of $\psi(x_n, t)$ on your spatial grid by taking the inverse discrete sine transformation of Re $\left[b_k \exp\left(i \frac{\pi^2 \hbar k^2}{2mL^2} t\right)\right]$.

(**c**) Plot $\psi(x,t)$ for several time steps and describe what you see.

Hint: No need to program the discrete sine transformation (or inverse) yourself, e.g., see:

`https://docs.scipy.org/doc/scipy/reference/generated/scipy.fftpack.dst.html`

and

`https://docs.scipy.org/doc/scipy/reference/generated/scipy.fftpack.idst.html`.

4. *Radioactive decay chain* (Based on Newman exercise 10.2) The isotope ^{213}Bi decays to a much more stable isotope ^{209}Bi via one of two different routes, with probabilities and half-lives shown in Fig. 1. Starting with a sample consisting of 10,000 atoms of ^{213}Bi, simulate the decay of atoms over 20,000 s using a time slices of 1 s. **Hint:** Start from the lower decay processes (^{209}Pb $\rightarrow^{209}$ Bi) and work your way up.

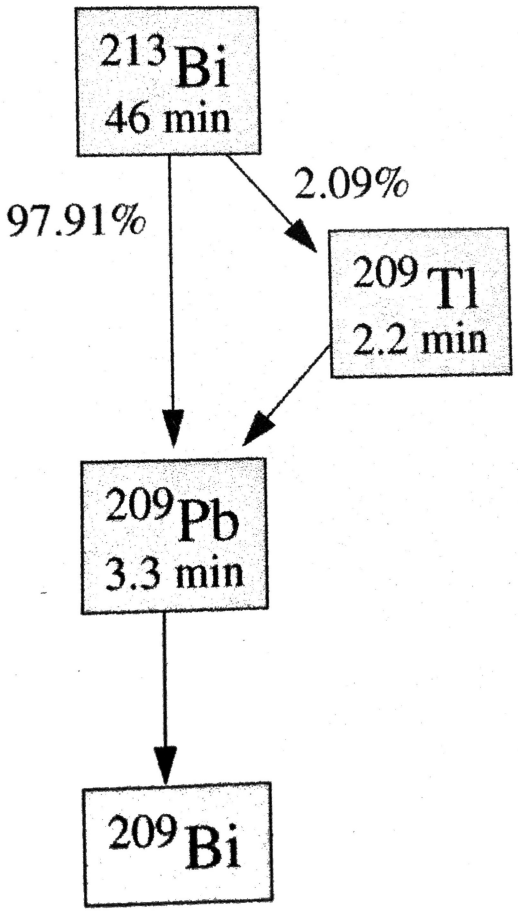

Figure 1: Decay paths from ^{213}Bi to ^{209}Bi