Diffractions and Scattering Techniques

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Secondary Structure Elucidation via X-Ray Cross Correlation Analysis

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We aim to measure substantial structural information via X-ray scattering in the absence of an ordered system. Instead of a crystal, which consists of N particles at a single orientation relative to the X-ray beam, our samples consist of N randomly oriented identical particles. Assume, in a given exposure, two (or more) photons scatter from the same particle in a time interval much less than the rotational diffusion time, i.e. while the particle orientation is fixed. These two photons are correlated via the structure of the particle. By time averaging intensity correlations from such measurements, one can hope to recover structural information of the single scatterer relative to the background of N randomly oriented scatterers. One can demonstrate the high-dimensional data obtained from such a correlation experiment exceeds that measured in small and wide angle X-ray scattering measurements.

We have performed measurements on gold nanoparticle solutions at the Linac Coherent Light Source (LCLS) and are using them to identify and overcome the challenges involved in CXS experiments. Imperfections in detector geometry and electronic response can contribute to false correlations in the data; we are developing ways of identifying and removing these artifacts. We are simultaneously gauging our ability to recover protein secondary structural information from such data. Nanoparticle scattering will serve as a benchmark for an upcoming experiment at the Spring-8 Angstrom Compact free electron laser (SACLA), where we will attempt to measure correlated scattering from F-actin. Thereafter we hope to refine current models of the F-actin polymer by fitting them against our high dimensional data.

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Diffuse X-Ray Scattering for Ensemble Modeling of Crystalline Proteins

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Ensemble models of proteins have been developed using X-ray crystallography, and important advances have been made using translation-libration-screw motions of locally rigid domains, detection of alternative side chain conformations and contact networks, and X-ray restrained molecular dynamics (MD) simulations. Experimental validation is hindered, however, because Bragg peak data are unable to distinguish among different models that yield the same mean electron density. By contrast diffuse X-ray scattering reports on correlated motions and can be used to distinguish models that yield the same Bragg data. In particular it has long been recognized that diffuse scattering could be used to validate MD simulations if adequate sampling of the conformational ensemble were achieved. We have performed a 1.1 microsecond MD simulation of crystalline *Staphylococcal* nuclease (SNase) and have evaluated the resulting ensemble using existing diffuse X-ray scattering data (Wall, Ealick, and Gruner, 1997). The global R-factor between the simulated and calculated diffuse intensity is 0.066, and the Pearson correlation coefficient is 0.86. Discrepancies are highlighted when comparing just the anisotropic component of the diffuse signal; this comparison reveals a strong resolution dependence of the agreement with the anisotropic component, which is best at about 5 Angstroms, and is worst at about 3.5 Angstroms. The diffuse R-factor is improved compared to an earlier 10 ns simulation of crystalline SNase (Meinhold and Smith, 2007), reflecting the 100-fold greater sampling of the conformational ensemble. Our results support the validity and feasibility of using diffuse X-ray scattering to model molecular motions.

M.E. Wall, S.E. Ealick and S.M. Gruner. 1997. Three-dimensional diffuse X-ray scattering from crystals of *Staphylococcal* nuclease. Proc. Natl. Acad. Sci. USA 94:6180-6184.

Reference:

L. Meinhold and J.C. Smith. 2005. Fluctuations and correlations in crystalline protein dynamics: A simulation analysis of *Staphylococcal* nuclease. Biophys. J. 88: 2554-2563.

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Classification Protocol of Projection Images by Manifold: Toward Analysis of Dynamics of Particles with Coherent X-Ray Diffraction Imaging

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Coherent x-ray diffraction imaging enables us to collect huge amounts of diffraction images of a single particle for a short time. Since images represent projections of snapshots of a particle, they reflect its dynamics. Thus, dynamics can be analyzed using the images. One of the requirements for the analysis is a classification of images. Usual classification methods, however, would generate a great deal of classes because there are images arising from snapshots with a subtle difference as well as those with a large difference. This makes the analysis difficult. Here we propose a classification protocol of projection images using the concept of manifold, by which the issue above can be solved. We demonstrate the usefulness of the protocol using the images constructed in a computer.

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SIMtoEXP: Software for Comparing Simulations to Experimental Scattering Data

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In recent years, high power neutron and X-ray scattering experiments have become important tools for investigating lipid bilayer systems found in biological membranes. These methods provide structural information for the bilayers by converting the scattering results into structure factors that provide some structural information, but are unfortunately limited in their scope and scale. The limitations arise due to the fluid nature of lipid bilayers, that unlike crystalline material do not have well defined periodic lattices and thus only produce broad peaked structure factors with essentially no long range order. A number of theoretical models have been developed to convert these structure factors into electron density and neutron scattering density functions across the bilayer, but these models are based on numerous assumptions and there is no way to confirm their correctness. To overcome the limitations of these models, the Simulation to Experiment (SIMtoEXP) software was developed. It converts simulation probability densities into structure factors for direct comparison with experiment, thus providing atomic level detail to the scattering results. Here we present an extended version of SIMtoEXP, rewritten in C^{++} and the 'Qt' GUI library in lieu of the original C/Tcl combination. A major extension has been added that reads molecular dynamics trajectories directly and calculates atomic probability densities across the bilayer. This eliminates much work for the user, and removes possible errors introduced through the calculation of the probability densities.

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Current Status of ABBIX Beamlines Developed for X-Ray Scattering and Macromolecular Crystallography at NSLS-II

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We present the current development status of the Advanced Beamlines for Biological Investigations with X-rays (ABBIX) at NSLS-II. This NIH-funded project includes an x-ray scattering beamline (LIX) and two macromolecular crystallography beamlines (FMX and AMX). User operations are scheduled to begin in 2016.

Facilitating x-ray scattering studies on proteins in solution, lipid membranes and biological tissues, the High Brightness X-ray Scattering for Life Sciences beamline - LIX - will be equipped with a single long undulator (IVU23). Via a two-stage demagnification scheme it will produce beams down to a size of ~1 μm, and up to several hundred microns. With a broad energy range of 2.1 - 18 keV (0.7 - 5.9 Å) and capable of simultaneously collecting data on 3 detectors, it will support a variety of x-ray scattering measurements.

In the neighboring sector are the pair of MX beamlines, equipped with two identical canted undulators (IVU21). The beamlines' specializations are complementary. The Frontier Microfocusing Macromolecular Crystallography - FMX - will deliver a high photon flux of 10^{13} ph/s at the Se K-edge into a spot of 1 μm width. It will cover a broad energy range from 5 - 30 keV, corresponding to wavelengths from 0.4 - 2.5 Å. Beam sizes up to 50 μm will be available. The Highly Automated Macromolecular Crystallography - AMX - will be optimized for high throughput applications, with beam sizes from 4 - 100 μm and an energy range of 5 −18 keV (0.7 - 2.5 Å). Together, FMX and AMX will cover a broad range of applications from serial crystallography on micron sized crystals, over very large unit cell complexes, to rapid sample screening, e.g. for ligand binding studies.

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Temperature-Pressure Phase Behavior of Triglycerides Revealed by Synchrotron X-Ray Scattering Studies

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Triglycerides, such as cocoa butter (also called theobroma oil), are widely used in food industry as they are a main part of foodstuff such as chocolate. This ingredient affects important properties like gloss, texture and mouth