

Workshop on Computational Modelling of Proteins

from ab-initio to coarse-grain methods

27 - 29 January 2010, School of Physics, University of Sydney

A three day workshop is organised to provide a hands-on introduction to modern computational methods used in modelling of proteins. Lectures in the mornings will be followed by practicals in the afternoons using the facilities of the computer lab at the School of Physics.

Workshop program:

January 27:	Computational approaches to protein structure determination (Ugur Sezerman)
8:30 - 9:00	Registration
9:00 - 10:30	Introduction to protein folding problem and lattice models
10:30 - 11:00	Tea break
11:00 - 12:30	Heuristic approaches to protein structure prediction: Homology modelling and threading
12:30 - 14:00	Lunch
14:00 - 17:30	Practicals in the computer lab
January 28:	Molecular dynamics (MD) simulations of proteins (Serdar Kuyucak)
9:00 - 10:30	Fundamentals of MD simulations and analysis of trajectory data
10:30 - 11:00	Tea break
11:00 - 12:30	Structure-function relations in proteins from MD simulations
12:30 - 14:00	Lunch
14:00 - 17:30	Practicals in the computer lab
January 29:	Ab initio approaches to protein modelling (Denis Bucher)
9:00 - 10:30	Basics of density functional theory and ab initio MD simulations
10:30 - 11:00	Tea break
11:00 - 12:30	QM/MM and free energy methods; applications to proteins
12:30 - 14:00	Lunch
14:00 - 17:30	Practicals in the computer lab

The lab sessions will be supervised by the lecturer of the session and the members of the Computational Biophysics Group: Alexandra De Castro, Poker Chen, Jeff Timko and Harun Rashid. If you would like to work with a specific protein during the lab sessions, please let us know in advance and we will try to cater to your needs.

There will be a \$50 registration fee to cover the costs of tea and lunches.

For inter-state participants, on-campus accommodation can be arranged if requested.

If you would like to attend, please register before Jan. 15, 2010 by sending an email to Serdar Kuyucak at serdar@physics.usyd.edu.au. Due to limited lab space, early registration is recommended.