PHYS6350 (Computational Physics)

Problem Set 4

Due:

Mon, Apr 17, 2023, end of the day

Instructions:

Send via Teams (preferably) or email. Should include code (or, where applicable, note) which solves the problems and, where applicable, plots and/or annotations. The preferred languages are Python/Jupyter notebook/C++ while other choices may be accepted on an individual basis.

Problem 4.1: Thermal diffusion in the Earth's crust (6 points)

Adapted from Exercise 9.4 from M. Newman "Computational Physics''

A classic example of a diffusion problem with a time-varying boundary condition is the diffusion of heat into the crust of the Earth, as surface temperature varies with the seasons. Suppose the mean daily temperature at a particular point on the surface varies as:

$$T_0(t) = A + B \sin \frac{2\pi t}{\tau},$$

where $\tau = 365$ days, $A = 10^{\circ}$C and $B = 12^{\circ}$C. At a depth of 20 m below the surface almost all annual temperature variation is ironed out and the temperature is, to a good approximation, a constant 11°C (which is higher than the mean surface temperature of 10°C---temperature increases with depth, due to heating from the hot core of the planet). The thermal diffusivity of the Earth's crust varies somewhat from place to place, but for our purposes we will treat it as constant with value $D = 0.1\,\mathrm{m}^2\,\mathrm{day}^{-1}$.

a) Write the corresponding heat equation and the boundary conditions described the temperature field $T(x,t)$ as function of depth x and time t.

b) Write a program to calculate the temperature profile of the crust as a function of depth up to 20 m and time up to 10 years. Start with temperature everywhere equal to 10°C, except at the surface and the deepest point, choose values for the number of grid points and the time-step h, then run your program for the first nine simulated years, to allow it to settle down into whatever pattern it reaches.

c) For the tenth and final year plot four temperature profiles taken at 3-month intervals on a single graph to illustrate how the temperature changes as a function of depth and time.

Problem 4.2: One-dimensional Ising model in magnetic field (6 points)

One-dimensional Ising model corresponds to a linear chain of N spins s_i.

If the system is placed in external magnetic field h, its energy for a given spin configuration s_i reads

$$E = -J \sum_{i=1}^{N} s_i s_{i+1} - h \sum_{i=1}^{N} s_i,$$

where, by convention, $s_{N+1} = s_1$ to enforce periodic boundary conditions.

Unlike the 2D-Ising model, this system does not exhibit a phase transition.

Analytic solution exists in the large N limit ($N \to \infty$). The average magnetization reads

$$m = \frac{M}{N} = \frac{\sum_{i=1}^{N} s_i}{N} = \frac{\sinh(h/T)}{\sqrt{[\sinh(h/T)]^2 + e^{-4J/T}}}$$

a) Write a program to simulate this system using the Metropolis algorithm for the following values of parameters,

$$J = 1, \qquad T = 1, \qquad h = 0.1,$$

and different values of N. By studying the system equilibration and comparing to the analytic solution, determine the value of N such that the average magnetization m from the Monte Carlo simulation (once equilibrium is reached) is within few percent from the $N \to \infty$ analytic solution.

b) Simulate the system for different values of magnetic field, e.g.

$$J = 1, \qquad T = 1, \qquad h = [-0.5, -0.2, -0.1, 0, 0.1, 0.2, 0.5],$$

and the sufficiently large value of N that you determined previously. Plot the results for m as a function of step number (*Hint: you may want to plot the solution after every N Metropolis steps rather than every single step*) and compare to the analytic solution.