

Integration of a Workflow Tool with MX Data Acquisition

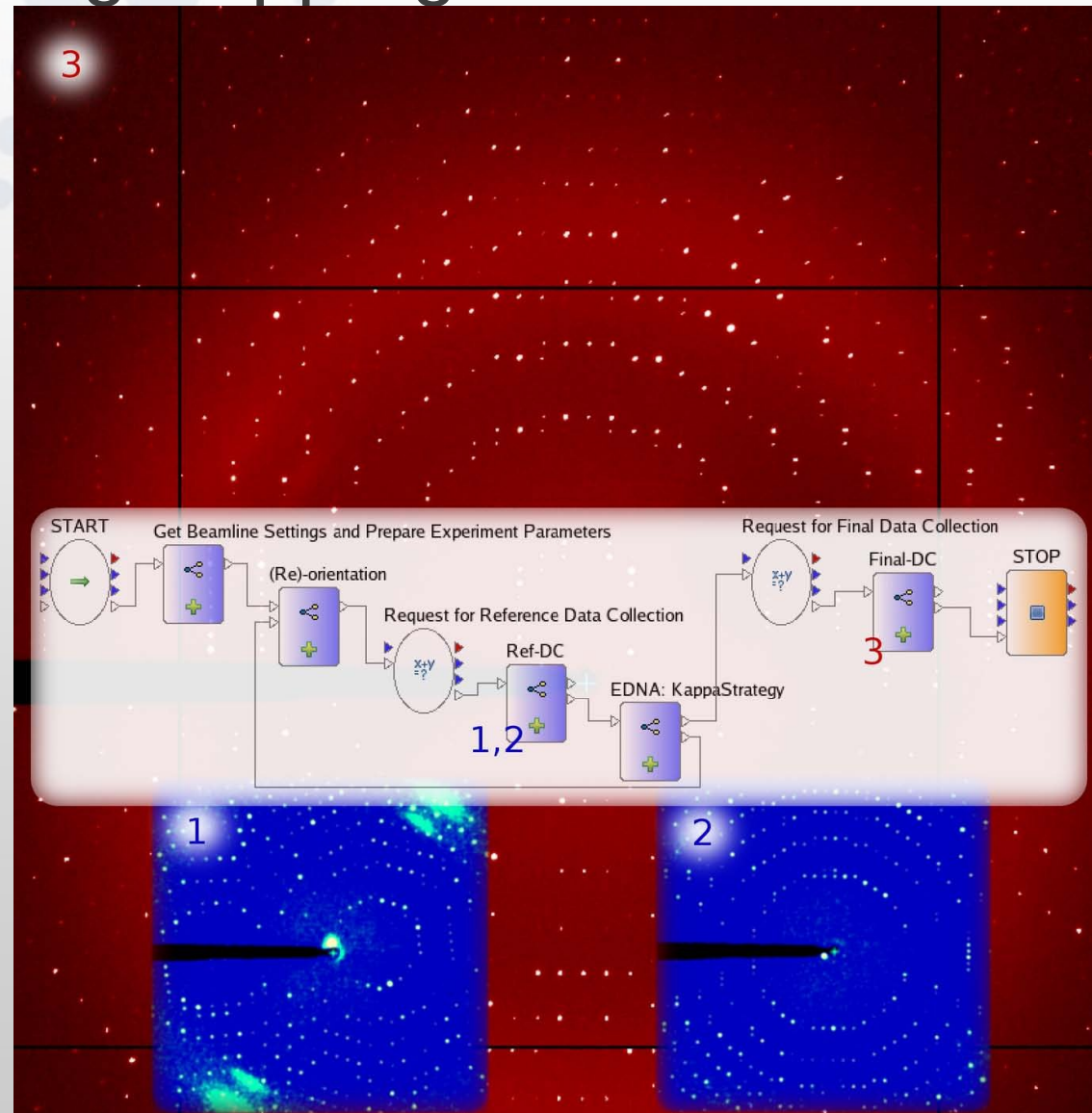
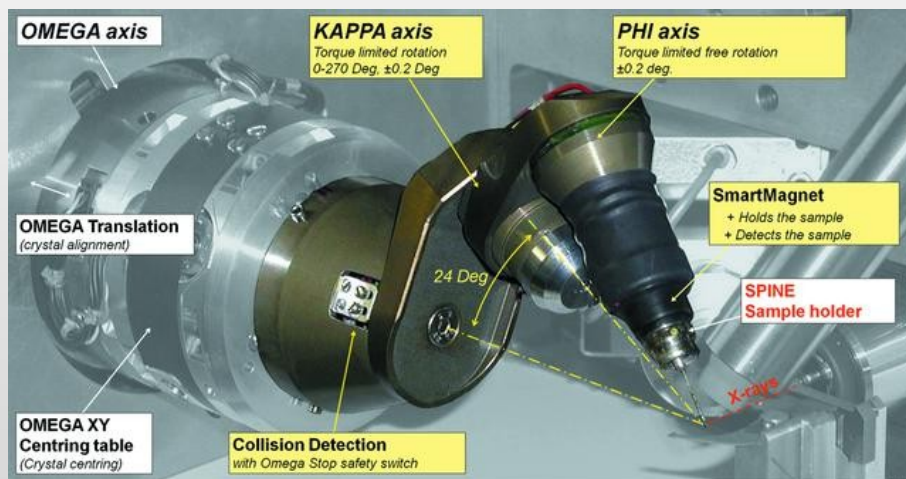
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Bowler², Max Nanao² and Matthew Gerring³

- 1) ESRF, France
- 2) EMBL Grenoble, France
- 3) DLS, UK

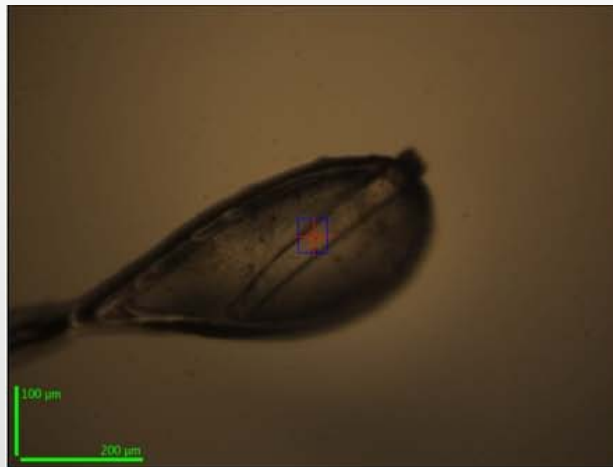
Overview

- On-line data analysis workflow examples:
 - Kappa goniostat reorientation
 - X-ray auto centring (mesh scan)
- Why use a workflow tool?
- DAWN vs EDNA
- Integration on ESRF MX beamlines
- Acknowledgements

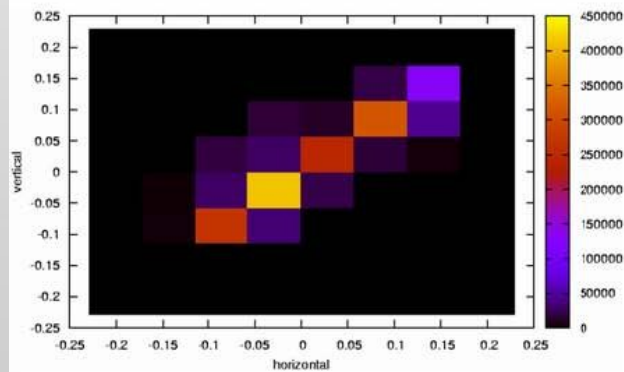
MX On-line data analysis 1 : Re-orientation using Kappa goniometer



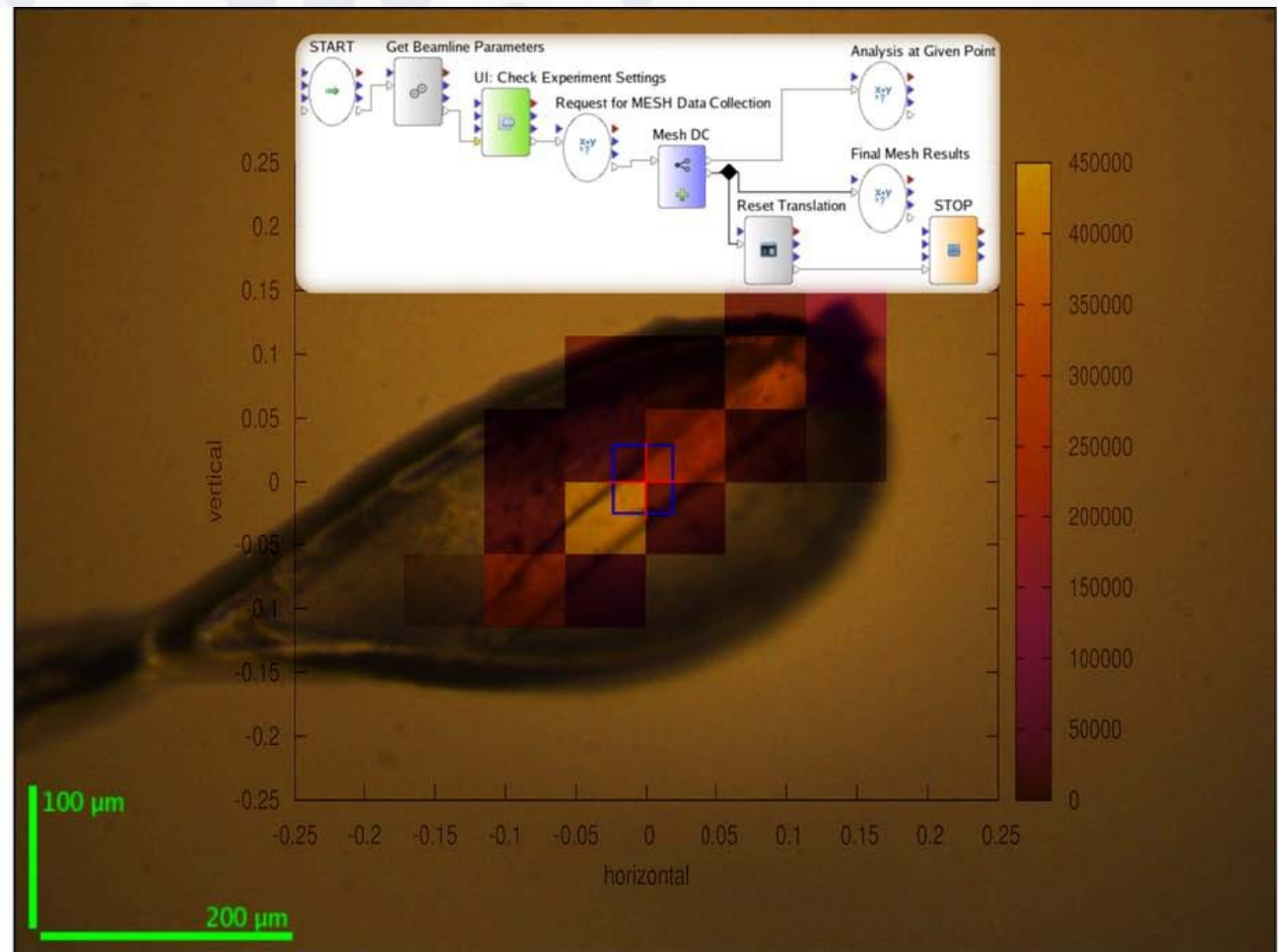
MX On-line data analysis 2 : Mesh / grid scan



(a)

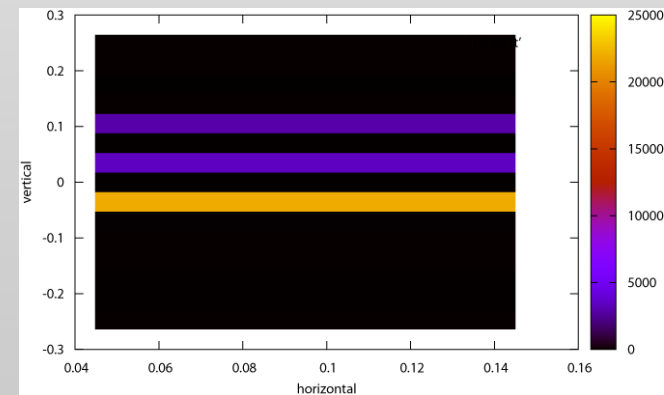
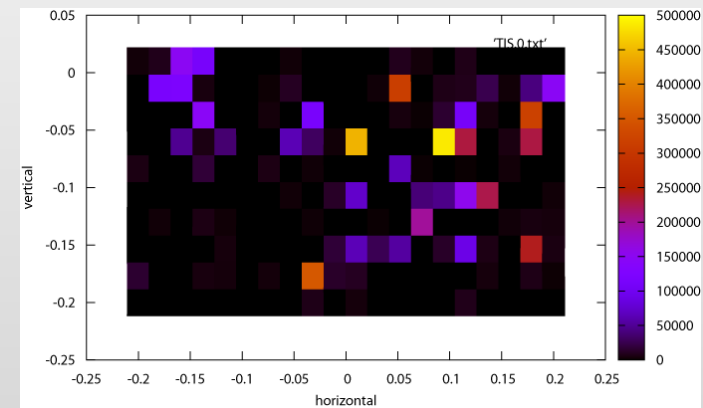
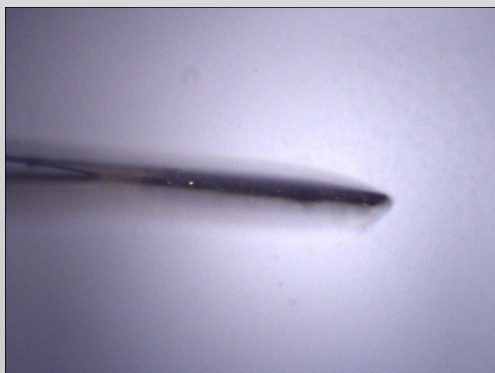
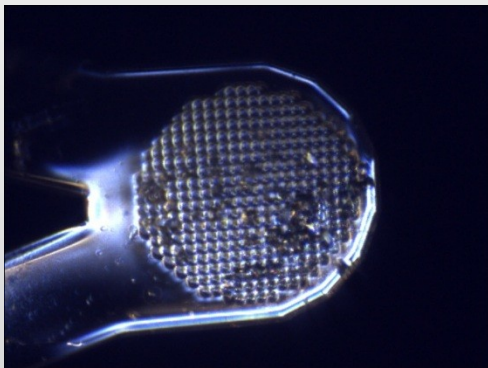
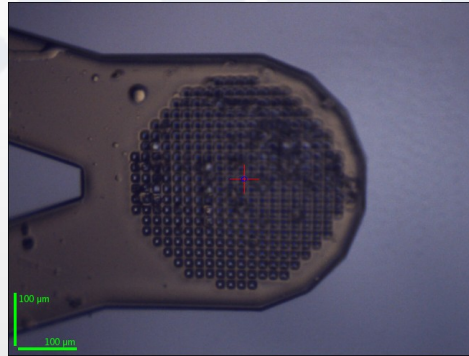


(b)

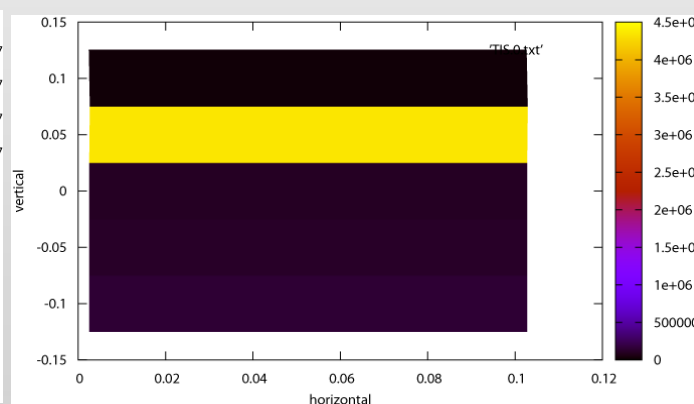
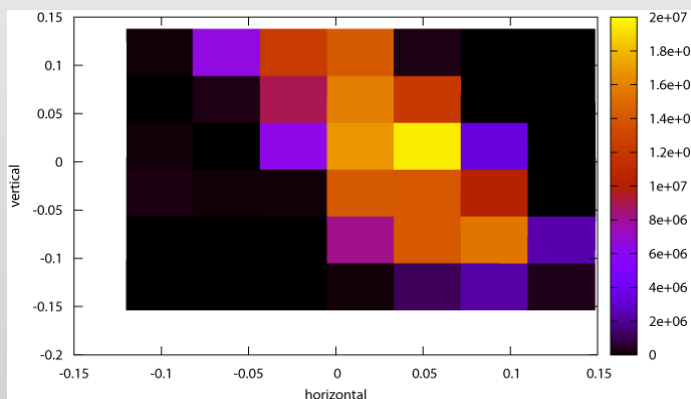
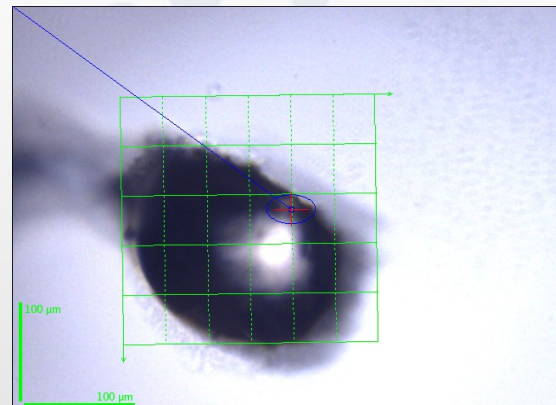
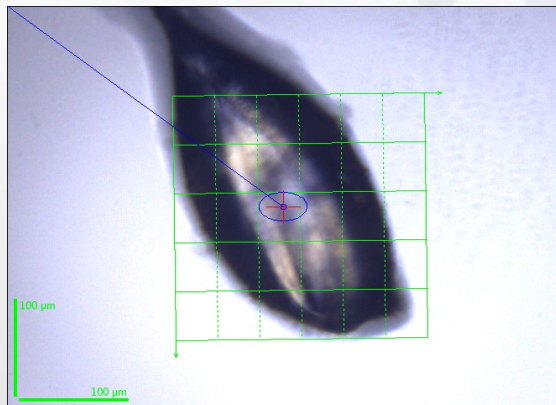


(c)

MX 3D Auto Centre



Combined workflows : Kappa reorientation and mesh scan



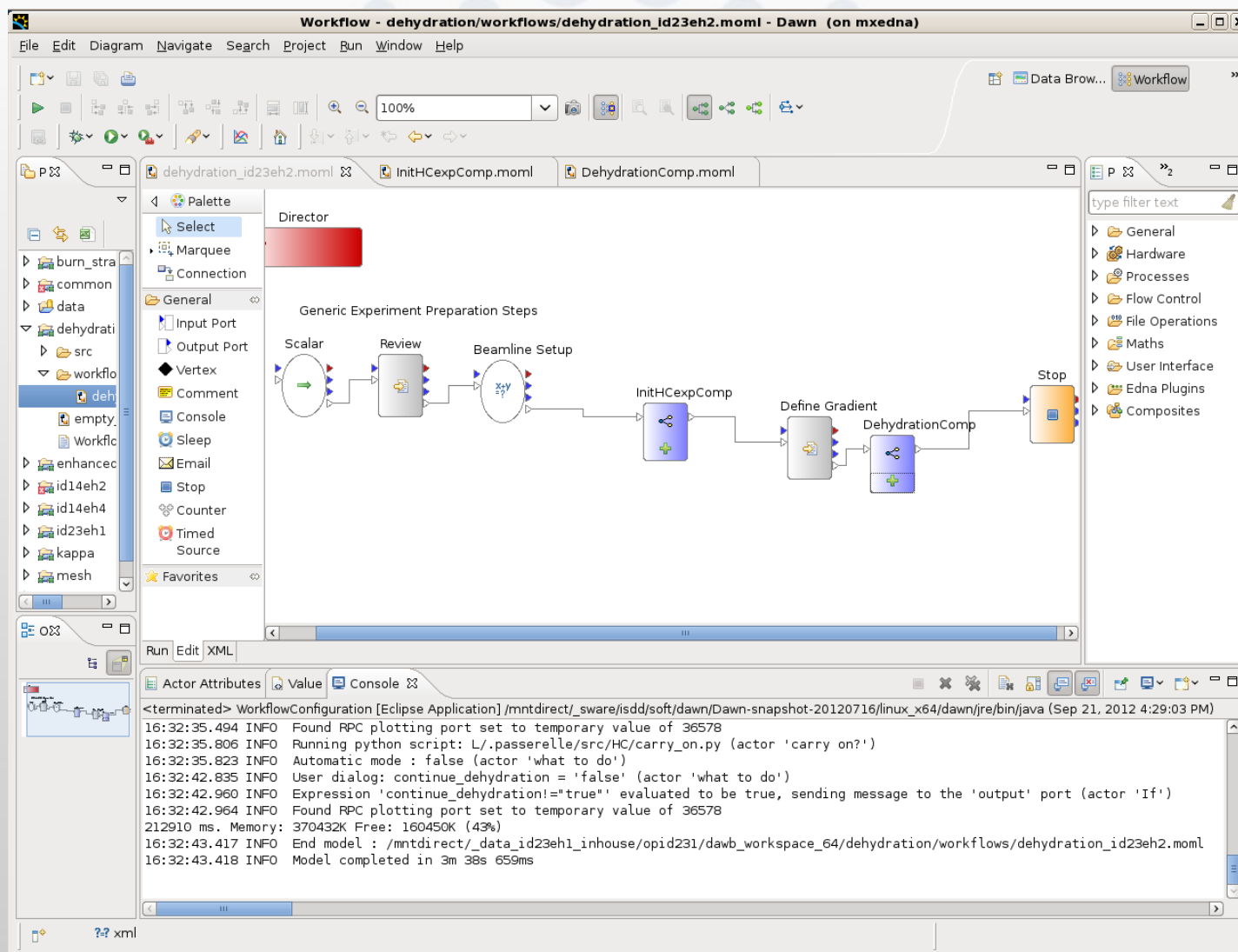
The orthorhombic sample was a very thin plate – difficult to visualise and very radiation sensitive – all standard data collections had resulted in low resolution at low completeness

Why use a workflow tool?

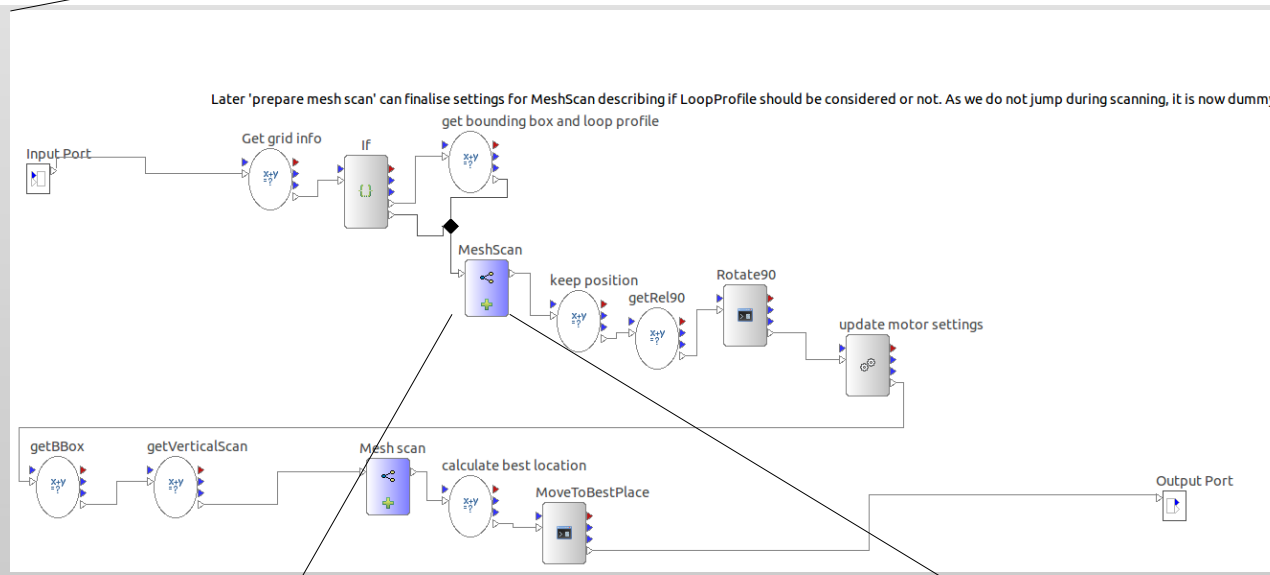
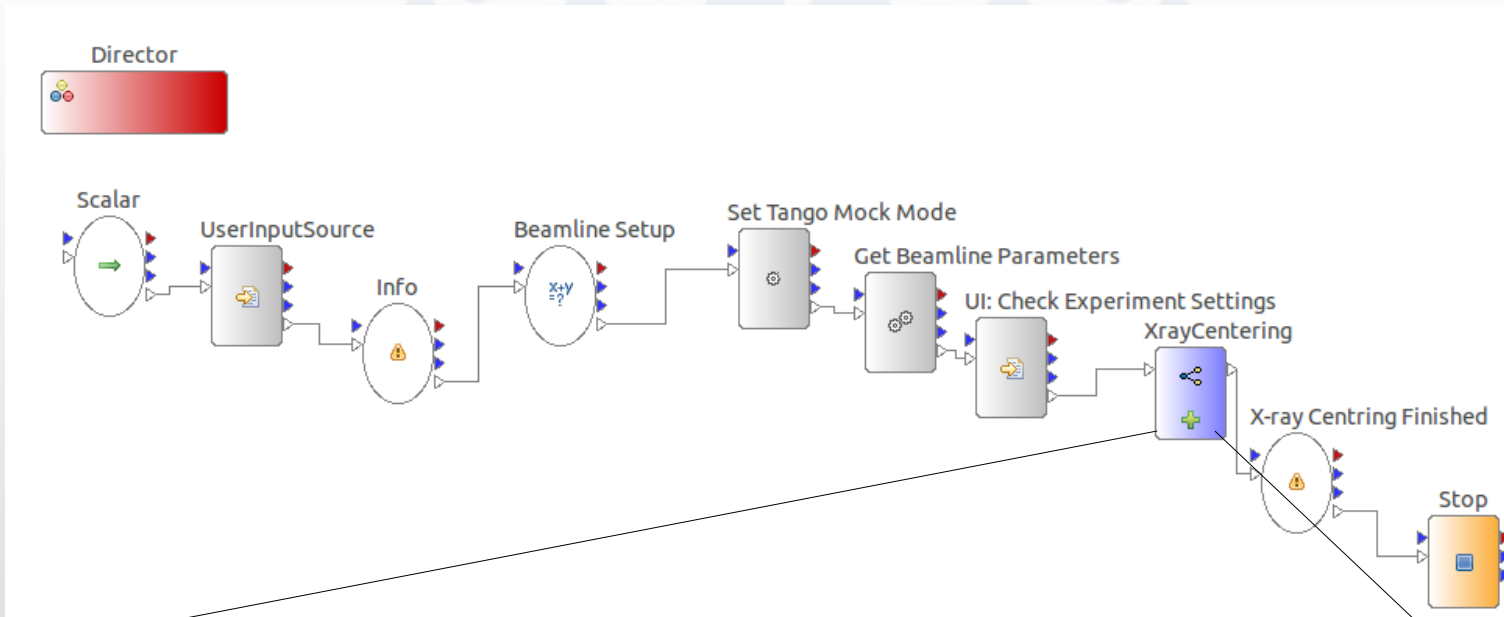
- Workflow tools for data analysis are new for synchrotron radiation facilities however they are widely used in other scientific fields e.g. biology
- They offer a higher level programming language than traditional languages like C, Python, Fortran etc
- The goal is not to replace these languages but to complement them
- Workflows facilitates development of the high level analysis:
 - Parallelism
 - Documentation
- Workflows \neq Labview

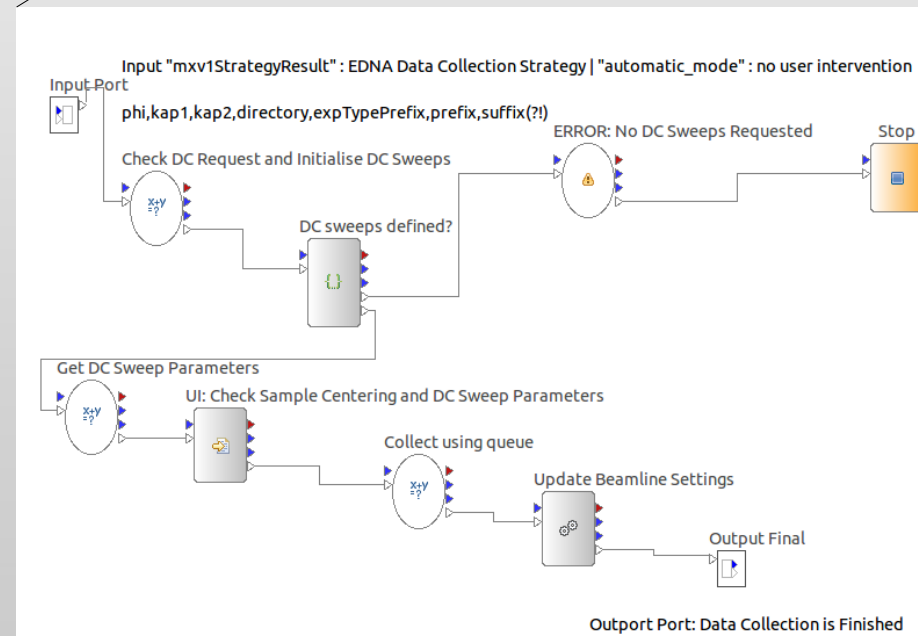
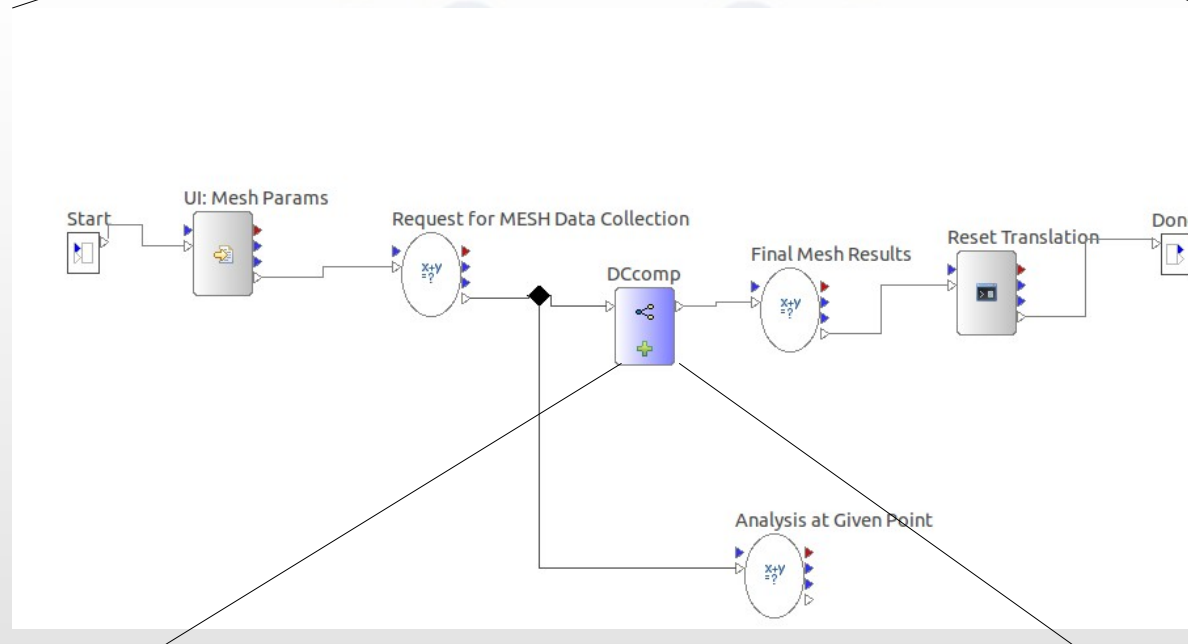


The workflow tool : DAWN and Passerelle



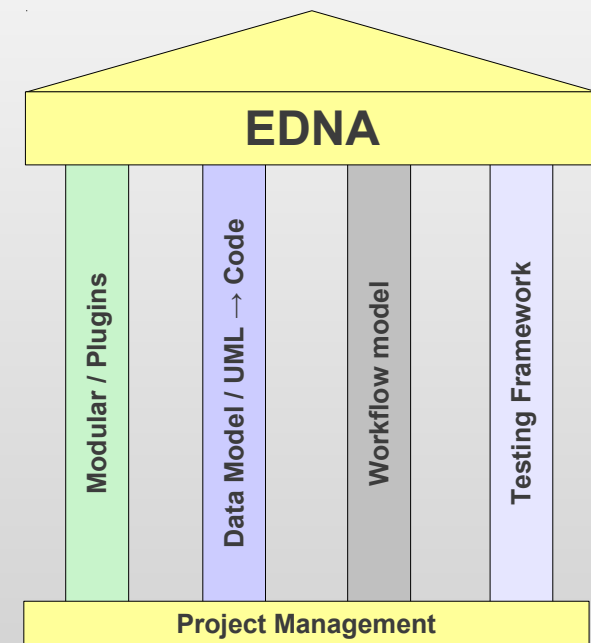
Workflow hierarchy



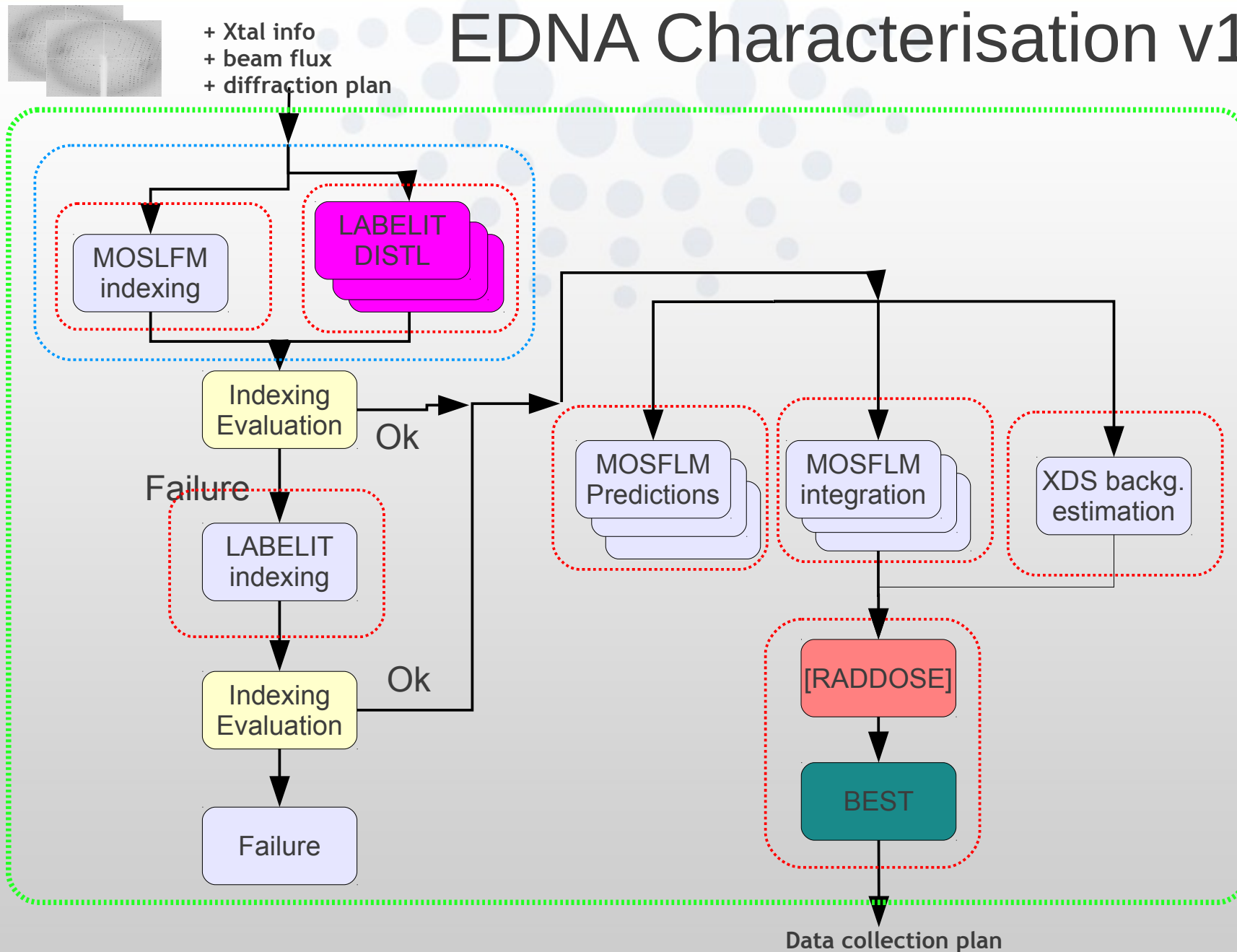


Workflows can implemented using EDNA, but EDNA is not a Workflow tool!

- EDNA is a framework aimed for online data analysis:
 - Python based
 - Data models
 - Modular / plugins
 - Workflows / pipelines
 - Strong testing
- No GUI!
 - All workflows must be programmed
 - No (built-in) visualisation of results



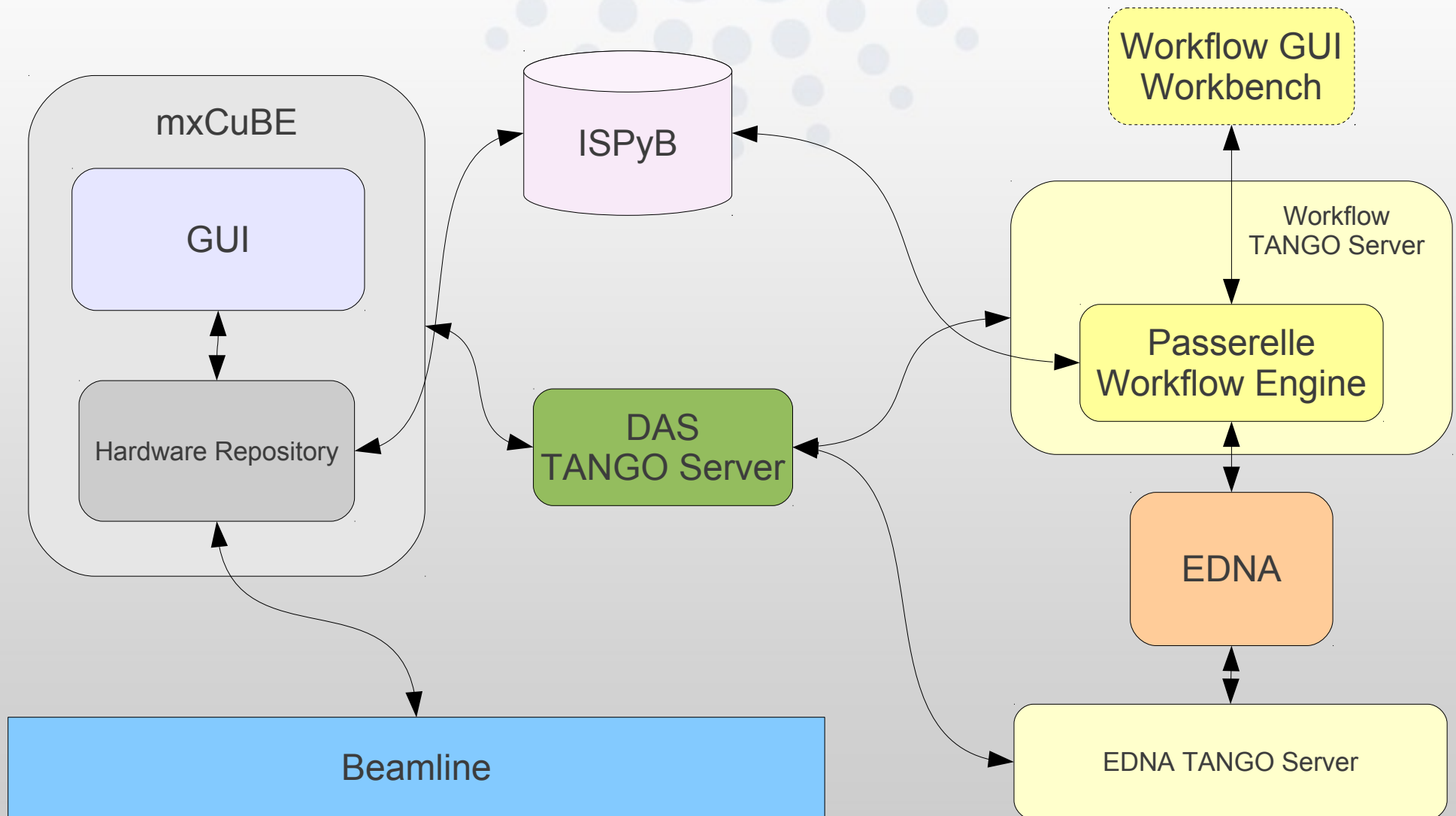
EDNA Characterisation v1.3



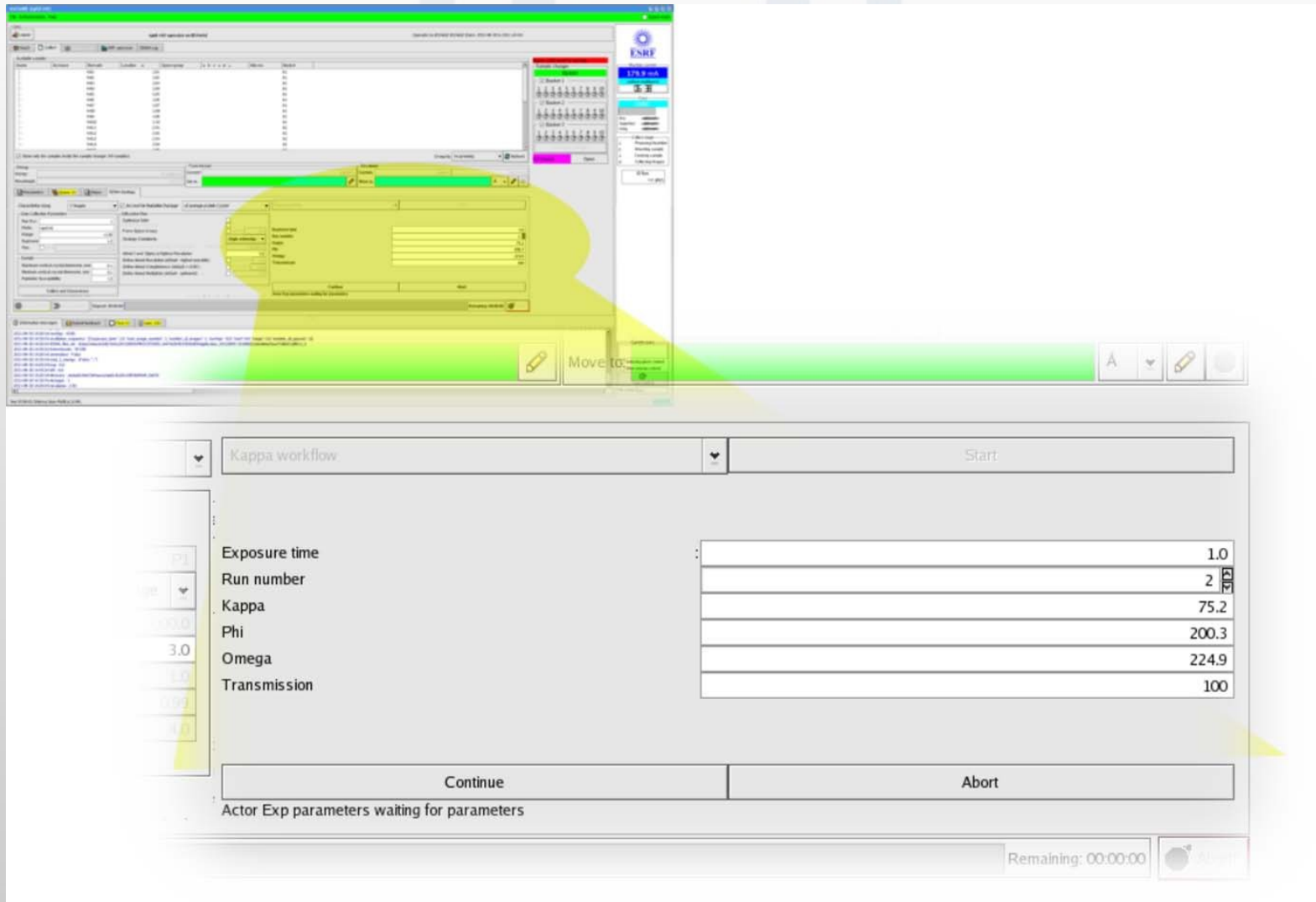
Integration of the workflow tool in beamline control / data acquisition

- Online without feedback to beamline control
 - Answers the question : "Did my experiment succeed?"
 - Fast data processing – if necessary approximative
 - Examples ESRF : BM29 (BioSAXS), ID24 (EXAFS), ID15 (High speed diffraction)
- Online with feedback to beamline control
 - Strategy calculations
 - Fast data processing but no corners cut!
 - Examples ESRF : MX

Beamline integration of EDNA and the Workflow tool



Integration of the workflow tool into mxCuBE



The screenshot displays the mxCuBE interface with the Kappa workflow tool integrated. The top window shows a workflow diagram with a yellow highlight on the 'Move to' button. The bottom window shows the 'Kappa workflow' parameters table.

| Parameter | Value |
|---------------|-------|
| Exposure time | 1.0 |
| Run number | 2 |
| Kappa | 75.2 |
| Phi | 200.3 |
| Omega | 224.9 |
| Transmission | 100 |

Buttons: Continue, Abort

Actor Exp parameters waiting for parameters

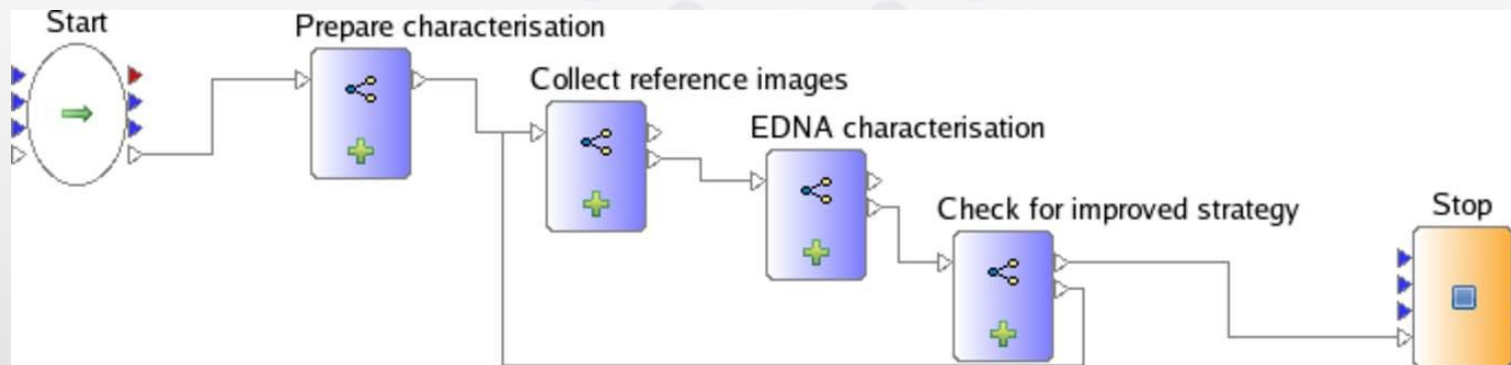
Remaining: 00:00:00

Future work

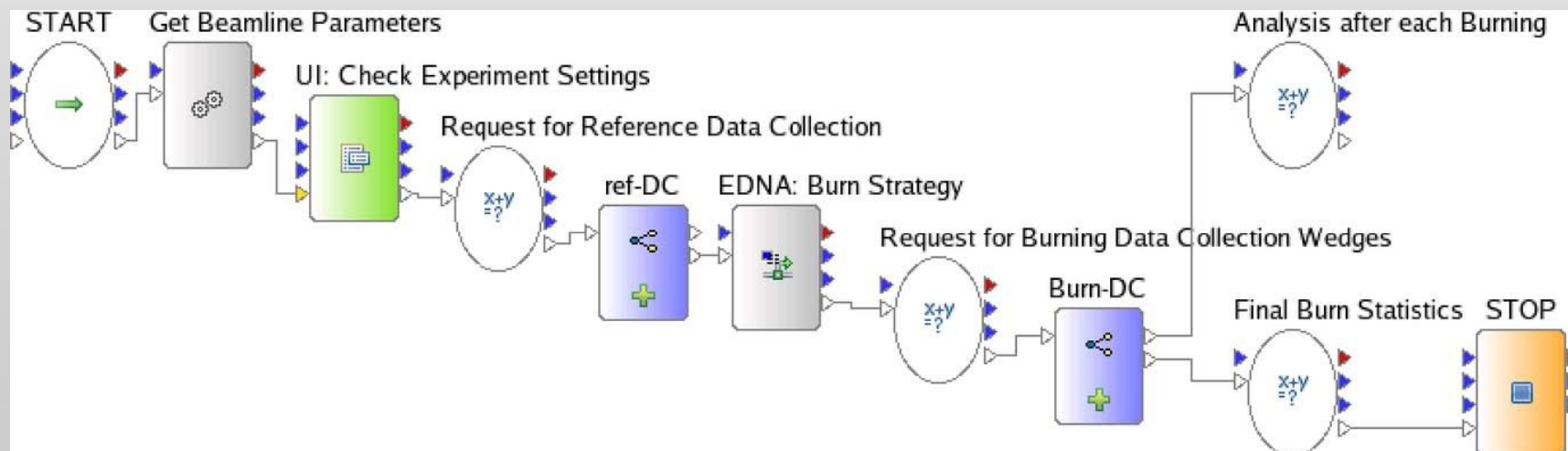
- DAWN / Passerelle :
 - Workflow-wide error handling
 - Abort
 - Debugging step execution
- MX :
 - Rapid development and deployment of more workflows
 - Improve result reports :
 - HTML pages
 - LIMS (ISPyB) integration
 - Integration into new mxCuBE

Other MX workflows

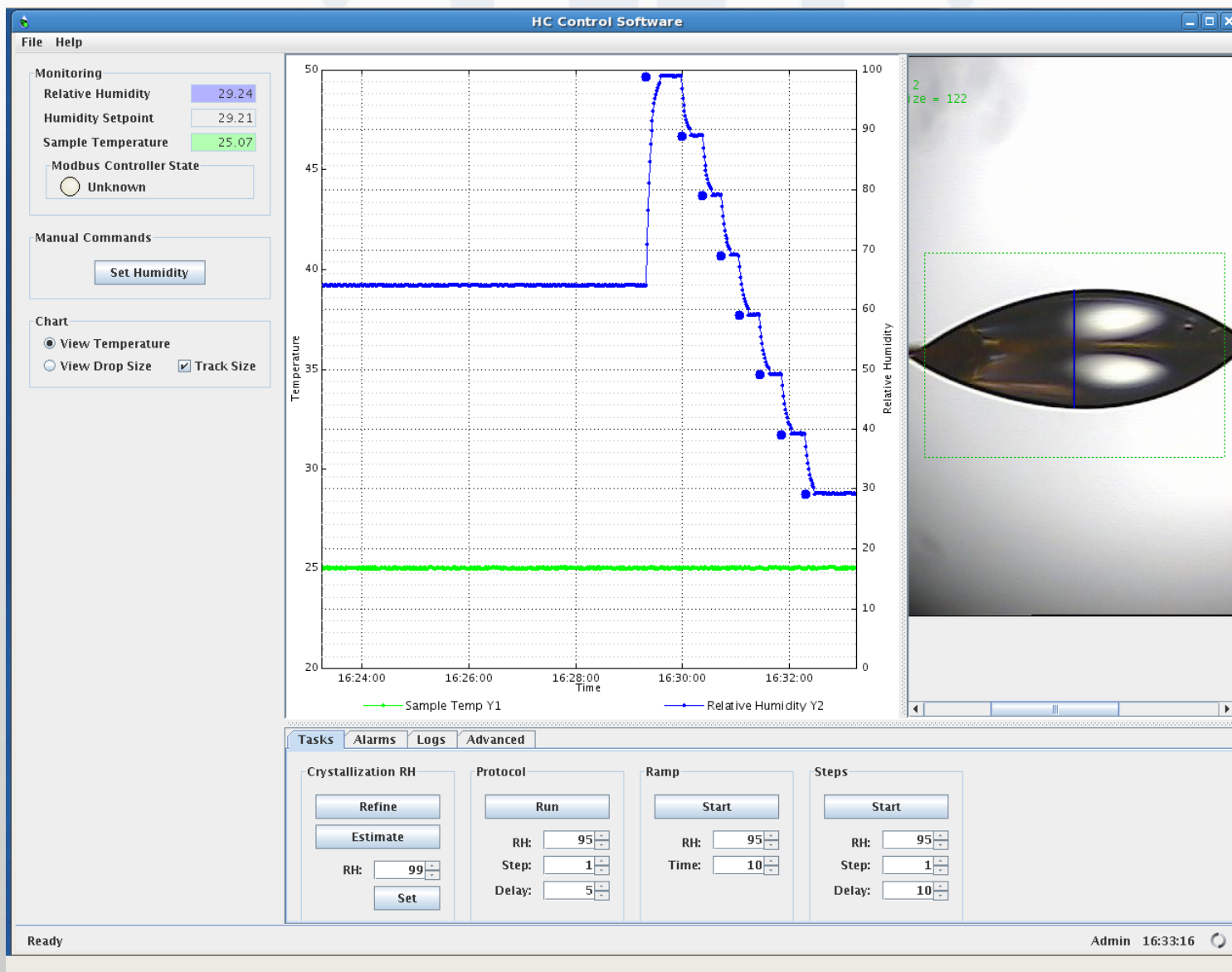
Enhanced characterisation



"Burning strategy" : Estimation of radiation damage susceptibility




Dehydration workflow



Acknowledgements

- Elspeth Gordon and Sasha Popov (ESRF MX)
- Andy Gotz and Jonathan Pommier (ESRF software)
- The DLS Scisoft Team
- The ESRF Data Analysis Unit and Beamline Control Unit

Further reading



Acta Cryst D68 (2012) 975-984
research papers

Acta Crystallographica Section D
Biological
Crystallography
ISSN 0907-4449

The use of workflows in the design and implementation of complex experiments in macromolecular crystallography

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The automation of beam delivery, sample handling and data analysis, together with increasing photon flux, diminishing focal spot size and the appearance of fast-readout detectors on synchrotron beamlines, have changed the way that many macromolecular crystallography experiments are planned and executed. Screening for the best diffracting crystal, or even the best diffracting part of a selected crystal, has been enabled by the development of microfocus beams, precise goniometers

Received 3 October 2011
Accepted 25 April 2012