Multiscale Modeling and Supercomputer Architectures
(Master program; 2nd year, 1-2 modules, 2019/2020)

Syllabus
The course «Multiscale Modeling and Supercomputer Architectures» 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.

Learning outcomes include the following:
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.

The Course develops the following competencies:

Skill	NC/NRU-HSE Code	Descriptors – the learning outcomes (the indicators of achievement)	Teaching methods that contribute to the development of a competence
Ability to reflect (to evaluate and to process) the mastered scientific methods and activity manners.	СК-	Capable to demonstrates the understanding which physics and mathematics models should be applied at different space and time scales. Capable to understand the details of the theoretical and computational approaches deployed in the published studies on multiscale modelling and fill the gaps in cases of absence of information for building similar models.	Lectures, seminars, practical classes and self-preparatory work.
Ability to offer concepts, models, to develop and to use new methods and tools for professional activity.	СК-2	Capable to offer concepts, models, to develop and to use new methods and tools for professional activity. Capable to analyse augmented dynamical systems for building the special variants of the molecular dynamics method.	Practical classes, seminars, presentations and self-preparatory work.
Ability to master the new research methods, to change of scientific and production activities profile	СК-3	Capable of mastering the new research methods, changing of scientific and production activities profile.	Lectures, seminars, presentations, practical classes and self-preparatory work.
Ability to take administrative decisions, estimating their possible consequences and taking responsibility for them	СК-5	Capable of taking administrative decisions, estimating their possible consequences and taking responsibility for them.	Lectures, seminars, practical classes, presentations and self-preparatory work.
Ability to conduct professional and research activity in the international environment	СК-8	Capable of conducting professional and research activity in the international environment.	Preparation of reports and presentations on the seminars by means of reviewing the articles in foreign scientific journals.
Ability to define and retranslate common purposes in professional and social activity	ПК-3	Capable to define and retranslate common purposes in professional and social activity.	Seminars, presentations.
Ability to produce radically new ideas and products, has the	ПК-8	Capable to produce radically new ideas and products, has the creativity, initiative.	Seminars, presentations.

Skill	NC/NRU-HSE Code	Descriptors – the learning outcomes (the indicators of achievement)	Teaching methods that contribute to the development of a competence
creativity, initiative			
Ability to present results of a study in a research report, academic article, executive summary or in oral presentation with multi-media presentation support tools	ПК-14	Capable to present results of a study in a research report and academic article or in oral presentation.	Preparation of reports and presentations on the course topics by means of reviewing the articles in foreign scientific journals and participation in group and individual discussions during seminars, presentations.
Able to use modern technology and the managerial develop new control technology to improve the efficiency of the organization	ПК-24	Capable to use modern computational tools to simulate biomolecular systems.	Seminars, presentations.
Ability to identify the data required for solving the management and the business tasks; to carry out data collection and processing	ПК-26	Capable to identify the data required for solving the task in biomedicine; to carry out data collection and processing.	Preparation of reports and presentations on the course topics by means of reviewing the articles in foreign scientific journals and participation in group and individual discussions during seminars

The Course is one of the courses to be provided education for "Applied Mathematics" curriculum to teach master students (area of study code 01.04.02, Educational program "Mathematical methods of modeling and computer technologies").

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

Summary of discipline should be used to further the study of the following disciplines:

- Research Seminar;
- Preparation and presentation of the thesis.

Evaluation criteria for knowledge and skills:

Evaluations of all intermediate forms of control are exhibited by the 10-point scale. Assessment for the Control work, Homework, and Exam are calculated as the percentage of successfully solved tasks by student from the total number of tasks multiplied by 10.

Content of the Course:

The content of the Course is divided into sections 1-4, for each section there are lectures and workshops.

Section 1. Multiscale levels of theoretical description of matter.

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

Reading List

1. Precision Physics of Simple Atomic Systems, S.G. Karshenboim V.B. Smirnov (Eds.), Springer, 2003.
2. Lepage G.P., Lattice QCD for novices, arXiv:hep-lat/0506036v1
3. Bertsch G.F., Dean D.J., Nazarewicz W., Computing atomic nuclei, SciDAC Review, 2007.
4. Цирельсон В. Г. Квантовая химия. Молекулы, молекулярные системы и твердые тела. М.:Бином, 2014.
5. Finnis M., Interatomic Forces in Condensed Matter. Oxford Series on Materials Modelling, 2003.
6. Gibbon P., Sutmann G. Long-Range Interactions in Many-Particle Simulation. In: Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms (eds. J. Grotendorst, et al), Julich: NIC, Vol. 10, pp. 467-506, 2002.
7. Sutmann G., Classical molecular dynamics. In: Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms (eds. J. Grotendorst, et al), Julich: NIC, Vol. 10, pp. 211-254, 2002.
8. Rapaport, D. C. (2004). The art of molecular dynamics simulation. Cambridge university press.

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

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

Reading List

1. Frenkel, D. and Smit, B., 2001. Understanding molecular simulation: from algorithms to applications (Vol. 1). Academic press.
2. Leach A.R., Molecular modelling: principles and applications. Prentice Hall, 2001.
3. 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.
4. Marx D., Hutter J. Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods, Cambridge University Press, 2012.
5. Goedecker S., Scuseria G.E., Linear Scaling Electronic Structure Methods in Chemistry and Physics // Computing in Science & Engineering. 2003. V.5. P.14.
6. Becquart C.S., Wirth B.D., Kinetic Monte Carlo Simulations of Irradiation Effects, Comprehensive Nuclear Materials, (5 Volume Set), 2012.

Section 3. Computational aspects of multiscale modelling and simulation.

3.1 Supercomputers of pre-exaflops era. SIMD and MIMD parallelisation strategies for computations. Interconnect topology. Moore’s law.

3.2 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.

3.3 Data processing at supercomputer calculations of multiscale models. Parallel input/output. On-the-fly data analysis.

Reading List

1. Dongarra J. et al., Sourcebook of parallel computing, Morgan-Kaufmann, 2003.
2. Стегайлов В.В., Норман Г.Э. Проблемы развития суперкомпьютерной отрасли в России: взгляд пользователя высокопроизводительных систем // Программные системы: теория и приложения. 2014. Т. 5. № 1(19). С. 111–152. URL: http://psta.psiras.ru/read/psta2014_1_111-152.pdf

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

4.1 Radiation damage of solids.

4.2 Fracture and movement of cracks.

4.3 Molecular machines.

4.4 Properties of polymer composites.

4.5 Active motion on complex systems and selforganisation.

Reading List

1. Weinan E., Principles of Multiscale Modeling, Cambridge University Press, 2011.
2. NIC Symposium 2014 Proceedings (12 –13 February 2014, Jülich, Germany), K. Binder, G. Münster, M. Kremer (Editors), John von Neumann Institute for Computing NIC Series, 2014.
3. Куксин А.Ю., Ланкин А.В., Морозов И.В., Норман Г.Э., Орехов Н.Д., Писарев В.В., Смирнов Г.С., Стариков С.В., Стегайлов В.В., Тимофеев А.В. ЗАЧЕМ и КАКИЕ нужны суперкомпьютеры эксафлопсного класса? Предсказательное

моделирование свойств и многомасштабных процессов в материаловедении. // Программные системы: теория и приложения. 2014. Т. 5. № 1(19). С. 191–244. URL: http://psta.psiras.ru/read/psta2014_1_191-244.pdf
4. Schweitzer F., Browning Agents and Active Particles Collective Dynamics in the Natural and Social Sciences, Springer, 2003.

Educational technologies

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.

Appraisal tools for current control and student assessment

a. 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».

b. Questions to assess the quality of learning:

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.

Guidelines for Knowledge Assessment:

The knowledge assessment is made in accordance with the aggregated sum: $K = 0{,}4H+0{,}6E$, where H is the accumulated score for intermediate controls, E is the score for the final exam (on the 10-points scale). The rating is rounded up. When the final exam grade is below 4 points, the final grade for the course equals the grade for the exam. Transfer to a 5-point scale is carried out according to the rule

- $0 \le K \le 3$ – unsatisfactory (2 points),
- $4 \le K \le 5$ – satisfactory (3 points),
- $6 \le K \le 7$ – good (4 points),
- $8 \le K \le 10$ – excellent (5 points).

Educational-methodical and information support of the Course

Basic reading List

Rapaport, D. C. (2004). The art of molecular dynamics simulation. Cambridge university press.

Frenkel, D. and Smit, B., 2001. Understanding molecular simulation: from algorithms to applications (Vol. 1). Academic press.

Sutmann G., Classical molecular dynamics. In: Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms (eds. J. Grotendorst, et al), Julich: NIC, Vol. 10, pp. 211-254, 2002.

Leach A.R., Molecular modelling: principles and applications. Prentice Hall, 2001.

Dongarra J. et al., Sourcebook of parallel computing, Morgan-Kaufmann, 2003.

Weinan E., Principles of Multiscale Modeling, Cambridge University Press, 2011.

Software

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 2-3 students is required for practical exercises.