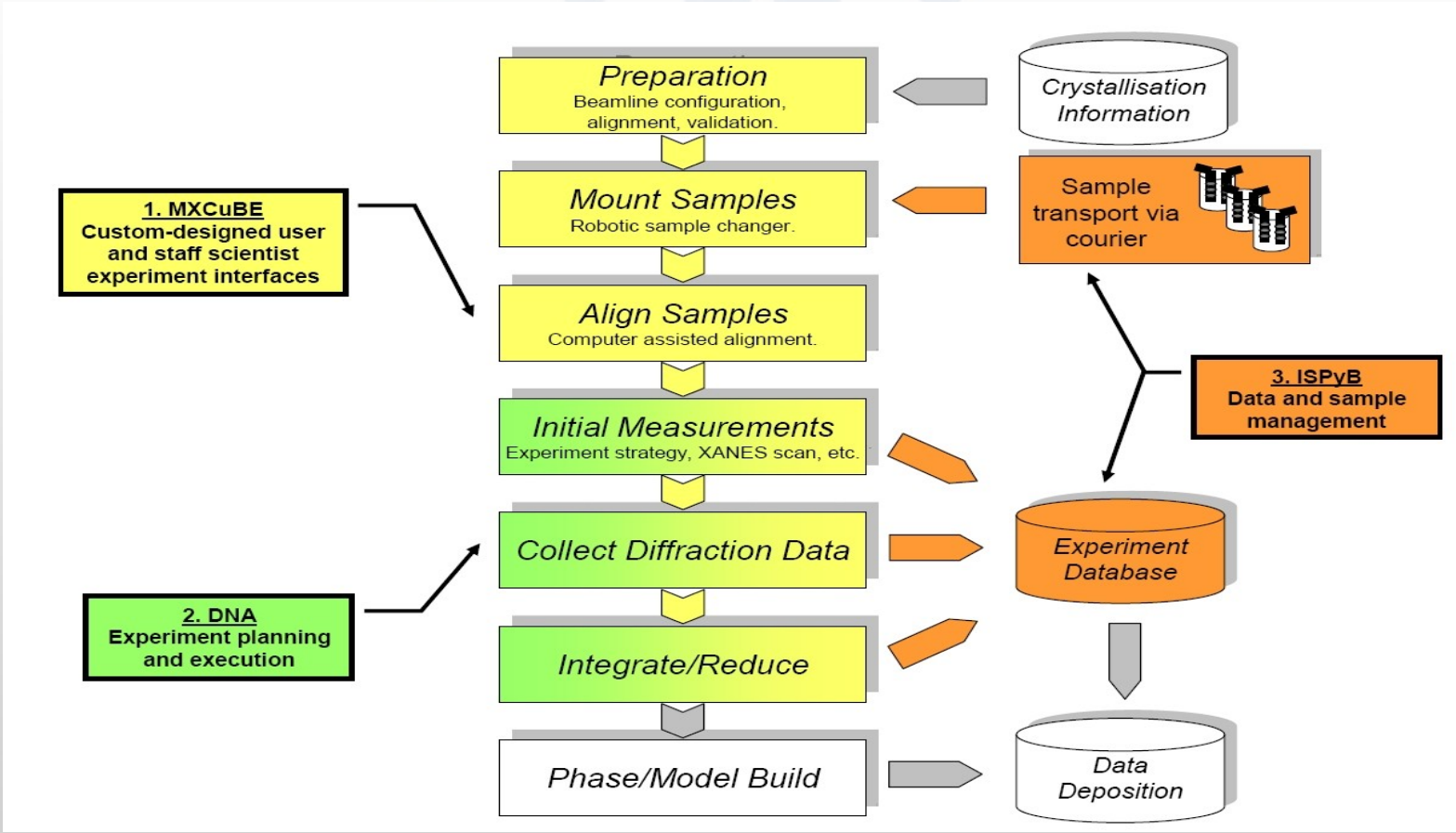
EDNA:
On-line Data Analysis for imaging and powder diffraction

Example of DiffractionCT

Layout

- Presentation of EDNA
  - On-line data analysis framework
  - Create pipeline by chaining plugins
  - Provides many useful building blocks
- Presentation of the diffractionCT experiment
- What has been implemented
  - Geometrical transformation of spline files
  - Test the equivalence of execution plugins (SPD / FIT2D)
  - 2D powder diffraction caking plugins
  - Storage of hyperspectal data-sets in HDF5/Nexus
- Ongoing developments
  - NiNa, HDF5, NeXus, ...

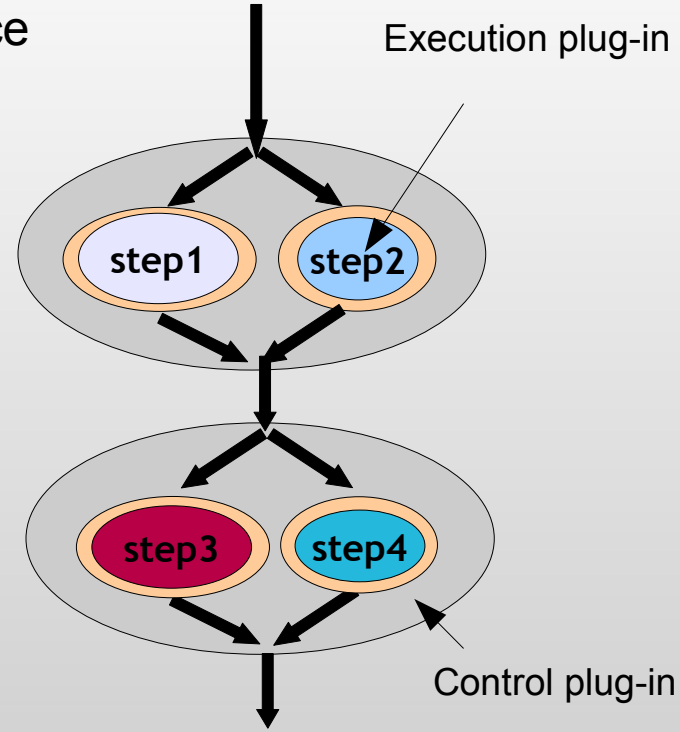
Example of an existing ODA implementation : The MX Data Collection Pipeline



Future challenges for MX ODA in the Upgrade Programme:
Large scale screening (MASSIF), multi-crystal data collection strategy etc.

Features of EDNA

- EDNA is a robust pipe-lining tool for on-line data analysis
  - It has been tested with thousands of tasks at once
- EDNA allows hi-performances
  - Multi-threaded implementation
- EDNA relies on data-models
  - Visual communication with scientists
  - Automatic bindings with the code
- EDNA has a strong testing framework
  - Unit & Execution tests
  - Non regression test before nightly builds
- EDNA is efficient to program
  - Plugin generator for execution plug-ins based on the data-model
  - Re-use of plug-ins already written (by others)
- EDNA is an international collaboration



EDNA is a versatile tool

- Run a plugin on the command line with a single input

  $ edna-plugin-launcher –execute EDPlugin –inputFile parameters.xml

- Run a plugin as a tango device server

  $ edna-tango-server

- Run a plugin in parallel on a set of inputs offline

  $ edna-SPD-Cake.py *.edf

- Run a plugin in parallel online on a set of incoming files

  $ edna-SPD-Cake.py –online

EDNA provides scientific building blocks

- Execution plugins:
  - MxExecPlugins: 24 exec plugins
  - Exec plugins: 14 exec plugins
    - SPD (4), FIT2D (2), EDF (2), HDF5 (2), thumbnail, video, …
- Control Plugins:
  - MX v1 26 control plugins, 7 exec plugins
  - MX v2 3 control plugins
  - DiffractionCT v1 6 control plugins
- Other projects:
  - CCP4 v0 3 plugins, 1 control, 2 exec
  - Dimple v0 20 plugins, 5 control, 15 exec
  - Darc v1 3 plugins, 1 control, 2 exec
- Total: 64 Execution plugins, 42 control plugins

Creating a pipeline is already easy

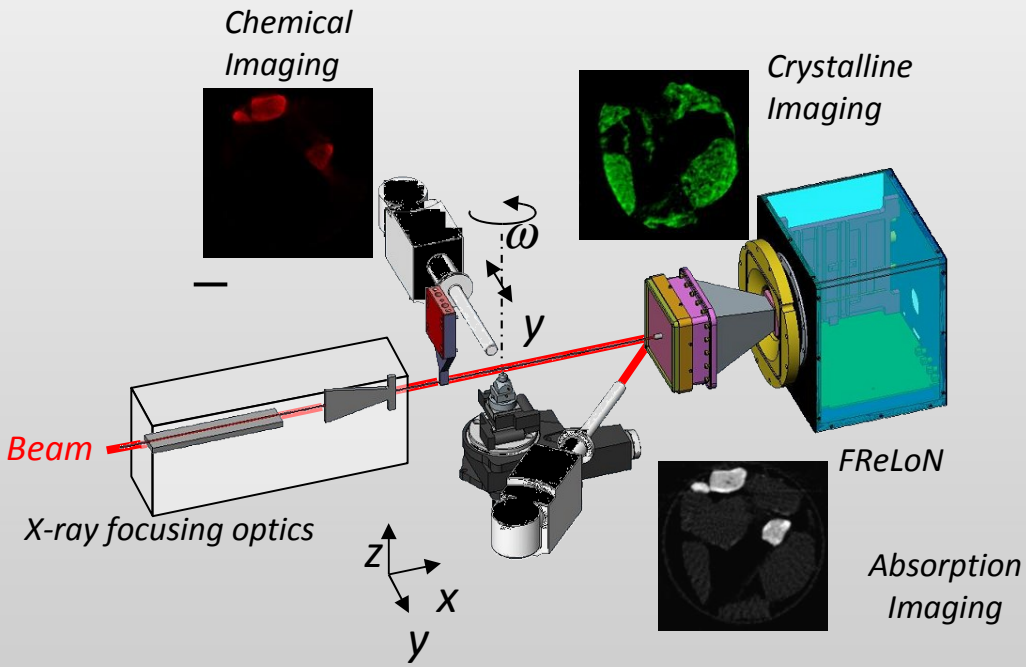
- Define the datamodel
  - What are the input and the output of your plugins (as XSD file)
- Use the plugin generator to create the structure
  - Tests are also automatically generated
- Re-use execution plugins as building blocks
- Chain them by connecting output from the first
  → To the input of the second

It will even be easier with the forthcoming workflow tool

Example of workflow:

DiffractionCT (ID22)

Part of UPBL4: Nano-imaging / Nano-analysis



Experimental setup @ ID22:

- KB optics with µ-/nano-focused beam
- FReLoN 2k taper: diffraction data
- Fluorescence (single element) detector
- Ion-chamber (I_o and attenuated I)

See e.g. Bleuet et al., Nature Mater. 2008

160 scanning steps/y-line,
60 angular steps/tomo scan

10-15h beam-time required/tomo scan
100 Go data generated/tomo scan

Slide from Pierre Bleuet

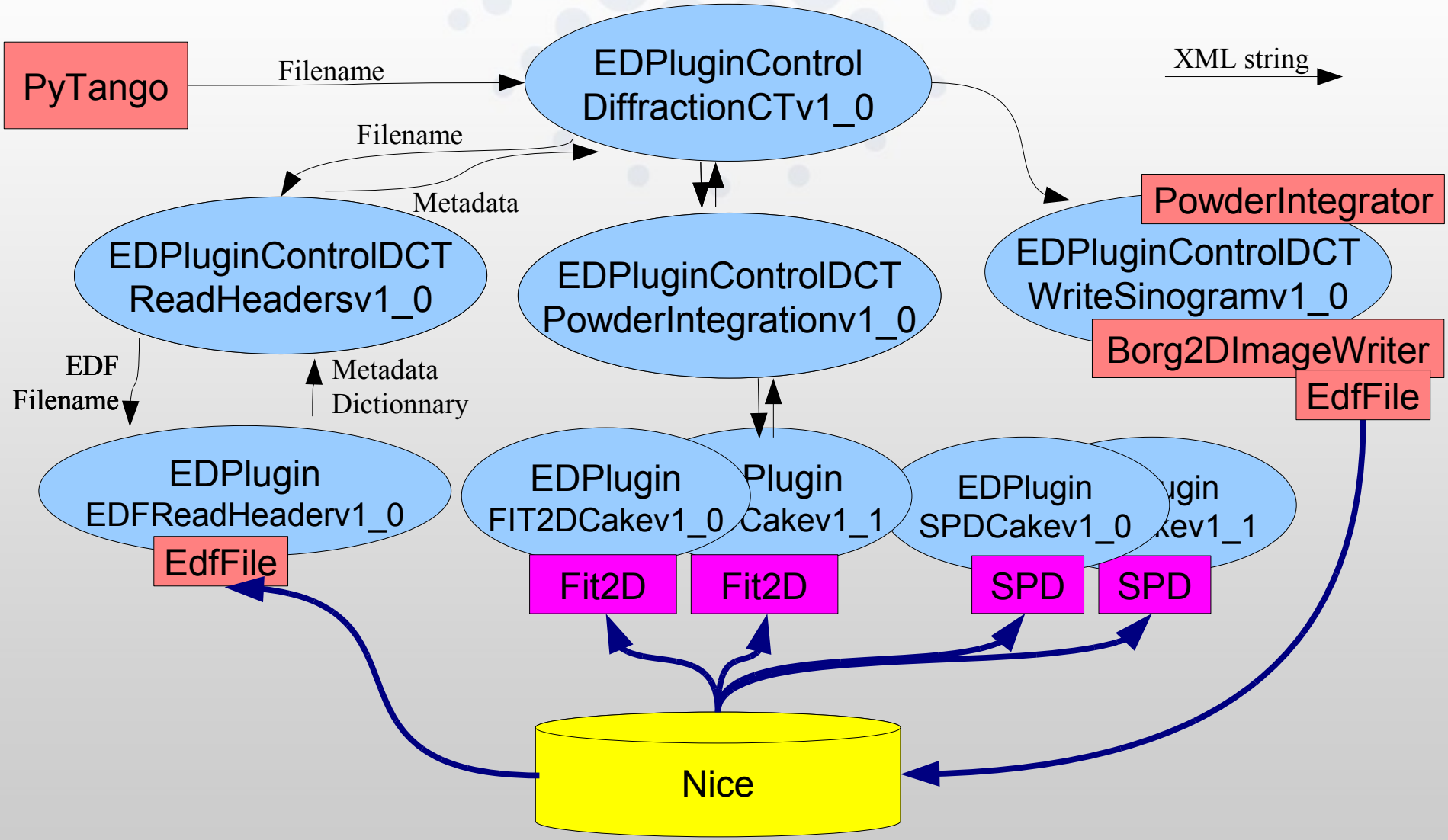
Towards combined contrast modes

- Absorption tomography:
  - record I_0 and attenuated I for each scanned position (point)
- Fluorescence tomography:
  - record a fluorescence spectrum (1D) for each position (point)
- Diffraction tomography:
  - record a (powder-)diffraction pattern (2D) for each position (point)

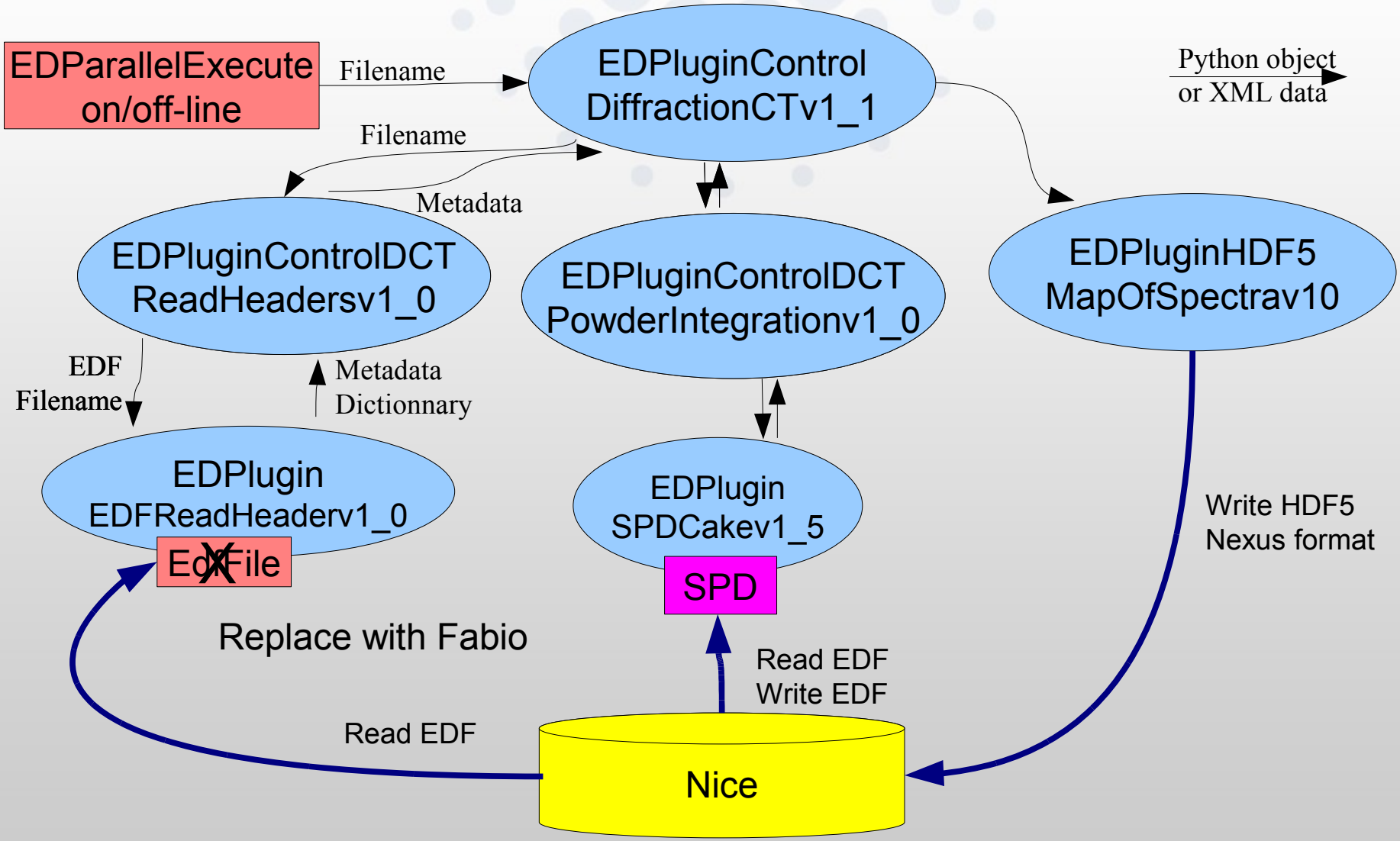
- Computational challenge:
  - Coherent data storage (HDF5/Nexus)
  - Large amount of data (10 000 datasets: each 0D, 1D and 2D)
  - Problems for archiving, transfer (to the user's location)

Work done up to now ...

First DiffractionCT implementation (11/2009)



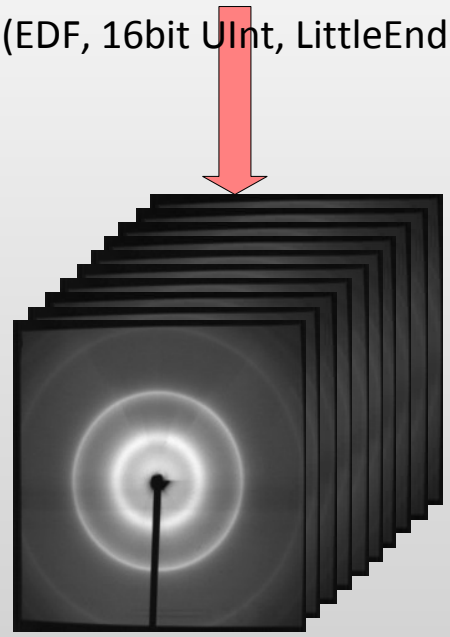
Second DiffractionCT implementation (06/2010)



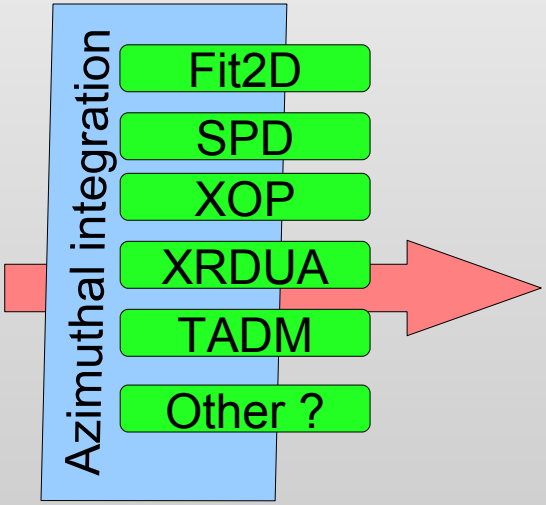
On-line data Analysis for NINA

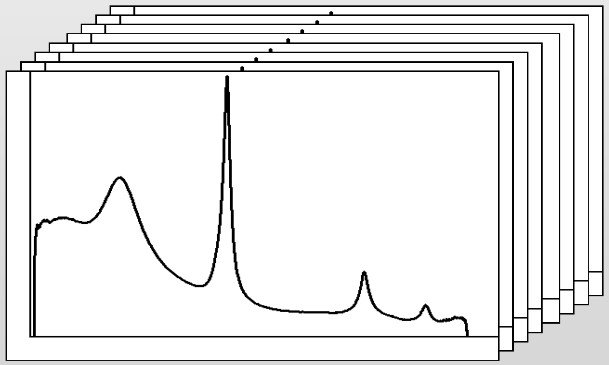
- Focus on most CPU demanding application: DiffractionCT

FReLoN2k
(EDF, 16bit UInt, LittleEndian)



N x **ω** 2D Diffraction Images



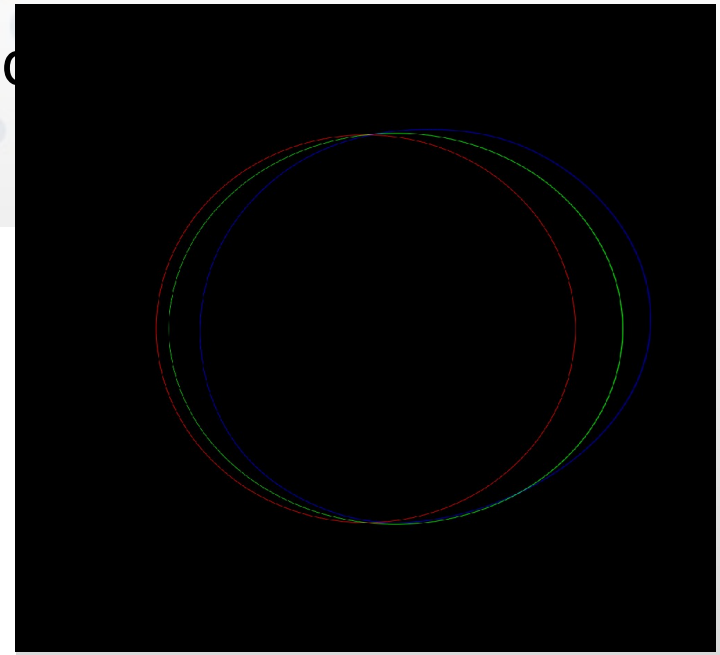


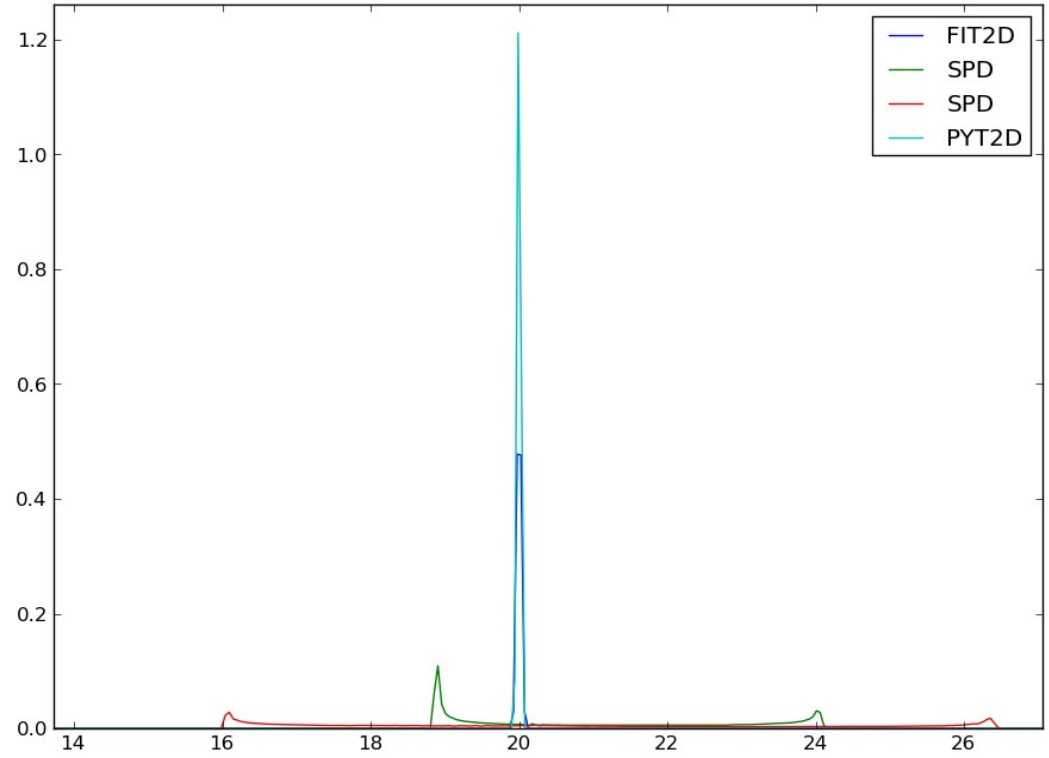
N x **ω** 1D diffraction patterns

Integration of many tools
Need plug-in management

Plug-ins for azimuthal integration
FIT2D / SPD / Python

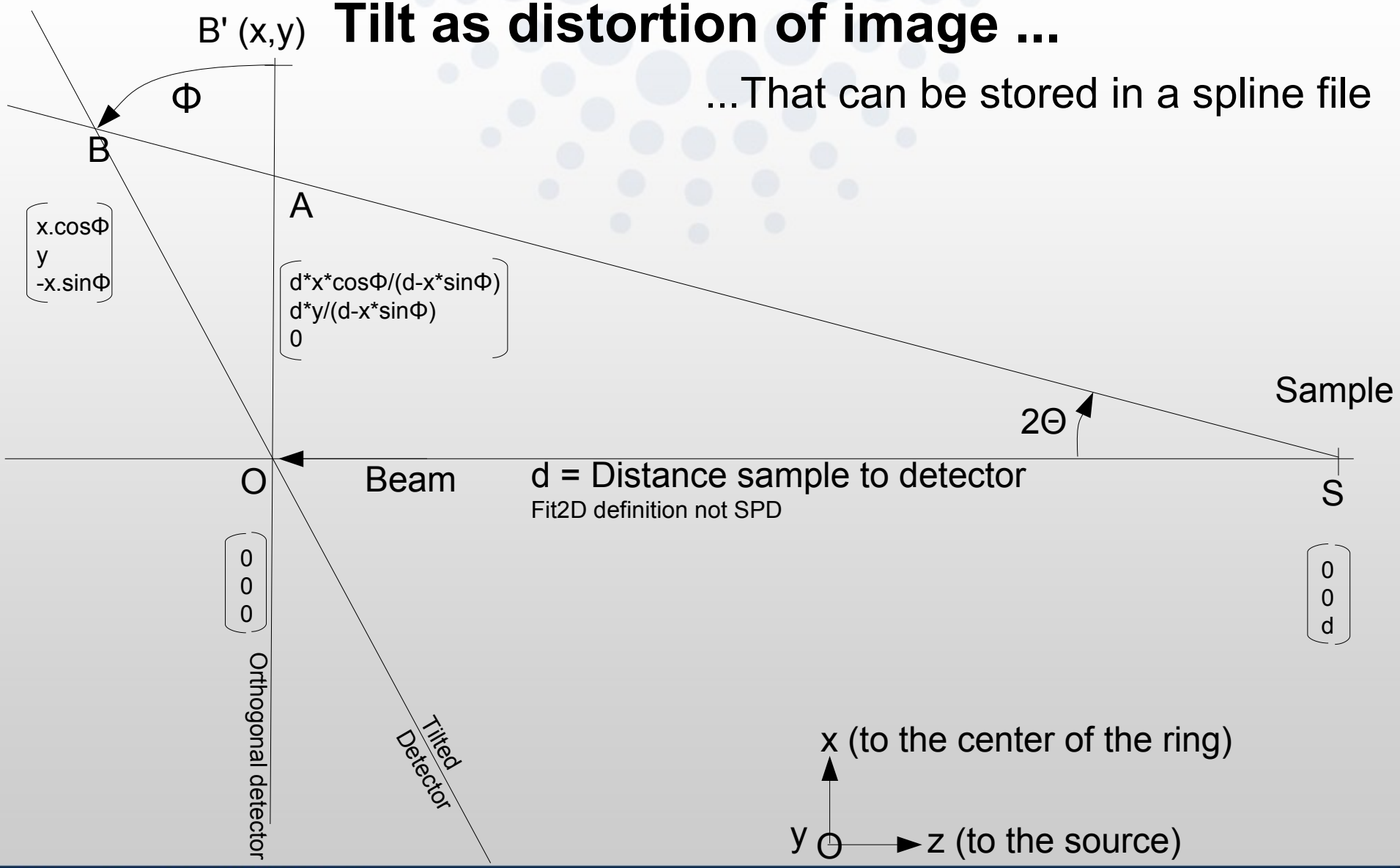
- They must all share the same data-mod
  - Dark noise & flat field subtraction
  - Converts the distance to the centre in 2Θ





Tilt as distortion of image ...

...That can be stored in a spline file



Testing & Profiling of EDNA

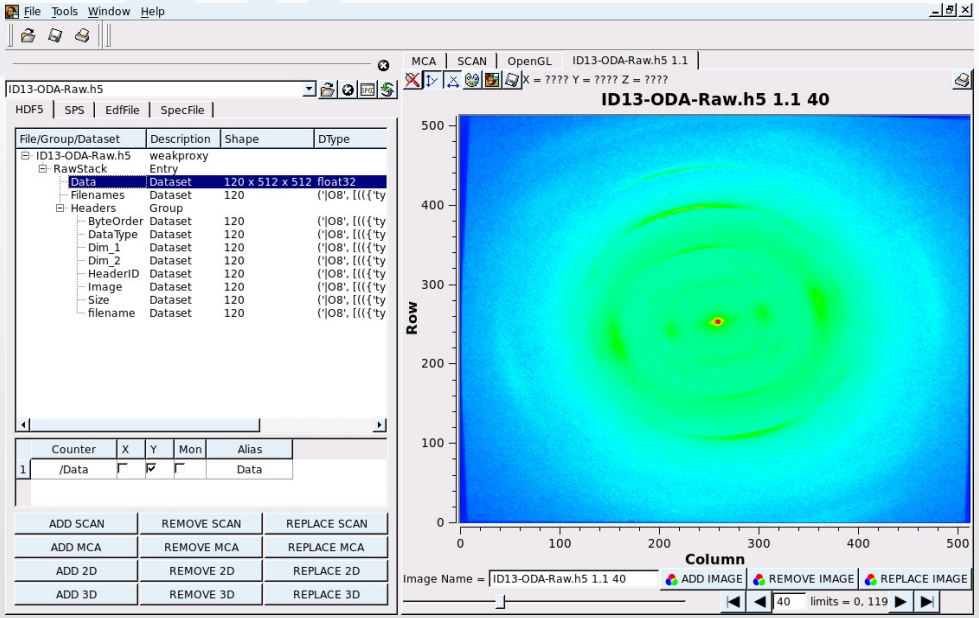
- Plug-ins in EDNA
  - Each plug-in should be usable alone (use of data-model)
  - Unit tests for each module with test suites (non regression tests)
  - Exchangeable plug-ins by sharing data-models (FIT2D / SPD)
- Profiling in EDNA
  - Global profiling using Python Profile
  - Performances evaluation using timings
- Performances (2k x 2k images on dual-Xeon 5500)
  - Fit2D:
    - < 5 sec / image with plug-in fit2dv1.1
    - Full sinogram at 1 point every 500ms
  - SPD:
    - < 2 sec / image with plug-in spdCakev1.5
    - multithreaded

Towards 3D and 4D data storage

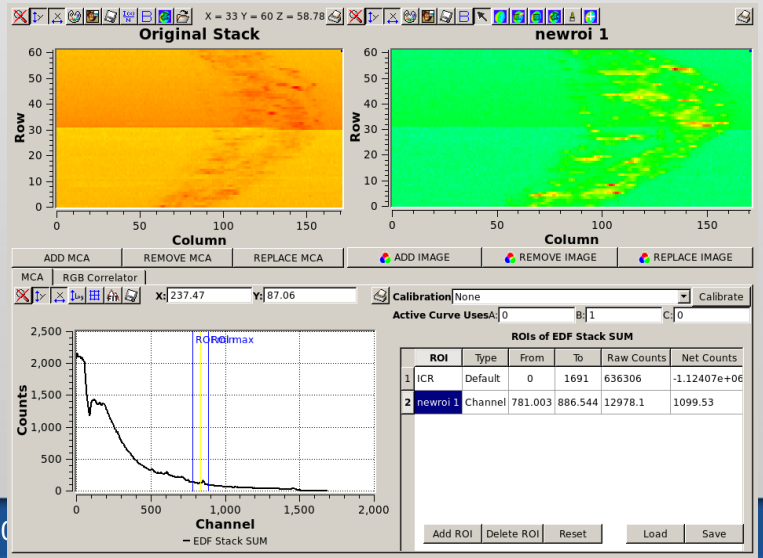
- Use HDF5 for data storage
  - Fewer files (currently hundred of thousands)
  - PyMCA can already read, visualize such data-sets
  - Need to get used to Nexus nomenclature
  - Compression is for free
- Store one experiments per HDF5 group / NXMeasurment
  - Absorption, Diffraction, Fluorescence …
  - Need to develop NeXus application definitions
- Problem of order for the data stored:
  - Stack of Images:[Index, y, x]
  - Map of Spectra : [SlowMotor, FastMotor, Spectrum]
- Live visualization of ROI with PyMca
  - No more ROI to be defined in the data-model !

Visualization of HDF5 files for DCT

- Images stored as a stack:
  Visualization with PyMca



- Live ROI selection for the sinograms with PyMca
- HDFview



Work currently in progress …
And long term milestones

Work in progress for NiNa

- Clean up plugins
  - HDF5 Map of Spectra is not (yet) NeXus compliant
  - SPD Cake is locked to single threaded
- New plugin for HDF5
  - HDF5 map of Images (4D data set !)
  - Extract data for HDF5
    - images to EDF or single image HDF5
    - spectra to spec or xy files
- Full Virtual Experiment
  - Full testing including the spec part, tango, ...
  - Needs especially a virtual camera...

TODO for Nina

- Other contrast modes:
  - NeXus application definitions do not exist at the moment
  - Datamodel to be defined as well
- Aggregation of data inside a single container
  - HDF5/Nexus file format (?)
  - Synchronisation issues
  - Rewrite the EDF-plug-ins in (HDF5)-plug-ins
  - keeping the same data models for all equivalent plug-ins
- On-line tomographic reconstruction with PyHST
- Absorption correction for diffraction data

Work in progress for EDNA

- Clean up in the source repository
  - Make it compatible with Windows (MacOSX is OK)
  - Refactor to new coding convention witch are lighter
- Interaction with scientists
  - EDNA plugins should be easily hackable
- Interaction with the beamline
  - Feed back to Spec (tango server, SpecClient? ...)
  - Use a data manager and stop transferring data through files on the disk
- Graphical feed-back of the processing
  - Matthew will work on a GUI for EDNA
  - Integration with a pipelining tool like Passerelle or Knime

Challenges for On-line data analysis

- Performances
  - Time constrained environment
  - Not slow down of the experiment (OK checked on ID22)
  - Use a data-manager (in the future)
- Development with and for scientists
  - Data-model for communication
  - Application definition for files (shared with other analysis software)
- Maintainability
  - Coding conventions
  - Testing framework
  - Shared SVN repository (www.edna-site.org)
- Sustainability and long term support
  - International and multi-site collaboration
  - Should be easy to install for external users (→ packaging)

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