APE Beamline @ Elettra as the first demonstrator for the NFFA data repository

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APE Beamline



Agenda

Introducing the NFFA project
 The NFFA DATA repository
 Introducing the APE Beamline
 <u>APE Beamline as a demonstrator</u>
 FUTURE designs studies by NFFA stuff



The NFFA project



Nanoscience Foundries and Fine Analysis

www.nffa.eu

- An EU-funded design study (2008-2010) for a European Research infrastructure enabling access to nanoscience, atomic precision and fine analysis with a unified metrology.
- MIUR funding (2011-2013) for a demonstrating phase
- Led by **CNR-IOM** (Trieste). The project coordinator is prof. **Giorgio Rossi (Università degli studi di Milano)**.
- It involves many scientists and users, mainly experimentalists.

Design study Consortium

• CNR-IOM (Coordinator)

Consiglio Nazionale delle Ricerche Istituto Officina dei Materiali *ITALY*

• STFC

Science and Technology Facility Council UNITED KINGDOM

• CSIC-CNM

Consejo Superior de Investigaciones Cientificas Centro Nacional de Microelectronica SPAIN

• PSI

Paul Scherrer Institute Laboratory for Micro- and Nanotechnology SWITZERLAND

• OEAW

Austrian Academy of Sciences Institute of Biophysics and Nanosystems Research AUSTRIA











NFFA Data Repository (DR)

Work Package #	Work Package Title
WP1	Management of NFFA Design Study
WP2	Analysis of users and science program, development of NFFA roadmap
WP3	Design study of NFFA-RI Centres, technical layout of instrumentation and tools
WP4	Development of management structure and format of user access for NFFA-RI Centres. <u>Design of NFFA Data Repository and its access criteria.</u>
WP5	Schemes of future dissemination activities

NFFA Data Repository goal

- NFFA has addressed the creation of the first Data Repository (DR) in nanoscience.
- Store all the data produced in the NFFA centres
- Less invasive as possible for the users: it doesn't change too much the user approach
- Make data accessible by appropriate search tools



APE beamline as a demonstrator

APE Existing scenario:

- The data acquisition occurs in **Labview** in **Windows** environment accessing a set of heterogeneous instruments
- The (row)data (*) and metadata (**) reside in text files within a folder structure organized by user and date (no binary home-made files, no third parties binary files, no HDF!)
- Data analysis tools are mostly these commercial products:
 Igor Pro by Wavemetrics and Origin by Originlab.
- Data exchange between users occurs mostly via network and USB sticks

(*) we mean: "data from the machine"(**) from Wikipedia: "refers to data about data"

Data acquisition PCs and data analysis PCs @ APE Beamline



A typical rowdata(set)

[Info 1] Region Name=Overview 86eV Excitation Energy=86 Energy Scale=Kinetic Acquisition Mode=Swept Center Energy=51 Low Energy=20 High Energy=82 Energy Step=0.05 Step Time=133 Detector First X-Channel=71 Detector Last X-Channel=992 Detector First Y-Channel=284 Detector Last Y-Channel=691 Number of Slices=204 Lens Mode=Angular Pass Energy=10 Number of Sweeps=1 File=D:\Data\Marangolo2013\S1\32 Sequence=D:\Ses-1.2.2-r5 101U\data\Seq Spectrum Name=Overview 86eV006 Instrument=SES 2002-101U Location=APE User=Marangolo Sample=32M0139B3 Comments=32M0139B3 overview 86 eV Date=7/20/2013 Time=3:25:11 PM Time per Spectrum Channel=1.862 [...]

[User Interface Information 1] Sample temperature [° K] = +77.300

[Data 1]

(SINGLE) FILE SIZE: Typically: < 1MB NUMBER OF FILES / 1 week-beamtime /1 APE branch : 1000-5000!!!

<u>Header</u>

It contains metadata about the experiment for future reproducibility
Sometimes resides in a separate files
Typically scalars:
It resembles Windows ini file: MagnitudeName = MagnitudeValue (MagnitudeUnit)

Dealing with many files and many users

Questions ?!?

- How to organize users and files?
- How to find a document of interest?
- How to design a system expandable to other NFFA laboratories / instruments

APE Future scenario (under development)

- The data and metadata are automatically uploaded into the database from an acquisition PC located at the experimental station via a <u>DR Plug-In</u>
 (*a minimal interaction with user is required!*)
- The database features a flexible architecture that can be adapted to different research facilities
- Users download the (row)data by accessing the DR for (subsequent) analysis
- Users then upload the analyzed data to be accessible for other participants





Ingredients for the DR (1)

- User name: (e.g. John Doe)
- Group name:(e.g XY university)
- Experimental Facility name: (e.g. Ape Beamline)
- Experimental Station name: (e.g. APE High energy experimental chamber)
- Description (e.g. topological insulators)
- Measurement technique (e.g. X-ray Magnetic Circular Dichroism)

Ingredients for the DR (2)

- Dataset (for a measurement)
 - Metadata and Rowdata (one or more text files)
 - "Data Analysis **blog**". It contains:
 - data analysis tools project files (e.g. .pxp files (Igor),
 .opj files (Origin)) sorted by date and user intervention.

> Data preview possibility on the web interface :

1. DR standard xy graphs	3. DR standard voxels
2. DR standard images	4.DR Animated data show









FUTURE design studies by NFFA stuff

Integrate into the demonstrator these experimental stations:

- The Scanning Electron Microscope instrument at CNR-IOM TASC laboratory
- The open package for first principle quantum simulation (Quantum Espresso) at CNR-IOM-Democritos.

THANK YOU!