International Workshop on Coarse-Grained Biomolecular Modeling

March 7-12 2010, Levi, Finland.

'International Workshop on Coarse-Grained Biomolecular Modeling' took place in picturesque fading winter of Levi from March 7-12, 2010. The workshop was organized by the Computational Soft Matter Research Group (Aalto University School of Science and Technology, Finland) and the CSC - Finnish IT center for Science. The course outline included basic as well as advanced applications of molecular dynamic simulations in biological areas. In molecular dynamics atoms and molecules are allowed to interact for a period of time based on by approximations of known physics and this all can be performed on computer giving a view of the motion of the particles.

The purpose of the workshop was to introduce the participants to different state-of-the-art methods in CG modeling of biomolecular systems. The course was lectured by the experts and innovators of the biomolecular simulation field including Prof. Siewert J Marrink and Alex de Vries University of Groningen, the Netherlands, Prof Markus Deserno Carnegie Mellon University, USA, Ilpo Vattulainen Tampere University of Technology, Finland, Will Noid Penn State University, USA Luca Monticelli INSERM, France etc. The workshop kicked off with a nice lecture 'Coarse Graining Basics' by Alex de Vries emphasizing basic concepts of computer simulations. Marrink explained the features of newly developed coarse grained MARTINI force field for molecular dynamics package GROMACS in determination of structural and functional properties of biomacromolecules like lipids, proteins and including sugars. Deserno group highlighted the concept of implicit water using molecular dynamics package 'Espresso' in studying vesicular fusion or budding. There were also other stimulating talks on the application of CG simulation in biological areas. All the methodologies targeted faster simulation by reducing computational power as well as time but still collect more information per simulation run. Lectures were followed by hands on experiments with full technical and scientific assistance to all its participants. Practical sessions on the featured CG methods provided the participants with hands-on experience on their application. In addition to exercises provided by the lecturers of the workshop, the participants were encouraged to work on their own systems of interest in the practical sessions. The course was an excellent learning experience for me.

The course selected 50 young researchers including PhD students and post docs from many countries. Generally CSC organizes this workshop after every one or two years (keep an eye on CSC website). I would recommend this course to researchers who want to have a basic knowledge of molecular dynamic simulation as well as for researchers and industrial scientists who wants to gain advanced knowledge of application of molecular simulation.

I gratefully acknowledge Åbo Akademi University and ISB for supporting my participation at this course.

Shishir Jaikishan
Department of Biochemistry and Pharmacy
Åbo Akademi University, Turku