Automation on FIP: what robots can do for you
Why automation of PX beamline

PX beamlines experiments
- Short (rapid turnover)
- Repetitive (boring...
Automation of local-contact tasks

⇒ Automation of beamline tuning

⇒ Remote control (nxclient)

⇒ Help for data processing

⇒ Virtual local-contact
Automation of the user tasks

What help for users?
Automation of the user tasks: drawback
Specifications

-1- use SPINE standard magnetic tubes, + data-matrix code reading (future)

-2- crystals frozen in LN2, propane, ethane…

-3- up to 40 vials stored (soon: 100) in a Dewar (24 h autonomy, automated refilling),
The choice to carry the cap + vial:

Advantage:
- Safer
- Faster

Drawback:
- Storage capacity
Specialized

EMBL-Grenoble/Maatel

Mar-Research
2/3 axis + translation
4/5 axis

Rigaku / Actor
6 axis
Integrated system

Versatile system:
may be upgraded or adapted

Robot: RX-60L
- 6 axis
- radius: 0.8 m without tool
- accuracy: ± 0.033 mm
- maximum speed: 12.5 m/s

Goniometer head

Robot
Actuator
Storage Dewar
### Sample unmounting

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Action</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Home position</td>
<td>'get sample' command sent</td>
</tr>
<tr>
<td>15</td>
<td>Sample holder covered by the vial</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>Sample holder in the vial back in Dewar</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>End of the trajectory</td>
<td>15 s warming</td>
</tr>
</tbody>
</table>

### Mounting of a new sample

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Action</th>
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<tbody>
<tr>
<td>0</td>
<td>Home position</td>
<td>'put sample' command sent</td>
</tr>
<tr>
<td>15</td>
<td>Sample holder covered by the vial</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>Sample holder in the vial back in Dewar</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>New sample holder mounted</td>
<td>= 25 s between the removal of the first sample holder and the mounting of the new one. The centring of the crystal can begin 40 s after the ‘put sample’ command</td>
</tr>
<tr>
<td>75</td>
<td>End of the trajectory</td>
<td>25 s warming</td>
</tr>
</tbody>
</table>
CATS 2.0 (IRELEC)

IRELEC guarantees a lead time for repairs of less than one week for most critical parts of the robot, grippers and the Dewar instrumentation.

In addition, Staubli® can offer fast and efficient support with business units in 20 countries and a comprehensive distribution network all over the world.

References


IRELEC

Engineering company for scientific and industrial equipment
Offers components and turnkey systems for:
synchrotron beamlines, neutron instruments, particle accelerators, high-voltage equipment, industrial applications
IRELEC is member of the BIB Group - www.groupebib.com

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CATS

Versatile and reliable Sample Changer

- Proven reliability
- High storage capacity
- Automatic Dewar
- Barcode reader
- Compatibility with most magazine and sample holder standards
- Open source programs and high level API for easy integration in control system
- High versatility for extended automation of the experimental station

Based on an industrial 6-axis robotic arm and control system, this sample changer offers an extended versatility, adapted to the various standards and to the forthcoming requirements of X-ray crystallography.

The CATS system is commercialised by IRELEC under CEA-CNRS licence.

CATS - Cryogenic Automated Transfer System - has demonstrated its high reliability and efficiency on the RIP-BM30A beamline at ESRF for more than three years.
CATS 2.0

Since Sept. 2006: 5 systems sold
- SLS, Switzerland (3)
- Bessy, Germany (1)
- Diamond, UK (1)

Options:
- 1 up-side down
- 2 with plate analysis
In situ analysis
The robot as a screening system of crystallization drops

Automated analysis of crystallization plates for challenging projects

(open to industrial users through the ESRF/ICU)

Microfluidic plates

Standard 96-plates
Analysis of crystallization drops

**Aim:**
look for diffraction
discrimination salt/protein
cell parameters, space group, …
data collection
precipitate analysis?

**Means:**
beam: 0.3x0.3 (soon 0.05x0.3) up to 1x1 mm, 0.8 Å
oscillations: 1 deg
10 to 30 sec / drop (1 to 2 h per box)
New services on FIP-BM30A
Protein vs. Salt

Protein crystal

Salt crystal
- screening of crystallization conditions
- precipitate analysis
- native data collection
- looking for derivatives
- screening compounds

Courtesy of I. Margiolaki (ESRF, Grenoble)
New X-Plate (09/2007)

Co-development of a new plate (shape, materials), better regarding:
- geometry (90 deg oscillation range)
- I/s (scattering / 2-3)
Structure of NDK from *A. Polyphaga Mimivirus* (C. Abergel) solved “in the drop”

- space group: p6(3)
- a/b/c: 70.8/70.8/106.3
- resolution: 2.3 Å
- completeness: 80%
- I/σ(I): 3.3
- Rsym: 19.6%
- Rfree: 27.4%

Membrane protein crystals:

- A bacterial pump of the internal membrane (Lab. Prot. Membr. at the IBS)
- detection of crystals
- indexation
Towards 'on chip' diffraction analysis (C. Sauter, Strasbourg)

Data collection (~25°C) on lysozyme
Nb of images 30
Oscillation 1°, 15 sec, 200 mm
Unit cell a=79.1 Å, c=38.8 Å
Space group P43212
Resolution range 2.15 – 20 Å
Completeness 72.4 % (72.7 %)*
Rsym 7.4 % (20.1 %)*

Tests performed on Fluidigm µChips

INDEXATION:

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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>oP</td>
<td>4.0</td>
<td>87.3</td>
<td>140.3</td>
<td>231.1</td>
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<tr>
<td>aP</td>
<td>0.1</td>
<td>87.3</td>
<td>140.3</td>
<td>231.1</td>
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</table>
No more diffractometer

The gonio-robot includes:
- Sample cryo-cooling
- Crystal centering
- Crystal orientation
- Single axis goniometer capability
- Beam monitoring
- Low price
- High reliability
- Faster
- Easier to use
**Test setup**

a goniometer head at the end of the arm

the robotized arm as a diffractometer

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**Data collection**

<table>
<thead>
<tr>
<th></th>
<th>sample</th>
<th>$R_{\text{sym}}$</th>
<th>comple.</th>
</tr>
</thead>
<tbody>
<tr>
<td>diffractometer</td>
<td>lysozyme</td>
<td>3.0</td>
<td>98.3</td>
</tr>
<tr>
<td>Robot, high acceleration</td>
<td>lysozyme</td>
<td>5.5</td>
<td>95.8</td>
</tr>
<tr>
<td>Robot, high acceleration + off axis oscil.</td>
<td>lysozyme</td>
<td>4.0</td>
<td>96.4</td>
</tr>
<tr>
<td>diffractometer</td>
<td>chs1</td>
<td>5.1</td>
<td>94.8</td>
</tr>
<tr>
<td>Robot, shutter controlled by the robot</td>
<td>chs2</td>
<td>7.7</td>
<td>87.7</td>
</tr>
<tr>
<td>Robot, <em>idem</em> + backslash</td>
<td>chs2</td>
<td>7.9</td>
<td>88.2</td>
</tr>
</tbody>
</table>

G-Rob

Mostly: **commercially available components**
- a 6-axis robotic arm TX60 from Staübli (#1),
- an automated Dewar for sample storage (IRELEC ?)
- a tools changer (Schunk Inc., #2),
- a protection device (Schunk Inc., #2).

+ **non commercial tools**, designed on FIP-BM30A
- a sample holder, with an automated magnet (#3),
- a sample gripper (#4),
- softwares.
What to do next…

Integrate a cryo-stream

Improve accuracy (ID beamline)
L. Jacquamet (crystallographer)
J. Joly (software/hardware)
P. Charrault (electronic)
M. Pirocchi (vacuum)
F. Bouis (drawings)
R. Kahn (adviser)
F. Borel (local contact)
X. Vernede (instrumentation)
J. Ohana (automation)
A. Bertoni (machining)