SOLEIL: STATUS REPORT IMPLEMENTATION OF SMARGON AND REMOTE ACCESS

Leo Chavas
PROXIMA-1
Synchrotron SOLEIL

10th 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

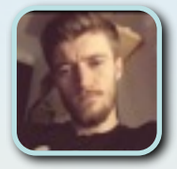
Gavin Fox
Beamline scientist

Martin Savko
Beamline scientist

Tiphaine Huet
Post-doctoral fellow

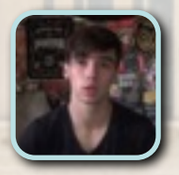
Pierre Montaville
Post-doctoral fellow

Igor Chaussavoine
PhD student



Adam Simpkin
PhD student

Enrico Stura
Associate scientist



Robin Lener
Apprenti

Ivan Polsinelli Nicolas Foos
James Torpey Nicolas Richet
Denis Duran **Laurent Gadea**

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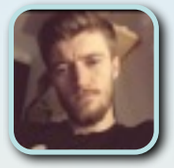

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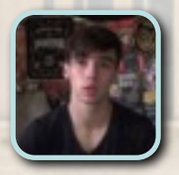

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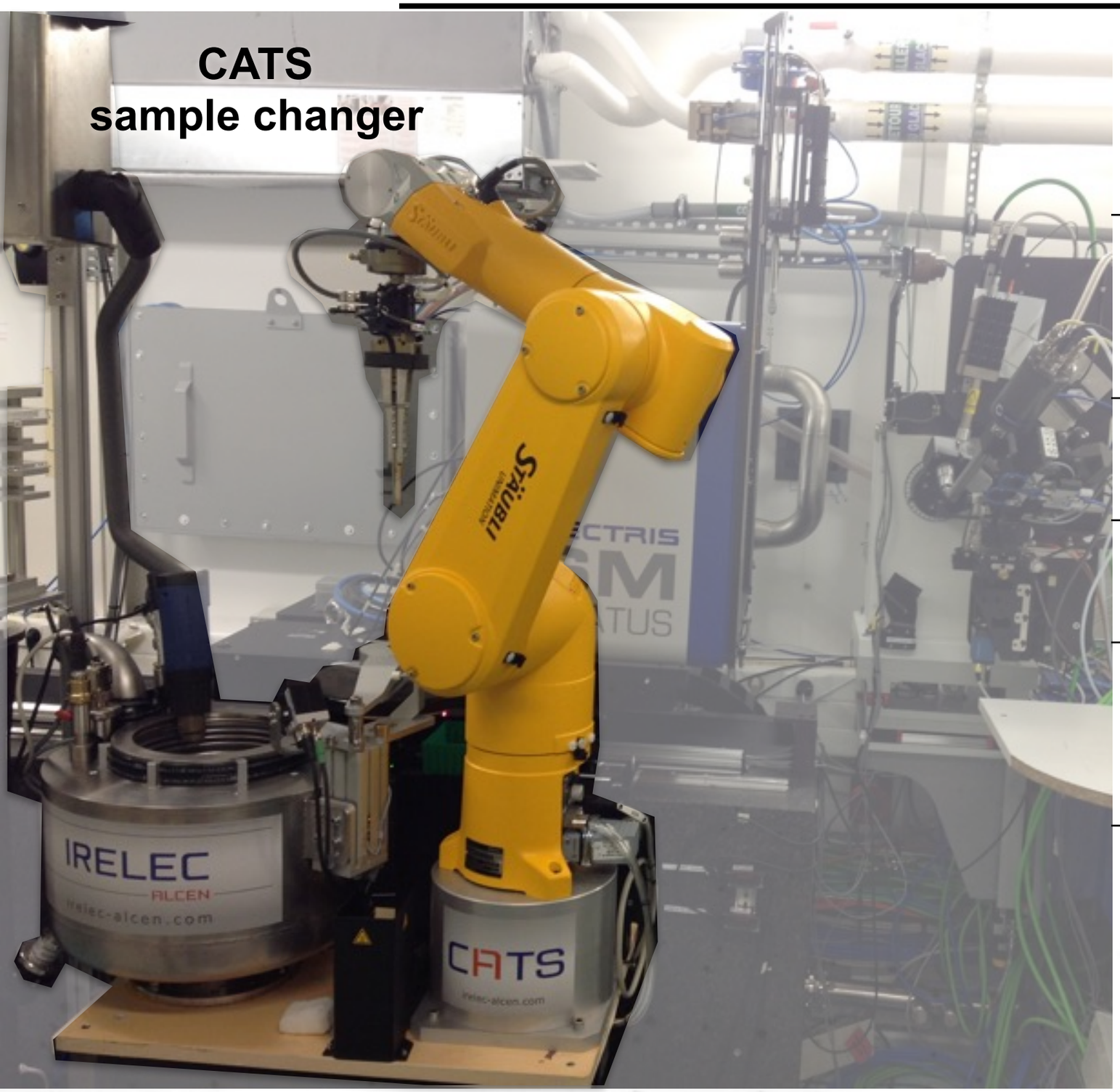
PROXIMA-I



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^2 (30x90μm^2 full beam)

FLUX AT SAMPLE

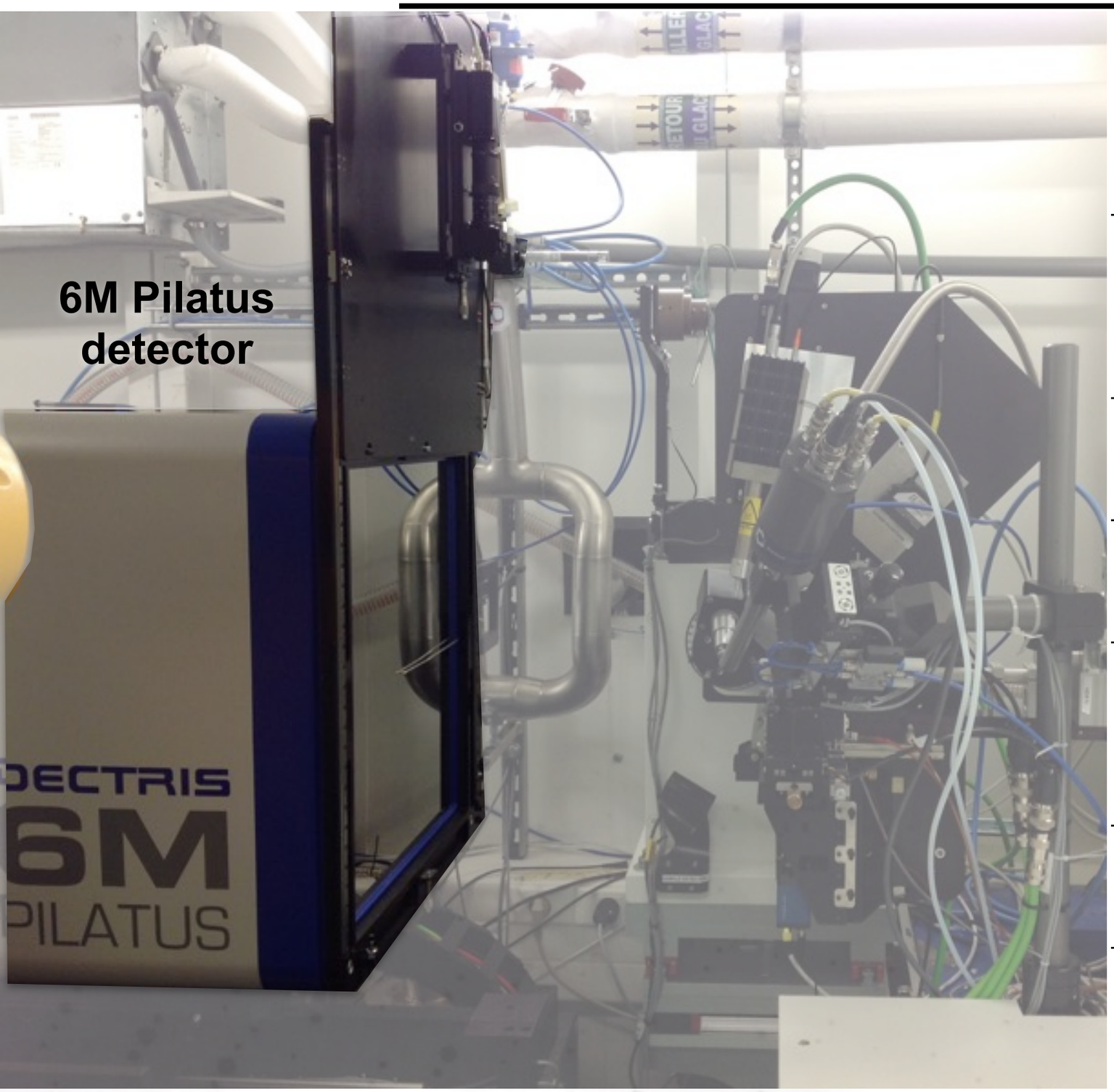
2.0E+12 phot/s/0.02% bw 500 mA

SAMPLE CHANGER

CATS (3 spine pucks)

possible *in situ* measurements

PROXIMA-I



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CAMERA

6M Pilatus

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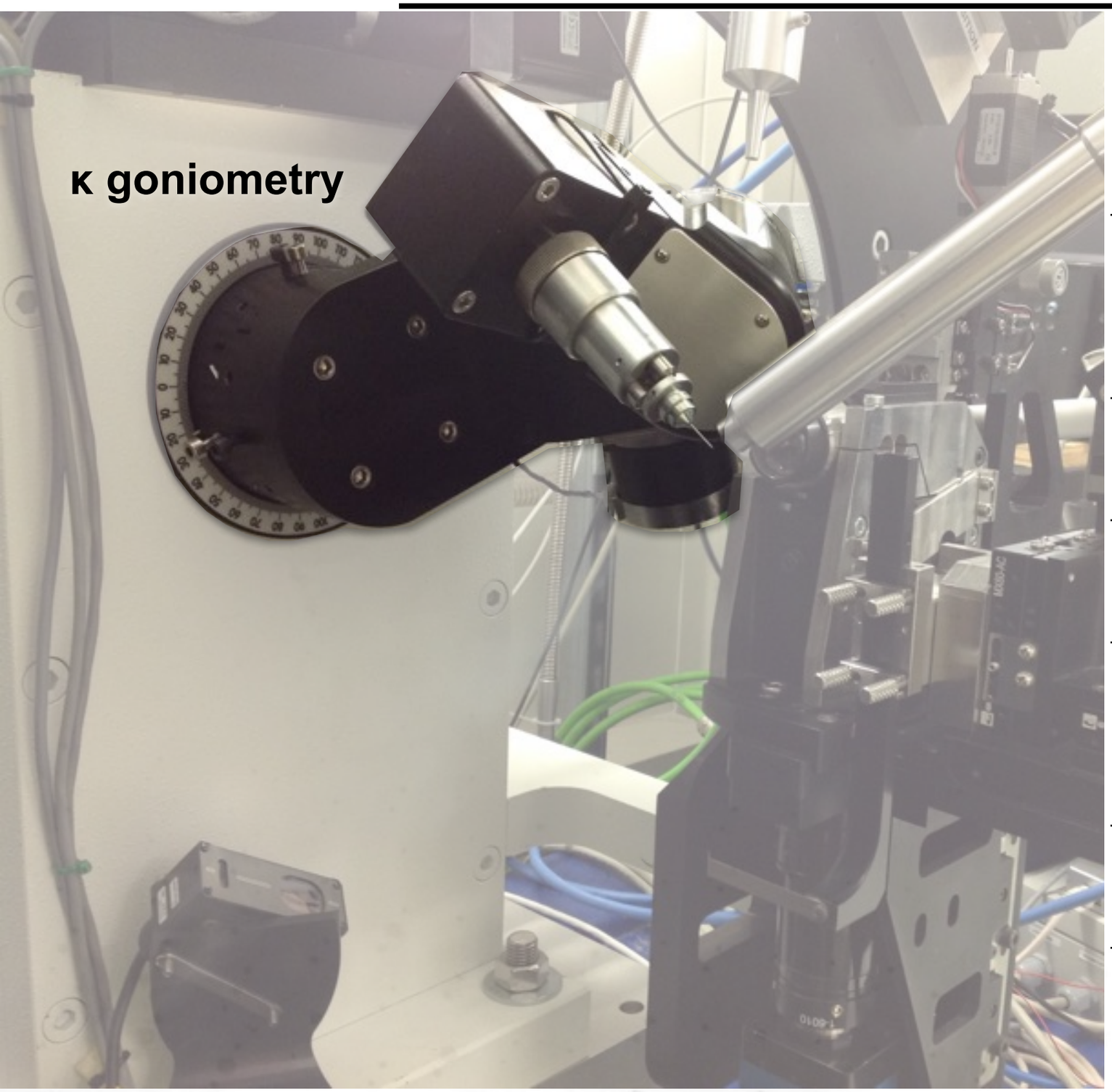

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SAMPLE ENVIRONMENT

3-axis κ-goniometre

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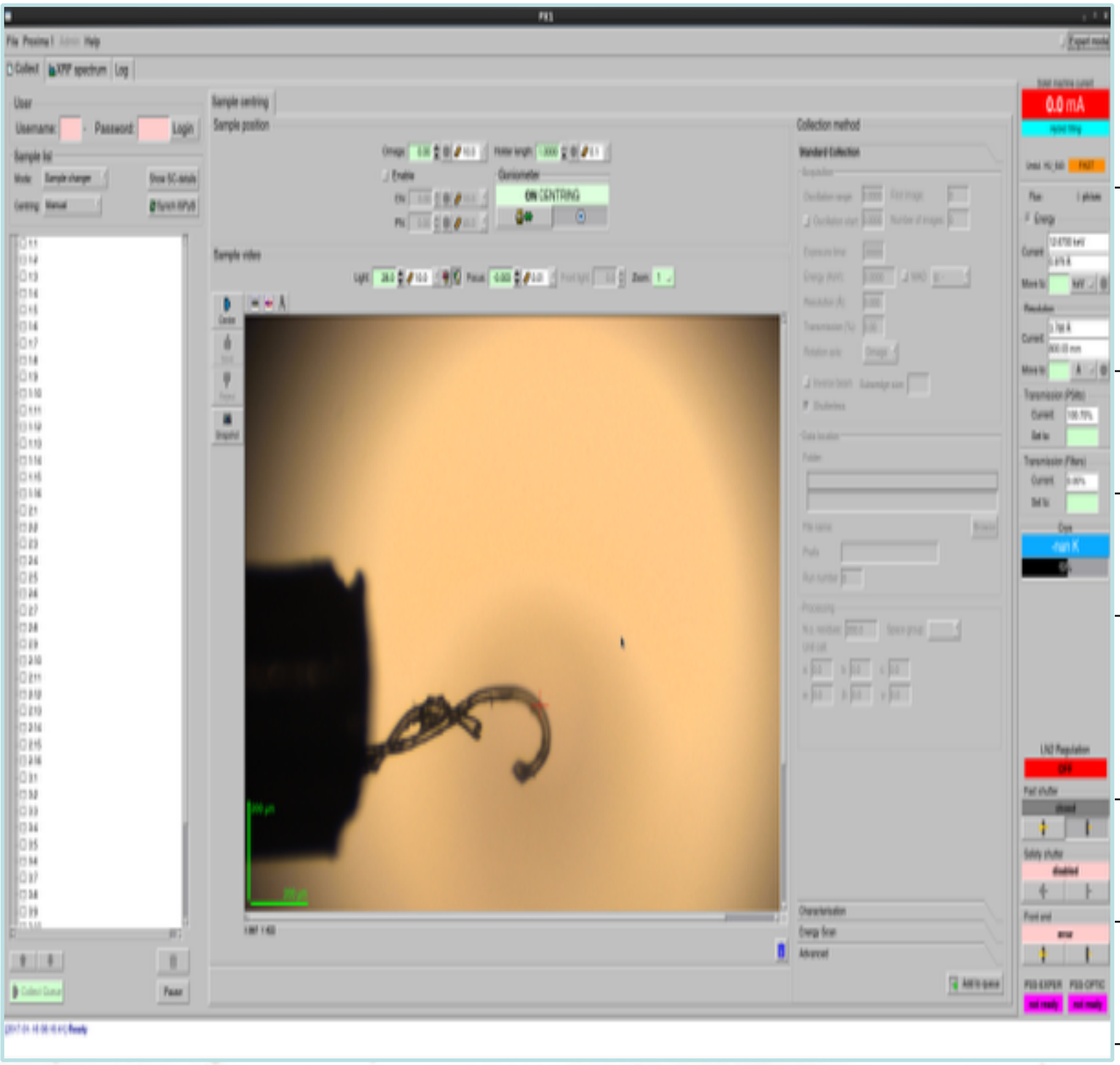

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MXCUBE VERSION

v2.1 Qt3

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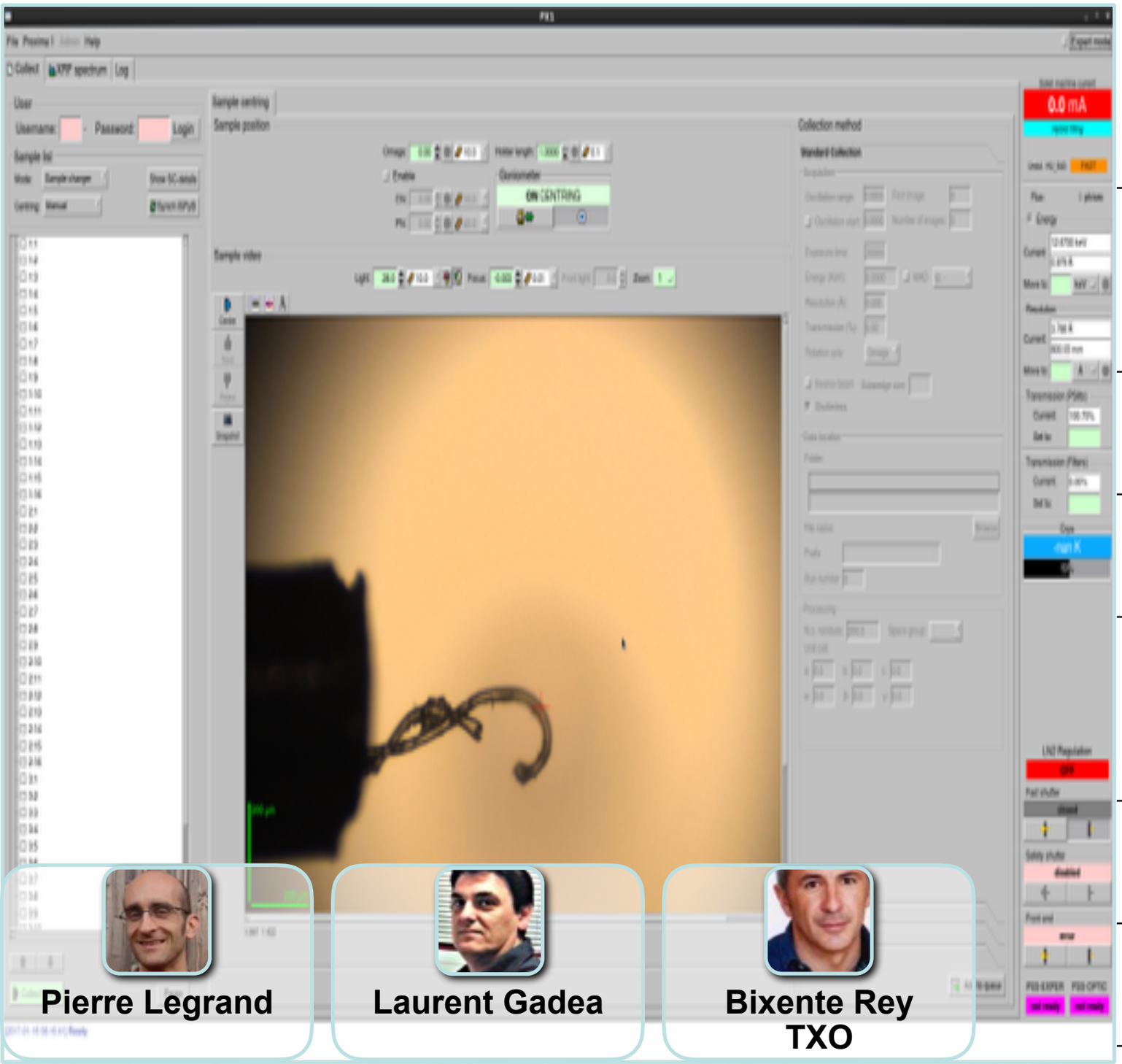

Pierre Legrand

Laurent Gadea

Bixente Rey
TXO

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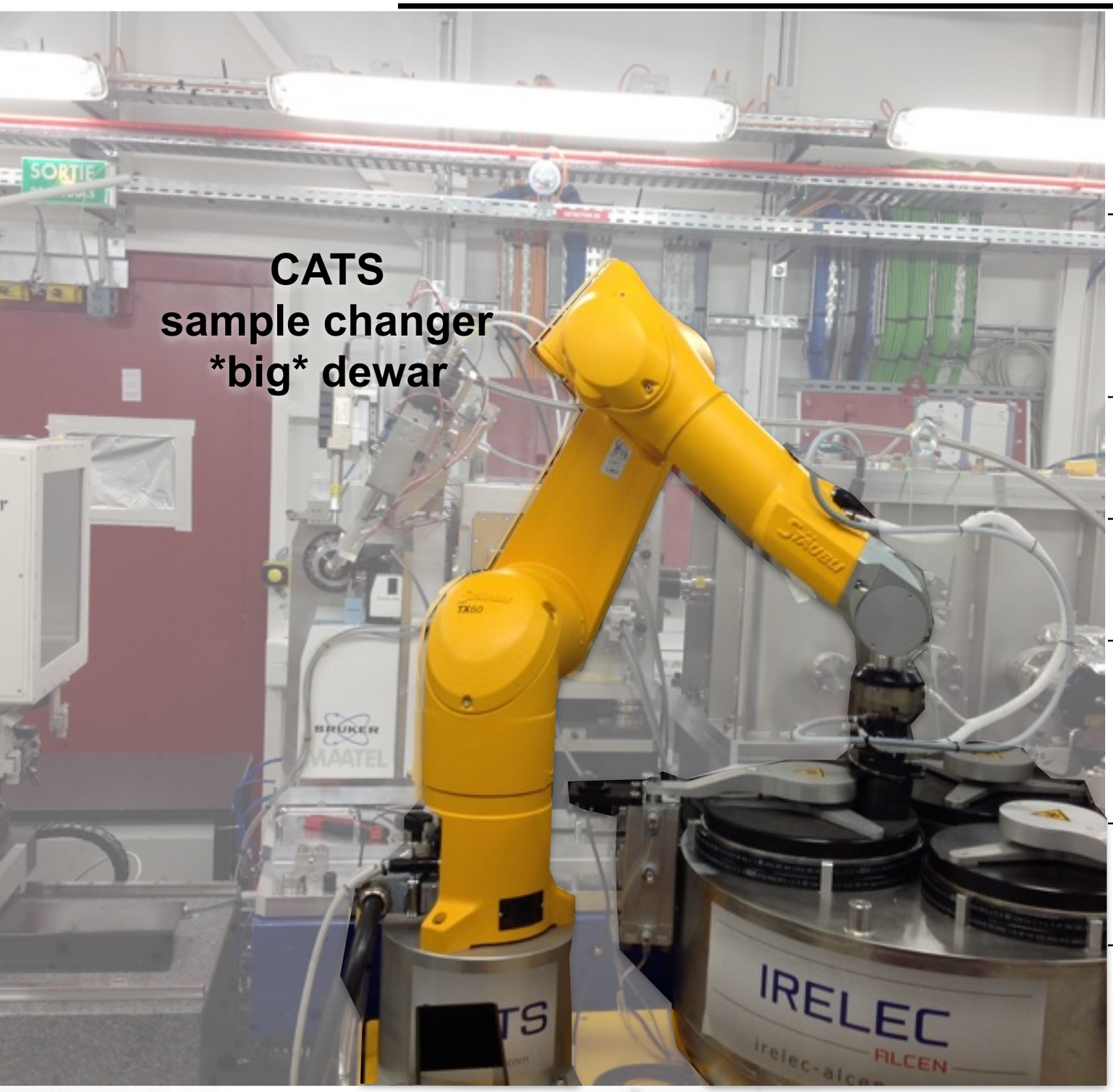
PROXIMA-2A



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 μm^2

FLUX AT SAMPLE

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

SAMPLE CHANGER

CATS (9 spine pucks)

in situ measurements available

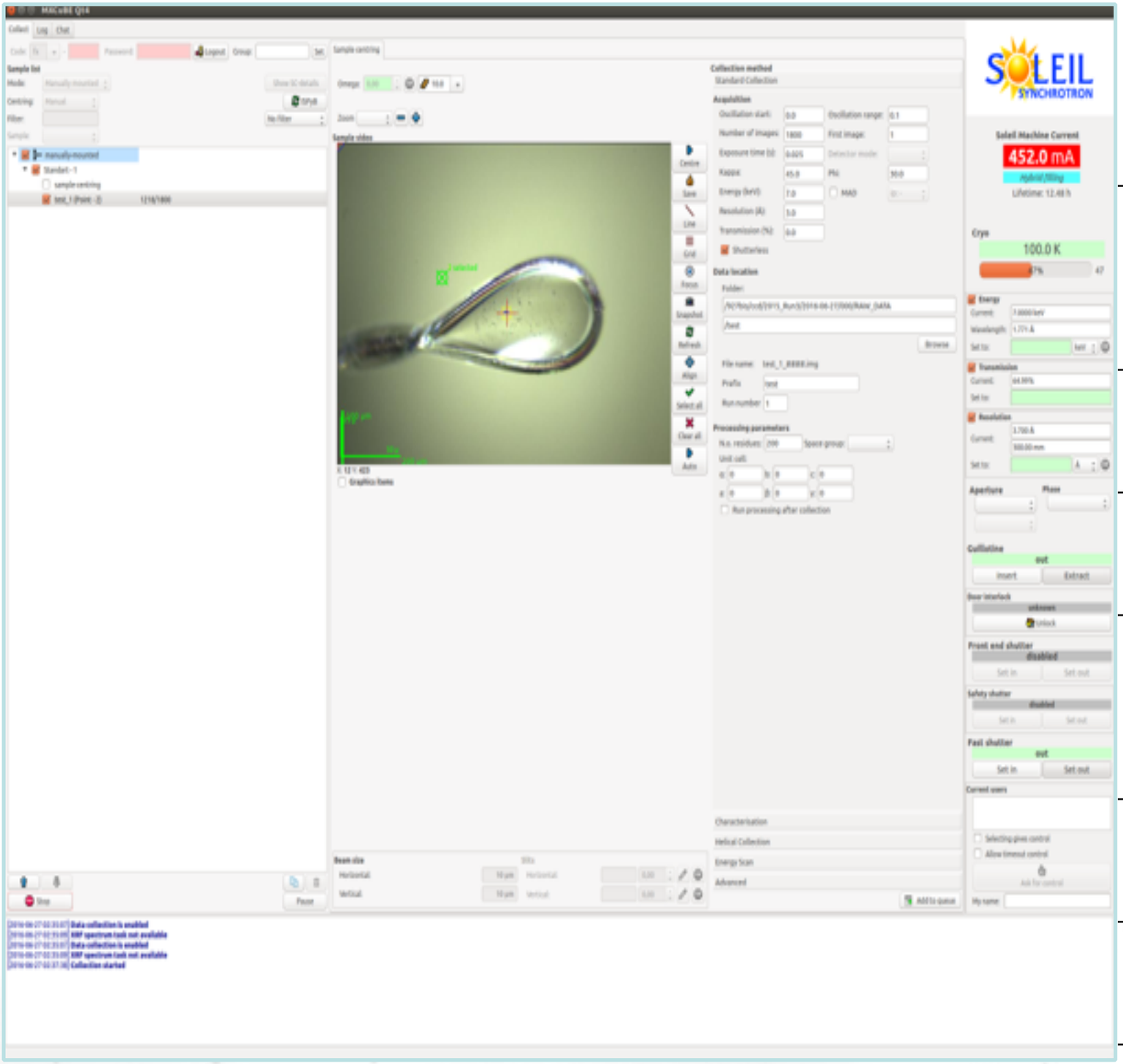
CAMERA

Eiger X-9M

SAMPLE ENVIRONMENT

microdiffractometer MD2

PROXIMA-2A



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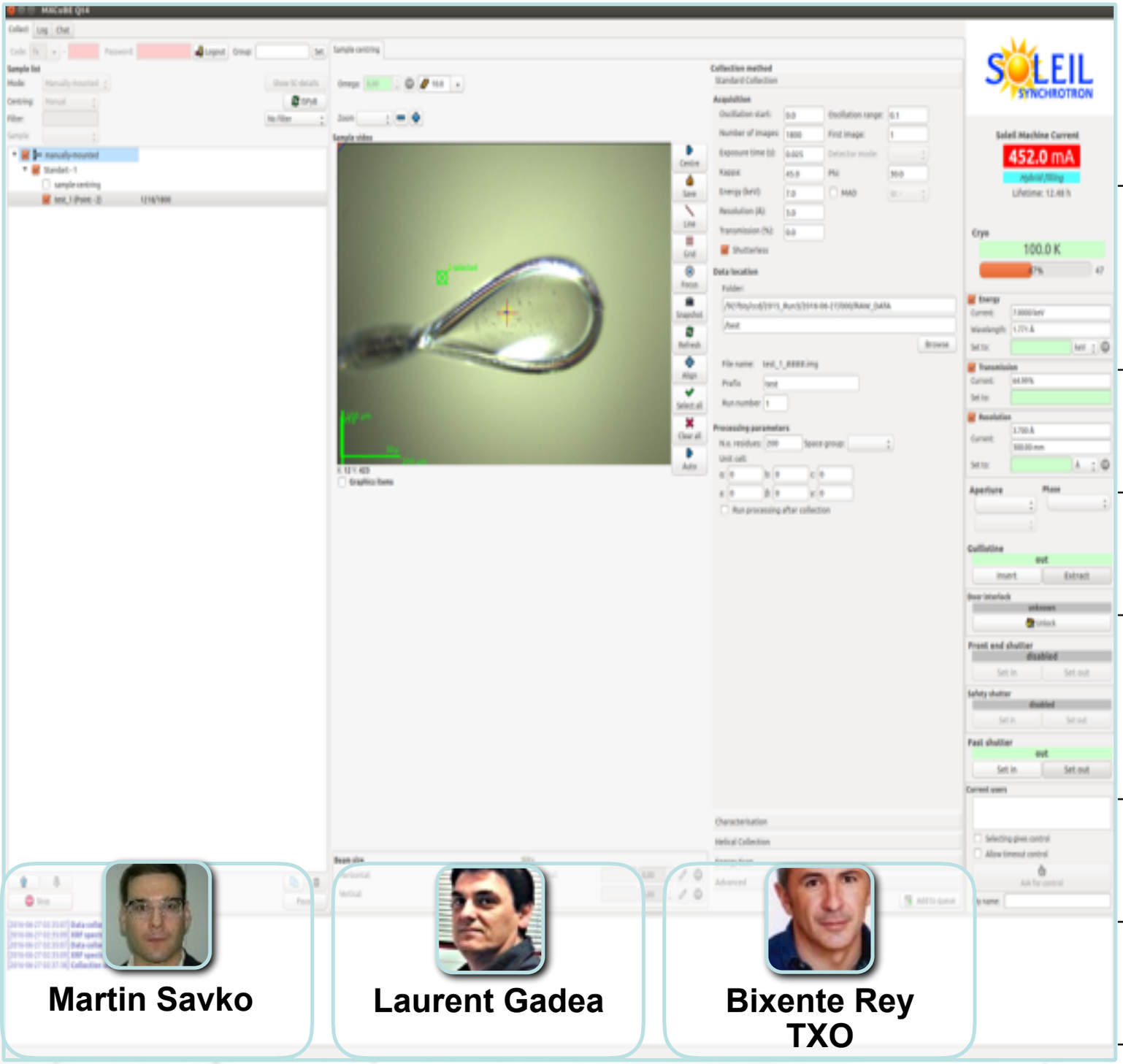
MXCUBE VERSION

v2.1 Qt3 in transition to Qt4

PROXIMA-2A



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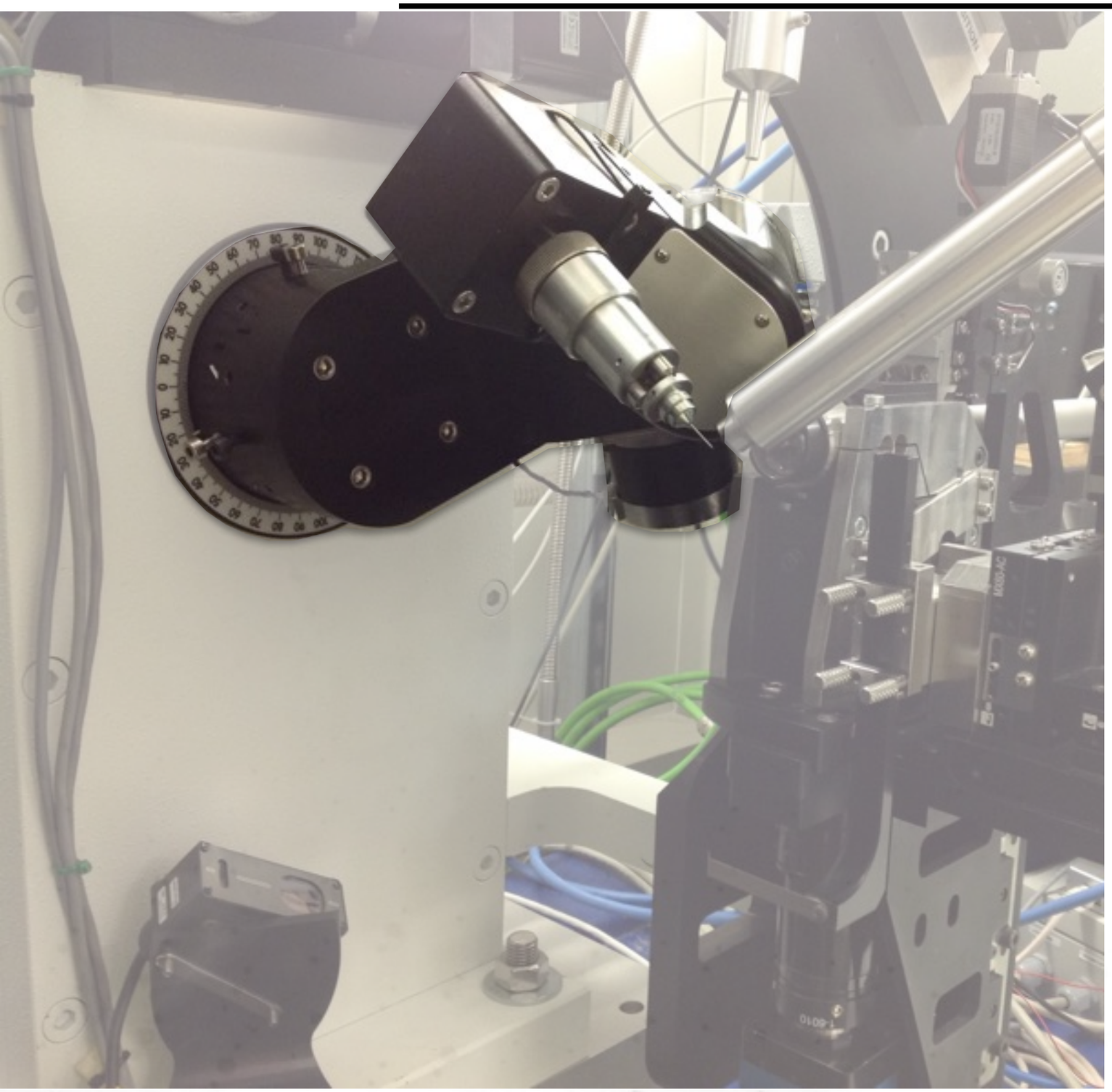
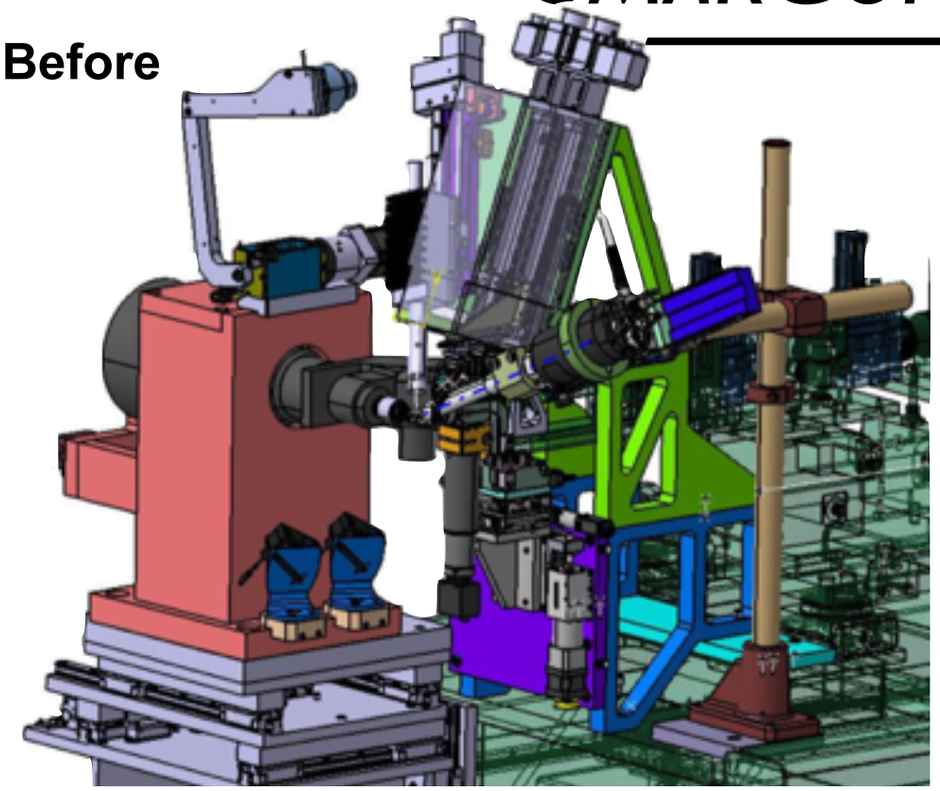
SmarGon implementation



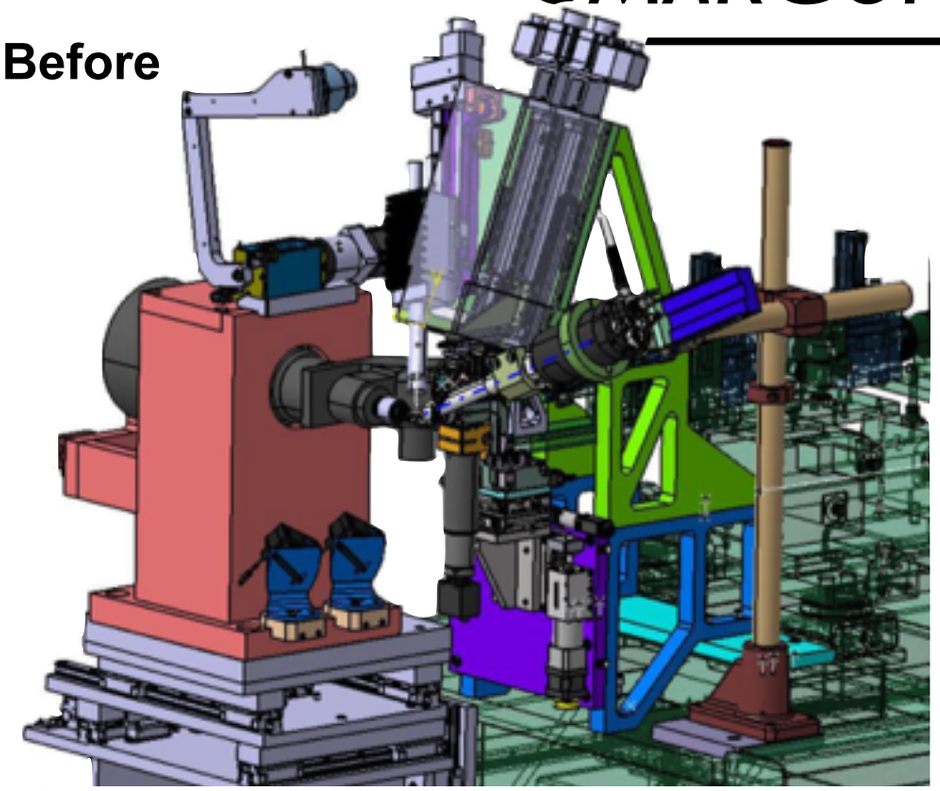
SmarGon implementation

Before



SmarGon implementation

Before



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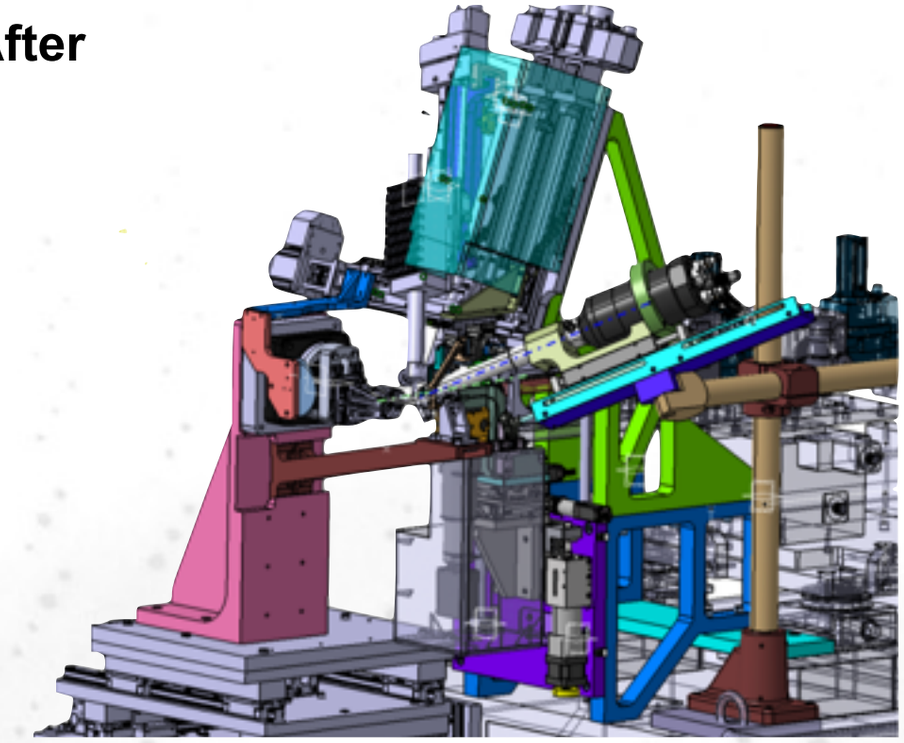

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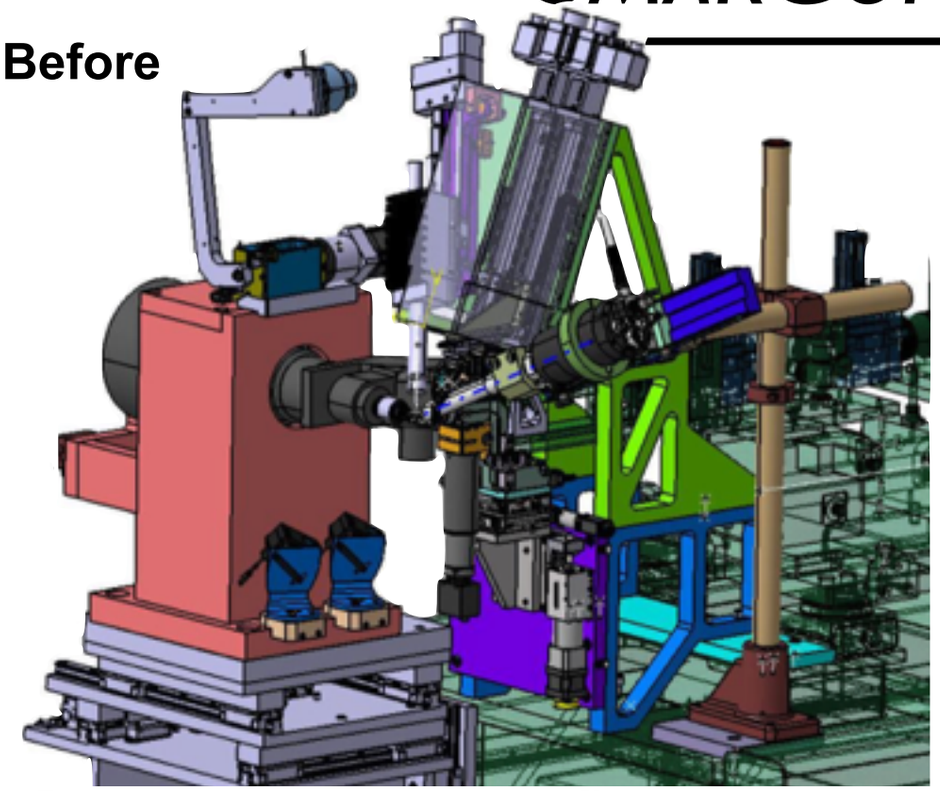

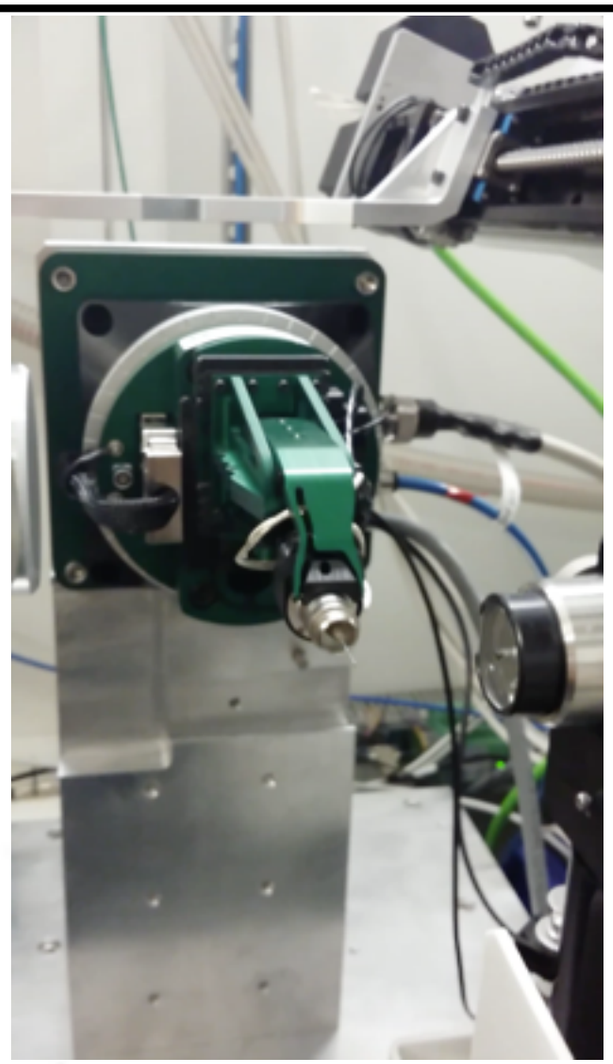

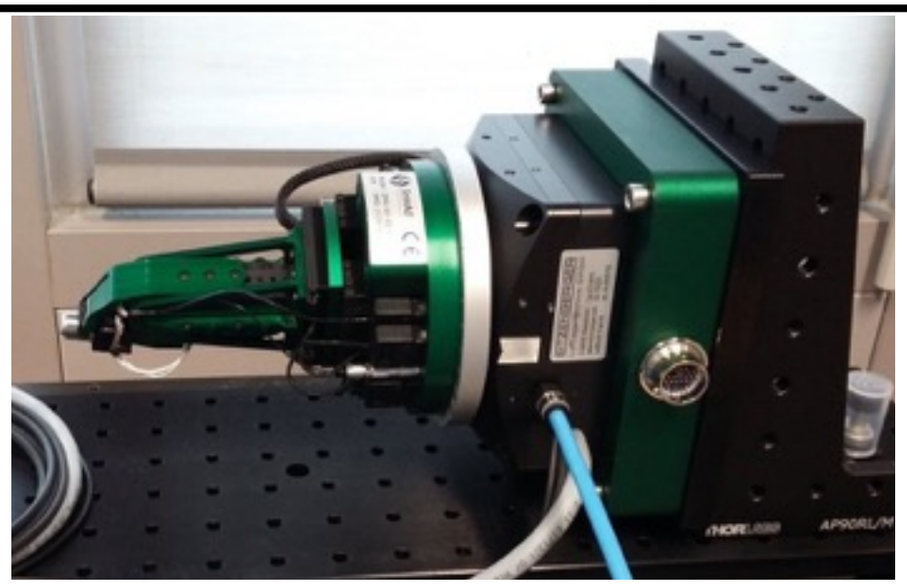

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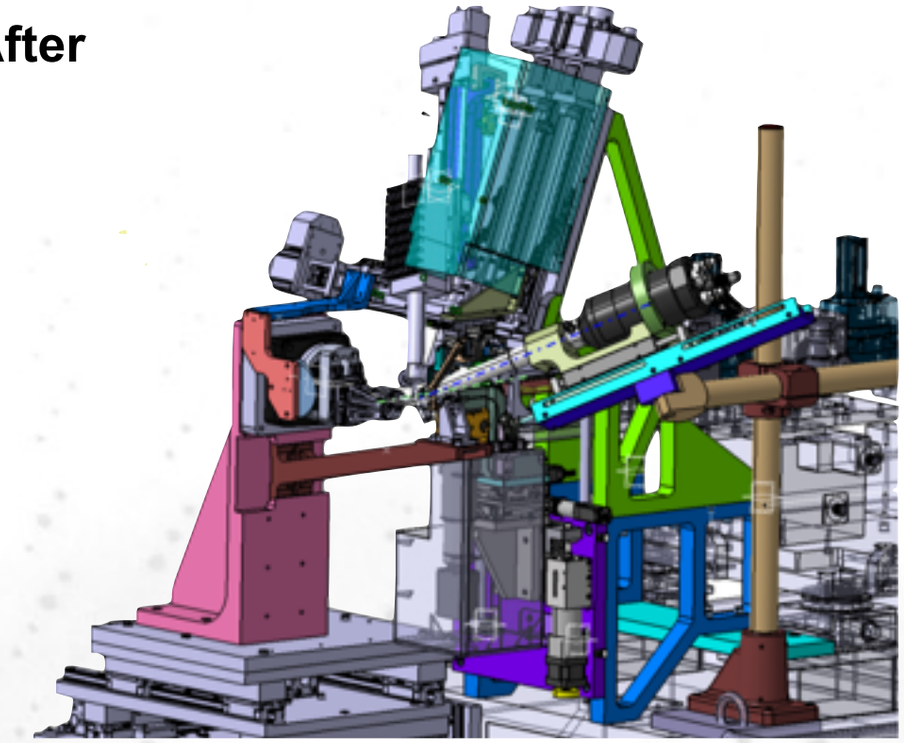

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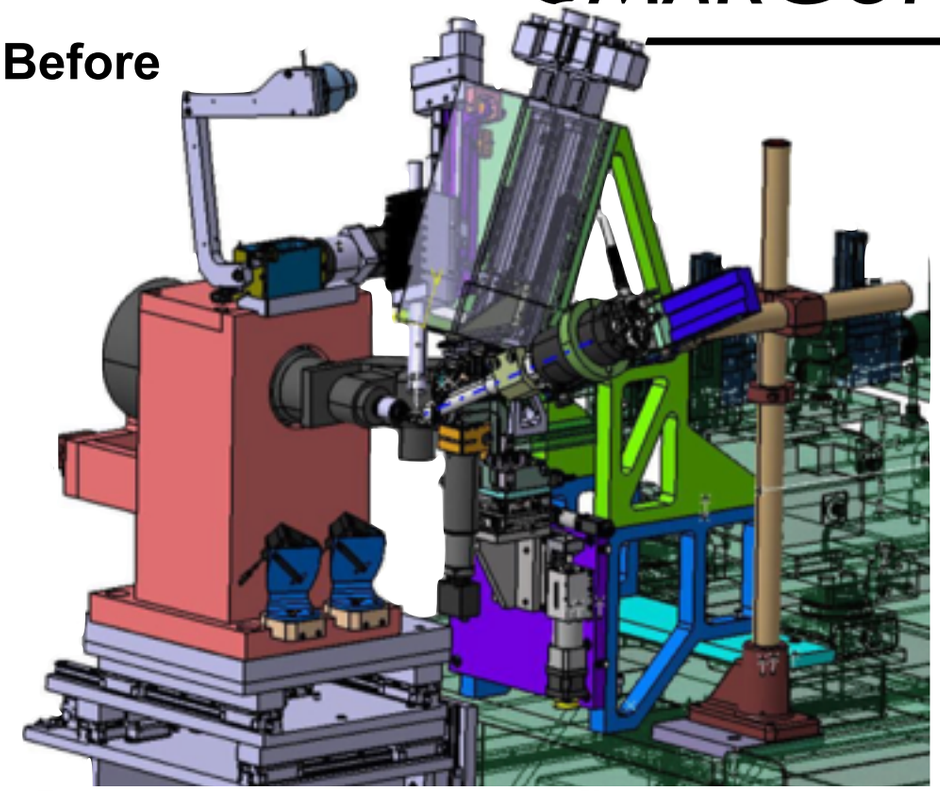

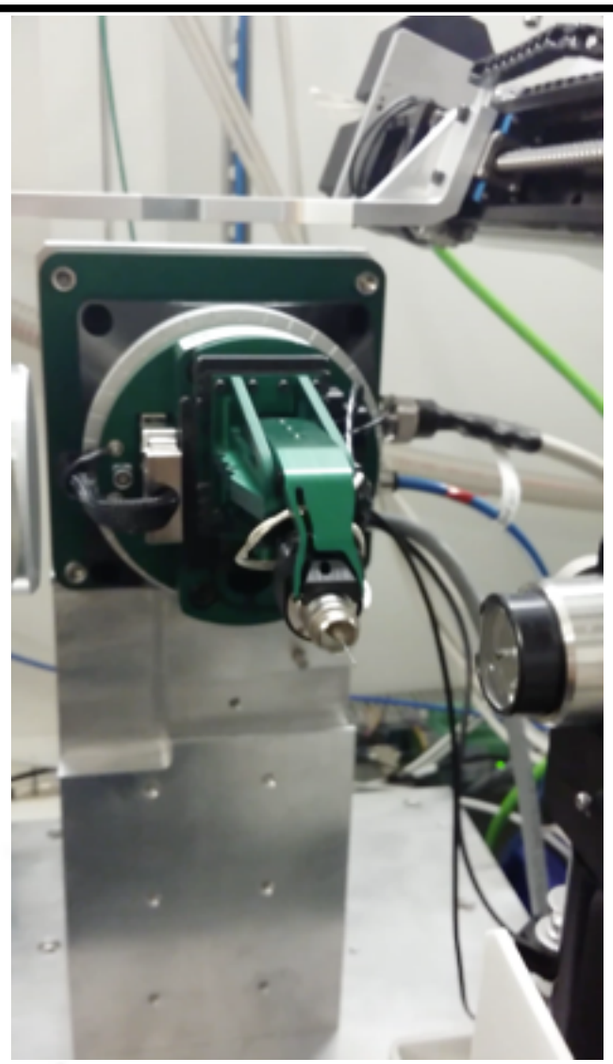

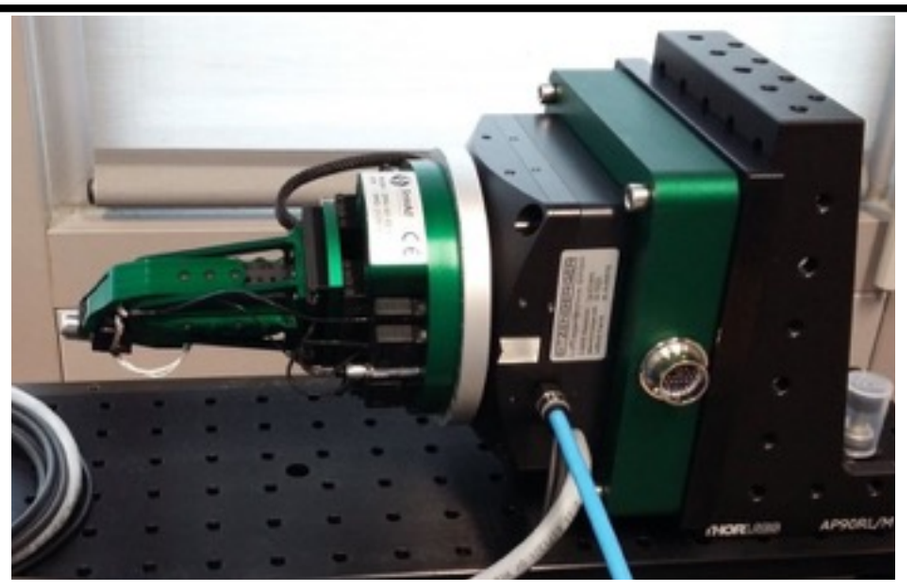

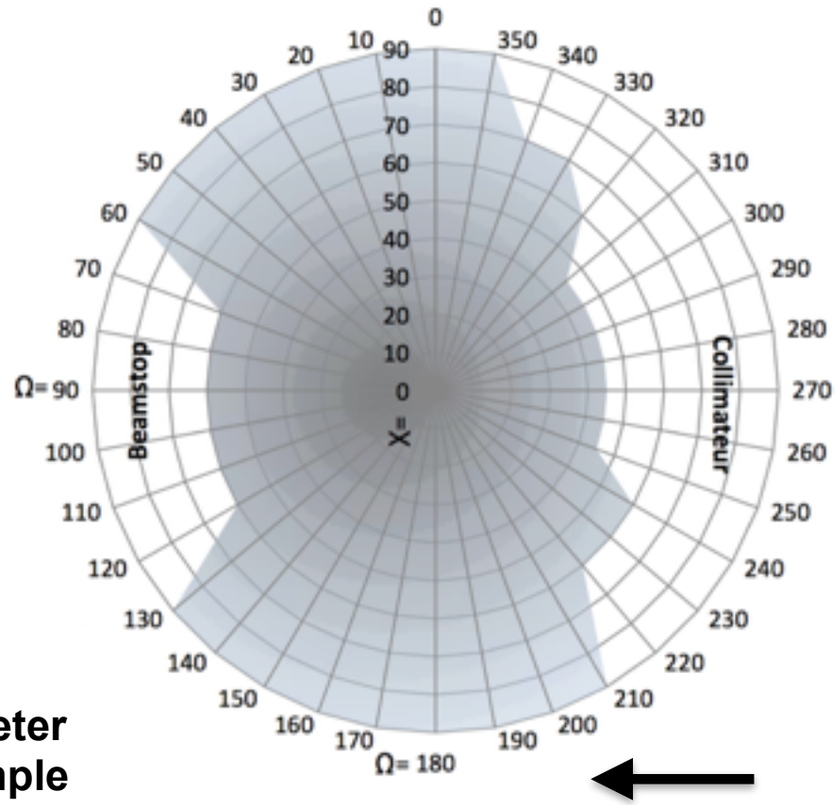

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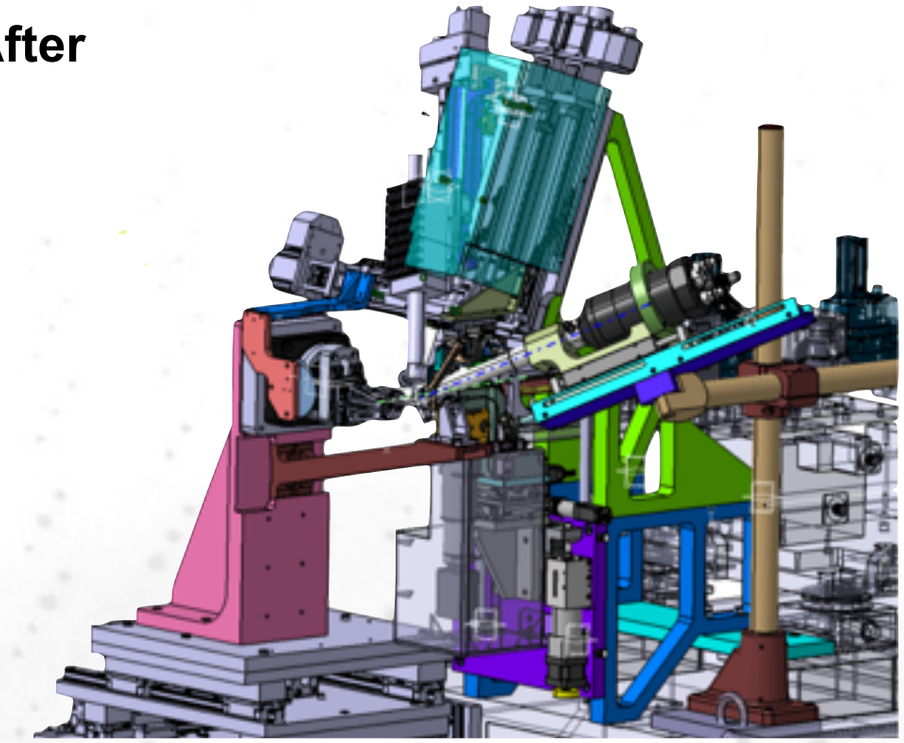
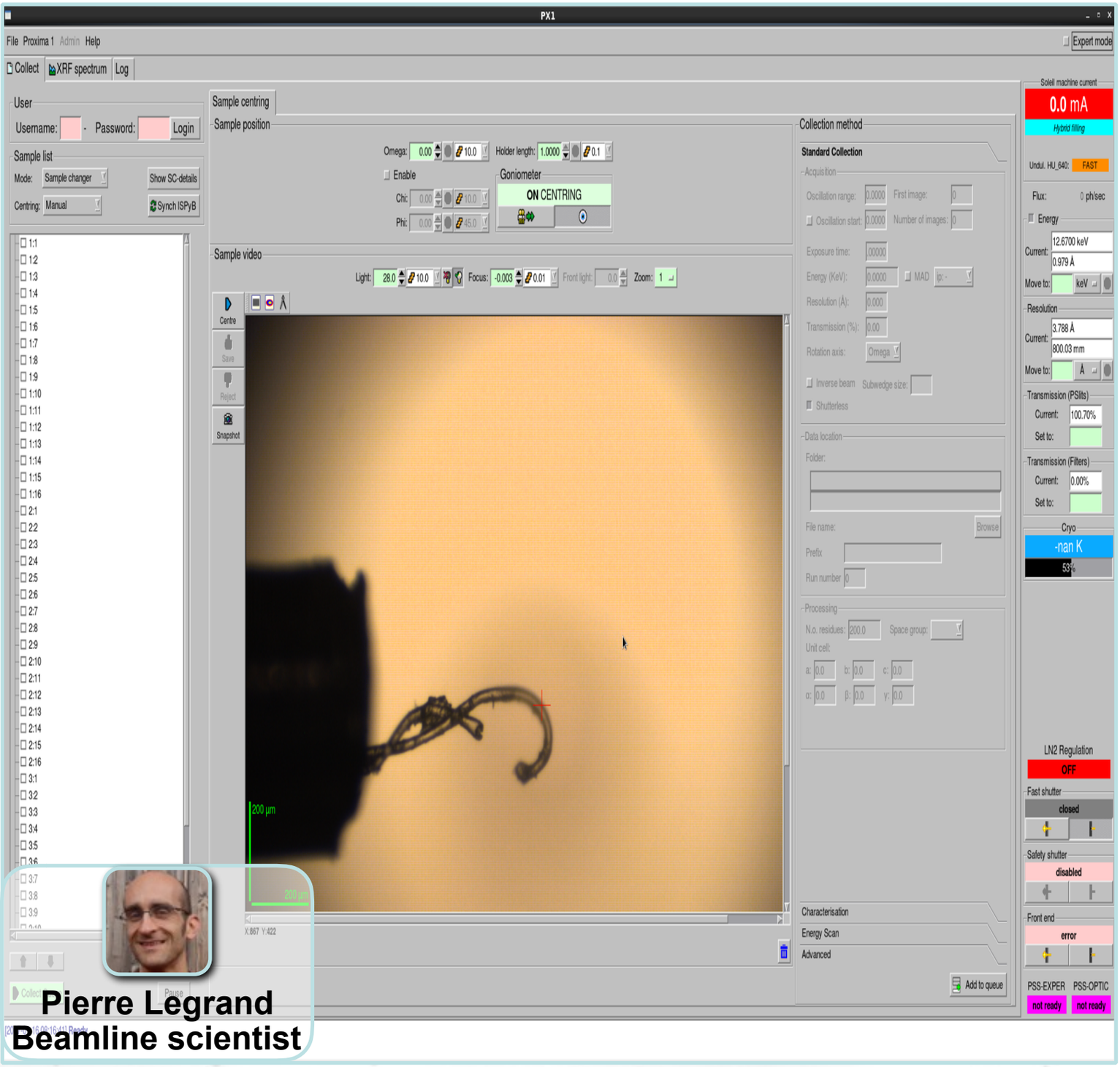


Sphere of possible goniometer movements around the sample position

Beam direction

SmarGon devices and MxCuBE setup



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Beamline scientist

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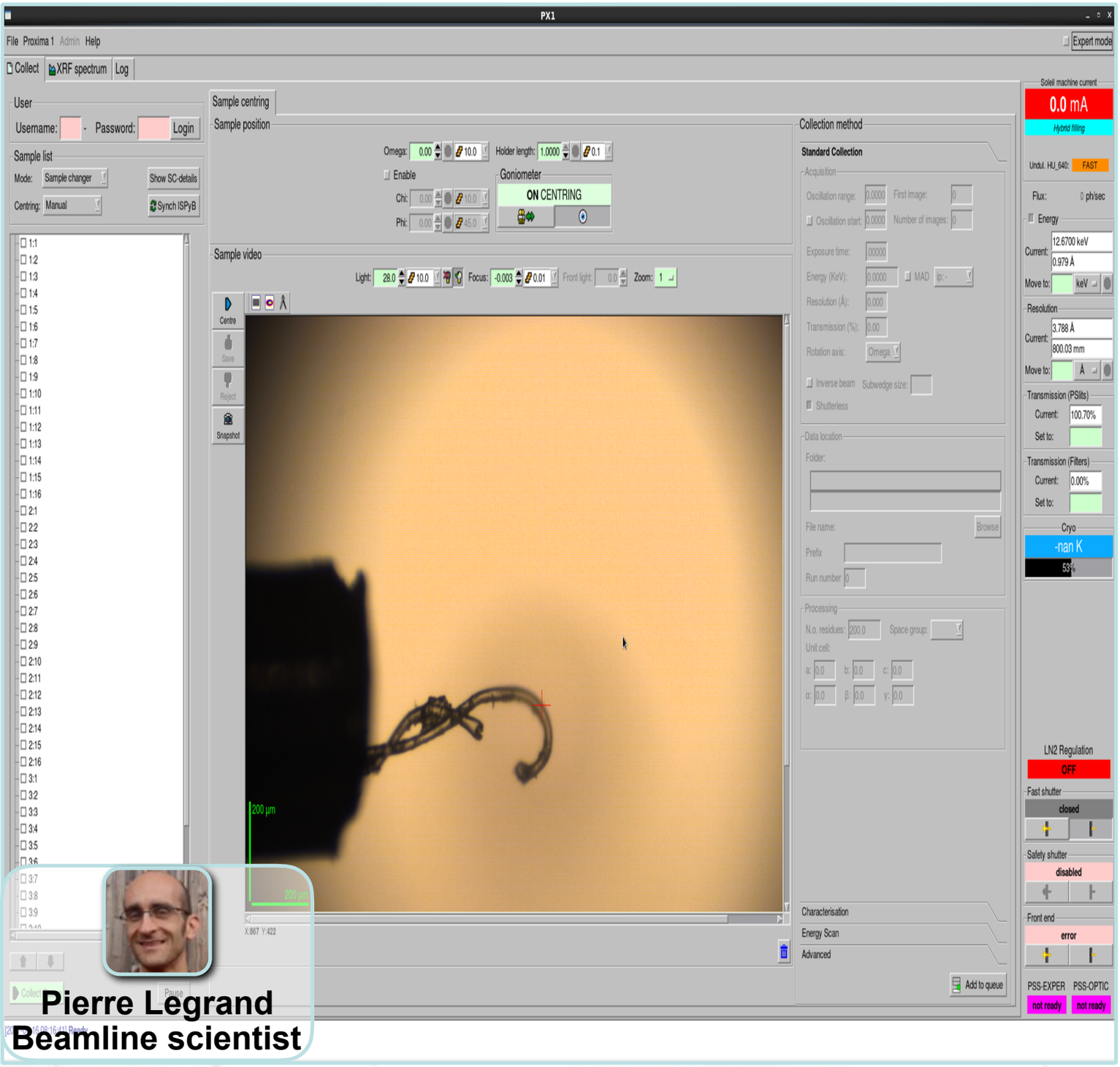

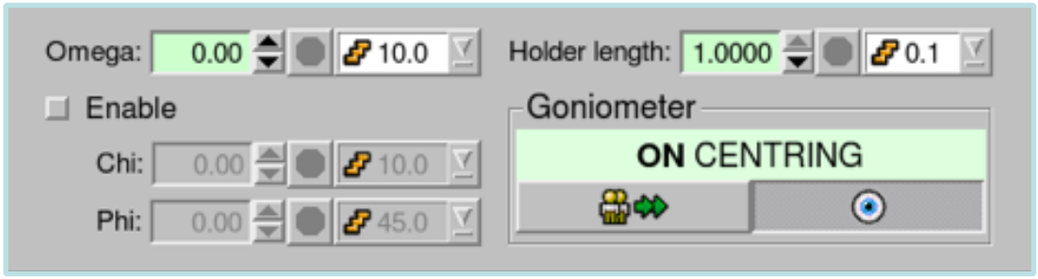

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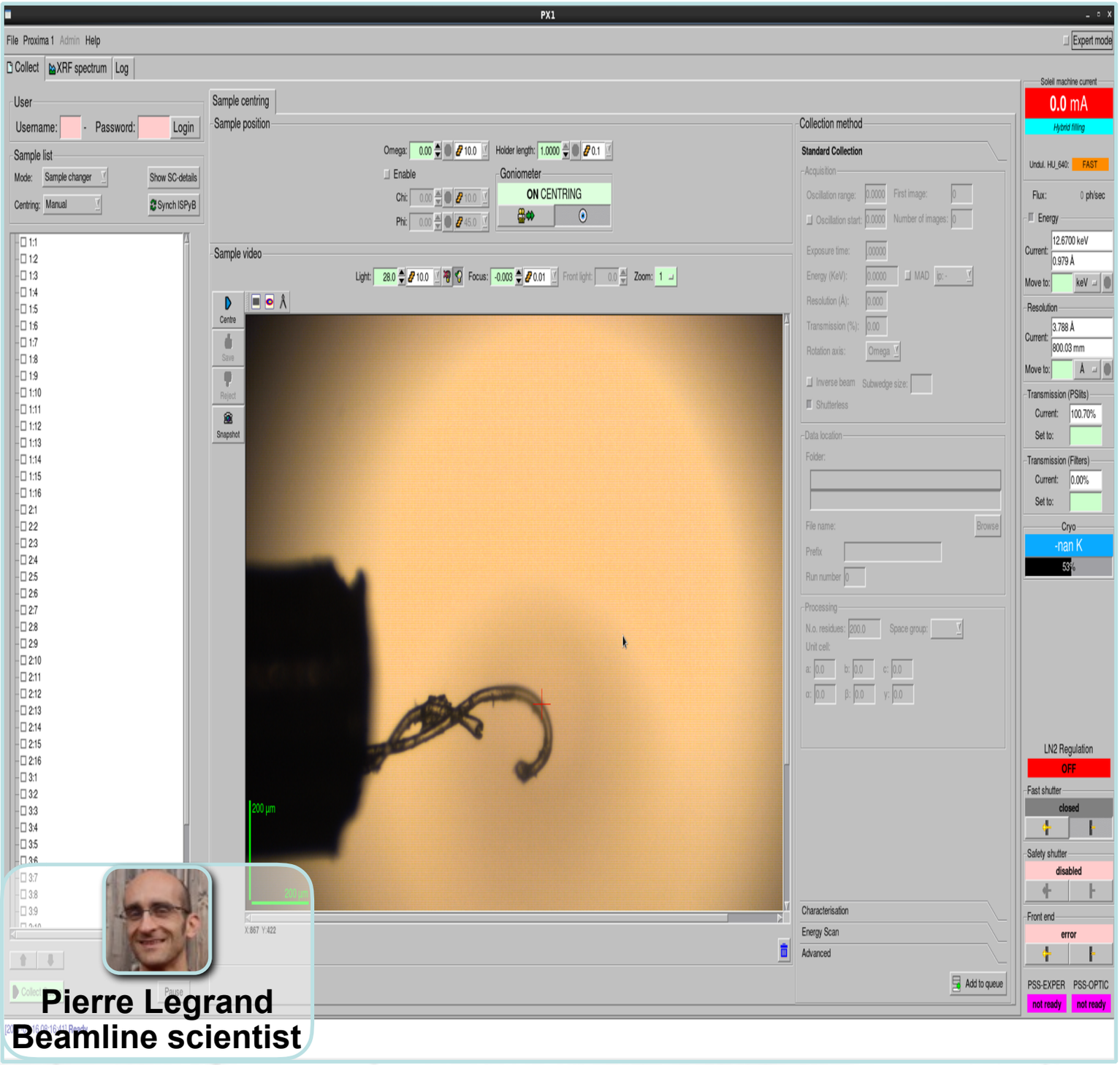

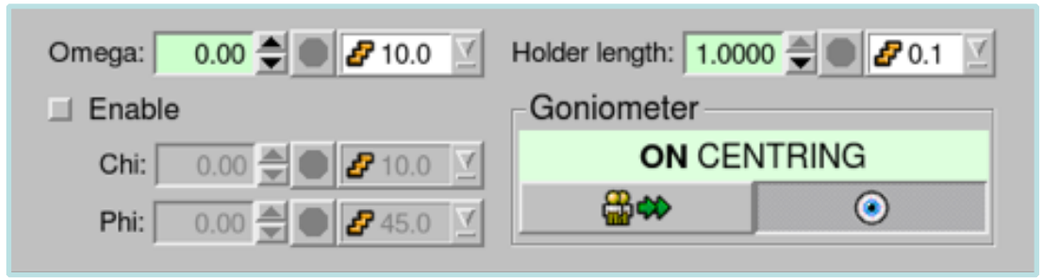

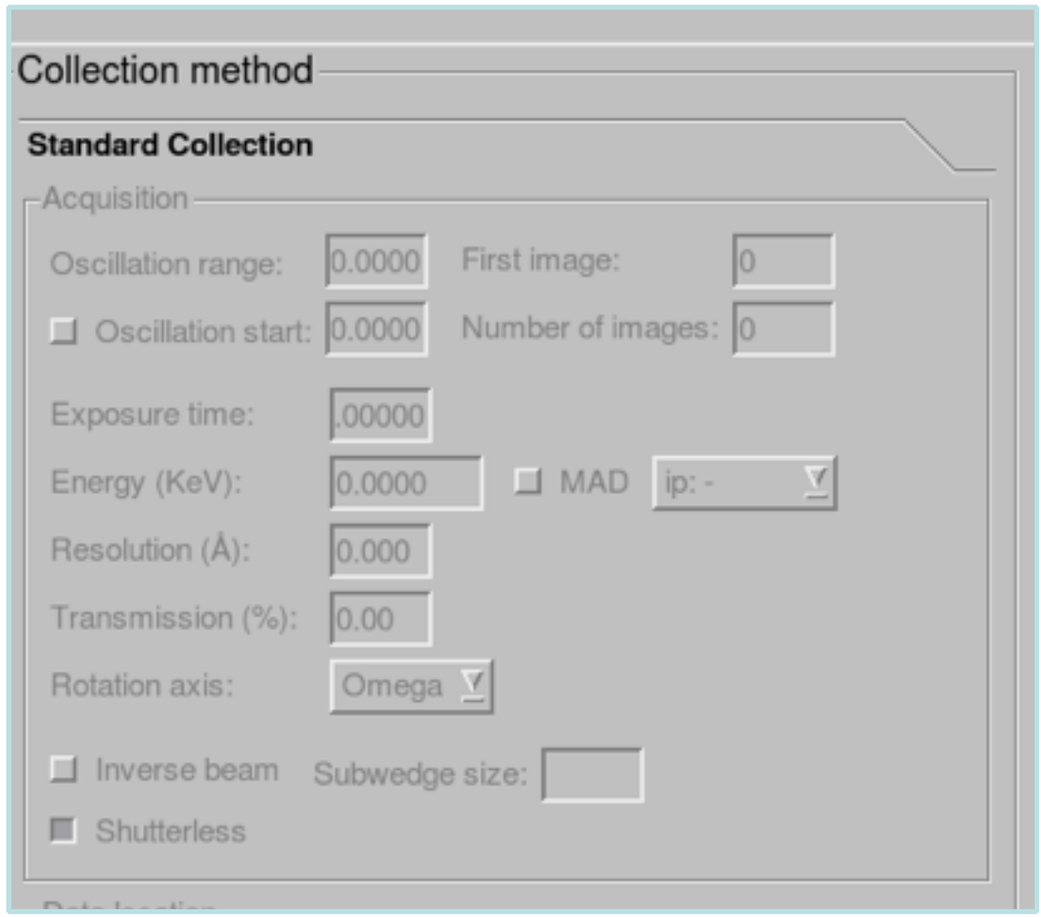

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QT4: MIGRATION STATUS

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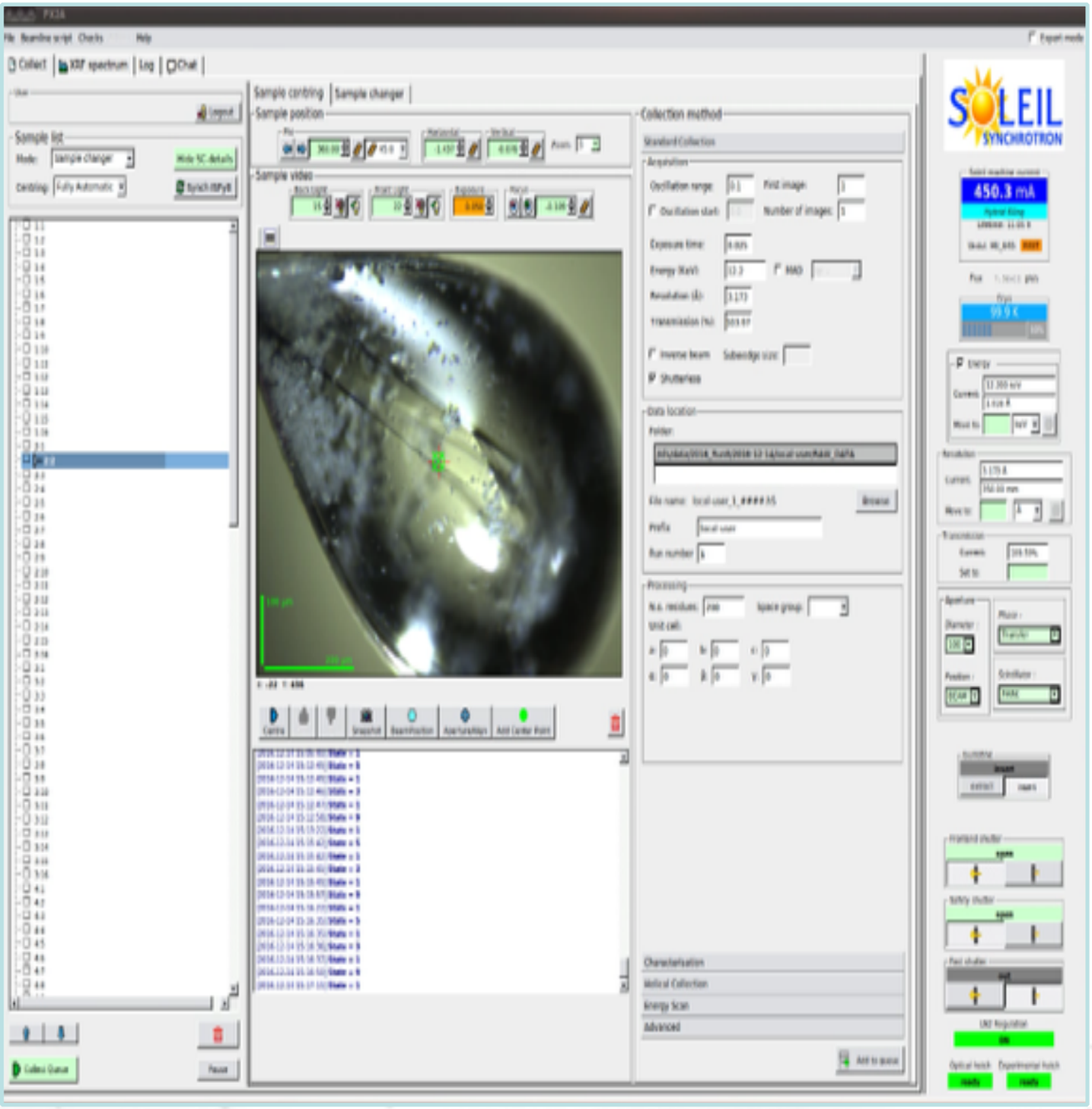

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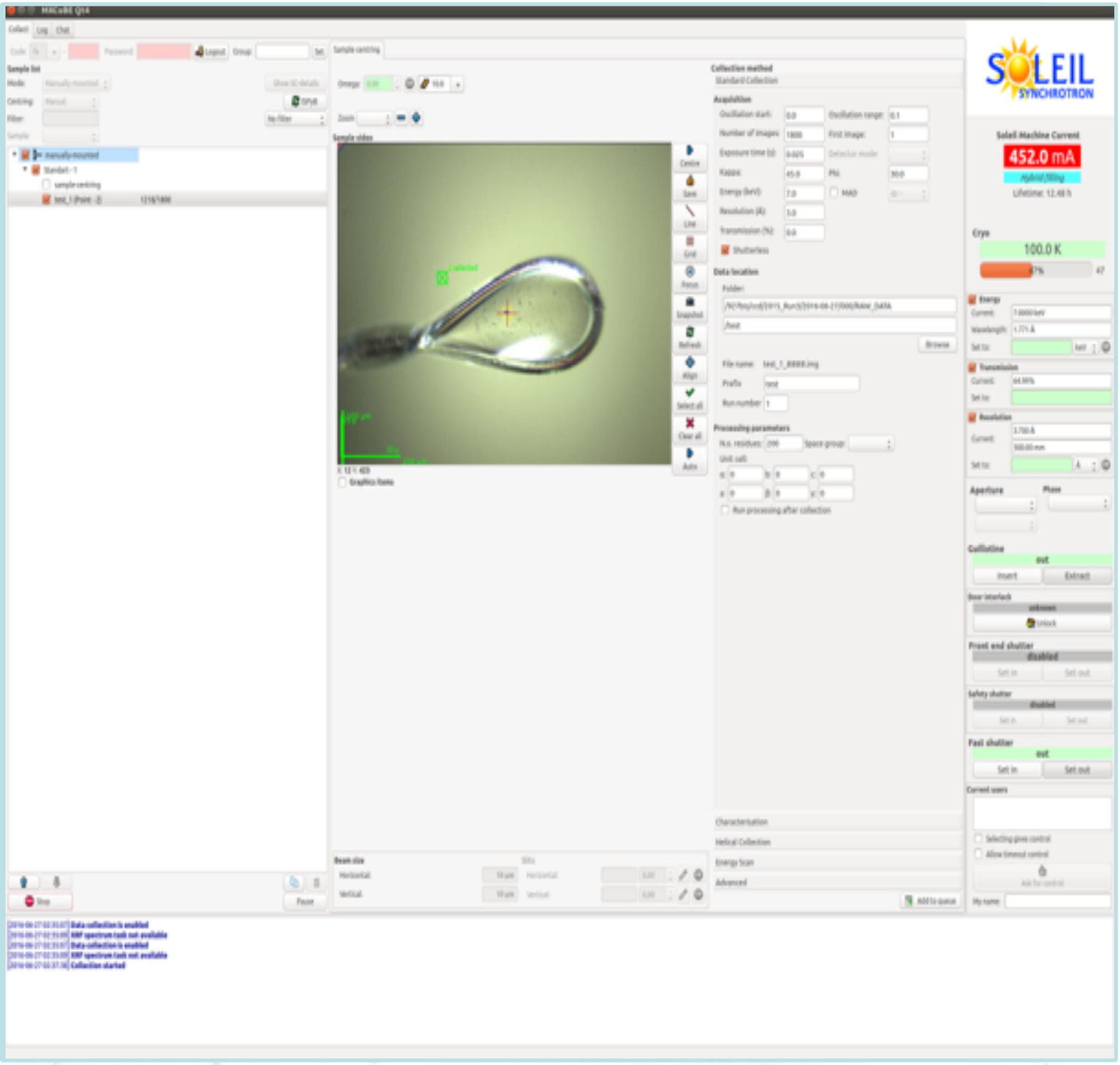

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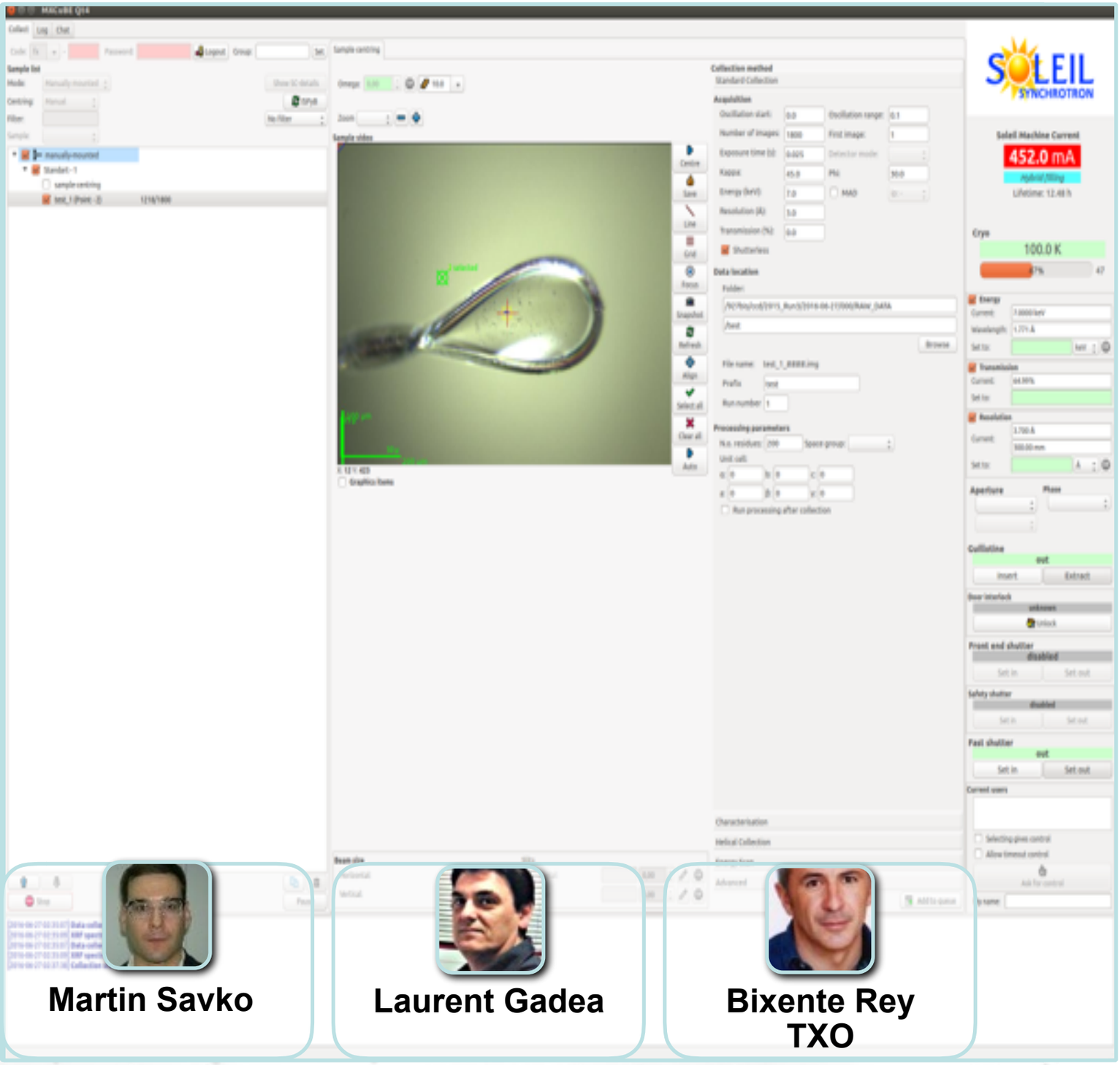

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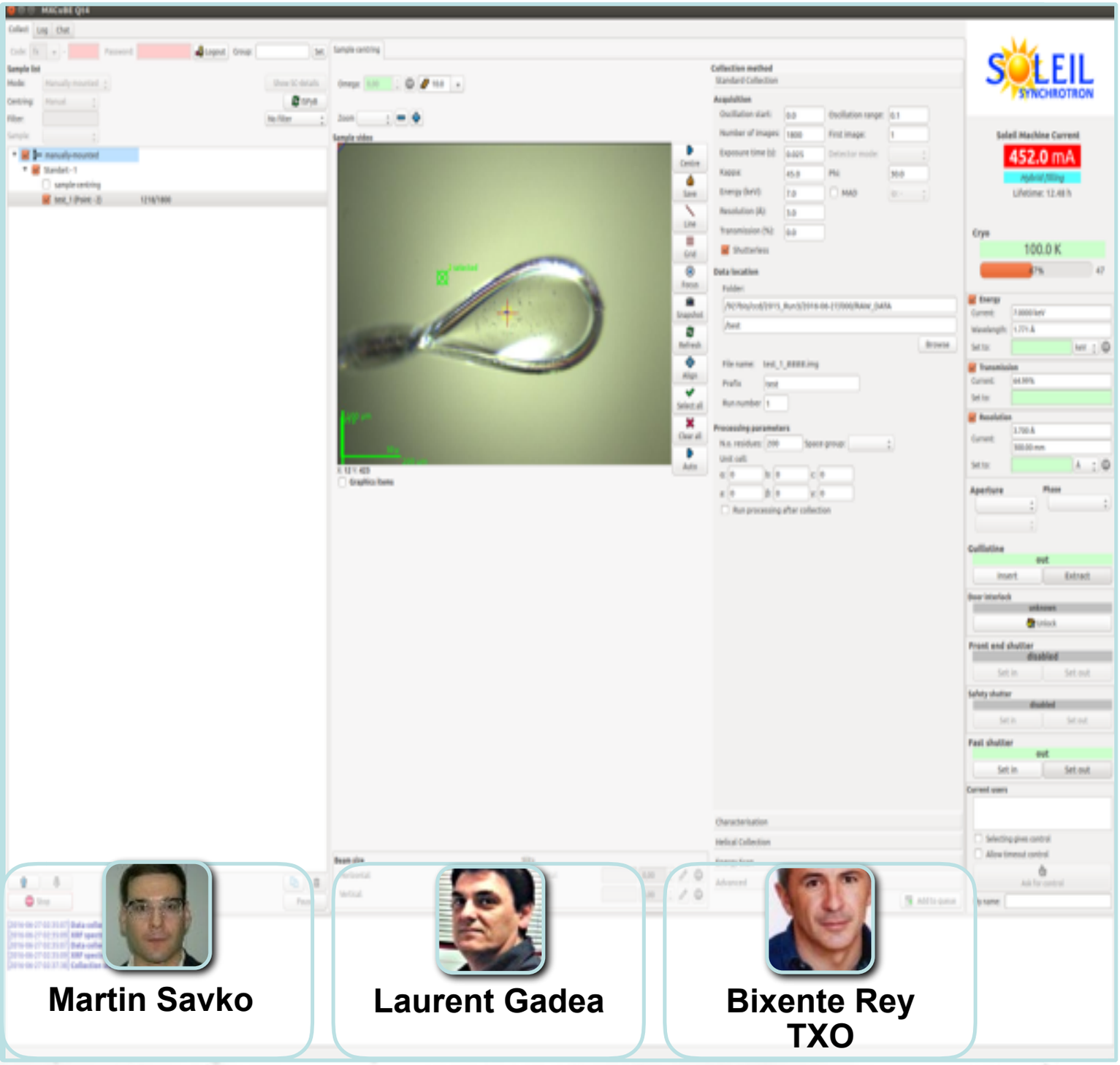

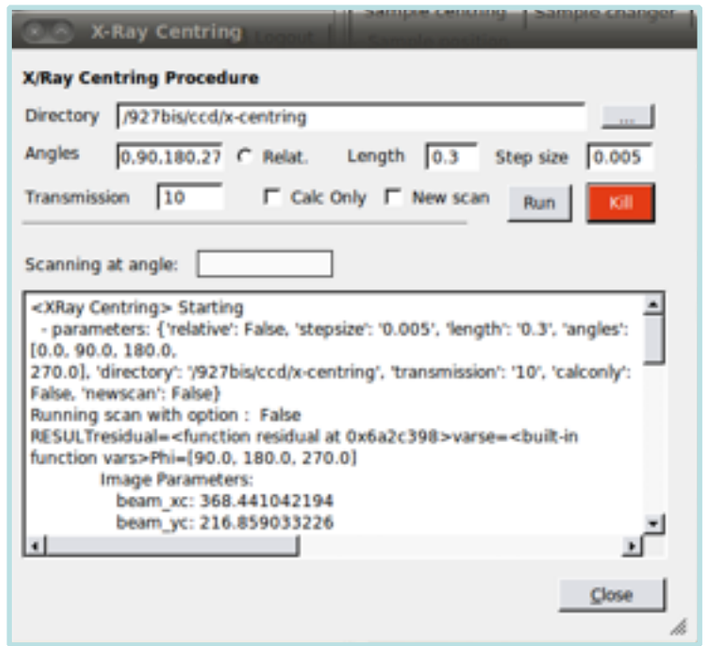

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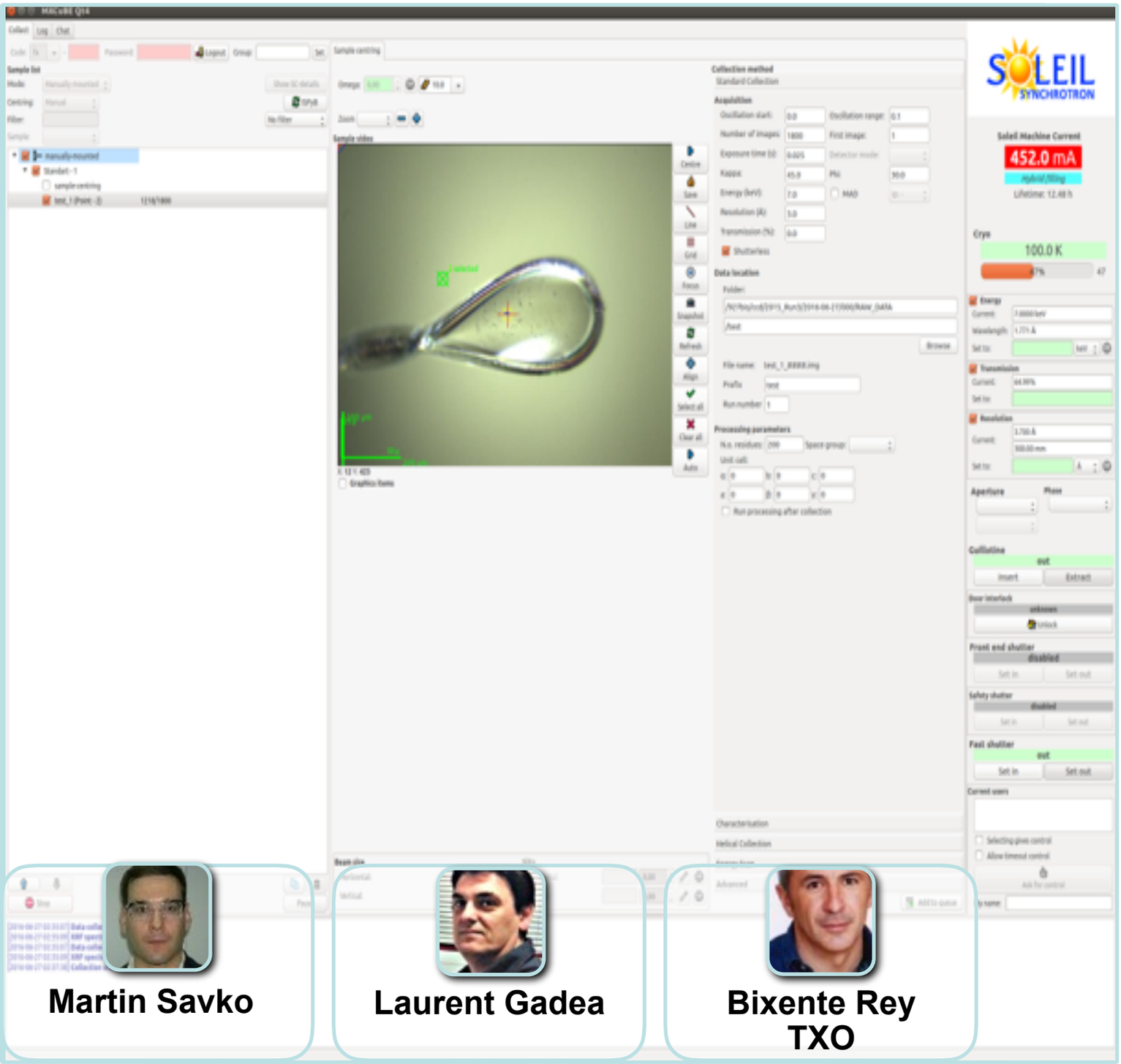

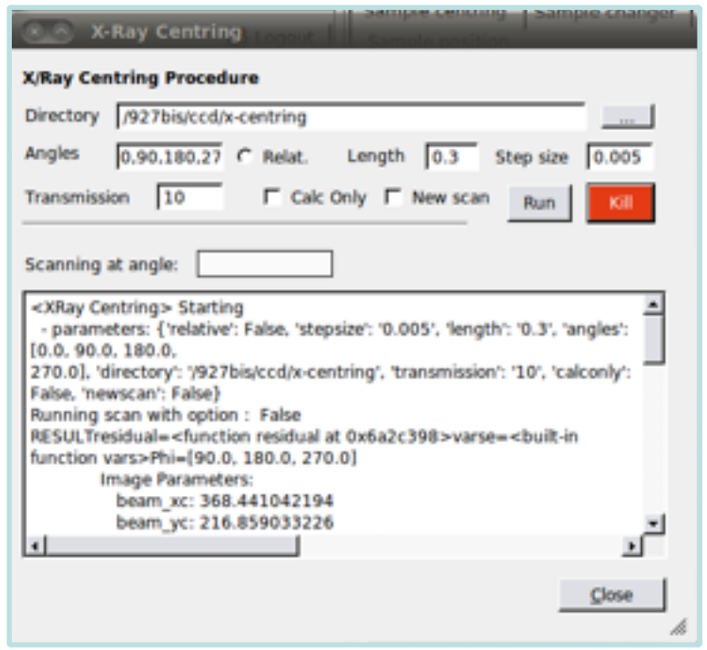

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TXO

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**

REMOTE ACCESS AT SOLEIL

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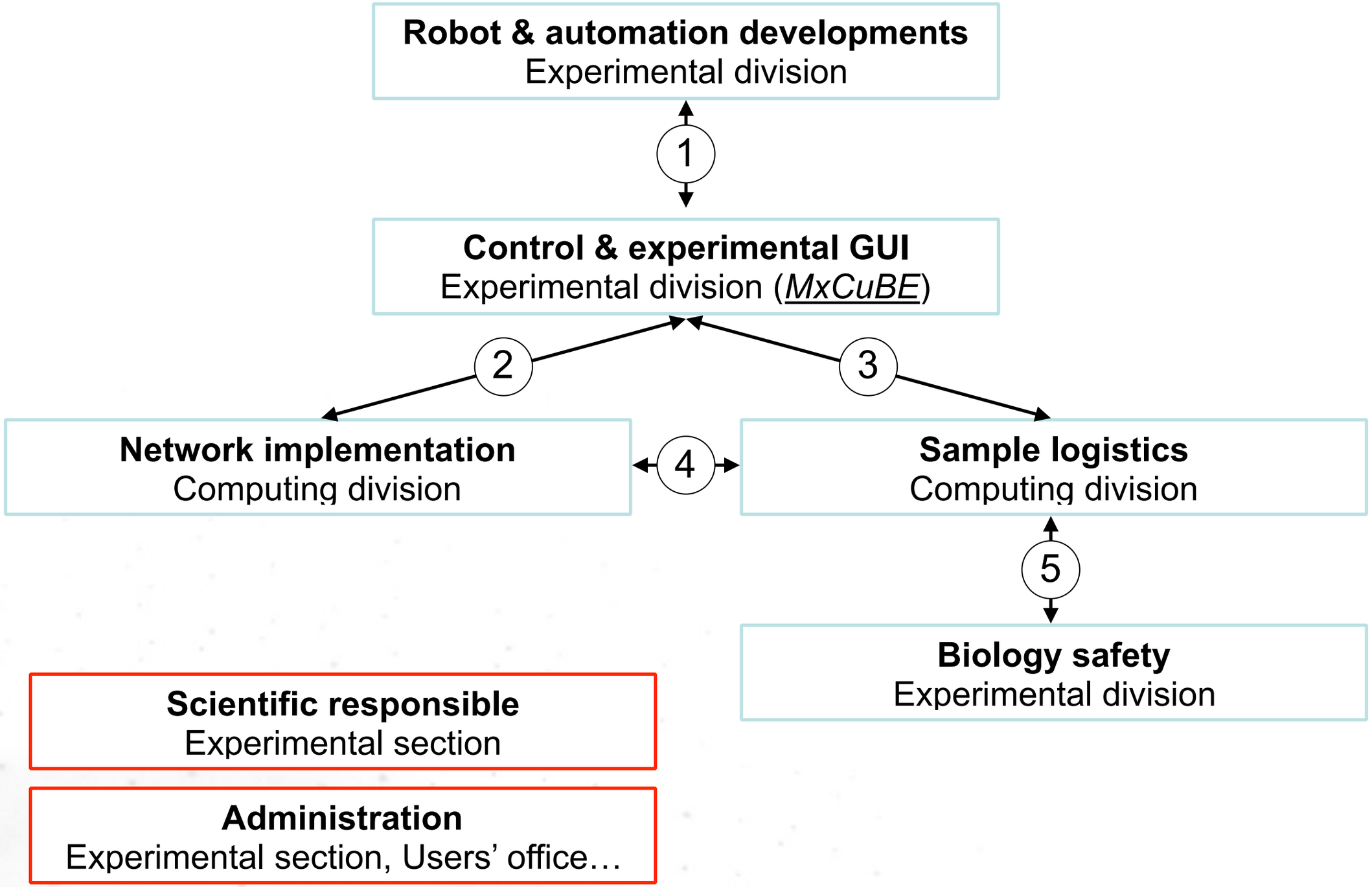

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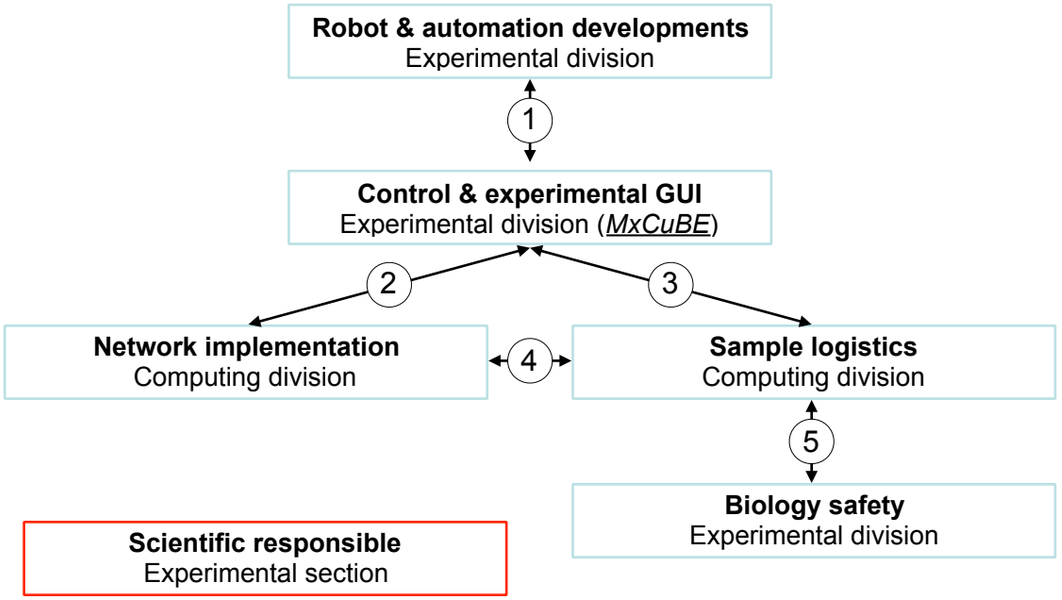


REMOTE ACCESS AT SOLEIL

Robot & automation
Experimental

1

Control & experi
Experimental divisi

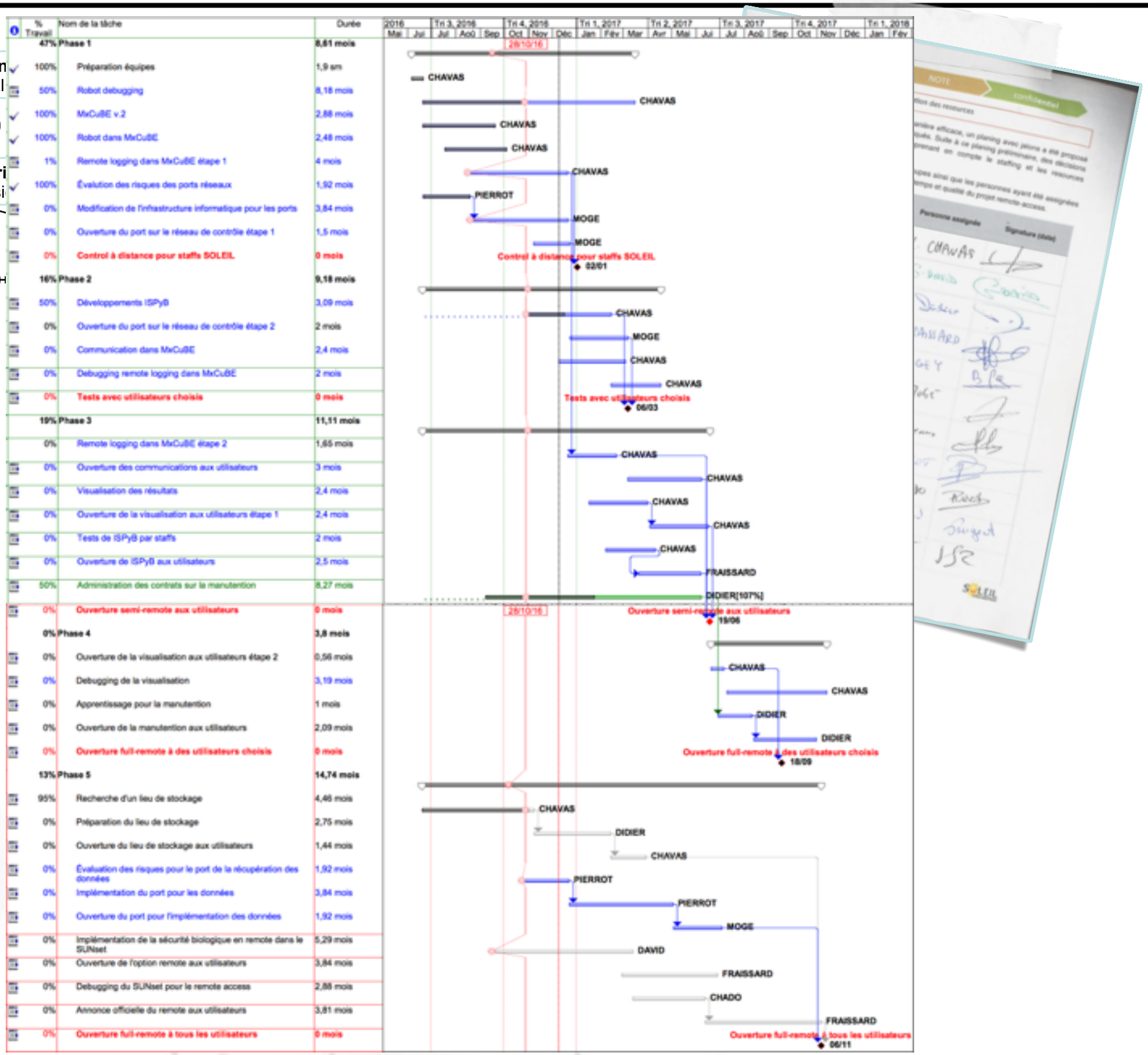
2

Network implementation
Computing division

4

Scientific responsible
Experimental section

Administration
Experimental section, Users' office…



REMOTE ACCESS AT SOLEIL

Robot & automation developments
Experimental division

1

Control & experimental GUI
Experimental division (*MxCuBE*)

SOLEIL SYNCHROTRON

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

- Home
- Proposal Management
  - Proposal Application
  - Management Before experiment
  - Management After experiment
- Experiment data
  - SOLEIL Data Retrieval
- Personal Management
  - Personal Information
  - Umbrella Information
  - Change password
- Other functions
- LogOff

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

Management After experiment
Management proposal after the experiment

Experiment data

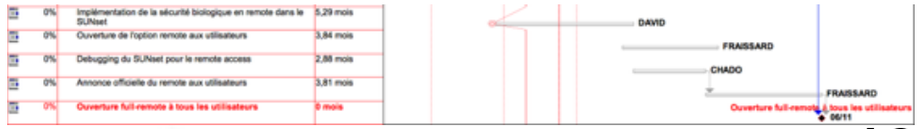
SOLEIL Data Retrieval
Consultation project experiment files (to see downloaded files you will need to download the databrowser from the help button)

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.

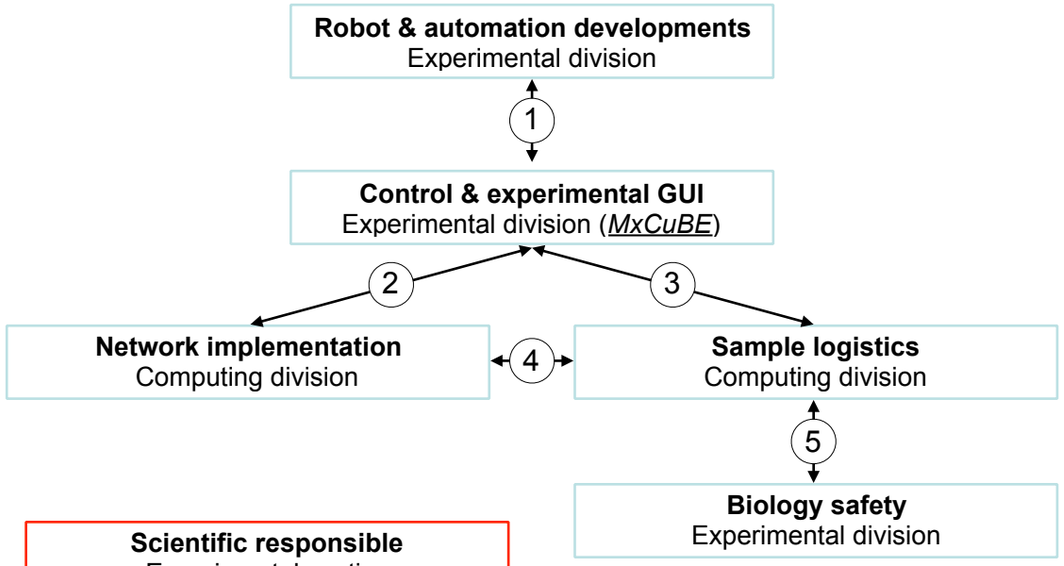
Umbrella Information
Click here to create an Umbrella account or to link it to your SUN set account if you were logged in through Umbrella.

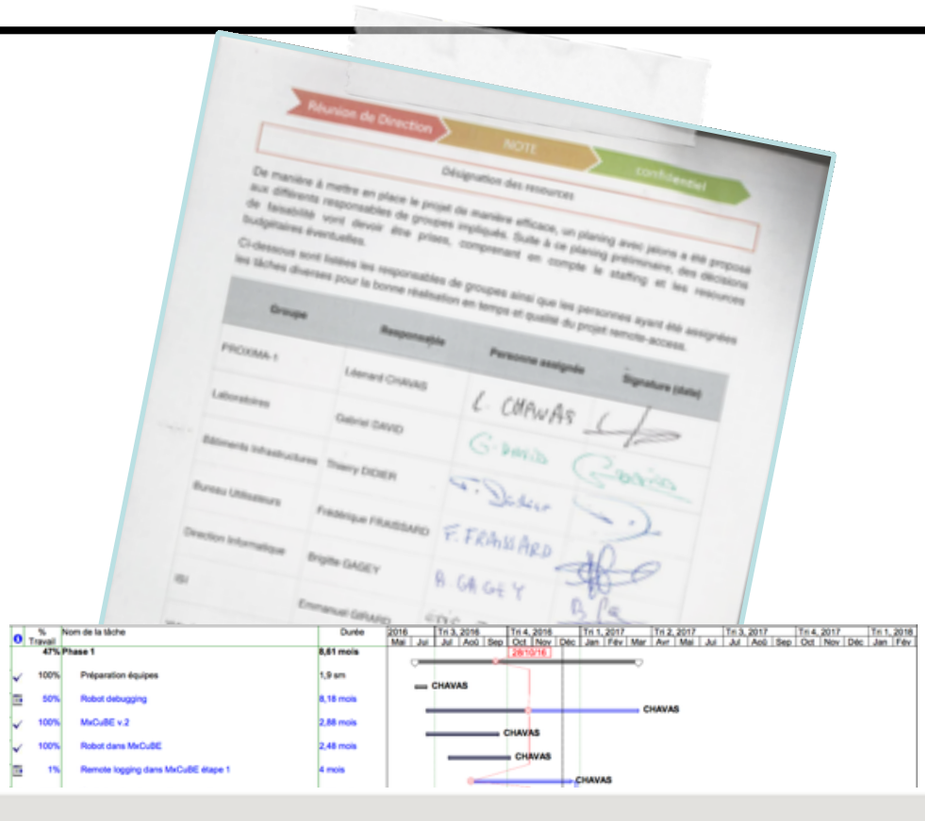
Change password
Click here to change your password. You will be asked for the current one for confirmation.



SOLEIL SYNCHROTRON

REMOTE ACCESS AT SOLEIL





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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	Compartimentation 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

REMOTE ACCESS AT SOLEIL

Robot & automation developments
Experimental division

1

Control & experimental GUI
Experimental division (*MxCuBE*)

2 3

Network implementation
Computing division

4

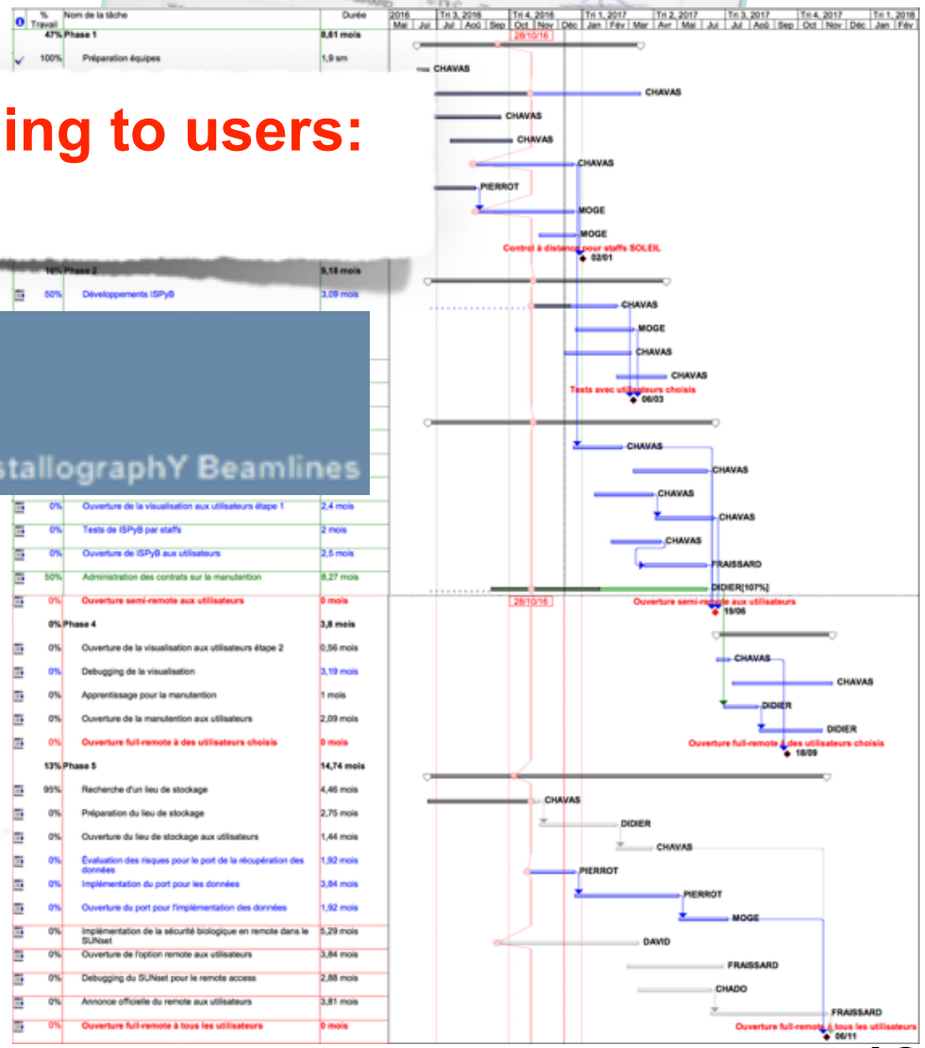
Sample logistics
Computing division

5

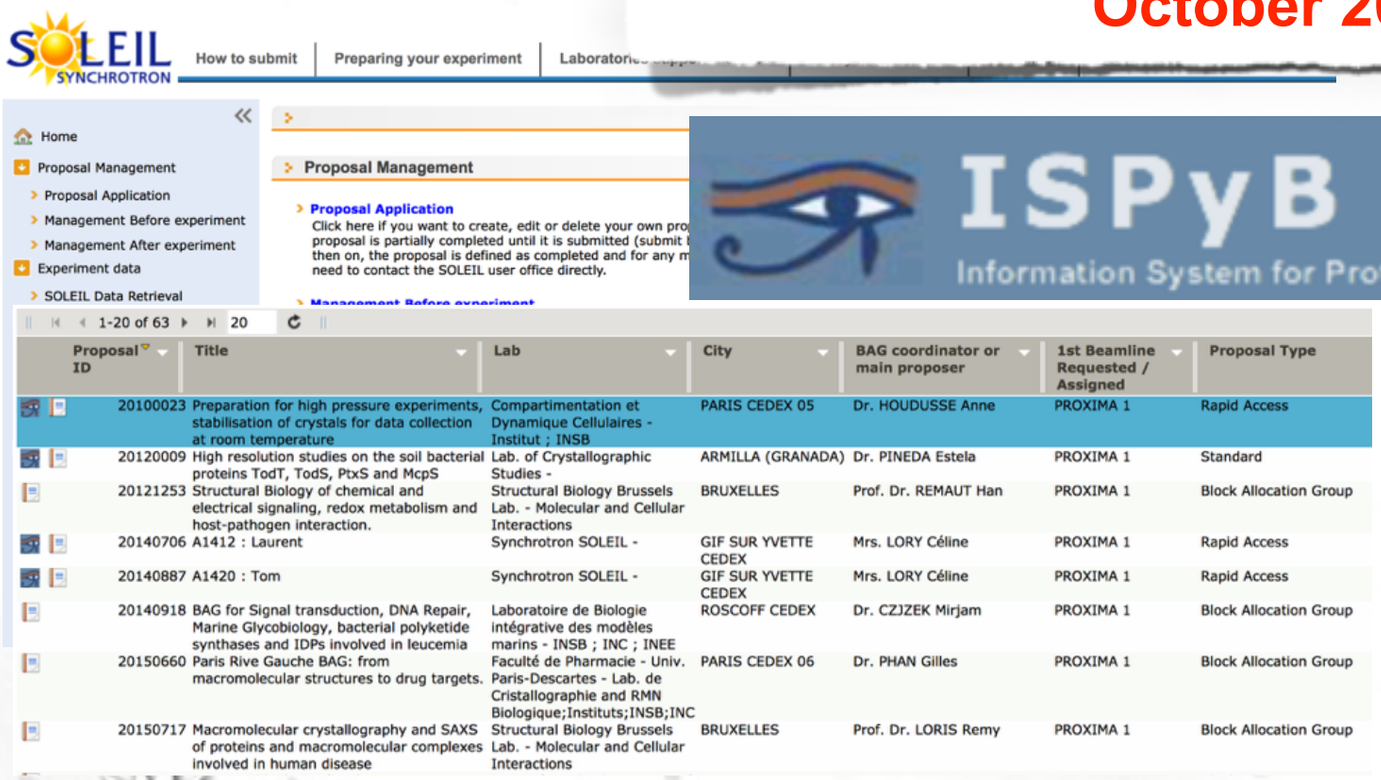
Biology safety
Experimental division

Scientific responsible
Experimental section

Administration
Experimental section, Users' office…

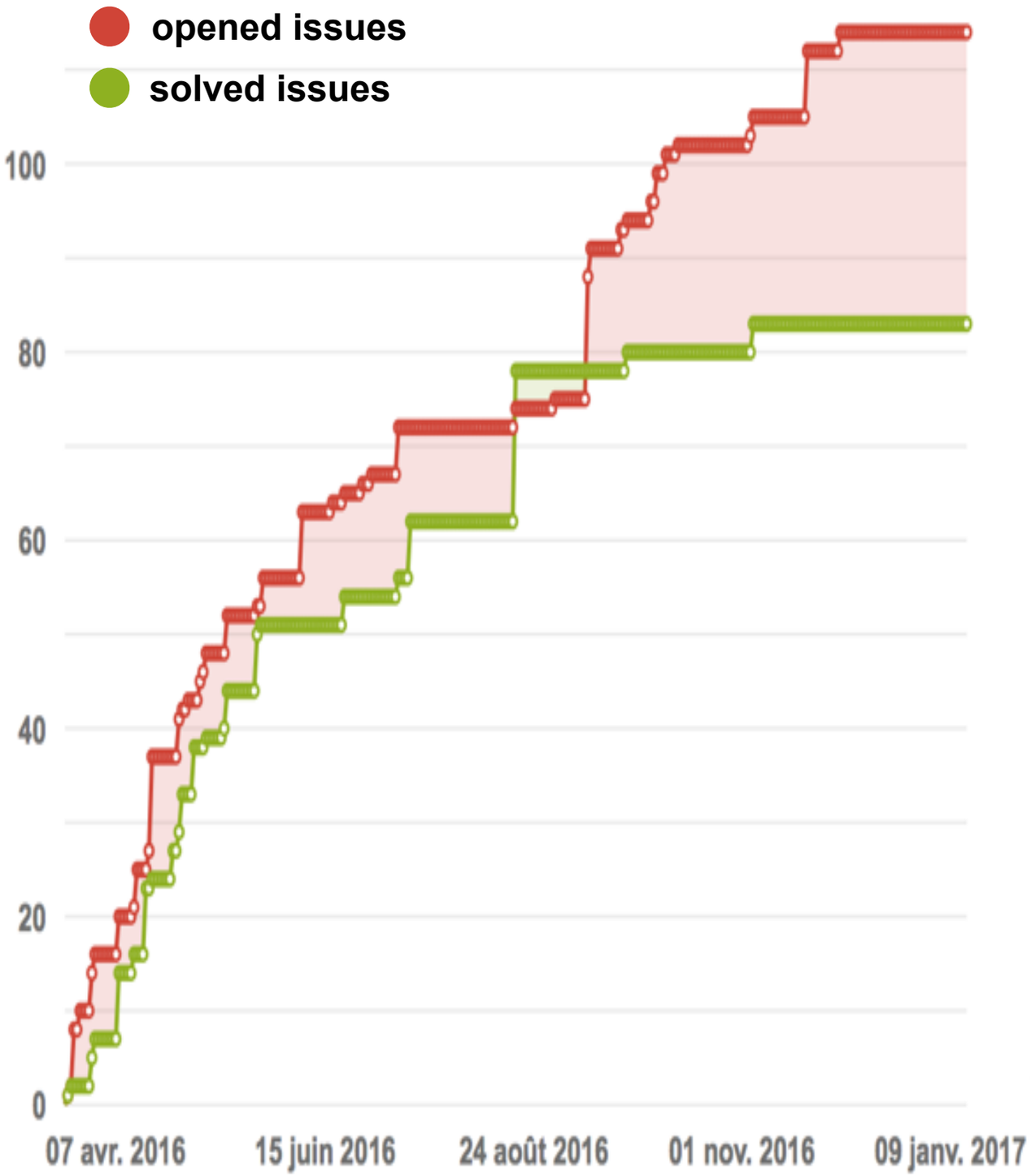


Proposed schedule for opening to users: October 2017

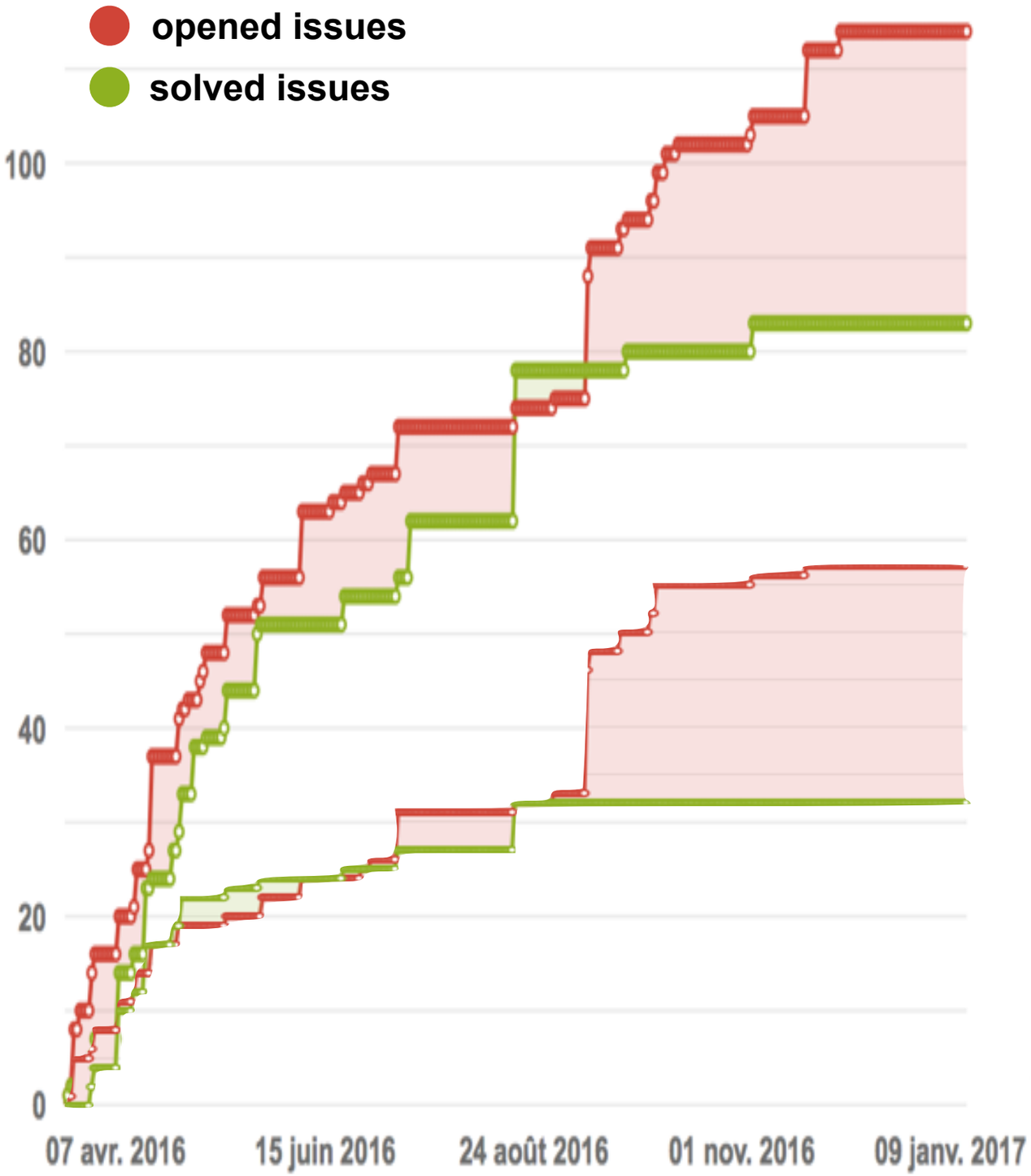


ISPyB
Information System for Protein crystallographY Beamlines

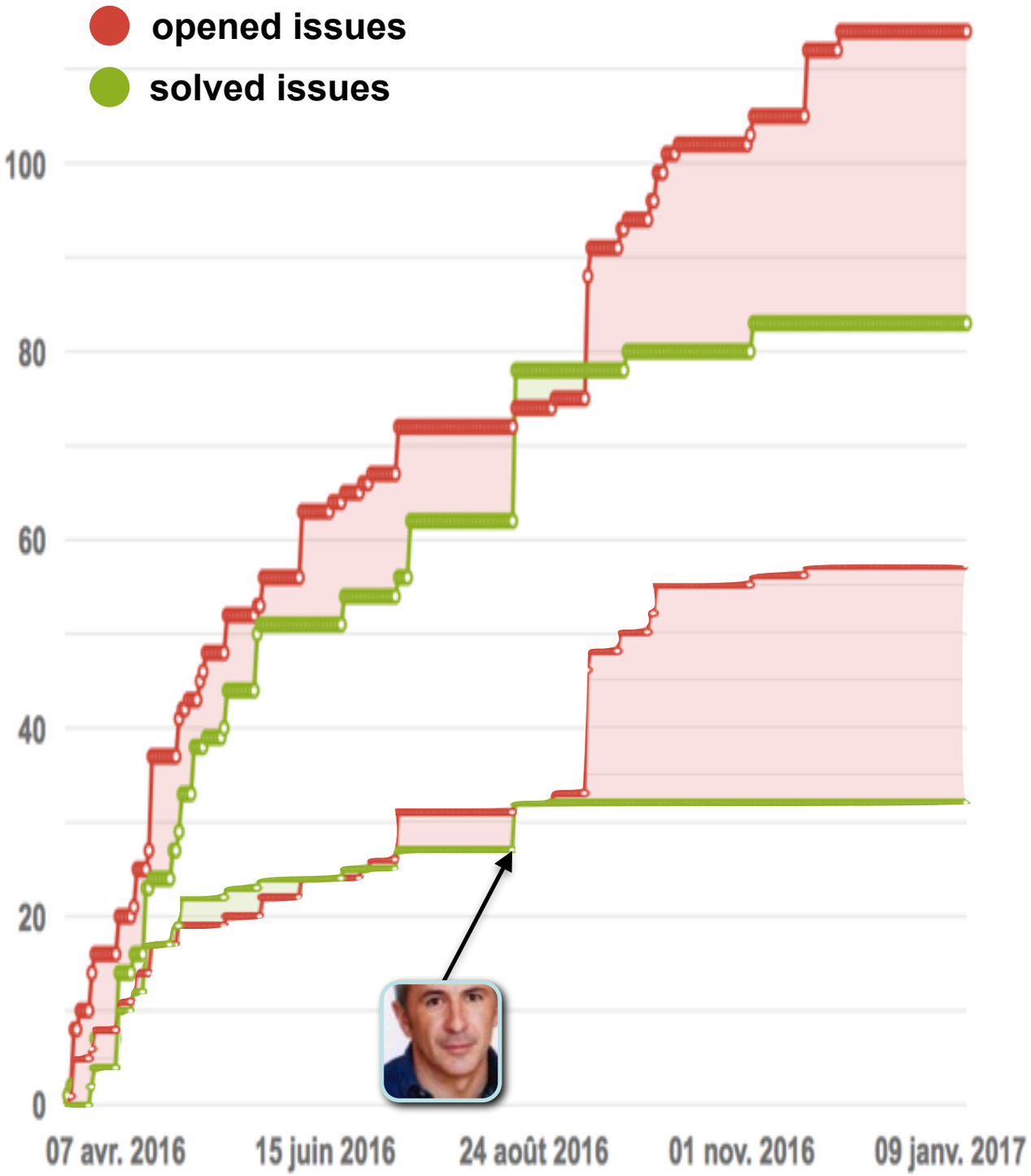
Evolution of Bug-fixes (PX1 only)



Evolution of Bug-fixes (PX1 only)



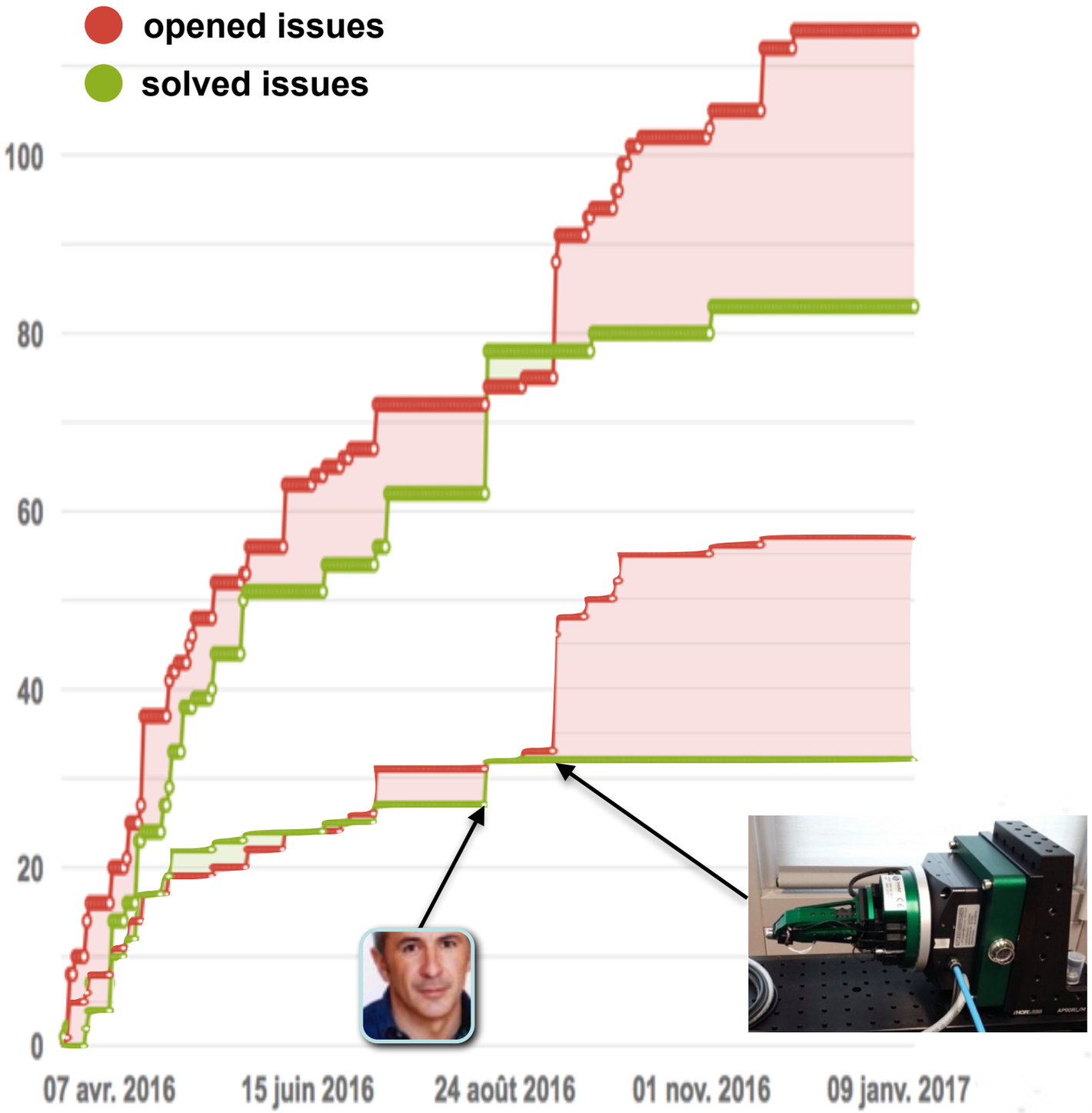
Evolution of Bug-fixes (PX1 only)



first series of issues related to:

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

Evolution of Bug-fixes (PX1 only)



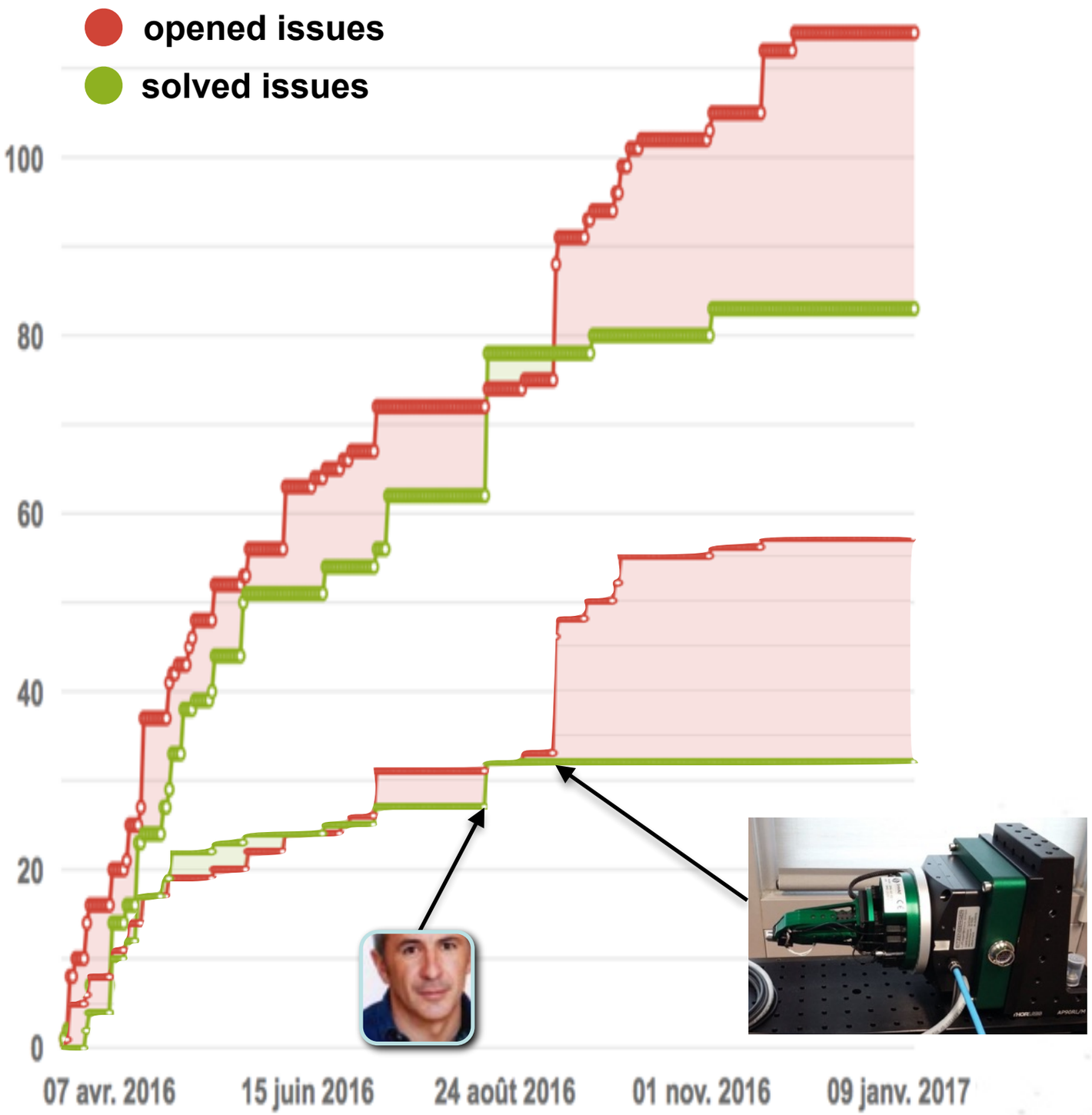
first series of issues related to:

- 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

Evolution of Bug-fixes (PX1 only)



first series of issues related to:

- robot operation 'smoothing'
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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

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

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Beamline manager

Damien Jeangerard
Assistant engineer

Pierre Legrand
Beamline scientist

Serena Sirigu
Beamline scientist

Tatiana Isabet
Responsible industry

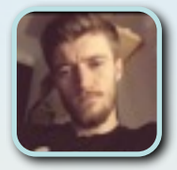
Gavin Fox
Beamline scientist

Martin Savko
Beamline scientist

Tiphaine Huet
Post-doctoral fellow

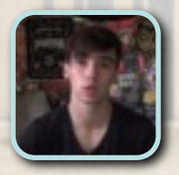
Pierre Montaville
Post-doctoral fellow

Igor Chaussavoine
PhD student



Adam Simpkin
PhD student

Enrico Stura
Associate scientist



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Apprenti

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James Torpey Nicolas Richet
Denis Duran **Laurent Gadea**