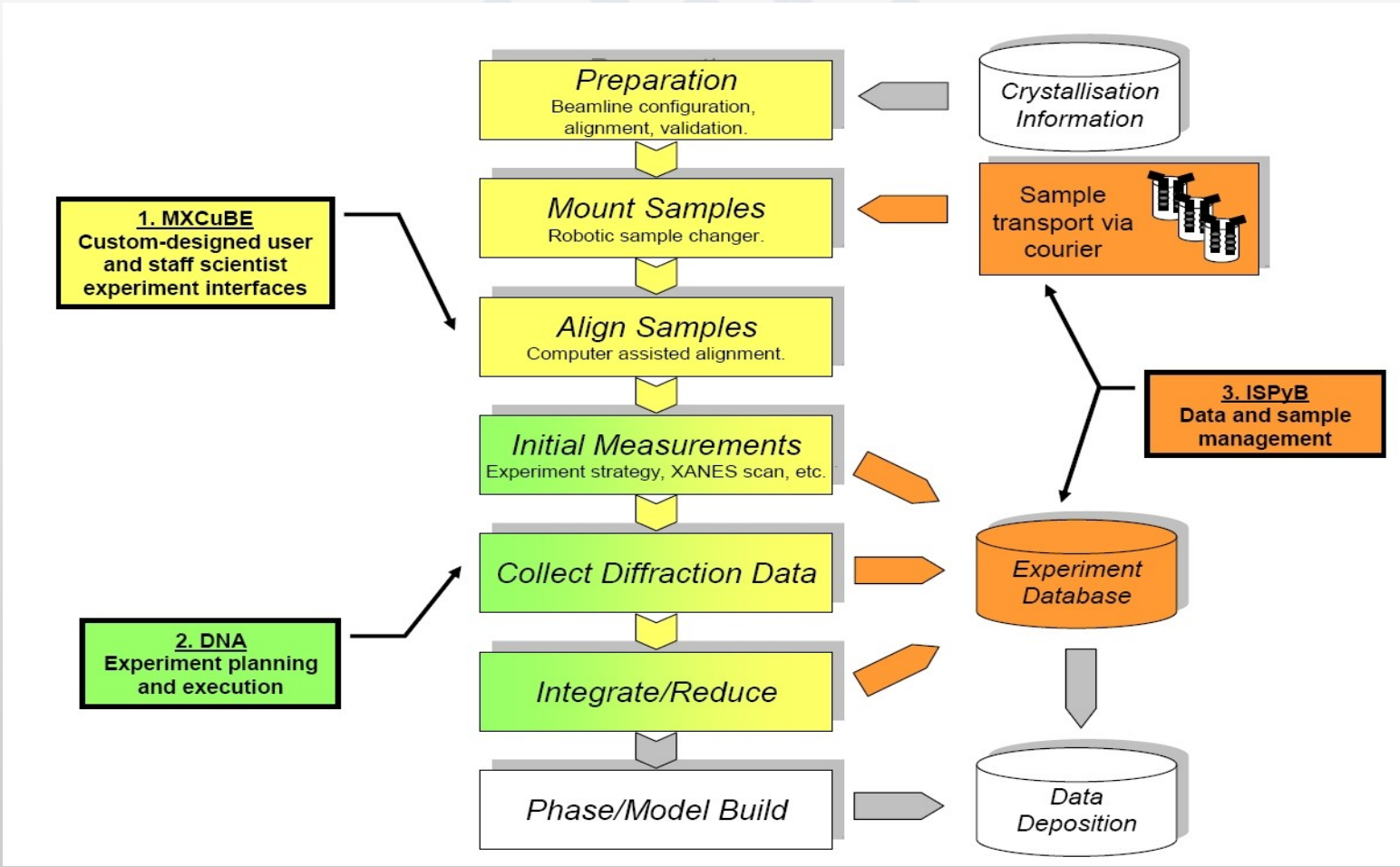
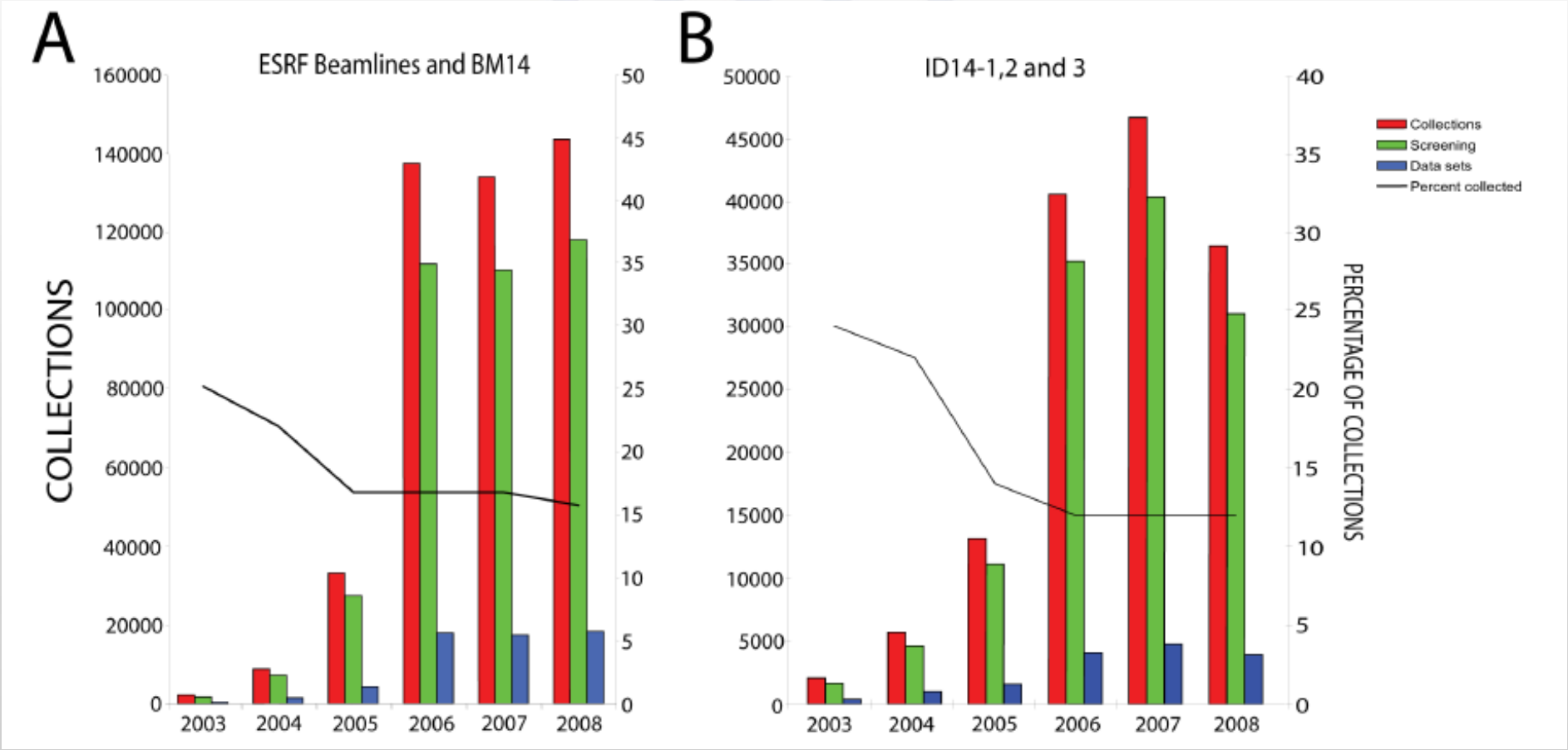
EDNA Workflows

MX Automation

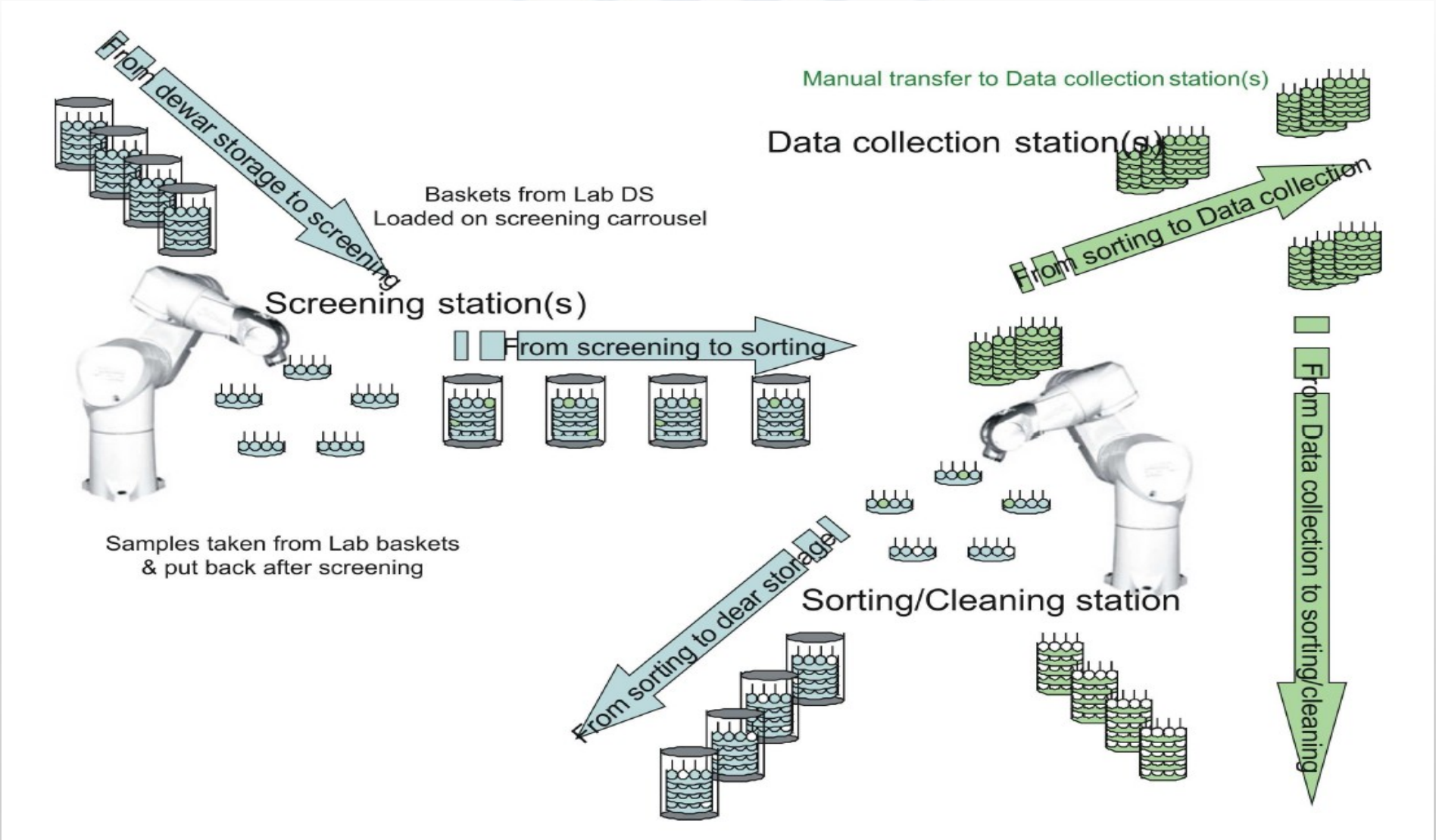
- Goal: Full automation from sample loading to reduced (integrated and scaled) data



Screening at the ESRF



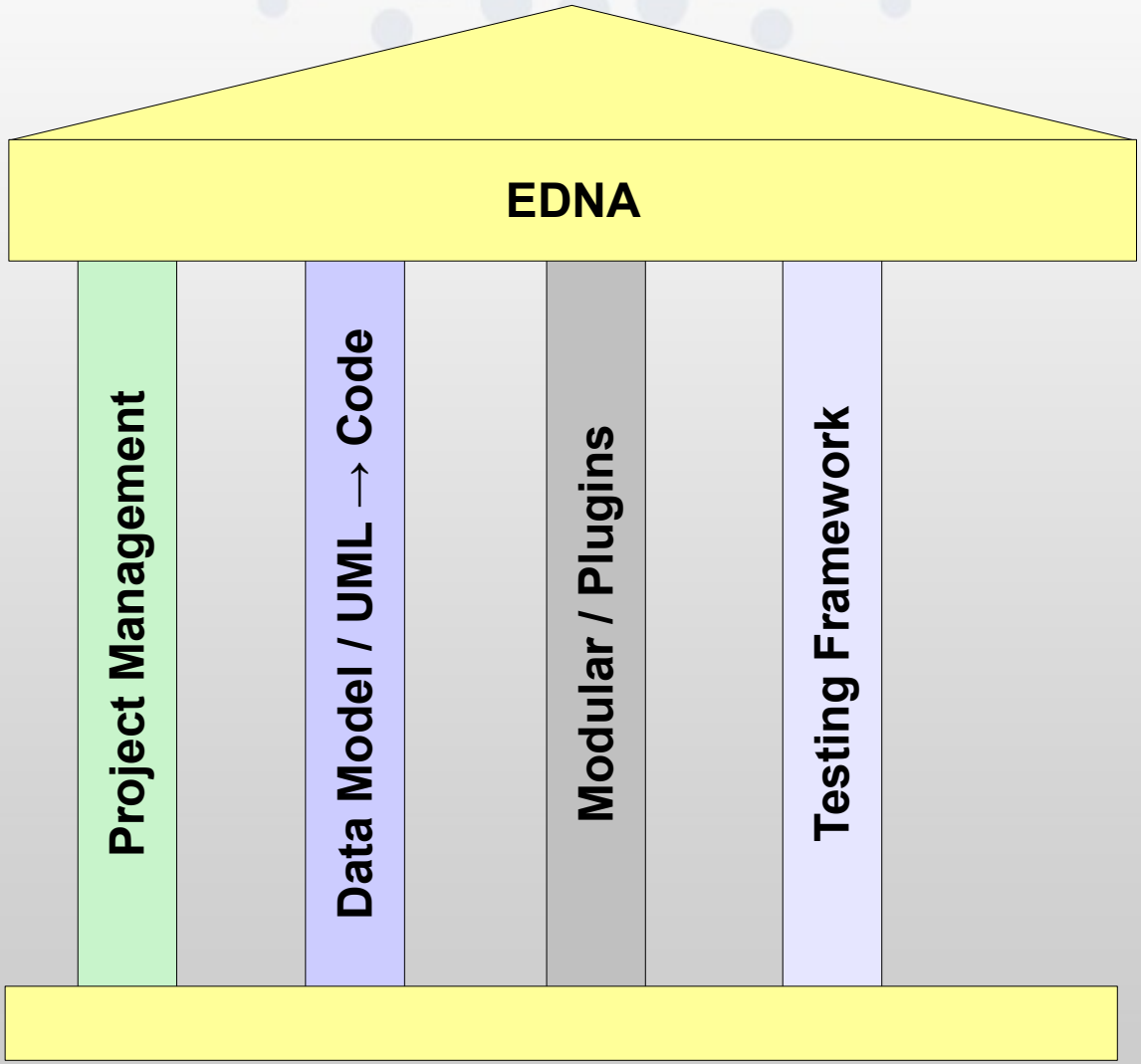
Massively Automated Sample Selection Integrated Facility



What is EDNA?

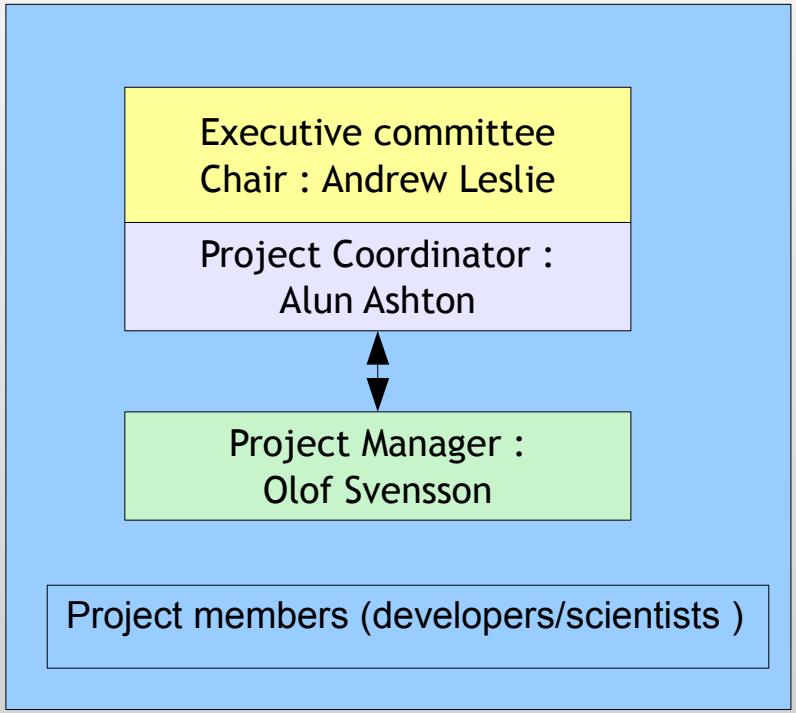
- EDNA is an international collaborative project between several institutes and synchrotron facilities.
- Developed on the foundation of the project automateD collectioN of datA (« DNA », www.dna.ac.uk)
- Designed to be a framework for Online Data Analysis (of X-ray experiments)

The EDNA Project / Framework



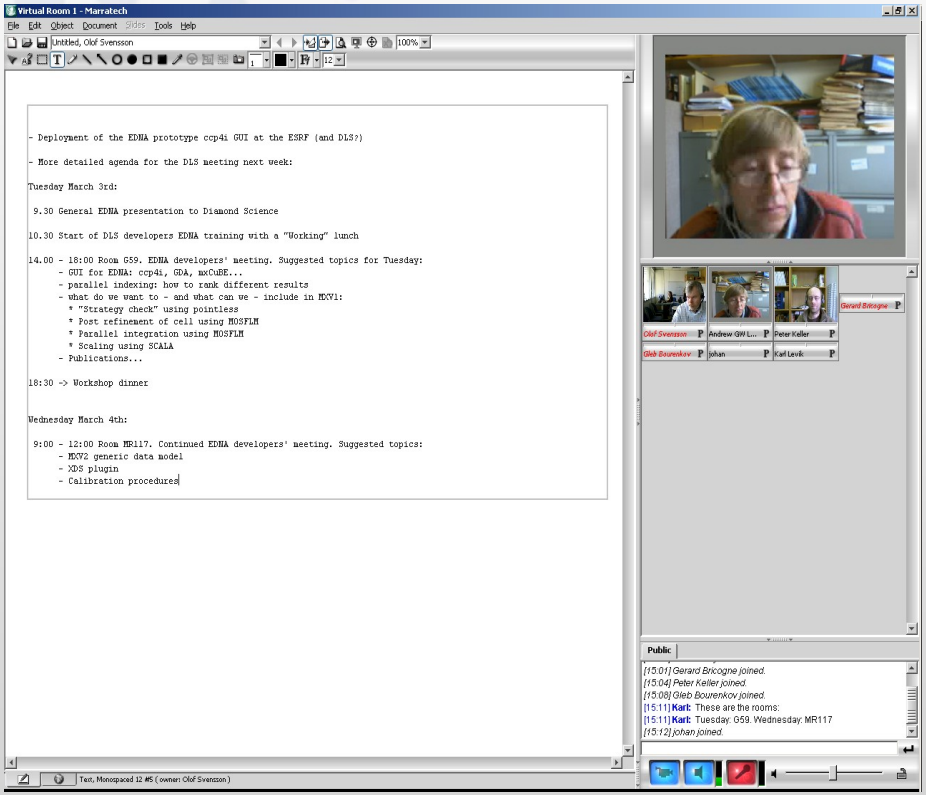
EDNA Project Management (1)

- 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, Switzeland
  - University of Sydney, Australia
  - University of York, UK



EDNA Project Management (2)

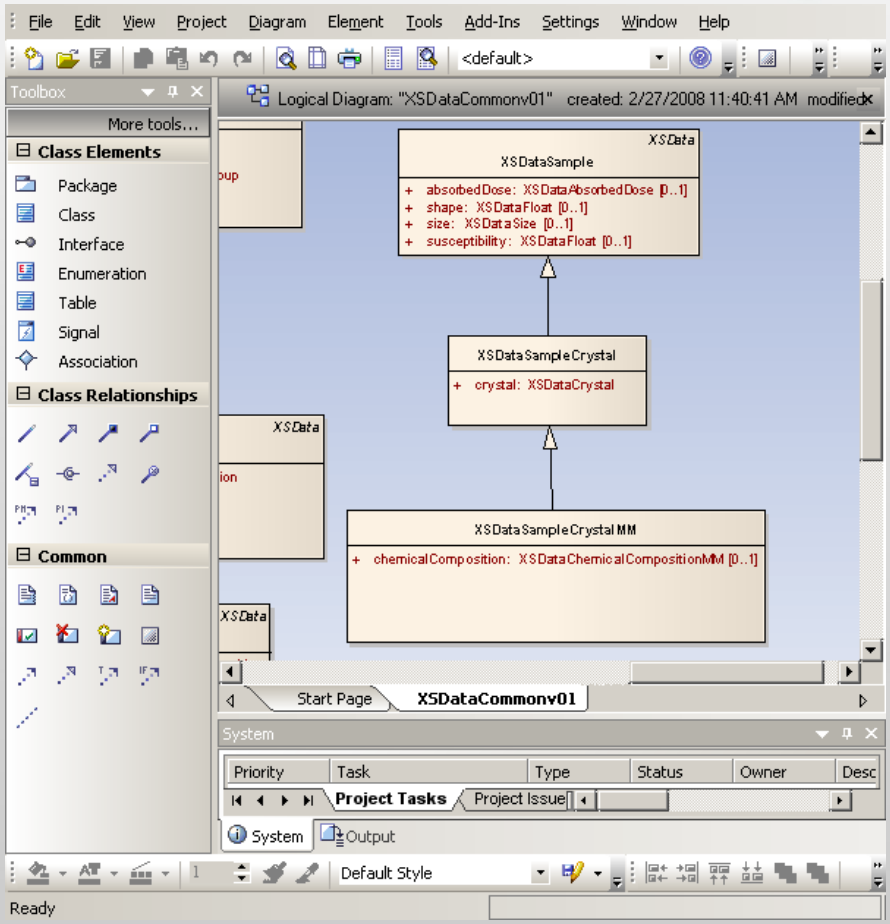
- Project agreement
- Coding conventions
- Code reviews
- Development tools
  - Eclipse
  - Enterprise architect
- Project portal
  - http://www.edna-site.org
  - Wiki documention
  - Bugzilla server
  - Subversion server
  - Discussion forum
- Executive committee
- Video conferences
- Developers' meetings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



Marratech video-conferencing tool

The EDNA Data Model Framework

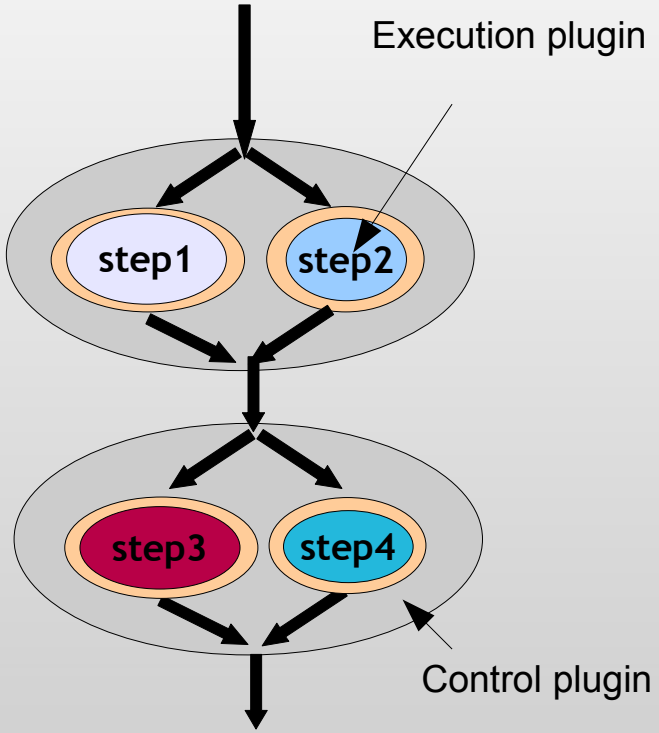
- From UML diagrams to generated code (data binding) :




```
<xs:element name="XSDataSample" type=
<xs:complexType name="XSDataSample">
     <xs:complexContent>
          <xs:extension base="XSData"
               <xs:sequence>
                    <xs:element name=
                    <xs:element name=
                    <xs:element name=
                    <xs:element name=
               </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 ][1.38881707
[SUCCESS] [ 4 ][ EDTestCasePluginExecuteControlSubWedgeAssemblev10NineImageSubWedge.execute ][2.38712
          [SUCCESS] [ 1 ][ EDTestCasePluginExecuteControlSubWedgeAssemblev10NineImageSubWedge.testExe

================================================================================


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

EDNA Collaborators

Alexander Popov(e)
Alun Ashton(b)
Andrew Leslie(h)
Andrew McCarthy(c)
Andrew Thompson(k)
Clemens Schulze(j)
Clemens Vonrhein(f)
Darren Spruce(e)
Elspeth Gordon(e)
Ezequiel Panepucci(j)
Gérard Bricogne(f)
Gerrit Langer(c)
Gleb Bourenkov(c)
Gordon Leonard(e)
Harry Powell(h)
Johan Turkenburg(m)
Johan Unge(g)
John Skinner(i)
Karl Levik(b)
Katherine McAuley(b)
Lucile Roussier(k)
Marie-Farnçoise Incardona(e)
Mark Basham(b)
Meitian Wang(j)
Michael Hellmig(a)
Olga Roudenko(k)
Peter Keller(f)
Peter Turner(l)
Pierre Legrand(k)
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Romeu Pieritz(e)
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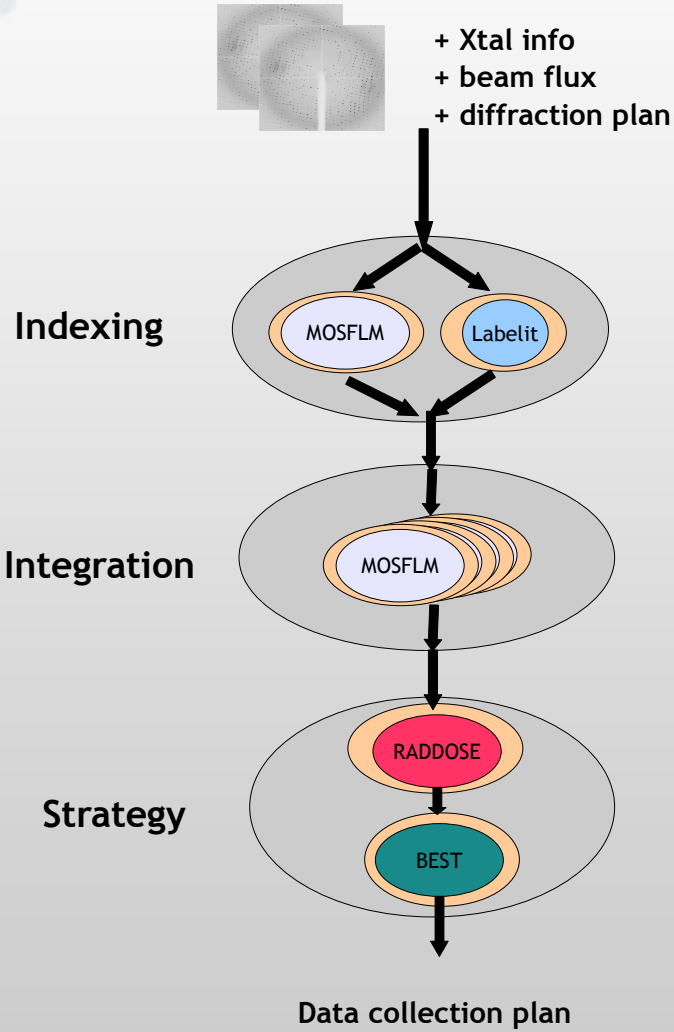
Sean McSweeney(e)
Takashi Tomizaki(j)
Thomas Schneider(c)
Uwe Mueller(a)

(a) BESSY, Berlin, Germany
(b) Diamond Light Source, UK
(c) EMBL, Grenoble, France
(d) EMBL, Hamburg, Germany
(e) ESRF, Grenoble, France
(f) Global Phasing, Cambridge, UK
(g) MAX LAB, Lund, Sweden
(h) MRC LMB, Cambridge, UK
(i) NSLS, Brookhaven, U.S.
(j) SLS, Villigen, Switzeland
(k) Synchrotron Soleil, France
(l) University of Sydney, Australia
(m) University of York, UK

EDNA developers
Executive committee

EDNA MXv1 Characterisation

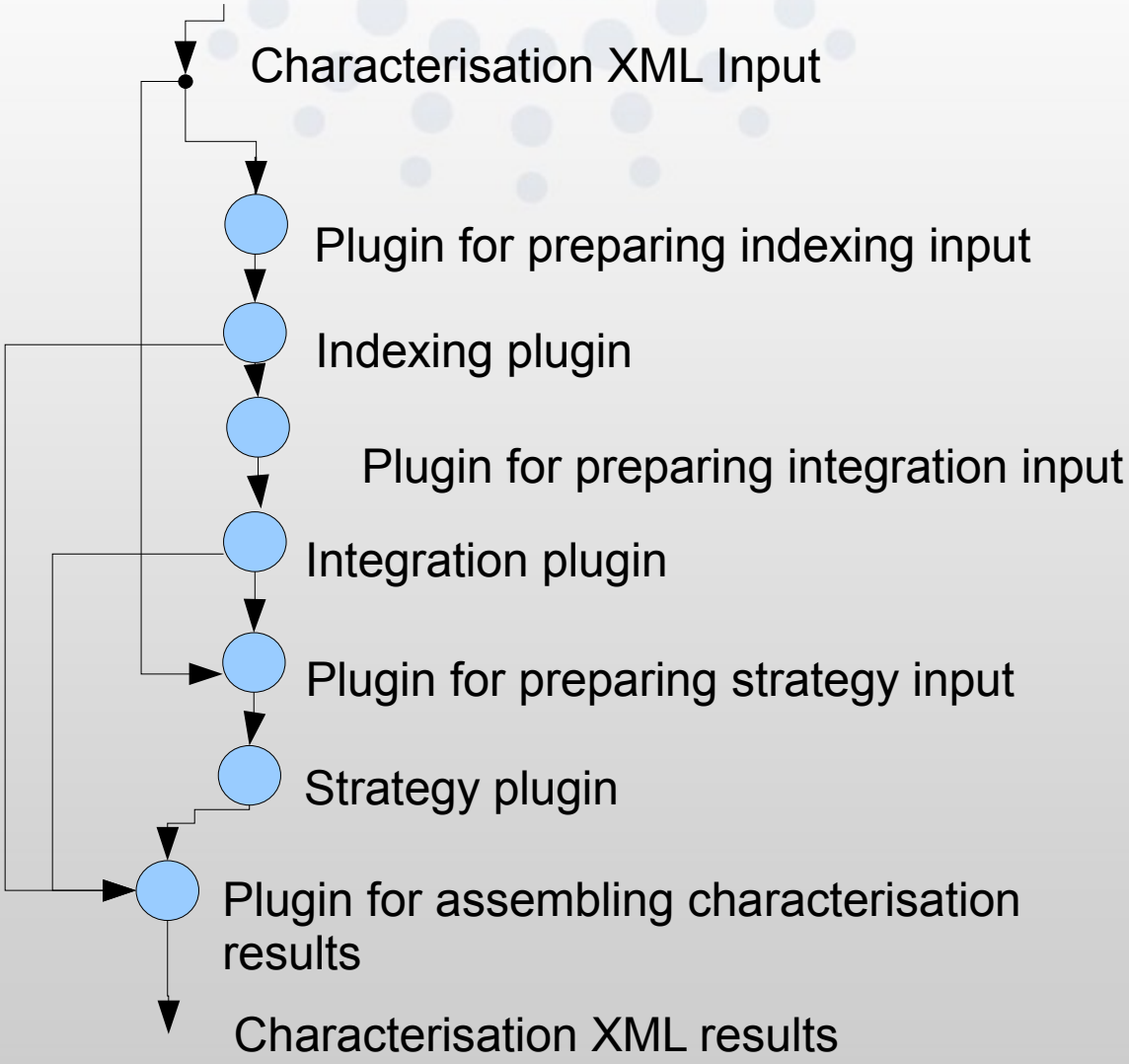
- MX sample characterisation taking into account radiation damage
  - Indexing using MOSFLM or Labelit
  - Parallel integration of reference images
  - If flux +beamsize + chemical composition: RADDOSE for estimating radiation damage
  - BEST strategy calculation
    - taking into account radiation damage
    - 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



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