SASSIE training course, Mohali, India. 18-19 September 2017

Course description

SAXS and SANS are highly effective experimental techniques for investigating a broad range of soft matter science. The primary bottleneck in the interpretation of the experimental data is that it requires the use of as much a priori knowledge about the system as possible. The experimental X-ray and neutron data need to be interpreted using atomic-level models. This will replace the relatively crude shape models used up to now, which are based on rather simplistic overall shapes. It is only by doing this atomistic modelling that the real significance of the experimental data becomes clear. Work to develop such a package called SASSIE has been made possible by the CCP-SAS project (Collaborative Computational Project for Small Angle Scattering). This is funded by the EPSRC in the UK and the NSF in the USA (www.ccpsas.org). Our open source software was released into the public domain in 2016, and easily accessible through a web interface. This package is being distributed to other centres outside the USA and UK.

SASSIE is a high-throughput, and user-friendly suite of software for the advanced atomistic and coarse-grained molecular modelling of SAXS and SANS data starting from physically accurate molecular structures. "SASSIE-Web" provides an online workflow framework into which modules are plugged to prepare structures, carry out simulations, calculate theoretical SAXS and SANS data and compare the outcome to experimental data. This provides a major step forward towards interpreting the experimental data down to atomistic level.

We are offering a two-day training course in Mohali on 18th/19th September 2017 that is suitable for PhD students, academics and scientists who want to interpret their small angle x-ray and neutron scattering (SAXS and SANS) data of soft matter polymer systems in order to obtain structural information down to the atomistic level.

In this training course, participants will get hands-on experience of using SASSIE-Web. They will perform molecular simulations of model polymer systems, calculate theoretical scattering curves for them and infer the best-fit atomistic structures with respect to the experimental data. There will also be opportunity to discuss participants' own polymeric systems (biological molecules) in order to help them set up for SASSIE-Web analysis.

Host: Dr Santanu Pal, Department of Chemical Sciences, IISER Mohali.
Venue: E-class Room, IISER Mohali
Trainers: Prof Stephen J. Perkins (UCL) and Dr Jayesh S. Bhatt (UCL)
CCP-SAS Website: http://www.ccpsas.org/

Schedule

Day 1 – 18th September

Time	Lead	Activity
09:30 – 10:10	JSB	Introduction to Molecular Dynamics & Monte Carlo.
10:10 – 10:50	SJP	SASSIE-web: Basic Usage.
10:50 – 11:20	**Tea/Coffee break**	
11:20 – 12:30	JSB, SJP	Lab 1: Introduction to VMD and NAMD. Running and visualising molecular dynamics simulation.
12:30 – 13:30	**Lunch**	
13:30 – 16:00	JSB, SJP	Lab 2: Use of SASSIE-web to analyse neutron scattering data of HIV-1 Gag protein. Involves Monte Carlo simulation.

Day 2 – 19th September

Time	Lead	Activity
09:30 – 11:00	JSB, SJP	Lab 3: ssRNA through SASSIE-web.
11:00 – 11:30	**Tea/Coffee break**	
11:30 – 13:00	JSB, SJP	Lab 4: Torsional Angle Monte Carlo.
13:00 – 14:00	**Lunch**	
14:00 – 16:00	JSB, SJP	Retreat session: Help with trainees' own projects.

JSB: Dr. Jayesh S. Bhatt (UCL)
SJP: Prof. Stephen J. Perkins (UCL)

A review of SASSIE and CCP-SAS is available to download from http://www.ccpsas.org/

Perkins, S. J., Wright, D. W., Zhang, H., Brookes, E. H., Chen, J., Irving, T. C., Krueger, S., Barlow, D. J., Edler, K. J., Scott, D. J., Terrill, N. J., King, S. M., Butler, P. D. & Curtis, J. E. (2016) Atomistic modelling of scattering data in the Collaborative Computational Project for Small Angle Scattering (CCP-SAS). *J. Appl. Crystall.* **49**, 1861-1875. DOI: 10.1107/S16005767160151X. Pubmed 27980506