SIMULATION COURSE FYSM350 / MOLECULAR DYNAMICS PART
23.3. – 20.4.2006

GENERAL INFO

CONTENT

7 lectures, student project and related numerical exercises. The task of the student project is to build a working molecular dynamics simulation program that can simulate a simple atomic system where interactions are described via a pair potential (Lennard-Jones). This program will be used to study thermal and dynamical properties of solid and liquid phase, melting transition, etc. The student projects will be presented (10 min) during lecture Thursday April 20. The project work can be done in groups of 2 students. The selection of the programming language is free (C, Fortran, Matlab). However example algorithms and pieces of codes shown in lectures will be mainly in Fortran 77/90.

Thursday 23.3. Lecture 1.

- **Fundamentals of molecular dynamic simulation, Hamiltonian dynamics, phase-space trajectories, dynamical systems, observables as trajectory averages, conservation principles, boundary conditions**
- **Introduction to the student project, general structure of a "good" MD code, programming hints. Workgroups (2 students in each) formed.**

Tuesday 28.3. Lecture 2.

- **Finite difference methods, prototypical Euler's method, errors and stability analysis, MD algorithms**
- **Project: programming the velocity-Verlet integrator, exercise: visualizing phase-space trajectories of modified 1D harmonic oscillators**

Thursday 30.3. Lecture 3.

- **Interaction models for atomic systems**
- **Project: programming the Lennard-Jones potential**

Tuesday 4.4. Lecture 4.

- **Simulations under various thermodynamic conditions (NVE, NVT, NPT,…)**
- **Project: testing the code**

Thursday 6.4. Lecture 5.

- **Analysis of simulations, static and dynamic observables, reliability analysis**

- **Project: static and dynamic correlation functions, analysis of atomic motion (vibrations, phonon spectra, diffusion),**

Tuesday 11.4. Lecture 6.

- **Introduction to quantum molecular dynamics**

Easter break

Thursday 20.4. Lecture 7.

- **Presentation of student projects. NOTE: it is absolutely necessary to start working on the project from the first week, 4 weeks is a short time! In an ideal case the development of the code should follow the "break points" discussed in the lectures above. If required, additional "workshop time" (where I am available to answer questions and give extra hints) can be arranged in the student PC room (Physics 3rd floor)**

PASSING THIS PART OF FYSM350

- **Presentation of the project work April 20.**
- **Documentation of the learning process in the "learning diary". Note that every student is required to update and return his/her individual "learning diary" although the project workload can be shared with another student. Solution to given exercises should also be documented in the "learning diary".**

OBJECTIVE OF THIS MODULE: to learn by doing hands-on simulations.

LITERATURE (books are available in student room Physics 2nd floor)

- **D.C. Rapaport: The art of molecular dynamics simulation (Cambridge University Press). This book has examples in C, many of them connected to simulating dynamics of particle flow.**
- **J.M. Haile: Molecular dynamics simulation, Elementary methods (Wiley). Example codes in Fortran. An excellent book about basics.**
- **M.P. Allen and D.J. Tildesley: Computer simulation of liquids (Oxford) Examples in Fortran. A good pedagogical book.**
- **Web material: lectures by K. Nordlund and Co. in Helsinki University: http://beam.helsinki.fi/~knordlun/atomistiset/**
- **Web: http://www.fz-juelich.de/nic-series/volume23/ (Introduction to MD by Allen)**
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