

AMS 321: Computer Projects in Applied Mathematics

Project 6

Assignment Date: Friday (11/06/2009)

Collection Date: Friday (12/11/2009) 5PM

Grade: See Individual Problems

This project is optional. Doing it or ignoring it should have no direct effect on most students. In rare occasions, I may lift the letter grade a little (for example, D to C- or C+ to B- or B+ to A-). If your schedule won't allow you to complete this project, please ignore it as the course load is already rather heavy for this semester. But if you do decide to submit, you must do it before the deadline for full consideration.

The following Problem (2) was assigned during 2008 and nobody had ever attempted it. The Problem (1) is assigned for 2009. Enjoy it.

- (1) For a system (whatever system, could be a supercomputer with N nodes or a town with N houses) with N components, each component is linked by a few line segment of varying but similar length (for example, no line should double the average length). Now, assume the time traveling from one component to another is proportional to the number of line segments it has to travel through. Find a way to connect the components ($N=100$) so that you use the smallest number of length segments to achieve shortest average distance for all components to all other components.
- (2) In physics or biology or other physical or life science areas, researchers like to use a method called molecular dynamics to study the dynamics of molecules by examining their micro movements. In this project, we consider N particles carrying charges with values uniformly randomly distributed in $[-1, 1]$ and fixed at sites that have random coordinates in a $10 \times 10 \times 10$ 3D cube. Any triplet of random numbers in $[0, 10]$ can be the coordinates of a particle. These particles interact under the Coulomb's law: $f_{ij} = q_i q_j / r_{ij}^2$ where f_{ij} is the force on particle i by

particle j whose charges are q_i and q_j and r_{ij} is the distance between these two particles.

We make the following assumptions:

- a) The mass of these particles is a constant which is normalized to "1";
- b) The components of the initial velocities of these particles follow Gaussian distribution centered at (0,0,0) with variance 4;
- c) Periodic boundary conditions in every dimension of the cube;
- d) These particles, as expected, move under the Newton's second law.

Write a program to compute the positions of these $N=1000$ particles after 100 steps with step size = 10^{-6} units.

Draw a 3D picture to show the force field of all $N=1000$ particles at the end of the 100th step.