



Joint Meeting  
Trieste 2018



ISPyB

# MXCuBE3 – Installation and User Experience

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- ✓ MXCuBE3 installation started in late August 2017 (almost no scientific activity during holidays around here...)
- ✓ Step by step:
  1. Installed a CentOS7 x64 virtual machine (with Tango)
  2. Downloaded MXCuBE3 from GitHub repository
  3. Followed “Installation and testing” instructions (GitHub wiki)
  4. It did not work: installed missing python packages
  5. mxcube3-server started !
  6. Strong help needed for the npm part (thanks Emiliano)
  7. MXCuBE3 login page works... and now?



# MXCuBE3@ELETTRA customization

```

google.com/search?client=ubuntu&hs=z116&channel=ts6el
x  _  Open  [?]  MxCube3_install_CentOS7_x64.log
/home/porro/mxcube3

===== MxCube3 INSTALLATION on CentOS7 x64 =====
as root on porro
sudo yum install epel-release
sudo yum install -y gcc
sudo yum install -y gcc-c++ make
sudo yum install git
sudo yum install redis
sudo yum install python-pip
cd /opt
git clone https://github.com/mxcube/mxcube3.git --recursive
cd /opt/mxcube3
sudo pip install -r requirements.txt
sudo pip install event==1.1.2 redis flask flask-socketio==2.8 Flask-Session
sudo pip install mock pydispatch PyDispatcher
sudo pip install numpy pillow v4l2 jsonpickle
curl -sL https://rpm.nodesource.com/setup_8.x | sudo -E bash -
sudo yum install -y nodejs
ln -s /opt/mxcube3/mxcube3/HardwareRepository/HardwareObjects/ mxcube3/
python setup.py build
sudo python setup.py install
===== MxCube3 STARTUP SERVER =====
redis-server &
(Note per monitorare l'attivita' di redis: 'redis-cli monitor')
Copio la directory di default test in ELETTRA
cp -r test ELETTRA
Questi due comandi di esecuzione lavorano in maniera diversa a seconda di come e' stata installata la libreria mxcube3
./mxcube3-server -r ELETTRA/HardwareObjects/Mockup.xml --log-file mxcube3.log
mxcube3-server -r ELETTRA/HardwareObjects/Mockup.xml --log-file mxcube3.log

Note:
Sembra che tutti i files in ELETTRA/HardwareObjects/Mockup.xml vengono caricati ed i relativi HardwareObjects sono di default in ./
HardwareRepository. Ci sono delle API particolari nell'HardwareObject per leggere la configurazione dal relativo XML, ad esempio:
- self.getProperty("image name")
oppure per postare un log message:
- logging.getLogger("HR").info("initializing camera object")
- se mi collego a localhost:8081 con il browser viene caricato il file ./mxcube3/routes/Main.py

===== MxCube3 STARTUP WEB CLIENT =====
npm install
npm install fabric
npm start
- se mi collego a localhost:8090 con il browser... MAGIA!
- se utilizzo la login 'user' tutto sembra OK ma non appare nulla...
Per capirci qualcosa installo l'ambiente di sviluppo (webpack, babel,...)
sudo npm install webpack-dev-server -g
sudo npm install webpack-dev-server webpack babel-loader babel-plugin-transform-es2015 babel-polyfill

==== Consulenza di Emiliano (sulla macchina virtualBOX) ====
npm lavora con un file di configurazione nella directory corrente che e':
package.json
questo file contiene le dipendenze che devono essere installate ed anche gli scripts a disposizione, ad esempio quando si lancia
'npm start' la keyword 'start' automaticamente viene interpretata come "npm run dev", che a sua volta esegue la keyword custom 'dev'
interpretata come ".".
(Note: Tutte le dipendenze si trovano nella cartella ./node_modules)
webpack-dev-server e' un'applicativo che compila un package JavaScript ed automaticamente implementa un HTML server per esportarlo.
Si basa su un file di configurazione che si chiama ./webpack.config.js. Nel file di configurazione ci sono diverse sezioni: "entry"
definisce il file .js o .jsx che rappresenta la root del progetto, "output" definisce la posizione dell'output della compilazione
del package, "devServer" definisce le caratteristiche per il server HTML.
Teoricamente il comando ./node_modules/.bin/webpack-dev-server dovrebbe compilare e lanciare il server ma in realta' non crea alcun
file di risultato. (da ricerca postuma di Emiliano webpack-dev-server si tiene il bundle in memoria e lo serve al percorso
specificato da publicPath, che attualmente dovrebbe essere una stringa vuota; PublicPath e' relativo al percorso specificato in
contentBase).
Per ottenere il package JavaScript compilato abbiamo dovuto eseguire ./node_modules/.bin/webpack
Per utilizzare il package appena compilato abbiamo dovuto modificare il file webpack.config.js sostituendo:
contentBase: path.join(__dirname, "mxcube3/ui")
Plain Text  Tab Width: 8  Ln 25, Col 35  INS
1. Row 1, Column 21  0.55 / 1.93  9.92 x 5.46

```

## Personal notes for a DIY approach:

- There is not so much documentation for developers
- The analysis of Python console errors is a good starting point for investigating the underlying architecture and object connections
- Use extensively "grep -r": following log messages helps in discovering who is doing what
- The customization process should concern only the XML configuration files and the HardwareObjects, other stuff is part of the 'core'
- An installation log file could be useful
- If you get stuck ask the MXCuBErs, they always help you

## January 2018

### - Login :

- still mockup

### - Data Collection Tab:

- Machine Status (Tango)
- Beamline Valves and shutters (Tango)
- Detector Distance (Tango)
- Beamline Actions
- Energy
- Wavelength
- Resolution
- Transmission
- Cryo
- Flux

### Diffractometer (MD2):

- Motors (Tango)
- Phase Control
- Aperture Control
- Lights (Tango)
- Zoom (Tango)
- Camera: MD2 JPG (Tango)
- 3 Click centering: MD2 command (Tango)
- Automatic centering

### - Sample Changer Tab:

- XRD2 sample changer under development

### - Sample Overview Tab:

- ISPyB, EDNA: not yet installed
- Tab content synchronized with SampleChanger Info
- Standard Data Collection
- Other Data Collection modes

## September 2018

### - Login :

- Rest authentication through ELETTRA VUO

### - Data Collection Tab:

- Machine Status (Tango)
- Beamline Valves and shutters (Tango)
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### - Sample Changer Tab:

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MxCuBE-3 Proposal: IDTEST000 - Mozilla Firefox

MxCuBE-3 Proposal: IDTEST X | annie.heroux@elettra.eu X

localhost:8090/datacollection

MXCuBE 3 | Sample Overview | **Data collection** | Sample Changer | System log | Help | RA | Sign out

Beamline Actions ▾

Energy: 13.4992 keV | Resolution: 1.528 Å | Transmission: 100.000 % | Cryo: 100.02 K  
 Wavelength: 0.9185 Å | Detector: 302.608 mm | Flux: 1331 ph/s

Sample chang: LOADED | Safety Shutter: CLOSED | Fast Shutter: CLOSED | Beamstop: IN | Ring Current: 160.3 mA

Beam size: 100

Omega: 271.18 | 90°

Kappa: -2 | 0.1°

Phi: 55.22 | 0.1°

Y: -1.835 | 0.1 mm

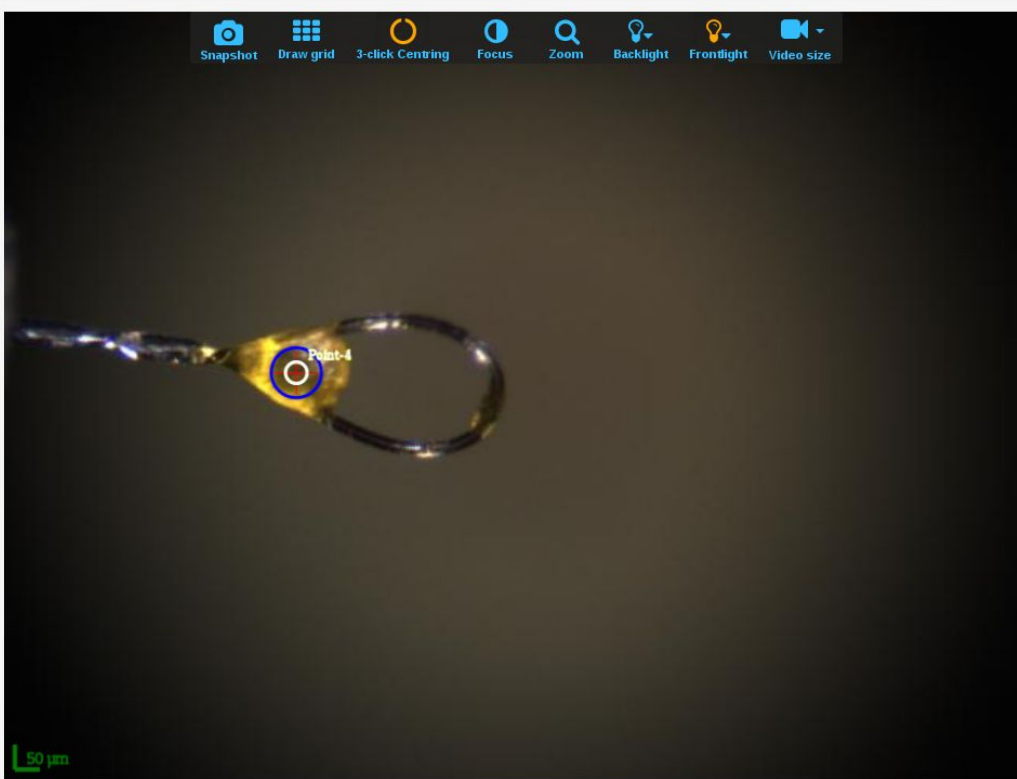
Z: -0.037 | 0.1 mm

Focus: -0.127 | 0.1 mm

Samp-X: 0.606 | 0.1 mm

Samp-Y: 1.216 | 0.1 mm

Snapshot | Draw grid | 3-click Centring | Focus | Zoom | Backlight | Frontlight | Video size



Run Queue | Finish | Settings ▾

Sample: CaBP101 - JNU11 | Queued Samples (0)

Point-1: Data Collection

Path: CaBP101\_1\_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
0.00	1.00	1.000	1	100.00	2.720	13.4991	57.21	-2.00

View Results in ISPyB

Point-1: Data Collection

Path: CaBP101\_2\_####.cbf

Start °	Osc. °	t (ms)	# Img	T (%)	Res. (Å)	E (KeV)	φ °	κ °
90.00	1.00	1.000	1	100.00	2.720	13.4991	57.21	-2.00

View Results in ISPyB

# MXCuBE3@ELETTRA authentication

- ✓ ISPyB not yet available
- ✓ 1<sup>st</sup> stage: the user logs in using a dedicated interface to setup the current investigation (info from the VUO)
- ✓ 2<sup>nd</sup> stage: the user logs in MXCuBE3 and can select only the current investigation



User Login

 Elettra Sincrotrone Trieste

**User Login**

Username

Password

Logged In

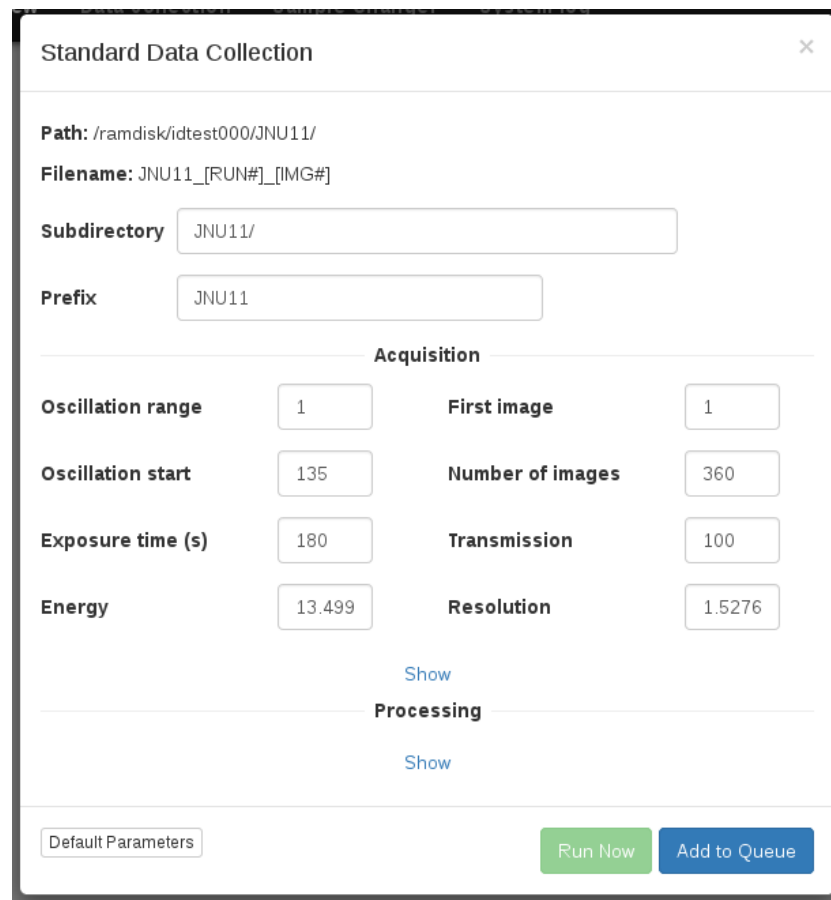
Investigations	
1	1111111
2	20180456
3	20180457
4	20180495
5	20180498

Active Investigation



 MXCuBE 3

- **Filenames:**
  - is it possible to modify current default naming (Sample XX:YY) ?
- **Data Collection:**
  - more info in the web gui (units, params meaning,...)
  - is it possible to modify the right-click menu when a sample is selected? (less options)
  - Is it possible to raise a popup box?
- **3-Click Centering:**
  - is it possible to customize it? (no multiple points)
- **Stop/Abort:**
  - is not clear to us which actions are triggered
- **Final installation:**
  - does exists a standard installation (Linux service?)



Standard Data Collection

Path: /ramdisk/idtest000/JNU11/  
Filename: JNU11\_[RUN#]\_[IMG#]

Subdirectory   
Prefix

**Acquisition**

Oscillation range	<input type="text" value="1"/>	First image	<input type="text" value="1"/>
Oscillation start	<input type="text" value="135"/>	Number of images	<input type="text" value="360"/>
Exposure time (s)	<input type="text" value="180"/>	Transmission	<input type="text" value="100"/>
Energy	<input type="text" value="13.499"/>	Resolution	<input type="text" value="1.5276"/>

[Show](#)

**Processing**

[Show](#)



## Fist external user experience

- ★ Period: 1-3 September 2018
- ✓ Samples mounted using the XRD2 samplechanger (dewar content described by a CSV file)
- ✓ Only standard Data Collection on the samples
- ✓ Data stored and shared on the ELETTRA central storage
- Data analysis pipeline implented manually
- Pilatus communication errors (under investigation)
- Abort actions raised problems with some instrumentation