

EDNA: Scientific workflows for synchrotron

**Example of existing pipelines
Developed by ESRF & DLS**

Scientific applications of EDNA

- Full Field X-Ray Absorption Spectroscopy
 - FF-XANES (ID21)
- Bio-Saxs collaboration
 - Up-stream data-reduction (ESRF + EMBL)
 - Down-Stream data processing (DLS + EMBL)
- Diffraction workflows
 - Diffraction Computed Tomography (ID22)
 - Material science (ID11)
 - Fiber diffraction (ID13)

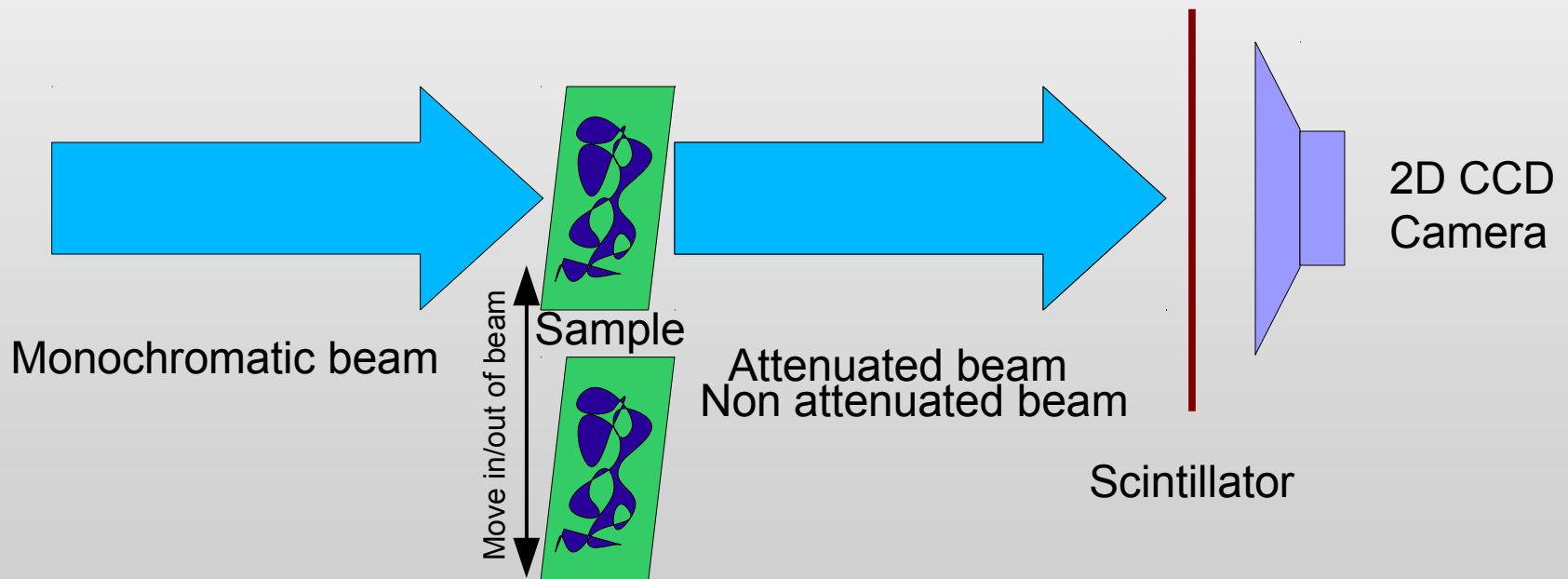
Full Field X-Ray Absorption Spectroscopy

First pure SciPy workflow

Scientific background

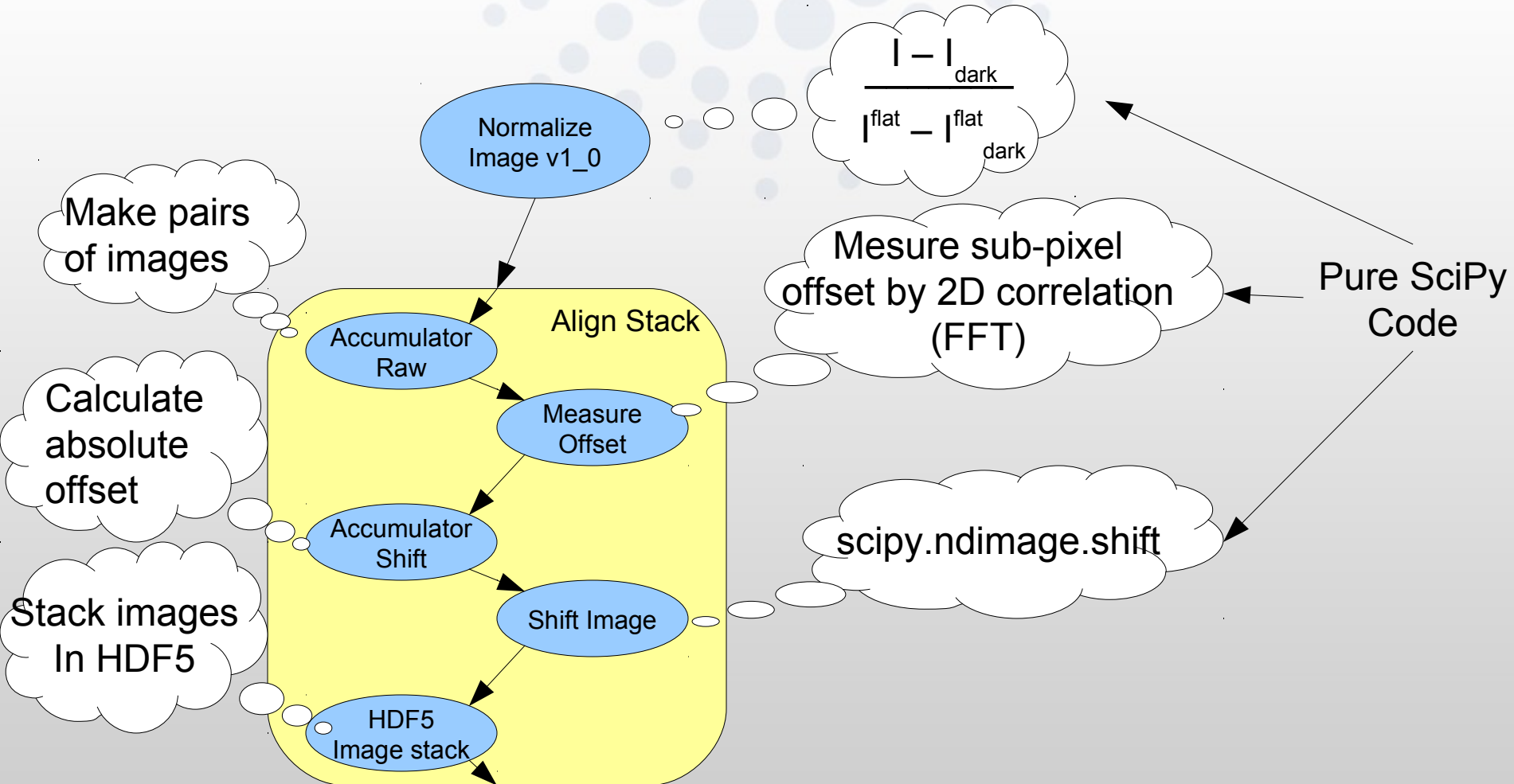
Scan in Energy on monochromator
around absorption edge of a given element

Sample size: 1 mm x 1 mm x 1 μm
Resolution: 500 nm



- Measure a (couple of) flats at each energy to correct for scintillator's response
- Align the sample at each position to correct sub-micron position change

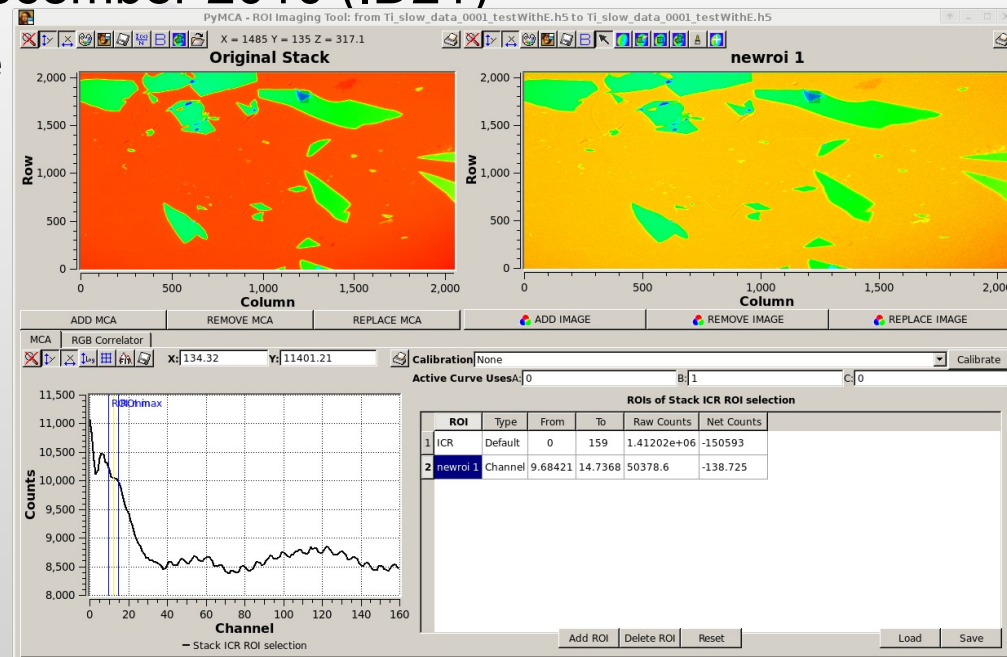
FullField XAS Pipeline



FullField XAS Results

Works:

- Tested online & offline in December 2010 (ID21)
- Towards Nexus compliance



Problems:

- Memory consumption for both EDNA & PyMca
- Distinction between feature of the image and artifacts (!)
- Limits of parallelism with the GIL (and/or) serialization of HDF5

Small Angle Scattering for Proteins

Collaboration with EMBL & Diamond

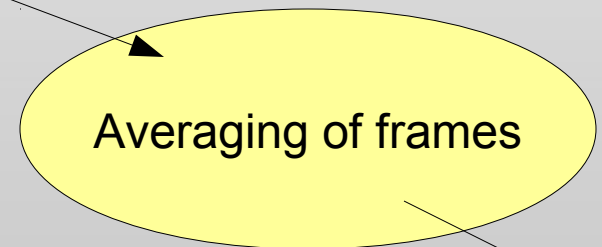
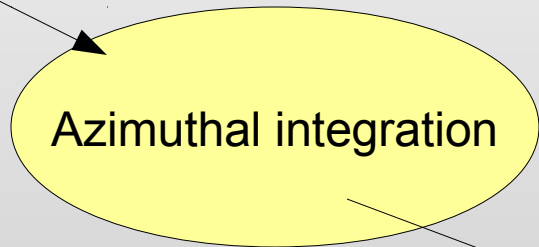
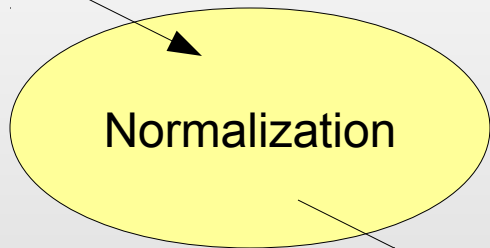
DLS-EMBL-ESRF BioSaxs Collaboration

Who does what ...

- ESRF & DLS collaborate on the maintenance of EDNA Kernel (port to windows asked by EMBL).
<http://www.edna-site.org>
- EMBL provides SAXS tools (as executable under unix & win)
<http://www.embl-hamburg.de/biosaxs/software.html>
- ESRF and DLS provide execution plugins for EMBL binaries
- ESRF focuses on data reduction EDNA plugins (→ AutoRG)
- DLS focuses on downstream processing (DAMMIF / DAMMIN)

Overview of the preprocessing pipeline (Existing but not used)

BSxCube



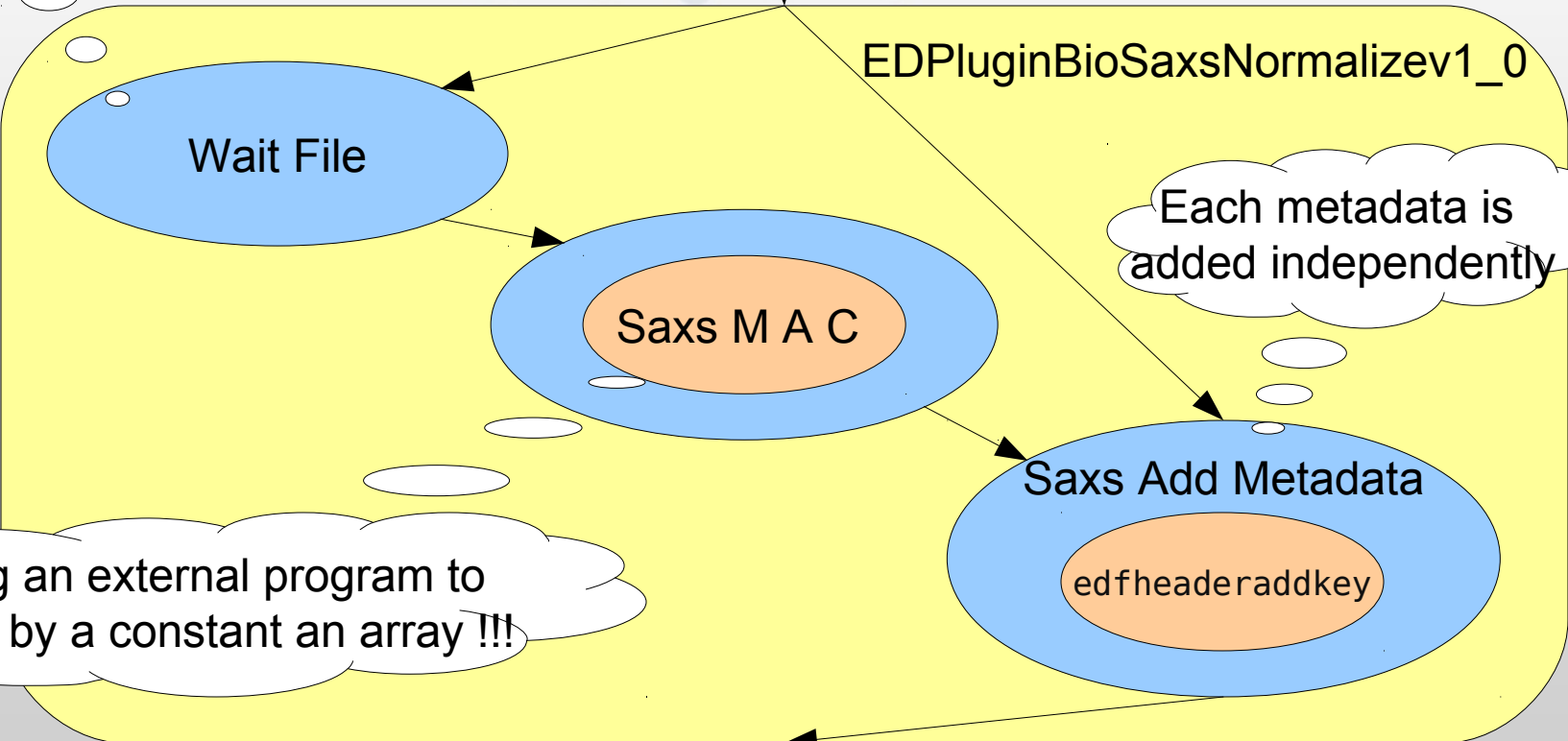
ESRF ID14-eh3

Focus on the Normalisation part

Work around for buggy NFS at ESRF

Raw Image + Metadata (Pilatus)

EDPluginBioSaxsNormalizev1_0



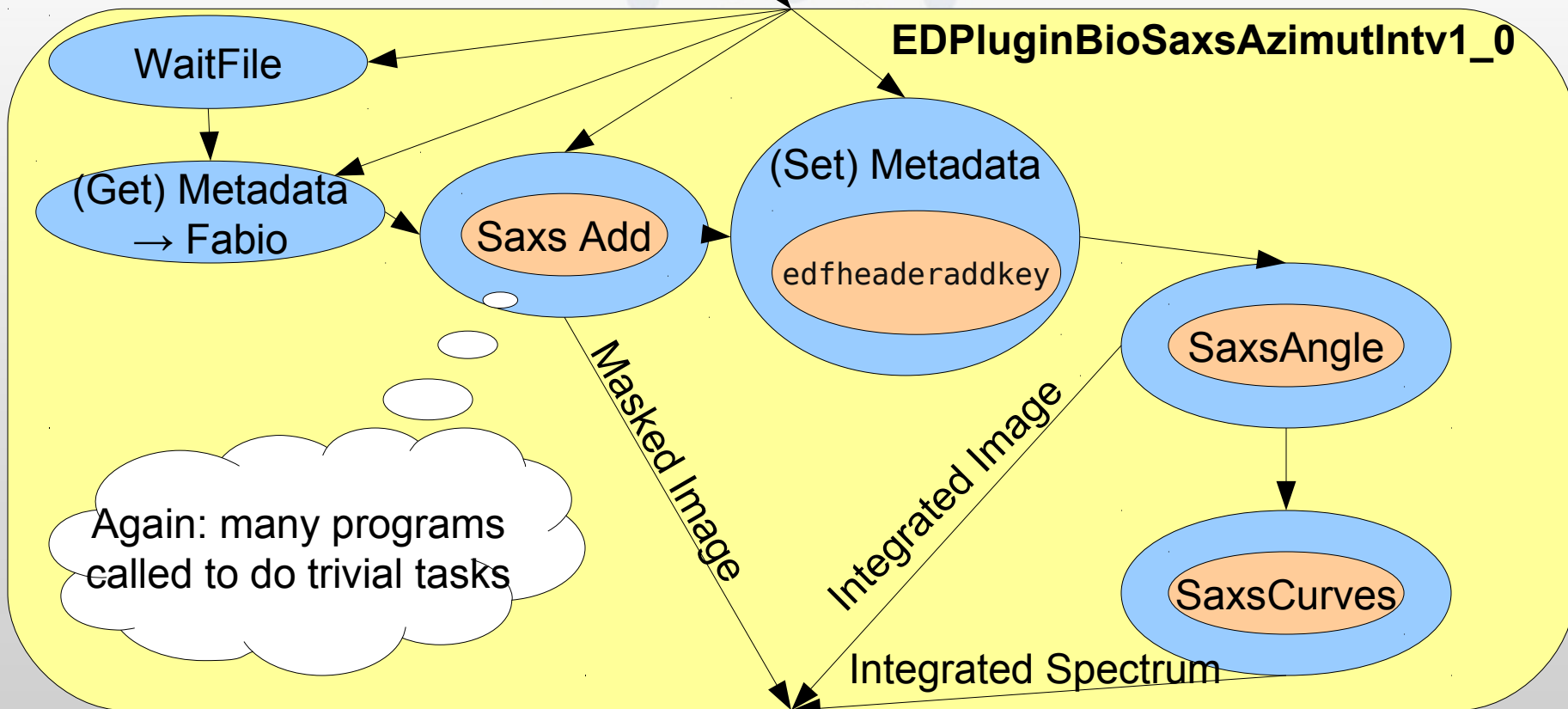
Each metadata is added independently

Calling an external program to Multiply by a constant an array !!!

Normalized Image

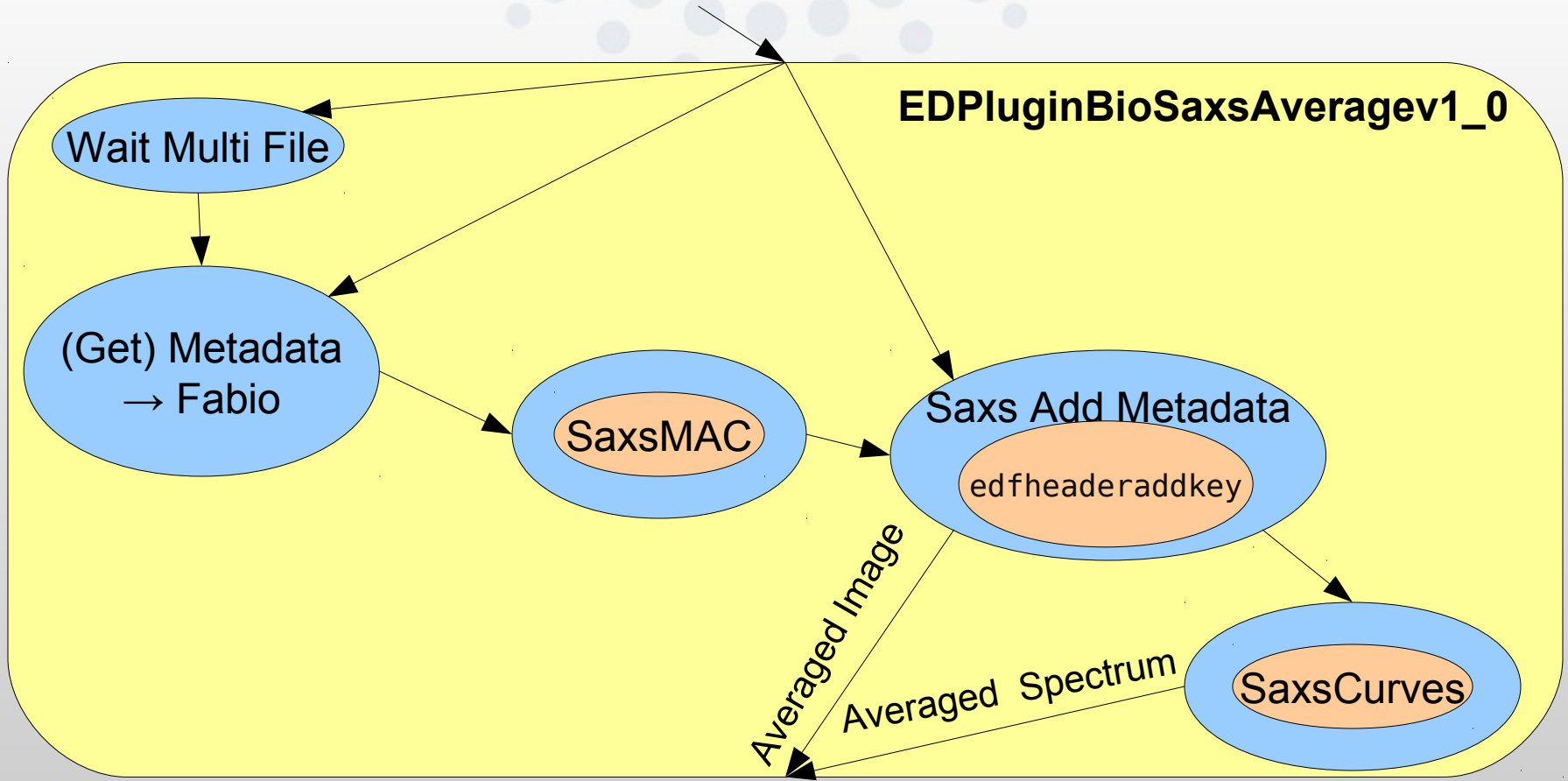
Focus on Azimuthal integration part

Normalized Image (+Metadata)



Focus on data averaging (basic version)

Integrated EDF + Metadata



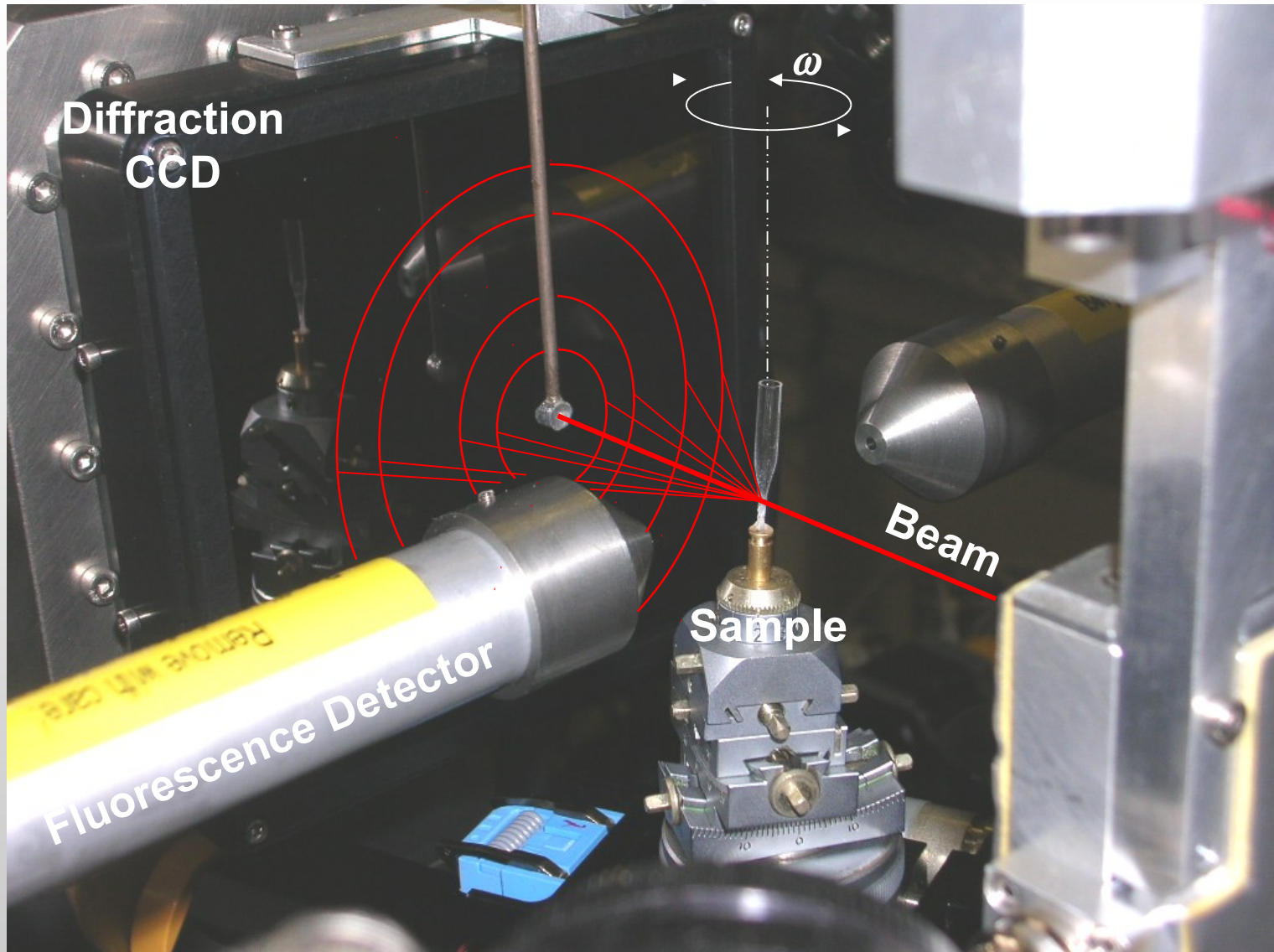
Pro / Cons / Future of the BioSaxs pipeline

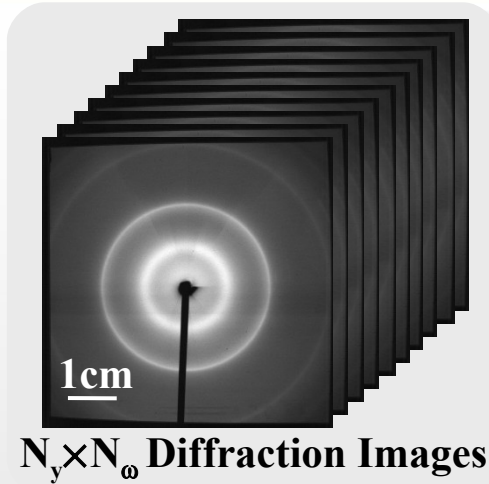
- Pro:
 - Reproduces the data of the existing pipeline
 - Adds proper metadata management
- Cons
 - Was not adopted because added value was too small
 - Dozens of external programs called (slow pipeline)
- Future:
 - Integration of new Fabio which is compatible with saxs* programs
 - Reduce external calls to a single program: saxs angle
 - Evaluation of radiation damage & AutoRg
→ Demo in May 2011

EDNA application around diffraction

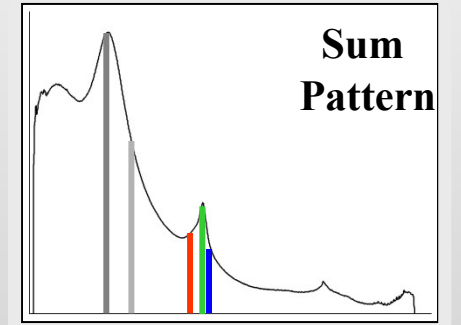
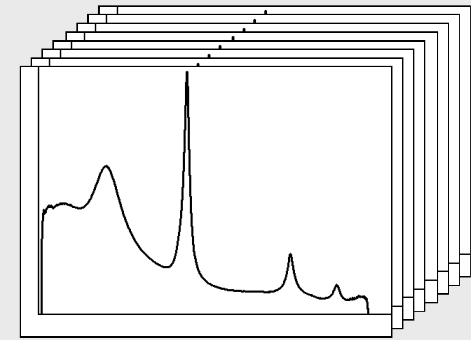
Making best use of SPD

ID22 – Fluorescence-Diffraction Tomography

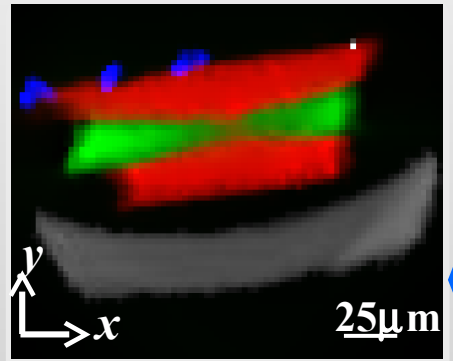
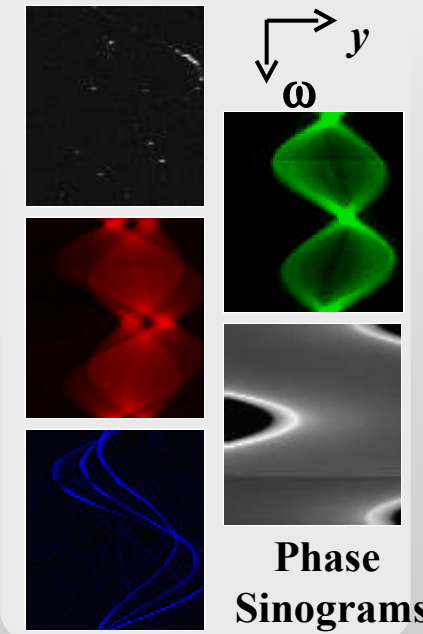
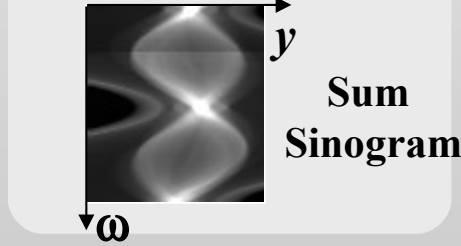




Azimuthal
Integrations
Fit2d software



PyMca
software

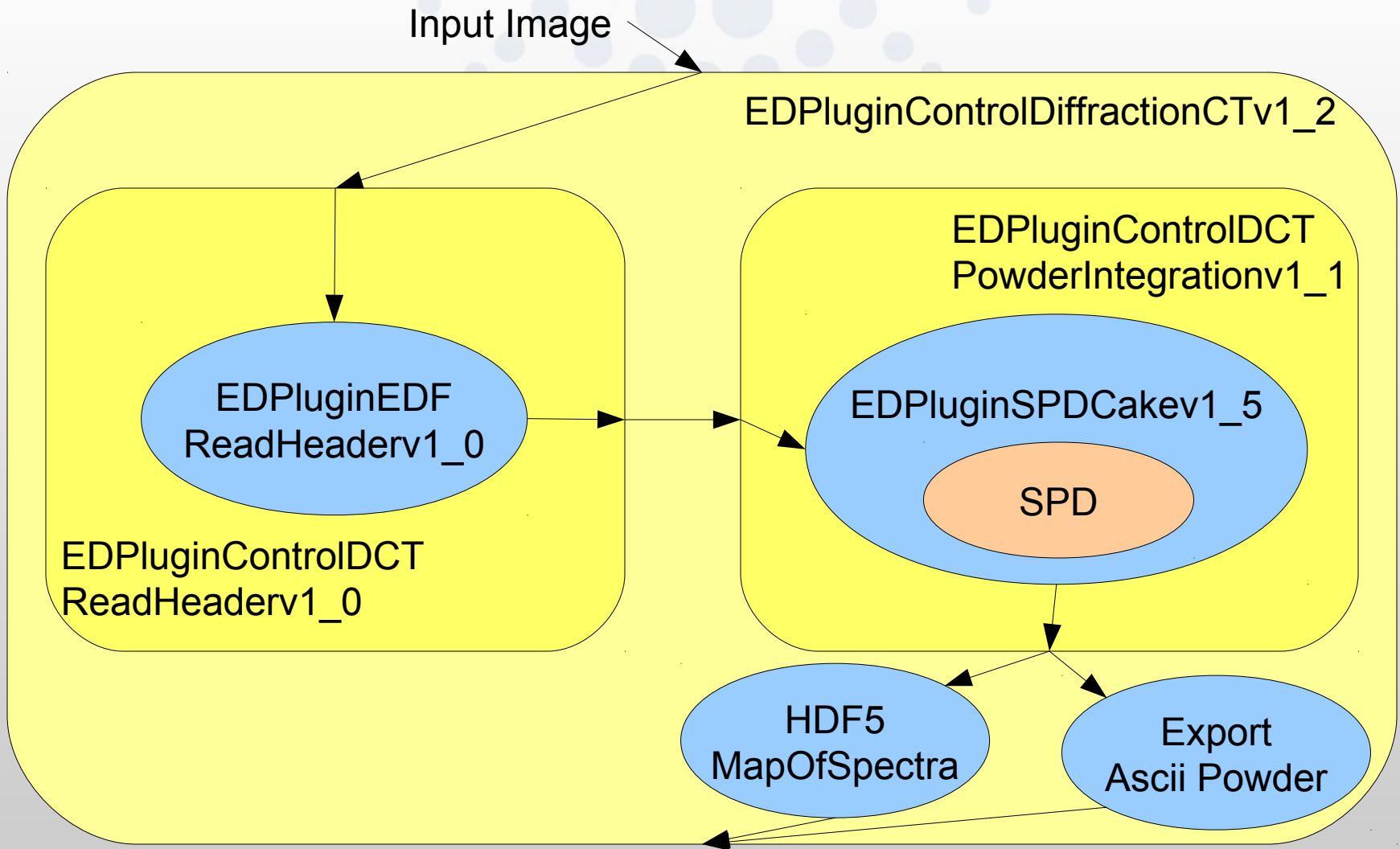


Reconstruction

Capillary	Ferrite
Calcite	sp3
	Cubic

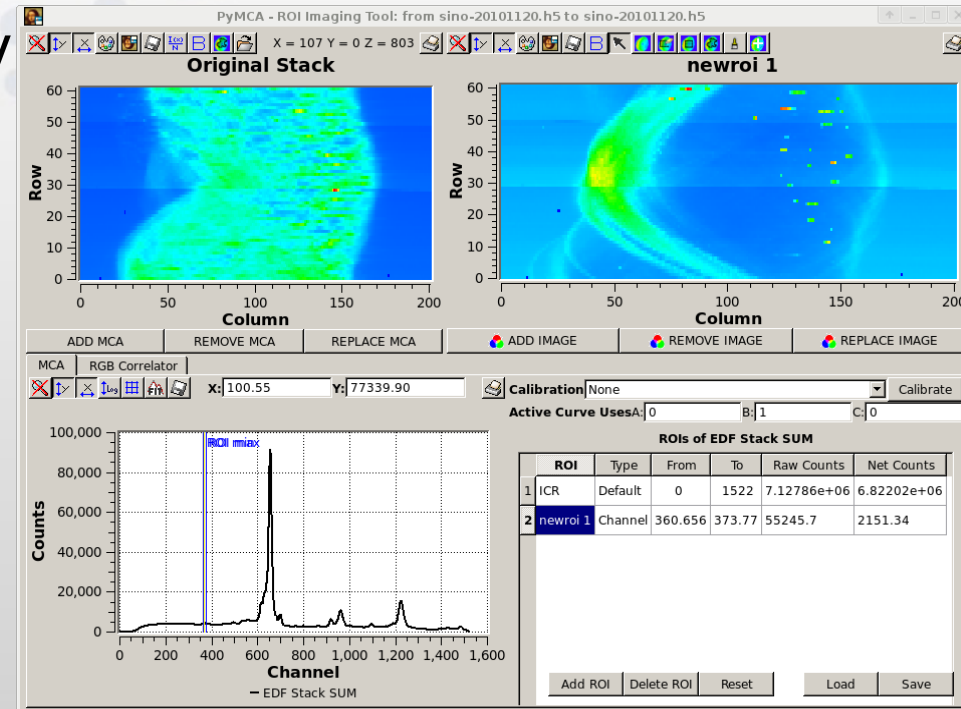
Acknowledgements: Pierre Bleuet CEA - Grenoble

EDNA - Diffraction Computed Tomography



Diffraction tomography on ID22

- Mesh 120 x 220 (26k images 2k x 2k)
- All data processed on the fly
 - Meta-data extraction
 - Dark & flat field correction.
 - Tilt & distortion corrections
 - Azimuthal integration (SPD)
 - Sinogram: HDF5 3D dataset,
 - live ROI with PyMca
 - Process time: 1.5 s/image
 - Throughput (8 cores): 4.3 fps
- Future:
 - PyMca will incorporate Algebraic Tomographic reconstruction
 - Nexus compliance of HDF5 data (axis, ...)



Spreading of the SPD-solution

- Soft Condensed Matter Nanofocus beamline (ESRF ID13)
 - SPD plugin tested with the online mode (EDNA Parallel Execute)
 - 10 frames per second (512 x 512 image)
 - 2 SPD processes under control on a 4-core computer
 - Image correction (dark, flat, distortion) + azimuthal integration
- Materials Science beamline (ESRF ID11)
 - SPD plugin tested with the offline mode (EDNA Parallel Execute)
 - Images coming from 3 different detectors
 - Selection of the right process for correction and azimuthal integration
 - Pipeline under evaluation

Acknowledgements

- ID11 (Materials Science):
 - Jon Wright & Andy King
- ID13 (NanoBeam):
 - Manfred Burghammer
- ID14-eh3 (BioSaxs):
 - Louiza Zerad & Adam Round
- ID21 (FF Xanes):
 - Barbara Fayard & Muriel Salomé
- ID22 (Diffraction computed tomography):
 - Rémi Tucoulou
- SPD developers:
 - Peter Boesecke & Rainer Wilcke
- ODA:
 - Cyril Guilloud, Armando Solé & Olof Svensson

A Light for Science



European Synchrotron Radiation Facility

List of EDNA Plugins

- Number of Control Plugins: 68
- Number of Execution Plugins: 88
- Number of Others Plugins: 21