
ESRF
The European Synchrotron

# AGENDA & OBJECTIVES

1. Make our User Community (more) aware of how facilities for Structural Biology are evolving and how they might evolve in the future.

2. For our User Community to let us know what they (i.e. you) want, both in the short and longer terms.

3. **Discussion!**

ESRF

ESRF Users' meeting 2016

MX BAG Meeting, Monday February 8th 2016

*Meeting Room MD-1-21*

Programme

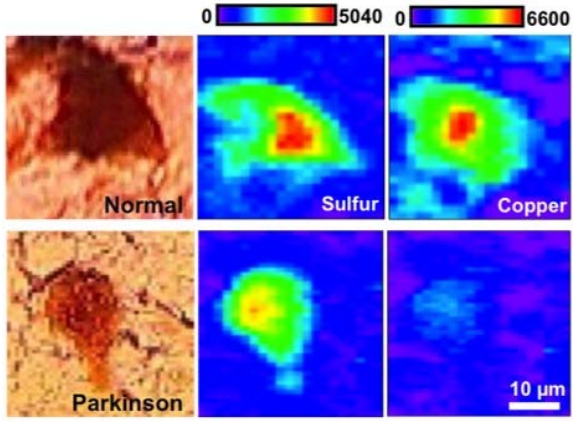
| | | |
|---|---|---|
| **8:30 – 9:00** | Registration and Welcome Coffee in the Marquee | |
| **Chairperson: C. Mueller Dieckmann** | | |
| **9:00 – 9:10** | Welcome<br>Meeting Room MD-1-21 | M. Mapelli (ESRF Users' Organisation)/J. Susini (Director Life Sciences, ESRF) |
| **9:10 – 9:20** | Agenda and Objectives | G. Leonard (SB Group Head) |
| **9:20 – 9:30** | ID23-1: News and the programme BEST | A. Popov |
| **9:30 – 9:45** | ID23-2: News and the upgrade plans | M. Nanao |
| **9:45 – 10:05** | Synchrotron Serial Crystallography: Opportunities and recent results | U. Zander |
| **10:05 – 10:25** | How to cluster partial data sets sensibly? | G. Santoni/M. Nanao |
| **10:25 – 10:45** | Coffee Break in MD-1-21 | |
| **Chairperson : G. Leonard** | | |
| **10:45 – 10:55** | ID29: News | D. de Sanctis |
| **10:55 – 11:05** | ID29S: News | A.Royant |
| **11:05 – 11:20** | BM29: News and microfluidics | P. Pernot |
| **11:20 – 11:30** | High pressure freezing | P. Carpentier |
| **11:30 – 11:40** | MASSIF-1: News | D. Nurizzo |
| **11:40 – 11:50** | MASSIF-3: News | D. Von Stetten |
| **11:50 – 12:00** | ID30B: News | A.McCarthy |
| **12:00 – 14:00** | Lunch at the ESRF canteen | |
| **14:00 – 16:30** | Visits & demonstrations | |
| | MASSIF-1/3 | |
| | ID30B/BM29 | |
| | ID29/ID29S | |
| | ID23-1/2 | |
| **15:00-15h30** | Coffee Break in 30.1.19 | |
| **Chairperson: Marina Mapelli** | | |
| **16:30 – 16:40** | Ligand screening | J. Marquez |
| **16:40 – 16:50** | Possibilities at the PSB: News | F. Bernaudat |
| **16:50 – 17:00** | SAXS-SANS platform | T.Forsyth |
| **17:00 – 17:20** | Forthcoming developments: Sample Changers; ESRF-EBS | G. Leonard |
| **17:20 – 18:00** | General Discussion | |
| **18:00** | Wine & Cheese in Marquee (general UM2016 event) | |

# When: December 2018 – Summer 2020

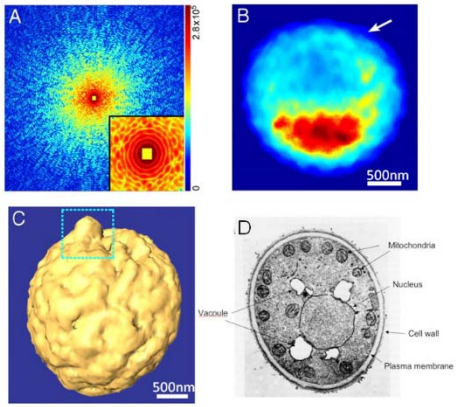
| ID29 Beam characteristics with current and Phase-II lattices | | | | |
|---|---|---|---|---|
| | Current | New Lattice (current optics) | New lattice (perfect optics) | **New Lattice (50:1)** |
| Source size (FWHM; H × V; μm²) | 115 × 13.2 | 59 x 11 | 59 x 11 | **59 x 11** |
| Divergence (r.m.s. H × V; μm²) | 104 × 6.1 | 7.4 x 5.3 | 7.4 x 5.3 | **7.4 x 5.3** |
| Demagnification ratio | 3:1 | 3:1 | 3:1 | **50:1** |
| Beamsize @ sample (μm²) | ~60 x 30 | 30 x 25 | 20 x 4 | **1.2 x 0.2** |
| Flux @ sample (ph/sec) | ~1 x $10^{13}$ | ~1 x $10^{14}$ | ~1 x $10^{14}$ | **~1 x $10^{14}$** |
| Flux density @ sample (ph/sec/μm²) | 7.0 x $10^{9}$ | 1.7 x $10^{11}$ | 2.1 x $10^{12}$ | **2.4 x $10^{14}$** |
| Absorbed dose rate (Gy/sec) | 3.2 x $10^{6}$ | 7.7 x $10^{7}$ | 9.6 x $10^{8}$ | **1.2 x $10^{11}$** |
| Time to Henderson Limit (sec)[c] | 6.3 | 0.26 | 0.021 | **0.0002** |

- **Smaller beams**
  - micro
  - nano
  - μradian divergence
- **Increase in flux density**
  - 2.5 orders of magnitude
  - 5 orders of magnitude

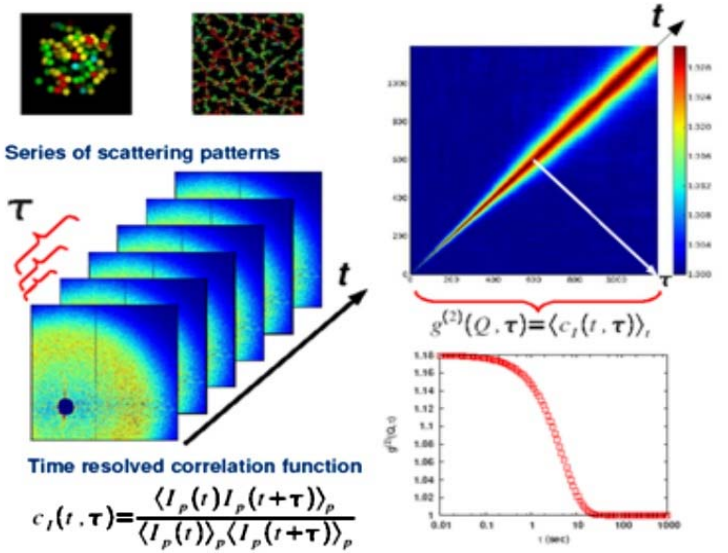
# EBS IS NOT JUST FOR MX & SAXS



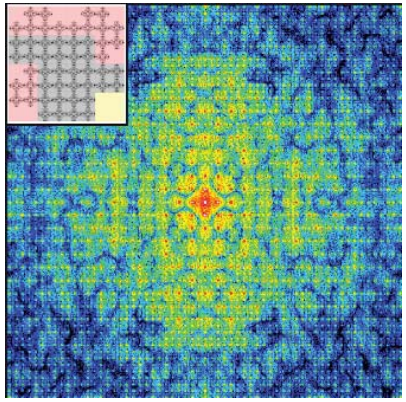

X-ray fluorescence microscopy of tissues and cells




Coherent Diffraction Imaging at resolution below 5 nm.




X-ray photon correlation spectroscopy (XPCS): dynamics of proteins on sub-µsecond time scales.



Use increased coherence in *ab initio* determination of macromolecular crystal structures

What to our User Community (i.e. you) want?

- **Do 'standard' things better?**
  - (fully) automatic data collection
  - finer probing of sample space
- **Faster, better & new experiments?**
  - SSX
  - RT data collection
  - micro-/millisecond TR
  - High energy (> 30 keV)
  - Low energy (< 6 k eV)
  - Exploit increased coherence
- **New scientific opportunities?**
  - mapping conformational space
  - dynamics

Expressions of interest

http://www.esrf.eu/home/about/upgrade/ESRF-EBS-call-expressions-of-interest.html

ESRF
The European Synchrotron

**ESRF EBS: EXTREMELY BRILLIANT SOURCE**
**Call for Expressions of interest**
**(5 pages maximum)**

Please send the completed form by 11th March 2016 to the Directors of Research (up2eoi@esrf.fr).

| | |
|---|---|
| Contact | |
| Title and Scientific area | |
| Scientific case | |
| Justification for the requesting ESRF-II capabilities | |
| Size of potential user community (including a list of interested groups) | |

For any further information, please contact the Directors of Research, Jean Susini (susini@esrf.fr) and Harald Reichert (reichert@esrf.fr).

# ESRF-EBS (+)

Cryo-Electron microscopy?

- High-end microscope in conjunction with IBS Platform
- Specific applications for projects requiring (at least) both MX & EM
- Is such a scenario of interest? Will send an e-mail asking for opinions, pleased start thinking about this.

# 2016-2017: FLEX-HCD SAMPLE CHANGERS


Will be installed on ID23-1, ID23-2, ID29, ID30A-3 (MASSIF-3), replacing current SC3s

Which sample formats?

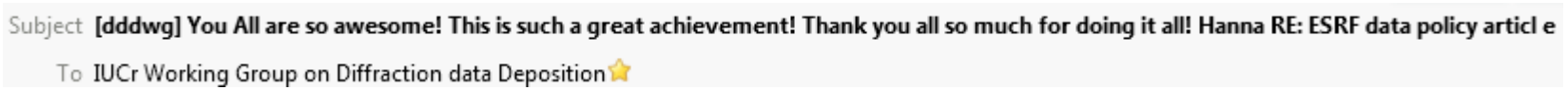
1. SPINE
    1. Vials
    2. 10 holders/puck
    3. 50 holders/transport dewar
    4. 120 holders/HCD
2. UniPuck (16 holders/puck)
    1. No vials
    2. 16 holders/puck
    3. 96 holders/transport dewar
    4. 192 holders/HCD
3. MiniSPINE
    1. No vials
    2. 36 holders/puck
    3. 192 holders/transport dewars
    4. 864 holders/HCD

# ESRF DATA POLICY

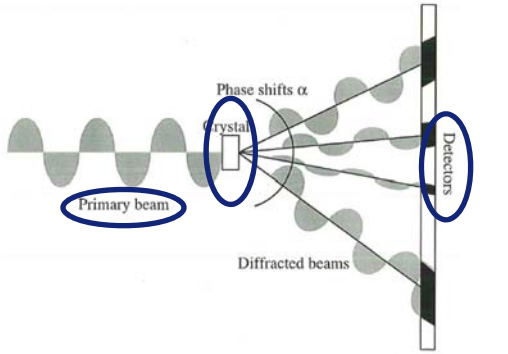
http://www.esrf.eu/home/news/general/content-news/general/esrf-takes-the-helm-in-saving-data.html

Based on the PaNdata Data Policy resulting from a European FP7 project delivered in 2011, the ESRF will be the custodian of raw data and metadata. **It will automatically collect metadata for all experiments carried out on its beamlines, including the beamlines from Collaborating Research Groups. The metadata will be stored in a metadata catalogue. The experimental team will have sole access to the data during a three-year embargo period, renewable if necessary. After the embargo, the data will be released into the public domain with open access.**

*"ESRF data will be traceable, verifiable and re-useable. The metadata and raw data will be archived for 10 years, with an option for longer archiving for more sensitive and unique data sets,"* says Rudolf Dimper, ESRF head of Technical Infrastructure. The cost of archiving data is in many cases only a fraction of the cost of preparing the sample, shipping it to the ESRF and collecting the data.



# WHAT METADATA IN ISPYB?




| Experiment parameters | Beamline parameters | AutoProcessing |
|---|---|---|
| **Img directory:** | /data/id29/inhouse/opid291/20150722/RAW_DATA/rory | |
| **Img prefix:** | rory_w1 | |
| **Nb of images:** | 1220 | |
| **Run no:** | 1 | |
| **Start Time:** | 22-07-2015 15:38:28 | |
| **End Time:** | 22-07-2015 15:39:16 | |
| **Type of experiment:** | OSC | |
| **Wavelength:** | 0.97625 Å | |
| **Energy:** | 12.7 keV | |
| **Phi start:** | 144 ° | |
| **Oscillation range:** | 0.1 ° | |
| **Overlap:** | 0 ° | |
| **Exposure Time:** | 0.02 s | |
| **Total Exposure Time:** | 24.4 s | |
| **Estimated Total Absorbed Dose:** | | |
| **Number of passes:** | 1 | |
| **Detector Distance:** | 218.61 mm | |
| **Resolution at edge:** | 1.30 Å | |
| **Resolution at corner:** | 1.07 Å | |
| **Xbeam:** | 212.36 mm | |
| **Ybeam:** | 215.73 mm | |
| **Kappa:** | 0 | |
| **Phi:** | 0 | |
| **Experiment comment:** | | |

+

| Experiment parameters | Beamline parameters | AutoProcessing |
|---|---|---|
| **Synchrotron name:** | ESRF | |
| **Synchrotron filling mode:** | 7/8 multibunch | |
| **Beamline name:** | ID29 | |
| **Undulator types:** | IVU21c_GAP U35a_GAP | |
| **Undulator gaps:** | 9.55 mm 50.0 mm | |
| **Beam transmission:** | 7 % | |
| **Slit gap Hor:** | 500 µm | |
| **Slit gap Vert:** | 200 µm | |
| **Detector type:** | PIXEL | |
| **Detector name:** | Pilatus3_6M | |
| **Detector manufacturer:** | DECTRIS | |
| **Detector mode:** | Unbinned | |
| **Detector pixel size Hor:** | 0.172 mm | |
| **Detector pixel size Vert:** | 0.172 mm | |
| **Focusing optics:** | Toroidal mirror | |
| **Monochromator type:** | Si(111) | |
| **Beam shape:** | ellipse | |
| **Flux:** | 3.7e+11 photons/sec | |
| **Flux end:** | 3.7e+11 photons/sec | |
| **Beam size at sample Hor:** | 50 µm | |
| **Beam size at sample Vert:** | 30 µm | |
| **Beam divergence Hor:** | 104 µrad | |
| **Beam divergence Vert:** | 6 µrad | |
| **Polarisation:** | 0.99 ° | |

Experiment parameters

```
JOB= ALL    !JOB= DEFPIX XPLAN INTEGRATE CORRECT
DATA_RANGE= 1 1220
SPOT_RANGE= 1 31
SPOT_RANGE= 580 610
BACKGROUND_RANGE= 1 4


!masking non sensitive area of Pilatus
UNTRUSTED_RECTANGLE= 487  495     0 2528
UNTRUSTED_RECTANGLE= 981  989     0 2528
UNTRUSTED_RECTANGLE=1475 1483     0 2528
UNTRUSTED_RECTANGLE=1969 1977     0 2528
UNTRUSTED_RECTANGLE=   0 2464   195  213
UNTRUSTED_RECTANGLE=   0 2464   407  425
UNTRUSTED_RECTANGLE=   0 2464   619  637
UNTRUSTED_RECTANGLE=   0 2464   831  849
UNTRUSTED_RECTANGLE=   0 2464  1043 1061
UNTRUSTED_RECTANGLE=   0 2464  1255 1273
UNTRUSTED_RECTANGLE=   0 2464  1467 1485
UNTRUSTED_RECTANGLE=   0 2464  1679 1697
UNTRUSTED_RECTANGLE=   0 2464  1891 1909
UNTRUSTED_RECTANGLE=   0 2464  2103 2121
UNTRUSTED_RECTANGLE=   0 2464  2315 2333
TRUSTED_REGION=0.0 1.41 !Relative radii limiting trusted detector region

!correction tables to compensate the misorientations of the modules

X-GEO_CORR= ../x_geo_corr.cbf
Y-GEO_CORR= ../y_geo_corr.cbf

MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT= 3
!STRONG_PIXEL= 3.0
OSCILLATION_RANGE= 0.1000
STARTING_ANGLE= 144.0
STARTING_FRAME= 1
X-RAY_WAVELENGTH=  0.97625
NAME_TEMPLATE_OF_DATA_FRAMES= ../../rory_w1_1_????.cbf !CBF
DETECTOR_DISTANCE= 218.61
DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE= 0.0 OVERLOAD= 1048500


SENSOR_THICKNESS=1.00
ORGX= 1234.63 ORGY= 1254.24
NX= 2463 NY= 2527
QX= 0.1720  QY= 0.1720
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 7000 30000

DIRECTION_OF_DETECTOR_X-AXIS= 1.0 0.0 0.0
DIRECTION_OF_DETECTOR_Y-AXIS= 0.0 1.0 0.0
ROTATION_AXIS= 1.0 0.0 0.0
INCIDENT_BEAM_DIRECTION= 0.0 0.0 1.0
FRACTION_OF_POLARIZATION= 0.99
POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0
!AIR= %.8f

SPACE_GROUP_NUMBER= 0
UNIT_CELL_CONSTANTS= 0 0 0 0 0 0
INCLUDE_RESOLUTION_RANGE= 50.0 0.0
!STRICT_ABSORPTION_CORRECTION=TRUE

REFINE(INTEGRATE)= BEAM ORIENTATION CELL
MAXIMUM_NUMBER_OF_PROCESSORS= 16
```

Data processing = input file/image header

# DO WE NEED TO ARCHIVE MORE METADATA?

- The metadata required in order to make raw data from ESRF MX beamlines intelligible are not extensive and are archived in ISPyB
  - Describes the experiment carried out on a given sample
  - Enables users to understand what happened during autoprocessing
  - Enables reprocessing of raw images by users.
  - Do we need a fuller description of the experiment?

- To make raw images fully intelligible for ‘non-owners’ further metadata are needed
  - Sample production/purification
  - Crystallisation
  - Post-crystallisation
  - Sequence/crystal composition
  - etc….
  - Requires linking of ISPyB and other databases (i.e. CRIMS, etc)

What do our users want?

# DATA CONFIDENTIALITY

- ESRF will soon (2016/2017) implement individual computer accounts, instead of the currently used BAG accounts (mx1234). The idea is that every user logs in with his/her personal credentials to collect his/her data. But, who should be able to ‘see’ the data?

- Only the individual user?
- Only those on A-Form?
- Entire BAG, as is currently the case?
- A subset of a BAG (i.e. the group of PI to whom the individual belongs)?

- Should it be possible to change this default behaviour, e.g. via a web interface to allow/disallow access for certain users? (...for all data of a given user, or per dataset, or per day?)