Major Project : N-Body Knows The Problems I've Seen

Due 12/8/2011 @ 12pm (noon)

TOPICS:

↳   N-Body Problem

↳   Data Visualization

BACKGROUND:
During class, we discussed how the motions of particles could be simulated using basics laws of physics such as gravitation. The progress of particle motion based on interactions with other particles is called the "N-Body Problem".

DIRECTIONS:
Using the CPU-based code that I provide as your guide, you will design and implement a CUDA program called NBody.cu.

The NBody program will use a single command line argument that corresponds to the number of timesteps to perform an n-body calculation. The program will then output the Cartesian coordinates of each of the n bodies in a PDB format. The CUDA program must compute the forces between the n bodies and update their positions via a kernel call.

You must check for 1) the appropriate number of command line arguments and 2) whether the command line argument corresponds to a positive number. Appropriate error messages must be issued, followed by a graceful exit.

You will then save the output of the program into a file called, "NBody.pdb", which you can load into VMD to generate a movie (see Appendix).

IMPLEMENTATION NOTES:
Any program that does not compile or does not have correctly constructed Makefiles will not be graded. The CUDA program must compile using nvcc.

COMMENTS AND STYLE:
Although there will be no formal policy on commenting and style, the reader should able to easily follow the main purpose of the code. Each set of code that does something significant must be commented. The variable names should be easily recognizable and acronyms should be avoided if possible.

Do not be surprised if help is not forthcoming if your code is poorly commented and/or difficult to follow. You have been warned.

PROJECT SUBMISSION:
The programs should be in appropriate directory named "NBody". The program must have a corresponding Makefile. The contents of the directory (+ the movie) must be archived in a tarball that is gzipped called BigOne.tar.gz. Do not submit your "NBody.pdb" file.

Place the gzipped tarball in your Drop Box on Sakai before it is due.

PLEDGED WORK POLICY:
Assignments in Computer Science courses may be specified as "pledged work" assignments by the professor of the course. When an assignment is specified as "pledged work" the only aid that the student may seek is from either the course professor or an assistant that the professor has explicitly specified. On "pledged work" assignments the student may not use the services of a tutor.

For this project, you may discuss only basic CUDA syntax with others. Any other discussions of the project are strictly prohibited except with the professor of the course. Your code and your implementation of the project must be the product of your own work.

APPENDIX:

## Visualizing MD Trajectories on VMD

Note: You are strongly encouraged to work together. However, each person is responsible for producing and submitting their own work.

Website References:

1. VMD Homepage: http://www.ks.uiuc.edu/Research/vmd/
2. VMD Tutorial: http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/index.html
3. Movie Making Tutorial: http://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/node3.html

Instructions:

1. **Start VMD:** Go to the Start Menu, All Programs, _WFU Academic Tools, Scientific Tools, VMD 1.8.7.
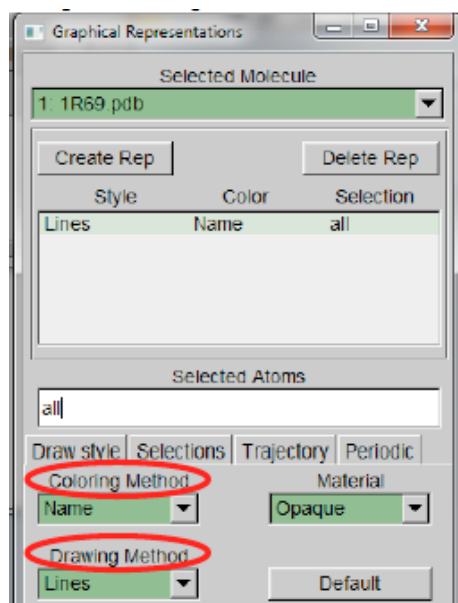
2. **Load PDB file:** File, New Molecule...,
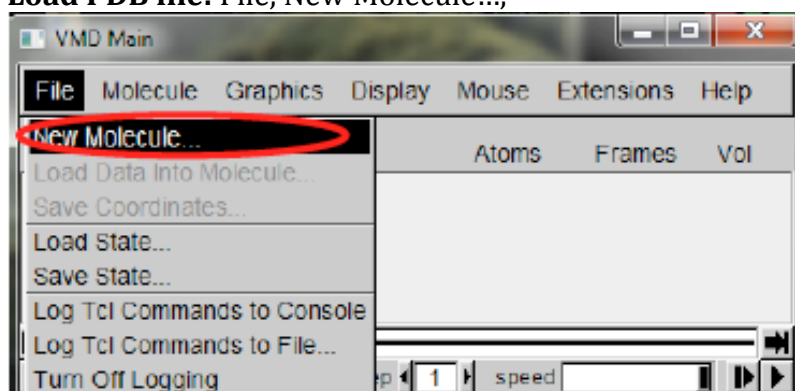
Filename: [insert file name] (or use "Browse..."),Load.
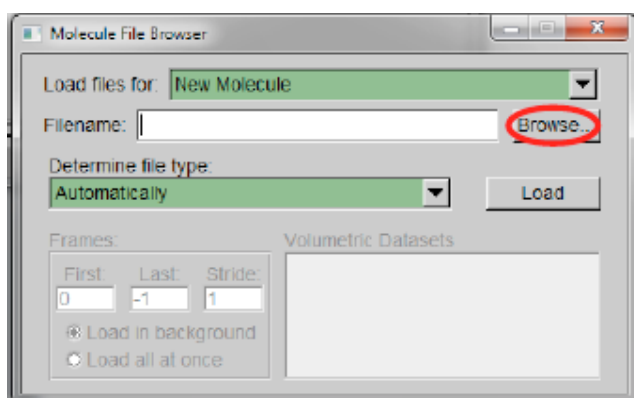
3. Using the instruction manual at the VMD website, learn to manipulate the structure. In particular, focus on rotation, translation, and zooming.
4. **Change the representation of the PDB structure:** Graphics, Representations...,
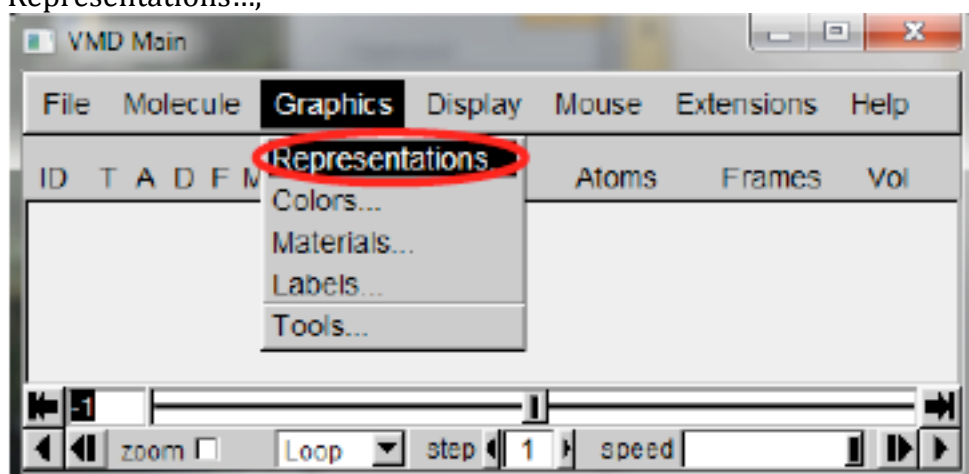
Drawing Method. Also, look at Coloring Method.

5. You can save a movie using the Movie Maker extension.