

Theory of a unified field

standard file formats and subroutine
libraries for diffraction imaging

Jan Steinbrener, SUNY Stony Brook

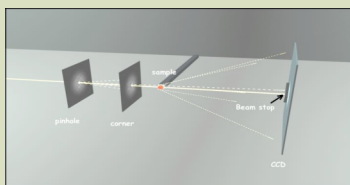
1. experiment

2. HDF5

3. API

4. collaboration

1. experiment 2. HDF5 3. API 4. collaboration



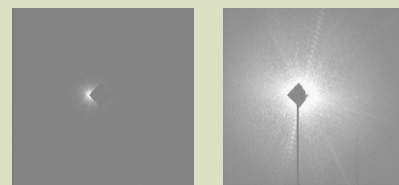
schematic of exp. setup at Beamline 9.0.1a at ALS, Berkeley

- 2D diffraction patterns recorded by CCD (1300 X 1340 px)
- rotate sample for 3D
- primary data format is *netCDF*

Jan Steinbrener, SUNY Stony Brook

imgCIF Workshop, BNL 05/24/07

1. experiment 2. HDF5 3. API 4. collaboration



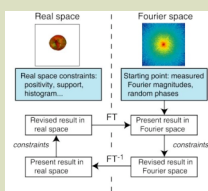
- due to saturation effects ~ 10^2 raw exposures per 2D assembled diffraction intensity (*ADI*) (10^4 for 3D)
- keep track of: raw datafiles, various experimental parameters, tilt angles for 3D \Rightarrow *ADI* is *HDF5* file

Jan Steinbrener, SUNY Stony Brook

imgCIF Workshop, BNL 05/24/07

1. experiment 2. HDF5 3. API 4. collaboration

- iterative reconstruction:
successively impose constraints in real space and in Fourier space
- ~ 10000 iterations \Rightarrow lots of FFTs
- \Rightarrow MPI-enabled cluster



- real space constraint is estimate of size of object in real space (support constraint)
- support is unique for each dataset and changes during reconstruction

Jan Steinbrener, SUNY Stony Brook

imgCIF Workshop, BNL 05/24/07

1. experiment 2. HDF5 3. API 4. collaboration

- self-contained, portable (C, C++, Fortran, Java, ...)
- groups, attributes, datasets
- data is binary, supports:
unlimited file size, # of dimensions
accessing subsets
extend dataset in any direction
- native MPI-support
- options for viewing data: *h5dump*, *hdfview*, ...
- more information @ <http://hdf.ncsa.uiuc.edu/HDF5/>

Jan Steinbrener, SUNY Stony Brook

imgCIF Workshop, BNL 05/24/07

