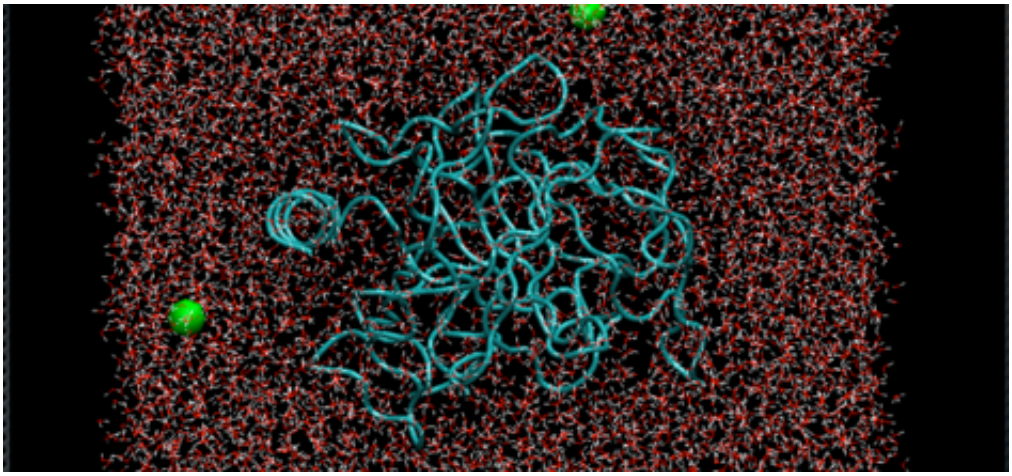
AUC 2015



SASSIE-web Based Framework for Atomistic Modeling to Interpret AUC & Scattering Data

December 8, 2015

La Trobe Institute of Molecular Science, Melbourne, Australia

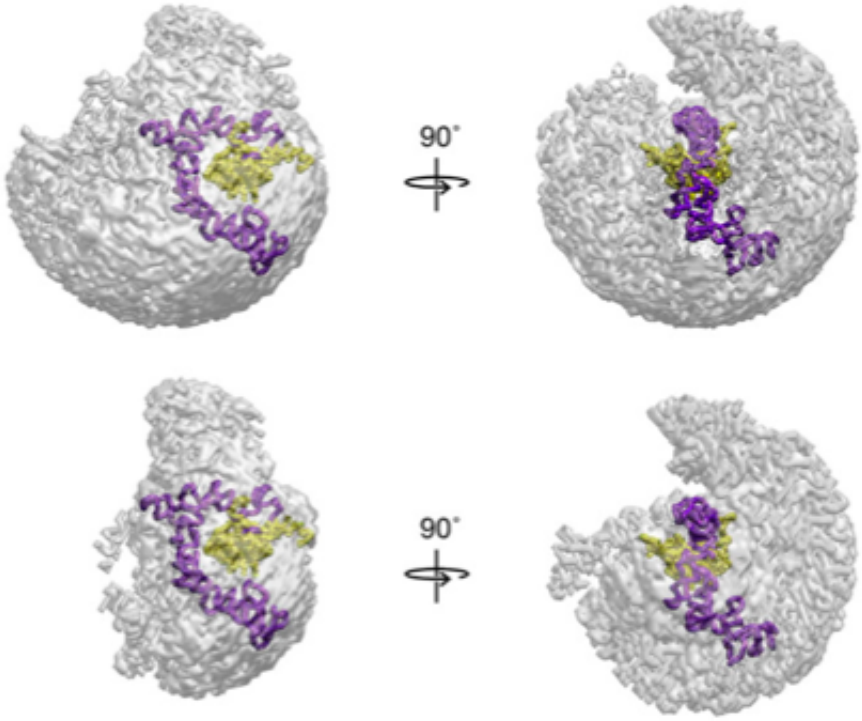
Molecular simulation is an important technique to analyze and interpret molecular phenomena across many disciplines. Analytical ultracentrifugation (AUC) & Small-angle scattering (SAS) utilizing either X-ray or neutron sources are valuable methods to characterize shape, interactions, and properties of many soft-matter systems. Modeling of AUC & 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 these studies to a wide variety of systems.

Atomistic modeling can be used to interpret AUC & 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 data.

The goal of this one day introductory course is to use modern simulation methods and software tools to predict

and analyze AUC & 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.

The course will involves the completion of "labs" by the students.
Examples will involve various protein, dna, and their complexes. The emphasis will be on ensemble molecular simulation, calculation of AUC & scattering profiles and comparison to experimental data.



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

Tuesday 12/8/2015

Time	Lead	Activity	File
8:30 - 9:00 AM	EHB	Software Installation and SASSIE-web	lab_0.pdf
9:00 - 10:30 AM	EHB	Lab I: VMD and PDB Scan	lab_I.pdf
10:30 - 11:00 AM		**Break**	
11:00 - 1:00 PM	EHB	Lab II: SASSIE-web Quick Start	lab_II.pdf
1:00 - 2:00 PM		**Lunch**	
2:00 - 3:45 PM	EHB	Lab III: SASSIE-web Advanced Monte Carlo & Simulation	lab_III.pdf
3:45 - 4:15 PM		**Break**	
4:15 - 6:00 PM	EHB	Links to US-SOMO	

SASSIE-web: Quick Start

How to Use Visual Molecular Dynamics (VMD)

Build

PDB Scan

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