**MX Automation**

- Goal: Full automation from sample loading to reduced (integrated and scaled) data
Screening at the ESRF

A. ESRF Beamlines and BM14

B. ID14-1,2 and 3

- Collections
- Screening
- Data sets
- Percent collected

<table>
<thead>
<tr>
<th>Year</th>
<th>Collections</th>
<th>Screening</th>
<th>Data Sets</th>
<th>Percent</th>
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Massively Automated Sample Selection Integrated Facility

- Baskets from Lab DS loaded on screening carrousel
- Screening station(s)
  - Samples taken from Lab baskets & put back after screening
- Sorting/Cleaning station
  - From sorting to data collection
  - From data collection to sorting/cleaning
- Manual transfer to Data collection station(s)

Diagram showing the workflow from storage to screening, screening to sorting, and sorting to cleaning.
What is EDNA?

• EDNA is an international collaborative project between several institutes and synchrotron facilities.

• Developed on the foundation of the project automateD collectioN of datA (« DNA », www.dna.ac.uk )

• Designed to be a framework for Online Data Analysis (of X-ray experiments)
The EDNA Project / Framework
EDNA Project Management (1)

- Executive Committee:
  - Alun Ashton, DLS, UK
  - Gérard Bricogne, Global Phasing, UK
  - Andrew Leslie, MRC LMB, Cambridge, UK
  - Andrew McCarthy, EMBL-Grenoble, France
  - Sean McSweeney, ESRF, Grenoble, France
  - Thomas Schneider, EMBL-Hamburg, Germany
  - Andrew Thompson, Synchrotron Soleil, France

- Other members from:
  - BESSY, Berlin, Germany
  - MAX LAB, Lund, Sweden
  - NSLS, Brookhaven, U.S.
  - SLS, Villigen, Switzerland
  - University of Sydney, Australia
  - University of York, UK
EDNA Project Management (2)

- Project agreement
- Coding conventions
- Code reviews
- Development tools
  - Eclipse
  - Enterprise architect
- Project portal
  - http://www.edna-site.org
  - Wiki documention
  - Bugzilla server
  - Subversion server
  - Discussion forum
- Executive committee
- Video conferences
- Developers' meetings & workshops

Marratech video-conferencing tool
The EDNA Data Model Framework

• From UML diagrams to generated code (data binding):

```xml
<xs:element name="XSDataSample" type="XSDataSample"/>
<xs:complexType name="XSDataSample">
    <xs:complexContent>
        <xs:extension base="XSData">
            <xs:sequence>
                <xs:element name="absorbedDose" type="XSDataAbsorbedDose" minOccurs="0" maxOccurs="1"/>
                <xs:element name="shape" type="XSDataFloat" minOccurs="0" maxOccurs="1"/>
                <xs:element name="size" type="XSDataSize" minOccurs="0" maxOccurs="1"/>
                <xs:element name="susceptibility" type="XSDataFloat" minOccurs="0" maxOccurs="1"/>
            </xs:sequence>
        </xs:extension>
    </xs:complexContent>
</xs:complexType>
```
EDNA Modularity: Plugins and their hierarchy

- **Plugin base class:**
  - Configuration, working directory, etc.

- **Execution plugins:**
  - Execution of external programs, e.g. (bash) scripts

- **Controller plugins:**
  - Control of execution plugins
  - Parallel execution
  - Synchronisation

- EDNA is partly based on AALib, however AALib is not a part of EDNA collaboration
EDNA Testing Framework

• The EDNA testing framework consist of three layers:
  • Kernel Unit tests
  • Plugin Unit tests
  • Plugin Execution tests

• Example: the EDNA Test Suite All result:

```
[SUCCESS] [ 3 ][ EDTestCasePluginExecuteControlSubWedgeAssemblev10.execute ][1.42272996902]
[SUCCESS] [ 1 ][ EDTestCasePluginExecuteControlSubWedgeAssemblev10.testExecute ][1.38881707191]
[SUCCESS] [ 4 ][ EDTestCasePluginExecuteControlSubWedgeAssemblev10NineImageSubWedge.execute ][2.38712197437]
[SUCCESS] [ 1 ][ EDTestCasePluginExecuteControlSubWedgeAssemblev10NineImageSubWedge.testExecute ]
```

-----------------------------------------------
[TestUnit]: ###################################################################
[TestUnit]: EDTestSuiteAll summary report:
[TestUnit]: TestSuites: 2
[TestUnit]: Total TestCases: 48
[TestUnit]: Total TestCases [SUCCESS]: 48
[TestUnit]: Total TestCases [FAIL]: 0
[TestUnit]: [Total TestMethods]: 96
[TestUnit]: Runtime: 444.1 [s]
[TestUnit]: Run: 00d:00h:07m:24s:096ms
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EDNA Collaborators

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Alun Ashton(b)
Andrew Leslie(h)
Andrew McCarthy(c)
Andrew Thompson(k)
Clemens Schulze(j)
Clemens Vornhein(f)
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(e) ESRF, Grenoble, France
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(l) University of Sydney, Australia
(m) University of York, UK

EDNA developers
Executive committee
EDNA MXv1 Characterisation

• MX sample characterisation taking into account radiation damage
  • Indexing using MOSFLM or Labelit
  • Parallel integration of reference images
  • If flux + beam size + chemical composition: RADDOSE for estimating radiation damage
  • BEST strategy calculation
    • taking into account radiation damage
    • multi-subwedge data collection strategies
Why use a workflow tool in EDNA?

- Implicit documentation of workflow
- Possibility to “easily” modify / construct new workflows
- Possibility to debug workflows
- Possibility to restart a stopped workflow
Example Characterisation Workflow

- Characterisation XML Input
  - Plugin for preparing indexing input
    - Indexing plugin
    - Plugin for preparing integration input
      - Integration plugin
      - Plugin for preparing strategy input
        - Strategy plugin
        - Plugin for assembling characterisation results
          - Characterisation XML results
EDNA plugin in workflows – current implementation

• Advantages :
  • Modular / plugins – easy to add new functionality
  • Data model framework
  • Testing framework

• Disadvantages :
  • Input / result data must be defined in data model
  • Only one input object and one result object for each plugin