EDNA ½ Day Introduction

- Agenda:

14:00 - 15:15 (Olof)

- Why EDNA?
- Collaboration
- Data model framework
- Modularity / plugins
- Workflows
- Testing framework

15:15 – 15:45 - Pause

15:45 - 17:00

- Azimuthal integration and diffraction tomography using EDNA (Jérôme)
- Workflow tools for EDNA (Matthew)
- MX applications (Olof, if time allows)

Why EDNA?

- EDNA is the best answer we (developers) have come up with so far for answering these questions :
  - How can we “pipeline” existing scientific software programs/packages for (online) data analysis workflows?
  - How can we make workflows that is easily adapted to new versions of scientific software packages?
  - How can we abstract certain calculations to be “generic”, e.g. indexing of a diffraction pattern?
  - How can we make “flexible” workflows, i.e. workflows that can be changed rapidly depending on the scientific needs?
  - How can we automate data analysis workflows?
  - How can we make these workflows robust?
  - How can we collaborate efficiently?
  - How can we re-use code developed by another facility without breaking existing functionality?

So – what is then EDNA?

- Short answer:

  A tool for Online Data Analysis

  and

  A Collaborative Effort

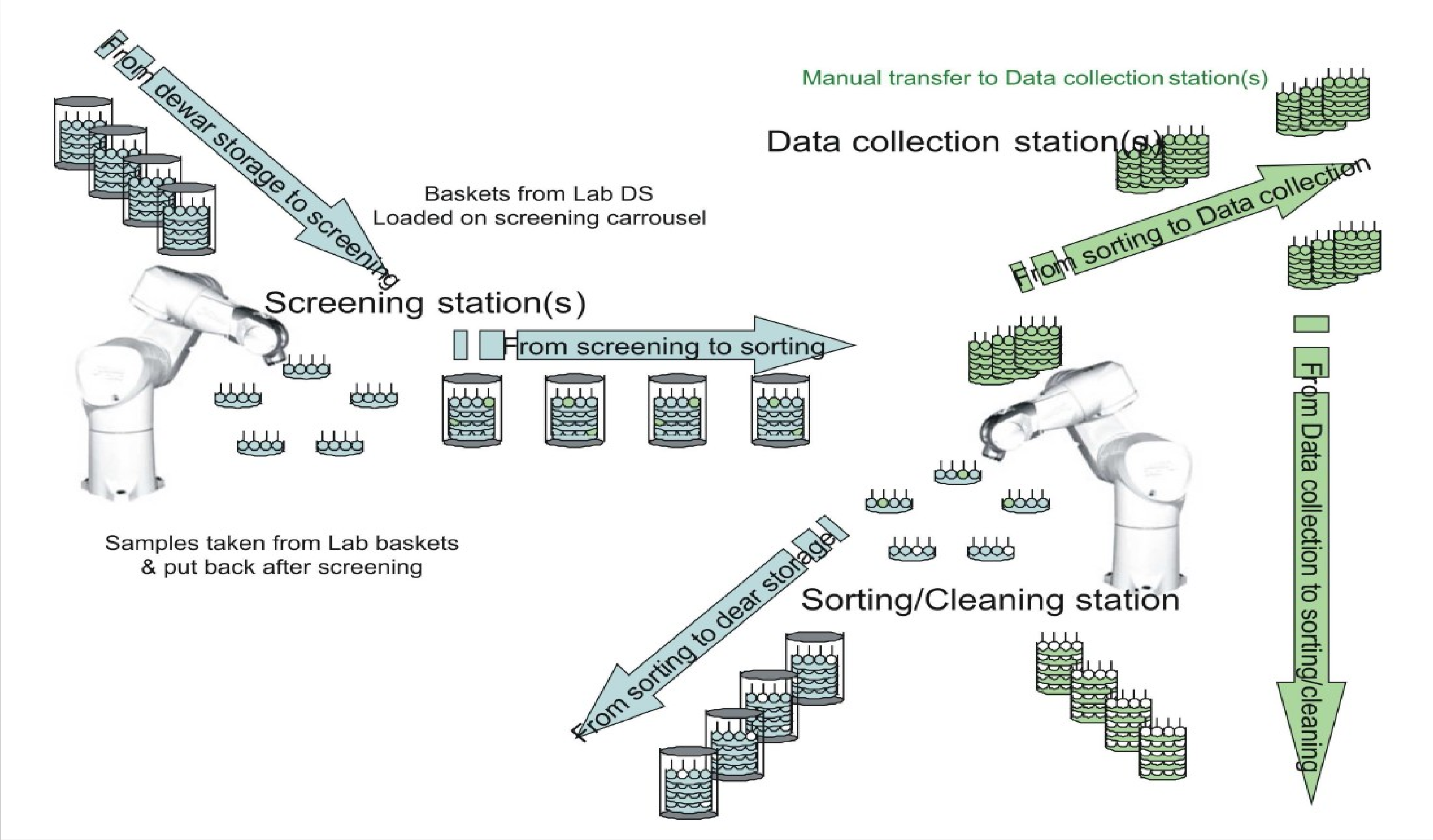
- Long answer :

  This introduction!

Online Data Analysis

- Data analysis performed as quickly as possible in order to provide feedback to the user(s):
  - Quick calculations for data visualisation
  - Quality of the data generated by the experiment – is the experiment successful?
  - Use of results for planning the experiment : e.g. MX strategy calculation
- Combination of data acquisition and data processing
- Automation - Workflow
- Meta data definitions important (data manager)
- Impact on beamline efficiency :
  - Should introduce added value
  - No slow-down of experiments
  - No or little impact on beamline scientists / users workload

Challenge for the Upgrade :
Massively Automated Sample Selection Integrated Facility

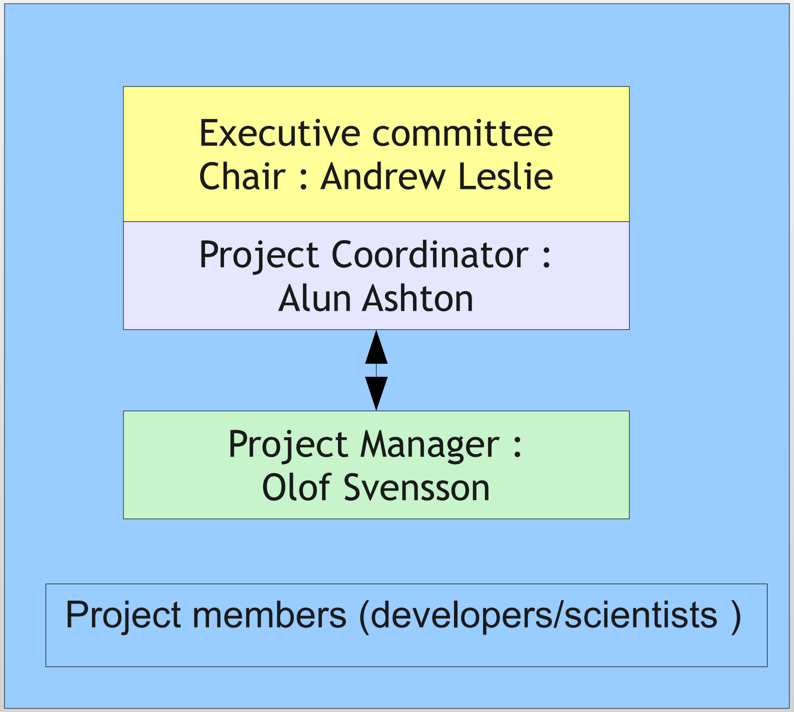


The EDNA foundation – the project management

Project Management

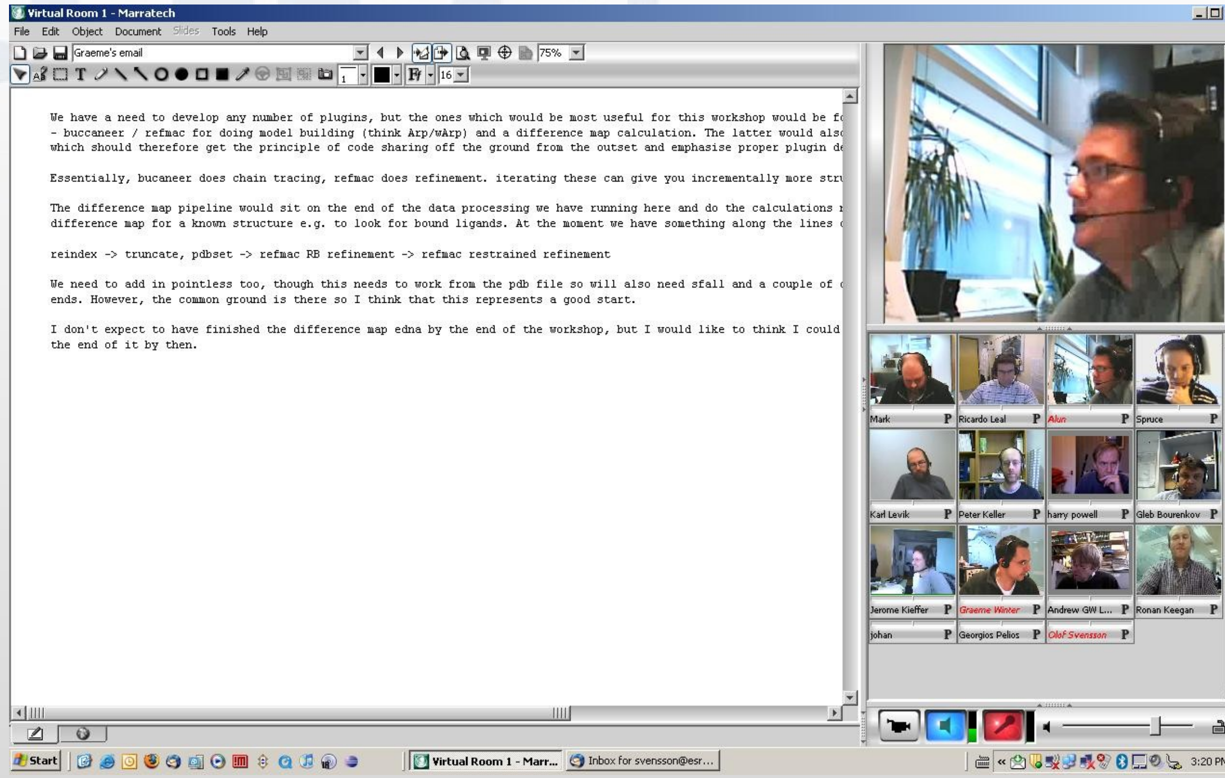
EDNA Project Management
To be revised on September 23rd 2010

- 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



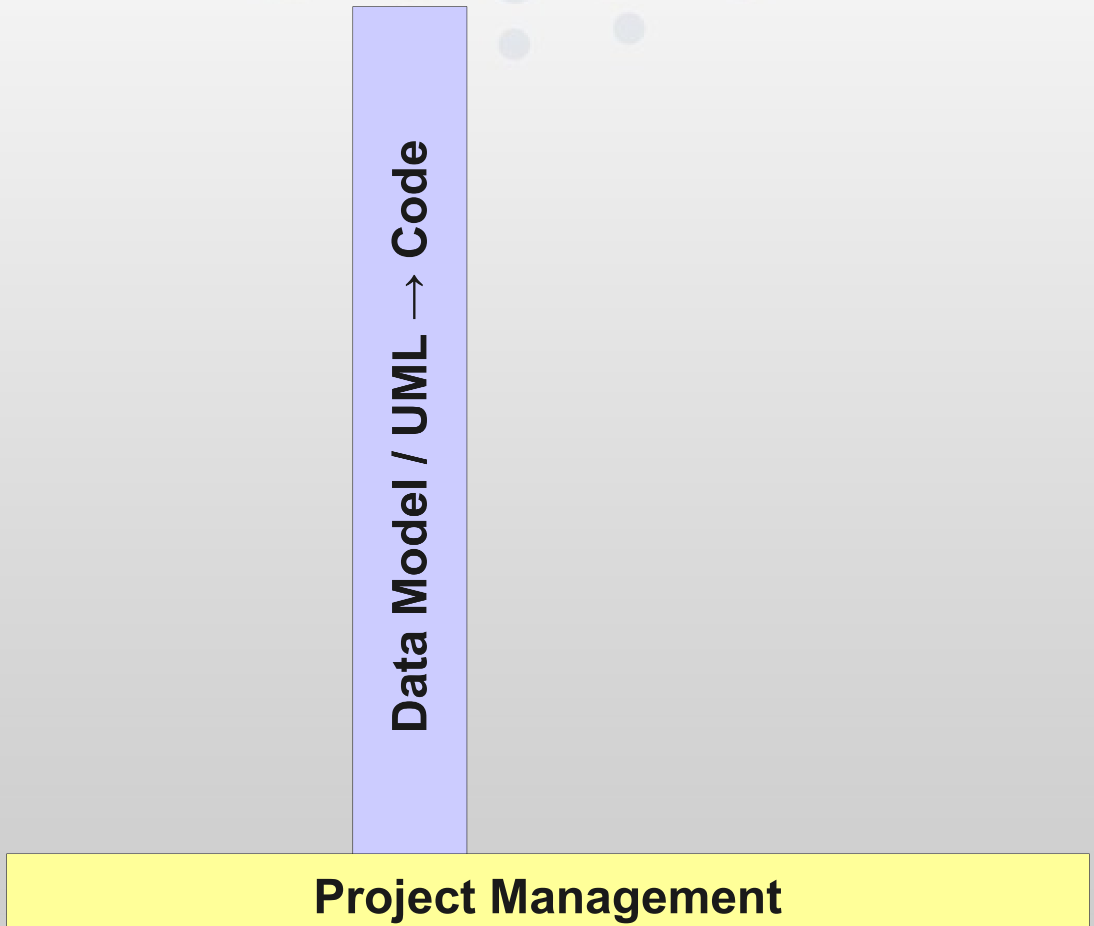
EDNA Project Management

- 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 (now replaced by EVO)

The first pillar – Data Model Framework



EDNA Data Model Framework

- What is a data model? From wikipedia:

  A data model in software engineering is an abstract model that describes how data are represented and accessed. Data models formally define data elements and relationships among data elements for a domain of interest.

  Communication and precision are the two key benefits that make a data model important to applications that use and exchange data.

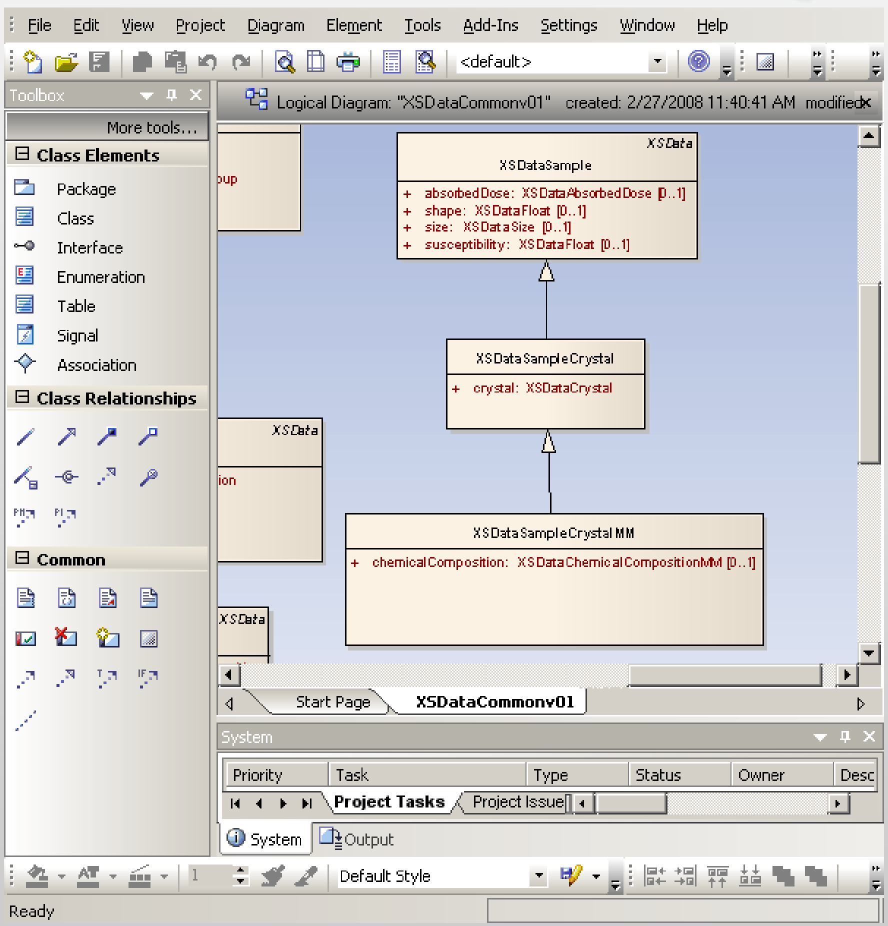
- Since we want to make workflows → communication between programs → data modelling is important

How are Data Models used in EDNA?

- The “common” data model :
  - This data model defines a set of simple basic types (e.g. double, string etc) and some more complex (3x3 matrix) which can be used by all other EDNA data models.
  - The common data model is a part of the EDNA kernel.
- The “specific” data models :
  - Data models which are specific for a certain task or program, e.g. data models for MOSFLM, XDS, FIT2D etc
  - The specific data models are typacilly used only by a few EDNA plugins (modules)
- The “generic” or “project” data models :
  - These data models should not be dependent on a single program but rather be developed for a certain scientific area, e.g. MX, tomography etc.

The EDNA Data Model Framework

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




```
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     <xs:complexContent>
          <xs:extension base="XSData">
               <xs:sequence>
                    <xs:element name="absorbedDose
                    <xs:element name="shape" type=
                    <xs:element name="size" type="
                    <xs:element name="susceptibil
               </xs:sequence>
          </xs:extension>
     </xs:complexContent>
</xs:complexType>
```
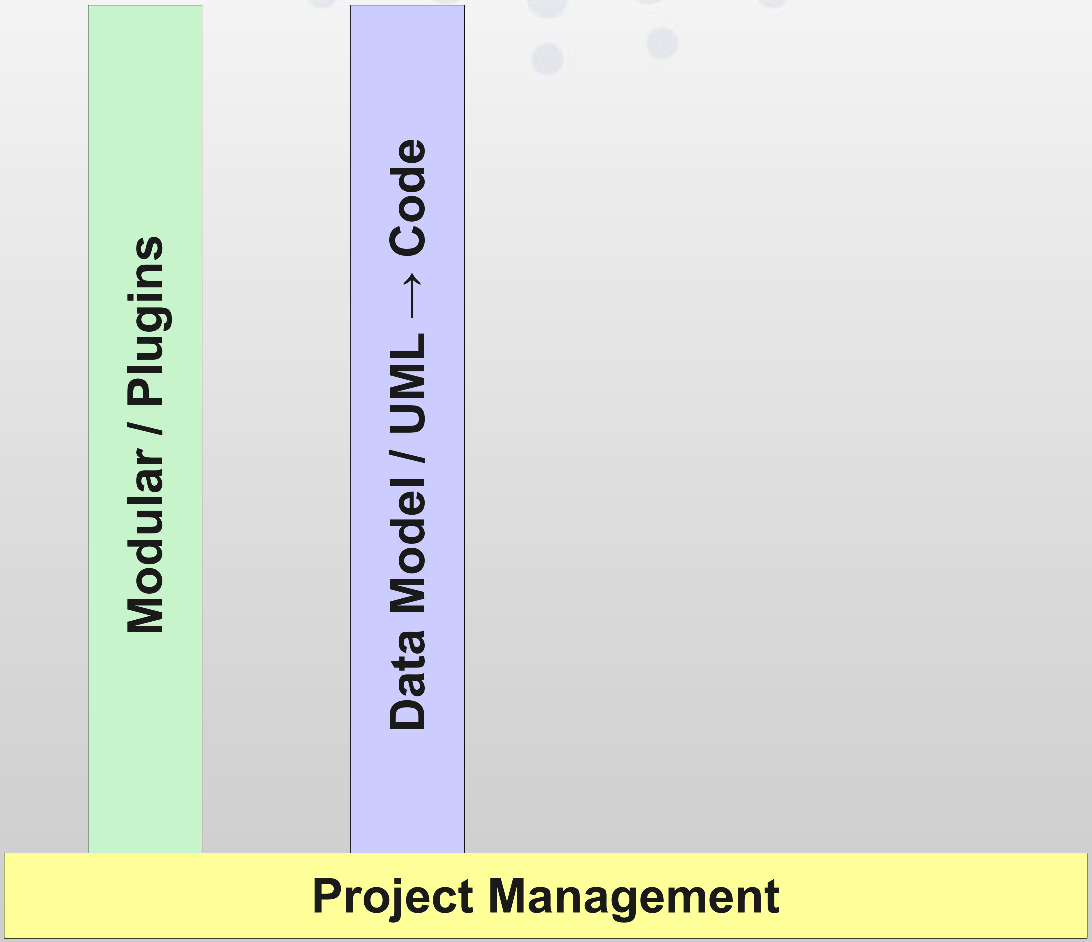

The second pillar – modularity / plugins



Why do we want modules / plugins ?

- Again from wikipedia:

  In computing, a plug-in is a set of software components that adds specific capabilities to a larger software application.

  Applications support plug-ins for many reasons. Some of the main reasons include:

  - *to enable third-party developers to create capabilities which extend an application*
  - *to support easily adding new features*
  - *to reduce the size of an application*
  - *to separate source code from an application because of incompatible software licenses.*

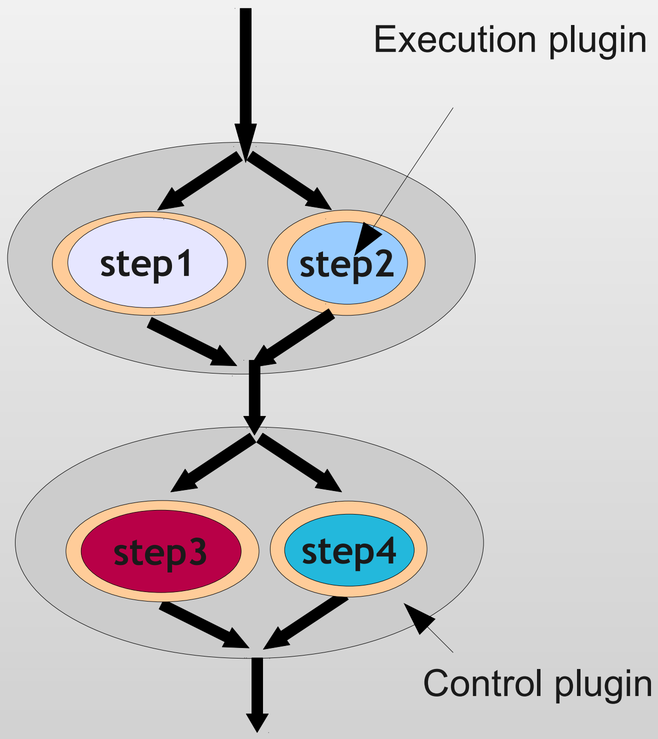
EDNA Framework : Kernel + Plugins

- The EDNA kernel contains:
  - The common data model and data binding generator code
  - Base classes for all EDNA plugins
  - Base classes for EDNA applications
  - Some utility/helper classes
  - The testing framework
  - The plugin generator
  - Plugin and test launcher scripts
  - The EDNA kernel is written in pure Python
  - No dependency on AALib any longer

- An EDNA application consists generally of:
  - One or several data model based on the common data model
  - A set of plugins derived from the kernel plugin base classes
  - One or several application classes
  - One or several scripts for launching the application

EDNA Modularity : Plugins and their hierarchy

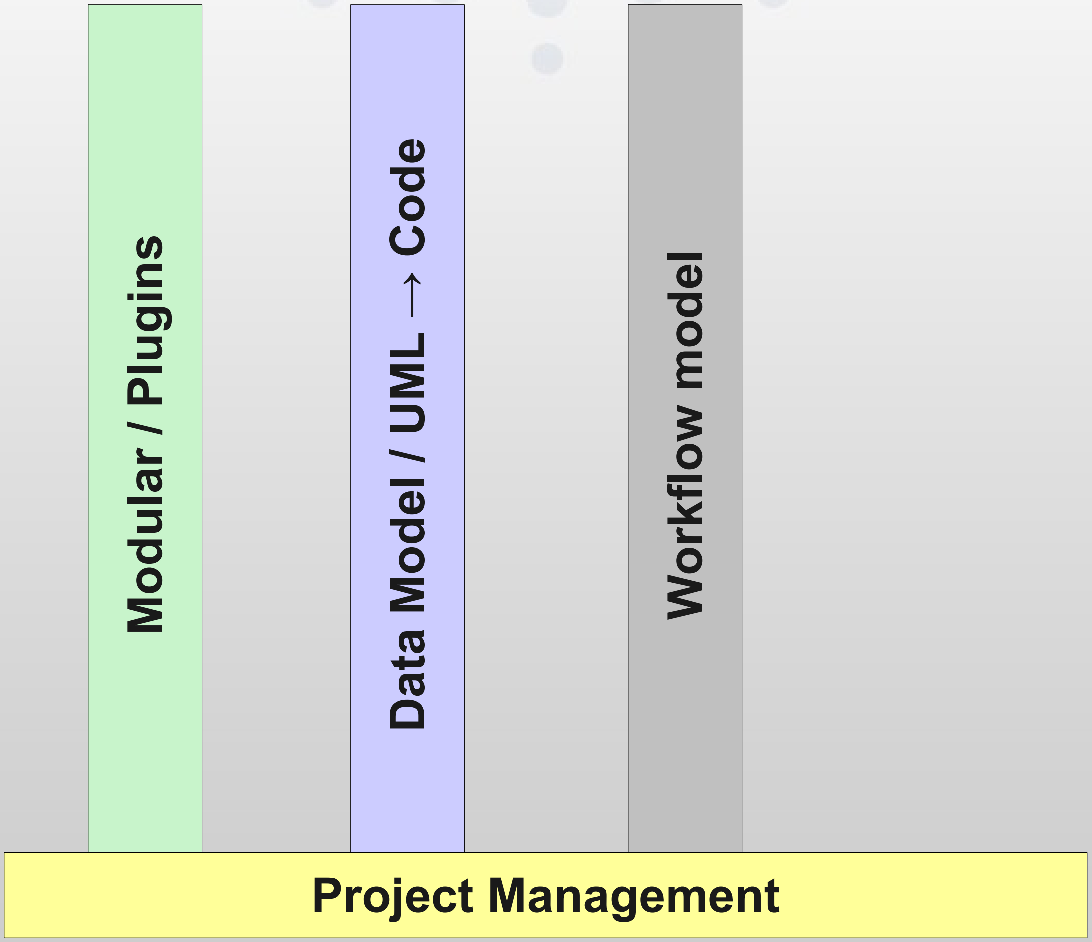
- Plugin base class :
  - Configuration, working directory, etc.
- Execution plugins :
  - Execution of external programs, e.g. (bash) scripts
- Controller plugins:
  - Control of execution plugins
  - Parallel execution
  - Synchronisation



EDNA Plugins Features :

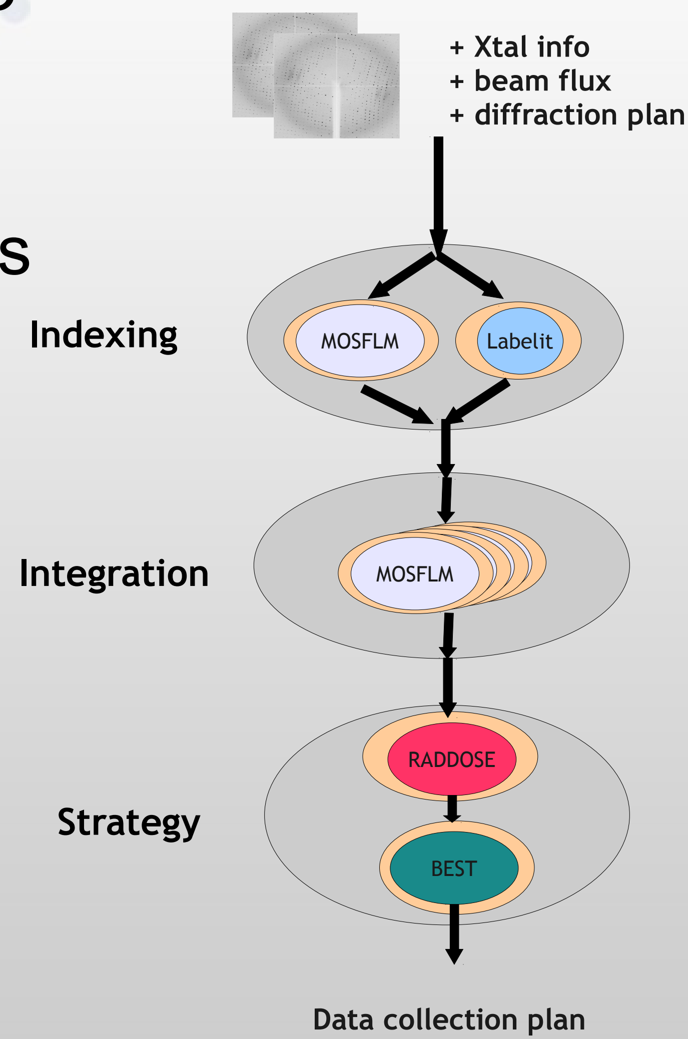
- Self-contained plugin structure:
  - Data model(s)
  - Plugin source code
  - Data binding objects
  - Unit and execution tests
  - Data for tests
  - Documentation
- Fast dynamic plugin loading (cache)
- Plugin execution and synchronisation (threadsafe)
- Plugin configuration
- Handling of input and output data

The third pillar - workflows

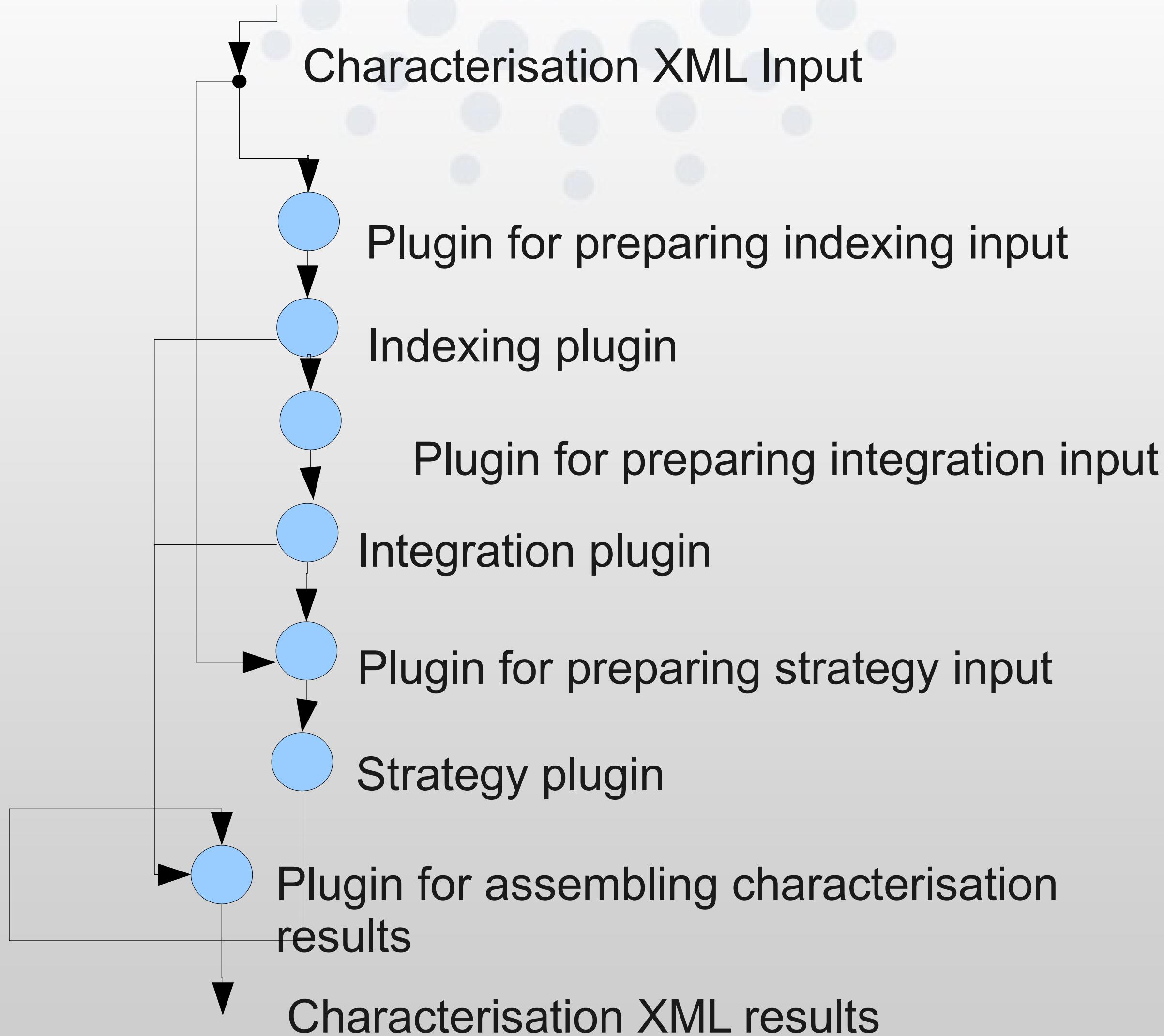


Example EDNA workflow : MXv1 Characterisation (1)

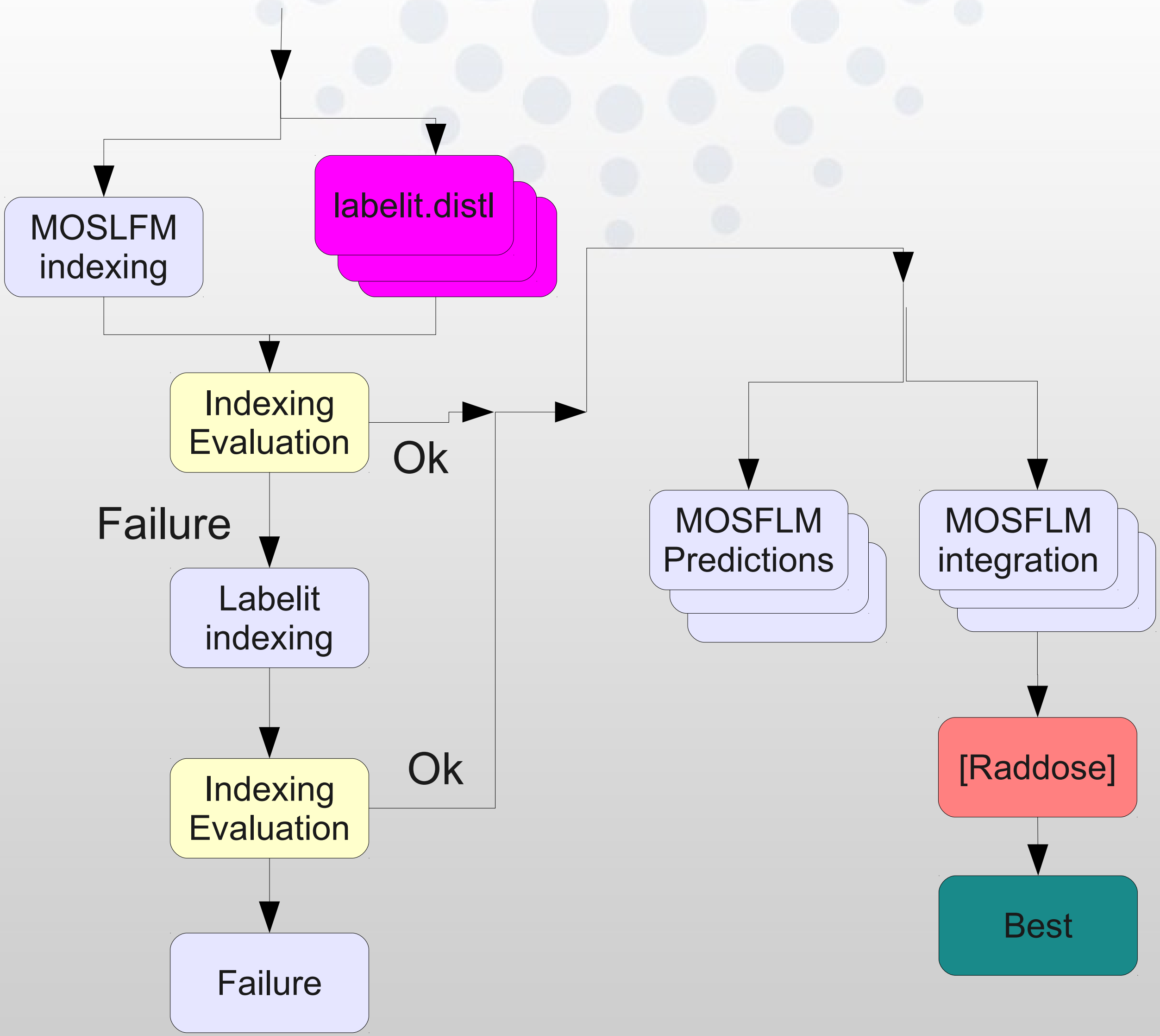
- MX sample characterisation taking into account radiation damage
- Indexing using MOSFLM or Labelit
- Parallel integration of reference images
- If flux + beamsize:
  - RADDOSE for estimating radiation damage
- BEST strategy calculation
  - taking into account radiation damage
  - multi-subwedge data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



Example Characterisation Workflow (1)

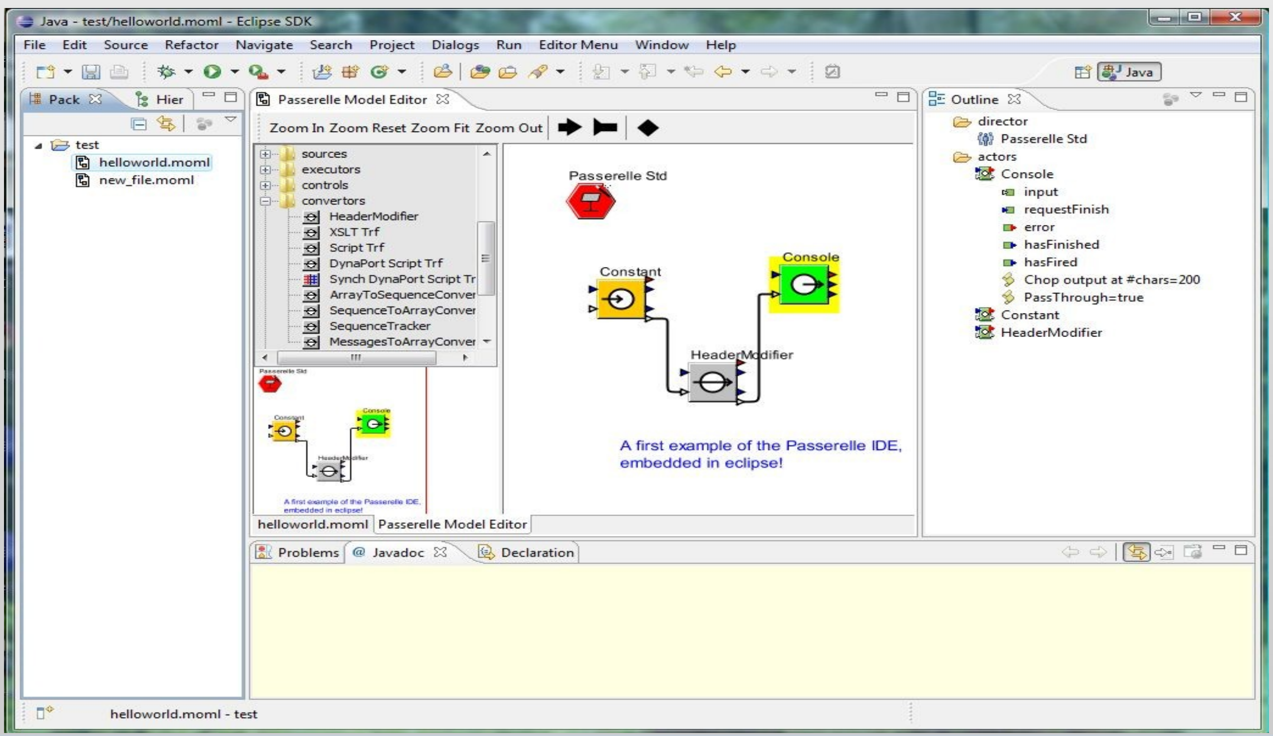


MXv1 Characterisation (2)

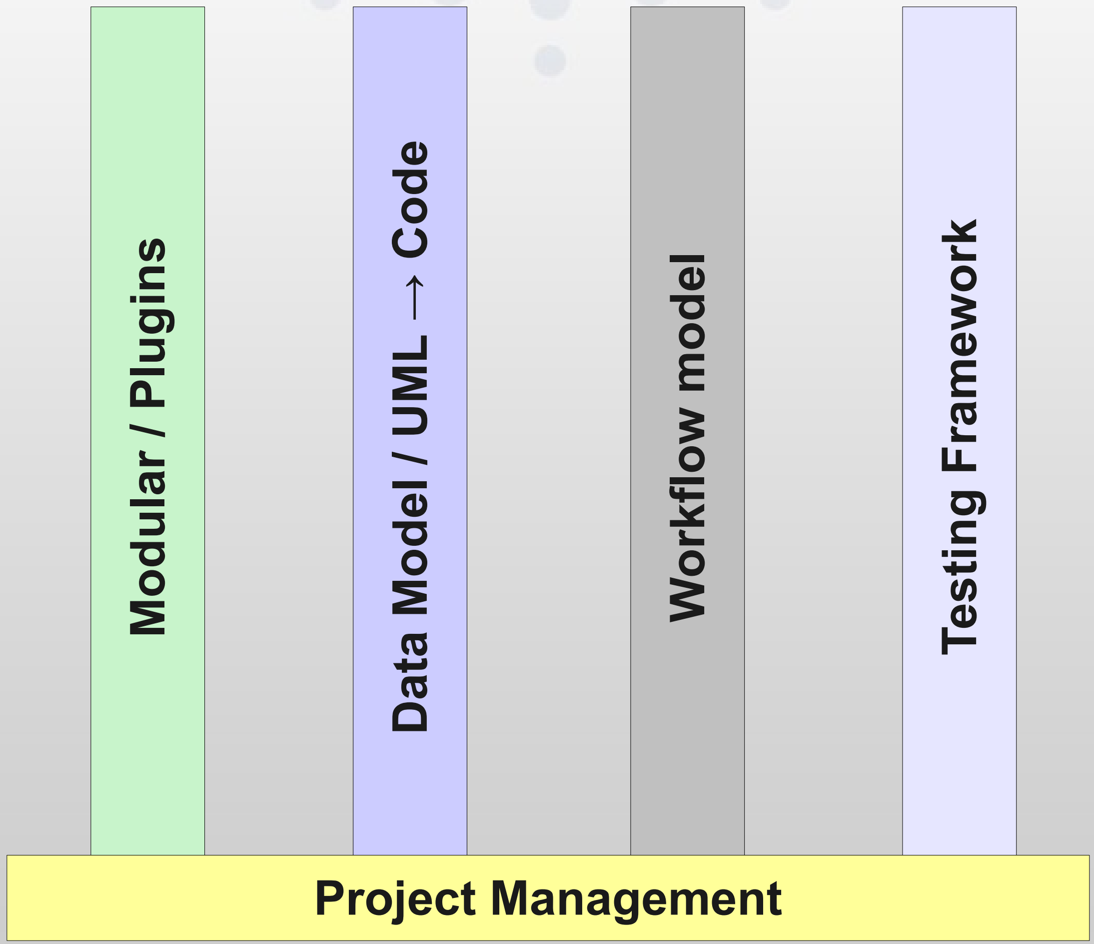


Why use a workflow tool in EDNA?

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



The fourth pillar – the testing framework

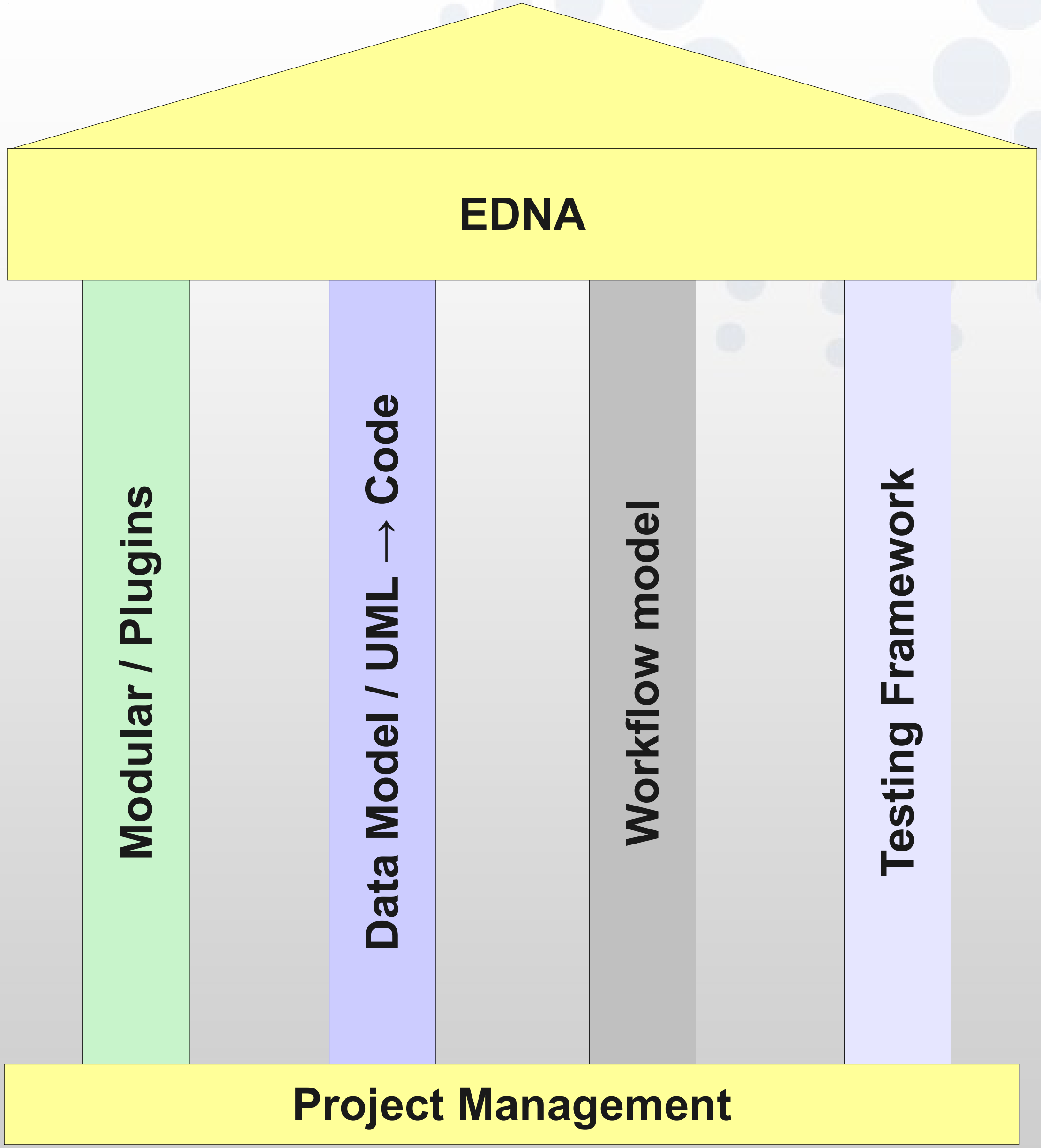


EDNA Testing Framework

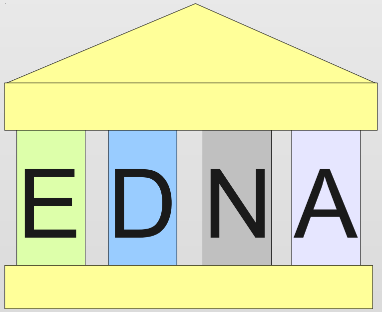
- The EDNA testing framework consist of three layers :
  - Kernel Unit tests
  - Plugin Unit tests
  - Plugin Execution tests

- Example of EDNA Plugin Execution tests result:

```
[UnitTest]: ###################################################################
[UnitTest]: Result for EDTestSuiteKernel : SUCCES
[UnitTest]:
[UnitTest]:
[UnitTest]:   Total number of test cases executed with SUCCESS : 10
[UnitTest]:   Total number of test cases executed with FAILURE : 0
[UnitTest]:
[UnitTest]: Total number of test methods executed with SUCCESS : 26
[UnitTest]: Total number of test methods executed with FAILURE : 0
[UnitTest]:
[UnitTest]:                                           Runtime : 4.420 [s]
[UnitTest]: ###################################################################
```

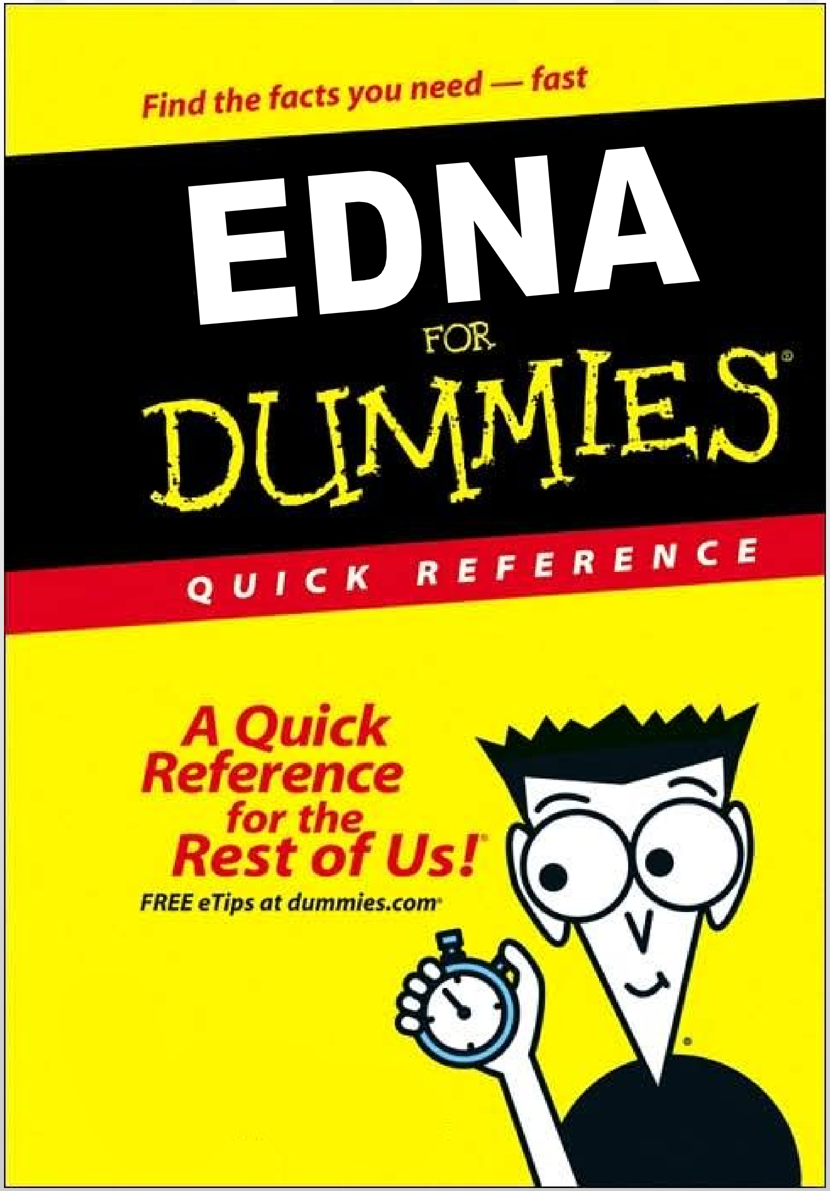

EDNA
Modular / Plugins
Data Model / UML → Code
Workflow model
Testing Framework
Project Management

New logo :


E D N A

To be avoided...

Documentation!



EDNA Documentation

- Available today :
  - Data models (png)
  - Automatic API doc generation
  - Wikipages with developers' “How-to”s
  - Minutes / presentations of previous meetings, code camps etc
- Planned :
  - Automatic plugin documentation repository (use cases etc)
  - Workflow documentation (workflow tool)

EDNA is not DNA...

- Same goals (initially)...
  - Automatic MX sample characterisation
  - Online data processing during MX data collection
  - Ranking
- ...however very different implementations
  - EDNA designed to not be specific to MX
  - No shared code base between DNA and EDNA
  - Different project management
  - Different collaborators

EDNA Collaborators 2009

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]
Jérôme Kieffer(e)
Johan Turkenburg[m]
Johan Unge(g)
John Skinner[i]

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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]
Robert Sweet[i]
Romeu Pieritz[e]
Sandor Brockhauser[c]
Sean McSweeney[e]
Takashi Tomizaki[j]
Thomas Schneider[c]
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(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