Syllabus

1. Course Description
    a. Title of a Course

    Multiscale Computer Simulation

    b. Pre-requisites

    The Course is to be based on the acquisition of the following Courses:
    - General physics;
    - Mathematical analysis;
    - Probability theory and mathematical statistics;
    - Numerical methods;
    - General English.

    c. Course Type (compulsory, elective, optional)

    compulsory

    d. Abstract

    The course «Computer multiscale modelling and simulation» is aimed at the teaching students with a wide spectrum of methods, technologies and problems in the field of multiscale modelling and simulation and material properties. Different levels of theoretical description at various space and time scales are considered as well as the connections between them and computational technologies oriented on the hardware of the pre-exaflops era supercomputers.
2. Learning Objectives

    The objectives of this course are at the suding of a wide spectrum of methods, technologies and problems in the field of multiscale modelling and simulation and material properties.
3. Learning Outcomes

    The student will know:
    - the principles of the theoretical and computational description of matter at various scales.
    - the basic algorithms for application of software for numerical solution of problems at each scale.
    - the principles of bridging the gaps between the scale for solving particular problems and to have the corresponding experience.

    The student will be capable of:
    - Estimation the computational complexity of the multiscale problems and the amount of computational resources for their solution;
    - Analyzing scientific problems and physical processes, realizing in practice fundamental knowledge obtained in the course of training;
    - Adaptation new problematics, knowledge, scientific terminology and methodology, to possess the skills of independent learning;
    - Application in the given subject area statistical methods of processing experimental data, numerical methods, methods of mathematical and computational modeling of complex systems;

- Understanding meaning of the tasks appearing in the course of professional activity and employment the related physico-mathematical apparatus for description and solving the above tasks;
- Using the knowledge of physical and mathematical subjects for further learning according to the training profile;
- Practical working with modern software in the field of computer modeling of complex systems.

The student will get experience in:

- Formulation of computational tasks in studies of complex systems;
- Preparing and running computer simulations of various systems;
- Correct processing of modeling results and their comparison with available experimental and literature data;
- Theoretical analysis of real problems related to atomic-scale studies.

4. Course Plan

Section 1. *Multiscale levels of theoretical description of matter.*

Quantum manybody problem and ab initio modelling and simulation. The notion of quantum chromodynamics and qantum electrodynamics. Introduction into the methods of quantum theory of solids and quantum chemistry. Hartry- Fock method and multiconfiguration approaches. Density functional theory. Classical many body problem. Molecular dynamics method and other particle methods. Horizon of predictability and stochastic properties. Empirical models of interatomic interaction. Pair potentials. Many body potentials. Central symmetric and non-central symmetric models. Force fields of molecular systems. Methods for development of coarse-grained models for complex molecular systems.

Section *2. Principles of bridging the gaps between the scales.*

Separation of fast and slow dynamics. Integrators that distinguish slow processes. Car-Parinello method. Combining first-principles calculation of forces with classical atomic dynamics. Division of a model into quantum and classical parts (QM/MM methods). Combining atomistic and continuum description in a single model. Calculation rare events barriers. Kinetic Monte Carlo methods.

Section *3. Computational aspects of multiscale modelling and simulation.*

Supercomputers of pre-exaflops era. SIMD and MIMD parallelisation strategies for computations. Interconnect topology. Moore's law. Parallel scaling of algorithms. Ahmdal's law. Parallel efficiency in strong and weak sense. Typical features of data transfers in classical and quantum molecular dynamics algorithms. Data processing at supercomputer calculations of multiscale models. Parallel input/output. On-the-fly data analysis.

Section *4. Examples of the development and deployment of multiscale models in different fields.*

Radiation damage of solids. Fracture and movement of cracks. Molecular machines. Properties of polymer composites. Active motion on complex systems and selforganisation.

5. Reading List

a. Required

1. Rapaport, D. C. The art of molecular dynamics simulation. – Cambridge university press, 2004. – URL: https://ebookcentral.proquest.com/lib/hselibrary-ebooks/detail.action?docID=259878 – ELS: ProQuest Ebook Central – Academic Complete.

b. Optional

1. Frenkel, D. and Smit, B. Understanding molecular simulation: from algorithms to applications (Vol. 1). – Academic press, 2001. – URL: https://ebookcentral.proquest.com/lib/hselibrary-ebooks/detail.action?docID=307221 – ELS: ProQuest Ebook Central – Academic Complete.
2. Voter A.F., Montalenti F., Germann T.C., Extending the time scale in atomistic simulation of materials // Annu. Rev. Mater. Res. 2002. V.32. P.321–46. URL: https://www.annualreviews.org/doi/pdf/10.1146/annurev.matsci.32.112601.141541 - ELS: Archive of Annual Revies.

6. Grading System

Evaluations of all intermediate forms of control are exhibited by the 10-point scale. Assessment for the Control work (C), Homework (H), and Exam (E) are calculated as the percentage of successfully solved tasks by student from the total number of tasks multiplied by 10.
The knowledge assessment is made in accordance with the aggregated sum:

$$K = 0,4*A+0,6E,$$

where A is the accumulated score for intermediate controls:

$$A= 0.5* (C + H),$$

and E is the score for the final exam (on the 10-points scale). The rating is rounded up.

7. Guidelines for Knowledge Assessment

Topics of the tasks for the current control
Sample questions/tasks of the current control carried out in the form of a Colloquium (in written form):
1. Question: «The transfer of information about a model of material from the electronic structure level to the level of many atomic classical dynamics is performed using: (variants for answer) A. By parameterizing of interatomic potentials. B. By using the data about equilibrium structure. C. By calculations of the rare events barriers».
2. Question: «Radial distribution function allows: (variants for answer) A. To determine an average concentration of atoms of specific type in the system. B. To describe the short-range order. C. To determine the valence angles values».

The approximate list of questions for the final exam
- Molecular dynamics method. Models of interatomic interaction. Plastic deformation of solids as an example of multiscale modelling.
- Sorting methods at computing of interatomic forces in the molecular dynamics method.
- Development of interatomic potentials. Embedded atom method, its functions and their transformations.
- Force field models for macromolecules. Radial distribution function.
- Stochastic properties of molecular-dynamics systems. Exponential instability of trajectories. Dynamical memory time.
- The partial sum and theoretical proof of the Nose-Hoover thermostat scheme.
- Force of friction. Langevin force (and thermostat).
- Models of melting of solids. Melting of graphite.
- Radiation damage of solids. Development of the multiscale approach for description of radiation defects.
- Development of supercomputers in Russia and abroad.
- Parallel programming for systems with distributed memory. MPI standart.

8. Methods of Instruction

In the course of study the following type of teaching are used: the analysis of applied research cases from the field of computer multiscale modelling, the acquaintance with modern software and independent practice on the set of examples.

9. Special Equipment and Software Support (if required)

For successful learning of the discipline, students use the following software:

LAMMPS (lammps.sandia.gov) – molecular-dynamics software package.

VMD (http://www.ks.uiuc.edu/Research/vmd/) – software fo molecular visualisation.

Logistics of the Course

Some lectures and practical classes require media-projector. Wireless access to the Internet is obligatory. One laptop per student is required for practical exercises.