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

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

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

- due to saturation effects ~ 10^2 raw exposures per 2D assembled diffraction intensity (ADI) (10^6 for 3D)
- keep track of: raw datafiles, various experimental parameters, tilt angles for 3D \( \Rightarrow \) ADI is HDF5 file

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- iterative reconstruction:
  - successively impose constraints in real space and in Fourier space
  - 10000 iterations \( \Rightarrow \) lots of FFTs
  - 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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- soft 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: ncdump, hview, ...
- more information @ http://hdf.ncsa.uiuc.edu/HDF5/
- existing programs in IDL (Windows, Linux, Mac OS X) number crunching on MPI enabled Apple cluster
  => enforce interoperability through API

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This talk and related information at:
http://xray.physics.sunysb.edu/~steinhre/implCIF.html

Community contributions/discussions encouraged