Course: MAE 496 Senior Thesis or MAE 495 Independent Study

Proposed Topic #3: **Molecular Dynamic Simulation**

Advisor: Ever Barbero
Term: Spring 2011
Standing: Senior AE/ME/MSE or equivalent
Pre/co-requisites: Proficiency in Fortran
Knowledge of materials science or engineering or metallurgy or equivalent

I am looking for a senior undergraduate student that wants to do MAE 495 (independent study) or MAE 496 (senior thesis) or a Senior Thesis for an approved external/foreign program. The project consists of developing a (basic) modular/parallel Fortran code for Molecular Dynamics Simulation and associated documentation. The student will have to study, ahead of time, the fundamentals of Molecular Dynamics Simulation in [1] and be proficient in Fortran 95.

The input/output must interface with existing model preparation and post-processing codes available at WVU. The code must be object oriented, so that modules such as the potential can be later substituted easily. The overall tasks must be broken down into clearly meaningful procedures. A top-level flowchart of major modules/tasks/objects and their interaction will be provided to the student as a guideline. The code must be written with parallelization in mind (Beowulf cluster available).

The expected deliverables are:

a) Object oriented Fortran code implementing MD and the Lennard-Jones potential [2], but ready for easy inclusion of different, n-body potentials.

b) A report demonstrating the use of the code to solve a specific problem: viscosity of a liquid using the Lennard-Jones potential [3—section VI] or similar problem.

The student should be aware that a lot of software exists (e.g., [4]) that can be used directly (with appropriate permission), or to learn from, but that we need complete understanding of the code delivered at the conclusion of this project.

The student will be mentored by Prof. Barbero plus two Ph.D. students near completion of their degrees in this same topic.

[1] Computer Simulation of Liquids, M. P. Allen & D. J. Tildesley,
ISBN: 978-0-19-855645-9
http://www.amazon.com/reader/0198556454?_encoding=UTF8&ref_=sib_dp_pt#reader-link
P.S. Here is a WEB SITE to DOWNLOAD THIS BOOK:
http://rs46.rapidshare.com/files/268493047/Computer_simulation_of_liquids_1991_-_Allen___Tildesley.djvu
[2] http://en.wikipedia.org/wiki/Lennard-Jones_potential

[3] Hess, B., Determining the shear viscosity of model liquids from molecular dynamics simulations, journal of chemical physics volume 116, number 1, January 2002, pp. 209—217.
[4] http://www.ccp5.ac.uk/librar.shtml