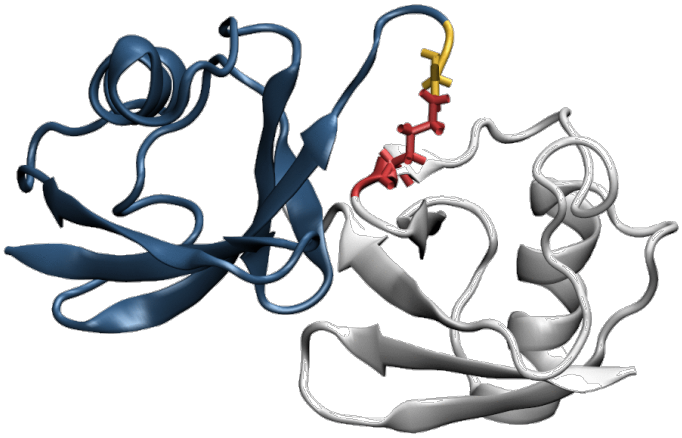
UK 2017

SASSIE CCP-SAS Workshop

January 23-25, 2017



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 atomic interactions that are unavailable using analytical or DB models. In addition, atomistic models can allow the use of experimental and computational constraints on the SAS data. The goal of this introductory course is to use modern simulation methods and software tools to predict and analyze small-angle scattering data of soft-matter systems, focusing particularly on biological systems. Participants will be introduced to modern simulation tools such as VMD and NAMD.

The bulk of the course will introduce SASSIE, a software framework designed to facilitate the use of atomistic modeling to interpret scattering data.

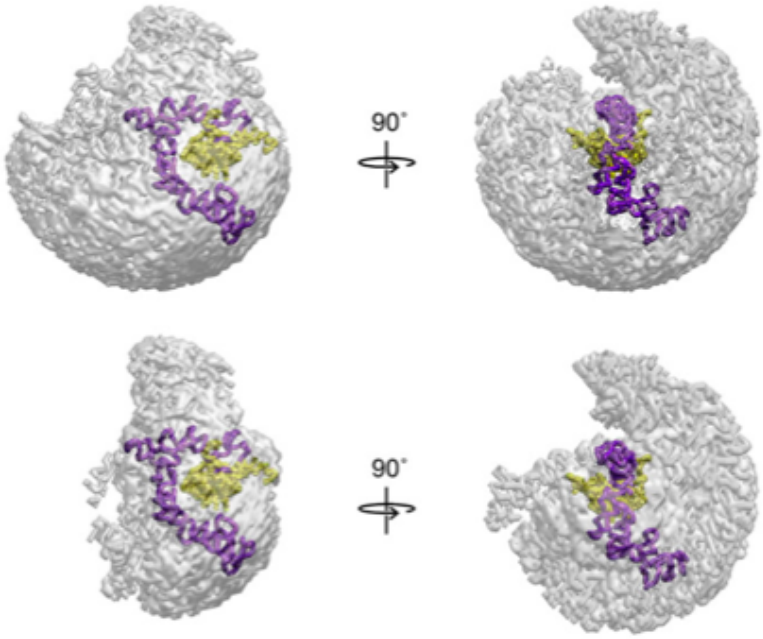
The course will involve a mixture of lectures and examples with student lessons. Examples will involve various protein and DNA molecules, as well as their complexes. Advanced simulation methods for glycosylated proteins, lipidic systems, and coarse-grain methods can be accommodated depending on demand. 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.

Day 2: SASSIE.

Day 3: Advanced building examples 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 initial models for their own projects.



Monday 1/23/2017

Time	Lead	Activity	File
Noon - 12:15 PM	SJP	Course Welcome	
12:15 - 12:30 PM	JEC	Course Introduction	lecture_0.pdf
12:30 - 1:30 PM	JEC	Lecture 1: Coordinates to Structure	lecture_1.pdf
1:30 - 1:45 PM		**Break**	
1:45 - 2:30 PM	JB	Lab I: VMD	lab_I.pdf
2:30 - 4:30 PM	JB	Lab II: PSFGEN/NAMD	lab_II_windows.pdf
4:30 - 5:30 PM	JEC	Lecture 2: MD	lecture_2.pdf
5:30 - 7:30 PM	DWW	Lab III: NAMD	lab_III_windows.pdf

Files needed for day 1: uk_2017_day_1_files.zip

Answers for labs on day 1: uk_2017_day_1_answers.zip

Tuesday 1/24/2017

Time	Lead	Activity	File
9:00 - 9:30 AM	JEC	Lecture 3: MMC & SASSIE Overview	lecture_3.pdf
9:30 - 10:00 AM	GKH/SJP	Lab IV: SASSIE-web Basics	lab_IV.pdf
10:00 - 10:15 AM		**Break**	
10:15 - Noon	DWW	Lab V: SASSIE-web Quick Start	lab_V.pdf
Noon - 1:00 PM		**Lunch**	
1:00 - 2:45 PM	SB	Lab VI: SASSIE-web Workflows	lab_VI.pdf
2:45- 3:00 PM		**Break**	
3:00 - 3:15 PM	SB	Lecture 4: Advanced SASSIE-web	lecture_4.pdf
3:15 - 6:00 PM	SB	Lab VII: Advanced SASSIE-web	lab_VII.pdf
6:00 - 7:30 PM	ALL	Extra time	

Files needed for day 2: uk_2017_day_2_files.zip

Answers for labs on day 2: uk_2017_day_2_answers.zip

Wednesday 1/25/2017

Time	Lead	Activity	File
9:00 - 9:20 AM	JEC	Lecture 5: Advanced Structure Building	lecture_5.pdf
9:20 - 10:00 AM	SB	Lab VIII: Advanced Structure Building	lab_VIII_windows.pdf
10:00 - 10:15 AM		**Break**	
10:15 - 11:30 AM	SB	Lab VIII-2: Advanced Structure Building	
11:30 - Noon AM	ALL	Breakout Sessions; Student Projects; Lab IX & X (optional)	lab_IX_membrane_builder.pdf lab_X_normal_modes.pdf
Noon - 1:00 PM		**Lunch**	

Files needed for Day 3: uk_2017_day_3_files.zip

Answers for labs on Day 3: uk_2017_day_3_answers.zip

Take-Home Exam: Antibody Build & Simulation

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