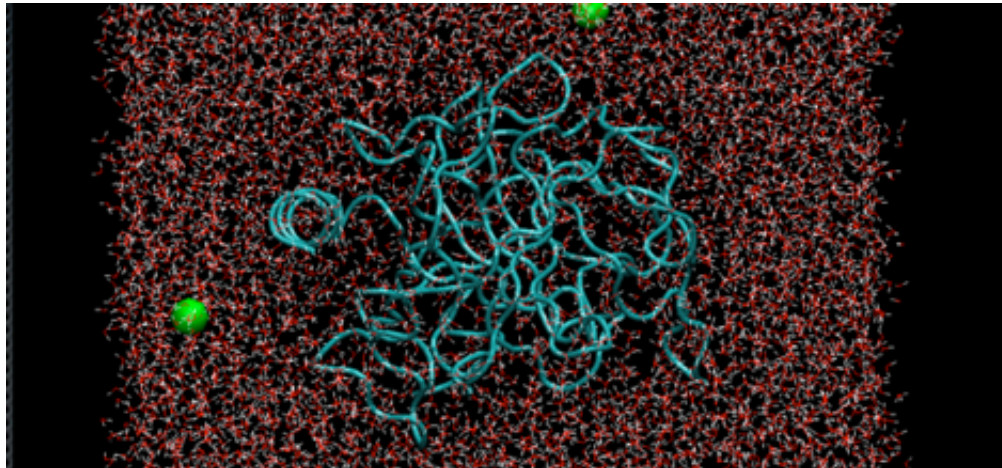


APS 2016



Atomistic Modeling of Small-Angle Scattering Data Using SASSIE-web

September 21-23, 2016

Advanced Photon Source, Argonne National Laboratory, Argonne, IL

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 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 gain experience with modern simulation tools such as VMD, NAMD. The latter half of the course will introduce SASSIE, a software framework designed to facility the use of atomistic modeling to

interpret scattering data.

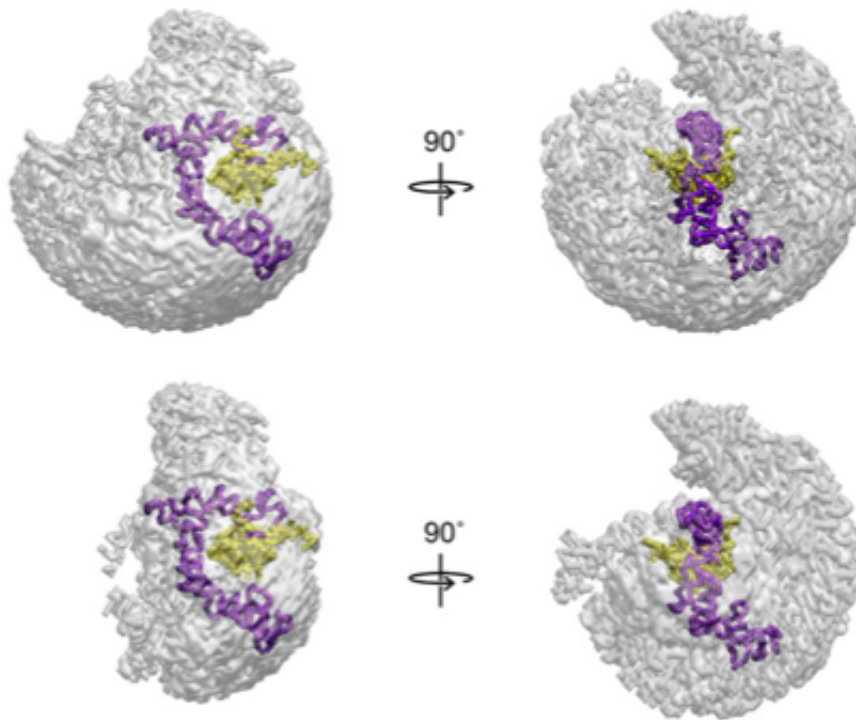
The course will involve a mixture of lectures and examples with student lessons. Examples will involve various protein, dna, and their complexes. Advanced simulation methods for glycosylated proteins, lipidic systems and coarse-grain methods can be accommodated depending on demand. The emphasis will 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: Intermediate MD, SASSIE and advanced building methods.

Day 3: Advanced MS, 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 initial models for their own projects.



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

Wednesday 9/21/2016

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	ALL	Lab 0: Software Installation and SASSIE-web Basics	lab_0.pdf ; basicoslinux_commands.pdf ; basicwindowscommands.pdf
Noon - 1:00 PM		Lunch	
1:00 - 2:45 PM	SK/ALL	Lab I: VMD	lab_1.pdf
2:45 - 3:00 PM		Break	
3:00 - 5:00 PM	SK/ALL	Lab II: PSFGEN/NAMD	lab/osx_linux.pdf ; lab/windows.pdf

Thursday 9/22/2016

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	SB/CJ	Lab III: NAMD	lab//osx_linux.pdf lab//windows.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	SK/ALL	Lab IV: SASSIE-web Quick Start	lab_IV.pdf
3:00 - 3:15 PM		Break	
3:15 - 5:00 PM	SK/ALL	Lab V: SASSIE-web Workflows	lab_V.pdf



Friday 9/23/2016

Time	Lead	Activity	File
9:00 - 9:30 AM	SCH	Lecture 4: Advanced SASSIE-web	lecture_4.pdf
9:30 - 10:00 AM	SCH/CJ	Lab VI-1: Advanced SASSIE-web	lab_VI.pdf lab_VI.html
10:00 - 10:15 AM		Break	
10:15 - 11:30 AM	SCH/CJ	Lab VI-2: Advanced SASSIE-web	lab_VI.pdf
11:30 - Noon AM	JEC	Lecture 5: Advanced Structure Building	lecture_5.pdf
Noon - 1:00 PM		Lunch	
1:00 - 3:00 PM	SK/ALL	Lab VII: Advanced Structure Building	lab VII/osx_linux.pdf lab VII/windows.pdf
3:00 - 3:15 PM		Break	
3:15 - 5:00 PM	SB/ALL	Lab VIII: Breakout Sessions: Student Projects and Advanced MD Labs	lab VIII/membrane_builder.pdf lab VIII/normal_modes.pdf

[Go to top](#)

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