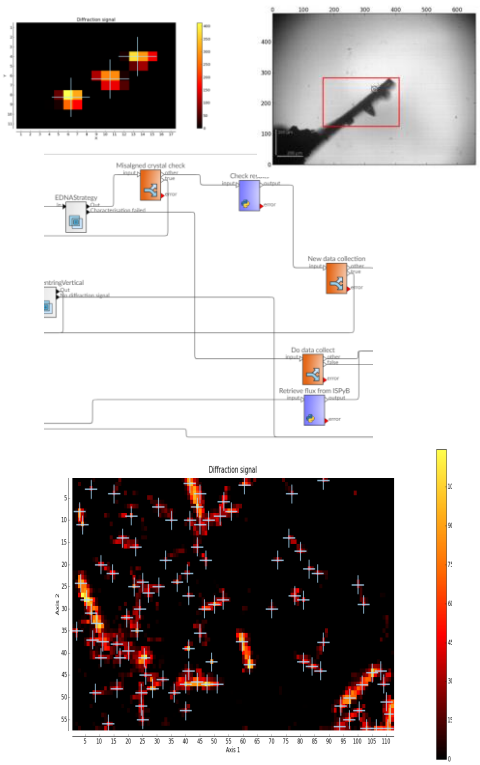
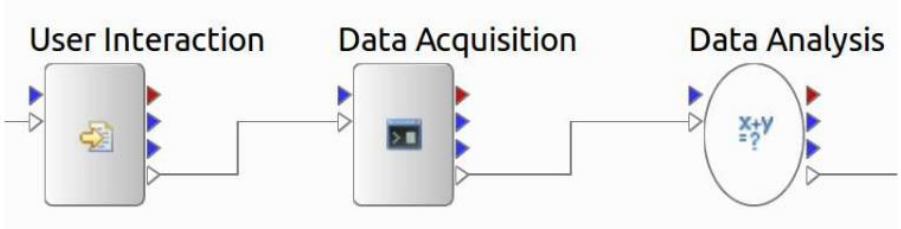



# Multi-crystal data collection capabilities at the ESRF

**Olof Svensson**

**Data Analysis Unit / ISDD**

- **Multi-crystal data collections implemented as workflows**

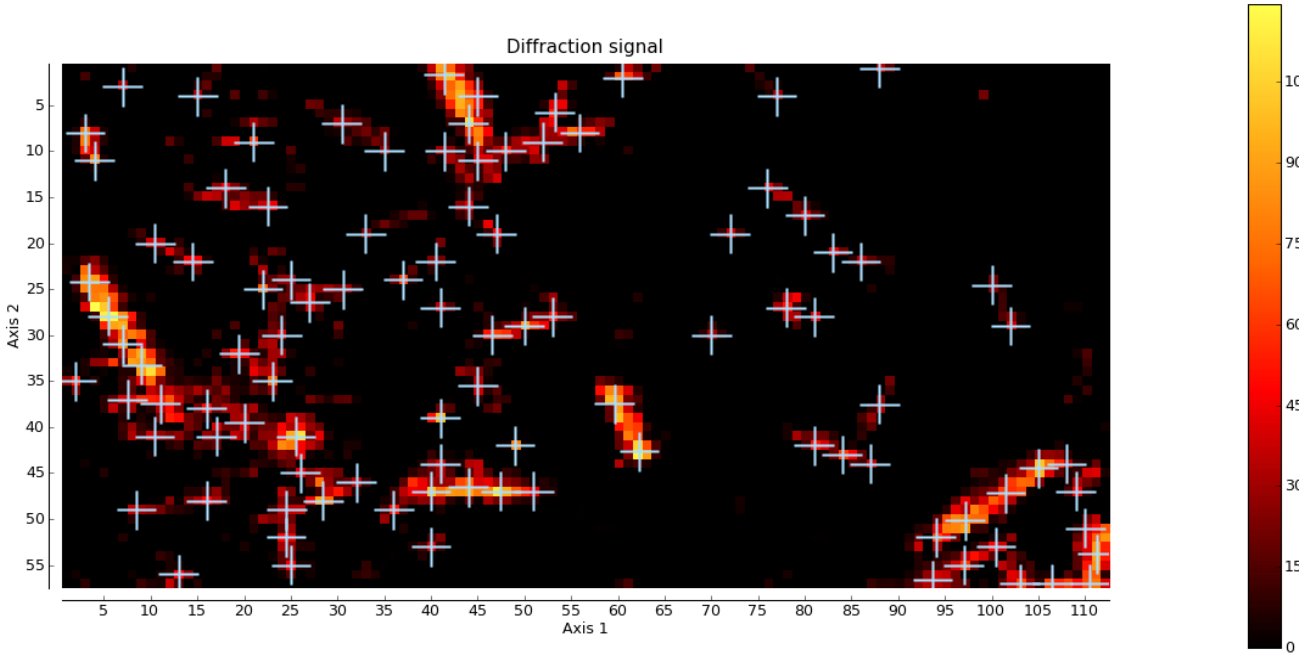



- **Mesh and collect – interactive**
- **Fully automatic workflows :**
  - MXPressE : Auto-mesh, X-ray centring, characterisation, data collection
  - MXPressO : Auto-mesh, X-ray centring, data collection 180 degrees
  - MXPressI : Auto-mesh, X-ray centring, characterisation, data collection 180 degrees with resolution from characterisation

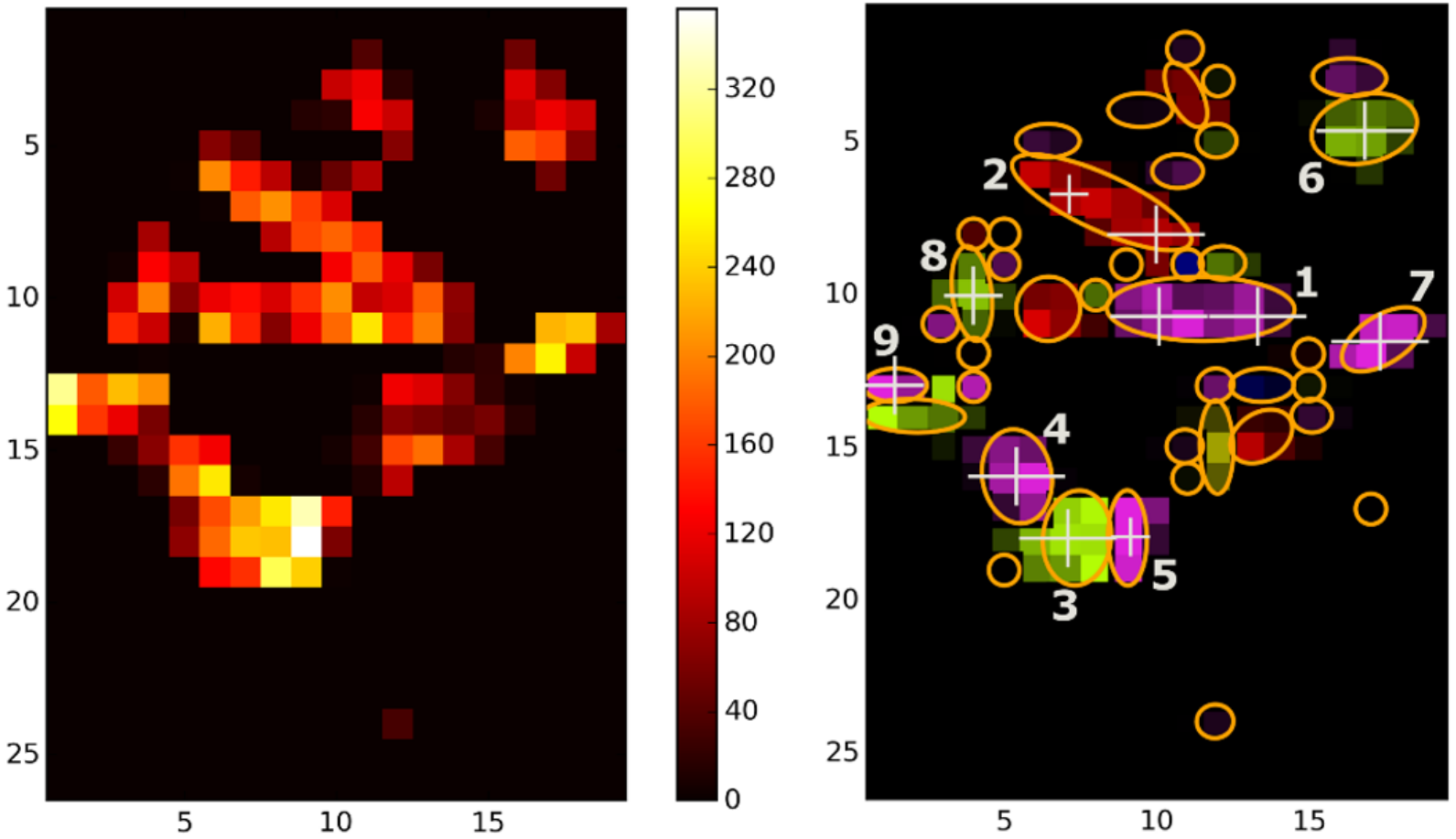
- **Manual grid selection in mxCuBE + initial parameters:**

| | |
|---|---|
| Diffraction signal detection | Dozor (macro-molecules) |
| Grid exposure time | 0.1 |
| Total oscillation range | 1.0 |
| Transmission | 50.0 |
| Take single snapshot at end of WF | true |

- **2D X-ray grid :**



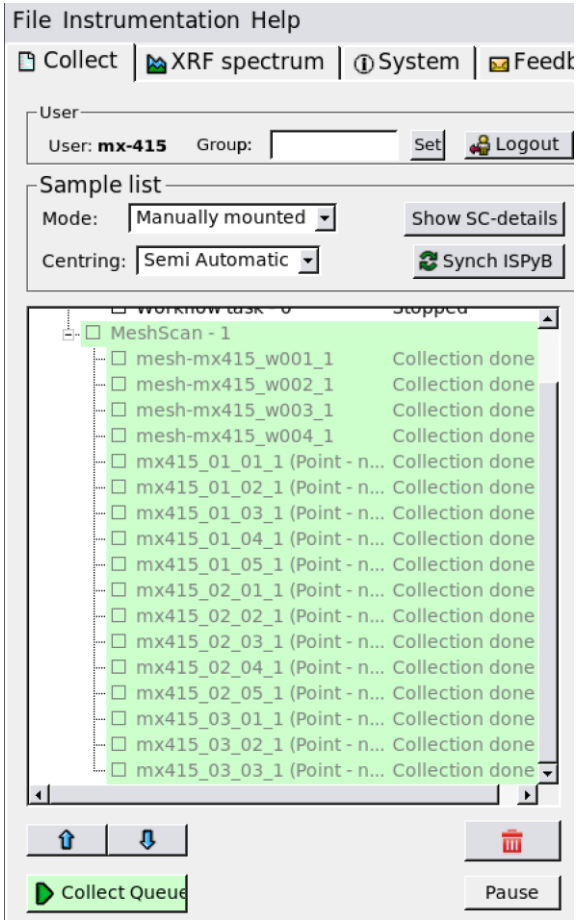
# MESHBEST OPTION (IGOR MELNIKOV)



# MESH AND COLLECT

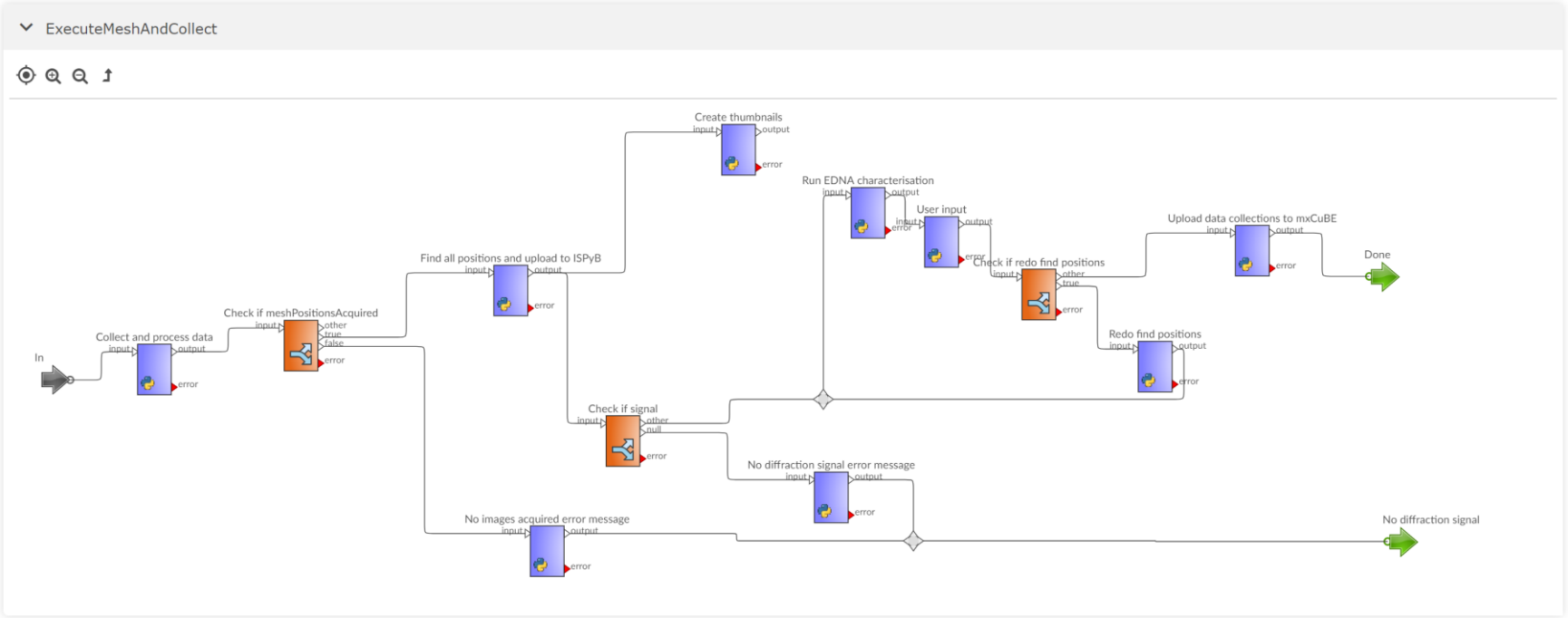
- **Characterisation on strongest grid image(s)**
- **User input :**

| | |
|---|---|
| Diffraction signal detection | Dozor (macro-molecules) |
| Resolution | 2.93 |
| Data threshold | 100000.0 |
| Redo find positions? | false |
| Exposure time | 5.41463414634 |
| Transmission | 50.0 |
| Total oscillation range | 10.0 |
| No images | 100 |
| Max no data collection positions | 5 |
| Number of data collection iterations | 1 |
| Radius | 3.0 |
| Aimed I/Sigma at highest resolution | 1.0 |
| Inverse beam data collection | false |
| Flux | 1e+12 |
| Time to reach Henderson limit | 541.5 |
| XDSAPP auto-processing | true |
| Grenades_fastproc auto-processing | true |
| Grenades_parallelproc auto-processing | false |
| EDNA_proc auto-processing | false |
| XIA2_DIALS auto-processing | false |
| autoPROC auto-processing | false |




- **Data collection on found positions :**

# BEAMLINE EXPERT SYSTEM – PASSERELLE EDM



# OUTLINE

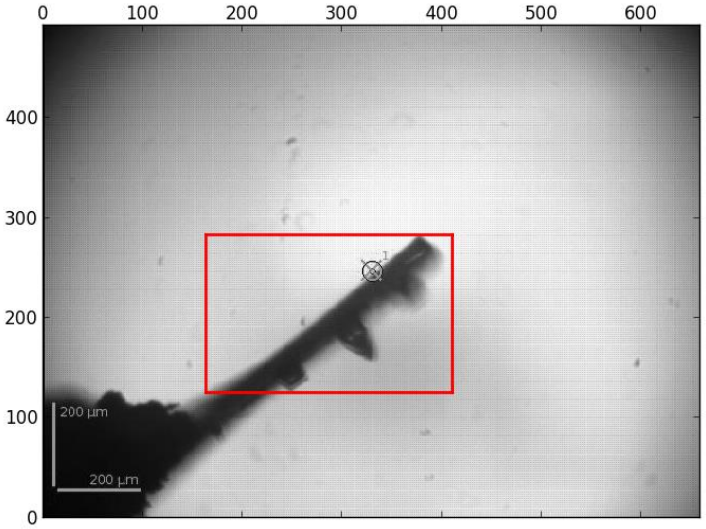
## MXPress diffraction plan choices:

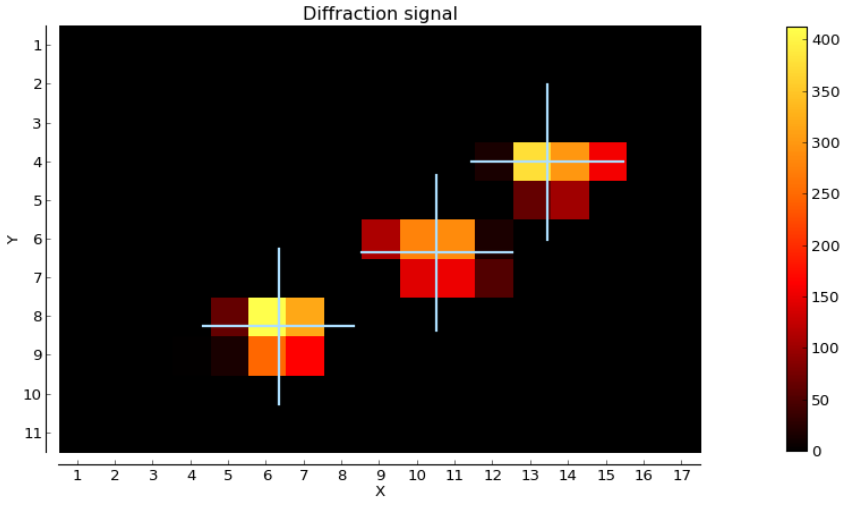
- Type of experiment:
  - MXPressE: automesh, X-ray centring, (EDNA) characterization, data collection
  - MXPressO : automesh, X-ray centring, 180 degree standard data collection
  - MXPressI : automesh, X-ray centring, characterization, 180 degree data collection at resolution given by characterization (ranking resolution), data collection
  - MXPressM : Loop screening; automesh, 2D mesh
  - MXPressP : Pseudo helical; automesh, X-ray centring with many point detection, characterization on strongest position, full data collection on strongest position, partial data collections on remaining positions

- Common choices:
  - SAD / no SAD
  - No positions
  - Beam size
  - Crystal space group and cell dimensions
  - Crystal susceptibility to radiation damage

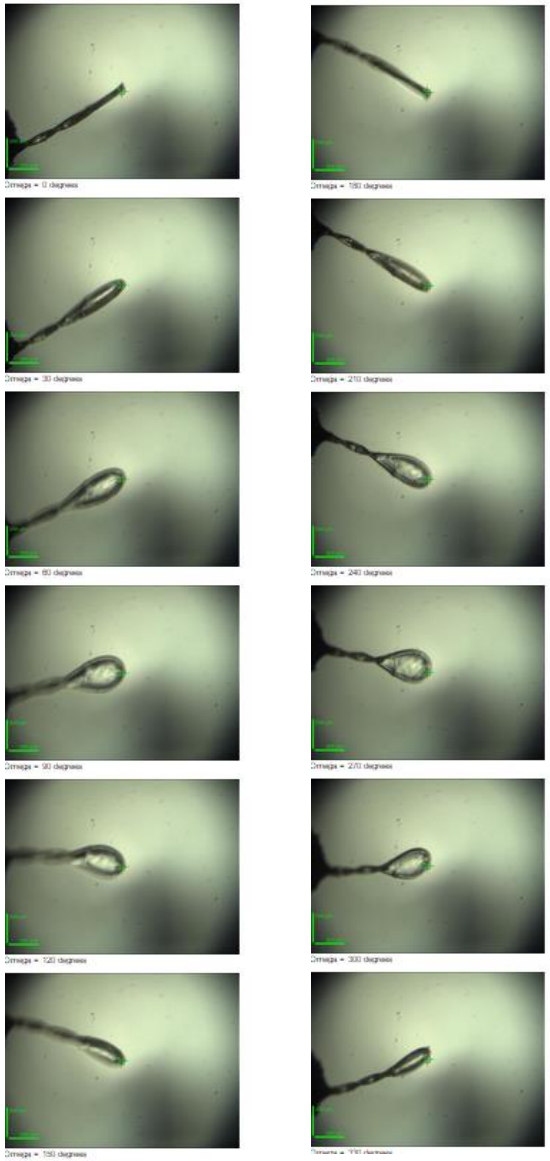
# MXPRESS-STYLE WORKFLOWS

- **Number of positions taken from ISPyB diffraction plan**
- **Auto mesh, max loop size**
- **2D X-ray grid**
- **For every position :**
  - Vertical centring 90 degrees apart from 2D mesh
  - Characterisation
  - Data collection

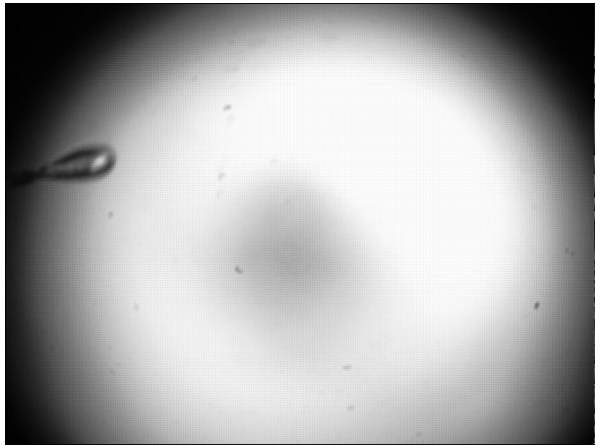


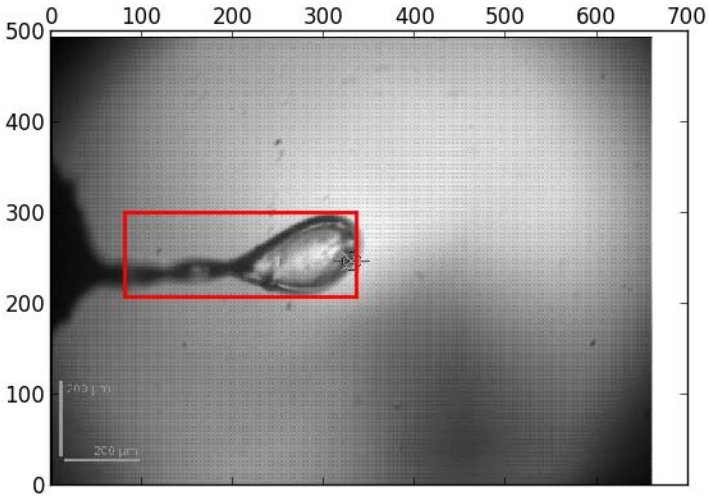



# AUTO MESH



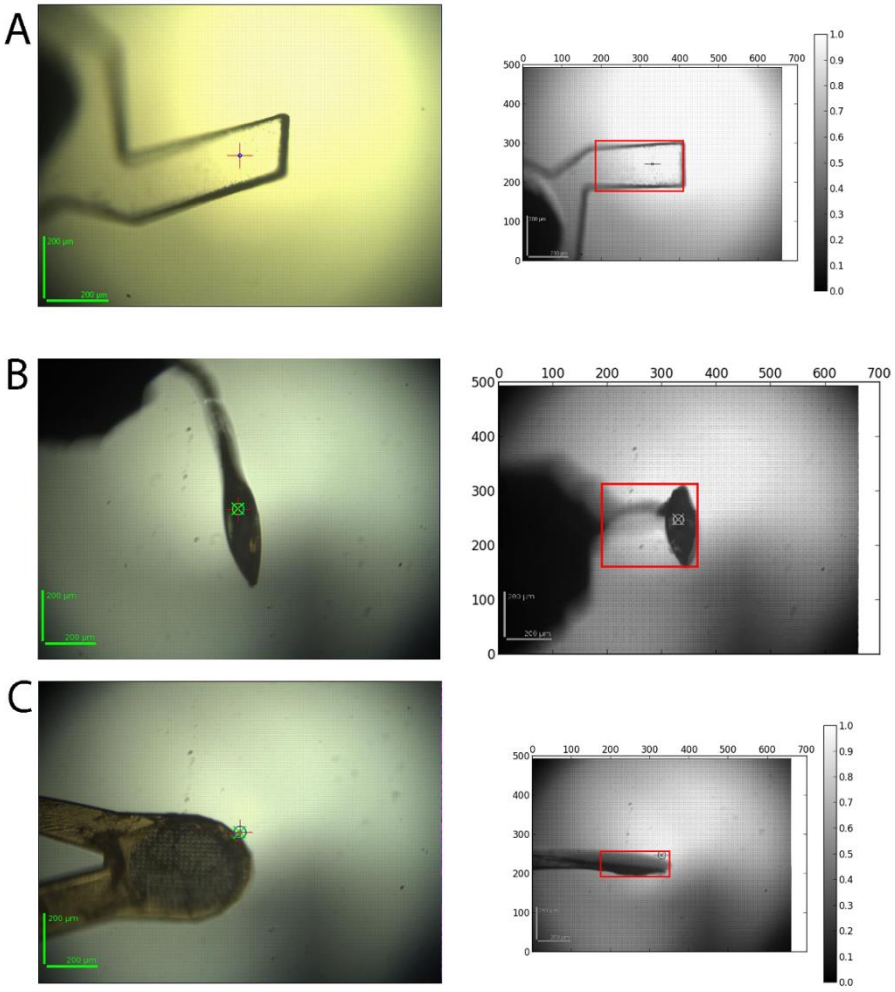
Auto loop centring with Lucid 2





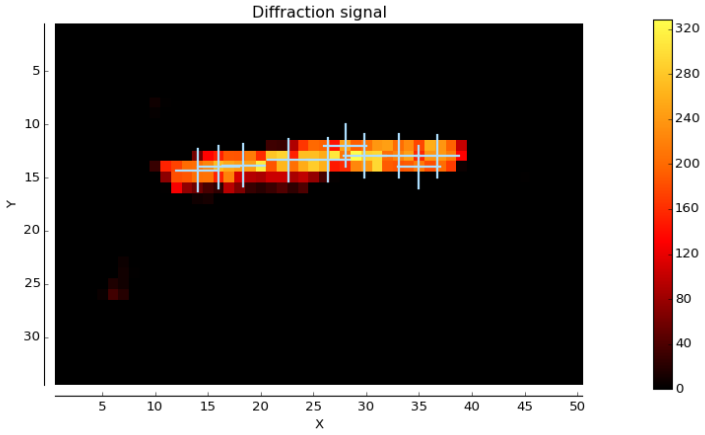
# AUTO MESH

## Code on github: https://github.com/olofsvensson/AutoMesh (→ mxCuBE?)



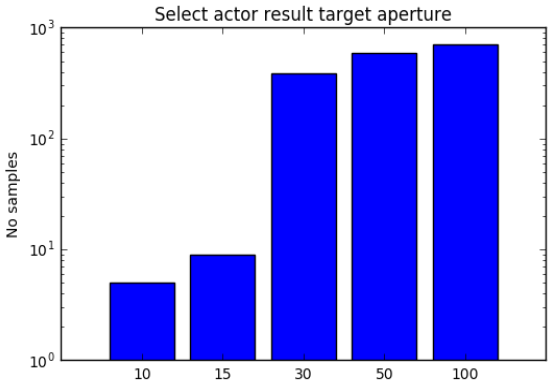
# PSEUDO-HELICAL

- **Number of positions taken from ISPyB diffraction plan, default 5**
- **Initial 2D mesh on max loop size**
- **Normal characterization and full data collection on first position**
- **Pseudo-helical characterization for remaining points**
- **For remaining positions :**
  - Vertical centring 90 degrees apart from 2D mesh
  - Partial data collection from pseudo-helical characterisation



## Dynamic aperture adjustment

- Aperture automatically set to match crystal size determined from X-ray centring
- Can be overridden by aperture desired by user




Auto selected beam size

## Improved error handling

- Automatic recovery in case of detection of non-centred crystal

# ACKNOWLEDGEMENTS


- David von Stetten, Max Nanao, Sasha Popov, Daniele de Sanctis, Stéphanie Monaco, Didier Nurizzo, Matias Guijarro, Solange Delagenière, Alejandro de Maria, Marcus Oskarsson, Pascal Theveneau, Christoph Mueller-Dieckmann, Gordon Leonard, David Flot, Igor Melnikov and Antonia Beteva (ESRF)
- Matthew Bowler, Andrew McCarthy and Michael Hons (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