



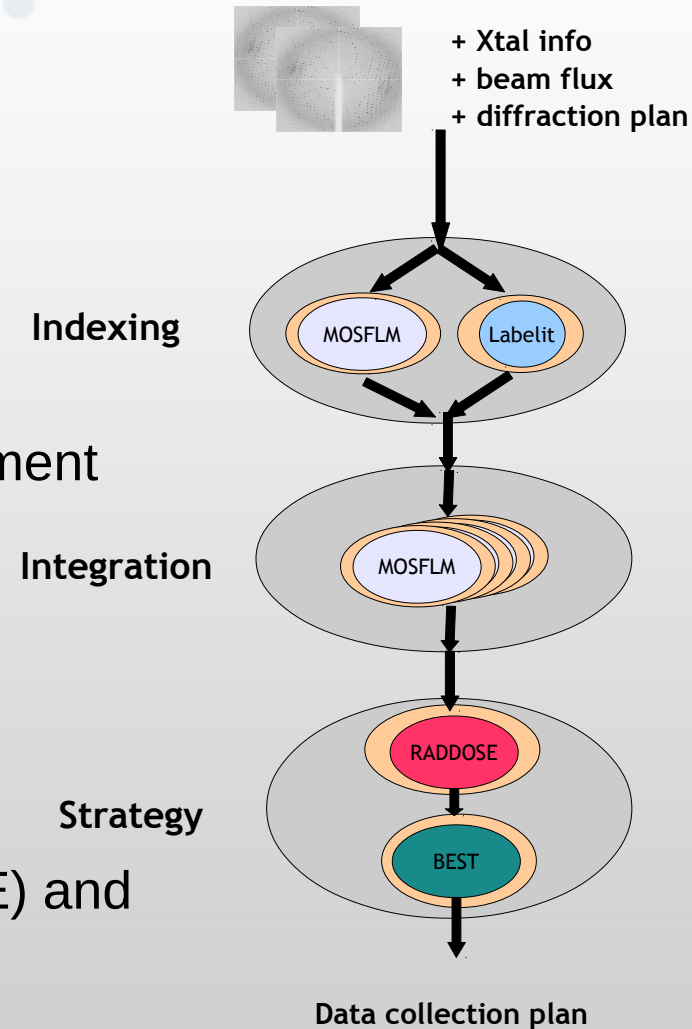
MxCuBE control of DAWN workflows

Olof Svensson

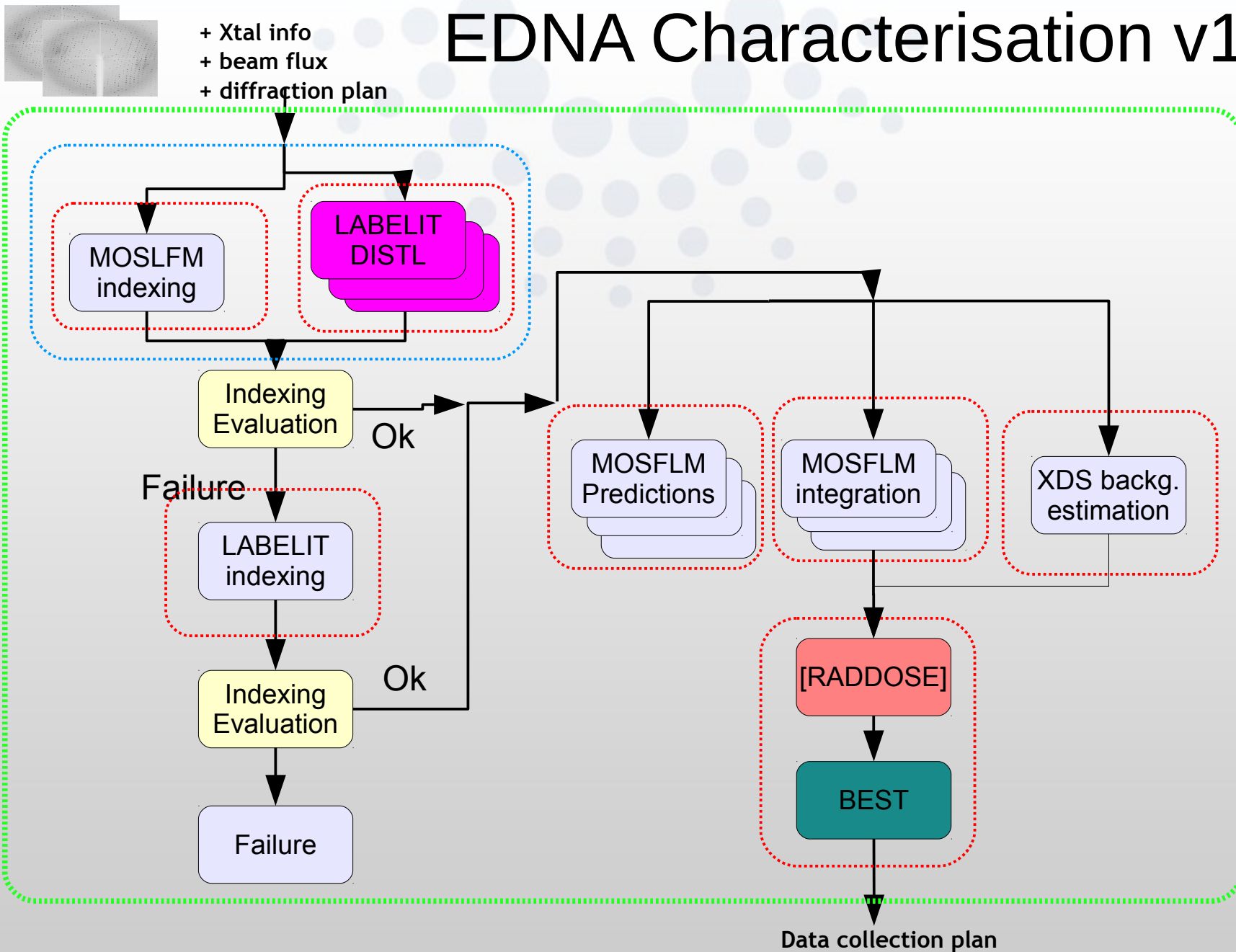
Data Analysis Unit
ISDD Software Group
ESRF

History of mxCuBE control of workflows

- DNA :
 - Separate GUI controlling prodc / mxCuBE
 - Confusing for user – two GUIs
- EDNA :
 - Processing library by design – no control of instrument
 - One GUI : mxCuBE
 - Difficult to collect data as result of processing, e.g. kappa, screening/ranking...
- DAWN :
 - Workflow tool – control of data collection (mxCuBE) and processing (EDNA)
 - One GUI : mxCuBE
 - Advanced on-line data analysis : kappa, mesh, burn strategy, dehydration etc.



EDNA Characterisation v1.3



Why use a workflow tool?

- They offer a visual, 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:
 - Visual programming → (beamline) scientists can participate in the design and make modifications
 - Parallelism, error handling
 - Documentation
- Workflow tools for data analysis :
 - Widely used in many scientific fields e.g. biology
 - New for synchrotron radiation facilities
- Workflows ≠ Labview



The workflow tool : DAWN and Passerelle



The screenshot displays the DAWN workflow tool interface. The main window shows a workflow diagram titled "Generic Experiment Preparation Steps". The workflow consists of the following components in sequence:

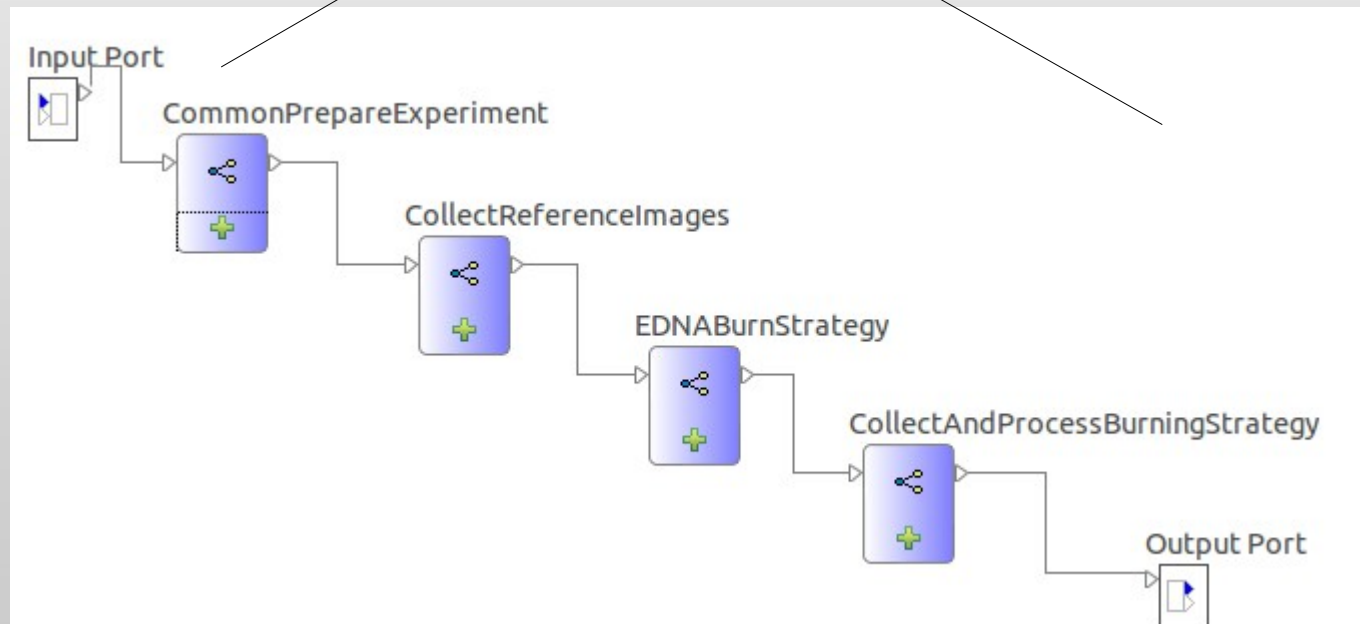
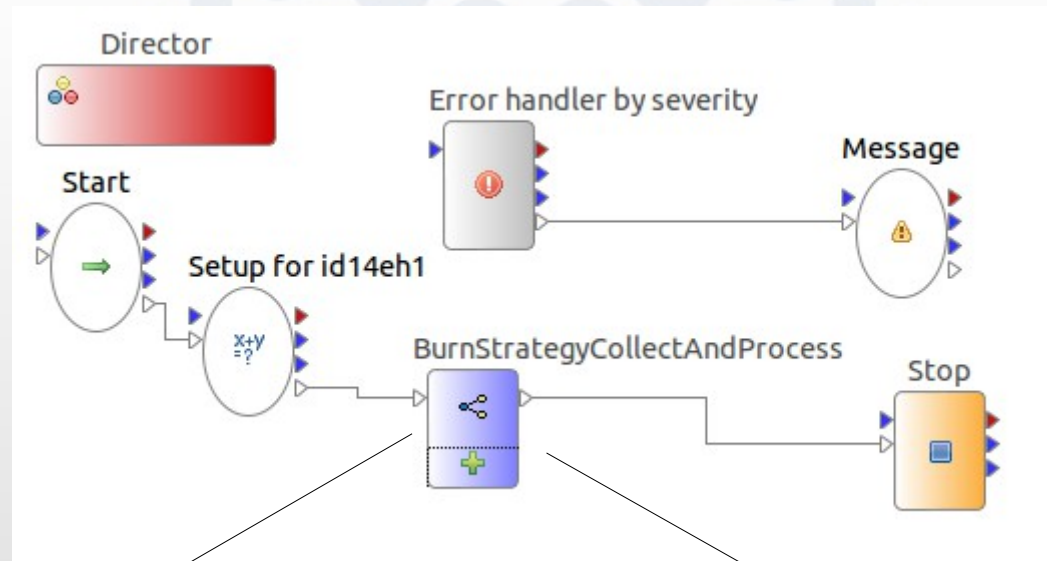
- Scalar (Input Port)
- Review (Vertex)
- Beamline Setup (Vertex)
- InitHCexpComp (Actor)
- Define Gradient (Actor)
- DehydrationComp (Actor)
- Stop (Actor)

The interface includes a Palette on the left with various components like Select, Marquee, Connection, and General. A right-hand pane shows a type filter and a list of categories including General, Hardware, Processes, Flow Control, File Operations, Maths, User Interface, Edna Plugins, and Composites.

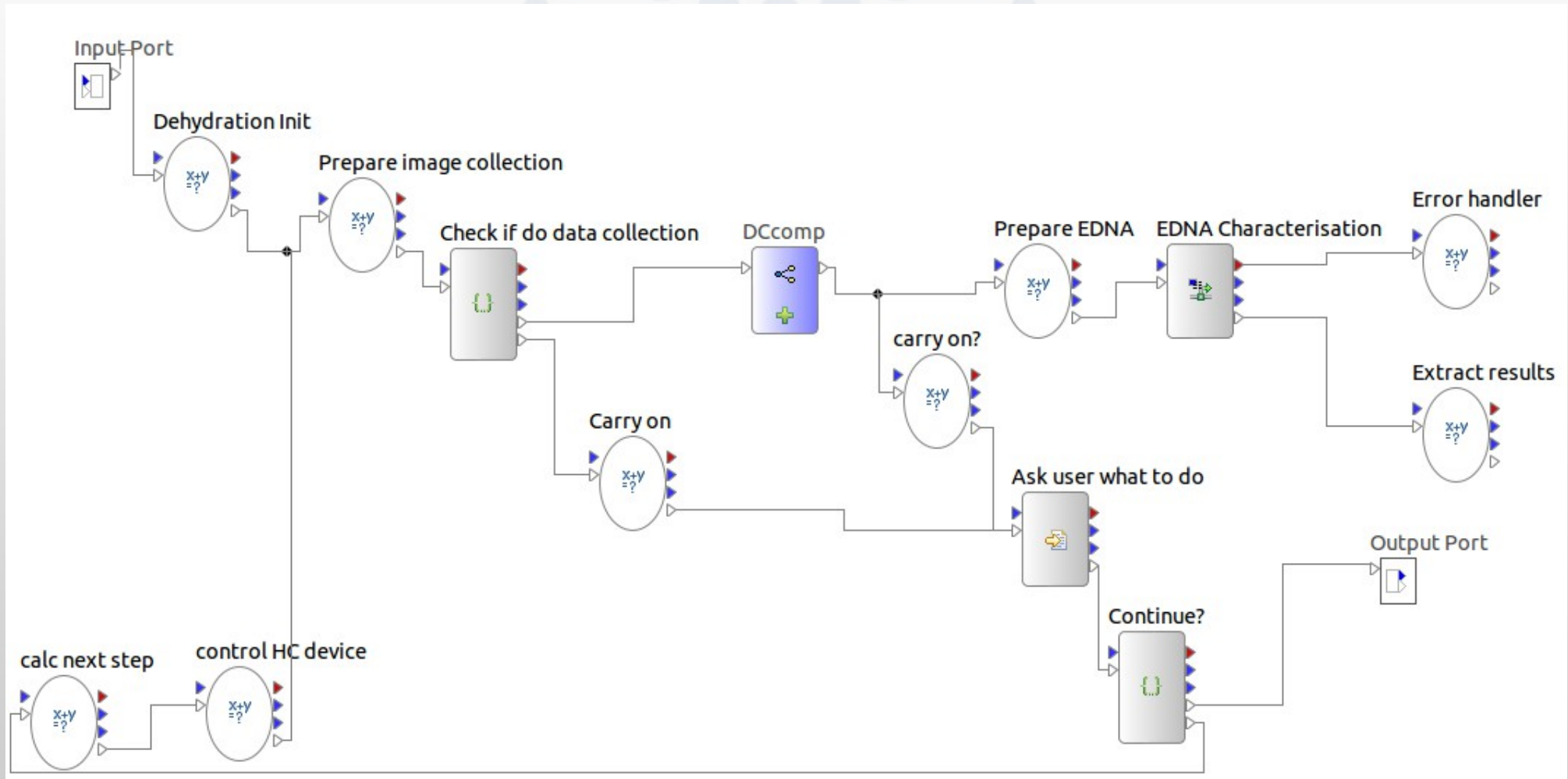
At the bottom, the console window shows the following log output:

```
<terminated> WorkflowConfiguration [Eclipse Application] /mntdirect/_sware/isdd/soft/dawn/Dawn-snapshot-20120716/linux_x64/dawn/jre/bin/java (Sep 21, 2012 4:29:03 PM)
16:32:35.494 INFO Found RPC plotting port set to temporary value of 36578
16:32:35.806 INFO Running python script: L:/passerelle/src/HC/carry_on.py (actor 'carry on?')
16:32:35.823 INFO Automatic mode : false (actor 'what to do')
16:32:42.835 INFO User dialog: continue_dehydration = 'false' (actor 'what to do')
16:32:42.960 INFO Expression 'continue_dehydration!=true' evaluated to be true, sending message to the 'output' port (actor 'If')
16:32:42.964 INFO Found RPC plotting port set to temporary value of 36578
212910 ms. Memory: 370432K Free: 160450K (43%)
16:32:43.417 INFO End model : /mntdirect/_data_id23eh1_inhouse/opid231/dawb_workspace_64/dehydration/workflows/dehydration_id23eh2.moml
16:32:43.418 INFO Model completed in 3m 38s 659ms
```

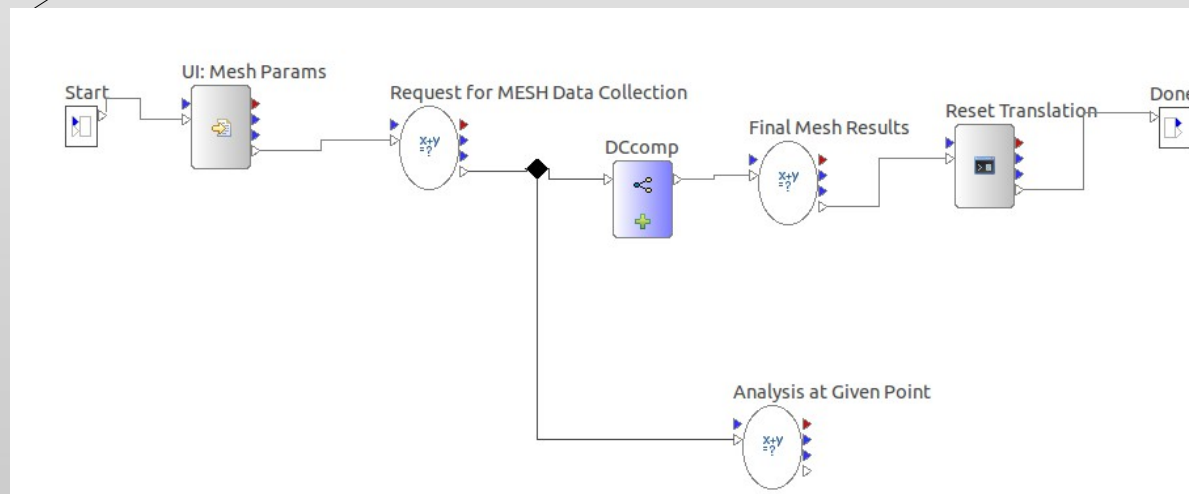
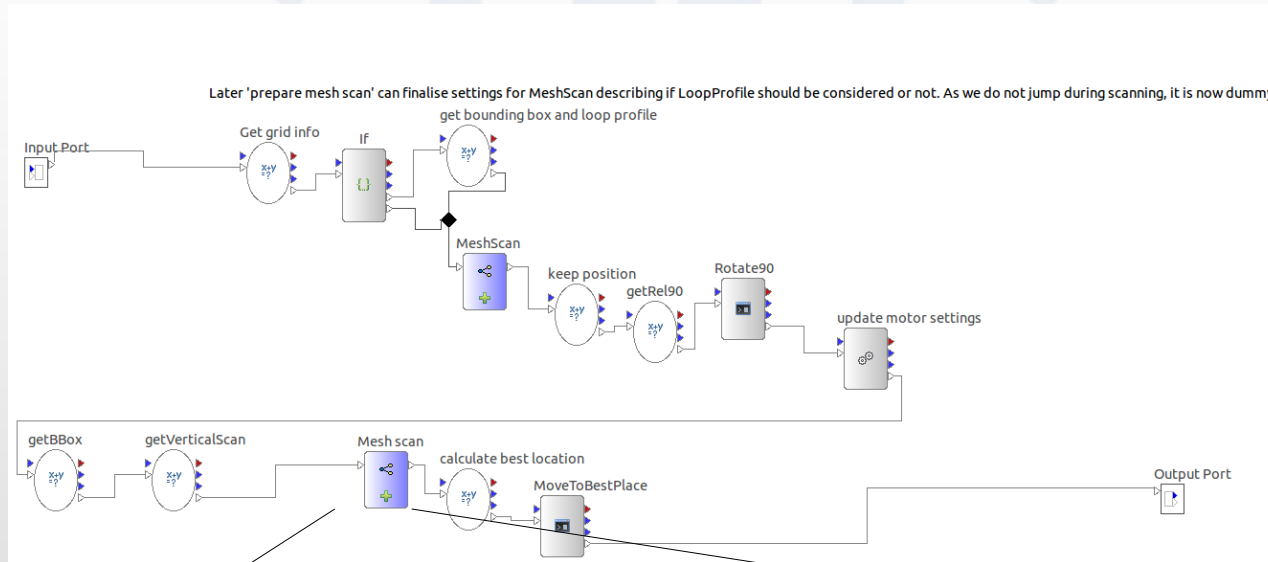
Examples: burning strategy workflow



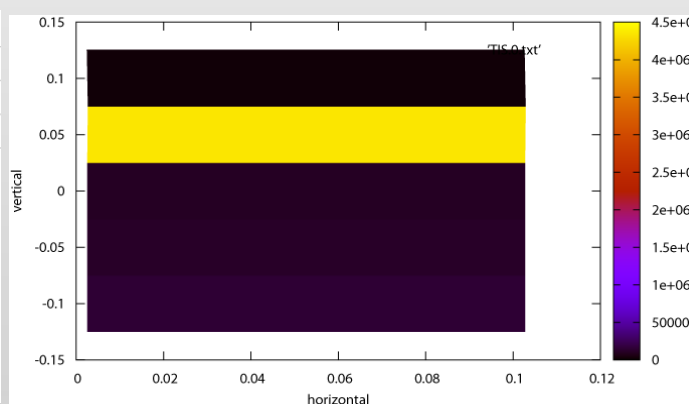
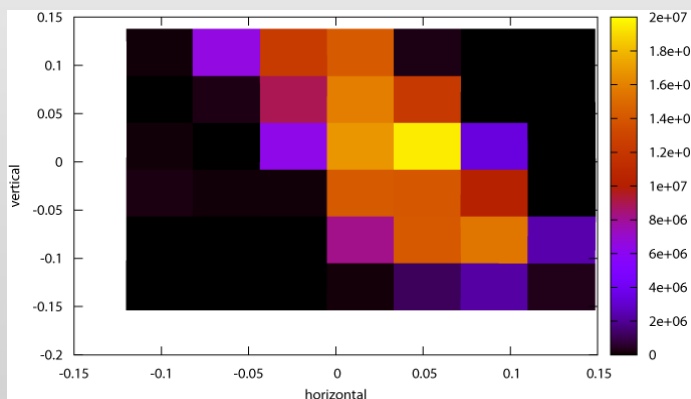
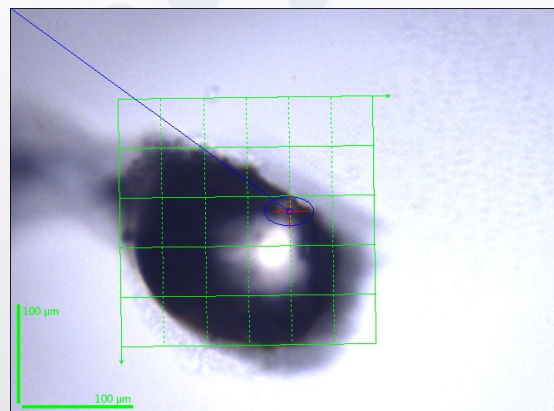
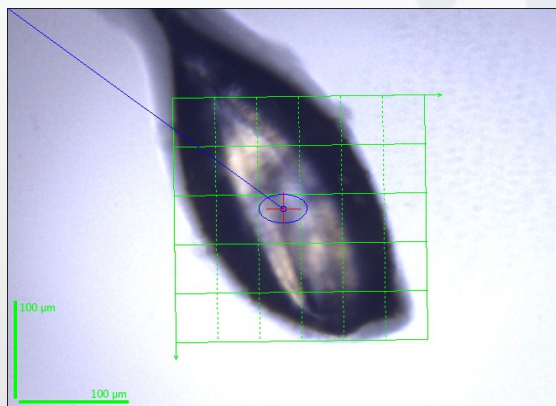
Dehydration workflow



X-ray centring (mesh) workflow

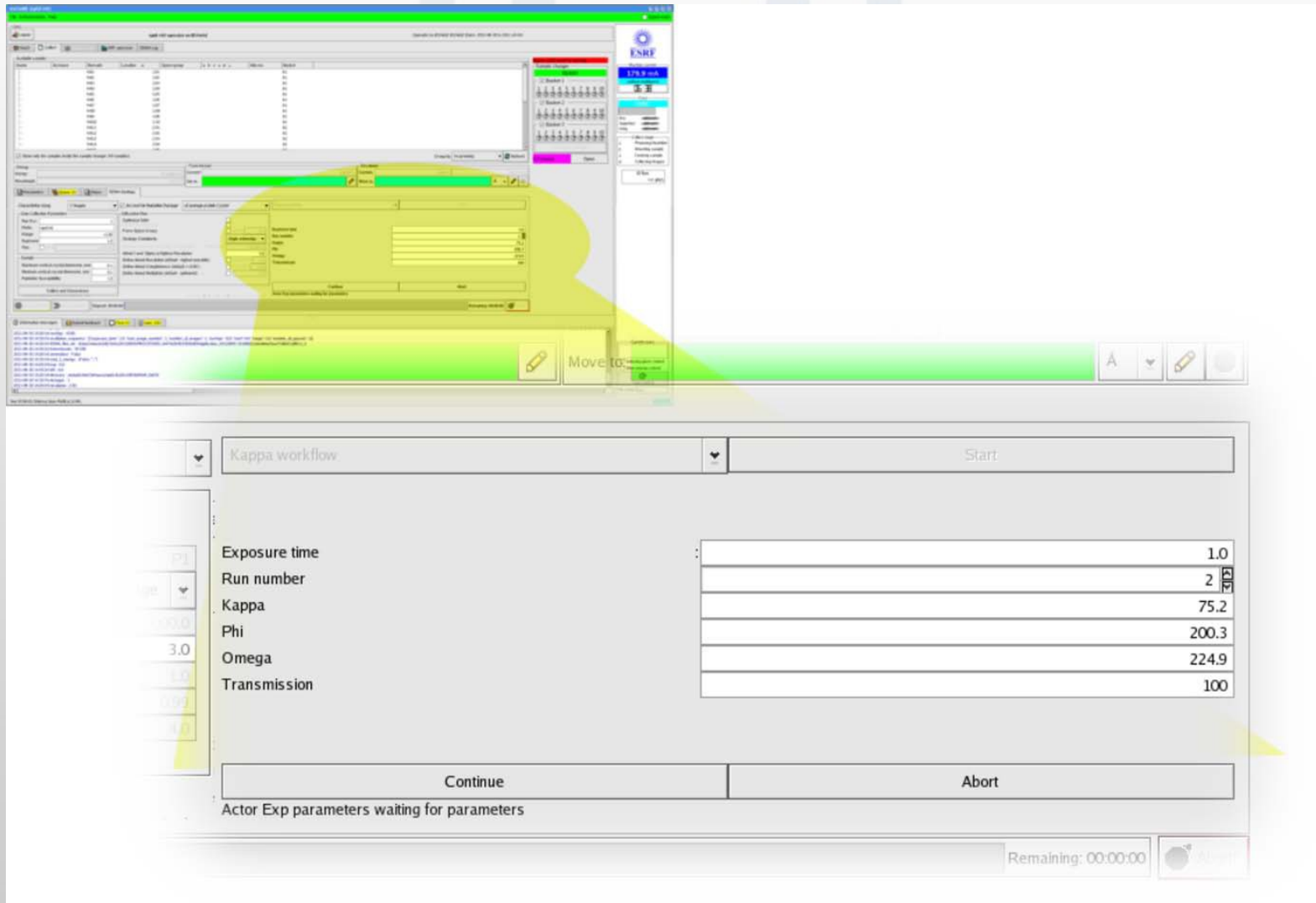


Combined workflows : Kappa reorientation and mesh scan



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

Integration of the workflow tool into (old) mxCuBE

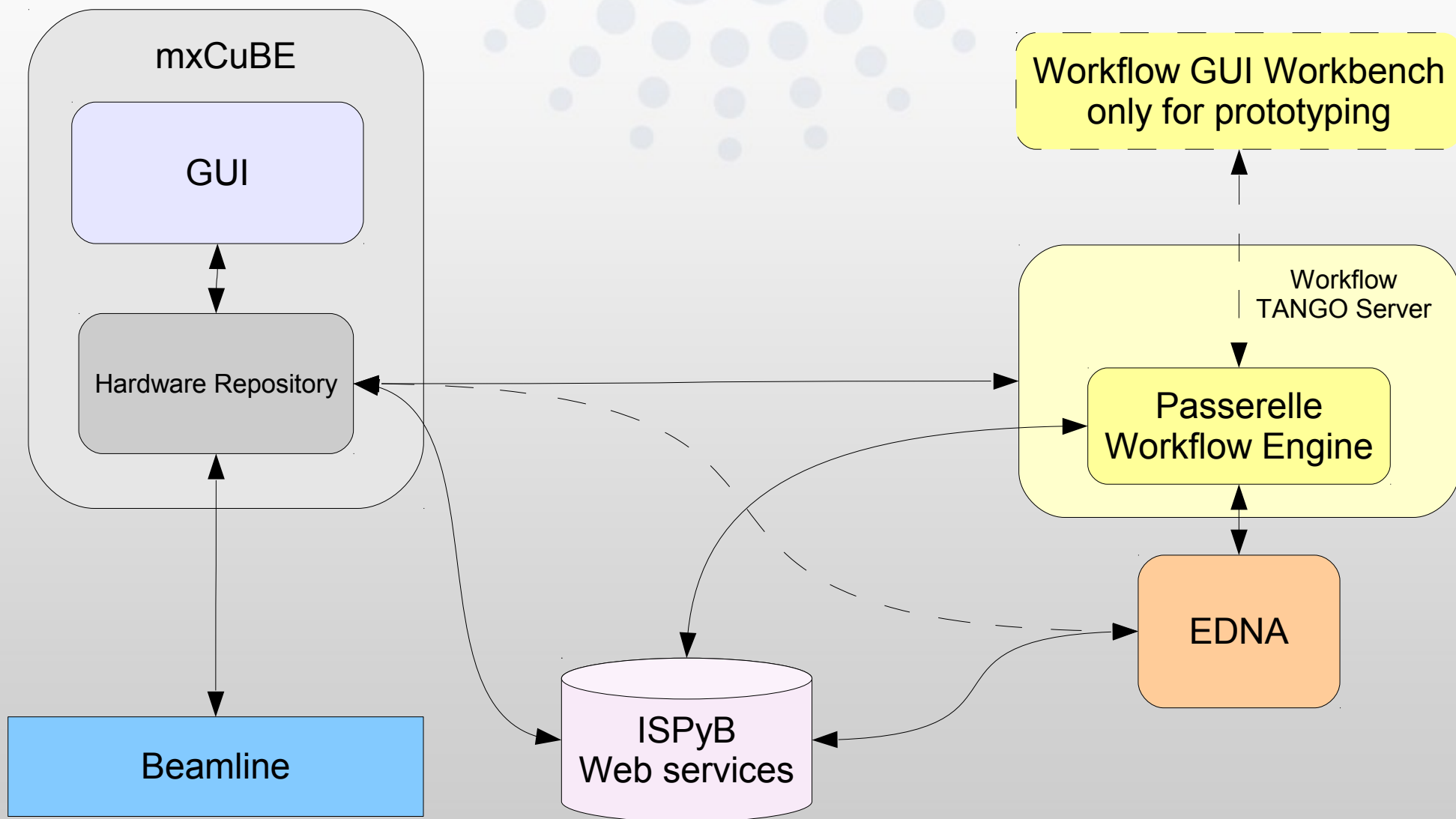


The screenshot displays the mxCuBE software interface. The top window shows a workflow configuration tool with a yellow highlight over a 'Kappa workflow' section. Below it, a parameter table is visible with the following data:

Exposure time	1.0
Run number	2
Kappa	75.2
Phi	200.3
Omega	224.9
Transmission	100

At the bottom of the interface, there are 'Continue' and 'Abort' buttons, and a status bar indicating 'Actor Exp parameters waiting for parameters' and 'Remaining: 00:00:00'.

Beamline integration of the workflow tool




Current / future developments

- Workflow in "production":
 - Improved error reporting / handling
 - Integration with ISPyB :
 - Workflow → 0..* data collection groups → 1..* data collections
 - Status : Started, success, failure etc.
 - Links to log file and results on pyarch
 - Documentation
- New MX workflows:
 - Fast mesh ID29 using 4dscan (first 1D)
 - 3D mesh scan → diffraction volume tomography
- New mxCuBE :
 - Bespoke workflow GUIs, e.g. Kappa, X-ray centring / mesh scan etc

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Further reading


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research papers

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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

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