EDNA at the ESRF

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Challenge for the ESRF Upgrade: Massively Automated Sample Selection Integrated Facility

1. Baskets from Lab DS Loaded on screening carrousel
2. Samples taken from Lab baskets & put back after screening
3. From screening to sorting
4. Sorting/Cleaning station
5. From sorting to cleaning
6. Manual transfer to Data collection station(s)
7. Data collection station(s)
8. From sorting to Data collection
9. From Data collection to sorting/cleaning
Challenge for the ESRF Upgrade: Nano-imaging / Nano-analysis

Experimental setup @ ID22:
- KB optics with μ-/nano-focused beam
- FReLoN 2k taper: diffraction data
- Fluorescence (single element) detector
- IonChamber (I₀ and attenuated I)

See e.g. Bleuet et al., Nature Mater. 2008

Commonly $N \approx 160$ scanning steps/y-line,
$\omega \approx 60$ angular steps/tomographic scan

10-15h beamtime required/tomo scan
100 Go data generated/tomo scan

Slide from Pierre Bleuet
MXv1 Characterisation v1.1

- MX sample characterisation taking into account radiation damage
- Indexing using MOSFLM or Labelit
- Parallel integration of reference images
- If flux + beamsize:
  - RADDJOSE for estimating radiation damage
- BEST strategy calculation
  - taking into account radiation damage
  - multi-subwedge data collection strategies
MXv1 Characterisation v1.2

+ Xtal info
+ beam flux
+ diffraction plan

MOSLFM indexing

LABELIT DISTL

Indexing Evaluation

Ok

Failure

LABELIT indexing

Indexing Evaluation

Ok

MOSFLM Predictions

MOSFLM integration

[RADDOSE]

BEST

Data collection plan
MxCuBE ↔ EDNA MXv1 Characterisation
Future challenges for the EDNA framework

- Replacement of Enterprise Architect with an Eclipse based modelling tool
- Replacement of generateDS for data binding code generation

Workflow editor:
- Implicit documentation of workflow
- Implicit parallel workflows
- Possibility to “easily” modify / construct new workflows
- Possibility to debug workflows
- Possibility to restart a stopped workflow
- Improved logging
What is EDNA?

- EDNA is about collaboration:
  - Code sharing (SVN)
  - Coding conventions
  - Code reviews
  - Open source (LGPL, GPL)
  - Bug tracker
  - Wiki: http://www.edna-site.org
  - Memorandum of Understanding
  - Executive committee
  - Project manager / coordinator
  - Regular meetings / video conferences

- EDNA is a framework:
  - “Generic” kernel
  - Data modelling framework
  - Support for multi-threaded modules (plugins) development
  - Support for workflow development
  - Testing framework
  - “Specific” applications (MXv1, bioSaxs etc.)
  - Automatic testing and nightly builds
  - Automatic API doc generation
  - No GUI