

Joint MXCuBE and ISPyB meeting, Hamburg 27/6/2016

MXCuBE @ ELETTRA



Elettra Sincrotrone Trieste

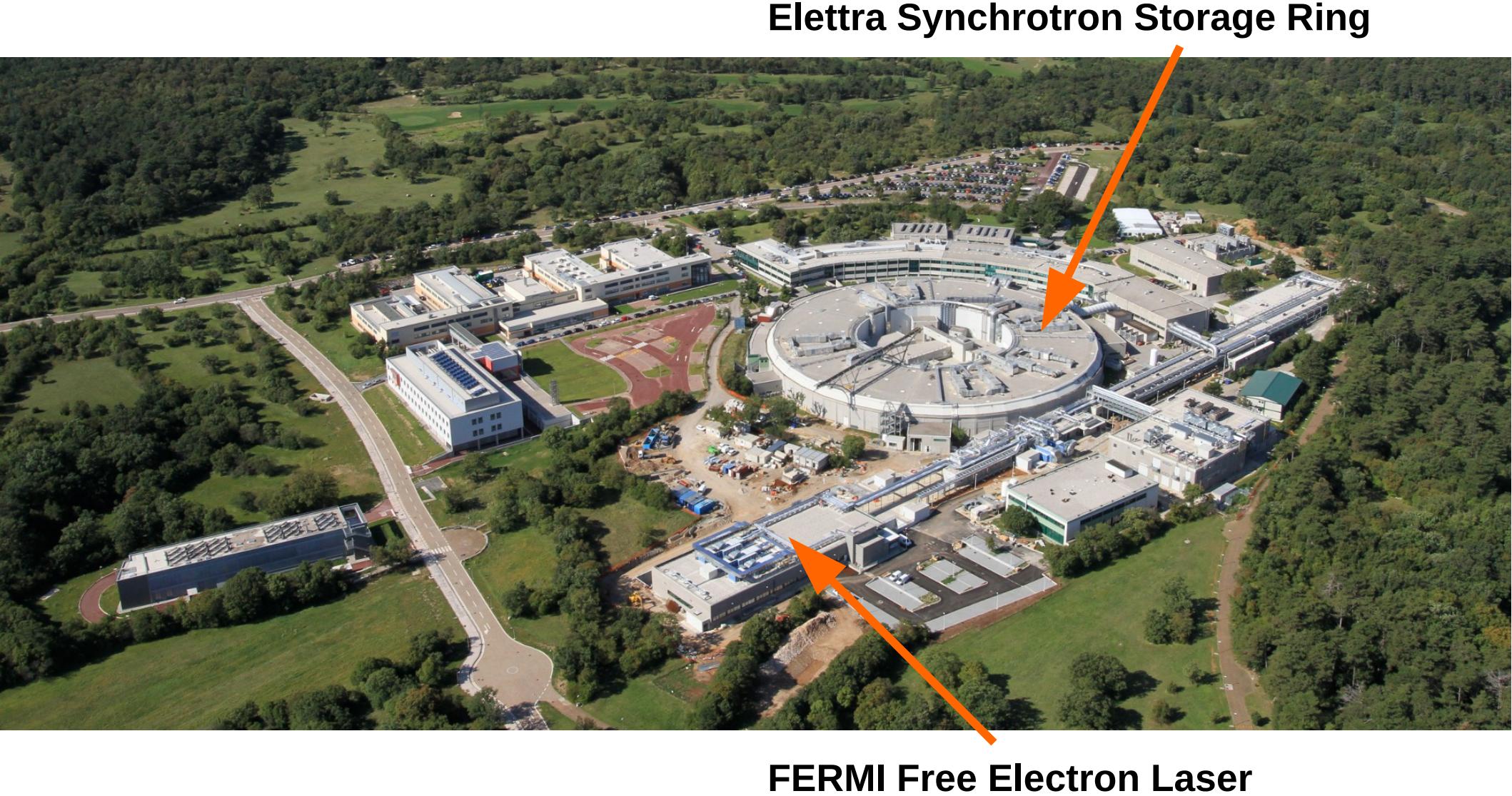
Milan Prica

www.elettra.eu

Introduction

- **Elettra** – 3rd generation synchrotron radiation facility
 - Operational since 1993
 - 28 beamlines
- **FERMI** – 4th generation light source is a linac based, single pass Free Electron Laser.
 - Operational since 2012
 - 6 beamlines (3 fully operational and 3 in development)
- Almost 1400 users/year
- Elettra – Sincrotrone Trieste is the statutory seat of **CERIC-ERIC** [www.ceric-eric.eu]

Light sources



Scientific Computing Group

- Support to beamlines and laboratories
 - TANGO-controls on all FERMI beamlines and all recent Elettra beamlines
 - Data acquisition
 - Automation of experimental sequences
 - Development of reusable tools and components (C++, Python, QT, Taurus,...)
 - Data management and reduction
- Virtual Unified Office (VUO)
- Participation in numerous EU projects

VUO – Virtual Unified Office

VUO - Investigation

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[He_10_bar_1s5p](#) / [He_10_bar_50-76](#) / [He_Meta_and_Fluo](#) / [He_VMI](#) / [TEST](#) / [VMI_and_Meta_HEn](#) / [Xe](#) / [test](#)

Investigation details	
Name:	20124009
Description:	20124009
Max 400 characters	
Principal investigator:	(14637) ZITNIK Matjaz [JSI - 20124009]
Proposal:	
[Edit]	

Other investigators	
[Delete]	AVALDI Lorenzo
[Delete]	BUCAR Klemen
[Delete]	CORENO Marcello
[Delete]	JURNEL Loic
[Delete]	MARCHENKO Tatiana
[Delete]	MIHELIC Andrej
[Delete]	O KEFFE Patrick
[Delete]	PIANCATELLI Maria Novella
[Delete]	PLEKAN Oksana Kudelich
[Delete]	PRINCE Kevin Charles
[Delete]	RICHTER Robert
[Delete]	RUBENSSON Jan Erik
[Delete]	SODERSTROM Johan

[\[Add a new investigator\]](#)

Experiments	
[View]	Code
[View]	He_10_bar_1s5p
[View]	He_10_bar_50-76
[View]	He_Meta_and_Fluo
[View]	He_VMI

Data access through Virutal Lab

VUO - Experiment

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Experiment details	
Name:	He_10_bar_1s5p
Description:	He_10_bar_1s5p
Max 400 characters	
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Datasets		
	Code	Status
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[View]	He_006	Filled
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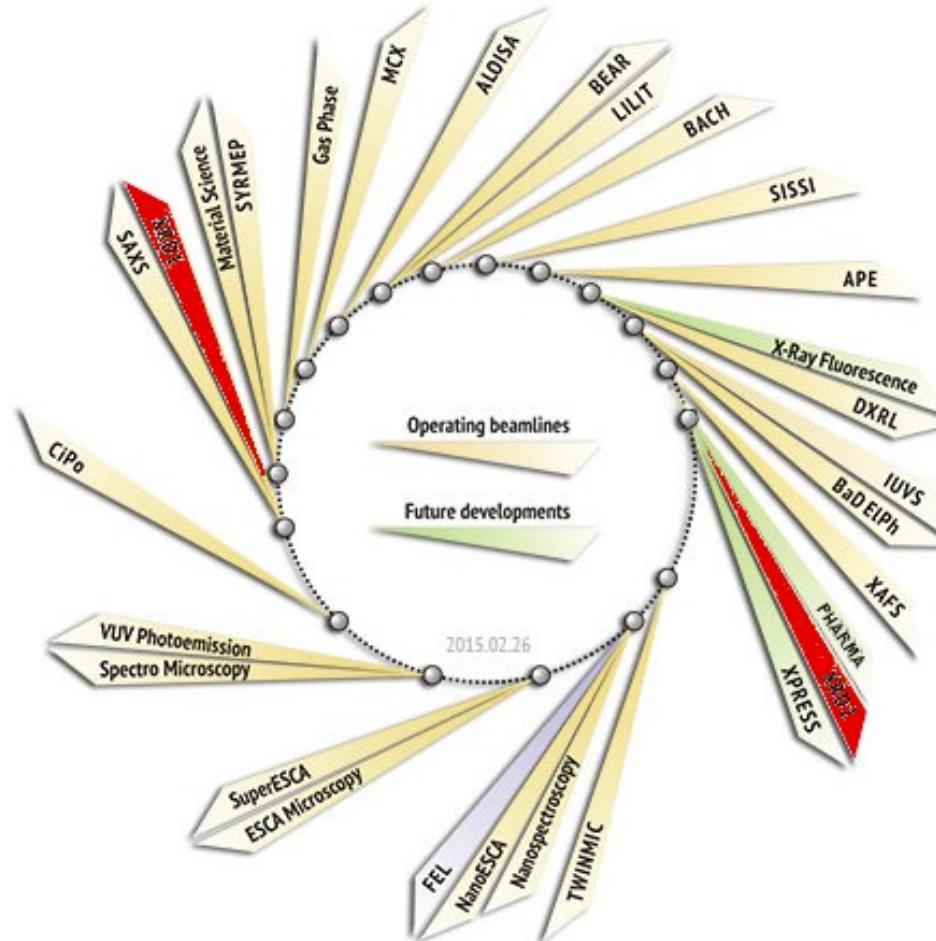
Beamlines for the structural biology

XRD1

A general-purpose X-rays diffraction BL offering MAD capabilities in a wide energy range: 4-21.5 KeV.

Operates since 1994 in cooperation with the CNR. BL is particularly suitable for data collections aiming to exploit the enhancement of weak signals from light elements.

Upgraded in 2014-15.



Starting from 2016 and in cooperation with IISc, a MX dedicated beamline offering MAD capabilities in a wide energy range: 7-35 KeV. The beamline particularly suits remote controlled, automatic data collections aiming to exploit the high flux produced by the SCW.

XRD2

XRD1 in a nutshell

Performance

70 papers/year in different X-ray diffraction fields:
Macromolecular crystallography
 Powder diffraction
 Grazing angle X-ray diffraction

30 PDB deposited/year.

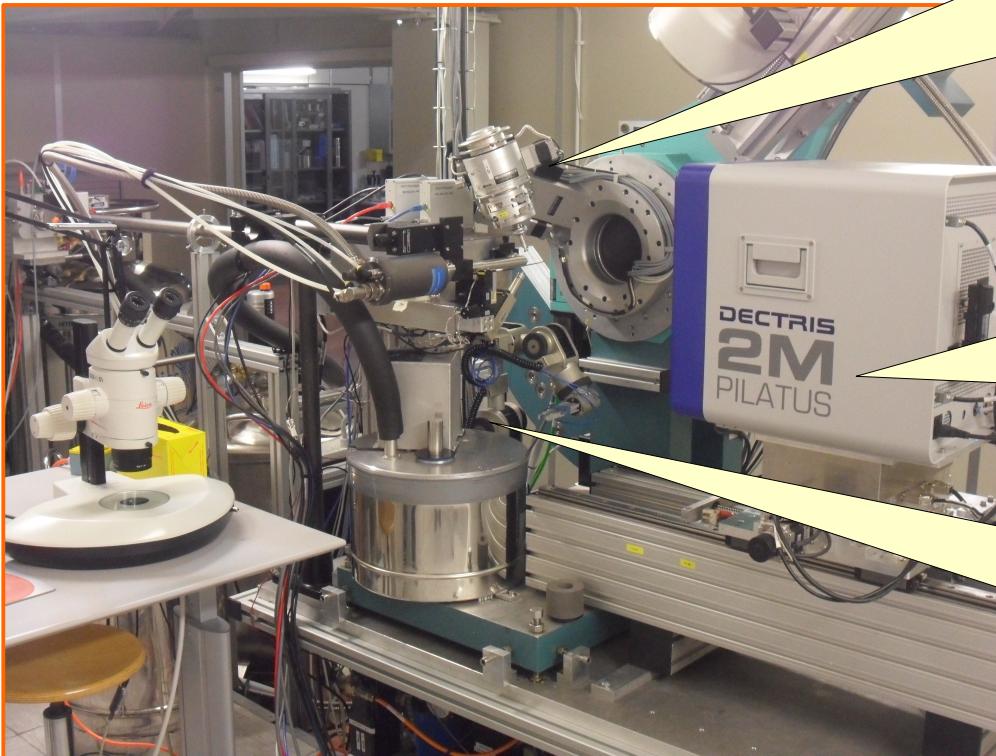
Software

Tango based SW architecture.
Pipelines for data integration and scaling.
Remote data collection.
Python scripting allows for rapid prototyping of experimental sequences.

Remote User Assistance

Wide Spectrum (4-21KeV, max at low energies)

The lower part (4-8 KeV) offers the enhancement of the signal from biologically relevant elements like Mn, K, Cl, I, Ca, S, P. and many edges for phasing (e.g. Xe).



Goniometer

(wide k-geometry)
Multiple crystal orientations for high quality data.
Very flexible set-up to Host non-conventional data collections.

Detectors

Wide area DECTRIS 2M detector. CCD detector on a 2theta arm.

Sample Changer

50 SPINE samples in ESRF punks.
Robust and reliable.
Katana robotic arm.

XRD2 in a nutshell

Status

Beam in experimental hutch, under commissioning.
Full beamline commissioning expected in Feb. 2017.
Remote data collection from July 2017.

Local & Remote User Assistance

Software

Tango based SW architecture. @TODO: **MXCuBE2** pipelines for data integration and scaling. Remote data collection (mandatory for the Indian community)

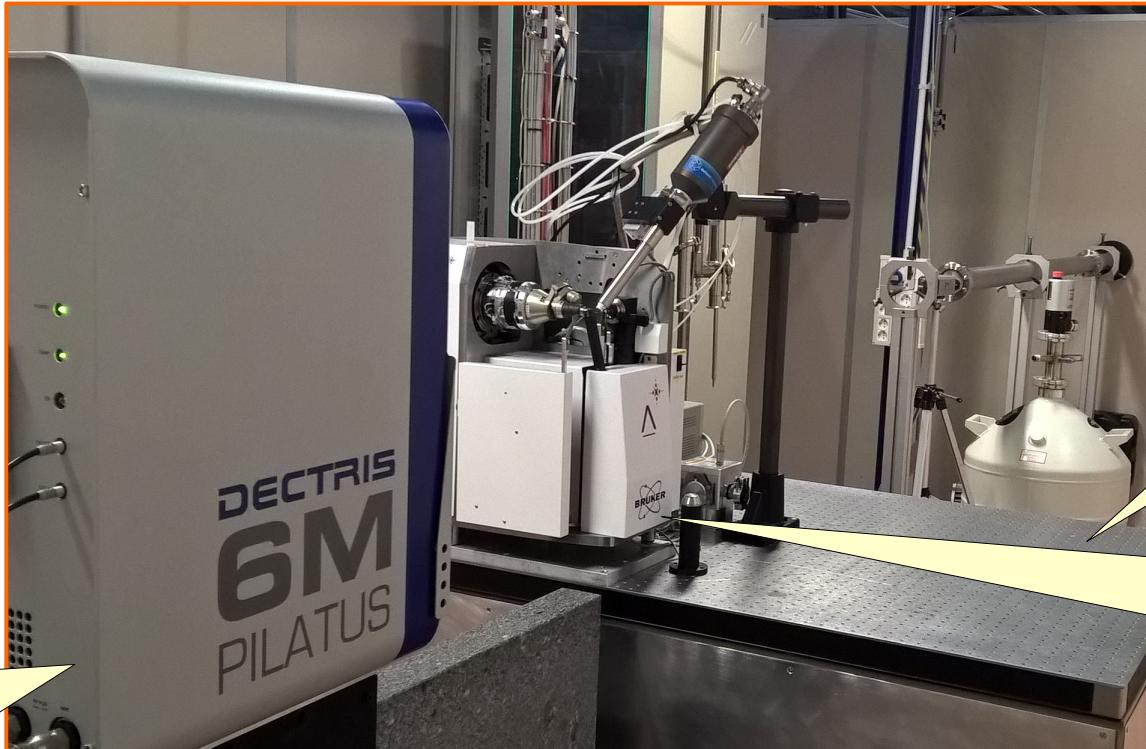
Wide Spectrum

The beamline offers a spectrum of 7-30 KeV peaked at 'typical' MX energies

Flux at the sample:
3.3 E13 ph/s/0.1%BW
(2GeV, 100mA)

Detector

Wide area **DECTRIS 6M** detector with PPU processing unit



Sample Changer

100 SPINE samples in ESRF punks.
XRD1 SC engineered (**under construction**).
New **Katana** robotic arm.

Goniometer

MD2s from Arinax (ESRF like) with minikappa for crystal re-orientation.

XRD2 – Work in progress



- Sample changer and robotic arm HW still to be completed
- Control of MD2s and Pilatus 6M from MXCuBE2
 - Same for sample changer and robotic arm, once ready
- Integration of ISPyB with VUO
- Remotization (large user community in India)
 - Strong interest in web version of MXCuBE
- Most of the above should be completed by Christmas

Thank you

Q: As newcomers,
what would you like
to see improved?

A: Documentation,
detailed examples
and more...
documentation!

