

Final project assignment 1.978

The project is due on February 5, 2007. You may submit electronically or drop it of at my office.

The final project includes molecular studies of three different systems, including (i) a nanowire, (ii) fracture of a single crystal of silicon and (iii) deformation and unfolding of a protein. All three examples serve the purpose of becoming more acquainted with MD, including setting up problems, analysis methods and interpretation of results.

The three problems represent broad application areas of MD in various areas of engineering and science. Typically, MD codes are implemented in Linux or Unix computing environments and require creation of specific input files, parameter selections and preprocessing steps. To make it easier for students and in order to improve the learning experience, here we use a web interface that provides a consistent interface to all three applications without having to learn the particularities of each individual code.

The problems all have open ended character, so I don't expect a unique answer. Try to be creative and play with this new tool. Articles and background material will be posted for each problem set. Try to read the articles, and you will understand much better what you are actually modeling.

In the beginning of each part of the problem set, we will explain the most important parameters. The simulations you will carry out can each take up to 8 hours, with a rough total estimate of 40 hours computing time necessary to complete the entire project. So please start early, as only 14 computers are available on the remote cluster your code will run on, and you share these resources with all others in the class.

The web interface is developed in collaboration with Ivica Ceraj from IS&T. This will make it easier for us to reply to requests. When we answer to any questions, all of you can take advantage of it.

You are welcome to work in groups, but I expect everyone to hand in their own problem set solution.

For now, good luck, and have fun!

Website for simulation codes: <http://starapp.mit.edu:8083/gp/index.jsp>

Note: Please provide a clear write-up with graphs and captions that clearly describe your observations. Provide intermediate steps when you do derivations – they should be done clearly.