INTERNATIONAL SUMMER SCHOOL:
UNDERSTANDING MOLECULAR SIMULATION

Institute of Physics, Chinese Academy of Sciences, Beijing

July 29 – August 5 2018

Organizers:
Daan Frenkel (University of Cambridge, UK)
Ignacio Pagonabarraga (CECAM, Switzerland)
Jure Dobnikar (Institute of Physics, CAS, Beijing)

School secretary:
Xie Zhaoping (Institute of Physics, CAS, Beijing)

This is a week-long school that offers a program focusing on numerical techniques for the study of properties of many-particle systems. It targets PhD and postdoctoral researchers who want to learn these techniques to study topics in physics, chemistry or biology. The course may also be followed by advanced BSc or MSc students. It offers a recap of the statistical mechanics relevant for molecular simulation and addresses basic and advanced simulation techniques including Monte Carlo, molecular dynamics, free energy calculations, rare events and coarse graining without discussing particular software packages.

The school consists of an integrated program of lectures and hands-on exercises. The book ``Understanding Molecular Simulation'' by Frenkel and Smit will provide the basis of the lectures. This will be supplemented by exercise handouts and copies of the lecture slides. A poster session will provide the participants an opportunity to present their research in an informal setting.

There will be two special additional topics, one on machine learning and its applications in condensed matter and biological physics and the second one on mesoscopic modelling of the colloidal interactions and the fluid flow.

The school will provide shared accommodation close to the venue for the participants. There is no registration fee. In order to participate, or if you require further information, please send an email to Xie Zhaoping at zpxie@iphy.ac.cn. Including your CV, background, a brief description of why you want to attend and what do you expect from the school. Please mention your programming experience, research interests, and whether you plan to bring your own laptop with you. We will inform the participants about their acceptance by the end of June.

SCHOOL SCHEDULE

The exercises will be done in Python programming language. We will distribute material needed to learn Python before the school and will have an introductory session on technical aspects of programming in Python.

Date	Activity	Lecturer
Sunday July 29th	Arrival Preparatory session: Programming in Python	James Farrell **(IoP CAS)**
Monday July 30th	Introduction Statistical Thermodynamics; Monte Carlo & Molecular Dynamics Basic Techniques & Ensembles	*Daan Frenkel* **(U. Cambridge)**
Tuesday July 31st	Free Energy and Phase Equilibria Coding Intro (Python, Compiling, Running)	*Daan Frenkel* **(U. Cambridge)**
Wednesday August 1st	Advanced MC: Gibbs Ensemble, Biased Sampling Methods, Lattice Models	*Daan Frenkel* **(U. Cambridge)**
Thursday August 2nd	Advanced MD: Constraints, Rare events Coding: g(r), correlations	*Erik Luijten* **(Northwestern U.)**
Friday August 3rd	Modelling long range interactions: electrostatics Mesoscopic modelling of fluid flow	*Erik Luijten* **(Northwestern U.)** *Ignacio Pagonabarraga* **(CECAM)** *Mincheng Yang* **(IoP CAS)**
Saturday August 4th	Machine learning / Exercise class: big data set, extract correlations; train simple neuron net	*Alpha Lee* **(U. Cambridge)**
Sunday August 5th	SOCIAL PROGRAM / DEPARTURE	