short x-ray free electron laser pulses. A special molecular dynamics model has been developed to describe the Coulomb explosion of the clusters [1]. We use numerical modeling based on the non-relativistic classical equation of motion. Quantum processes are taken into account by the respective cross sections. The explosion dynamics is examined for various conditions: pulse length, constituent atomic number, number of photons in a pulse. We use our model to get an estimate of the time available for imaging before the cluster deteriorates significantly. Based on these results we calculate the continuous elastic scattering pattern of the sample and try to reconstruct the original atomic order from this pattern. We use a density modification type algorithm analogous to the Fienup hybrid input output reconstruction method [2,3]. Since this method needs a 3D dataset in the reciporocal space, scattering patterns have to be taken at various sample orientations. That requirement leads to a multi shot experiment. Therefore the full dataset have to be built from scattering patterns of several independent exploding clusters. We included this complication in the calculations. We found that the shorter the pulse the higher the ratio of the photons useable for imaging. The conclusion of the calculations is that the pulse length of the presently planed x-ray free electron lasers is too long.

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Keywords: X-ray free-electron lasers, clusters, molecular dynamics simulations

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Three-dimensional Data merging of Randomly Oriented Continuous Diffraction Patterns

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We have developed methods for the assembly of three-dimensional diffraction data from noisy and randomly oriented continuous diffraction images. Before a structural reconstruction is possible, the patterns must be oriented with respect to each other and the signal to noise ratio must be increased by averaging of redundant data. While certain aspects of this problem are similar to problems in single-particle electron tomography, there are also significant differences. In single-particle electron tomography, similar images are located based on their correlation and the mutual orientation of the averaged images is determined from the common lines of intersection of their Fourier transforms. We present an extension of this scheme to the case of diffraction images, which intersect in spherical sections in Fourier space rather than in planar sections and which have statistical properties different from those of tomograms. We study how our scheme works on both real and simulated sets of three-dimensional data.

Keywords: three dimensional image, imaging, fourier transform

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MS23 PUTTING THE PEDAL TO THE METAL: SPEEDING UP BIOLOGICAL STRUCTURE DETERMINATION

Chairpersons: E. Yvonne Jones, Peer R. Mittl

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Development of a High-throughput Structure Determination Pipeline at BM14

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The basic operations to be performed for the collection of MAD and SAD data from protein crystals are well established and have been implemented successfully at beamlines across the world. There is now, however, intense activity aimed at revolutionizing the possibilities via a series of improvements, centered around (i) the mechanical aspects of automation, improved precision and improved visualization and (ii) the software aspects of automation and integration.

BM14 is a tunable bending magnet beamline at the ESRF operated by the UK research councils in collaboration with the EMBL Grenoble outstation. A high-throughput pipeline for structure determination by SAD and MAD phasing is being developed through our participation in the BBSRC e-science project e-HTPX (www.e-htpx.ac.uk).

An overview of the hardware and software implemented at BM14 for automation of macromolecular data collection will be presented. In particular, software developments which allow the user to keep track of the sample from their home lab to and from the beamline, as well as management of experimental data acquired, through the development of an easy to use beamline Laboratory Information Management System (LIMS) will be described. Our experiences in the use of SAD phasing with naturally occurring light atoms, such as sulphur and manganese, and their application for use in a high-throughput structure determination pipeline are summarized.

Keywords: MAD phasing, automation, LIMS

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Automating Crystallographic Structure Determination Calculations

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Structural genomics efforts require a high throughput at all stages of the structure determination process. Simultaneously, it is important to reduce the cost per structure, which means reducing the time spent on each structure. We have focused on the structure determination calculations going from processed, merged data through to initial model. The Automated Crystallography System (ACrS) utilizes existing software and algorithms but a distributive program interface administers the programs for determining protein structures. A relational data base stores initial data for starting the process as well as harvesting and warehousing data generated during the structure determination process.

The ACrS default mode of operation is to try several defined pathways in parallel. Analysis of the results in the database provides information for improving the pathways and for selecting software with complementary strengths.

An example is a recently determined structure of a member of the ROK family of transcription regulators that used a “native” data set and SAD phasing from one bound zinc to automatically built 384 residues of 405 without any intervention or optimization of parameters.

Keywords: structural genomics, automatic structure solution, macromolecular structure

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HT Structure Determination at SER-CAT: Five Structures in 23 Hours

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Researchers at the University of Georgia (UGA) have developed an optimizing, high throughput structure determination pipeline (SCA2Structure) capable of providing fitted or partially refined structures in a matter of hours from anomalous scattering (MAD or SAD) data [1]. This powerful structure determination engine coupled with the excellent data collection facilities provided by the SER-CAT, beamlines at the Advanced Photon Source (www.ser-cat.org) provides the basis for high-throughput structure determination.

Using prescreened crystals and data collected at SER-CAT, UGA researchers were able to determine five SAS structures on-site during a recent 24-hour run. Data were processed at SER-CAT and input to