Brief description of the course on

"Numerical Modeling and Simulation in Condensed Matter (NMS)" at the School of Nano Science, IPM 2020-2021

Lecturer: Jalal Sarabadani

Description:

CFirst we learn how some simple experiments can be modeled in computer. Then a short review on how differential equations are numerically solved is presented. After that, different ensembles such as NVE, NVT, NPT and \muVT are shortly reviewed, and coarse grain molecular dynamics (MD) simulation is introduced. Using the above knowledge we will learn how some quantities (coming from stat. phys.) are calculated for quite a few examples. Finally, we will focus on Monte Carlo simulation. Moreover, to perform MD simulations we learn how to install and use LAMMPS (a software package), and for visualization we will use visual molecular dynamics (VMD) package, and to present the results xmgrace and gnuplot are employed. It is assumed that the students know at least one programming language such as C, C++ or Fortran etc. .

References:

- Understanding Molecular Simulation, by D. Frenkel and B. Smit.
- Computer Simulation of Liquids, by: M. P. Allen and D. J. Tildesley.
- LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator): https://lammps.sandia.gov/.
- Lecture notes, by: M. Ejtehadi.