TITLE: Computational methods in materials' science

LECTURER: dr Panagiotis Theodorakis
email: panos@ifpan.edu.pl

PLACE AND TIME: Institute of Physics of the Polish Academy of Sciences, Room: SALA **D**, Mondays 12:00 – 14:00 (First class is on the 6th of March 2017)

BOOK: There will be no specific book and course will be based on the notes given in the class. Supplementary literature is suggested below.

LANGUAGE: English

AIMS/OBJECTIVES OF THE MODULE: This module provides an excellent opportunity for familiarizing graduate students with classical computational methods in materials science, such as Monte Carlo and Molecular dynamics methods in different statistical ensembles, as well as various coarse-grained models and techniques:

This module aims to:

a) Provide the highest standard of training for natural sciences and engineering scientists, who will become leaders to their field, whether in academia, consultancy, research, government bodies, non-government organizations or industry and commerce, both nationally and internationally.
b) Deliver a comprehensive understanding of the interdisciplinary concepts of computational materials science with in-depth education in the more specific areas as described in the course structure
c) Attract motivated students
d) Develop new areas of teaching in response to the needs of the Institute and vocational training

The module objectives are:

a) To introduce and describe the main concepts and a range of computational methodologies to resolve problems in materials science and the ability to apply the knowledge to practical issues
b) Specialization on certain areas of soft matter and biophysics
c) Development of the ability of conducting independent research in materials science

LEARNING OUTCOMES: The module provides opportunities for graduate and postgraduate students to develop and demonstrate knowledge and understanding, qualities, skills, and other attributes in becoming professionals in the area of computational materials science with a focus on soft matter and biological physics with a number of obvious implications in different research areas.

The students will develop knowledge and understanding of

a) The current status and essential breadth of computational materials science, particularly in soft

matter and biological research areas and their interdisciplinary nature

b) The underlying principles of statistical principles enabling to develop computational and theoretical models in soft matter and biological physics, as well as in other scientific areas

c) Practical knowledge of computational research techniques

d) Management and communication skills, including problem definition, project design, decision processes, teamwork, and written reports.

TEACHING/LEARNING METHODS AND STRATEGIES:

The course is organised in twelve lectures. Each lecture will last 2 hours with a 20 minute break in between. The module will be based on blackboard teaching and will not contain any kind of laboratory demonstrations. The students are expected to acquire the main knowledge from the lectures. Throughout the students are encouraged to undertake independent reading both to supplement and consolidate what they are taught in the class and to broaden their individual knowledge and understanding of computational materials science. The lecturer will be available to answer questions of the students anytime via email communication, and will also arrange for a regular time once per week, when the students can meet with the lecturer.

CRITERIA FOR ADMISSION:

The course is open to graduate and postgraduate students within and outside IF PAN and it may be of particular interest to students of international PhD studies programme.

METHODS FOR EVALUATING AND IMPROVING THE QUALITY AND STANDARDS OF TEACHING AND LEARNING:

The course evaluation will be based on the opinion of the students. For this reason, a questionnaire will be given to the students in the end of each lecture. The evaluation of each course will be taken into account for improving the subsequent lectures.

ASSIGNMENTS:

Students are expected to prepare a presentation on a research topic at the end of the semester either in their area of research or in topics related to soft matter/biophysics.

COURSE STRUCTURE:

Lecture 1

Dynamic trajectories in phase space, probability density of a statistical ensemble, Liouville equation, ergodicity, thermodynamic equilibrium.

Lectures 2 and 3

Equilibrium statistical ensembles (e.g. mircrocanonical, canonical, etc.), Calculation of thermodynamic properties, pressure as a mean of a statistical ensemble (virial theorem), chemical potential as a mean

value of a statistical ensemble (Widom theorem).

Lecture 4

Grand-canonical ensemble for open systems (density fluctuations and other properties). Distribution functions for the characterization of structure, their connection to thermodynamic properties and scattering experiments.

Lecture 5

Molecular models, potential functions, periodic boundary conditions. Calculation of energy. Mean field approximations.

Lectures 6 and 7

Monte Carlo integration and Monte Carlo sampling. Connection to stochastic chains. Metropolis algorithm and extensions to different statistical ensembles. Advanced-sampling methods.

Lectures 8 and 9

Molecular dynamics simulations. Algorithms for integration of the equations. Molecular dynamics simulations with geometrical constraints. Molecular dynamics simulations in various statistical ensembles.

Lecture 10

Analysis of results obtained by computer simulations to calculate thermodynamic and dynamics properties of systems. Auto-correlation functions and relation to spectroscopy measurements. Calculation of transport properties.

Lecture 11

Coarse-grained models for large time and length scales. Equations of motion as functions of slow varying degrees of freedom. Elements of Brownian kinetic theory. Principles of Brownian dynamics simulations. Kinetic Monte Carlo.

Lecture 12

Discussion of various applications in soft matter and biological physics.

SUPPLEMENTARY LITERATURE:

D. Frenkel and B. Smit, *Understanding molecular simulation: From algorithms to applications*, Academic Press: New York, 2002.

M.P. Allen and D.J. Tildesley, *Computer simulations of liquids*, Clarendon Press: Oxford, 1999.

A.R. Leach, *Molecular modelling*: *Principles and applications*, Pearson-Prentice Hall: London, 2001.

P. Nielaba, M. Mareschal, G. Ciccotti, *Bridging times scales: Molecular simulations for the next decade*, Springer: Berlin, 2002.

D. Chandler, *Introduction to modern statistical mechanics*, Oxford University Press: Oxford, 1987.