

# **SOLEIL: STATUS REPORT IMPLEMENTATION OF SMARGON AND REMOTE ACCESS**

**Leo Chavas  
PROXIMA-I  
Synchrotron SOLEIL**

**I0<sup>th</sup> MxCuBE meeting at ESRF, Grenoble, France**



# Acknowledgments



**Patrick Gourhant**  
Assistant engineer



**Leo Chavas**  
Beamline manager



**Bill Shepard**  
Beamline manager



**Damien Jeangerard**  
Assistant engineer



**Pierre Legrand**  
Beamline scientist



**Serena Sirigu**  
Beamline scientist



**Tatiana Isabet**  
Responsible industry



**Gavin Fox**  
Beamline scientist



**Martin Savko**  
Beamline scientist



**Tiphaine Huet**  
Post-doctoral fellow



**Pierre Montaville**  
Post-doctoral fellow



**Igor Chaussavoine**  
PhD student



**Adam Simpkin**  
PhD student



**Enrico Stura**  
Associate scientist

Ivan Polzinelli    Nicolas Foos  
James Torpey    Nicolas Richet  
Denis Duran    Laurent Gadea

Robin Lener  
Apprenti

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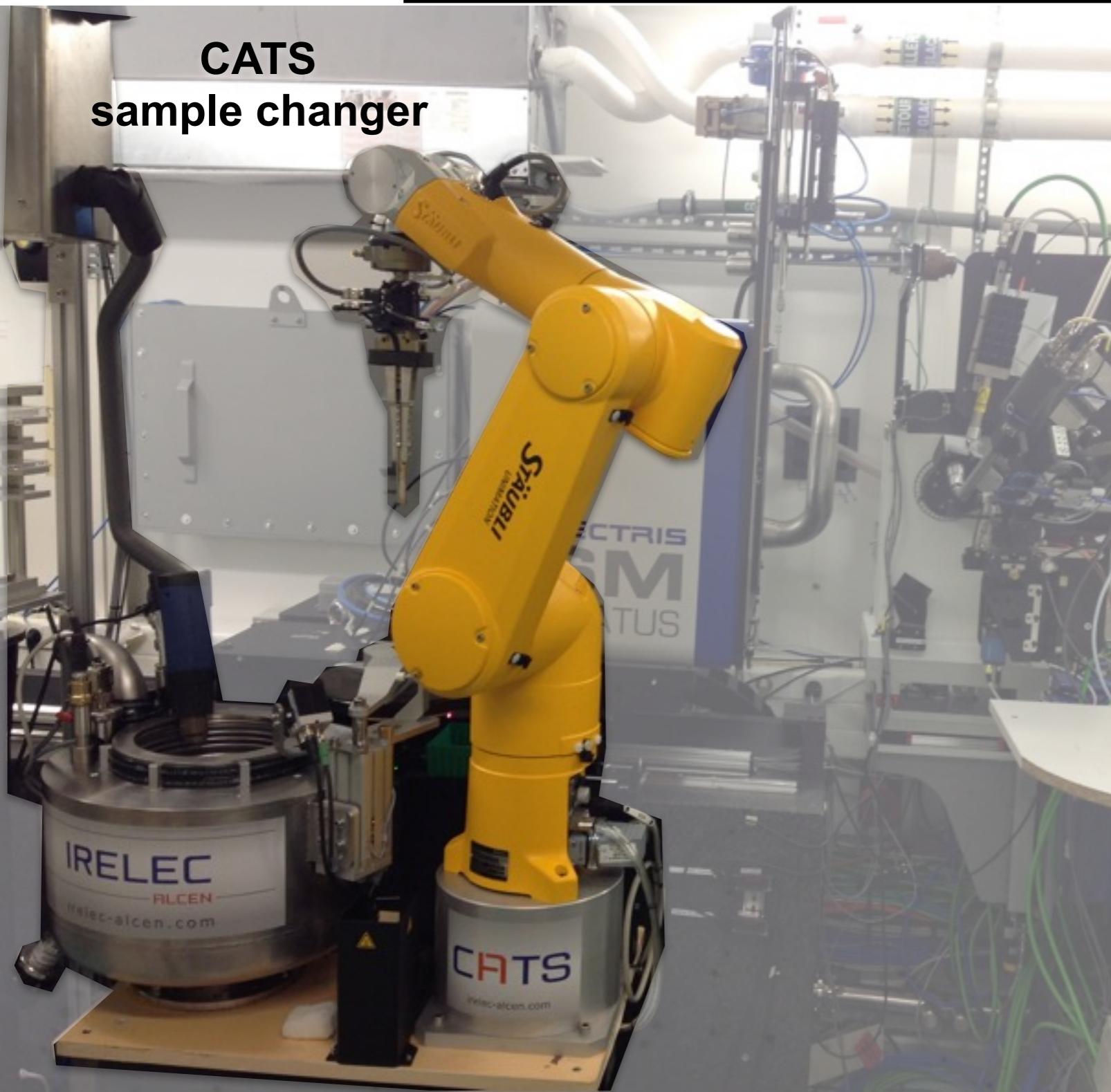
Ivan Polzinelli    Nicolas Foos

James Torpey    Nicolas Richet

Denis Duran    Laurent Gadea

# PROXIMA-I

CATS  
sample changer



ENERGY RANGE

5.5 ~ 15.5 keV  
0.8 ~ 2.25 Å

OPTICS

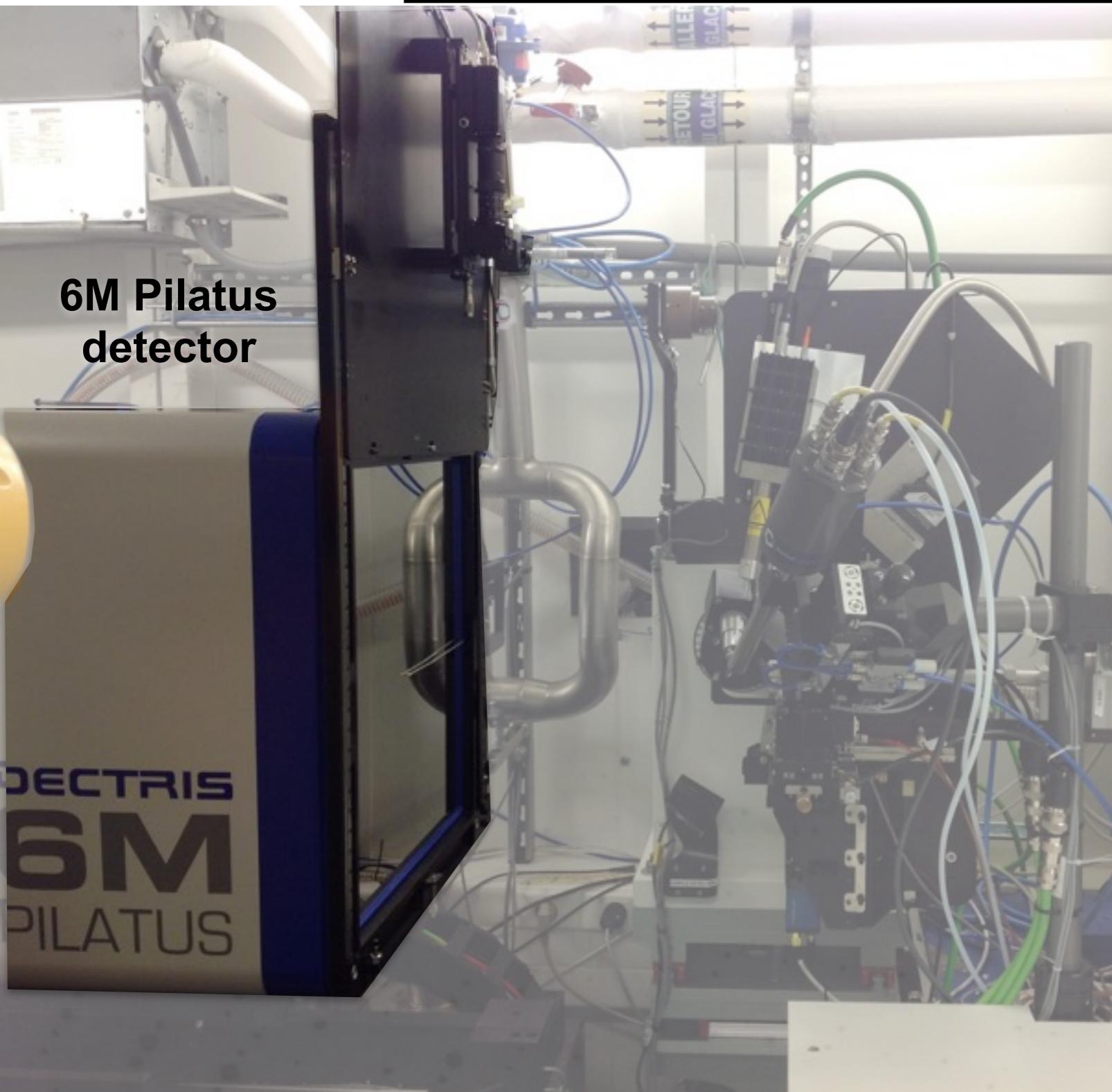
Channel cut monochromator  
K/B bi-morph mirrors

TYPICAL BEAM SIZE AT SAMPLE  
 $20 \times 40 \mu\text{m}^2$  ( $30 \times 90 \mu\text{m}^2$  full beam)

FLUX AT SAMPLE  
 $2.0 \times 10^{12}$  phot/s/0.02% bw 500 mA

SAMPLE CHANGER  
CATS (3 spine pucks)  
possible *in situ* measurements

# PROXIMA-I



6M Pilatus  
detector

**ENERGY RANGE**

**5.5 ~ 15.5 keV**  
**0.8 ~ 2.25 Å**

**OPTICS**

**Channel cut monochromator**  
**K/B bi-morph mirrors**

**TYPICAL BEAM SIZE AT SAMPLE**

**20 x 40  $\mu\text{m}^2$  (30x90 $\mu\text{m}^2$  full beam)**

**FLUX AT SAMPLE**

**2.0E+12 phot/s/0.02% bw 500 mA**

**SAMPLE CHANGER**

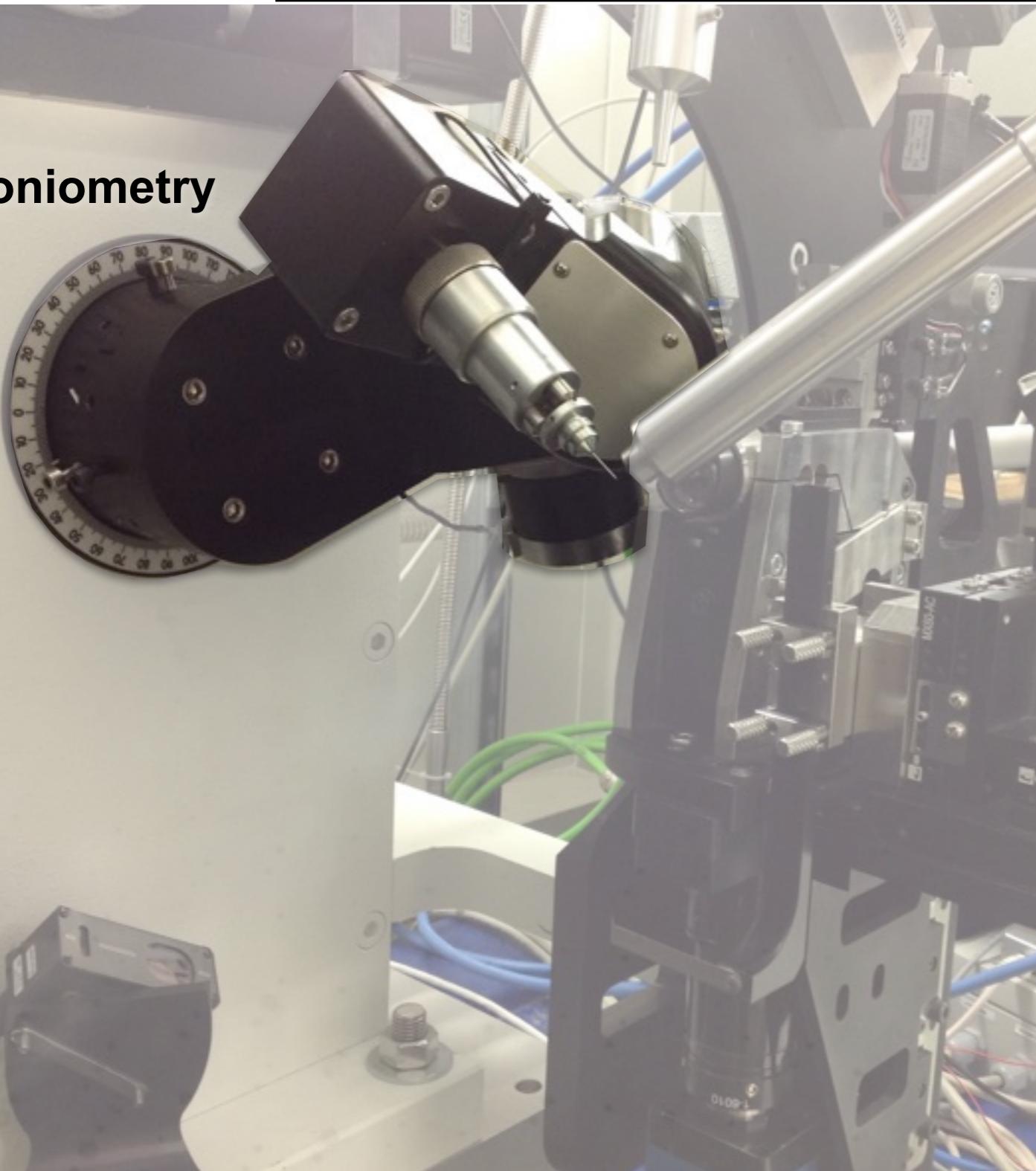
**CATS (3 spine pucks)**  
**possible *in situ* measurements**

**CAMERA**

**6M Pilatus**

# PROXIMA-I

$\kappa$  goniometry



**ENERGY RANGE**

**5.5 ~ 15.5 keV**  
**0.8 ~ 2.25 Å**

**OPTICS**

**Channel cut monochromator**  
**K/B bi-morph mirrors**

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**FLUX AT SAMPLE**

**2.0E+12 phot/s/0.02% bw 500 mA**

**SAMPLE CHANGER**

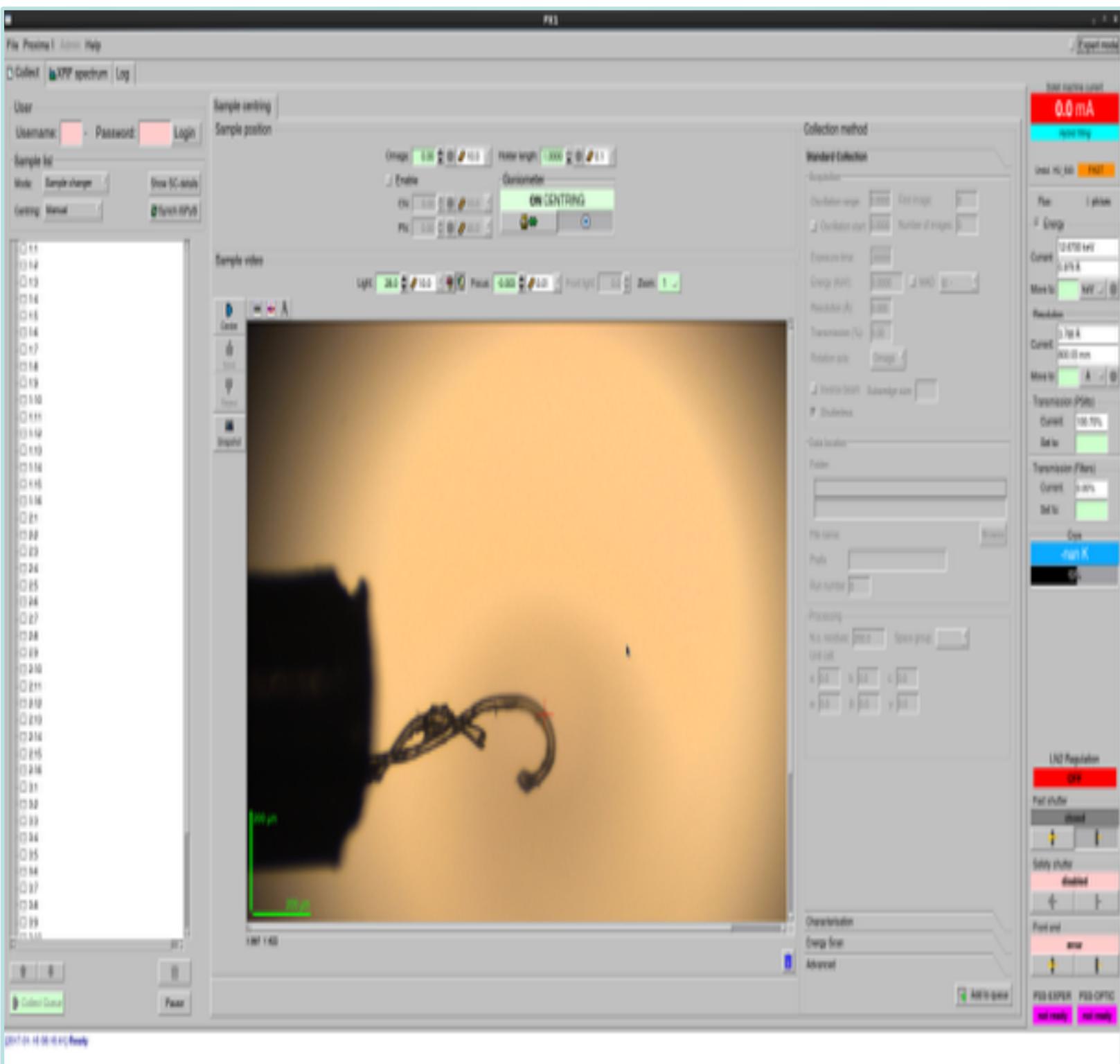
**CATS (3 spine pucks)**  
**possible *in situ* measurements**

**CAMERA**

**6M Pilatus**

**SAMPLE ENVIRONMENT**  
**3-axis  $\kappa$ -goniometre**

# PROXIMA-I



**ENERGY RANGE**

**5.5 ~ 15.5 keV**

**0.8 ~ 2.25 Å**

**OPTICS**

**Channel cut monochromator**

**K/B bi-morph mirrors**

**TYPICAL BEAM SIZE AT SAMPLE**

**20 x 40 μm<sup>2</sup> (30x90μm<sup>2</sup> full beam)**

**FLUX AT SAMPLE**

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**SAMPLE CHANGER**

**CATS (3 spine pucks)**

**possible *in situ* measurements**

**CAMERA**

**6M Pilatus**

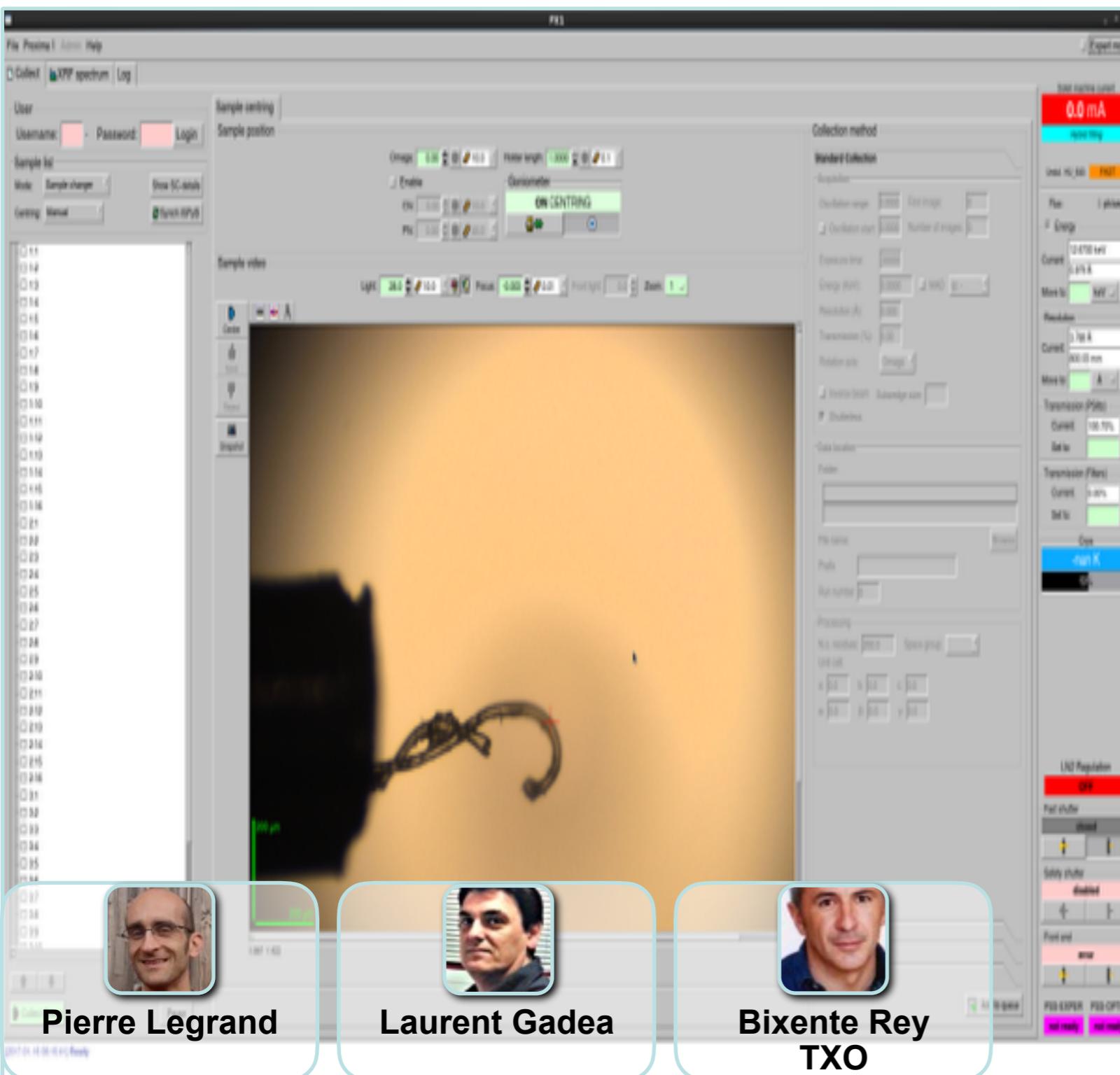
**SAMPLE ENVIRONMENT**

**3-axis κ-goniometre**

**MXCUBE VERSION**

**v2.1 Qt3**

# **PROXIMA-I**



# ENERGY RANGE

5.5 ~ 15.5 keV

0.8 ~ 2.25 Å

OPTICS

## Channel cut monochromator

## K/B bi-morph mirrors

## **TYPICAL BEAM SIZE AT SAMPLE**

**20 x 40  $\mu\text{m}^2$  (30x90 $\mu\text{m}^2$  full beam)**

# FLUX AT SAMPLE

**2.0E+12 phot/s/0.02% bw 500 mA**

# SAMPLE CHANGER

## CATS (3 spine pucks)

**possible *in situ* measurements**

# CAMERA

6M Pilatus

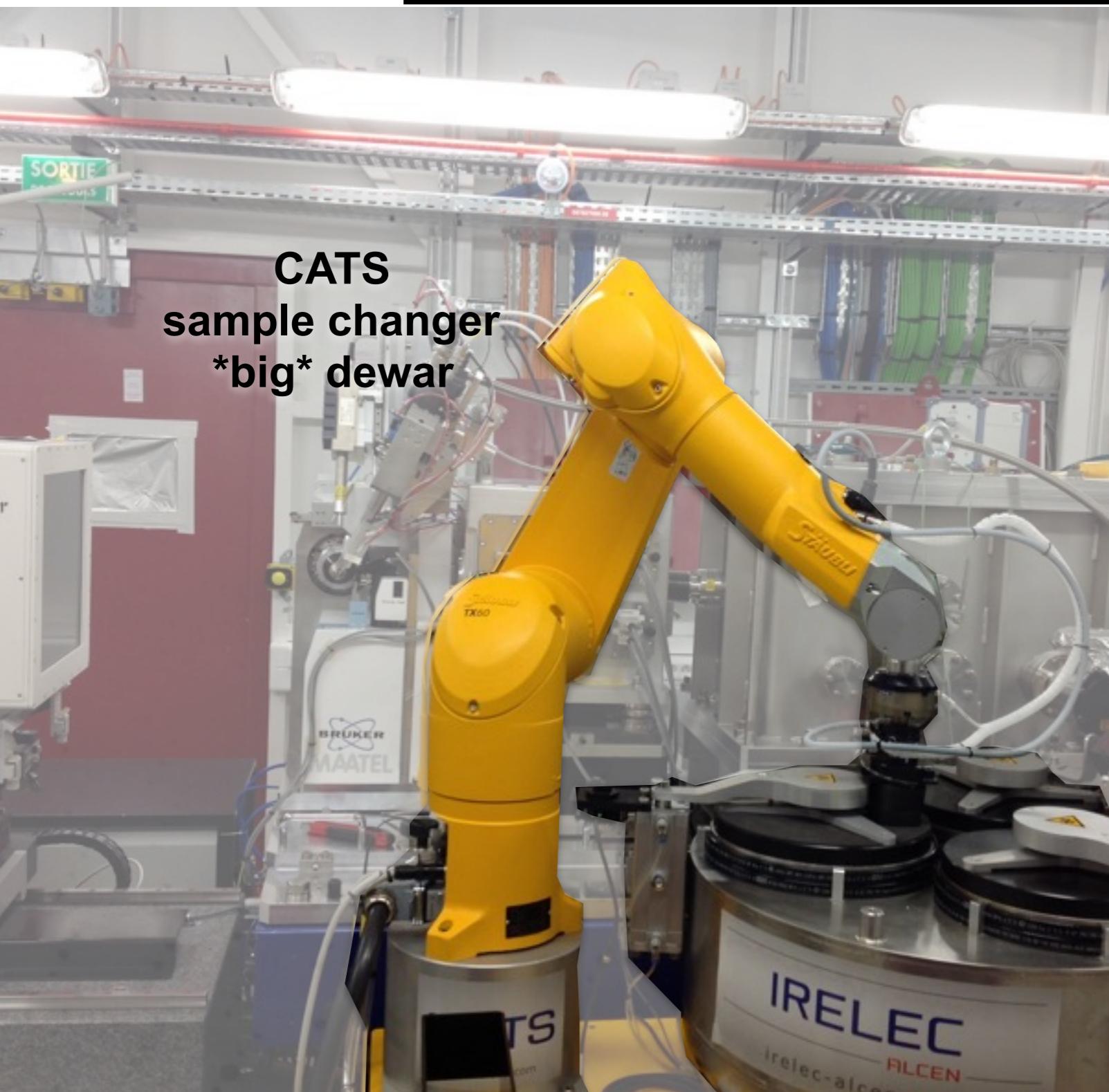
# SAMPLE ENVIRONMENT

## 3-axis κ-goniometre

# MXCUBE VERSION

v2.1 Qt3

# PROXIMA-2A



**ENERGY RANGE**

**6 ~ 15 keV**

**0.8 ~ 2.0 Å**

**OPTICS**

**Channel cut monochromator**

**Convex & K/B bi-morph mirrors**

**TYPICAL BEAM SIZE AT SAMPLE**

**3 x 5  $\mu\text{m}^2$**

**FLUX AT SAMPLE**

**3.5E+12 phot/s/0.02% bw 500 mA**

**SAMPLE CHANGER**

**CATS (9 spine pucks)**

***in situ* measurements available**

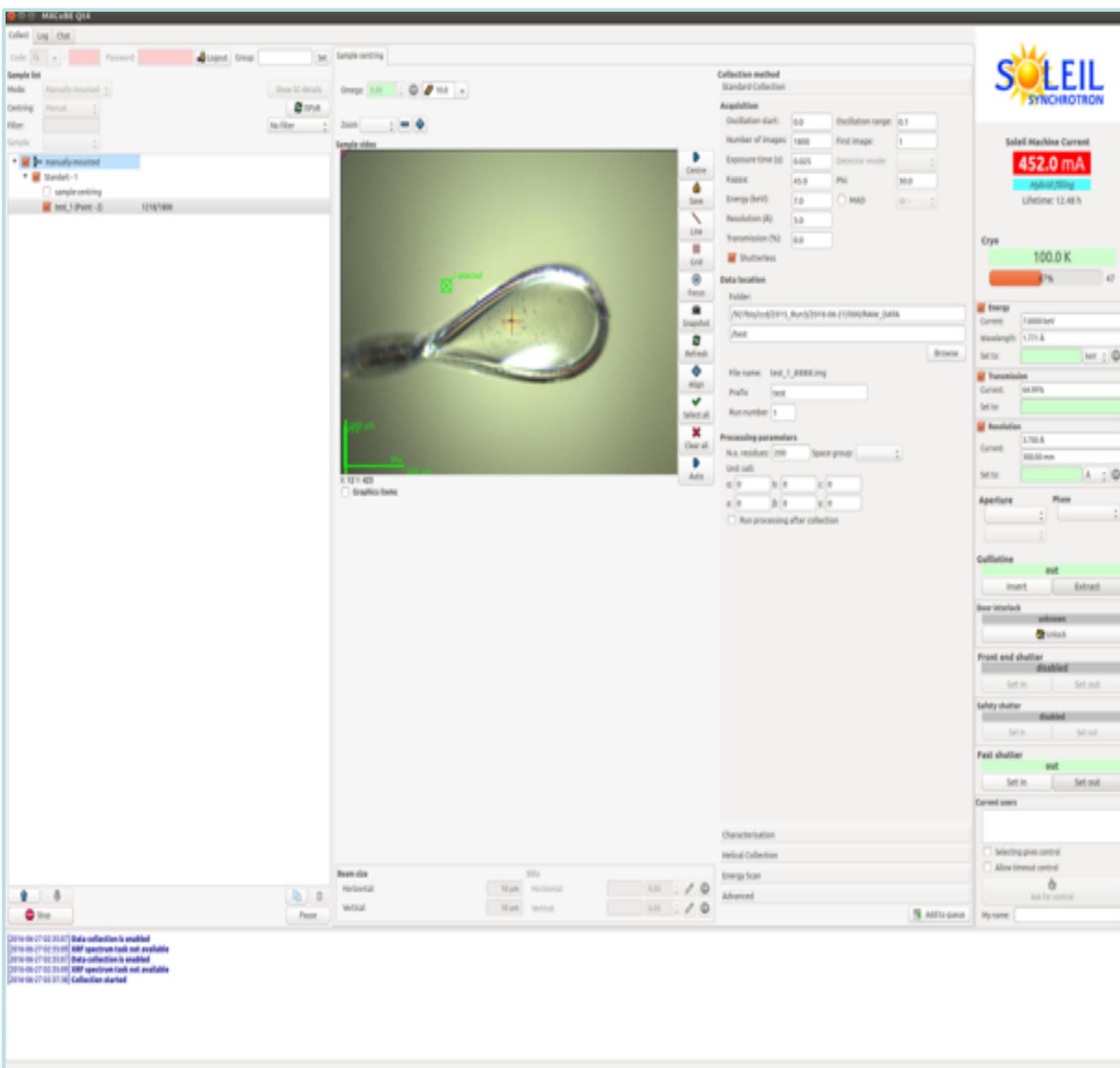
**CAMERA**

**Eiger X-9M**

**SAMPLE ENVIRONMENT**

**microdiffractometer MD2**

# PROXIMA-2A



**ENERGY RANGE**

**6 ~ 15 keV**

**0.8 ~ 2.0 Å**

**OPTICS**

**Channel cut monochromator**

**Convex & K/B bi-morph mirrors**

**TYPICAL BEAM SIZE AT SAMPLE**

**3 x 5  $\mu\text{m}^2$**

**FLUX AT SAMPLE**

**3.5E+12 phot/s/0.02% bw 500 mA**

**SAMPLE CHANGER**

**CATS (9 spine pucks)**

***in situ* measurements available**

**CAMERA**

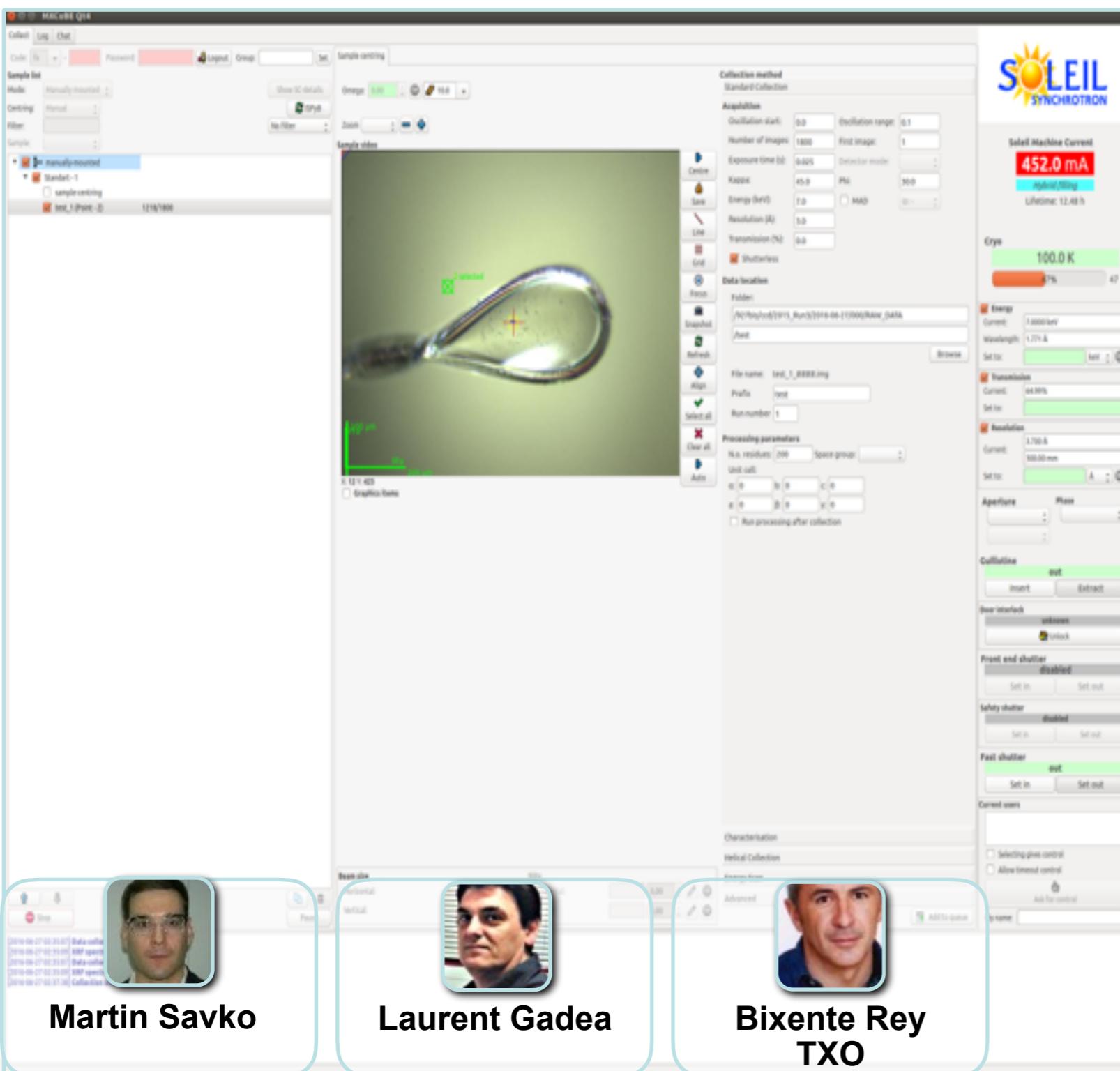
**Eiger X-9M**

**SAMPLE ENVIRONMENT**  
**microdiffractometer MD2**

**MXCUBE VERSION**

**v2.1 Qt3 in transition to Qt4**

# PROXIMA-2A



Martin Savko



Laurent Gadea



Bixente Rey  
TXO

**ENERGY RANGE**

**6 ~ 15 keV**

**0.8 ~ 2.0 Å**

**OPTICS**

**Channel cut monochromator**

**Convex & K/B bi-morph mirrors**

**TYPICAL BEAM SIZE AT SAMPLE**

**3 x 5 μm<sup>2</sup>**

**FLUX AT SAMPLE**

**3.5E+12 phot/s/0.02% bw 500 mA**

**SAMPLE CHANGER**

**CATS (9 spine pucks)**

***in situ* measurements available**

**CAMERA**

**Eiger X-9M**

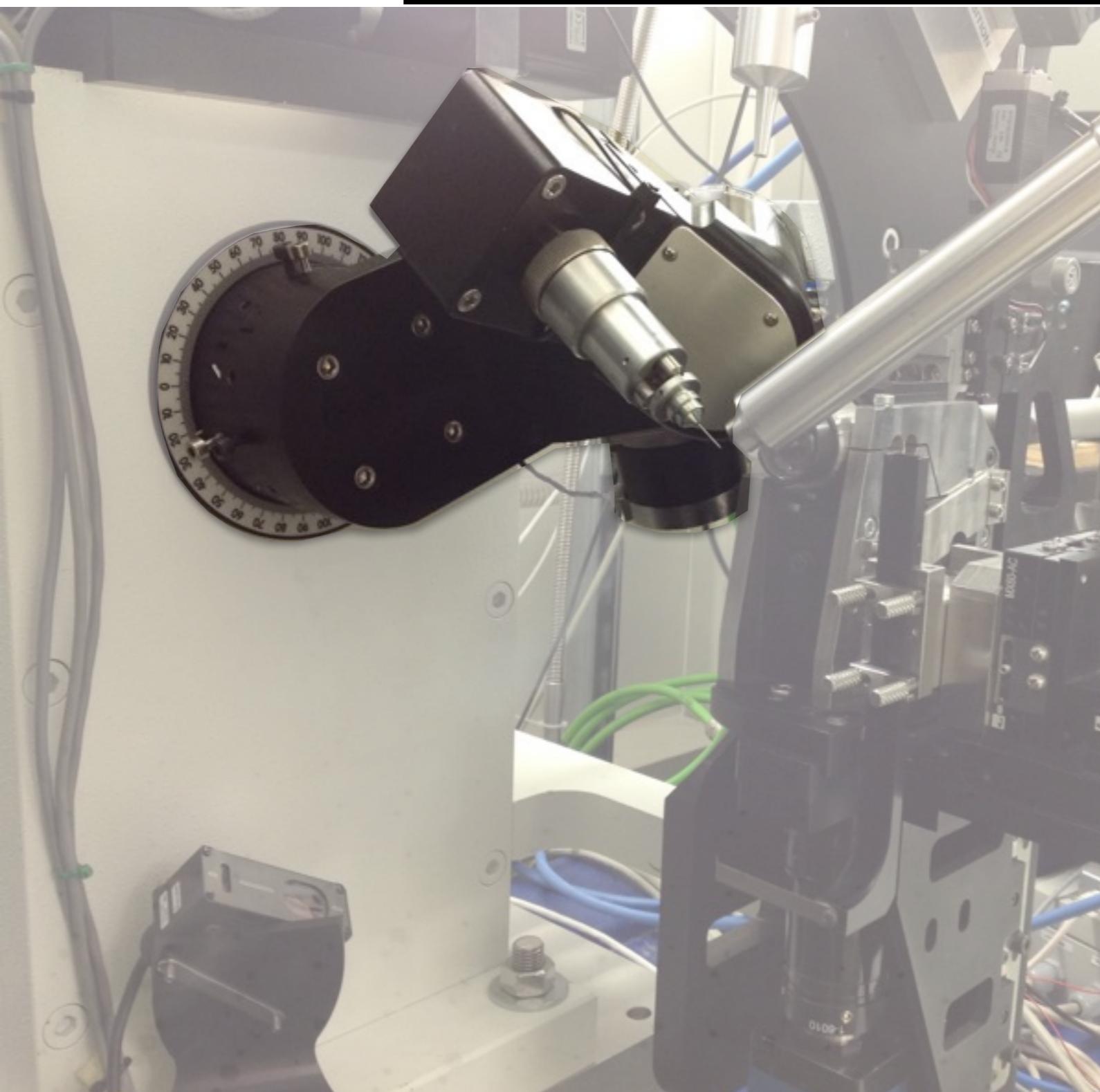
**SAMPLE ENVIRONMENT**  
**microdiffractometer MD2**

**MXCUBE VERSION**

**v2.1 Qt3 in transition to Qt4**

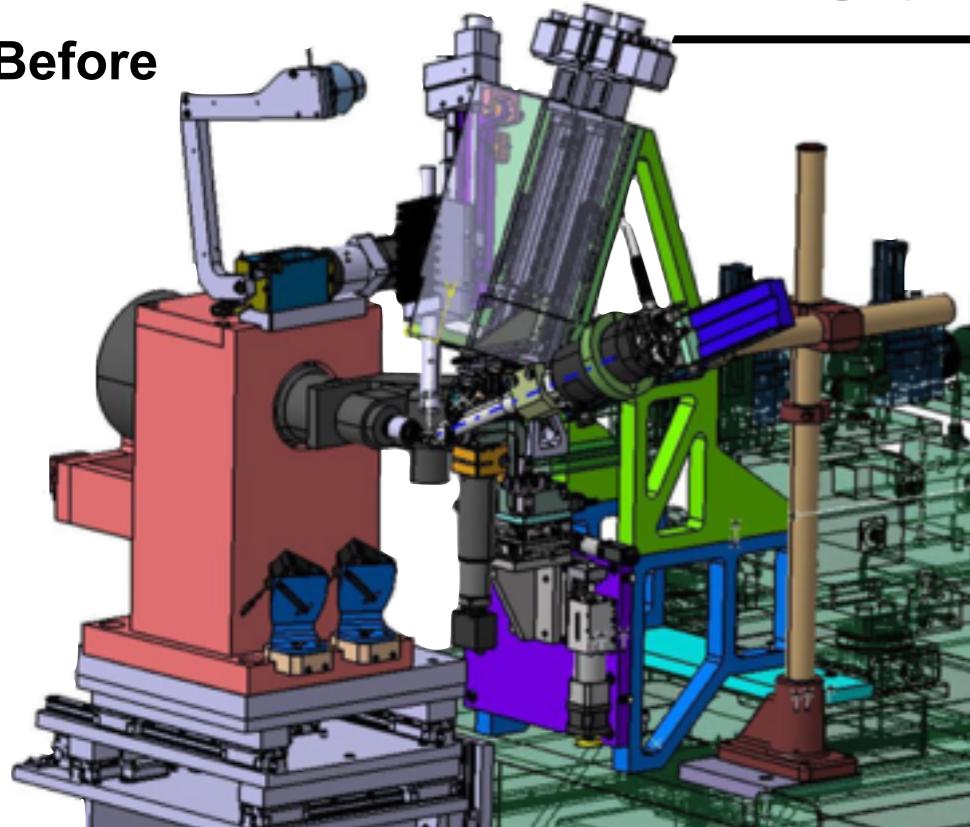


# SMARGON IMPLEMENTATION



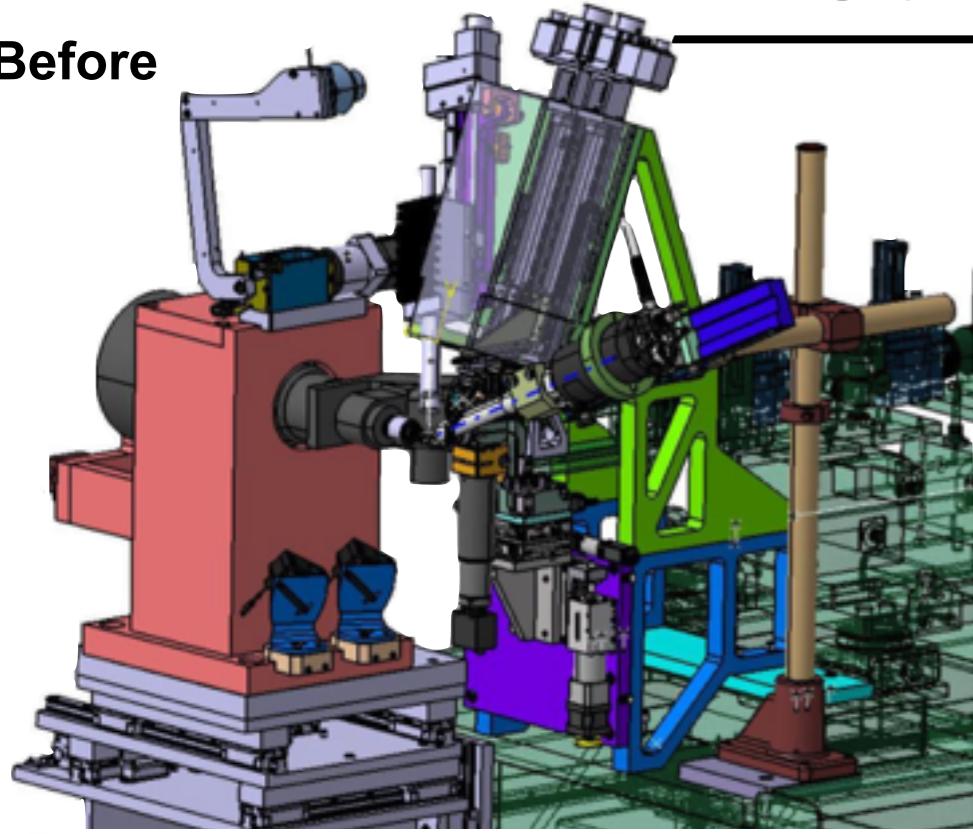
# SMARGON IMPLEMENTATION

Before

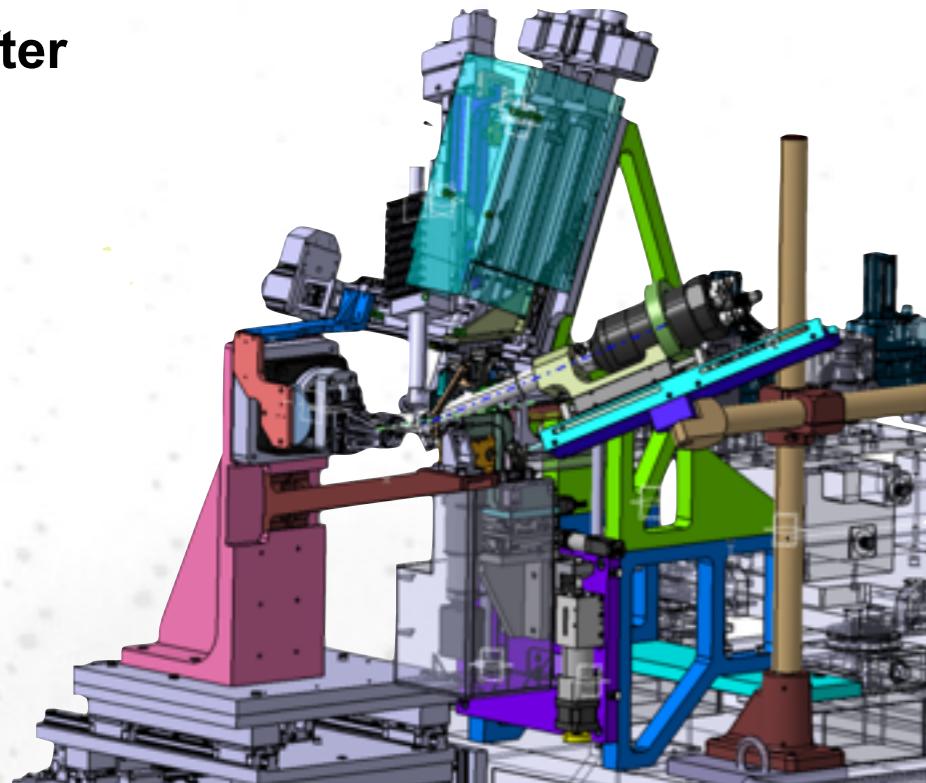


# SMARGON IMPLEMENTATION

Before

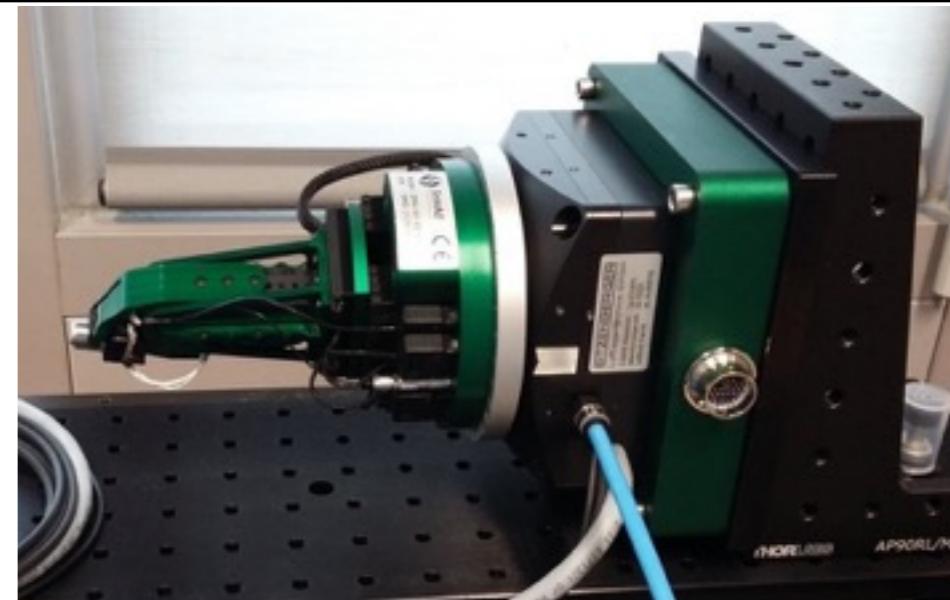
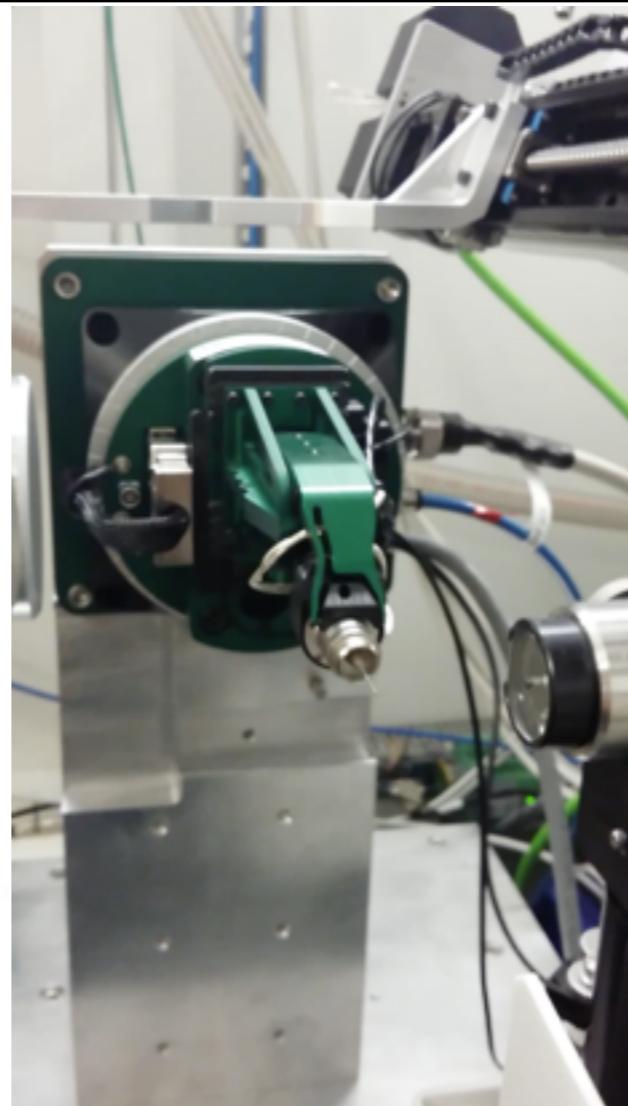
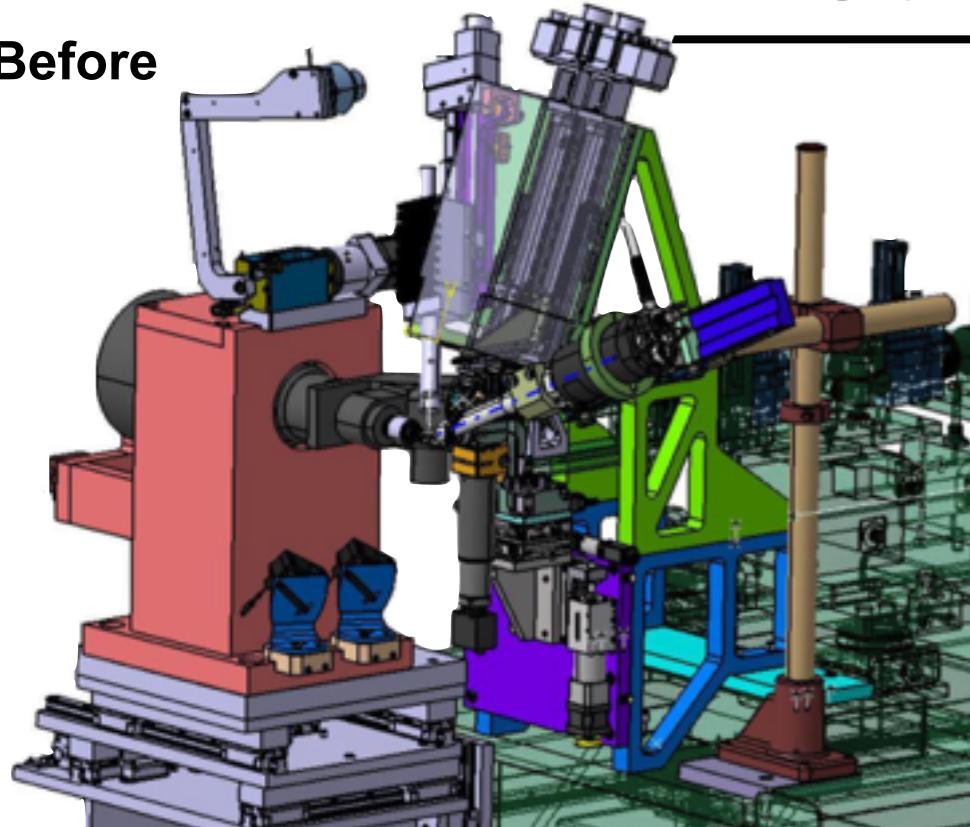


After

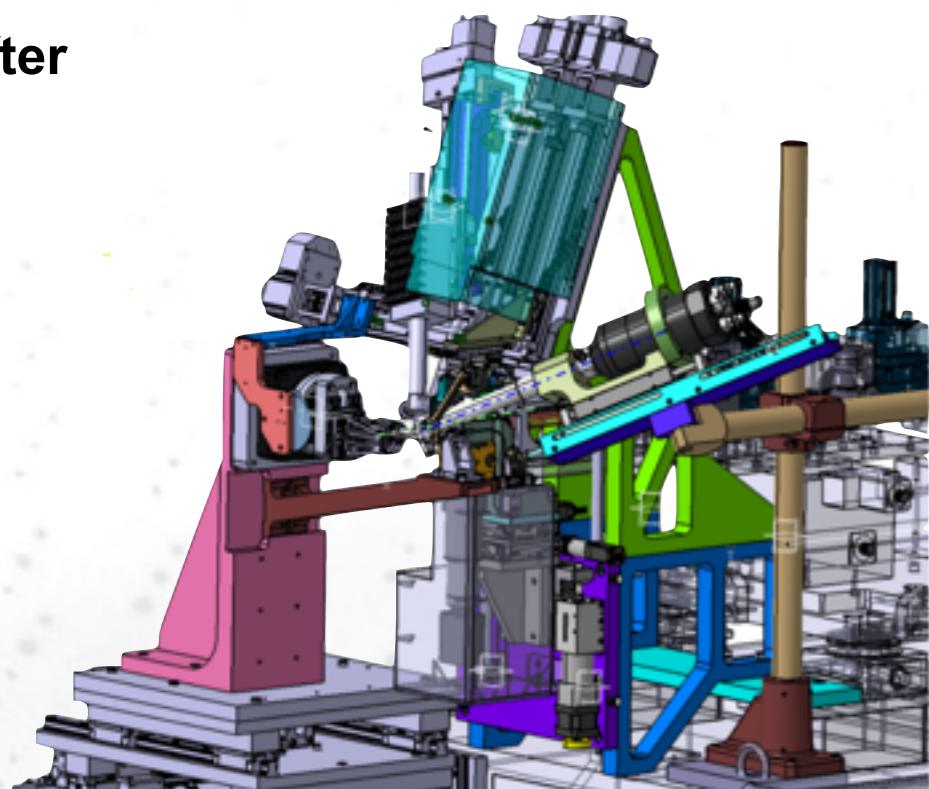


# SMARGON IMPLEMENTATION

Before

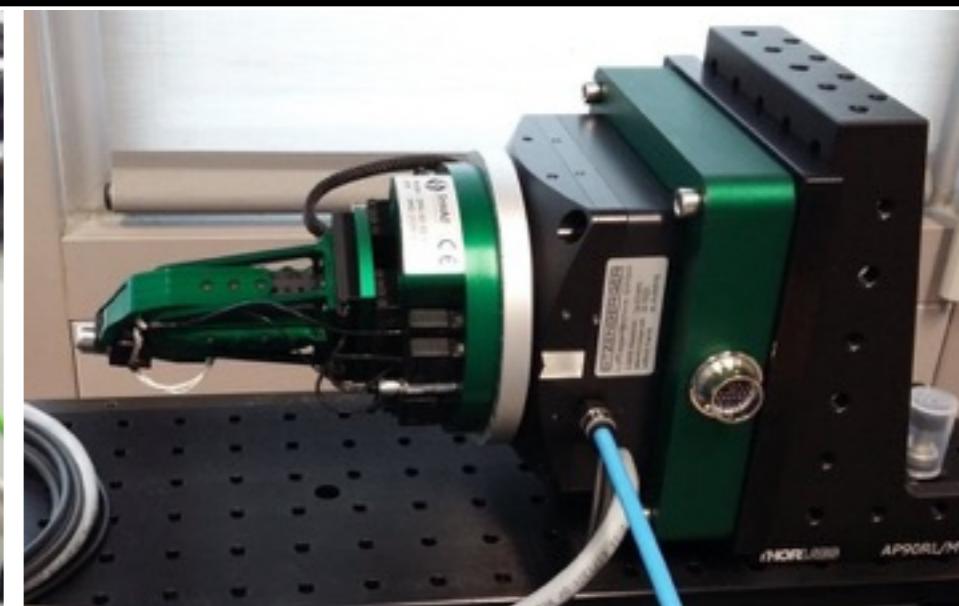
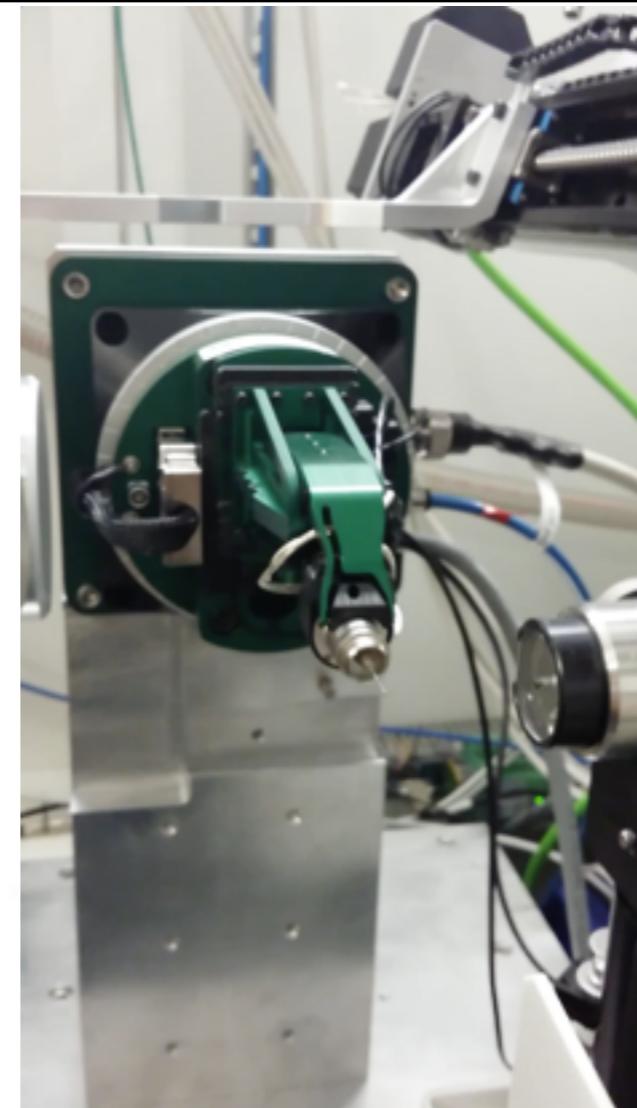
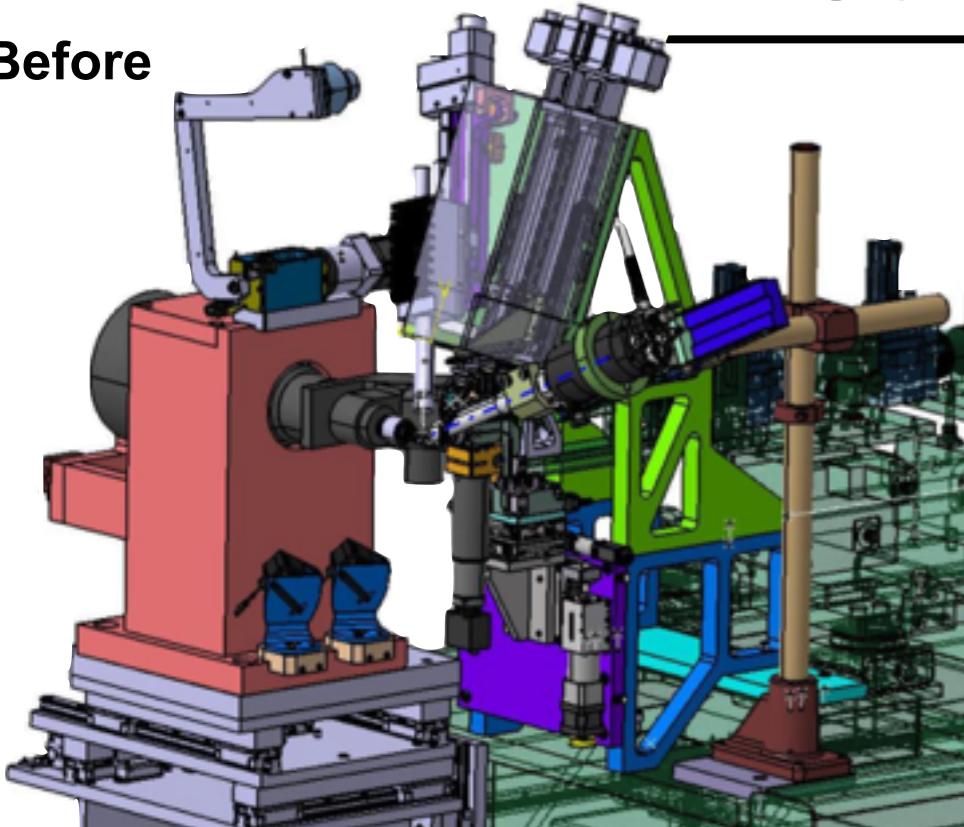


After

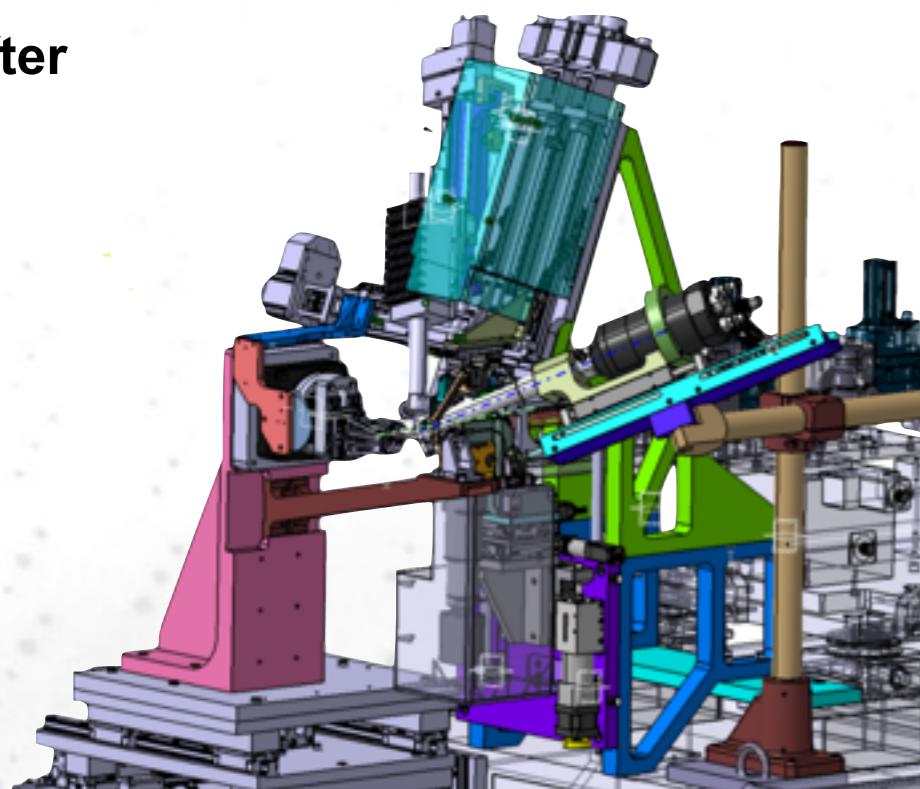


# SMARGON IMPLEMENTATION

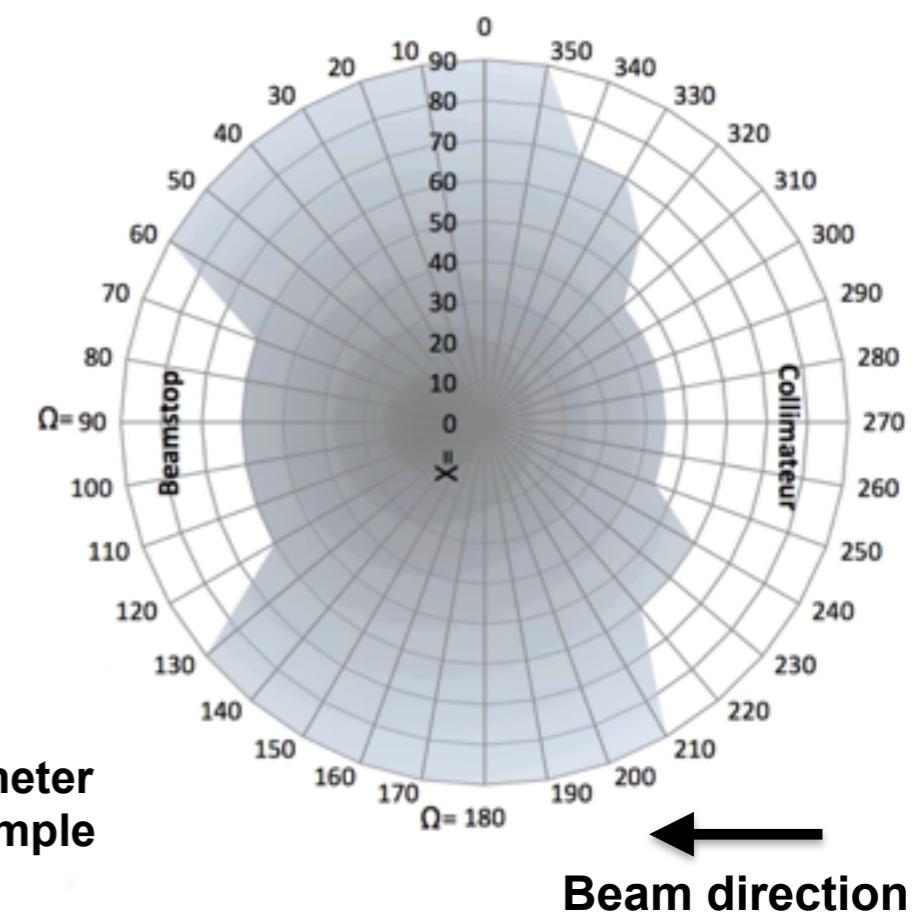
Before



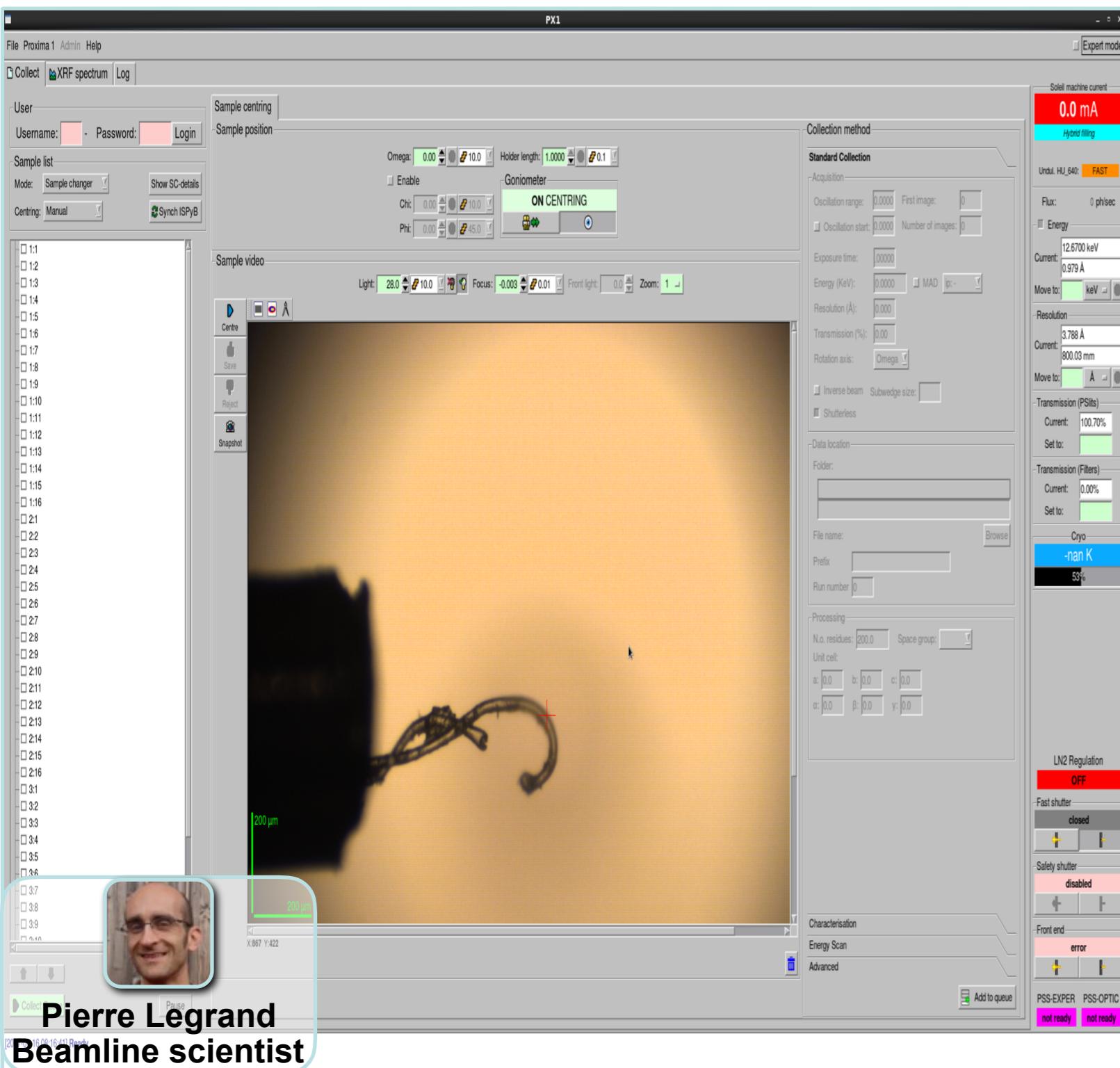
After



Sphere of possible goniometer movements around the sample position



# SMARGON DEVICES AND MxCUBE SETUP



Pierre Legrand  
Beamlime scientist



# SMARGON DEVICES AND MxCUBE SETUP

The screenshot displays the MxCube software interface for the PX1 beamline at the Soleil Synchrotron. The main window shows a video feed of a sample being centered, with a 200 µm scale bar and coordinates X:867 Y:422. The control panel includes sections for User (Username: Pierre Legrand, Password: [redacted], Login), Sample centring, Sample position, Collection method (Standard Collection, Omega: 0.00 mA, Holder length: 1.0000 mm), and various experimental parameters like Energy (12.6700 keV), Resolution (3.788 Å), and Transmission (100.70%). On the right, a Goniometer panel shows 'ON CENTRING' status with controls for Omega, Chi, and Phi angles. A bottom banner identifies Pierre Legrand as a Beamlime scientist.

**PX1**

User  
Username: **Pierre Legrand** - Password: **[redacted]** Login

Sample centring  
Sample position

Collection method  
Standard Collection

Soleil machine current: **0.0 mA**  
Holder length: **1.0000 mm**

Goniometer  
ON CENTRING

Omega: **0.00** Chi: **0.00** Phi: **0.00**

Sample video  
Light: **28.0** Focus: **-0.003** Front light: **0.0** Zoom: **1**

Sample list  
Mode: **Sample changer** Show SC-details  
Centring: **Manual** Sync ISPyB

Sample list (partial list):  
1:1, 1:2, 1:3, 1:4, 1:5, 1:6, 1:7, 1:8, 1:9, 1:10, 1:11, 1:12, 1:13, 1:14, 1:15, 1:16, 2:1, 2:2, 2:3, 2:4, 2:5, 2:6, 2:7, 2:8, 2:9, 2:10, 2:11, 2:12, 2:13, 2:14, 2:15, 3:1, 3:2, 3:3, 3:4, 3:5, 3:6, 3:7, 3:8, 3:9, 3:10

Centre Save Reject Snapshot

Folder: **A**

File name: **[redacted]** Browse  
Prefix: **[redacted]**  
Run number: **0**

Processing  
N.o. residues: **200.0** Space group: **[redacted]**  
Unit cell:  
a: **0.0** b: **0.0** c: **0.0**  
α: **0.0** β: **0.0** γ: **0.0**

Characterisation  
Energy Scan  
Advanced

Add to queue

Omega: **0.00** Chi: **0.00** Phi: **0.00**

Holder length: **1.0000** Goniometer  
ON CENTRING

LN2 Regulation: **OFF**

Fast shutter: **closed**

Safety shutter: **disabled**

Front end: **error**

PSS-EXPER PSS-OPTIC  
not ready not ready

**Pierre Legrand**  
Beamlime scientist

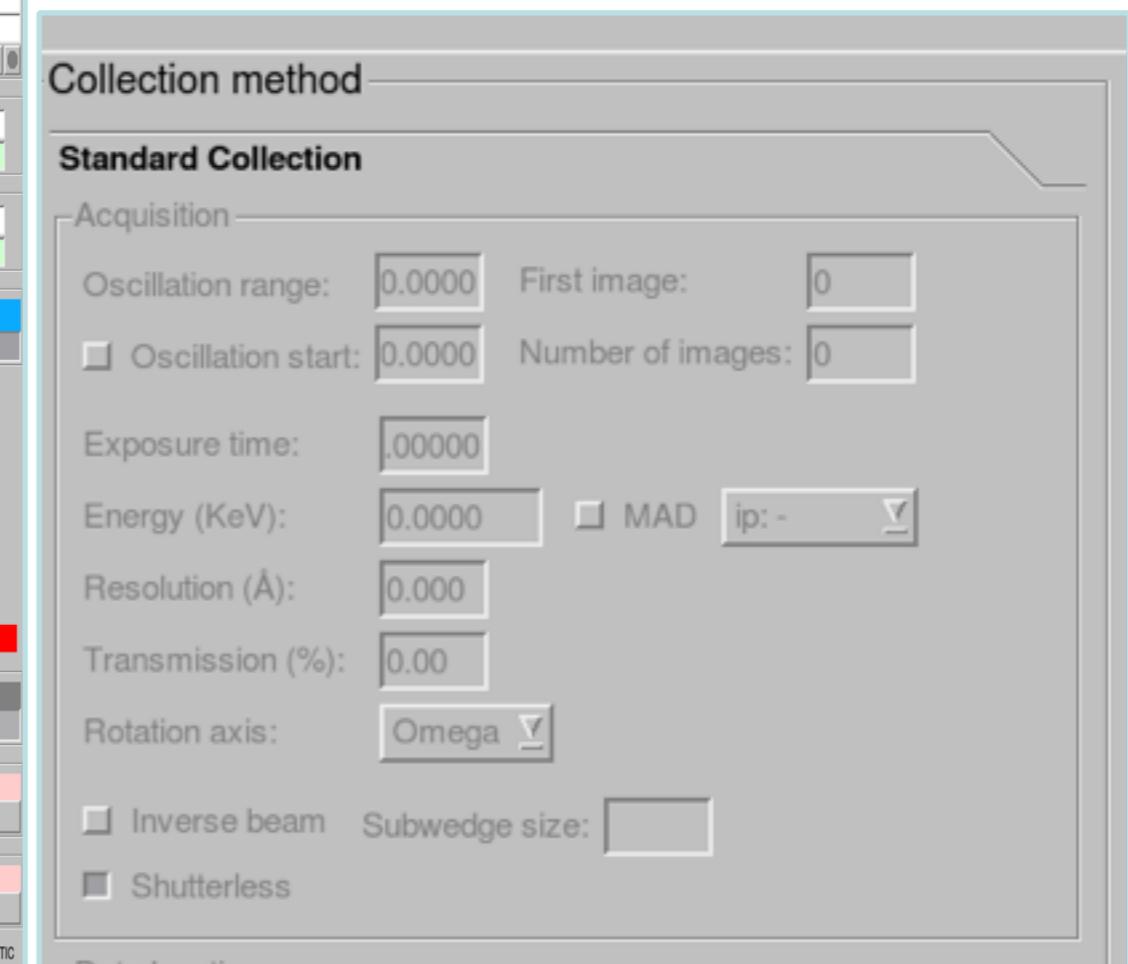


# SMARGON DEVICES AND MxCUBE SETUP

The screenshot displays the MxCube software interface for the PX1 beamline at the Soleil Synchrotron. The main window shows a video feed of a sample being centered, with a 200 μm scale bar and coordinates X:867 Y:422. The control panel includes sections for User (Username: Pierre Legrand, Password: [redacted], Login), Sample centring, Sample position, Collection method (Standard Collection, Acquisition, Energy, Resolution, Transmission, Processing), and Characterisation. On the right, the Goniometer status is shown as "ON CENTRING". A zoomed-in view of the "Collection method" section highlights the "Standard Collection" parameters:

Parameter	Value
Oscillation range	0.0000
First image	0
Oscillation start	0.0000
Number of images	0
Exposure time	.00000
Energy (KeV)	0.0000
MAD	[disabled]
Resolution (Å)	0.000
Transmission (%)	0.00
Rotation axis	Omega
Inverse beam	[unchecked]
Subwedge size	[disabled]
Shutterless	[unchecked]

Below the collection method, the LN2 Regulation is set to OFF. The fast shutter is closed and the safety shutter is disabled. The front end status is error. The data location section includes fields for Folder, File name, Prefix, and Run number.



Pierre Legrand  
Beamline scientist

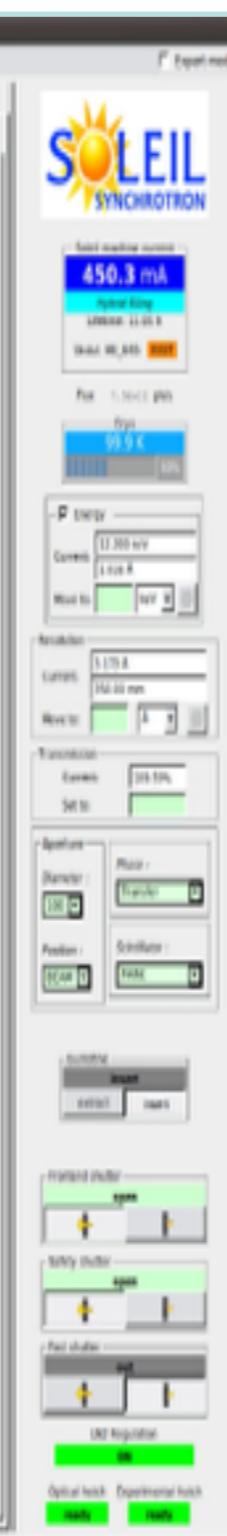
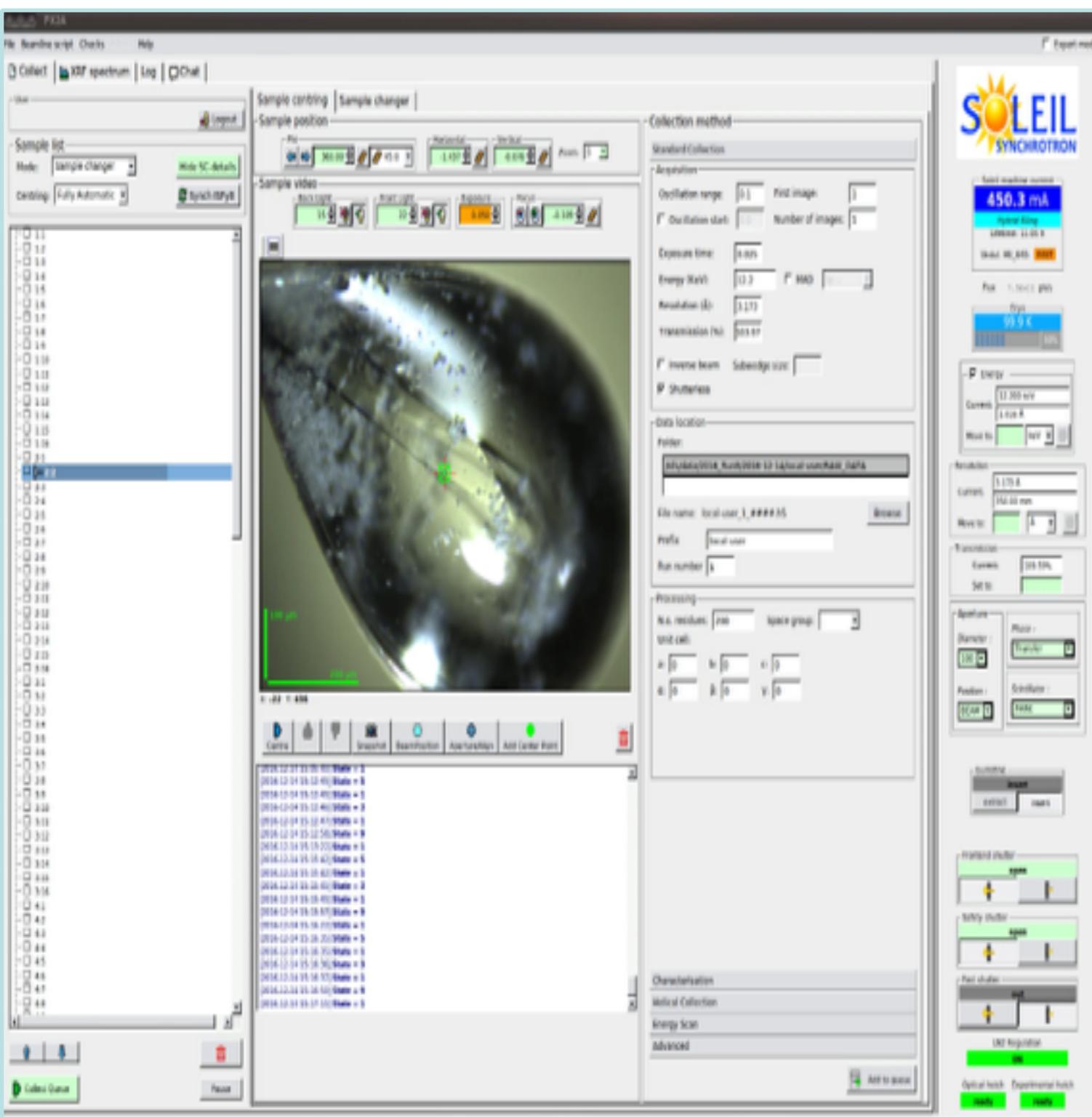


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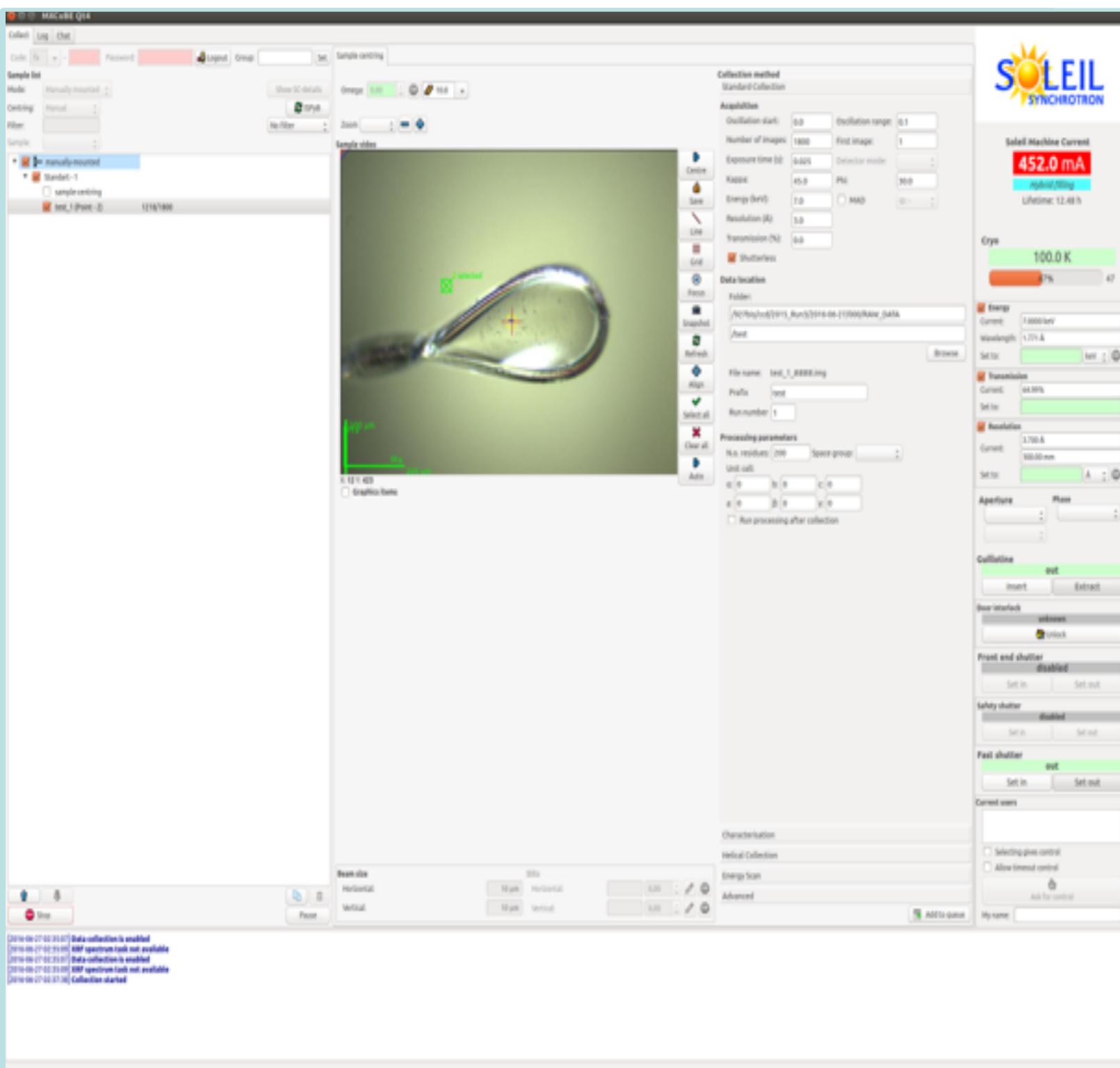
# QT4: MIGRATION STATUS

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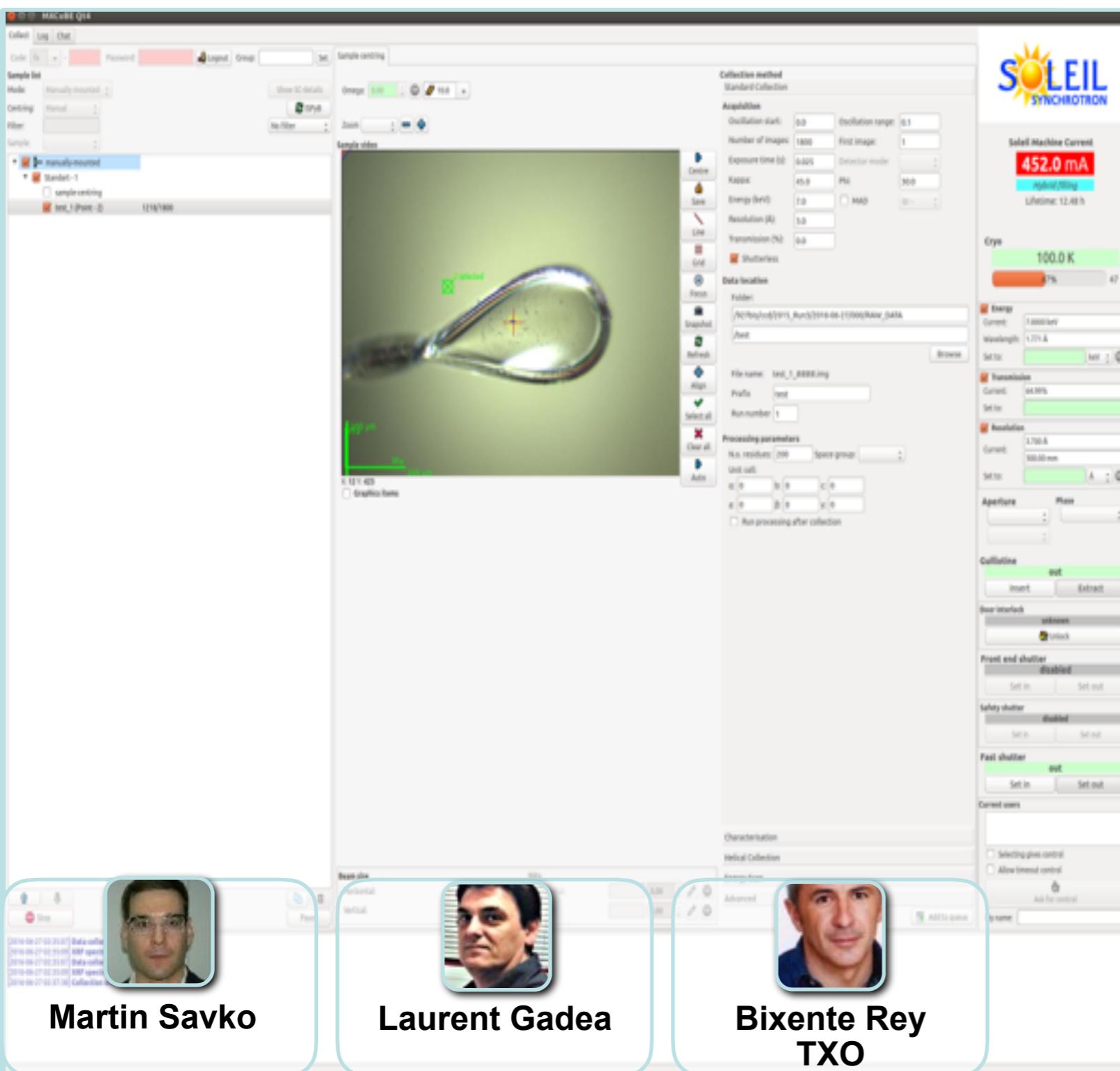
# QT4: MIGRATION STATUS



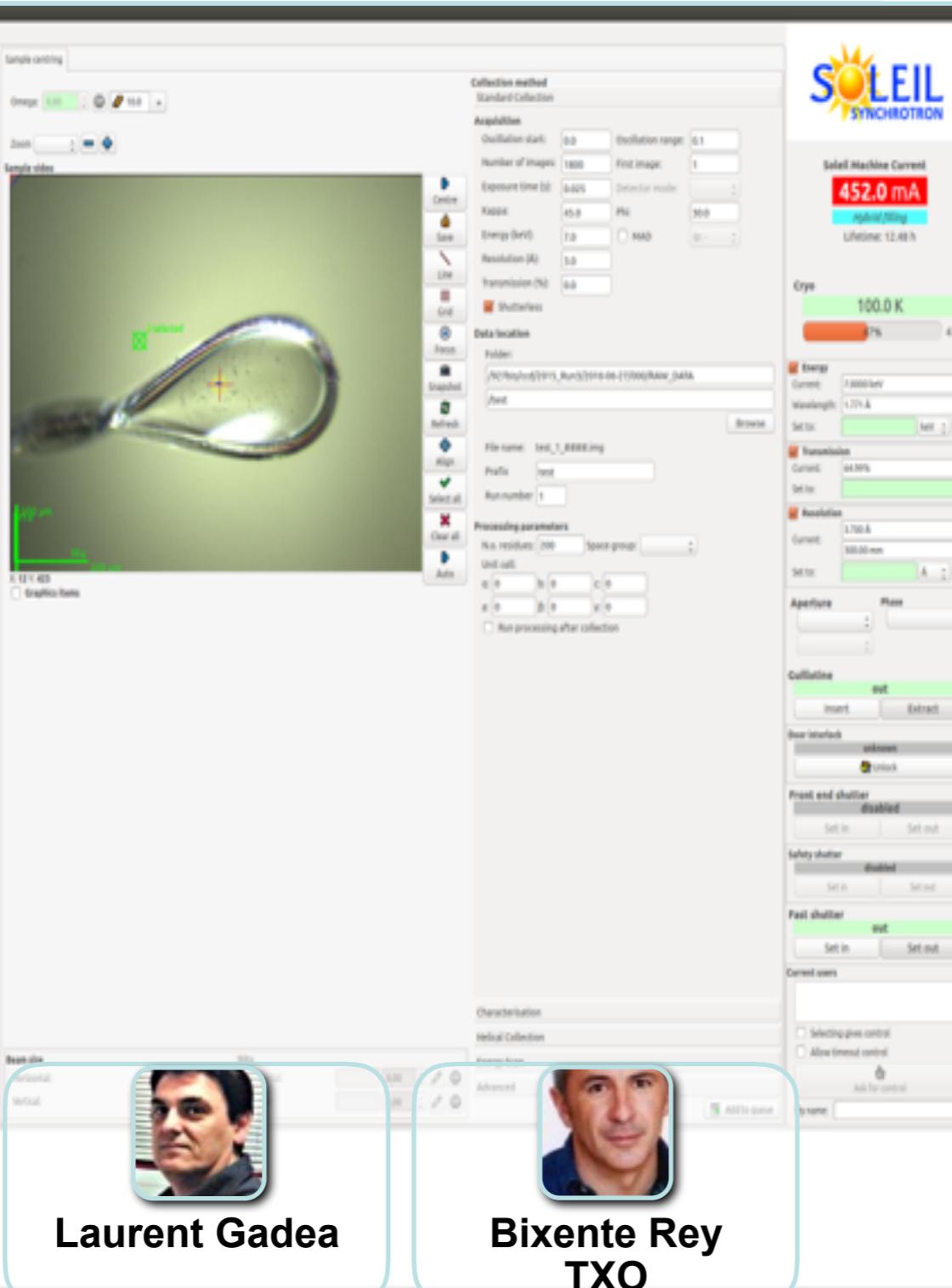
# QT4: MIGRATION STATUS



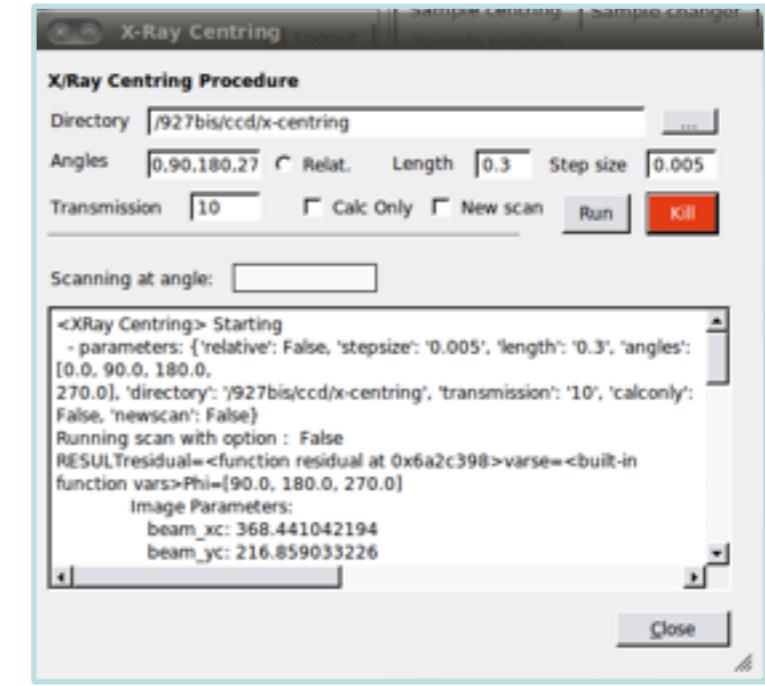
# QT4: MIGRATION STATUS



# QT4: MIGRATION STATUS



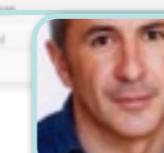
The screenshot shows the Soleil Synchrotron software interface. On the left, there's a 'Sample list' panel with a tree view showing 'manually-mounted' and 'Standart-1' categories. A central window displays a sample image of a protein crystal in a capillary, with a green crosshair indicating the beam position. To the right of the image are 'Collection method' and 'Acquisition' settings, including oscillation start (0.0), oscillation range (0.1), number of images (1000), first image (1), exposure time (0.005), detector mode (PIL), kappa (45.0), energy (keV) (7.0), resolution (Å) (1.0), transmission (%), and shutterless. Below these are 'Data location' fields for folder and file name (set to 'test'), processing parameters (no. resolutions: 200, space group: P1, unit cell: a=6.0, b=6.0, c=6.0), and a checkbox for 'Run processing after collection'. At the bottom, there's a 'Characterisation' section with tabs for 'Helical Collection' and 'Advanced'.



The dialog box is titled 'X-Ray Centring Procedure'. It shows the directory '/927bis/ccd/x-centring', angles [0.90, 180, 270], length 0.3, step size 0.005, and transmission 10. It includes checkboxes for 'Relat.', 'Calc Only', and 'New scan', and buttons for 'Run' and 'Kill'. The main text area displays log output: '<XRay Centring> Starting - parameters: {relative: False, 'stepsize': '0.005', 'length': '0.3', 'angles': [0.0, 90.0, 180.0, 270.0], 'directory': '/927bis/ccd/x-centring', 'transmission': '10', 'calconly': False, 'newscan': False} Running scan with option : False RESULTresidual=<function residual at 0x6a2c398>varse=<built-in function vars>Phi=[90.0, 180.0, 270.0] Image Parameters: beam\_xc: 368.441042194 beam\_yc: 216.859033226'. There's also a 'Close' button.

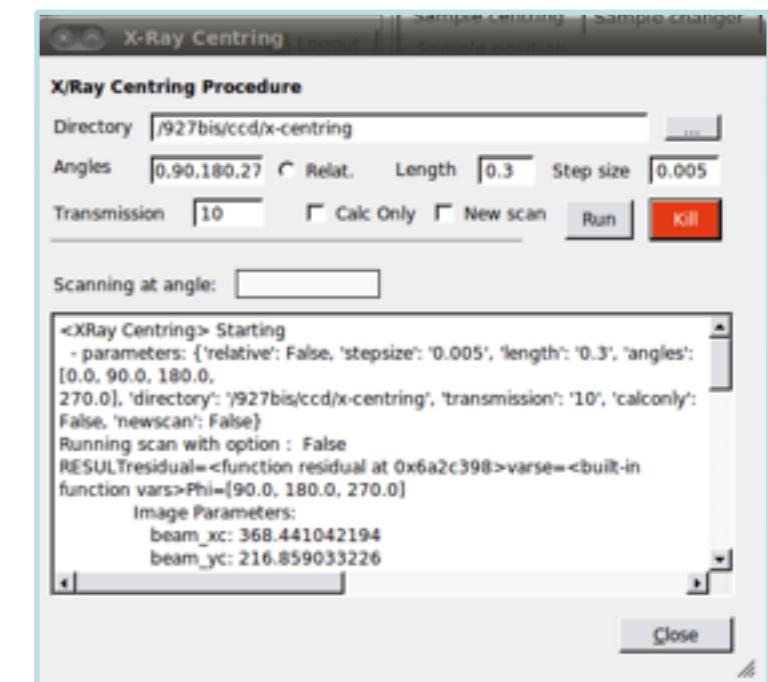
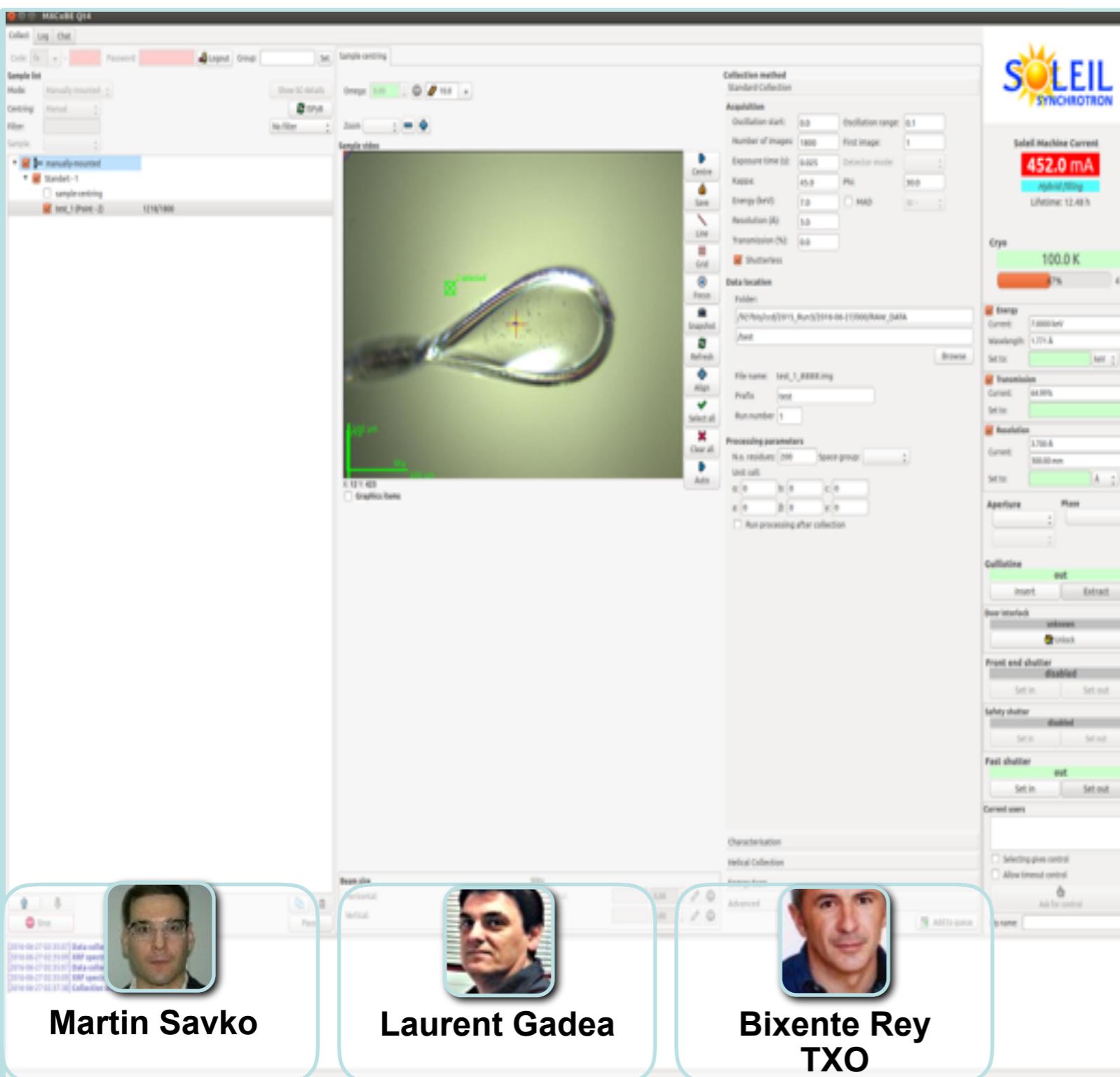
**Martin Savko** 

**Laurent Gadea** 

**Bixente Rey  
TXO** 



# QT4: MIGRATION STATUS



## Migration status...

- all devices connected
- collection, helical scan etc. okay
- ISPyB connected
- many 'minor' bugs to be corrected
- interface still slow
- mesh-scan yet to be implemented

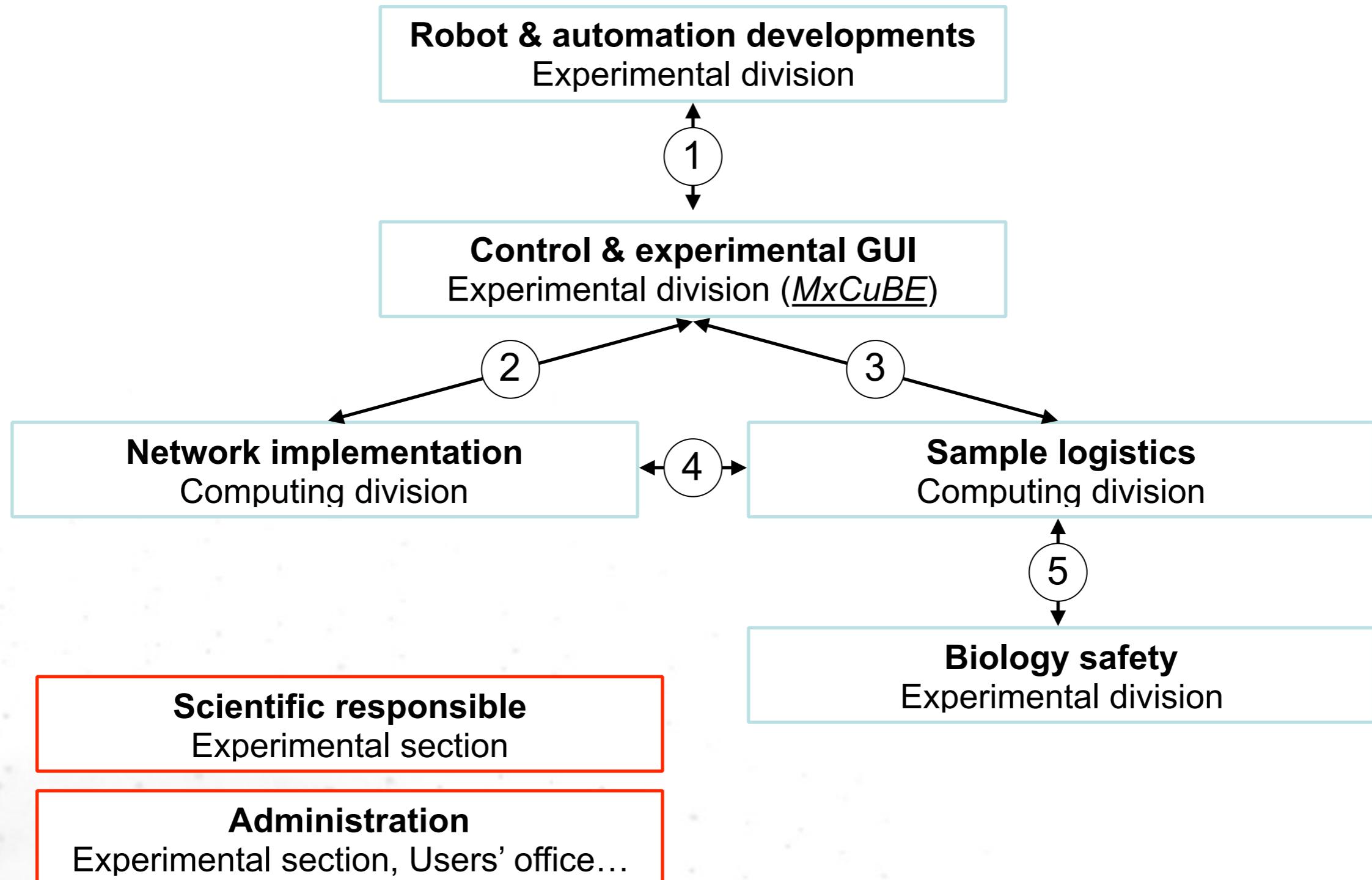


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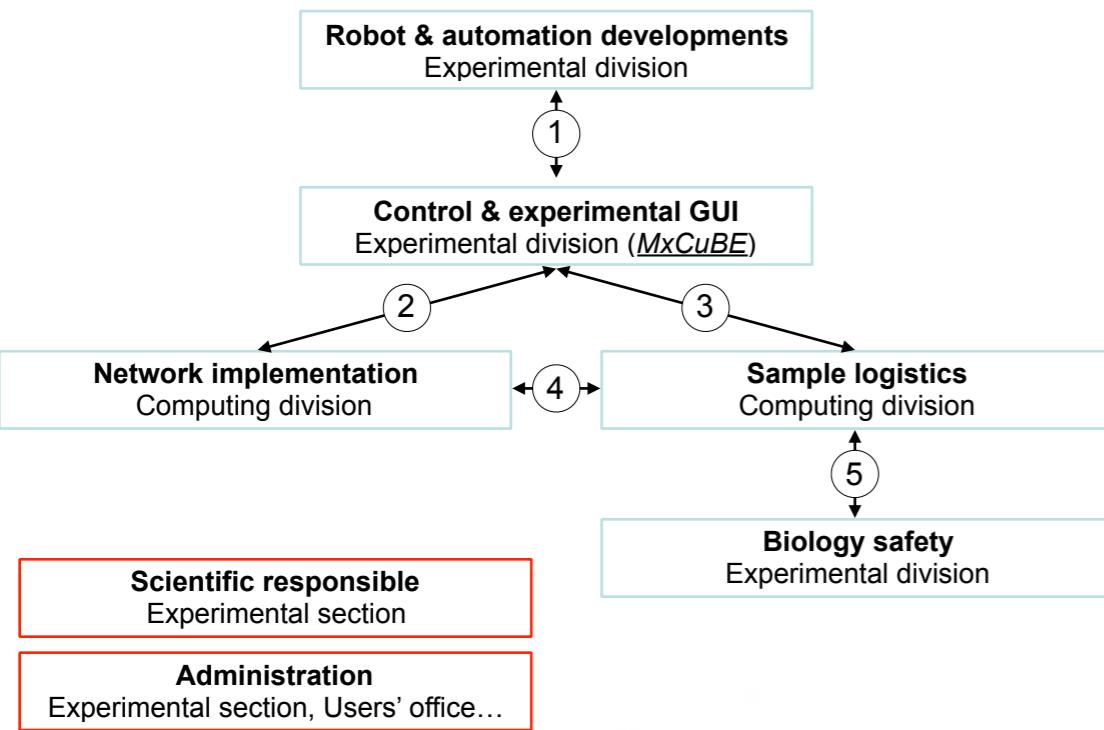
# **REMOTE ACCESS AT SOLEIL**

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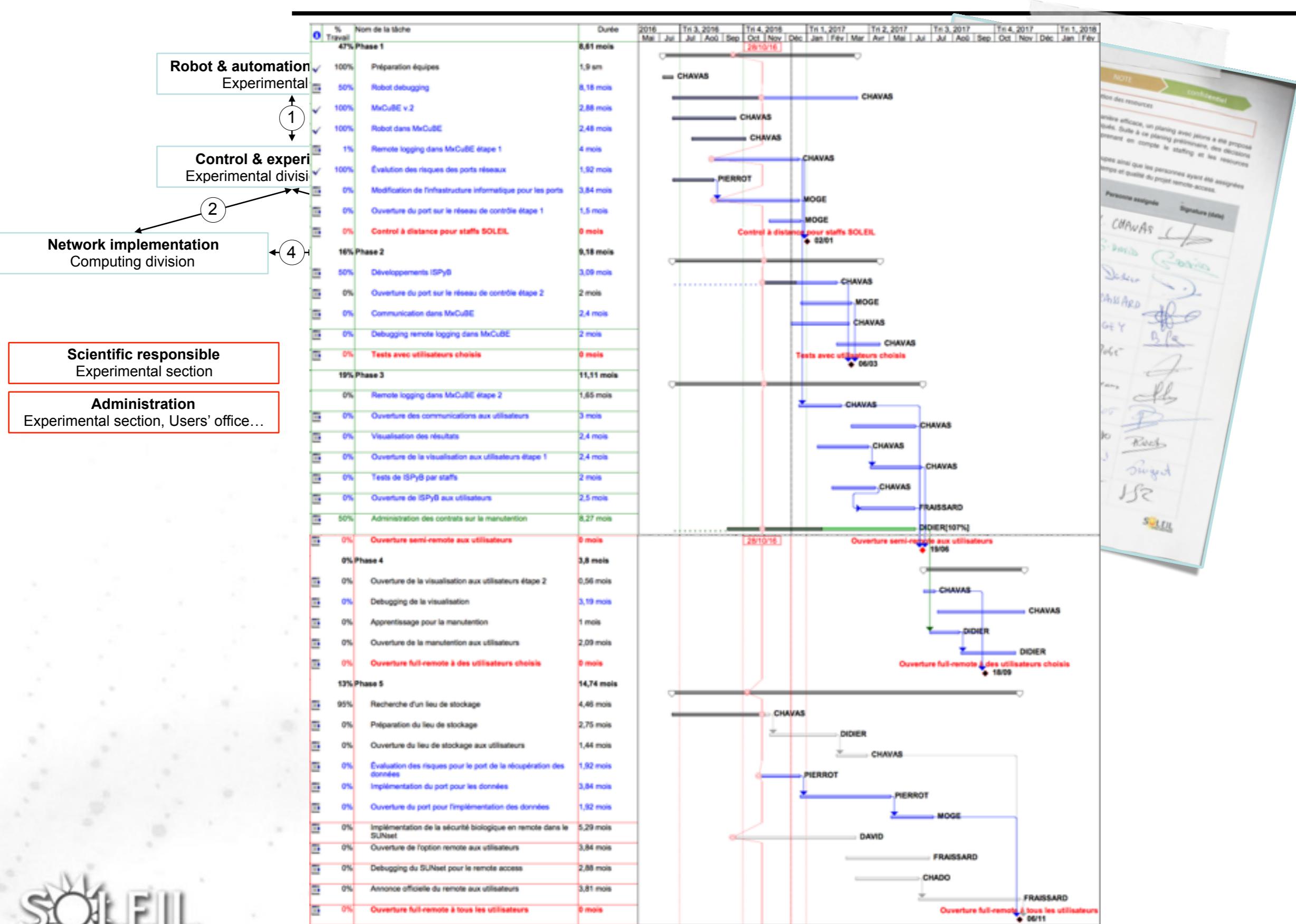
# REMOTE ACCESS AT SOLEIL



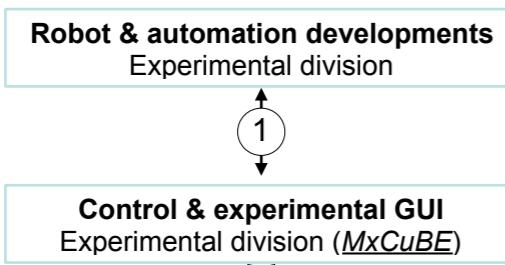
# REMOTE ACCESS AT SOLEIL



# REMOTE ACCESS AT SOLEIL



# REMOTE ACCESS AT SOLEIL



How to submit | Preparing your experiment | Laboratories support facilities | Safety requirements | Beamlines | User Office

<<

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  - [Proposal Application](#)
  - [Management Before experiment](#)
  - [Management After experiment](#)
- [Experiment data](#)
  - [SOLEIL Data Retrieval](#)
- [Personal Management](#)
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  - [Umbrella Information](#)
  - [Change password](#)
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## Proposal Management

[Proposal Application](#)  
Click here if you want to create, edit or delete your own proposal. A proposal is partially completed until it is submitted (submit button). From then on, the proposal is defined as completed and for any modification you need to contact the SOLEIL user office directly.

[Management Before experiment](#)  
Management proposal before the experiment

## Experiment data

[SOLEIL Data Retrieval](#)  
Consultation project experiment files (to see downloaded files you will need to download the databrowser from the help button)

## Personal Management

[Personal Information](#)  
Click here for changing your personal information like institute, phone number, email address or to create an Umbrella account and/or linked it to your SUN set account.

[Umbrella Information](#)  
Click here to create an Umbrella account or to link it to your SUN set account if you were logged in through Umbrella.

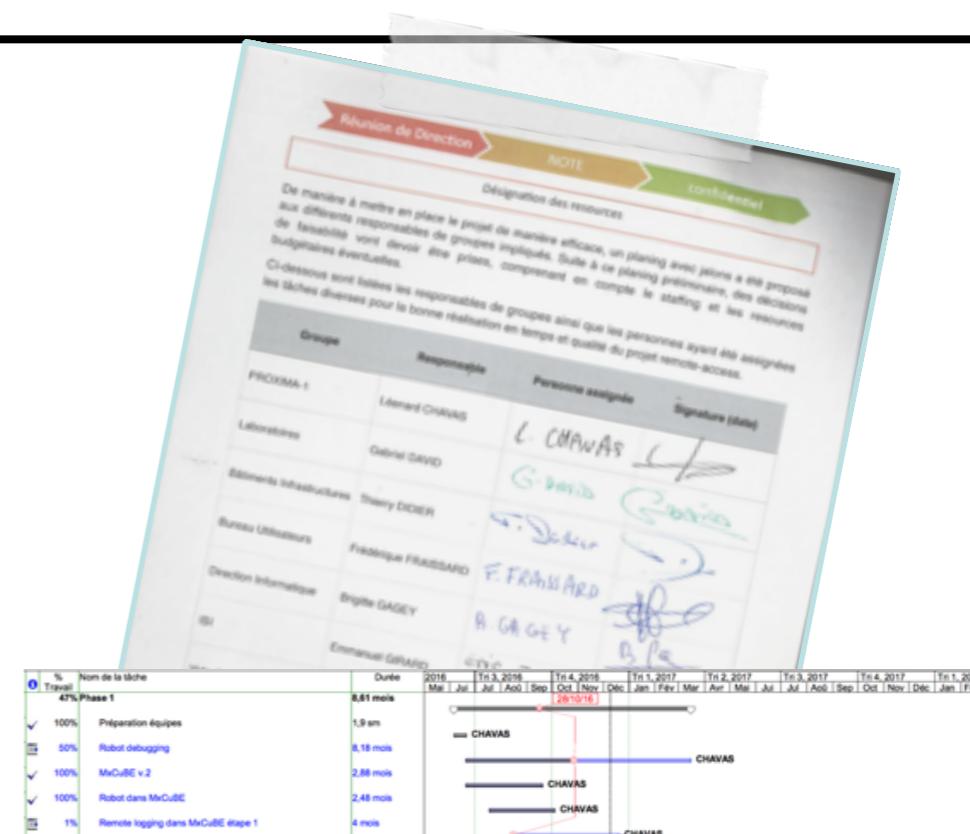
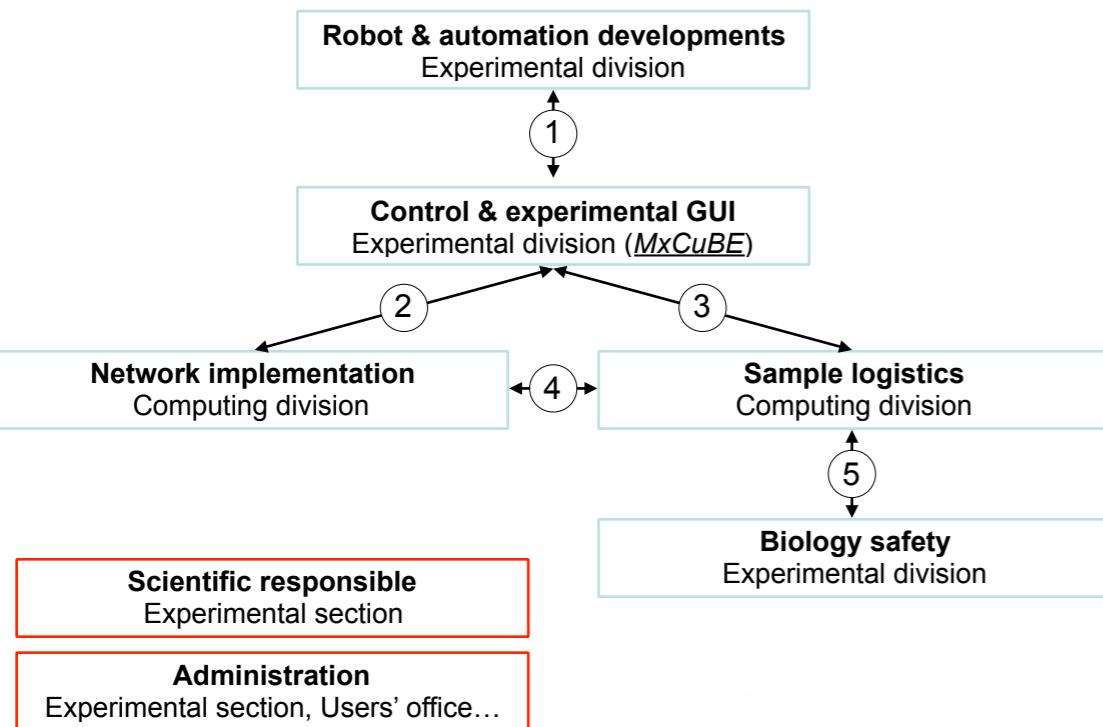
[Management After experiment](#)  
Management proposal after the experiment



0%	Implémentation de la sécurité biométrique en remote dans le SUNet	0,29 mois
0%	Ouverture de l'option remote aux utilisateurs	3,84 mois
0%	Debugging du SUNet pour le remote access	2,88 mois
0%	Annonce officielle du remote aux utilisateurs	3,81 mois
0%	Ouverture full remote à tous les utilisateurs	8 mois



# REMOTE ACCESS AT SOLEIL



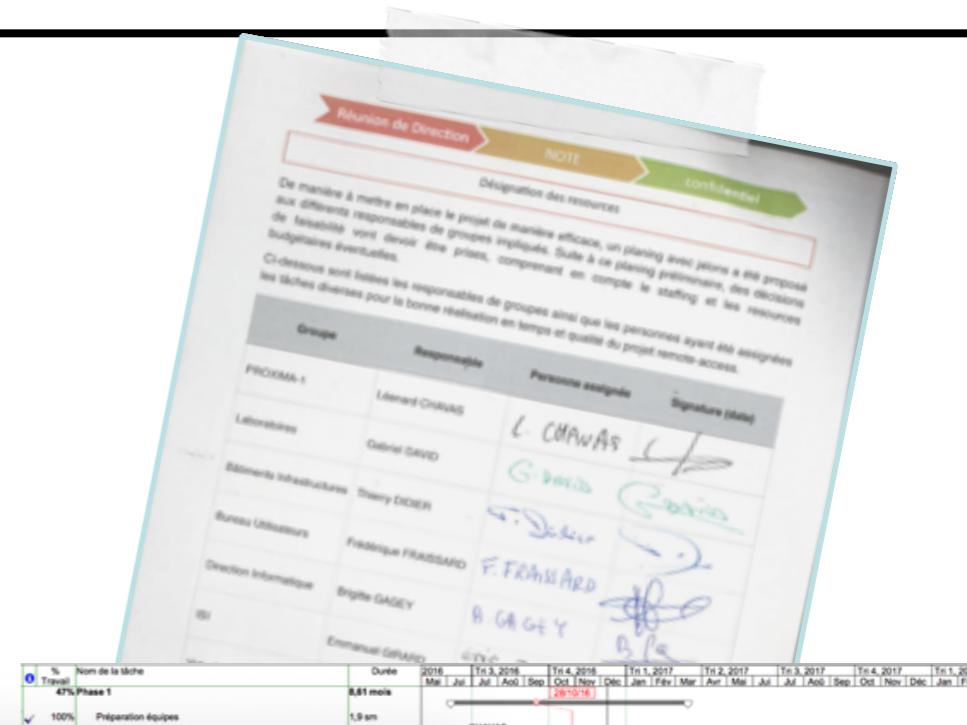
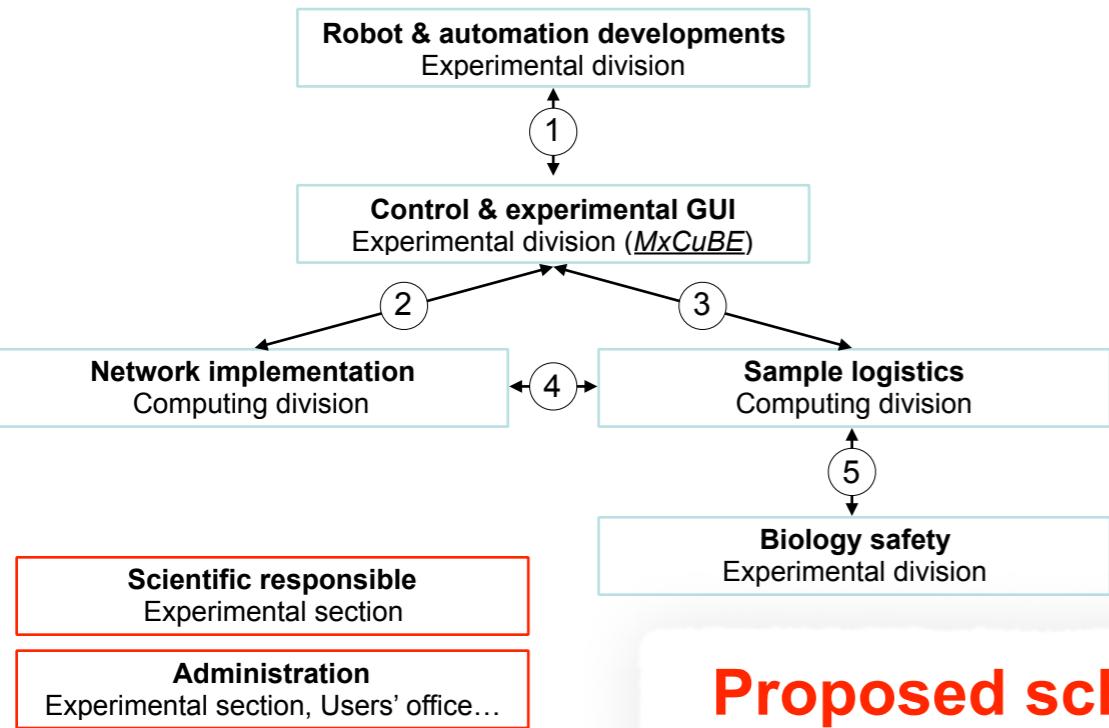
1-20 of 63 | 20 | 🔍

Proposal ID	Title	Lab	City	BAG coordinator or main proposer	1st Beamline Requested / Assigned	Proposal Type
20100023	Preparation for high pressure experiments, stabilisation of crystals for data collection at room temperature	Compartmentation et Dynamique Cellulaires - Institut ; INSB	PARIS CEDEX 05	Dr. HOUDUSSE Anne	PROXIMA 1	Rapid Access
20120009	High resolution studies on the soil bacterial proteins TodT, TodS, PtxS and McpS	Lab. of Crystallographic Studies -	ARMILLA (GRANADA)	Dr. PINEDA Estela	PROXIMA 1	Standard
20121253	Structural Biology of chemical and electrical signaling, redox metabolism and host-pathogen interaction.	Structural Biology Brussels Lab. - Molecular and Cellular Interactions	BRUXELLES	Prof. Dr. REMAUT Han	PROXIMA 1	Block Allocation Group
20140706 A1412 : Laurent		Synchrotron SOLEIL -	GIF SUR YVETTE CEDEX	Mrs. LORY Céline	PROXIMA 1	Rapid Access
20140887 A1420 : Tom		Synchrotron SOLEIL -	GIF SUR YVETTE CEDEX	Mrs. LORY Céline	PROXIMA 1	Rapid Access
20140918	BAG for Signal transduction, DNA Repair, Marine Glycobiology, bacterial polyketide synthases and IDPs involved in leucemia	Laboratoire de Biologie intégrative des modèles marins - INSB ; INC ; INEE	ROSCOFF CEDEX	Dr. CZJZEK Mirjam	PROXIMA 1	Block Allocation Group
20150660	Paris Rive Gauche BAG: from macromolecular structures to drug targets.	Faculté de Pharmacie - Univ. Paris-Descartes - Lab. de Cristallographie and RMN Biologique;Instituts;INSB;INC	PARIS CEDEX 06	Dr. PHAN Gilles	PROXIMA 1	Block Allocation Group
20150717	Macromolecular crystallography and SAXS of proteins and macromolecular complexes involved in human disease	Structural Biology Brussels Lab. - Molecular and Cellular Interactions	BRUXELLES	Prof. Dr. LORIS Remy	PROXIMA 1	Block Allocation Group

Ouverture full-remote à tous les utilisateurs 8 mois 06/11

**SOLEIL SYNCHROTRON**

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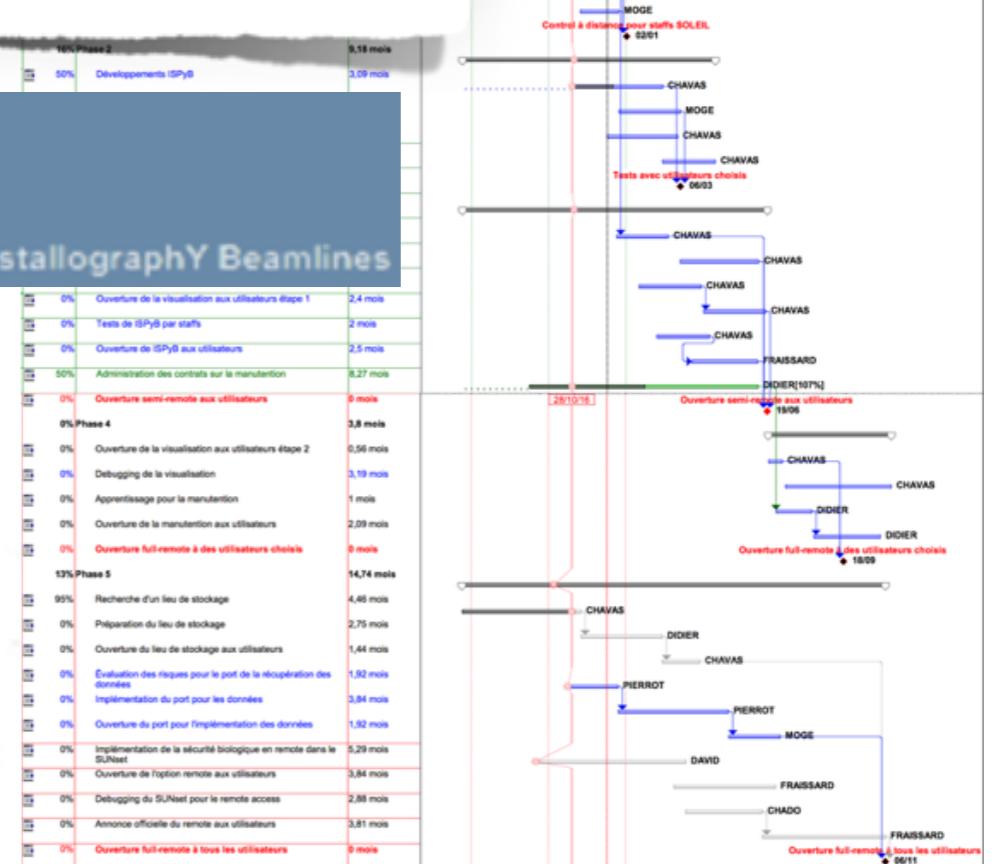


**Proposed schedule for opening to users:**  
**October 2017**

The screenshot shows the Soleil Synchrotron website with a navigation bar for 'How to submit', 'Preparing your experiment', and 'Laboratory'. The main content area is titled 'ISPyB' with a subtitle 'Information System for Protein crystallographY Beamlines'. It features a large eye icon. Below is a table of proposals:

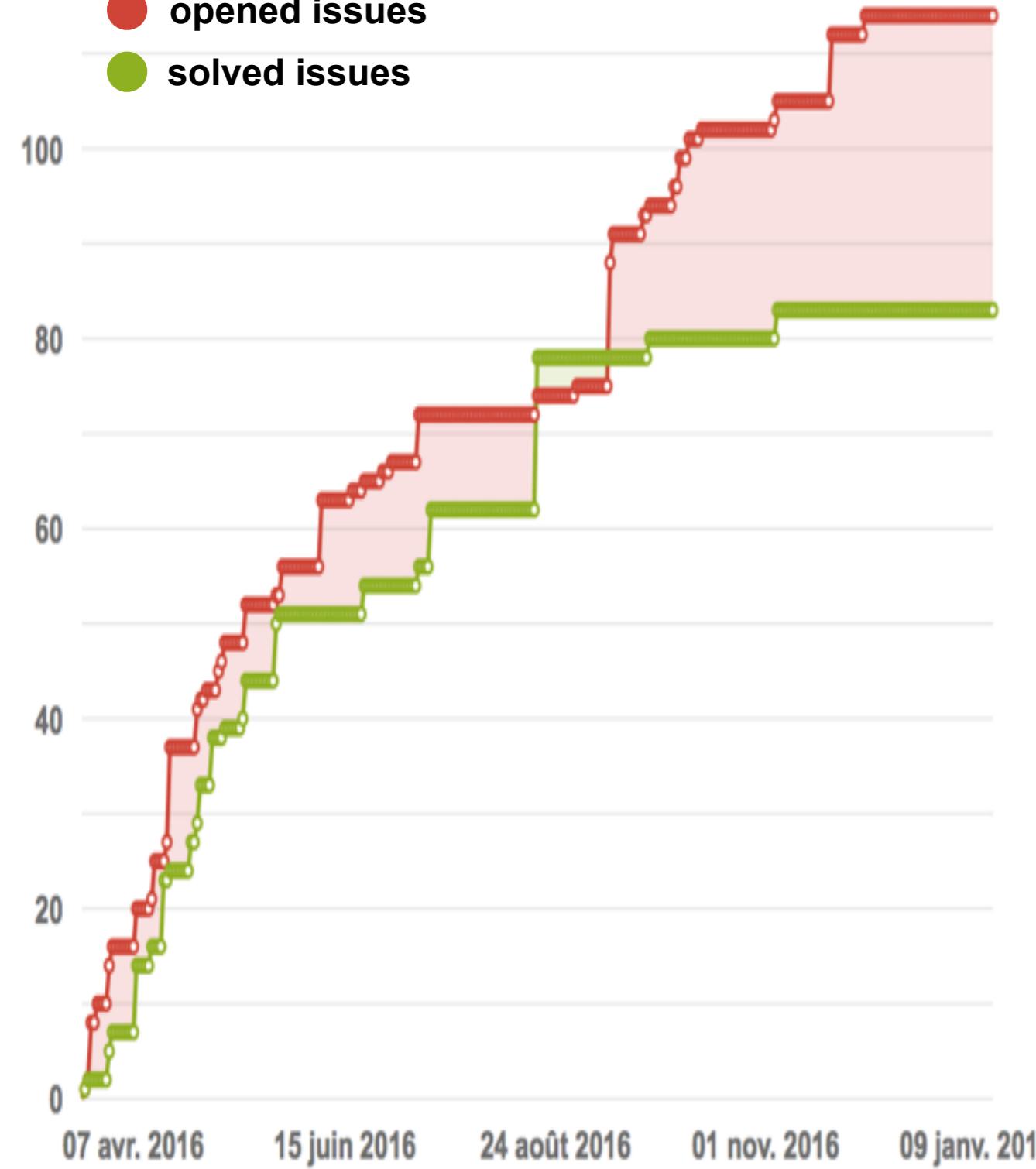
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The Soleil logo is visible at the bottom left.



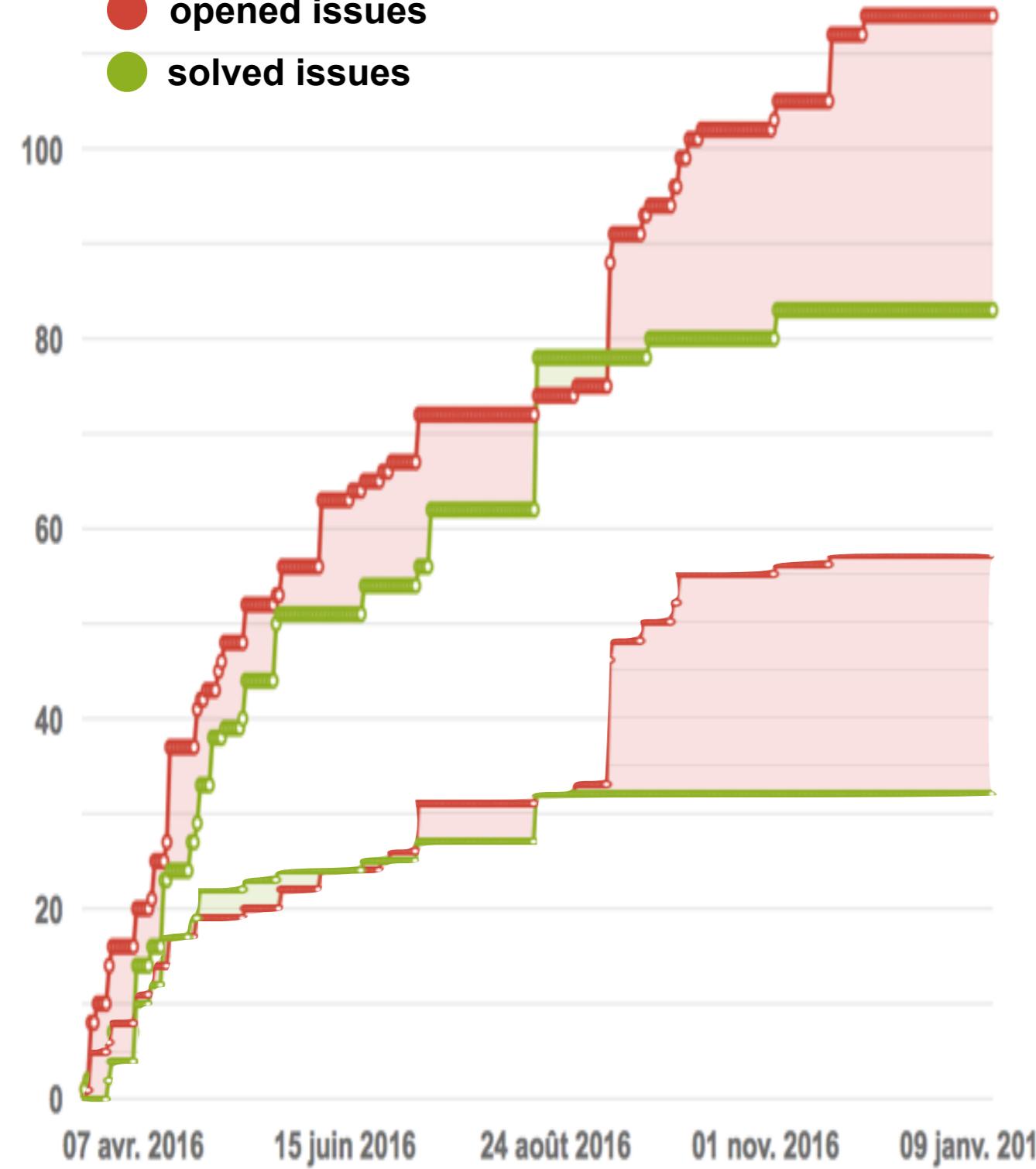
# EVOLUTION OF BUG-FIXES (PXI ONLY)

- opened issues
- solved issues



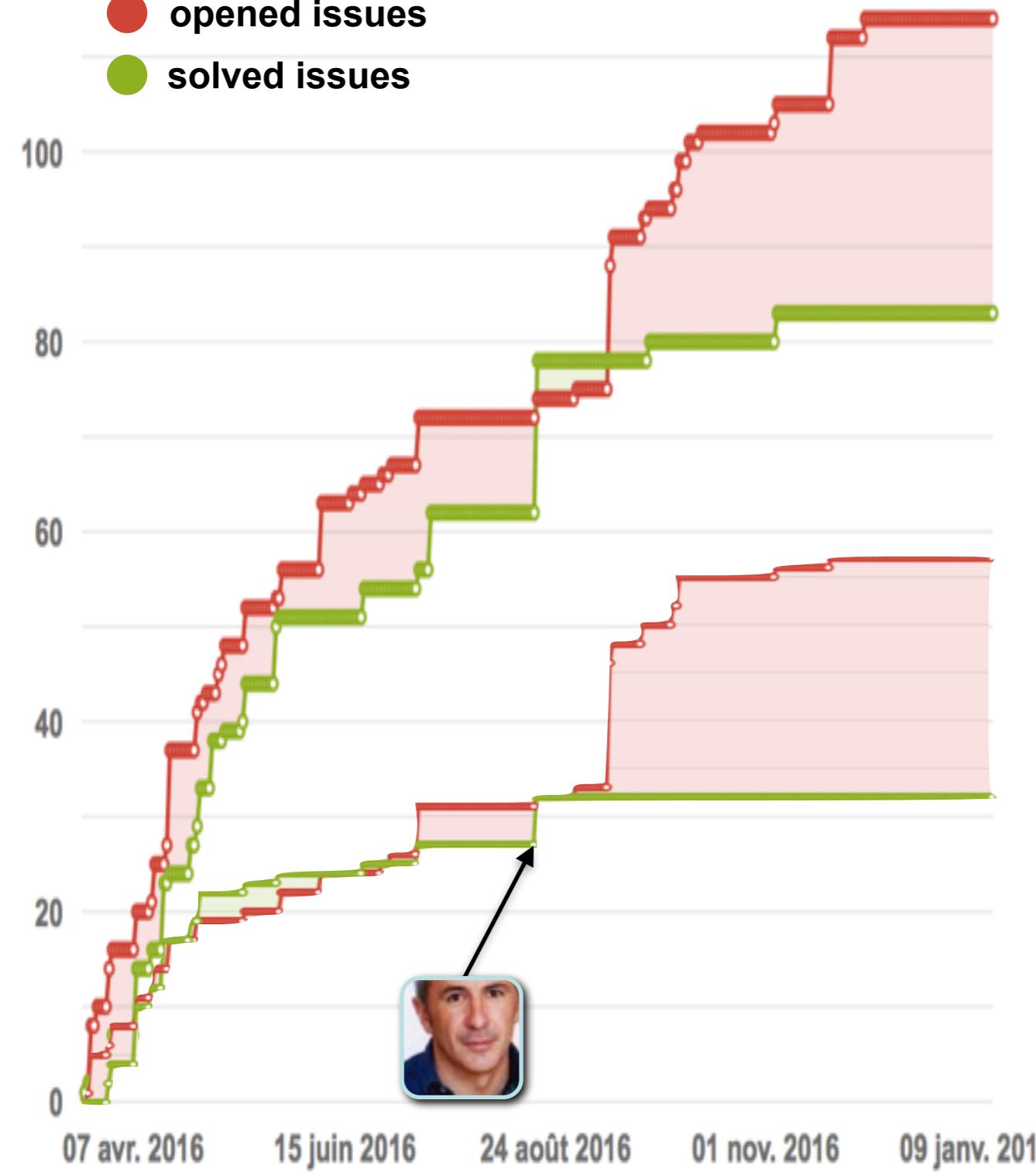
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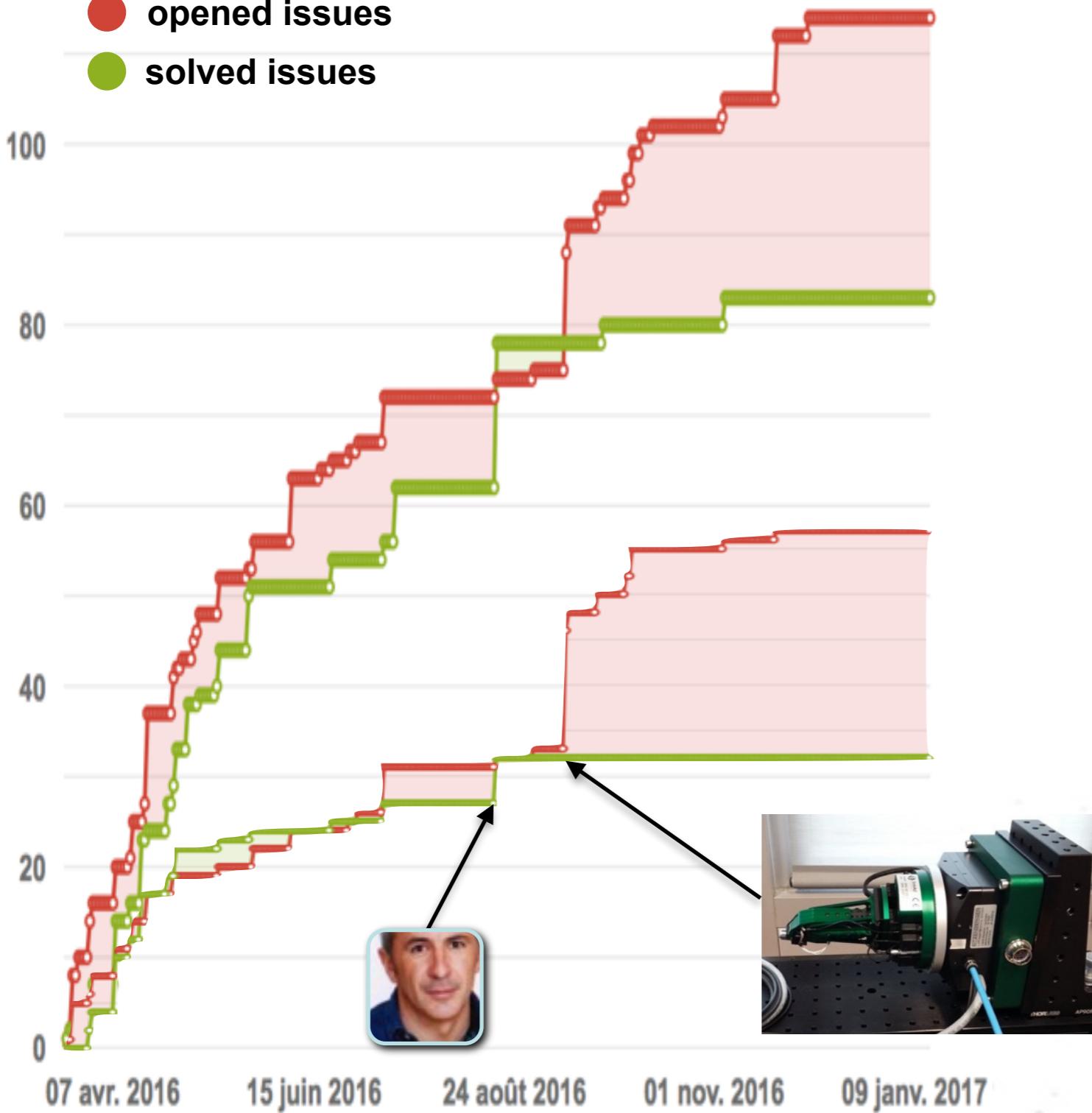


first series of issues related to:

- robot operation 'smoothing'
- slow-down of the interface

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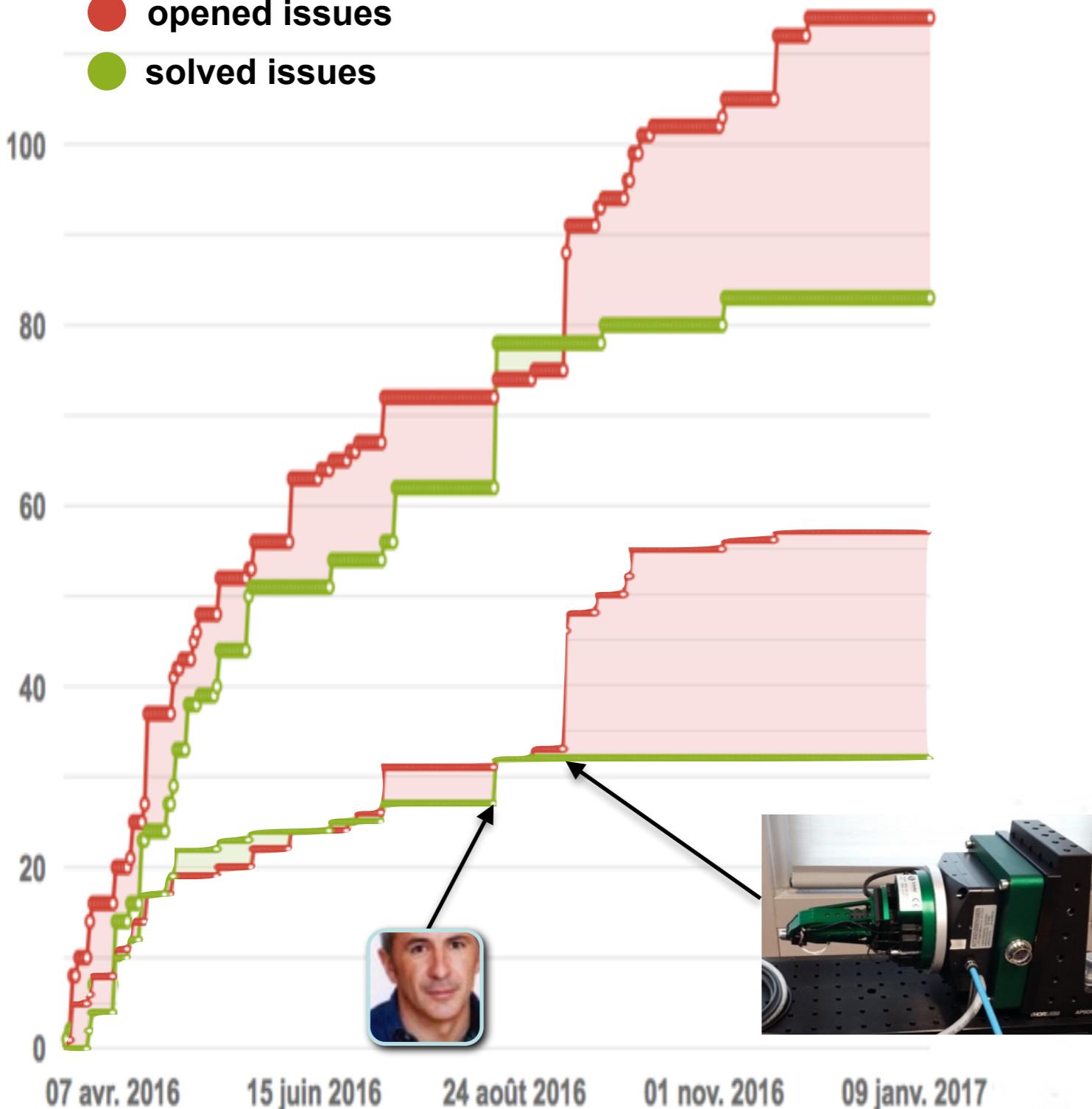
- robot operation 'smoothing'
- slow-down of the interface

second series of issues related to:

- implementation of SmarGon
- all devices surrounding SmarGon
- new slow-down of the interface
- XDS results linked to ISPyB
- neighbouring beam line status

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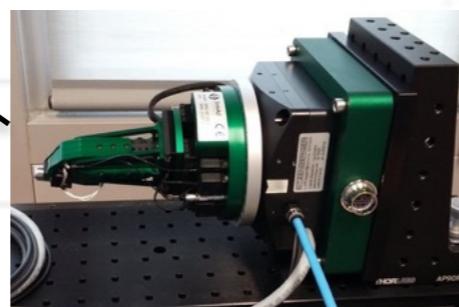
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current plans for upcoming period:

- fix most of above issues
- addition of 'basic' functions
  - ~ on-the-fly indexing (new server)
  - ~ *in situ* data measurements
  - ~ remote access options



# Acknowledgments



**Patrick Gourhant**  
Assistant engineer



**Leo Chavas**  
Beamline manager



**Bill Shepard**  
Beamline manager



**Damien Jeangerard**  
Assistant engineer



**Pierre Legrand**  
Beamline scientist



**Serena Sirigu**  
Beamline scientist



**Tatiana Isabet**  
Responsible industry



**Gavin Fox**  
Beamline scientist



**Martin Savko**  
Beamline scientist



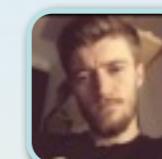
**Tiphaine Huet**  
Post-doctoral fellow



**Pierre Montaville**  
Post-doctoral fellow



**Igor Chaussavoine**  
PhD student



**Adam Simpkin**  
PhD student



**Enrico Stura**  
Associate scientist

Ivan Polzinelli    Nicolas Foos  
James Torpey    Nicolas Richet  
Denis Duran    Laurent Gadea

Robin Lener  
Apprenti