

Automating complex data collection using workflows

Olof Svensson
Data Analysis Unit
ISDD / ESRF

- **Automation of complex data collection**
 - Examples
 - Motivation and short history
- **The Beamline Expert System / Passerelle EDM**
 - Overview
 - Why Passerelle EDM?
 - Screenshots
 - Statistics
- **Interfaces to mxCuBE and ISPyB**
- **Implementation**
- **Future developments**

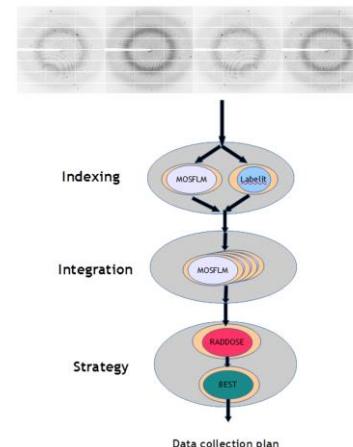
EXAMPLES OF COMPLEX DATA COLLECTION

- **Combination of:**

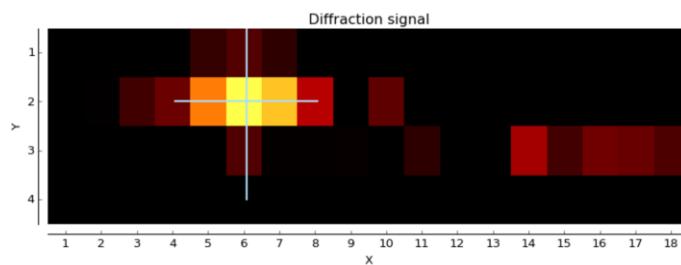
- Data collection
- Data processing
- [User interaction]



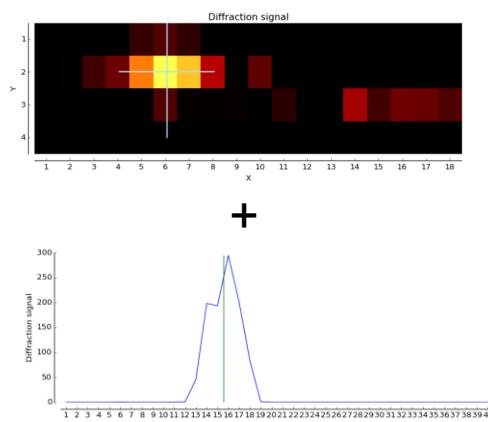
Characterisation (~64000)



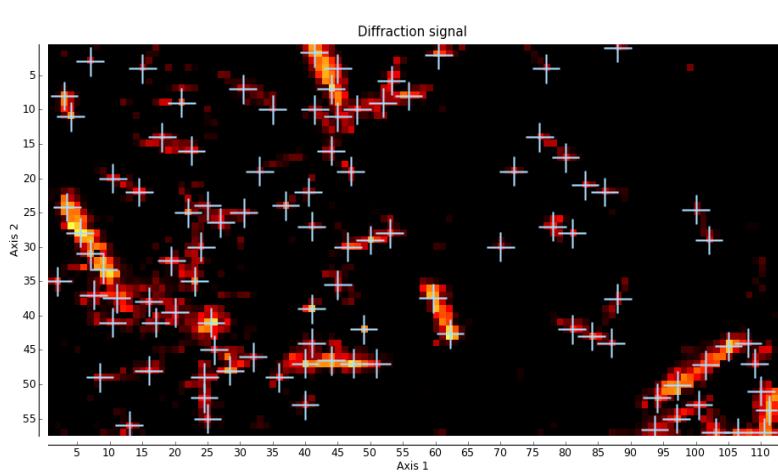
MeshScan (~2700)



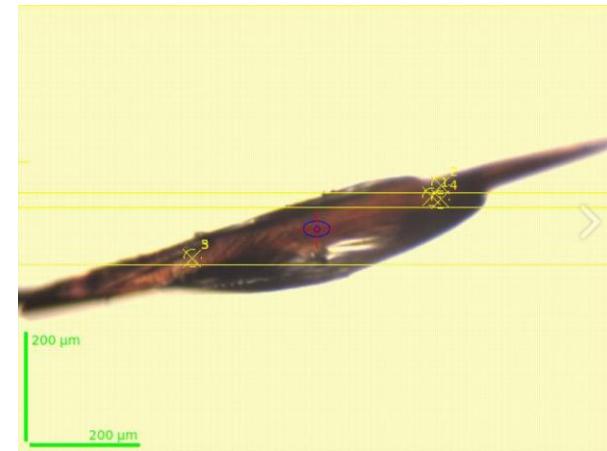
X-ray centring (~5900)



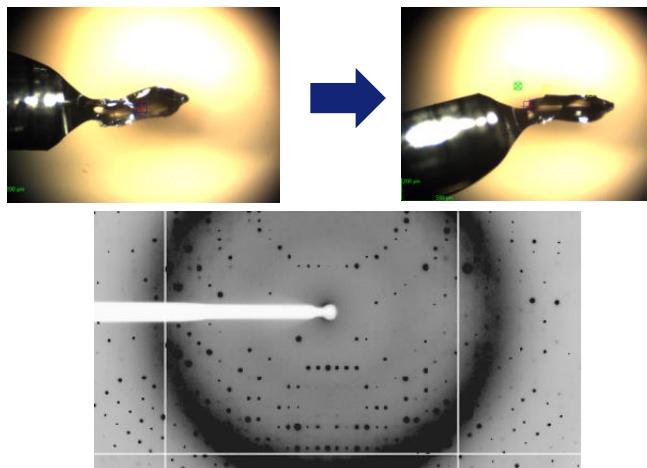
Mesh and collect (~600)



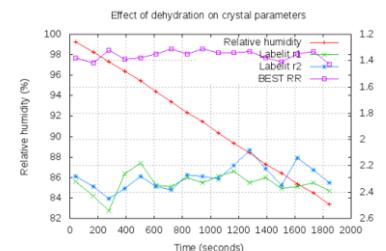
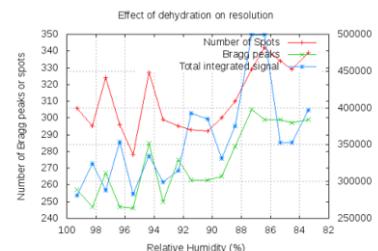
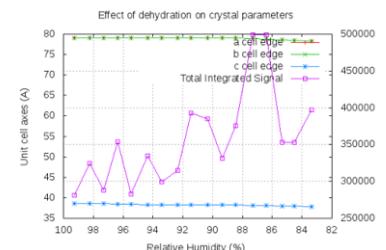
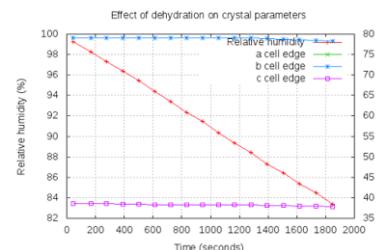
Helical characterisation (~370)



Visual + cell re-orientation (~360)

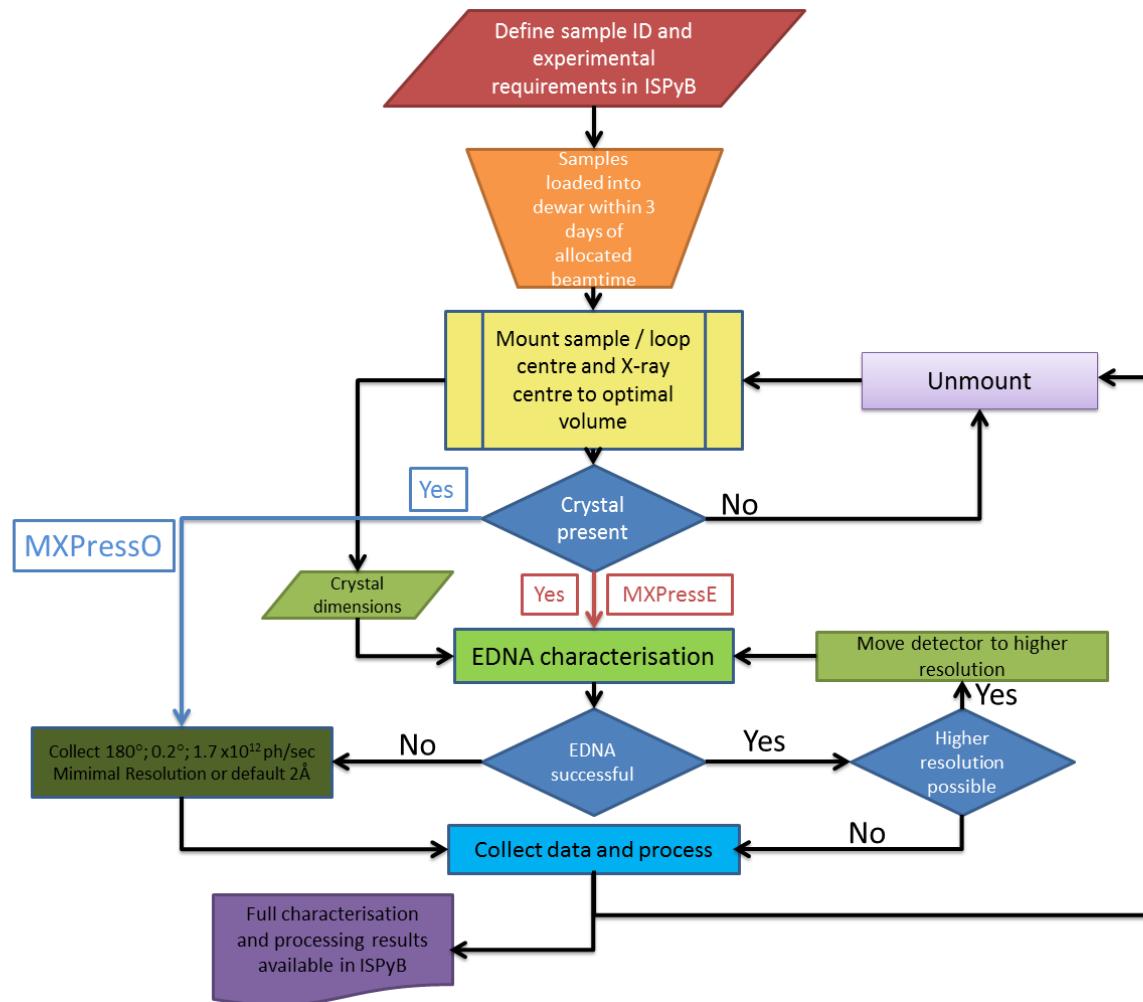


Dehydration (~80)



THE MOST COMPLEX DATA COLLECTION: MXPRESSA

MXPressA (~10000)



OTHER COMPLEX DATA COLLECTION WORKFLOWS

- **Interleaved MAD**
- **Burn strategy**
 - Carefully kills the crystal and measures the radiation damage
- **Spectroscopy**

- **Why automation?**

- Complex data collection is often tedious and time-consuming
- Avoid human errors
- Increase speed
- “Hands-off” data collections

- **Short history:**

- 2003 -> 2007 : DNA – automateD collectioN of datA. Dedicated to MX crystal characterization, dedicated GUI
- 2007 -> : EDNA – Enhanced DNA. Framework based on data models, plugins and testing facilities. Today used in MX for thumbnail generation, characterisation, automatic data processing and many other processing tasks.
- 2012 -> 2014 : Passerelle workflow tool (design and execution) in DAWN (open source)
- 2015 -> : Passerelle EDM (Entreprise Decision Manager, not open source)

- **The BES (Beamline Expert System)**
 - A customized version of Passerelle EDM for the ESRF
 - Similar to the SES (Soleil Expert System)
- **Passerelle EDM:**
 - Based on the open-source passerelle workflow engine, which is based on the Ptolemy II workflow engine (written in Java)
 - Combines the passerelle workflow engine with a workflow design tool
 - Both the engine and the design tool are connected to a data base
 - Accessed via a web GUI (JBoss Application Server 7)
- **Passerelle EDM is a commercial product:**
 - Initial one-off purchase followed by one-year maintenance contracts
 - ESRF license costs shared between the ESRF and EMBL Grenoble
 - Contact person: Erwin de Ley (erwin.de.ley@isencia.be)

BES DESIGN TOOL

Beamline Expert System Olof

mxhpc2-1705:8090/BES/bridge/app/ ABP V S ...

BES 3.2.0 ? Olof Svensson

Design Configuration Testing Support Admin

Commit Save Lock General Validate Flow Run Customize Gear

Selected Submodel MXPressDataCollection (2.1) Original layout

Editor Debug

Palette

- Throttling Delay
- Error Observer
- Error Catcher
- Router
- > Transform
- > I/O
- > Expert
- > Cluster
- > Events
- > Monitoring
- > Continuation
- > ESRF actors
 - !● Error Handler by Causing actor
 - !● Error Handler by ErrorCode raise
 - !● Error Handler by Severity
 - Python Actor
- > Shared Submodels
 - AnalyseKappa
 - CenterRotationAxis
 - CollectAndProcessBurningStrat
 - CollectReferenceImages
 - CollectWithoutStrategy
 - CommonDataCollection

MXPressDataCollection

The workflow diagram illustrates a complex data collection process. It begins with an 'In' node, followed by a 'Select aperture' node. This leads to a 'Do characterisation' node, which then triggers a 'Prepare automatic characterisation and data collection' submodel. Inside this submodel, the flow goes through 'CollectReferenceImages', 'EDNAStrategy', 'Characterisation failed', 'Check results', and 'New data collection' nodes. The 'Characterisation failed' path leads to a 'Do data collect_1' node. The 'Check results' path leads to a decision diamond. From this diamond, the flow can lead to 'Do data collect_2' or 'Only EDNA resolution'. The 'Only EDNA resolution' path leads to 'Pre collect with resolution and phi start' and 'Load msCuBE queue'. The 'Do data collect_2' path leads to 'Retrieve flux from ISPyB' and then to 'Do data collect_1'. Finally, the flow leads to 'Load msCuBE queue', 'Collection with', and 'Collection without' nodes, concluding with a 'No data collection' node.

- **Advantages of using a workflow design tool:**
 - Modularity by design
 - Easy to get global overview – documentation “built in”
 - Easier discussions with non-programmers
 - Of course if “spaghetti”-like workflows avoided
- **Further advantages of using Passerelle EDM:**
 - Built-in revision handling of workflows
 - Workflow and actor execution details in database
- **Disadvantages:**
 - Proprietary software which needs an annual budget
 - Hence collaborations difficult

SCREENSHOTS BES – PASSERELLE EDM

Beamline Expert System Olof

mxhpc2-1705:8090/BES/bridge/app/ ABP

BES 3.2.0 Olof Svensson

Design Configuration Testing Support Admin

Flows Original configuration

Enter search string here ? Gear icon

Name: Group: Comment:
Type: Flow Submodel Status: New In Progress Translate Done Stand By

+ Create Edit View Delete General Import Export : « < 1-20 of 85 rows > » 20 C

| | Rev | Type | Name | Status | Last Updated By | Modify date | Comment |
|---|-----|------|----------------------------|-------------|-----------------|---------------------|--|
| ✓ | 4.1 | Flow | BurnStrategy | Done | MASTER | 2015-01-28 10:21:39 | message_text |
| ✓ | 2.1 | Flow | Characterisation | Done | SVENSSON | 2015-09-09 08:21:46 | Changed status to "Done". |
| ✓ | 1.0 | Flow | CollectAndSpectra | New | SVENSSON | 2015-11-23 11:06:22 | Added sampleInfo to do collect input |
| ✓ | 1.2 | Flow | CreateLucidBackgroundImage | Done | SVENSSON | 2015-09-09 08:21:59 | Changed status to "Done". |
| ✓ | 3.1 | Flow | CreateThumbnails | Done | SVENSSON | 2015-09-09 08:22:12 | Changed status to "Done". |
| ✓ | 2.3 | Flow | Dehydration | Done | SVENSSON | 2015-02-03 11:25:45 | Renamed to Dehydration |
| ✓ | 1.7 | Flow | EDNA_dp | Done | SVENSSON | 2015-09-09 08:22:24 | Changed status to "Done". |
| ✓ | 1.1 | Flow | EDNA_proc | Done | SVENSSON | 2016-05-03 09:44:18 | Renamed from EDNA_dp |
| ✓ | 2.0 | Flow | EDNA_proc_OAR | New | SVENSSON | 2016-10-12 16:28:03 | Added wait for first and last image |
| ✓ | 1.1 | Flow | EnergyInterleavedMAD | Done | SVENSSON | 2016-04-14 11:15:48 | First version |
| ▲ | 3.1 | Flow | EnhancedCharacterisation | Done | SVENSSON | 2015-02-03 11:26:13 | Renamed to EnhancedCharacterisation |
| ✓ | 2.2 | Flow | HelicalCharacterisation | Done | SVENSSON | 2015-12-03 14:05:43 | Changed user input python script path |
| ✓ | 5.1 | Flow | KappaReorientation | Done | MASTER | 2015-01-28 10:22:32 | message_text |
| ✓ | 2.1 | Flow | LowDoseDC | In Progress | SVENSSON | 2015-11-24 09:23:38 | Renamed redo low dose DC input python script |
| ✓ | 6.0 | Flow | MXPressA | Done | SVENSSON | 2015-11-17 10:00:38 | Removed stop actor. |
| ✓ | 1.1 | Flow | MXPressA_aperture_100um | Done | SVENSSON | 2015-12-01 14:17:48 | First revision |
| ✓ | 1.1 | Flow | MXPressA_aperture_10um | Done | SVENSSON | 2015-12-01 14:18:14 | First revision |
| ✓ | 1.1 | Flow | MXPressA_aperture_15um | Done | SVENSSON | 2015-12-01 14:18:43 | First revision |
| ✓ | 1.1 | Flow | MXPressA_aperture_30um | In Progress | SVENSSON | 2015-12-01 14:11:58 | First revision |

BES EXECUTION LOG

Beamline Expert System Olof

mxhpc2-1705:8090/BES/bridge/app/ ABP

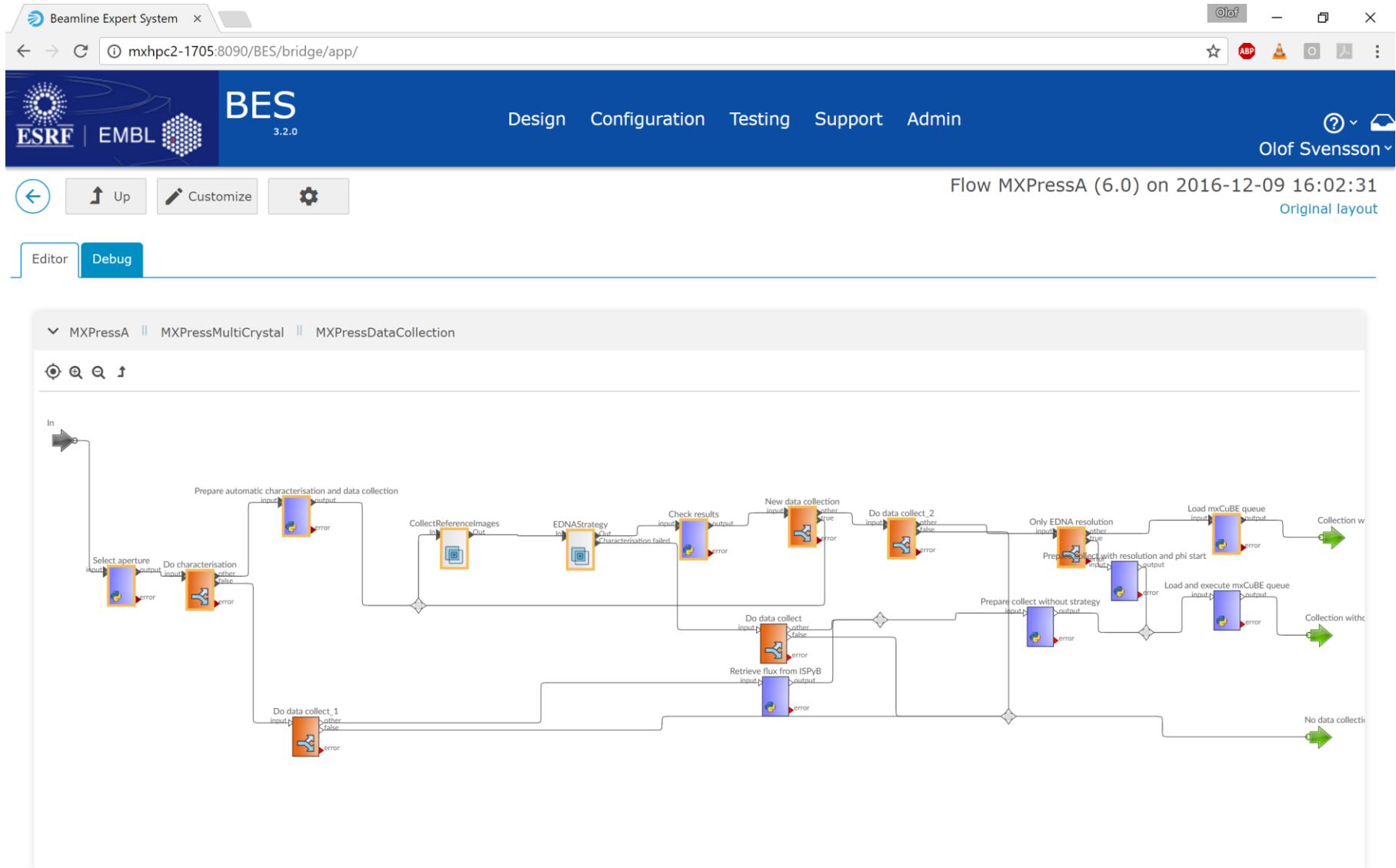
BES 3.2.0 Olof Svensson

Design Configuration Testing Support Admin Requests My settings

CreateThumbNails ⚙️

Reference: Id: Correlation Id:
Type: External Reference:
Initiator: bm14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b
Status: Created Error Finished Cancelled Started Timeout
Creation Date: 2016-12-08 00:00:00 To 2016-12-09 16:04:59

| View | Export | ⋮ | « | < | 1-200 of ? rows | > | » | 200 | C |
|--------------------------|----------------------|-------------------------|------------------|---------------------|-----------------|--------------------|----------|--------------|---|
| | Reference | Id | Type | Creation Date | Initiator | External Reference | Status | Duration(ms) | + |
| <input type="checkbox"/> | 3841 | 4734310 | EDNA_proc_OAR | 2016-12-09 16:03:06 | id23eh1 | mx1777 | Finished | 200,355 | |
| <input type="checkbox"/> | 3841 | 4734303 | dozor_OAR | 2016-12-09 16:03:04 | id23eh1 | mx1777 | Finished | 131,912 | |
| <input type="checkbox"/> | 3841 | 4734302 | XIA2_DIALS_OAR | 2016-12-09 16:03:04 | id23eh1 | mx1777 | Finished | 3,707,707 | |
| <input type="checkbox"/> | 3841 | 4734301 | autoPROC_OAR | 2016-12-09 16:03:04 | id23eh1 | mx1777 | Finished | 2,219,649 | |
| <input type="checkbox"/> | 9070 | 4734179 | MXPressA | 2016-12-09 16:02:31 | id30a1 | fx57 | Finished | 1,010,921 | |
| <input type="checkbox"/> | 4191 | 4734243 | Characterisation | 2016-12-09 16:01:47 | id29 | mx1833 | Finished | 26,202 | |
| <input type="checkbox"/> | 4191 | 4734254 | dozor_OAR | 2016-12-09 16:01:22 | id29 | mx1833 | Finished | 49,588 | |
| <input type="checkbox"/> | 4191 | 4733359 | Characterisation | 2016-12-09 15:57:41 | id29 | mx1833 | Finished | 33,214 | |
| <input type="checkbox"/> | 4191 | 4733650 | dozor_OAR | 2016-12-09 15:57:14 | id29 | mx1833 | Finished | 46,688 | |
| <input type="checkbox"/> | 3661 | 4734186 | EDNA_proc_OAR | 2016-12-09 15:56:50 | id30a1 | fx57 | Finished | 389,262 | |
| <input type="checkbox"/> | 3661 | 4734181 | XIA2_DIALS_OAR | 2016-12-09 15:56:48 | id30a1 | fx57 | Finished | 661,905 | |
| <input type="checkbox"/> | 3661 | 4734130 | dozor_OAR | 2016-12-09 15:56:48 | id30a1 | fx57 | Finished | 221,346 | |
| <input type="checkbox"/> | 1523 | 4734147 | EDNA_proc_OAR | 2016-12-09 15:56:19 | id30a2 | mx415 | Finished | 52,785 | |
| <input type="checkbox"/> | 1523 | 4734135 | XIA2_DIALS_OAR | 2016-12-09 15:56:17 | id30a2 | mx415 | Finished | 478,871 | |
| <input type="checkbox"/> | 1523 | 4734134 | autoPROC_OAR | 2016-12-09 15:56:17 | id30a2 | mx415 | Finished | 568,424 | |
| <input type="checkbox"/> | 1523 | 4734141 | XDSAPP_OAR | 2016-12-09 15:56:17 | id30a2 | mx415 | Finished | 467,971 | |



BES – WORKFLOW EXECUTION LOG

Beamline Expert System Olof

mxhpc2-1705:8090/BES/bridge/app/ ABP

BES 3.2.0 Olof Svensson

Design Configuration Testing Support Admin

Request details
Request (id= 4734179, type = MXPressA)

Reference: 9070
Id: 4734179
Type: MXPressA
Creation Date: 2016-12-09 16:02:31
Status: Finished
External Reference: fx57
Correlation Id:
Initiator: id30a1
Executor:

Result Item

| Name | Value | Data Type | + |
|---------------------|---|-----------|---|
| collection_software | mxCuBE_ - _2.0 | STRING | |
| directory | /data/visitor/fx57/id30a1/20161209/RAW_DATA/BIPDE1/BIPDE1-CD014403_H04-3_DI01318464 | STRING | |
| modelpath | MXPressA | STRING | |
| prefix | BIPDE1-CD014403_H04-3_DI01318464 | STRING | |
| run_number | 1 | STRING | |
| sample_lims_id | 575403 | STRING | |
| sample_node_id | 119 | STRING | |

Event

Enter search string here 🔍

Id: Status: Created Error Finished Cancelled Started Timeout

Type: Discriminator: Initiator:

View 101 rows 400 C

| | ID | Creation Date | Duration(ms) | Status | Type | Initiator |
|--------------------------|---------|---------------------|--------------|----------|------------------------------|---|
| <input type="checkbox"/> | 4734180 | 2016-12-09 16:02:31 | 8 | Finished | Start | actor:/MXPressA.Start |
| <input type="checkbox"/> | 4734291 | 2016-12-09 16:02:31 | 632 | Finished | eu.esrf.services.python.v2.6 | actor:/MXPressA.Beamline%20setup |
| <input type="checkbox"/> | 4734292 | 2016-12-09 16:02:32 | 576 | Finished | eu.esrf.services.python.v2.6 | actor:/MXPressA.Prepare%20MXPressA |
| <input type="checkbox"/> | 4734293 | 2016-12-09 16:02:32 | 1850 | Finished | eu.esrf.services.python.v2.6 | actor:/MXPressA.CommonPrepareExperiment.Init%20workflow |
| <input type="checkbox"/> | 4734294 | 2016-12-09 16:02:34 | 768 | Finished | eu.esrf.services.python.v2.6 | actor:/MXPressA.CommonPrepareExperiment.Read%20motor%20positions |
| <input type="checkbox"/> | 4734295 | 2016-12-09 16:02:35 | 299 | Finished | eu.esrf.services.python.v2.6 | actor:/MXPressA.CommonPrepareExperiment.Default%20parameters |
| <input type="checkbox"/> | 4734296 | 2016-12-09 16:02:35 | 2295 | Finished | eu.esrf.services.python.v2.6 | actor:/MXPressA.MXPressMultiCrystal.Interpretation%20of%20diffract%20 |
| <input type="checkbox"/> | 4734297 | 2016-12-09 16:02:37 | 315 | Finished | eu.esrf.services.python.v2.6 | actor:/MXPressA.MXPressMultiCrystal.Contact%20user%20if%20first%20across%20 |

BES – ACTOR EXECUTION LOG

Beamline Expert System mxhpc2-1705:8090/BES/bridge/app/ Olof ABP Olof Svensson

BES 3.2.0 Design Configuration Testing Support Admin Task details Request (id= 4734179, type = MXPressA)

Id: 4734296
Creation Date: 2016-12-09 16:02:35
Status: Finished
Type: eu.esrf.services.python.v2.6
Initiator: actor:/MXPressA.MXPressMultiCrystal.Interpretation%20of%20diffraction%20plan
Executor:

| Name | Value | Data Type |
|----------|--------|-----------|
| beamline | id30a1 | STRING |
| Case ID | 9070 | STRING |

Resultitems Resultblocks Event Task

Enter search string here

Result Block Type: Name: Value: Colour:

| Colour | Name | Value | Discriminator | + |
|---------------------------------------|-------------------------|---------------|---------------|---|
| Resultblock [id=3809818, type=python] | | | | |
| aimedCompleteness | | NULL_RESULT | | |
| aimedMultiplicity | | NULL_RESULT | | |
| anomalousData | false | STRING_RESULT | | |
| dataCollectionGroupComment | Number of positions: 2. | STRING_RESULT | | |
| do2DMeshOnly | false | STRING_RESULT | | |
| doCharacterisation | true | STRING_RESULT | | |
| doOnlyEDNAResolution | false | STRING_RESULT | | |
| do_data_collect | true | STRING_RESULT | | |
| findLargestMesh | false | STRING_RESULT | | |
| minOscWidth | | NULL_RESULT | | |

14 rows 30

Page 15 | I Automating complex data collection using workflows | 2017-01-17 | Olof Svensson | The European Synchrotron | ESRF

WORKFLOW EXECUTION STATISTICS

- **Shipped with Passerelle EDM:**

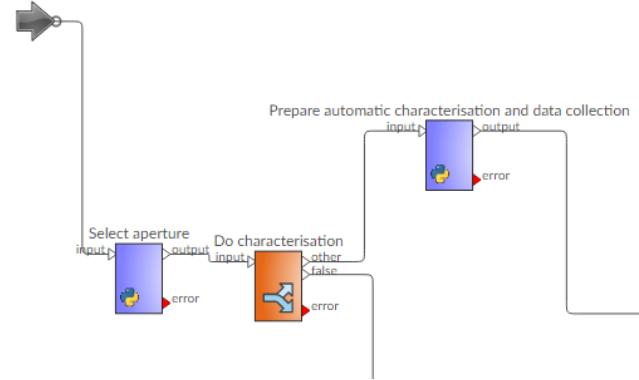
Enter search string here

Type: Day(Creation Day): 01/12/2016 To 07/12/2016

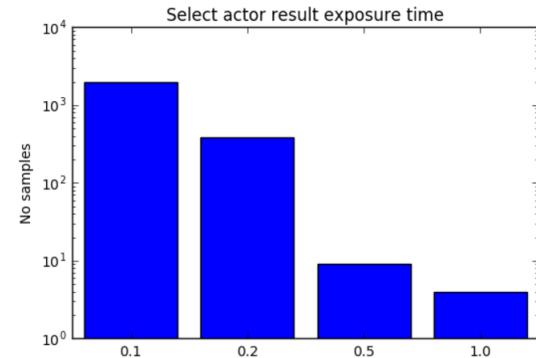
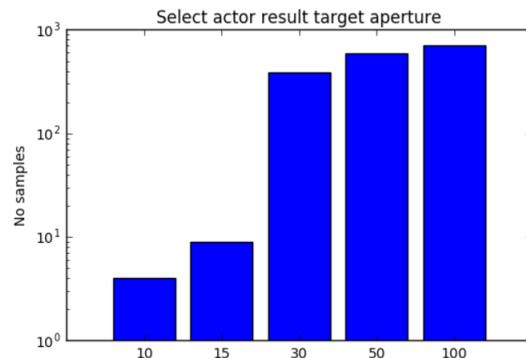
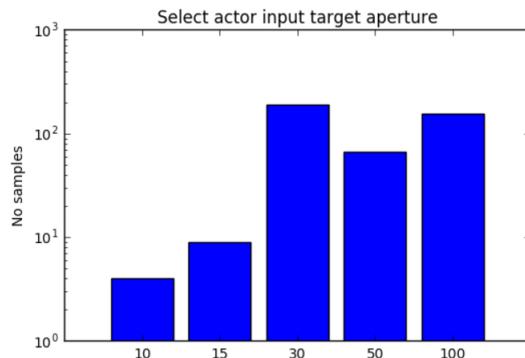
Initiator: bm14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b

⋮

| Creation Date/Day | | 71 rows | | | | | | | | | | | | | | | | |
|-------------------|-------|-----------|--------------|---------------|----------------|------------|---------------------|-----------------|----------|----------------|------------------------|--------------------|-------------------------|---------------|------------------|------------------|--------|--|
| | | dozor_OAR | autoPROC_OAR | xray_Centring | XIA2_DIALS_OAR | KDSAPP_OAR | VisualReorientation | TroubleShooting | MeshScan | MeshAndCollect | MXPressA_aperture_30um | KappaReorientation | HelicalCharacterisation | EDNA_proc_OAR | CreateThumbnails | Characterisation | Sum | |
| 01/12/2016 | 303 | 113 | 1 | 139 | | 2 | 91 | | 29 | | 139 | 2565 | 154 | 3,536 | | | | |
| 02/12/2016 | 408 | 107 | 17 | 107 | | 1 | 93 | | 40 | | 2 | 107 | 3371 | 300 | 4,553 | | | |
| 03/12/2016 | 253 | 127 | 18 | 140 | | 2 | | | 94 | | 140 | 2787 | 117 | 3,678 | | | | |
| 04/12/2016 | 406 | 81 | 1 | 81 | | | | | 29 | 11 | | 80 | 1974 | 325 | 2,988 | | | |
| 05/12/2016 | 580 | 108 | 2 | 108 | | 10 | 1 | 28 | 9 | 5 | | 108 | 1799 | 463 | 3,221 | | | |
| 06/12/2016 | 162 | 49 | | 49 | 6 | | | 5 | | | | 42 | 518 | 111 | 942 | | | |
| 07/12/2016 | 276 | 66 | 38 | 71 | | 1 | 11 | | 8 | 6 | 1 | 68 | 1821 | 203 | 2,570 | | | |
| Sum | 2,388 | 651 | 77 | 695 | 6 | 10 | 7 | 228 | 9 | 29 | 187 | 6 | 3 | 684 | 14,835 | 1,673 | 21,488 | |



- **Custom statistics with Python script accessing BES database:**



WORKFLOW ERROR STATISTICS

Enter search string here 

Type: Day(Creation Day):  To 

Initiator: bm14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b

9 rows

| Type | Error | Finished | Started | Sum |
|------------------|-------|----------|---------|-------|
| dozor_OAR | | 35 | | 35 |
| autoPROC_OAR | | 24 | | 24 |
| XIA2_DIALS_OAR | | 35 | | 35 |
| MXPressA | 4 | 34 | 1 | 39 |
| EDNA_proc_OAR | | 35 | | 35 |
| CreateThumbnails | 6 | 923 | | 929 |
| Sum | 10 | 1,086 | 1 | 1,097 |

WORKFLOW TROUBLESHOOTING

Enter search string here

Reference: Id: Correlation Id:
 Type: External Reference:

Initiator: bmr14 id23eh1 id23eh2 id29 id30a1 id30a2 id30a3 id30b
 Status: Created Error Finished Cancelled Started Timeout
 Creation Date: To 08:00:00 08:30:00

| | Reference | Id | | Type | Creation Date | Initiator | External Reference | Status | Duration(ms) | + |
|--------------------------|---|----------|------------------|---------------------|---------------|-----------|--------------------|---------|--------------|---|
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47556048 | CreateThumbnails | 2016-12-10 08:29:50 | id30a1 | fx1 | Finished | 6,055 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47556044 | CreateThumbnails | 2016-12-10 08:29:36 | id30a1 | fx1 | Finished | 6,913 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47556020 | CreateThumbnails | 2016-12-10 08:28:56 | id30a1 | fx1 | Finished | 5,674 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47556016 | CreateThumbnails | 2016-12-10 08:28:42 | id30a1 | fx1 | Finished | 6,801 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47556012 | CreateThumbnails | 2016-12-10 08:28:08 | id30a1 | fx1 | Finished | 5,684 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47556008 | CreateThumbnails | 2016-12-10 08:28:01 | id30a1 | fx1 | Finished | 7,557 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47556003 | CreateThumbnails | 2016-12-10 08:27:44 | id30a1 | fx1 | Finished | 5,580 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559999 | CreateThumbnails | 2016-12-10 08:27:37 | id30a1 | fx1 | Finished | 6,588 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559995 | CreateThumbnails | 2016-12-10 08:27:22 | id30a1 | fx1 | Finished | 5,578 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559991 | CreateThumbnails | 2016-12-10 08:27:15 | id30a1 | fx1 | Finished | 6,844 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559987 | CreateThumbnails | 2016-12-10 08:26:59 | id30a1 | fx1 | Finished | 5,631 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559983 | CreateThumbnails | 2016-12-10 08:26:49 | id30a1 | fx1 | Finished | 8,640 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559979 | CreateThumbnails | 2016-12-10 08:26:32 | id30a1 | fx1 | Finished | 5,601 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559975 | CreateThumbnails | 2016-12-10 08:26:23 | id30a1 | fx1 | Finished | 9,346 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559971 | CreateThumbnails | 2016-12-10 08:26:06 | id30a1 | fx1 | Finished | 5,777 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559967 | CreateThumbnails | 2016-12-10 08:25:56 | id30a1 | fx1 | Finished | 8,553 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559963 | CreateThumbnails | 2016-12-10 08:25:39 | id30a1 | fx1 | Finished | 5,596 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559959 | CreateThumbnails | 2016-12-10 08:25:30 | id30a1 | fx1 | Finished | 9,293 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559954 | CreateThumbnails | 2016-12-10 08:25:15 | id30a1 | fx1 | Finished | 5,657 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559951 | CreateThumbnails | 2016-12-10 08:25:06 | id30a1 | fx1 | Finished | 9,592 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559947 | CreateThumbnails | 2016-12-10 08:24:49 | id30a1 | fx1 | Finished | 6,195 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559943 | CreateThumbnails | 2016-12-10 08:24:42 | id30a1 | fx1 | Finished | 6,608 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559938 | CreateThumbnails | 2016-12-10 08:24:25 | id30a1 | fx1 | Finished | 5,727 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559935 | CreateThumbnails | 2016-12-10 08:24:18 | id30a1 | fx1 | Finished | 7,336 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559931 | CreateThumbnails | 2016-12-10 08:24:00 | id30a1 | fx1 | Finished | 5,805 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559917 | CreateThumbnails | 2016-12-10 08:23:51 | id30a1 | fx1 | Finished | 7,809 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 9100 | 47558877 | MXPressA | 2016-12-10 08:22:41 | id30a1 | fx1 | Error | 490,444 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47559904 | CreateThumbnails | 2016-12-10 08:20:03 | id30a1 | fx1 | Finished | 6,632 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47558890 | CreateThumbnails | 2016-12-10 08:18:28 | id30a1 | fx1 | Finished | 5,944 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47558887 | EDNA proc_OAR | 2016-12-10 08:18:28 | id30a1 | fx1 | Finished | 139,347 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47558870 | XIA2_DIALS_OAR | 2016-12-10 08:18:26 | id30a1 | fx1 | Finished | 282,136 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47558869 | dozor_OAR | 2016-12-10 08:18:26 | id30a1 | fx1 | Finished | 131,598 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47558868 | autoPROC_OAR | 2016-12-10 08:18:26 | id30a1 | fx1 | Finished | 562,360 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47558863 | CreateThumbnails | 2016-12-10 08:17:42 | id30a1 | fx1 | Finished | 6,305 | | |
| <input type="checkbox"/> | <input type="button" value="Search"/> <input type="checkbox"/> 2832 | 47558849 | CreateThumbnails | 2016-12-10 08:17:37 | id30a1 | fx1 | Finished | 5,634 | | |

| | | | |
|------------------------|----------------|---------------|--------|
| External Reference:fx1 | modpath | MXPressA | STRING |
| Correlation Id: | prefix | AV147-D_679_1 | STRING |
| InitiatorId30a1 | run number | 1 | STRING |
| Executor: | sample_lims_id | 575875 | STRING |
| | sample_node_id | 136 | STRING |

Task Result Item Event

Enter search string here

Status: Created Error Finished Cancelled Started Timeout
Type: Discriminator: Initiator:

| View | Id | Creation Date | Duration(ms) | Status | Type | Initiator |
|-------------------------------------|---------|---------------------|--------------|----------|------------------------------------|--|
| Q | 4755878 | 2016-12-10 08:22:41 | 9 | Finished | Start | actor:/MXPressA,Start |
| Q | 4755879 | 2016-12-10 08:22:41 | 692 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,Beamline#v2Setup |
| Q | 4755880 | 2016-12-10 08:22:42 | 586 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,Prepare%20MXPressA |
| Q | 4755891 | 2016-12-10 08:22:43 | 2904 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,CommonPrepareExperiment,Init%20workflow |
| Q | 4755922 | 2016-12-10 08:22:46 | 772 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,CommonPrepareExperiment,Read%20motor%20positions |
| Q | 4755923 | 2016-12-10 08:22:46 | 290 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,CommonPrepareExperiment,Default%20parameters |
| Q | 4755924 | 2016-12-10 08:22:47 | 1461 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,Interpretation%20of%20diffraction%20plan |
| Q | 4755925 | 2016-12-10 08:22:48 | 310 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,Contact%20user%20if%20first%20acronym%20collection |
| Q | 4755926 | 2016-12-10 08:22:48 | 40139 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,PrepareAutoMesh,Auto%20mesh |
| Q | 4755927 | 2016-12-10 08:23:29 | 1434 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,Get%20grid%20positions |
| Q | 4755928 | 2016-12-10 08:23:30 | 280245 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,ExecuteMesh2D,Collect%20and%20process%20data |
| Q | 4755929 | 2016-12-10 08:28:10 | 29 | Finished | Check if meshPositionsAcquired | actor:/MXPressA,MXPressMultiCrystal,ExecuteMesh2D,Check%20if%20meshPositionsAcquired |
| Q | 4755930 | 2016-12-10 08:28:10 | 2212 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,ExecuteMesh2D,Find%20best%20position |
| Q | 4756021 | 2016-12-10 08:28:12 | 43961 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,ExecuteMesh2D,ISPy%20upload |
| Q | 4756022 | 2016-12-10 08:28:13 | 13924 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,ExecuteMesh2D,Send%20results%20to%20mxCuBE |
| Q | 4756023 | 2016-12-10 08:28:13 | 62 | Finished | Check if signal | actor:/MXPressA,MXPressMultiCrystal,ExecuteMesh2D,Check%20if%20signal |
| Q | 4756024 | 2016-12-10 08:28:13 | 338 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,ExecuteMesh2D,Extract%20best%20position |
| Q | 4756025 | 2016-12-10 08:28:13 | 25 | Finished | Check if 2D mesh only | actor:/MXPressA,MXPressMultiCrystal,Check%20if%202D%20mesh%20only |
| Q | 4756026 | 2016-12-10 08:28:13 | 7661 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Move%20to%20new%20sample%20position |
| Q | 4756027 | 2016-12-10 08:28:21 | 594 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Correct%20for%20d30a1%20phi |
| Q | 4756028 | 2016-12-10 08:28:21 | 28 | Finished | Extra vertical scan | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Extra%20vertical%20scan |
| Q | 4756029 | 2016-12-10 08:28:21 | 17 | Finished | Check if center rotation axis | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Check%20if%20center%20rotation%20axis |
| Q | 4756030 | 2016-12-10 08:28:21 | 1583 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,Prepare%20first%20line%20scan |
| Q | 4756031 | 2016-12-10 08:28:23 | 36506 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,Collect%20and%20process%20data |
| Q | 4756032 | 2016-12-10 08:29:00 | 27 | Finished | Check if meshPositionsAcquired | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,Check%20if%20meshPositionsAcquired |
| Q | 4756033 | 2016-12-10 08:29:00 | 2611 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,Find%20best%20position |
| Q | 4756034 | 2016-12-10 08:29:02 | 47900 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,ISPy%20upload |
| Q | 4756035 | 2016-12-10 08:29:02 | 17778 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,Send%20results%20to%20mxCuBE |
| Q | 4756036 | 2016-12-10 08:29:02 | 55 | Finished | Check if signal | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,Check%20if%20signal |
| Q | 4756037 | 2016-12-10 08:29:02 | 383 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,Extract%20best%20position |
| Q | 4756038 | 2016-12-10 08:29:03 | 12415 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,Move%20to%20sample%2080%20degrees |
| Q | 4756039 | 2016-12-10 08:29:15 | 1679 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,Prepare%20second%20line%20scan |
| Q | 4756040 | 2016-12-10 08:29:17 | 36642 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,Collect%20and%20process%20data |
| Q | 4756051 | 2016-12-10 08:29:53 | 40 | Finished | Check if meshPositionsAcquired | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,Check%20if%20meshPositionsAcquired |
| Q | 4756052 | 2016-12-10 08:29:54 | 2070 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,Find%20best%20position |
| Q | 4756053 | 2016-12-10 08:29:56 | 15513 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,ISPy%20upload |
| Q | 4756054 | 2016-12-10 08:29:56 | 7929 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,Send%20results%20to%20mxCuBE |
| Q | 4756055 | 2016-12-10 08:29:56 | 31 | Finished | Check if signal | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,Check%20if%20signal |
| Q | 4756056 | 2016-12-10 08:29:56 | 485 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,No%20diffraction%20signal%20error%20message |
| Q | 4756057 | 2016-12-10 08:29:56 | 31 | Finished | Check if more positions to collect | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,1,Check%20if%20more%20positions%20to%20collect |
| Q | 4756058 | 2016-12-10 08:29:56 | 6679 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,Move%20to%20next%20position |
| Q | 4756059 | 2016-12-10 08:30:03 | 9326 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Move%20to%20new%20sample%20position |
| Q | 4756060 | 2016-12-10 08:30:12 | 592 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Correct%20for%20d30a1%20phi |
| Q | 4756071 | 2016-12-10 08:30:13 | 44 | Finished | Extra vertical scan | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Extra%20vertical%20scan |
| Q | 4756072 | 2016-12-10 08:30:13 | 17 | Finished | Check if center rotation axis | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,Check%20if%20center%20rotation%20axis |
| Q | 4756073 | 2016-12-10 08:30:13 | 1508 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,Prepare%20first%20line%20scan |
| <input checked="" type="checkbox"/> | 4756074 | 2016-12-10 08:30:14 | 34323 | Error | eu.esrf.services.python,v2.6 | actor:/MXPressA,MXPressMultiCrystal,XrayCentringVertical,CenterRotationAxis,ExecuteMesh1D,Collect%20and%20process%20data |
| Q | 4756075 | 2016-12-10 08:30:49 | 279 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,CommonErrorReporter,Log%20error%20message |
| Q | 4756076 | 2016-12-10 08:30:49 | 1723 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,CommonErrorReporter,Set%20SP%20status%20to%20failure |
| Q | 4756077 | 2016-12-10 08:30:51 | 749 | Finished | eu.esrf.services.python,v2.6 | actor:/MXPressA,CommonErrorReporter,Display%20error%20message%20in%20mxCuBE |

Id:4756074

Creation Date: 2016-12-10 08:30:14

Status: Error

Type: eu.esrf.services.python.v2.6

initiator:actor:/MXPressA/MXPressMultiCrystal/XrayCentringVertical.CenterRotationAvis.ExecuteMesh1D.Collect%20and%20process%20data

xecutor:

| Name | Value |
|----------------------------|---|
| beamline | id30a1 |
| Case ID | 9100 |
| Creator | MXPRESSA#sep4755877.MXPressMultiCrystal.XrayCentringVertical.CenterRotationAvis.ExecuteMesh1D.Collect and process data |
| dataCollectionGroupComment | |
| directory | /data/visitor/fx1/id30a1/20161210/RAW DATA/AV147/AV147-D_679_1/MXPressA_01 |
| expTypePrefix | line- |
| firstImagePath | /data/visitor/fx1/id30a1/20161210/RAW DATA/AV147/AV147-D_679_1/MXPressA_01/line/AV147-D_679_1_3_0001.cbf |
| grid_info | {"x1": 0.0, "y1": -0.300, "dx_mm": 0.1, "dy_mm": 0.600, "steps_x": 1, "steps_y": 60, "angle": 0.0} |
| meshPositionFile | /data/visitor/fx1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/meshPositionsAvisCentring_fudfl.json |
| meshQueueListFile | /data/visitor/fx1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/meshQueueListFileAvisCentring_shM9w.json |
| meshZigZag | false |
| motorPositions | {"SampX": -0.5485013623978202, "phy": -0.377, "zoom": 2.0, "chi": 0.0, "phi": 0.3727583333333336, "kappa_phi": null, "kappa": null, "focus": -0.6, "z": -0.075, "y": -0.178, "phi": 60.0, "sampy": 0.016893732970027248} |
| prefix | AV147-D_679_1 |
| pyarch_html_dir | /data/pyarch/id30a1/fx1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/html |
| raw_directory | /data/visitor/fx1/id30a1/20161210/RAW DATA/AV147/AV147-D_679_1 |
| Request ID | 4755877 |
| resolution | 2.0 |
| Result type | |
| run_number | 2 |
| sampleInfo | {"cellBeta": 0.0, "nodeId": 136, "limsId": 575875, "cellC": 0.0, "numberOfPositions": 2, "cellB": 0.0, "experimentKind": "Default", "crystalSpaceGroup": "Undefined", "cellAlpha": 0.0, "groupNodeId": 346, "cellGamma": 0.0, "cellA": 0.0} |
| script_asset | |
| script_path | execute_mesh_startDataCollection.py |
| suffix | cbf |
| useFastMesh | false |
| workflowParameters | {"index": 1, "stackTraceFile": "/data/visitor/fx1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/stackTrace_tv_crs5", "workflowWorkingDir": "/data/visitor/fx1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/", "logFile": "/data/visitor/fx1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/workflow.log", "tempDir": "/tmp/ds3498", "yamlFile": "/data/pyarch/id30a1/fx1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/workflow.yaml", "workflows": "None", "workflowLog": "/data/pyarch/id30a1/fx1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/workflow.log.txt", "workflowYamlLog": "/data/pyarch/id30a1/fx1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/Workflow_log.txt", "workflowLogFile": "/data/pyarch/id30a1/fx1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/workflow.log", "workDir": "/data/visitor/fx1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224", "title": "MXPressA: X-centre, eEDNA + dc on id30a1", "workflowLogTitle": "/data/pyarch/id30a1/fx1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224/workflow.log.txt", "workingDir": "/data/visitor/fx1/id30a1/20161210/PROCESSED DATA/AV147/AV147-D_679_1/MXPressA_01/Workflow_20161210-08224"} |
| workflow_id | 63498 |

ResultItems Resultblocks Event Task

| | Creation Date | Topic | Message |
|--|---------------------|---------------|---|
| | 2016-12-10 08:30:14 | CREATED | |
| | 2016-12-10 08:30:14 | STARTED | |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | raw_directory |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | meshZigZag |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | resolution |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | pyarch_html_dir |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | run_number |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | workflow_id |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | sampleInfo |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | meshQueueListFile |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | grid_info |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | useFastMesh |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | meshPositionFile |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | firstImagePath |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | motorPositions |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | suffix |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | beamline |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | expTypePrefix |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | workflowParameters |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | dataCollectionGroupComment |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | directory |
| | 2016-12-10 08:30:14 | ADD ATTRIBUTE | prefix |
| | | | com.scienc...passerelle.edm.request.service.ServiceException: TASK_ERROR - ERROR - [PASS_FUNC-5000] - Task processing error - Error from python script Traceback (most recent call last): File "/usr/local/bin/workflow/pythonserverscripts/scisoft/pypy/python/pyrpy.py", line 86, in pyrpyhandler.common ret = handler('unlabeled') File "/usr/local/BES5/id30a1/workflow/pythonserverscripts/python_service/runscript.py", line 77, in runScript result = vars[funcName](**inputs) |

- **Start of workflows:**

- Hardware object “EdnaWorkflow”
- Corresponding XML file “ednaparameters.xml” contains host/port of BES and list of available workflows:

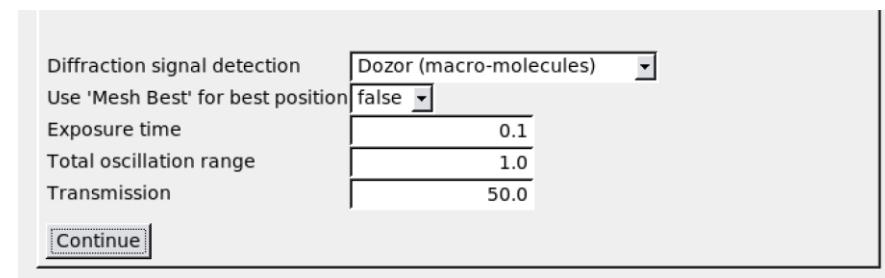
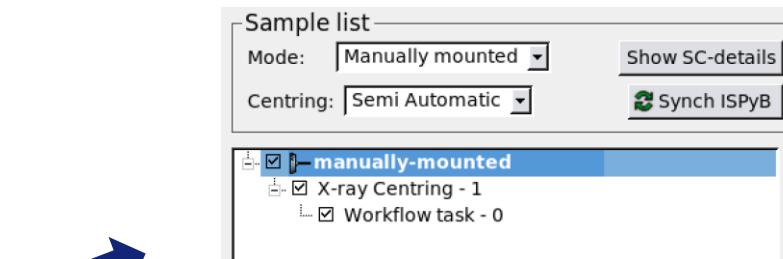
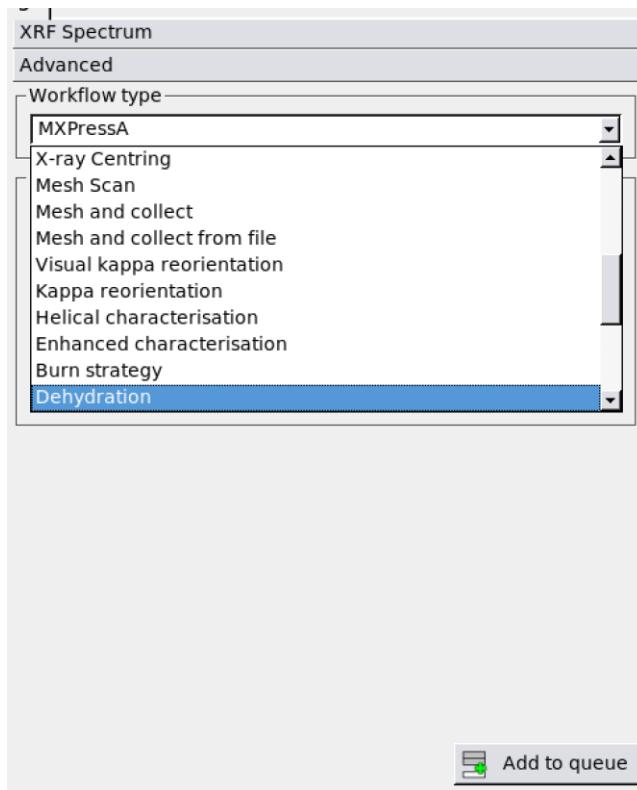
```
<object class = "EdnaWorkflow" role = "workflow">
    <bes_host>mxhpc2-1705</bes_host>
    <bes_port>38180</bes_port>
    <object href="/session" role="session"/>
    <workflow>
        <title>MXPressA</title>
        <path>MXPressA</path>
    </workflow>
    <workflow>
        <title>MXPressE</title>
        <path>MXPressE</path>
    </workflow>
    ...
</object>
```

- **Call-back from Workflows to mxCuBE:**

- Handled by the XMLRPCServer hardware object
- Almost all methods used (start_queue, log_message, shape_history_get_grid, open_dialog, workflow_end etc)

GUI INTERFACE TO MXCUBE

- **Interface to mxCuBE v2:**



- **Interface to mxCuBE v3:**

- Better integrated, context driven
- Improved dialogs

MXCUBE WORKFLOW RESULT

mxCuBE (mx-415) (on ub1004)

File Instrumentation Help

Collect XRF spectrum System Feedback Chat

User: mx-415 Group: Set Logout

Sample centring Data collection

Results

Diffraction signal

Manually mounted

- X-ray Centring - 1
- Workflow task - 0
- XrayCentering - 1
 - mesh-t1_1 Collection done
 - mesh-t1_1 Collection done
 - mesh-t1_1 Collection done
 - mesh-t1_1 Collection done
 - line-t1_2 Collection done

Grid size

Machine current: -1.0 mA
unknown
00:00

Flux: ? ph/s

Energy: Energy: Wavelength:

Resolution: Current: Move to:

Transmission: Current: Set to: Filters

Current users: Selecting gives control Allow timeout control Ask for control My name:

[2017-01-16 09:42:09] Workflow: Sending email
[2017-01-16 09:42:09] Workflow: Storing workflow mesh
[2017-01-16 09:42:10] Workflow: ISPyB uploading finished.

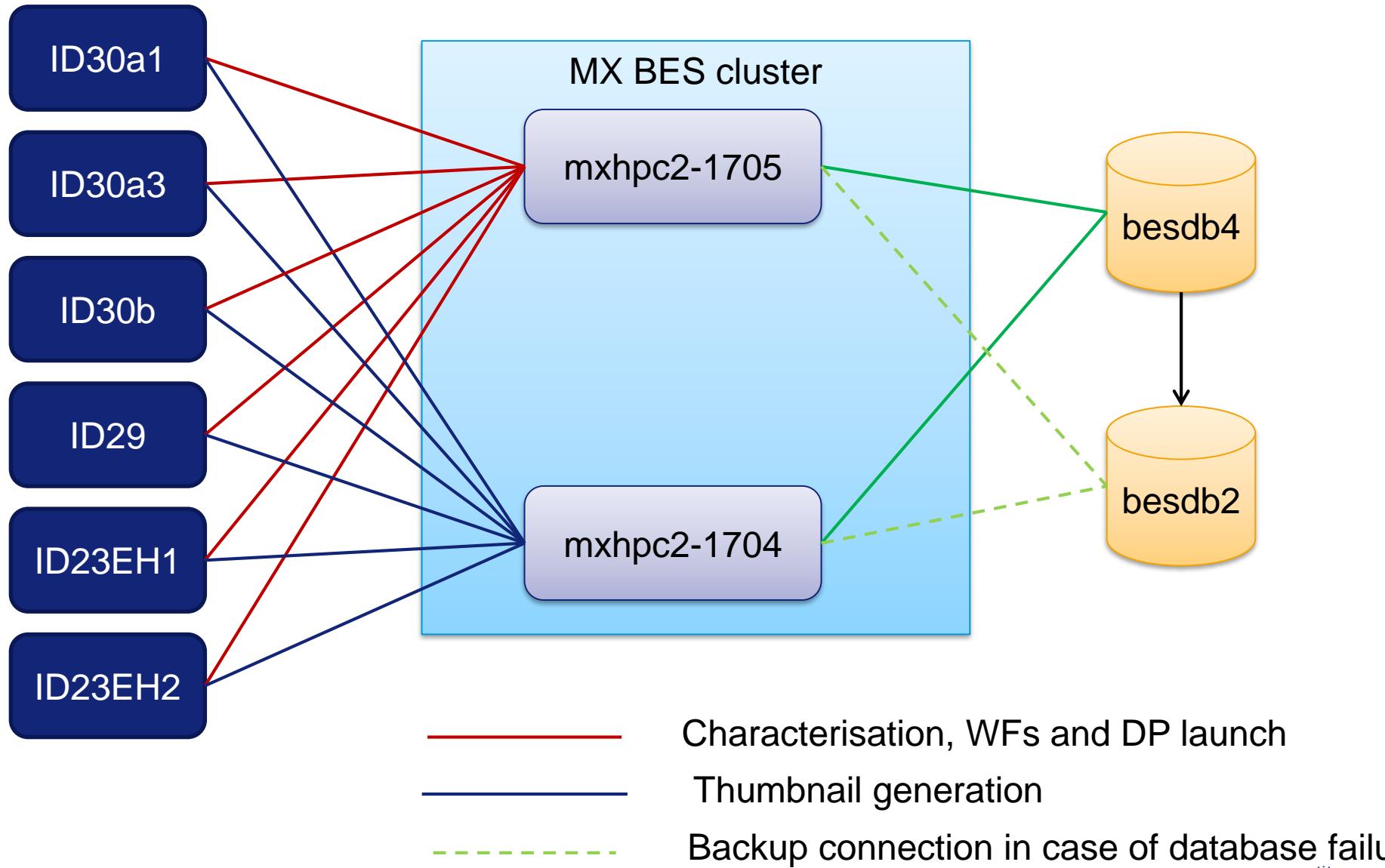
INTERFACE TO ISPYB

- Same type of web services as mxCuBE for retrieving and uploading data
- (Old) ISPyB GUI and (new) EXI result pages:

The screenshot shows the ISPyB interface. At the top, there are two boxes: 'Selected Session' (Proposal: mx415, Start Date: 16-01-2017, Beamline: ID30A-2) and 'Selected Workflow' (Workflow Type: X-rayCentering, Title: X-ray centering on id30a2). Below these are tabs for DataCollections, Workflow Log, and Results. The Results tab is active, displaying a 'Diffraction signal' plot with axes x and y from 1 to 15. A 'Mesh plot' section below it shows a grid size of 18x4 steps, resulting in a size of 0.635 mm. A note says 'Best position - the sample has automatically been moved to this position'. Motor positions listed are sampx.move(0.000), sampy.move(-0.063), phiy.move(-0.250), phiz.move(0.000). The bottom status bar shows various beamline controls.

The screenshot shows the ExiMX interface. At the top, it says 'Version: 0.9.8 Released: 2016/12/22' and features the ESRF logo. The main area has tabs for Home, Shipment, Proteins and Crystals, Prepare Experiment, Data Explorer, Offline Data Analysis, Help, and search by p. The 'Results' tab is active, showing a 'Workflow' section with a 'Mesh' plot and a 'Line' plot. Below is a 'Grid size' table: Steps x: 18, Steps y: 4, Size x [mm]: 0.635, Size y [mm]: 0.194. A note says 'Best position - the sample has automatically been moved to this position'. Motor positions listed are sampx.move(0.000), sampy.move(-0.063), phiy.move(-0.250), phiz.move(0.000). To the right, there is a large grid of grayscale images labeled 'mesh-t1_1_0024.cbf'.

CURRENT BES INSTALLATION



ACKNOWLEDGEMENTS

- David von Stetten, Max Nanao, Sasha Popov, Daniele de Sanctis, Stéphanie Monaco, Didier Nurizzo, Matias Guijarro, Solange Delageneire, Alejandro de Maria, Marcus Oskarsson (ESRF)
- Matthew Bowler (EMBL Grenoble)
- Erwin de Ley and Koen Heunick (Isencia, Belgium)
- The ESRF Data Analysis Unit, Beamline Control Unit and Structural Biology group

Further reading:

- **Fully automatic characterization and data collection from crystals of biological macromolecules**, Svensson, O., Malbet-Monaco, S., Popov, A., Nurizzo, D., & Bowler, M. W. (2015). *Acta Crystallographica Section D: Biological Crystallography*, 71(Pt 8), 1757–1767. <http://doi.org/10.1107/S1399004715011918>
- **MeshAndCollect: an automated multi-crystal data-collection workflow for synchrotron macromolecular crystallography beamlines**, Ulrich Zander · Gleb Bourenkov · Alexander N Popov · Daniele De Sanctis · Olof Svensson · Andrew A McCarthy · Ekaterina Round · Valentin Gordeliy · Christoph Mueller-Dieckmann · Gordon A Leonard, *ACTA CRYSTALLOGRAPHICA SECTION D BIOLOGICAL CRYSTALLOGRAPHY* 71(11):2328-2343 · NOVEMBER 2015
- **Facilitating best practices in collecting anomalous scattering data for de novo structure solution at the ESRF Structural Biology Beamlines**, Daniele de Sanctis · Marcus Oscarsson · Alexander Popov · Olof Svensson · Gordon Leonard, *Acta Cryst.* (2016). D72, 413-420
- **The use of workflows in the design and implementation of complex experiments in macromolecular crystallography**, 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,, *Acta Cryst.* (2012). D68, 975-984