



| The European Synchrotron

Wikipedia workflow definition:

“A workflow consists of a sequence of connected steps where each step follows without delay or gap and ends just before the subsequent step may begin”

Therefore, any experiment (manual or automated) and most computer programs can be described as a workflow!

The work described in this presentation uses a workflow tool for designing and executing the workflows for complex structural biology experiments at ESRF MX beamlines

WHY USE A WORKFLOW TOOL?

They offer a visual, higher level programming language than traditional programming 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
- Easy to implement parallelism, error handling, LIMS connection etc.
- Documentation by design!

Workflow tools for data analysis :

- Widely used in many scientific fields e.g. biology
- New for synchrotron radiation facilities

THE WORKFLOW TOOL : DAWN AND PASSERELLE

The screenshot displays the Dawn workflow tool interface. The main window shows a workflow diagram titled "Enhanced Characterisation" with the following steps: CommonPrepareExperiment, CollectReferenceImages, EDNAStrategy, and Check results. The "Check results" step is highlighted, and its properties are shown in the "Actor Attributes" panel below. The "Check results" actor has the following properties:

Property	Value
Name	Check results
Create Separate Interpreter	<input type="checkbox"/>
Dataset Outputs	newDataCollection, resolution, run_number, doRefDataCollectionReview
Interpreter Type	Python
Pass Inputs On	<input checked="" type="checkbox"/>
Python Interpreter Command	python
Python Script	mx_submodels/less/EDNACheckResults.py

To the right of the workflow diagram, a diffraction image is displayed with axes ranging from 0 to 3000 and a color scale from 0 to 1500. The image shows a central spot with a surrounding diffuse ring. The "Image Info" panel is visible below the image.

The left sidebar shows a project tree with the following structure:

- beamline
 - src
 - doc
 - macros
 - workflows
 - BeamlineBurnStrategy.moml
 - BeamlineDehydration.moml
 - BeamlineEnhancedCharacter
 - BeamlineKappa.moml 12 KB
 - BeamlineMesh1D.moml 12 K
 - BeamlineMesh2D.moml 12 K
 - BeamlineTroubleShooting.m
 - BeamlineVisualKappaAlignm
 - BeamlineXrayCentring.moml
 - WorkflowConfiguration.launch
 - python (/usr/bin/python2.7)



<http://www.dawnsci.org>



The following workflows have been deployed on ESRF MX beamlines:

Sample positioning:

- Mesh scan
- X-ray centring

Kappa goniostat re-orientation:

- Cell re-orientation using STAC (align lattice vector with rotation axis, optimise anomalous signal etc)
- Visual sample re-orientation

Sample characterisation:

- Enhanced EDNA characterisation
- Helical EDNA characterisation

Automatic control of dehydration device

Automatic estimate of crystal radiation damage susceptibility (burn strategy)

VISUAL KAPPA GONIOSTAT RE-ORIENTATION

mxCuBE (opid-144) Expert mode

File Instrumentation Help Collect XRF spectrum System Feedback Chat

User
Logout **opid-144**

Sample list
Mode: Sample changer Show SC-details
Centring: Automatic loop centring Synch ISPyB

- 1.1
- 1.2
- 1.3
- 1.4
- 1.5
- 1.6
- 1.7
- 1.8
- 1.9
- 1.10
- 2.1
- 2.2
- 2.3
- 2.4
- 2.5
- 2.6
- 2.7
- 2.8
- 2.9
- 2.10
- 3.1
- 3.2
- 3.3
- 3.4
- 3.5
- 3.6
- 3.7
- 3.8
- 3.9
- 3.10
- 4.1
- 4.2
- 4.3
- 4.4
- 4.5
- 4.6
- 4.7
- 4.8
- 4.9
- 4.10

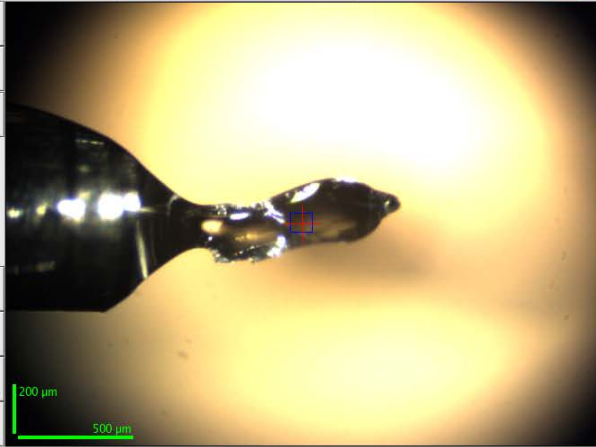
Collect Queue Pause

Sample centring

Sample position
Omega: 59.96 20 Kappa: 0.0 10 Phi: 0.0 10.0

Holder length: 21.768 0.1

Sample video
Light: 0.6 Focus: -0.096 0.05 Front light: 2.0 Zoom: 1



200 μ m
500 μ m

Hor: 0.1 Ver: 0.1 0.01 Move: Offsets

Collection method

Discrete
Characterise
Helical
Energy Scan

Advanced
Workflow type
Burn Strategy

Data location
Folder: /data/id14eh4/inhouse/opid144/20131030/RAW_DATA/
Prefix: opid144
Run number: 1

Grid
Nb points

	points per line	steps (mm)	distance
Axis 1	2		
Axis 2	2		

Show Grab

Add to queue

Machine current
177.0 mA
7/8 multibunch
05:03
Flux: +0.00 ph/s

Energy
Current: 12.694 keV 0.976
Move to: keV

Resolution
Current: 2.302 Å 330.61 mm
Move to: Å

Transmission
Current: 100.00%
Set to: Filters

Cryo
-1.0 K

Safety shutter closed

Fast shutter closed

Beamstop in

Current users
 Selecting gives control
 Allow timeout control
Take control
My name: artemis2

[2013-10-30 14:27:33] Cannot find appropriate attenuation, scan aborted

[2013-10-30 14:27:33] Queue execution was aborted, queue stopped.

[2013-10-30 14:30:35] The current path settings will overwrite data from another task. Correct the problem before adding to queue

VISUAL KAPPA GONIOSTAT RE-ORIENTATION

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: opid-144

Logout

Sample list

Mode: Sample changer Show SC-details

Centring: Automatic loop centring Synch ISPyB

- 1.1
 - Visual Re-orientation - 1
 - sample-centring
 - opid144 - 0
- 1.2
- 1.3
- 1.4
- 1.5
- 1.6
- 1.7
- 1.8
- 1.9
- 1:10
- 2.1
- 2.2
- 2.3
- 2.4
- 2.5
- 2.6
- 2.7
- 2.8
- 2.9
- 2:10
- 3.1
- 3.2
- 3.3
- 3.4
- 3.5
- 3.6
- 3.7
- 3.8
- 3.9
- 3:10
- 4.1
- 4.2
- 4.3
- 4.4
- 4.5
- 4.6
- 4.7

Collect Queue Pause

Sample centring

Sample position

Omega: 59.96 20 Kappa: 0.0 10 Phi: 0.0 10.0

Holder length: 21.768 0.1

Sample video

Light: 0.6 Focus: -0.096 0.05 Front light: 2.0 Zoom: 1

Centre

Save

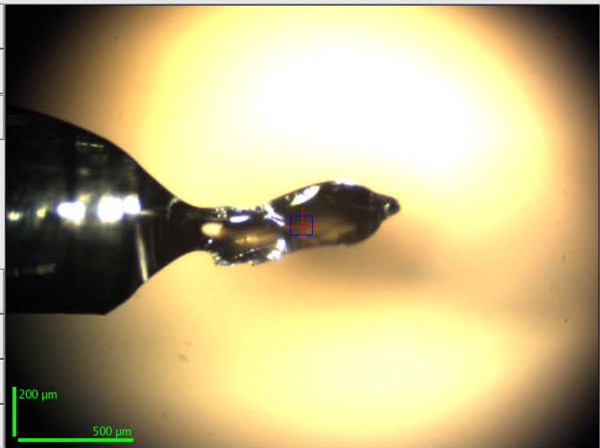
Snapshot

Centre beam

Quick realign

Take snapshots

Anneal



Hor: 0.1 0.01 Ver: 0.1 0.01 Move: Offsets

Collection method

Discrete

Characterise

Helical

Energy Scan

Advanced

Workflow type: Visual Re-orientation

Data location

Folder: /data/id14eh4/inhouse/opid144/20131030/RAW_DATA/ Browse

Prefix: opid144

Run number: 2

Grid

	points per line	steps (mm)	distance
Axis 1	2		
Axis 2	2		

Show Grab

Add to queue

Machine current

176.9 mA

78 multibunch

06:02

Flux: +0.00 ph/s

Energy

Current: 12.694 keV 0.976

Move to: keV

Resolution

Current: 2.302 Å 330.61 mm

Move to: Å

Transmission

Current: 100.00%

Set to: Filters

Cryo

-1.0 K

Safety shutter: closed

Fast shutter: closed

Beamstop: in

Current users

Selecting gives control

Allow timeout control

Take control

My name: artemis2

[2013-10-30 14:27:33] Cannot find appropriate attenuation, scan aborted!

[2013-10-30 14:27:33] Queue execution was aborted, queue stopped.

[2013-10-30 14:30:35] The current path settings will overwrite data from another task. Correct the problem before adding to queue

mxCuBE ISPyB

Front End & Vacuum

Shell - Konsole

Shell - Konsole <2>

mxCuBE (opid-144)

jidappli 2.3

Vacuum Viewer 1.11 [users/h]

Dserver

VISUAL KAPPA GONIOSTAT RE-ORIENTATION

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: **opid-144** [Logout]

Sample list: Mode: Sample changer [Show SC-details] Centring: Automatic loop centring [synchronise]

Sample centring: Sample position Omega: 59.96 Kappa: 0.0 Phi: 0.0 Holder length: 22.108

Sample video: Light: 0.6 Focus: -0.096 Front light: 2.0 Zoom: 1

Collection method: Discrete, Characterise, Helical, Energy Scan. Advanced: Workflow type: Visual Re-orientation

Data location: Folder: /data/nd14eb4/inhouse/opid144/20131030/RAW_DATA/ Prefix: opid144 Run number: 2

Grid: No points table with columns: points_per_line, steps (mm), distance

Machine current: 176.9 mA Flux: 7/8 multibunch 05:01 Flux: +0.00 ph/s Energy: 12.694 keV Current: 0.976 Move to: keV Resolution: 2.302 Å Current: 330.61 mm Move to: Å Transmission: 100.00% Set to: Filters Cryo: -1.0 K

Safety shutter: closed Fast shutter: closed Beamstop: in Current users: [empty] [Take control] My name: artemis2

Log: [2013-10-30 14:27:33] Queue execution was aborted, queue stopped. [2013-10-30 14:30:35] The current path settings will overwrite data from another task. Correct the problem before adding to queue. [2013-10-30 14:57:19] Please select a centred position.

VISUAL KAPPA GONIOSTAT RE-ORIENTATION

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: opid-144

Sample list:

- 1:1
 - Visual Re-orientation - 1
 - sample-centring Input accepted
 - opid144 - 0
 - VisualKappa - 0
 - Centre first position Input accepted
 - Centre second position Waiting for input
- 1:2
- 1:3
- 1:4
- 1:5
- 1:6
- 1:7
- 1:8
- 1:9
- 1:10
- 2:1
- 2:2
- 2:3
- 2:4
- 2:5
- 2:6
- 2:7
- 2:8
- 2:9
- 2:10
- 3:1
- 3:2
- 3:3
- 3:4
- 3:5
- 3:6
- 3:7
- 3:8
- 3:9
- 3:10
- 4:1
- 4:2
- 4:3
- 4:4

Sample centring

Sample position: Omega: 59.97, Kappa: 0.0, Phi: 0.0, Holder length: 21.439

Sample video: Light: 0.6, Focus: -0.096, Front light: 2.0, Zoom: 1

Collection method: Discrete, Characterise, Helical, Energy Scan

Advanced: Workflow type: Visual Re-orientation

Data location: Folder: data\nd14eb4\inhouse\opid144\20131030\RAW_DATA/

Prefix: opid144, Run number: 2

Grid:

No. points	points per line	steps (mm)	distance
Axis-1	2		
Axis-2	2		

Machine current: 176.6 mA, Flux: +0.00 ph/s, Energy: 12.694 keV, Resolution: 2.302 Å, Transmission: 100.00%, Cryo: -1.0 K

Safety shutter: closed, Fast shutter: closed, Beamstop: in

Current users: artemis2

Hor: 0.1, Ver: 0.1, Move: Offsets

200 µm, 500 µm

Stop, Continue

Workflow: First position: sampx=-1.562 mm, sampy=-1.069 mm and phiy=22.147 mm
 Workflow: Please centre the second position
 Please select a centred position.

VISUAL KAPPA GONIOSTAT RE-ORIENTATION

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: **opid-144** [Logout]

Sample list: Mode: Sample changer [Show SC-details] Centring: Automatic loop centring [Synch ISPyB]

Sample centring: Sample position Omega: 139.95 [20] Kappa: 55.47 [10] Phi: 59.52 [10.0] Holder length: 21.545 [0.1]

Sample video: Light: 0.6 [Focus: -0.096 [0.05] Front light: 2.0 [Zoom: 1]

Centre beam Quick realign Take powder Anneal

Hor: 0.1 [Ver: 0.1 [Move: Offsets]

Collection method: Discrete Characterise Helical Energy Scan Advanced Workflow type: Visual Re-orientation Data location: Folder: [data\d14eb\inhouse\opid144\20131030\RAW_DATA] Prefix: opid144 Run number: 2 Grid: No points: [points_per_line: 2, steps (mm):, distance:] [Show] [Grab]

Machine current: 176.6 mA Flux: +0.00 ph/s Energy: [Current: 12.694 keV 0.976] Move to: [keV] Resolution: 2.302 Å [330.61 mm] Move to: [Å] Transmission: Current: 100.00% Set to: [Filters] Cryo: -1.0 K

Safety shutter: closed Fast shutter: closed Beamstop: in Current users: [Selecting gives control] [Allow timeout control] Take control My name: artemis2

1:1 Visual Re-orientation - 1 Input accepted sample-centring opid144 - 0 VisualKappa - 0 Centre first position Input accepted Centre second position Input accepted 1:2 1:3 1:4 1:5 1:6 1:7 1:8 1:9 1:10 2:1 2:2 2:3 2:4 2:5 2:6 2:7 2:8 2:9 2:10 3:1 3:2 3:3 3:4 3:5 3:6 3:7 3:8 3:9 3:10 4:1 4:2 4:3 4:4

Collect Queue Pause

[2013-10-30 15:03:38] Workflow: Second position: sampx=-1.729 mm, sampy=-0.851 mm and phiy=21.440 mm
 [2013-10-30 15:03:38] Workflow: Kappa angle calculated to be 55.5 degrees
 [2013-10-30 15:03:38] Workflow: Phi angle calculated to be 59.5 degrees

VISUAL KAPPA GONIOSTAT RE-ORIENTATION

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: **opid-144** [Logout]

Sample list: Mode: Sample changer [Show SC-details] Centring: Automatic loop centring [Synch ISPyB]

Sample centring: Sample position Omega: 12.04 [90] Kappa: 55.47 [10] Phi: 59.52 [10.0] Holder length: 21.841 [0.1]

Sample video: Light: 0.6 [Focus: -0.096 [0.05] Front light: 3.0 [Zoom: 1]

Centre Save Snapshot

Centre beam Quick realign Fake powder Anneal

Grid grab, select the area Hor: 0.05 [Ver: 0.05 [0.01] Move: Offsets

Collection method: Discrete Characterise Helical Energy Scan Advanced Workflow type: X-ray Centring

Data location: Folder: /data/id14eh4/inhouse/opid144/20131030/RAW_DATA/ Prefix: opid144 Run number: 2

Grid: Nb points

	points per line	steps (mm)	distance
Axis 1	15	0.054690	0.765659
Axis 2	3	0.085942	0.171883

Show Grab

Machine current: 175.2 mA Flux: +0.00 ph/s Energy: 12.694 keV [0.976] Resolution: 2.302 Å [330.64 mm] Transmission: 100.00% [Set to: Filters] Cryo: -1.0 K

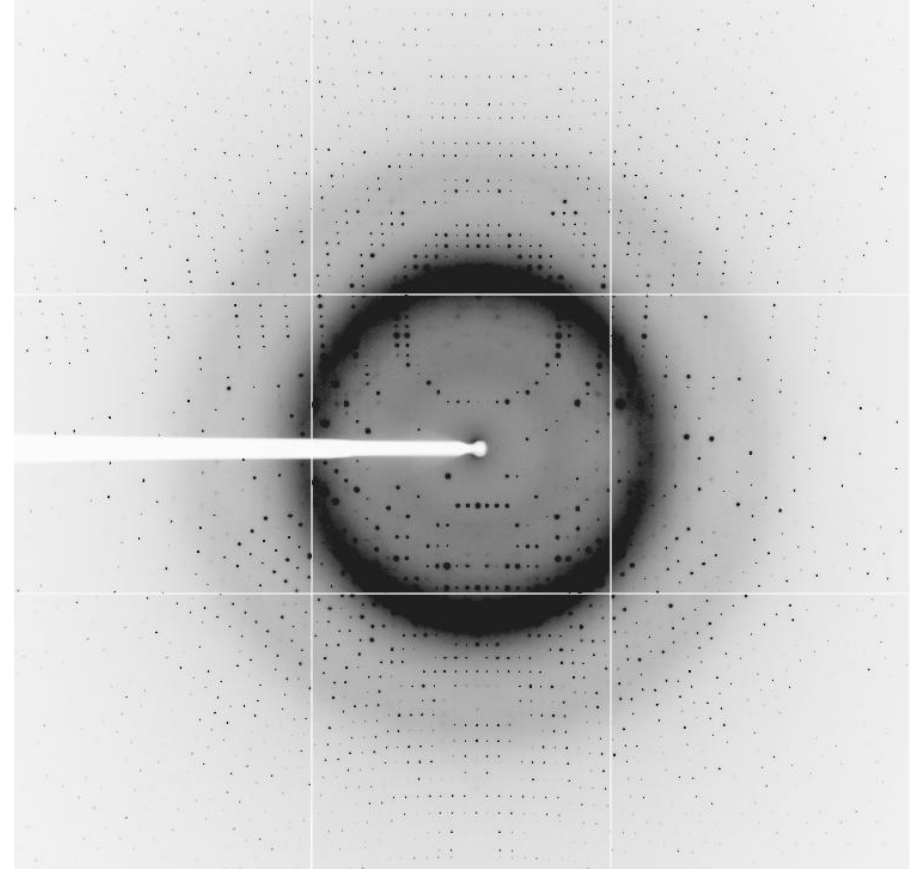
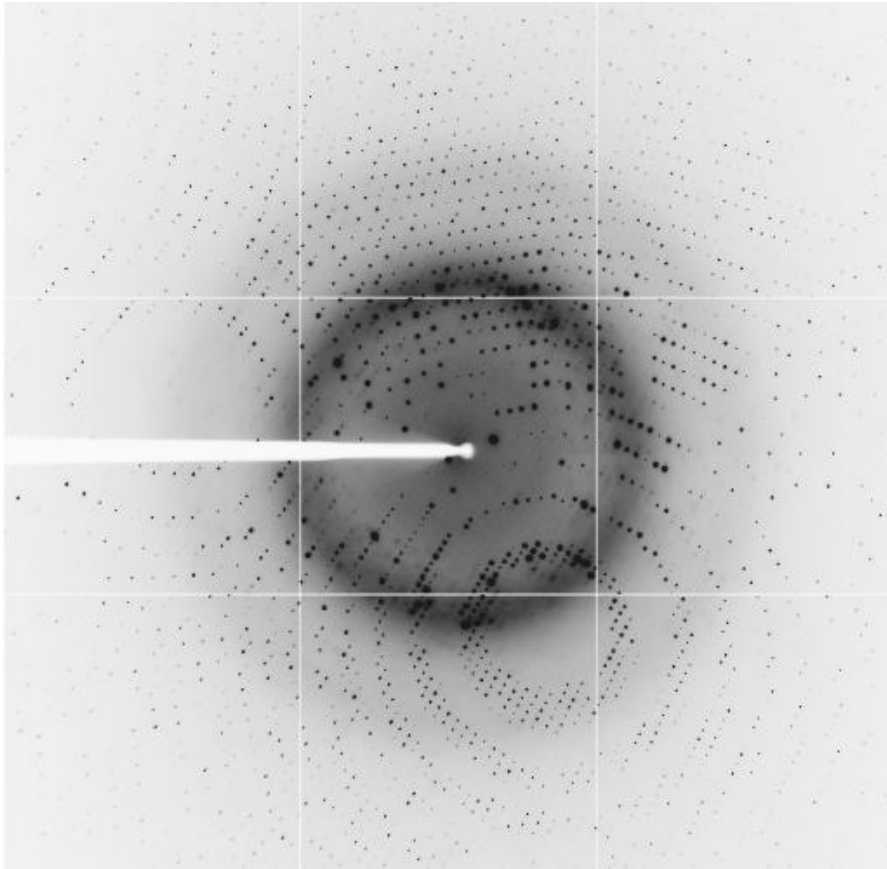
Safety shutter: closed Fast shutter: closed Beamstop: in Current users: [Selecting gives control] [Allow timeout control] Take control My name: artemis2

Collect Queue Pause

[2013-10-30 15:23:59] The current path settings will overwrite data from another task. Correct the problem before collecting

[2013-10-30 15:23:59] The current path settings will overwrite data from another task. Correct the problem before collecting

KAPPA GONIOSTAT CELL RE-ORIENTATION



X-RAY CENTRING

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: opid-144

Sample list: Mode: Sample changer, Centring: Automatic loop centring

Sample centring: Sample position (Omega: 89.99, Kappa: 55.47, Phi: 59.52), Holder length: 21.998

Sample video: Light: 0.6, Focus: -0.096, Front light: 3.0, Zoom: 1

Collection method: Discrete, Characterise, Helical, Energy Scan

Advanced: Workflow type: X-ray Centring

Data location: Folder: /data/d14eh4/inhouse/opid144/20131030/RAW_DATA/, Prefix: opid144, Run number: 2

Grid: Nb points table

	points per line	steps (mm)	distance
Axis 1	10	0.096355	0.867195
Axis 2	5	0.107423	0.429691

Machine current: 170.7 mA, Flux: +0.00 ph/s, Energy: 12.694 keV, Resolution: 2.302 Å, Transmission: 100.00%, Cryo: -1.0 K

Safety shutter: closed, Fast shutter: closed, Beamstop: in

Current users: Artemis2

Log: [2013-10-30 16:51:27] Workflow: phiz: -2.942, [2013-10-30 16:51:28] Workflow waiting for input

mxCuBE (opid-144)

File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: opid-144

Sample list: Mode: Sample changer Show SC-details Centring: Automatic loop centring synchronise ISP/B

Tree view:

- [-] 1:1
 - X-ray Centring - 1
 - sample-centring
 - opid144 - 0
 - XrayCentring - 0
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - line-opid144_2 Collecting
- 1:2
- 1:3
- 1:4
- 1:5
- 1:6
- 1:7
- 1:8
- 1:9
- 1:10
- 2:1
- 2:2
- 2:3
- 2:4
- 2:5
- 2:6
- 2:7
- 2:8
- 2:9
- 2:10
- 3:1
- 3:2
- 3:3
- 3:4
- 3:5
- 3:6
- 3:7
- 3:8
- 3:9
- 3:10

Sample centring Data collection

Mesh Results

Total integrated signal and Bravais lattice

Best position

Grid index Y	Grid index Z	Image file	sampx	sampy	phly	Total Integrated Intensity	Bravais lattice
3	3	mesh-opid144_1_0023.img	-2.173	-0.737	21.667	8.4e+05	C2221

All positions

Grid index Y	Grid index Z	Image file	sampx	sampy	phly	Total Integrated Intensity	Bravais lattice
1	1	mesh-opid144_1_0001.img	-1.957	-0.737	21.475	393	-
2	1	mesh-opid144_1_0002.img	-1.958	-0.737	21.571	667	-
3	1	mesh-opid144_1_0003.img	-1.958	-0.737	21.667	328	-
4	1	mesh-opid144_1_0004.img	-1.958	-0.737	21.764	630	-
5	1	mesh-opid144_1_0005.img	-1.959	-0.737	21.860	342	-
6	1	mesh-opid144_1_0006.img	-1.959	-0.737	21.957	795	-

Machine current: 170.5 mA, 7/8 multibunch, 03:59

Flux: 8.62e+10 ph/s

Energy: Energy Current: 12.694 keV 0.976 Move to: keV

Resolution: Current: 2.302 Å 330.64 mm Move to: Å

Transmission: Current: 100.00% Set to: Filters

Cryo: -1.0 K

Safety shutter: opened

Fast shutter: closed

Beamstop: in

Current users: Selecting gives control Allow timeout control Take control My name: artemis2

Stop Pause View parameters

[2013-10-30 17:00:12] The current path settings will overwrite data from another task. Correct the problem before collecting
 [2013-10-30 17:00:12] The current path settings will overwrite data from another task. Correct the problem before collecting

mxCuBE (opid-144) File Instrumentation Help Expert mode

Collect XRF spectrum System Feedback Chat

User: opid-144

Sample list: Mode: Sample changer, Centring: Automatic loop centring

1:1

- X-ray Centring - 1
- sample-centring
 - opid144 - 0
 - XrayCentring - 0
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - mesh-opid144_1 Collection done
 - line-opid144_2 Collection done

- 1:2
- 1:3
- 1:4
- 1:5
- 1:6
- 1:7
- 1:8
- 1:9
- 1:10
- 2:1
- 2:2
- 2:3
- 2:4
- 2:5
- 2:6
- 2:7
- 2:8
- 2:9
- 2:10
- 3:1
- 3:2
- 3:3
- 3:4
- 3:5
- 3:6
- 3:7
- 3:8
- 3:9
- 3:10

Mesh Results

Result and Bravais lattice

Total integrated signal

mm

Best position

Grid index Y	Grid index Z	Image file	sampx	sampy	phiy	Total integrated intensity	Bravais lattice
10	1	line-opid144_2_0010.img	-2.172	-0.790	21.667	7.24e+05	C2

All positions

Grid index Y	Grid index Z	Image file	sampx	sampy	phiy	Total integrated intensity	Bravais lattice
1	1	line-opid144_2_0001.img	-2.176	-0.549	21.667	519	-
2	1	line-opid144_2_0002.img	-2.176	-0.576	21.667	465	-
3	1	line-opid144_2_0003.img	-2.175	-0.603	21.667	461	-
4	1	line-opid144_2_0004.img	-2.175	-0.629	21.667	940	-
5	1	line-opid144_2_0005.img	-2.174	-0.656	21.667	6.85e+03	-
6	1	line-opid144_2_0006.img	-2.174	-0.683	21.667	2.95e+04	-

Machine current: 170.4 mA, 7/8 multibunch, 03:58

Flux: +0.00 ph/s

Energy: Energy, Current: 12.694 keV, 0.976, Move to: keV

Resolution: Current: 2.302 Å, 330.64 mm, Move to: Å

Transmission: Current: 100.00%, Set to: Filters

Cryo: -1.0 K

Safety shutter: closed

Fast shutter: closed

Beamstop: in

Current users: Selecting gives control, Allow timeout control, Take control, My name: artemis2

Collect Queue Pause

View parameters

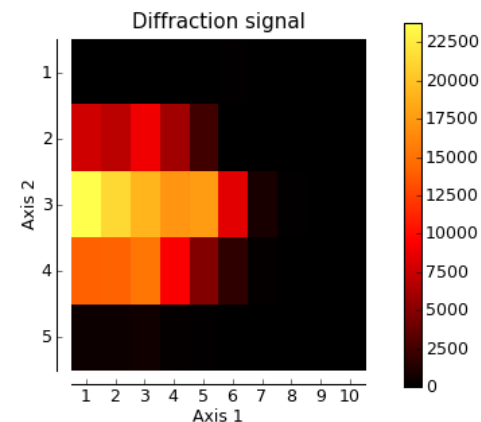
2013-10-30 17:01:20 Workflow: Sample position after move: sampx=-2.172 sampy=-0.790 phiy=21.667

2013-10-30 17:01:20 Workflow: Sample moved to the best position!

Two programs are run in parallel for each mesh scan image:

- Background 3D (written by Sasha Popov, ESRF)
- Labelit / Phenix spot finder (<http://www.phenix-online.org>)

For the five mesh scan images with the highest score MOSFLM indexing is executed:



Best position

The sample has automatically been moved to the best position.

In order to move the sample to an other position please copy/paste the commands from the right column into SPEC EXP.

Axis 1	Axis 2	Image file	Signal 1	Signal 2	Bravais lattice	SPEC command for moving sample to position
1	3	mesh-opid232_1_0021.cbf	2.38e+04	1016817	P222	mv sampx 0.182; mv sampy -0.807; mv phiy 21.380

Signal 1: Criteria that uses intensities over background vs resolution. Popov 2014, to be published.

Signal 2: Labelit distl spotfinder total integrated intensity.

All positions

Axis 1	Axis 2	Image file	Signal 1	Signal 2	Bravais lattice	SPEC command for moving sample to position
1	3	mesh-opid232_1_0021.cbf	2.38e+04	1016817	P222	mv sampx 0.182; mv sampy -0.807; mv phiy 21.380
2	3	mesh-opid232_1_0022.cbf	2.14e+04	714677	P222	mv sampx 0.182; mv sampy -0.807; mv phiy 21.402
3	3	mesh-opid232_1_0023.cbf	1.92e+04	726267	P222	mv sampx 0.182; mv sampy -0.807; mv phiy 21.424
5	3	mesh-opid232_1_0025.cbf	1.75e+04	537506	P222	mv sampx 0.182; mv sampy -0.807; mv phiy 21.469
4	3	mesh-opid232_1_0024.cbf	1.72e+04	541746	P1	mv sampx 0.182; mv sampy -0.807; mv phiy 21.446
3	4	mesh-opid232_1_0033.cbf	1.53e+04	423657	_	mv sampx 0.182; mv sampy -0.757; mv phiy 21.424
2	4	mesh-opid232_1_0032.cbf	1.4e+04	521400	_	mv sampx 0.182; mv sampy -0.757; mv phiy 21.402
1	4	mesh-opid232_1_0031.cbf	1.4e+04	688343	_	mv sampx 0.182; mv sampy -0.757; mv phiy 21.380

DEHYDRATION

mxCuBE (opid-144)

File Instrumentation Help

Collect XRF spectrum System Feedback Chat

User: opid-144

Sample list: Mode: Manually mounted, Centring: Automatic loop centring

manually-mounted

- Dehydration - 1
- sample-centring
- Lys0.1 - 0
- Dehydration - 3
 - hc1-Lys0.1_1
 - hc1-Lys0.1_2
 - hc1-Lys0.1_3
 - hc1-Lys0.1_4
 - hc1-Lys0.1_5
 - hc1-Lys0.1_6
 - hc1-Lys0.1_7
 - hc1-Lys0.1_8
 - hc1-Lys0.1_9
 - hc1-Lys0.1_10
 - hc1-Lys0.1_11
 - hc1-Lys0.1_12
 - hc1-Lys0.1_13
 - hc1-Lys0.1_14
 - hc1-Lys0.1_15
 - hc1-Lys0.1_16
 - hc1-Lys0.1_17

Sample centring Data collection

Dehydration Results

Effect of dehydration on crystal parameters

Effect of dehydration on crystal parameters

Effect of dehydration on resolution

Effect of dehydration on crystal parameters

Effect of dehydration on resolution

Effect of dehydration on resolution

Effect of dehydration on resolution

Machine current: 193.7 mA

Flux: +0.00 ph/s

Energy: Current: 13.3000 keV, 0.932

Resolution: 2.399 Å, 365.26 mm

Transmission: Current: 1.16%

Cryo: 100.0 K

Safety shutter: closed

Fast shutter: closed

Beamstop: in

Current users:

My name: artemis2

Log: [2013-12-02 10:14:55] Workflow: Target RH = 82.0, current RH = 82.8
 [2013-12-02 10:14:56] Workflow: Current RH = 82.5
 [2013-12-02 10:14:56] Workflow: Target RH = 82.0, current RH = 82.5

DEHYDRATION

mxCuBE (opid-144)

File Instrumentation Help

Collect XRF spectrum System Feedback Chat

User: opid-144

Sample list: Manually mounted, Automatic loop centring

Dehydration - 1, Lys0.1 - 0, Dehydration - 3

Effect of dehydration on resolution

Effect of dehydration on resolution

Rel. hum. [%]	Time [s]	Image	Res. 1	Res. 2	Spots	Bragg cand.	Cell a	Cell b	Cell c	Mosaicity	Rangin res.	Sym.
99.28	42.2	hc1-Lys0_1_1_0001.img	2.32	2.28	306	257	79.017	79.017	38.520	0.3	1.38	P4
98.26	167.8	hc1-Lys0_1_2_0001.img	2.43	2.36	295	247	79.022	79.022	38.517	0.25	1.42	P4
97.32	276.6	hc1-Lys0_1_3_0001.img	2.54	2.45	324	267	79.026	79.026	38.505	0.35	1.32	P4
96.38	390.0	hc1-Lys0_1_4_0001.img	2.26	2.37	296	247	79.045	79.045	38.451	0.2	1.39	P4
95.46	501.4	hc1-Lys0_1_5_0001.img	2.18	2.28	278	246	79.073	79.073	38.376	0.2	1.38	P4
94.37	612.5	hc1-Lys0_1_6_0001.img	2.35	2.36	327	285	79.112	79.112	38.334	0.2	1.35	P4
93.4	721.4	hc1-Lys0_1_7_0001.img	2.36	2.38	299	250	79.113	79.113	38.324	0.2	1.31	P4
92.34	832.2	hc1-Lys0_1_8_0001.img	2.29	2.27	295	275	79.113	79.113	38.319	0.25	1.35	P4
91.45	943.6	hc1-Lys0_1_9_0001.img	2.33	2.28	293	263	79.101	79.101	38.334	0.5	1.31	P4
90.34	1055.2	hc1-Lys0_1_10_0001.img	2.28	2.3	292	263	79.089	79.089	38.342	0.25	1.34	P4
89.36	1167.7	hc1-Lys0_1_11_0001.img	2.24	2.2	300	265	79.084	79.084	38.341	0.15	1.34	P4
88.44	1279.9	hc1-Lys0_1_12_0001.img	2.33	2.08	310	283	79.010	79.010	38.296	0.2	1.33	P4
87.31	1392.2	hc1-Lys0_1_13_0001.img	2.29	2.22	329	305	78.885	78.885	38.182	0.1	1.38	P4
86.41	1505.7	hc1-Lys0_1_14_0001.img	2.37	2.35	342	299	78.770	78.770	38.084	0.2	1.41	P4
85.35	1618.0	hc1-Lys0_1_15_0001.img	2.36	2.14	334	299	78.600	78.600	37.982	0.25	1.35	P4
84.52	1734.1	hc1-Lys0_1_16_0001.img	2.33	2.23	329	297	78.439	78.439	37.891	0.35	1.33	P4
83.38	1847.2	hc1-Lys0_1_17_0001.img	2.39	2.33	339	299	78.264	78.264	37.808	0.25	1.43	P4

File info

Machine current: 193.7 mA, Flux: +0.00 ph/s, Energy: 13.3000 keV, Resolution: 2.399 Å, Transmission: 1.16%, Cryo: 100.0 K

Safety shutter: closed, Fast shutter: closed, Beamstop: in

Current users: Artemis2

Workflow: Target RH = 82.0, current RH = 82.5
 Workflow: Current RH = 82.4
 Workflow: PAUSE: 60.000000 s

AUTOMATIC ESTIMATE OF CRYSTAL RADIATION DAMAGE SUSCEPTIBILITY

mxCuBE (opid-232)

File Instrumentation Help Expert mode

Collect XRF spectrum System Chat Feedback

User: **opid-232**

Sample list
 Mode: Manually mounted Show SC-details
 Centring: Automatic loop centring Synch ISPyB

manually-mounted
 Burn strategy - 1
 sample-centring
 Burn1 - 0
 BurnStrategy - 0
 ref-Burn1_1 Collection done
 burn-Burn1w1_1 Collection done
 burn-Burn1w2_1 Collection done
 burn-Burn1w3_1 Collection done
 burn-Burn1w4_1 Collection done
 burn-Burn1w5_1 Collection done
 burn-Burn1w6_1 Collection done
 burn-Burn1w7_1 Collection done
 burn-Burn1w8_1 Collection done
 burn-Burn1w9_1 Collection done
 burn-Burn1w10_1 Collection done
 burn-Burn1w11_1 Collection done
 burn-Burn1w12_1 Collection done
 burn-Burn1w13_1 Collection done
 burn-Burn1w14_1 Collection done
 burn-Burn1w15_1 Collection done
 burn-Burn1w16_1 Collection done
 burn-Burn1w17_1 Collection done
 burn-Burn1w18_1 Collection done
 burn-Burn1w19_1 Collection done
 burn-Burn1w20_1 Collection done
 burn-Burn1w21_1 Collection done

Collect Queue Pause

Sample centring Data collection

Burn Strategy Results

B-factor vs. dose $\beta = 0.06 \text{ \AA}^2/\text{MGy}$

Dose (MGy)	B-factor (\AA^2)
0	22.9
2	23.1
4	23.3
6	23.4
8	23.5

Scale vs. dose $\gamma = 0.00 \text{ MGy}^{-1}$

Dose (MGy)	Scale
0	1.01
2	0.995
4	1.005
6	1.002
8	0.998
10	0.992

Relative Intensity total vs. Dose, $D1/2 = 147.14 \text{ MGy}$

Dose (MGy)	Relative Intensity
0	1.01
2	1.00
4	0.99
6	0.98
8	0.97
10	0.96

View parameters

Machine current
175.5 mA
7/8 multibunch
05:04

Flux: +0.00 ph/s

Energy: 14.2037 keV
Wavelength: 0.873 \AA

Resolution
Current: 2.840 A 349.85 mm
Move to: A

Transmission
Current: 100.00%
Set to: Filters

Cryo
100.0 K

Safety shutter closed

Fast shutter closed

Beamstop in

Current users

Selecting gives control
 Allow timeout control

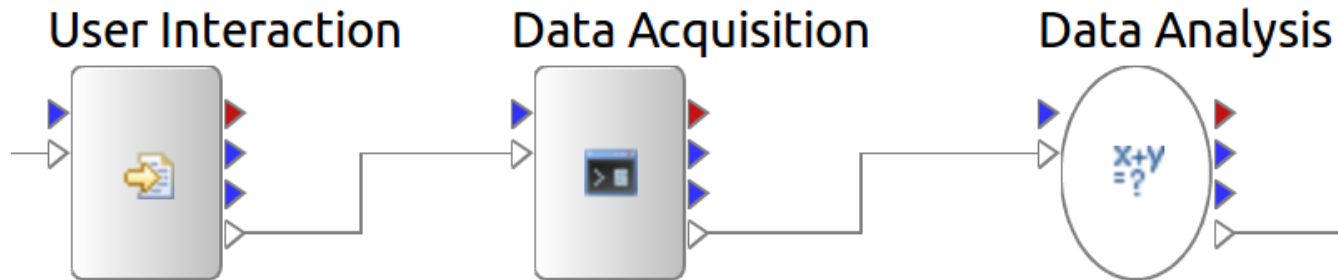
Take control

My name: sybil

[2013-11-18 15:55:18] Workflow: Dose_half: 147.13
 [2013-11-18 15:55:18] Workflow: Relative_radiation_sensitivity: 0.07
 [2013-11-18 15:55:19] Workflow waiting for input

Taskbar: mxCuBE ISPyB Shell No. 2 - Konsole mxCuBE (opid-232) jvacuum 2.0 emacs@sybil.esrf.fr jidappli 2.3 Dserver

15:55 18/11/2013



- Executed from mxCuBE
- Log and working directories created in PROCESSED_DATA
- Result HTML page displayed in mxCuBE
- Connected to ISPyB:
 - > *Status and workflow meta data uploaded automatically*
 - > *Log and result HTML pages uploaded to pyarch (long time archive)*
- Robust error catching / handling

Improvements of existing workflows:

- Interaction with mxCuBE
- Error handling / recovery
- Mesh scan data analysis

The following workflows are currently under development:

- Diffraction tomography
- Fully automatic X-ray centring, enhanced characterisation and data collection
- Inter-leaved MAD data collection

AUTOMATIC X-RAY CENTRING, CHARACTERISATION AND DATA COLLECTION

mxCuBE (opid-232) File Instrumentation Help Expert mode

Collect XRF spectrum System Chat Feedback

User: User: opid-232 Group: Set Logout

Sample list
 Mode: Sample changer Show SC-details
 Centring: Automatic Syncr ISPyB

1:1
1:2
 Massif 1 - 1
 opid232 - 0
 Massif1 - 1
 mesh-opid232_1 Collection done
 mesh-opid232_1 Collection done
 mesh-opid232_1 Collection done
 mesh-opid232_1 Collection done
 line-opid232_2 Collection done
 ref-opid232_2 Collection done
 opid232_2 Collection done
 1:3 **Centring done!**
 Massif 1 - 1
 opid232 - 0
 Massif1 - 1
 mesh-opid232_1 Collection done
 mesh-opid232_1 Collection done
 mesh-opid232_1 Collection done
 mesh-opid232_1 Collection done
 line-opid232_2 Collection done
 ref-opid232_2 Collection done
 opid232_2 Collection done
 1:4
 Massif 1 - 1
 opid232 - 0
 1:5
 Massif 1 - 1
 opid232 - 0
 1:6
 Massif 1 - 1
 opid232 - 0
 1:7
 1:8
 1:9

Stop Pause

Characterisation Results

Data collection info

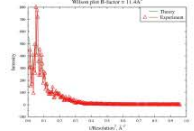
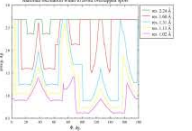
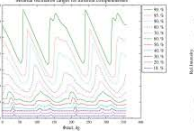
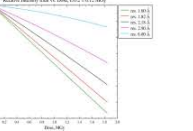
Data collection date	2014/Jan/29 17:02:49.673
Image prefix	ref-opid232_2
Directory	/data/id23eh2/inhouse/opid232/20140129/RAW_DATA/1-3/Massif1_01

Diffraction Plan

Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed I/sigma at highest res.	Aimed resolution (Å)
None	False	Default (optimized)	Default ($\nu > 0.99$)	BEST Default	Default (highest possible)

Collection plan strategy ([RADDOSE log file](#) , [BEST log file](#))

Resolution limit is set by the radiation damage								
Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	102.00	0.10	1110	0.01	1.60	22.55	202.84

Indexing summary: Selected spacegroup: P222

Refined unit cell parameters (Å/degrees)					
a (Å)	b (Å)	c (Å)	alpha (°)	beta (°)	gamma (°)
59.551	64.276	69.931	90.000	90.000	90.000

[Indexing log file](#)

ref-opid232_2_0001.cbf

[Integration log file 1](#)

View parameters

Machine current: 195.1 mA
7/8 multibunch
03:55

Flux: +0.00 ph/s

Energy: 14.2037 keV
Wavelength: 0.873 Å

Resolution: 1.599 Å 137.83 mm
Move to: A

Transmission: 23.16%
Set to: Filters

Cryo: 100.0 K

Safety shutter: closed

Fast shutter: closed

Beamstop: in

Current users:

Selecting gives control
 Allow timeout control

Take control

My name: sybil

[2014-01-29 17:04:06] Collection completed
 [2014-01-29 17:04:08] Workflow: Optimal strategy has been calculated and been transferred to the mxCuBE queue.
 [2014-01-29 17:04:08] Workflow: Workflow finished with status success.

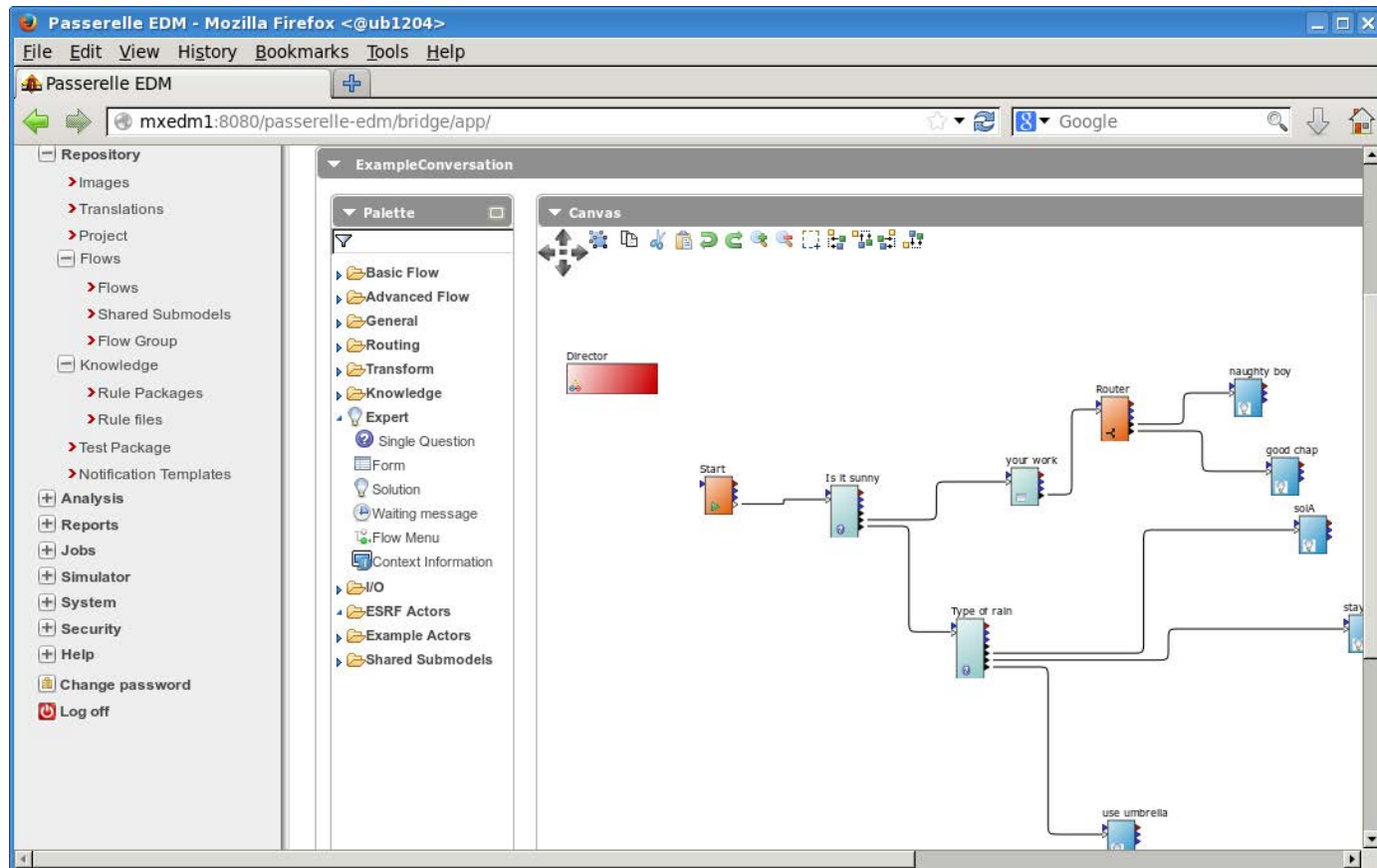
mxCuBE ISPyB
Shell - Konsole
jidappli 2.3
Temperature control
Front End & Vacuum
mxCuBE (opid-232)
jvacuum 2.0


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FUTURE DEVELOPMENTS – PASSERELLE EDM

Workflows for downstream processing – Passerelle Enterprise Decision Manager:

- Web based / collaborative workflow management
- Connection with ISPyB
- Goal: allow remote re-processing via ISPyB web interface



The following workflows have been proposed to be implemented for the ESRF bioSAXS beamline BM29:

- Burn strategies to assess radiation sensitivity and optimize acquisition parameters.
- Comparison of separate concentrations and extrapolation to zero concentration
- Merging of regions not affected by radiation damage
- Comparison of separate concentrations and taking actions to produce additional dilutions and triggering data collections
- Advanced HPLC analysis
- Automated water calibration

- Sandor Brockhauser, Matthew Bowler and Max Nanao (EMBL Grenoble)
- Andy Götz, Elspeth Gordon and Sasha Popov (ESRF)
- Erwin de Ley and Koen Heunick (Isencia, Belgium)
- Matthew Gerring and the DLS Scisoft Team
- The ESRF Data Analysis Unit, Beamline Control Unit and Structural Biology group

Further reading:

- S. Brockhauser, O. Svensson, M. W. Bowler, M. Nanao, E. Gordon, R. M. F. Leal, A. Popov, M. Gerring, A. A. McCarthy and A. Gotz, The use of workflows in the design and implementation of complex experiments in macromolecular crystallography, *Acta Cryst.* (2012). D68, 975-984