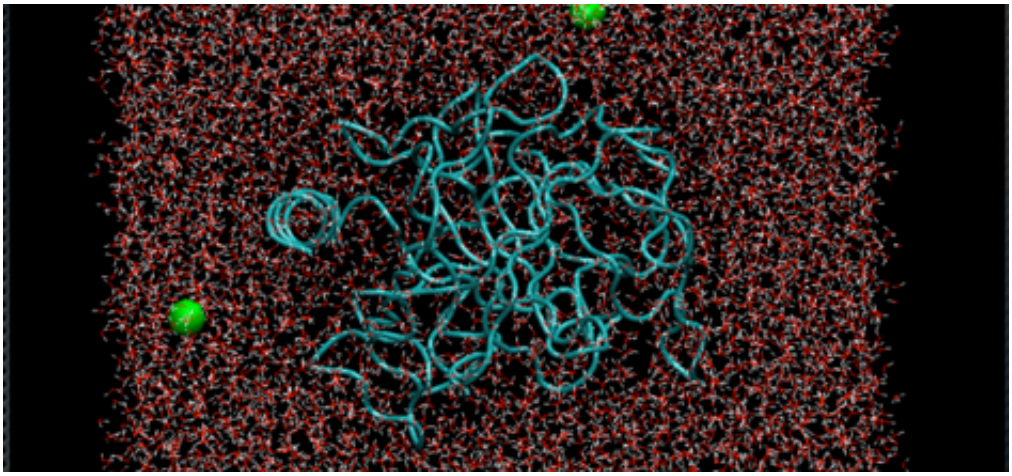
CCP-SAS 2015



Atomistic Modeling for Small-Angle Scattering ‹ A Short Course

May 26-28, 2015

Institut Laue-Langevin, Grenoble, France

Molecular simulation is an important technique to analyze and interpret molecular phenomena across many disciplines. Small-angle scattering (SAS) utilizing either X-ray or neutron sources is a valuable method to characterize shape, interactions, and properties of many soft-matter systems. Modeling of SAS data is typically done using analytical functions and/or dummy-ball (DB) models. While these methods are simple, they have proven to be quite robust and have allowed for a tremendous expansion of SAS studies to a wide variety of systems. Atomistic modeling can be used to interpret SAS data and inherently provides structural and physical knowledge that are unavailable using analytical or DB models. In additional, atomistic models can allow the use of experimental and computational constraints on the SAS data.

The goal of this three day introductory course is to use modern simulation methods and software tools to predict and analyze small-angle scattering data of soft-matter systems, focussing particularly on biological systems. Participants will be familiarized with SASSIE, a software framework designed to facility the use of atomistic modeling to interpret scattering data. SASSIE-web, a product of the CCP-SAS consortium, will be the

primary tool used during the course and will be freely available to the community after the course.

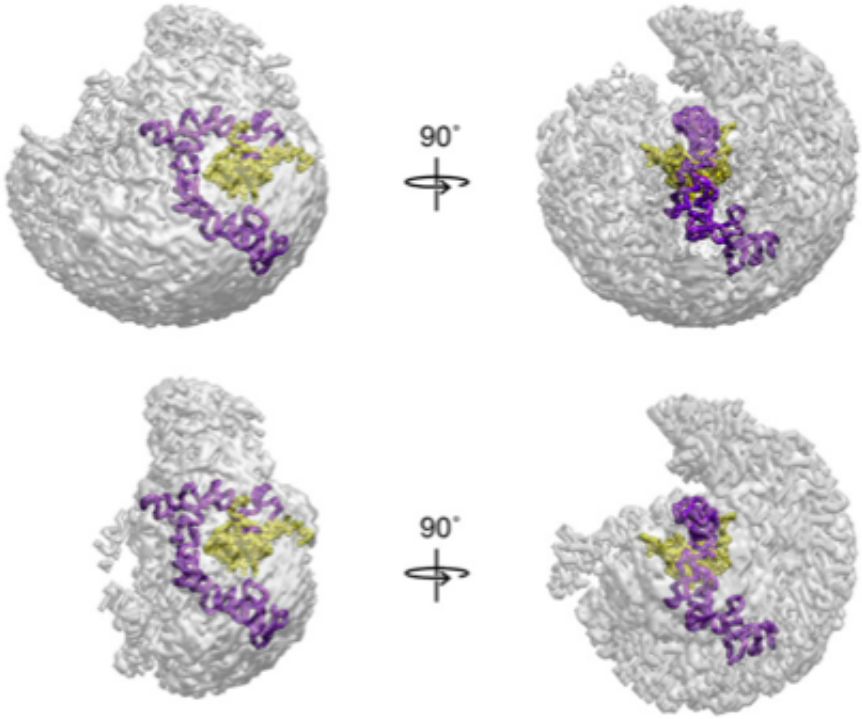
The course will involve a mixture of lectures and examples with student lessons. Examples will involve various protein, dna, and their complexes. The emphasis will be on structure building, ensemble molecular simulation, calculation of scattering profiles and comparison to experimental data.

Day 1: Introduction to molecular modeling using force-fields and SASSIE

Day 2: Intermediate MD, SASSIE and student projects.

Day 3: Advanced SASSIE and student projects.

Students are encouraged to contact the course organizers in advance to discuss their systems as a portion of the course will involve helping students set-up and model their project.



NOTE: Files to carry out the labs are no longer available below. Please see more recent courses for updated labs and files.

Tuesday 5/26/2015

Time	Lead	Activity	File
9:00 - 9:30 AM	JEC	Course Introduction	lecture_0.pdf
9:30 - 10:30 AM	JEC	Lecture 1: Coordinates to Structure	lecture_1.pdf
10:30 - 10:45 AM		**Break**	
10:45 - Noon	DWW/JEC/EHB	Lab 0: Software Installation & SASSIE-web	lab_0.pdf
Noon - 1:00 PM		**Lunch**	
1:00 - 2:45 PM	DWW/HZ/EHB	Lab I: VMD and PDB Scan	lab_I.pdf
2:45 - 3:00 PM		**Break**	
3:00 - 5:00 PM	DWW/HZ/EHB	Lab II: PSFGEN/NAMD	lab_II.pdf

Wednesday 5/27/2015

Time	Lead	Activity	File
9:00 - 10:00 AM	JEC	Lecture 2: MD II	lecture_2.pdf
10:00 - 10:15 AM		**Break**	
10:15 - Noon	DWW/HZ/EHB	Lab III: NAMD	lab_III.pdf
Noon - 1:00 PM		**Lunch**	
1:00 - 1:30 PM	JEC	Lecture 3: MMC & SASSIE Overview	lecture_3.pdf
1:30 - 3:00 PM	DWW/HZ/EHB	Lab IV: SASSIE-web Quick Start	lab_IV.pdf
3:00 - 3:15 PM		**Break**	
3:00 - 4:00 PM	DWW/HZ/EHB	Lab V: SASSIE-web Analysis	lab_V.pdf
4:00 - 5:00 PM	ALL	Breakout sessions for student projects	-

Thursday 5/28/2015

Time	Lead	Activity	File
9:00 - 10:15 AM	DWW/HZ	Lab VI: Advanced SASSIE-web	lab_VI.pdf
10:15 - 10:30 AM		**Break**	
10:30 - 10:45 AM	JEC	Lecture 4: Advanced Building	lecture_4.pdf
10:30 - Noon	DWW	Lab VII: Advanced Building	lab_VII.pdf
Noon - 1:00 PM		**Lunch**	
1:00 - 2:45 PM	ALL	Lab VIII: Breakout sessions for student projects	-
2:45 - 3:00 PM		**Break**	
3:00 - 5:00 PM	ALL	Lab IX: Breakout sessions for student projects	-

SASSIE-web: Quick Start

How to Use Visual Molecular Dynamics (VMD)

Build

PDB Scan

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