Scientifc Computing. Fall 2010

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Assignment 4. Due: Nov. 27, 2010.
Each problem is of equal value.

Problem 1. Show that the Metropolis transition rate satisfies the detailed balance condition.

Problem 2. Find out examples at least 6 different applications of Monte Carlo – preferably from different fields in science and engineering. Give a detailed explanation of (at least) one of your examples.

Problem 3. Using simple Monte Carlo integration, estimate the the volume of a sphere of radius r. Do this by selecting points randomly in a square in range $([-r, r], [-r, r])$. Use $z = \sqrt{r^2 - (x^2 + y^2)}$. You need a random number generator and to write a program to do this. Use 10, 100, 1000, 10000, 100000 and 1000000 points and compare the results to the exact answer.

Problem 4. Let us compare direct numerical integration and MC integration. For MC: use the approach as in the above problem, and compute the volume of a "sphere"in 2-10 dimensions. For MC, do this using 100,000 samples. Next, compute the same volumes using direct numerical integration (e.g. the midpoint method or comparable). In both cases, record the times needed for calculation. When presenting results, make a table using the following format:

dim.	exact value	MC result	MC time	integration result	time

What can you say about the speeds of the methods as a function of dimension?

Problem 5. Write a Monte Carlo code for simulated annealing of the travelling salesman problem for 42 cities located randomly in 2-dimensions.

Problem 6. Use your MD program (Lennard-Jones particles) as a starting and modify it so that it uses Metropolis Monte Carlo. Notice: instead of forces, you have to use energies. Tune the program so that it reaches about 50% acceptance ratio. Use the same densities as in the MD problems, plot the time development of the total energy and 3-5 snapshots of the system during the simulation.