

Theory of a unified field

standard file formats and subroutine libraries for diffraction imaging

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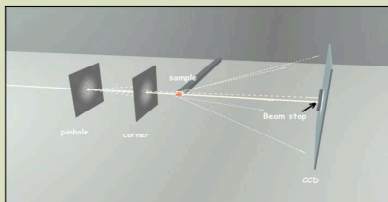
1. experiment

2. HDF5

3. API

4. collaboration

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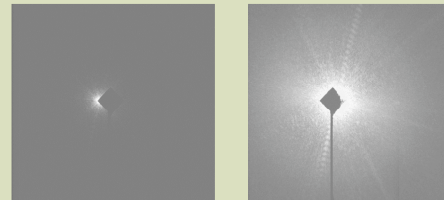
schematic of exp. setup at Beamline 9.0.1a at ALS, Berkeley

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

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- due to saturation effects $\sim 10^2$ 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

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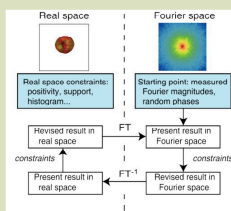
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- iterative reconstruction:

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

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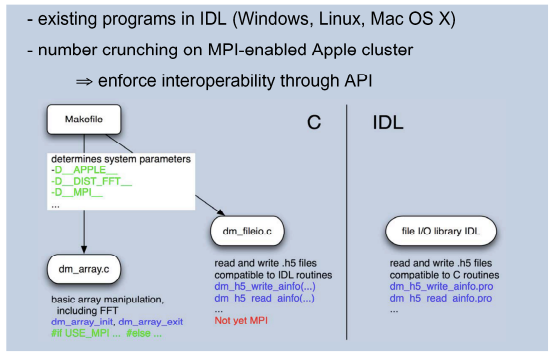
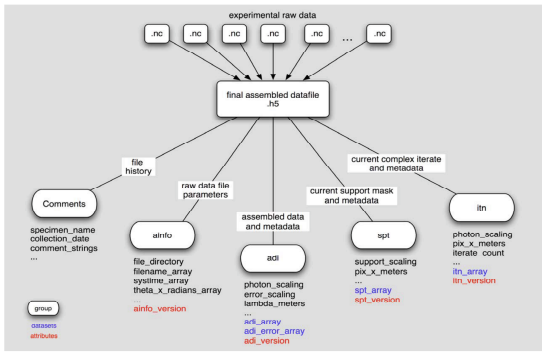
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- self-contained, portable (C, C++, Fortran, Java, ...)
- groups, attributes, datasets
- data is binary, supports:
 - unlimited file size, # of dimensions
 - accessing subsets
 - extend dataset in any direction
- native MPI-support
- options for viewing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

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 LBNL: Janos Kirz, Stefano Marchesini, David Shapiro
 Cornell: Veit Elser, Duane Loh, Pierre Thibault

This talk and related information at:
<http://xray.physics.sunysb.edu/~steinbre/imgCIF.html>

Community contributions/discussions encouraged