Molecular Modeling 2015

from first principles to mesoscopic simulations

Department of Biophysics, Košice

23th – 27st February

Course I Principles of molecular modeling – from *ab initio* simulations to nano objects at mesoscopic spatial scales   [c1]

Course II Development of mesoscopic models and their implementation in high-performance computing environment   [c2]

The aim of two interrelated courses is to bring state of the art knowledge in the area of multi-scale modeling of mesoscopic biological object, with an emphasis on DNA structures for the target group – students and researchers from the Pavol Jozef Safarik University. Leading researchers and experts in the field will provide international level training in the field of molecular simulation modeling in the established form of lectures on topic (mornings), followed by hands-on training (afternoons) and seminars (early evenings) from invited experts. The School will run 5 days and will cover general concepts and techniques of : first principles simulations (using Material Studio for practical exercises), molecular dynamics simulation of bio-polymers (using MD simulation package AMBER), mesoscale simulation techniques and development strategies (demonstrated using dedicated software framework MagiC), all in the context of interaction with X-ray imaging (coherent diffraction) experiments. Due to the rapid development in the area of single particle imaging, interrelations between the large-scale computing – both for particle simulations and the interpretation of scattering experiments will be also discussed, together with practical aspect of high-performance computing and related large data management. For all subjects, lecture materials comprise examples from contemporary literature and personal lecturers experience, reflecting actual state in given topics. The participants of course will gain experience of the algorithms at the nuts and bolts level of the software knowledge in high performance computing environments.

Foreign experts
Aatto Laaksonen, SU, Sweden   *aatto.laaksonen@mmk.su.se*
Alexander Lyubartsev, SU, Sweden   *alexander.lyubartsev@mmk.su.se*
Francesca Mocci, CU, Italy   *fmocci@unica.it*
Robert Harakaly, SA, Switzerland   *robert.harakaly@harakalyconsulting.eu*

Location
UPJS, Jesenná 5, Laboratory of molecular simulations and advanced visualizations

www.biophysics.sk

Time schedule :

Monday   *23.02.2015*

08:30 - 09:00 *opening of courses* [*Jozef Uličný*]
09:00 - 10:30 First principle simulations - **c1 lecture** [*Aatto Laaksonen*]
10:30 - 10:45 *coffee break*
10:45 - 12:00 Multiscale Modeling Framework - **c2 lecture** [*Aatto Laaksonen*]
12:00 - 13:00 *lunch*
13:00 - 15:00 Material Studio - **c1 workshop** [*Aatto Laaksonen*]
15:00 - 15:30 *coffee break*
15:30 - 17:00 Material Studio - **c2 workshop** [*Aatto Laaksonen*]
17:00 - 18:00 Summary, concluding remarks and discussion - **seminar**

Tuesday   *24.02.2015*

09:00 - 10:30 Molecular Dynamics - **c1 lecture** [*Francesca Mocci*]
10:30 - 10:45 *coffee break*
10:45 - 12:00 Biopolymers (DNA) - **c2 lecture** [*Francesca Mocci*]
12:00 - 13:00 *lunch*
13:00 - 15:00 Amber (atomistic aspects) - **c1 workshop** [*Francesca Mocci*]
15:00 - 15:30 *coffee break*
15:30 - 17:00 Amber (CG aspects) - **c2 workshop** [*Francesca Mocci*]
17:00 - 18:00 Summary, concluding remarks and discussion - **seminar**

Wednesday   *25.02.2015*

9:00 - 10:30 Mesoscale simulations - **c1 lecture** [*Alexander Lyubartsev*]
10:30 - 10:45 *coffee break*
10:45 - 12:00 Inverse Monte Carlo method - **c2 lecture** [*Alexander Lyubartsev*]
12:00 - 13:00 *lunch*
13:00 - 15:00 MagiC - **c2 workshop** [*Alexander Lyubartsev*]
15:00 - 15:30 *coffee break*
15:30 - 17:00 MagiC - **c2 workshop** [*Alexander Lyubartsev*]
17:00 - 18:00 Summary, concluding remarks and discussion - **seminar**

Thursday   *26.02.2015*

9:00 - 10:30 X-ray imaging experiments - **c2 lecture** [*Robert Harakaly*]
10:30 - 10:45 *coffee break*
10:45 - 12:00 High volume Data storage solutions - **c2 lecture** [*Robert Harakaly*]
12:00 - 13:00 *lunch*
13:00 - 15:00 Large data storage (CERN) - **c2 workshop** [*Robert Harakaly*]
15:00 - 15:30 *coffee break*
15:30 - 17:00 Hight performance computing - **c2 workshop** [*Robert Harakaly*]
17:00 - 18:00 Summary, concluding remarks and discussion - **seminar**

Friday   *(recent and future work,* **c1/c2***)*   *27.02.2015*

9:00 - 10:30 Challenges for multiscale modeling - interaction between the X-ray imaging experiments and simulations [*Jozef Uličný*]
10:30 - 12:00 Ionic liquids [*Aatto Laaksonen*]
12:00 - 13:00 *lunch*
13:00 - 14:30 NMR technique [*Francesca Mocc*]
14:30 - 16:00 Coarse Graining of Lipids [*Alexander Lyubartsev*]
16:00 - 17:30 Data storage and data management - Dcache [*Robert Harakaly*]
17:30 - 18:00 Concluding remarks and future work directions in light of XFEL SPB and SFX [*Jozef Uličný*]