EDNA – building on the experiences from MX automated strategy determination

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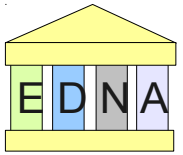
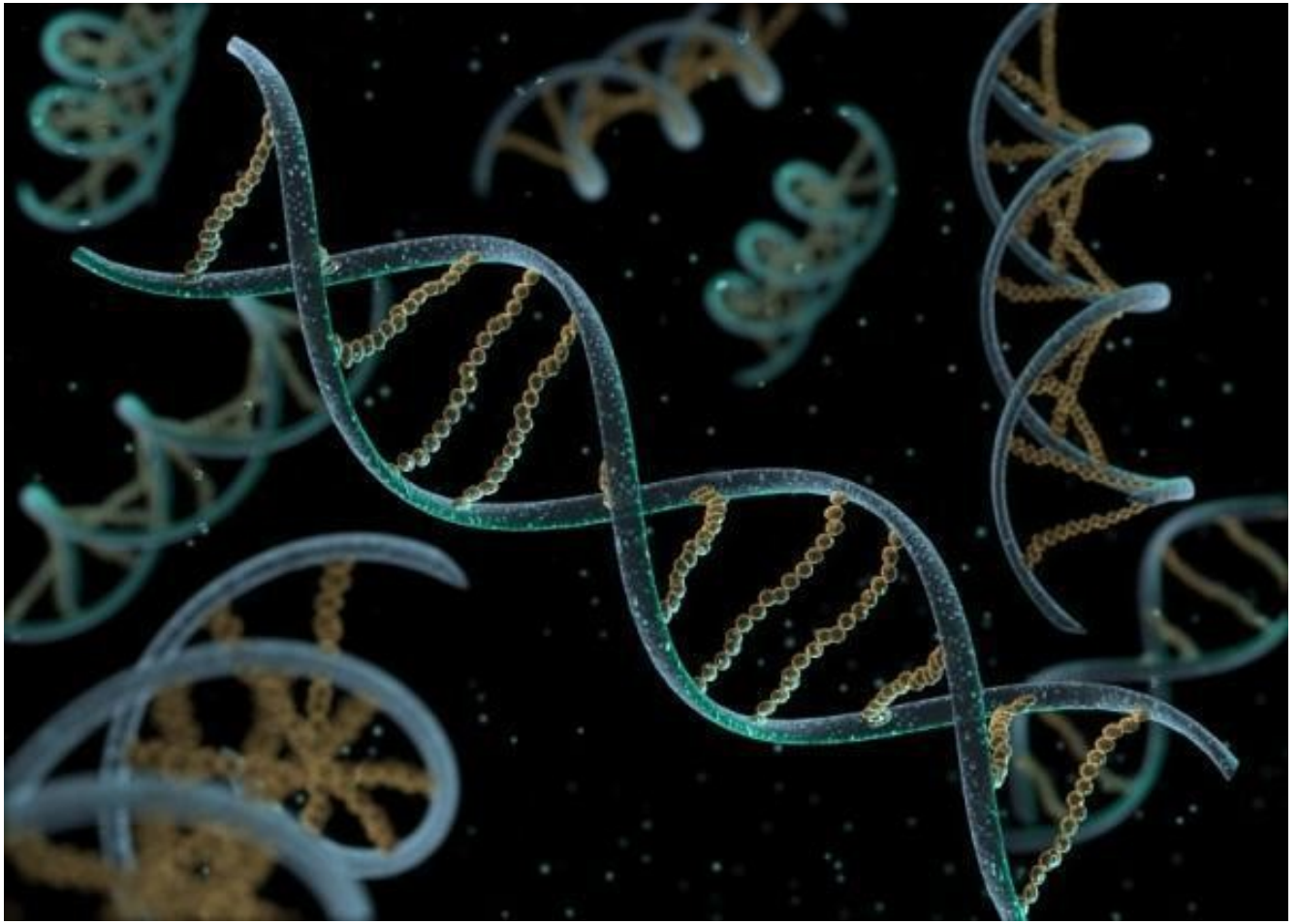
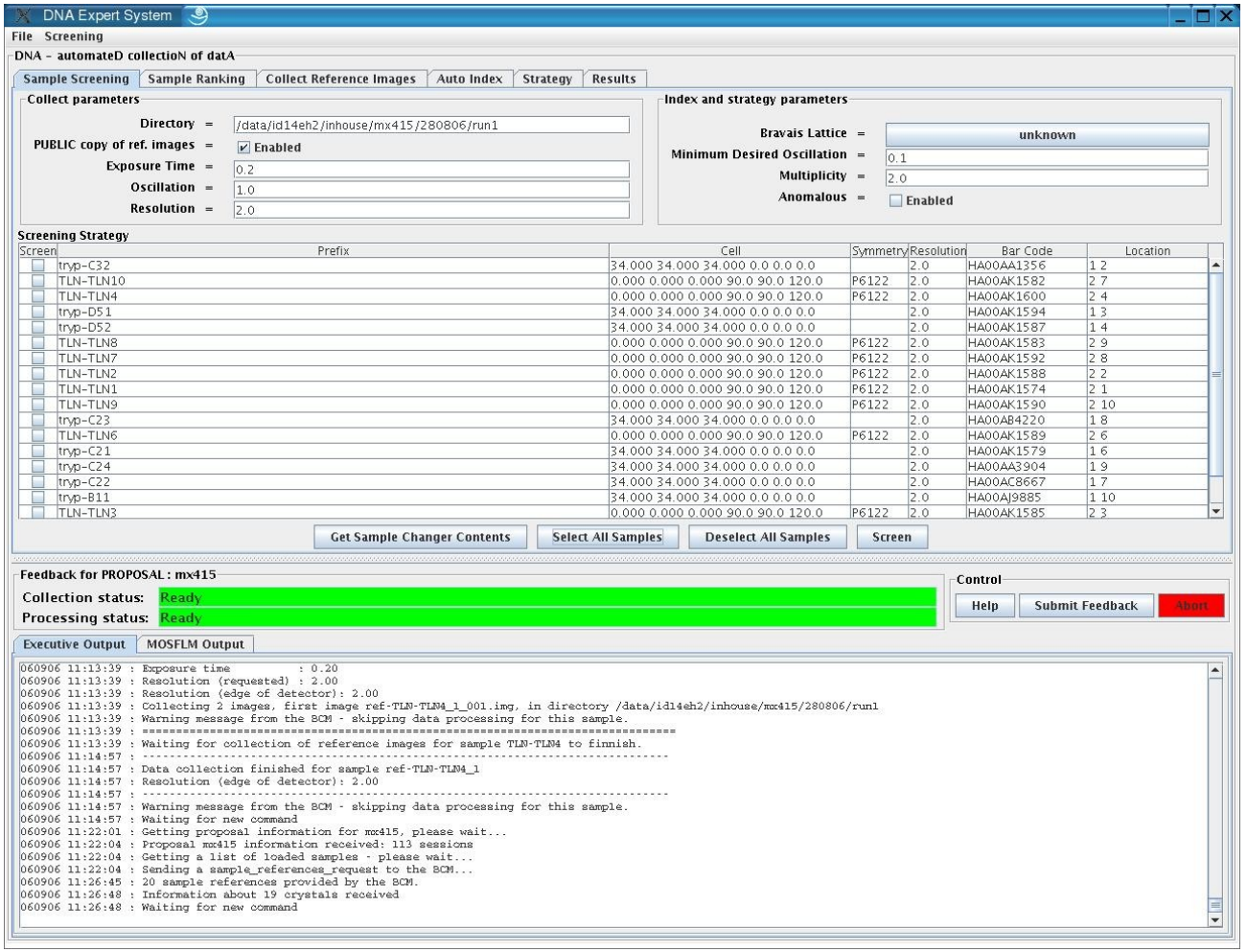


In the beginning there was DNA...



… or RNA or something else, if you speak about life...

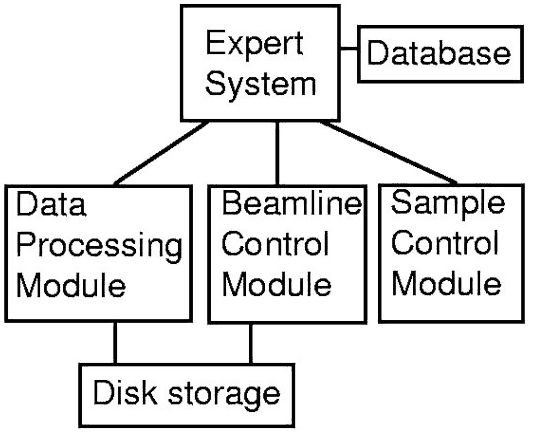
In the beginning there was DNA...

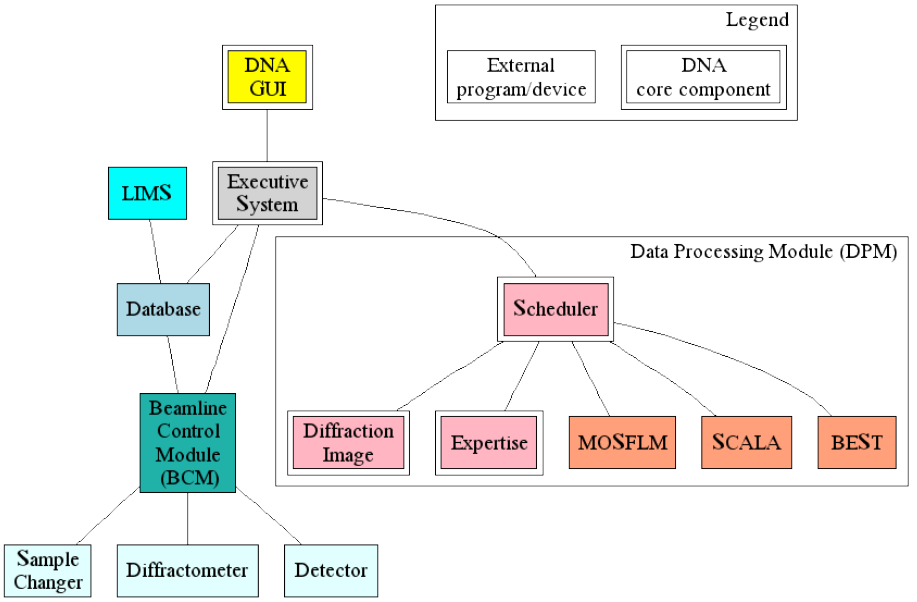


… if you speak about EDNA!

Beginning of automated MX characterisation... … or DNA in one slide

- Kick-off meeting in 2001
- Initial collaborators :
  - ESRF
  - Daresbury SRS
  - MRC LMB Cambridge
- Initially no external funding
- Meaning of ”DNA” :
  - automate**D** collectio**N** of dat**A**
- **Main development period 2001 – 2005**
- More collaborators and more developers entered the project, mainly thanks to external fundings : BioXHIT and e-HTPX.
- Since 2005 an integral part of the ESRF ”data collection pipeline”
- Installed and used at :
  - ESRF
  - Diamond
  - Recently used at NSLS (Brookhaven), now using EDNA
- **Major component of the 2008 BESSY innovation award**





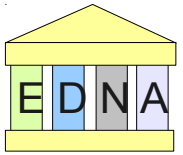
...so – why not DNA?

Good things learned from DNA:

- Collaboration :
  - Scientists involved in design and testing
  - Executive committee for setting milestones / deliverables and for resolving conflicts between developers
- Two major Use Cases implemented :
  - Characterisation + data collection with online integration and quick scaling
  - Automatic screening and ranking

Not so good things learned from DNA...:

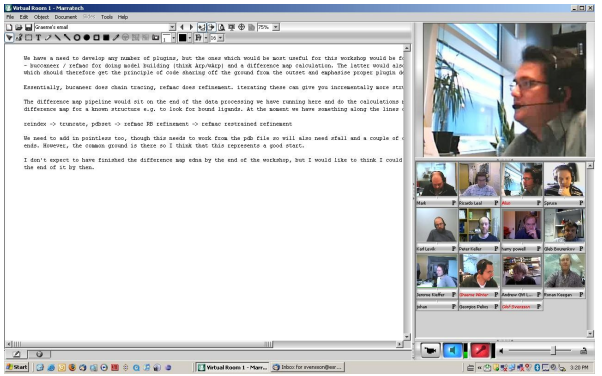
- The choice of name...
- Collaboration :
  - No project agreement
  - Minimal project management
- Not modular:
  - Too costly to change work flow
  - Poorly designed data model
  - Difficult for new developers to enter the collaboration
- MX hardwired!

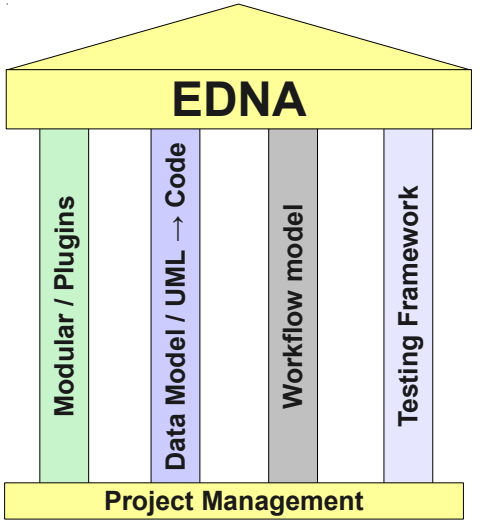


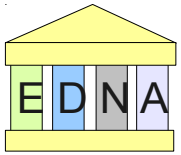
What is then EDNA?

- EDNA is about collaboration:
  - Code sharing (SVN)
  - Coding conventions
  - Code reviews
  - Open source (LGPL, GPL)
  - Bug tracker
  - Wiki
  - 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 builts
  - Automatic API doc generation

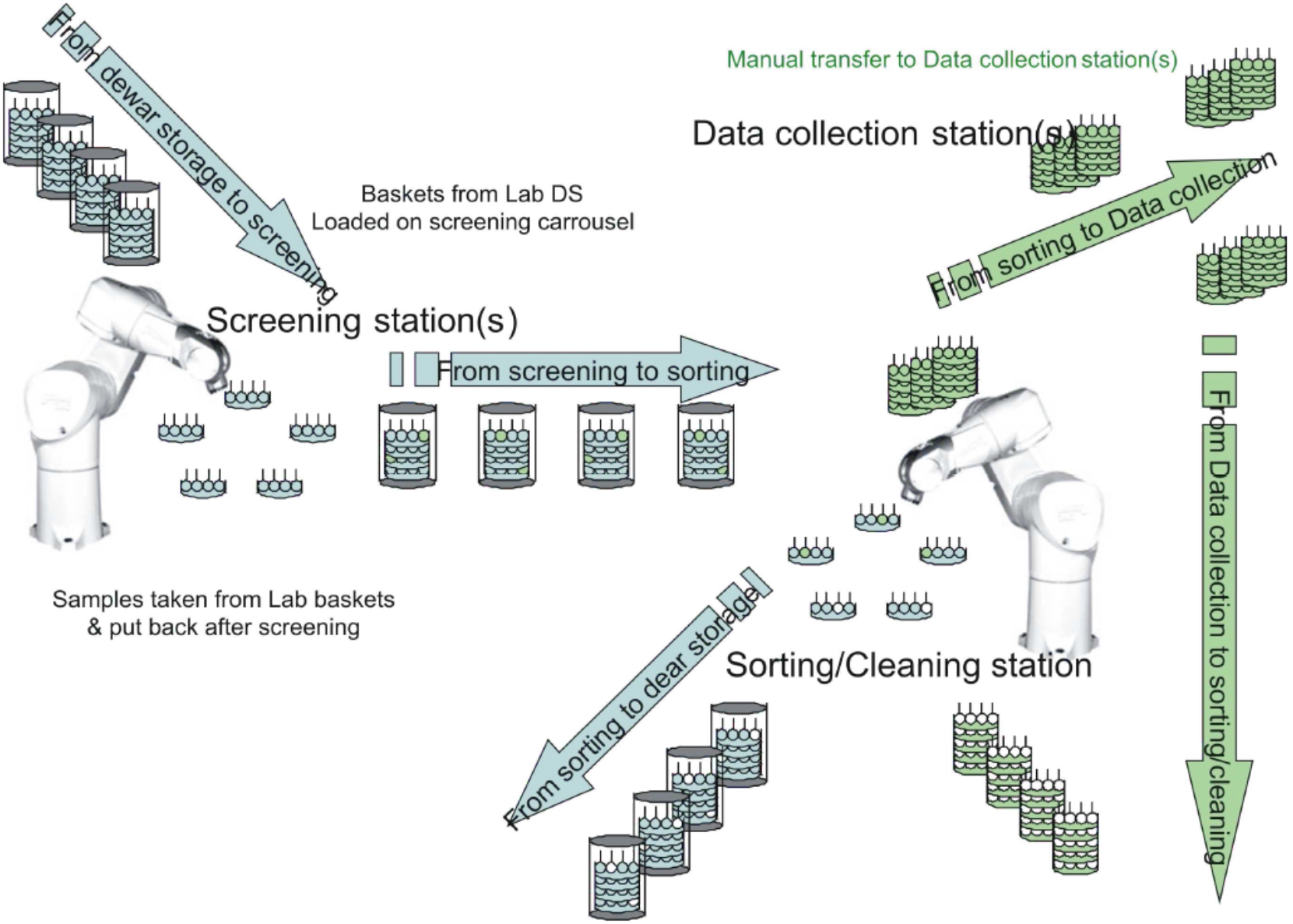






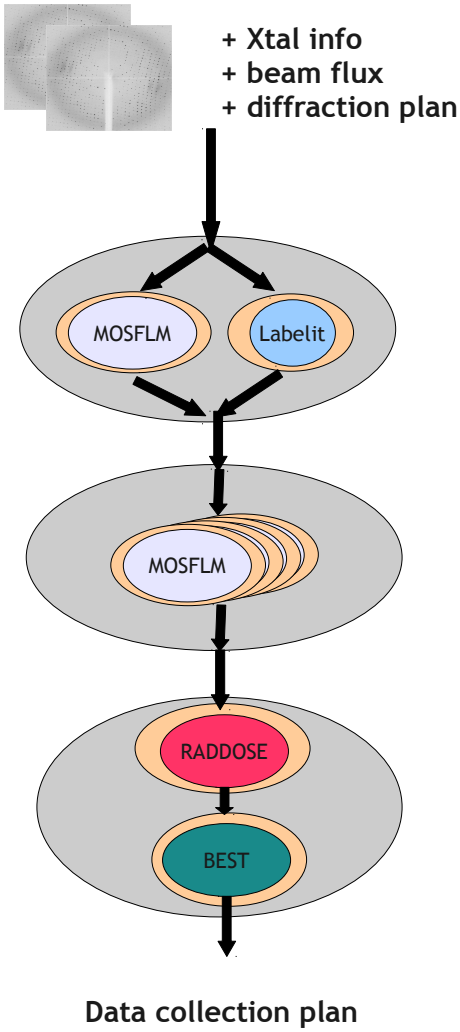
… what's mentioned above are lessons learned from the DNA collaboration

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

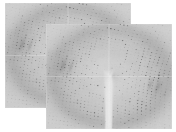


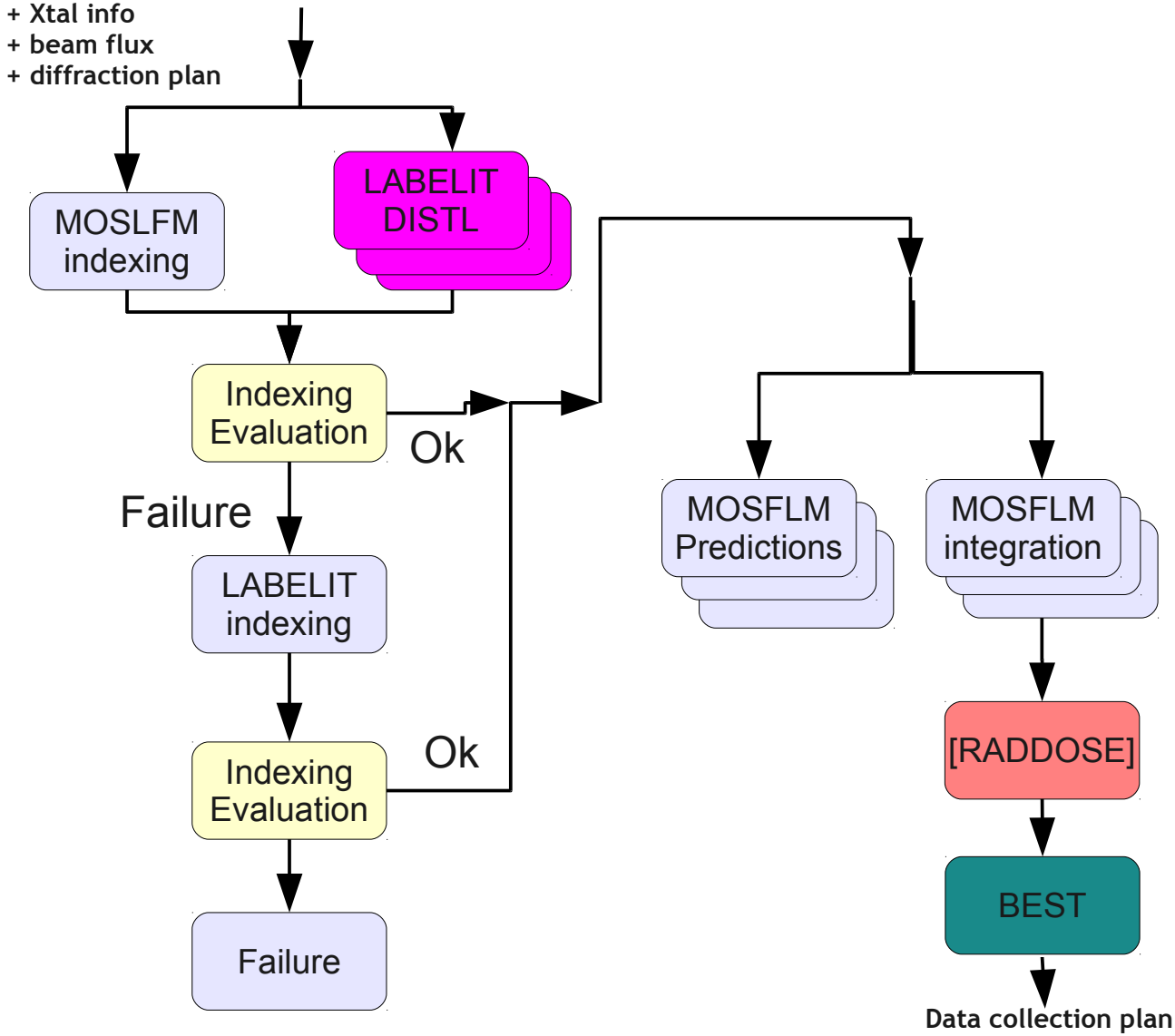
Example EDNA workflow : MXv1 Characterisation v1.1

- MX sample characterisation taking into account radiation damage
- Indexing using MOSFLM or Labelit
- Parallel integration of reference images
- If flux + beamsize : RADDOSE for estimating radiation damage (not in DNA!)
- BEST strategy calculation
  - taking into account radiation damage
  - multi-subwedge data collection strategies



Example EDNA workflow : MXv1 Characterisation v1.2





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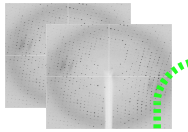
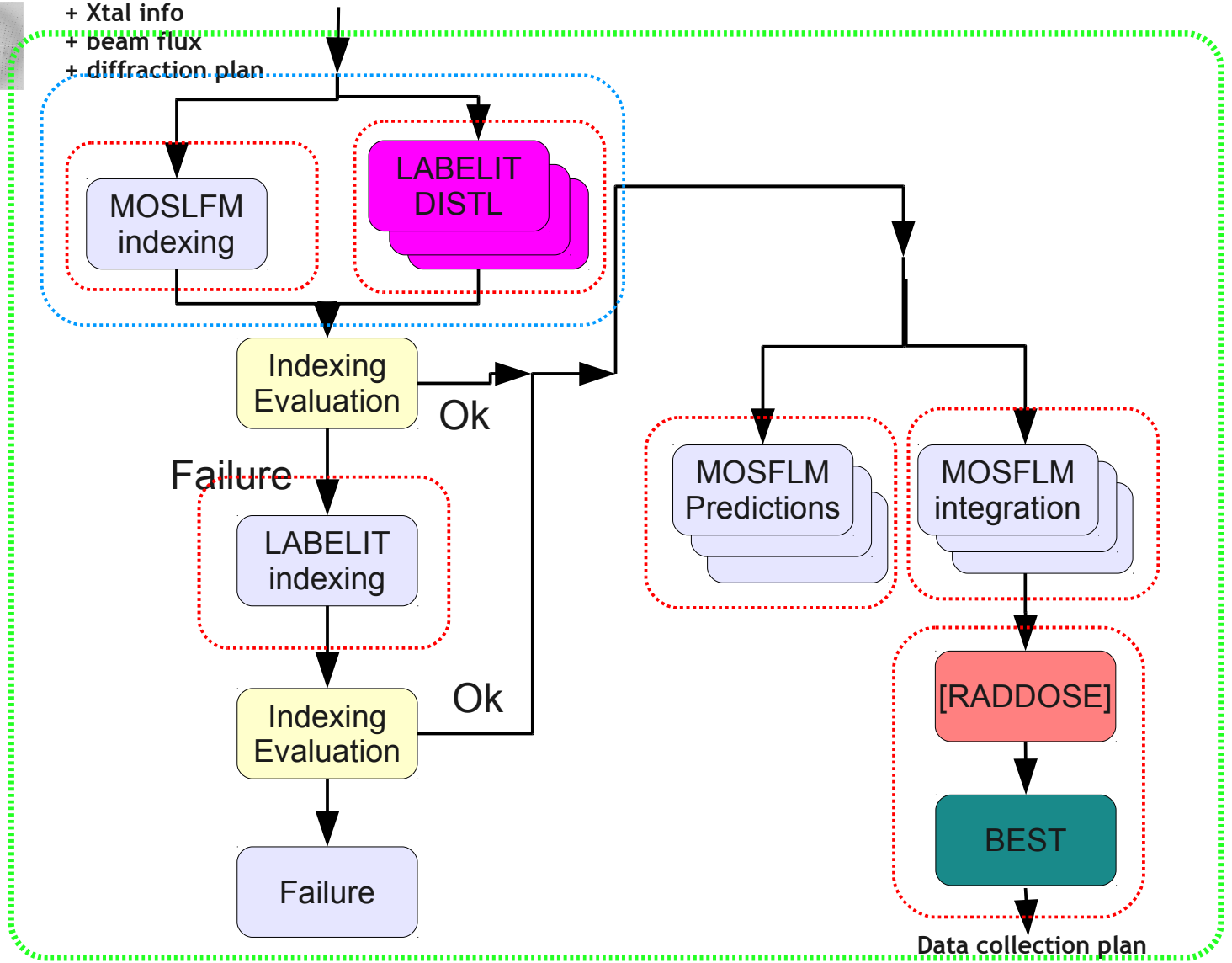
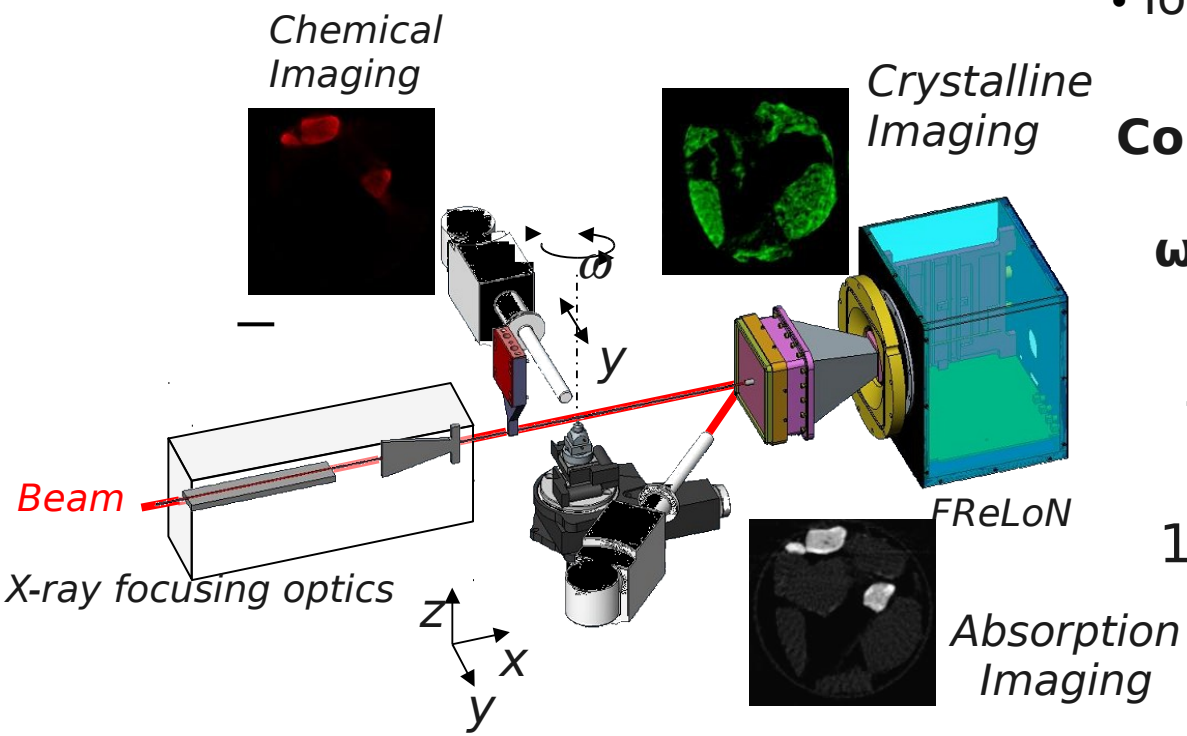




Part of ESRF upgrade project UPBL4: Nano-imaging / Nano-analysis



Experimental setup @ ID22:

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

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

Commonly N ≈ 160 scanning steps/y-line,
ω ≈ 60 angular steps/tomographic scan

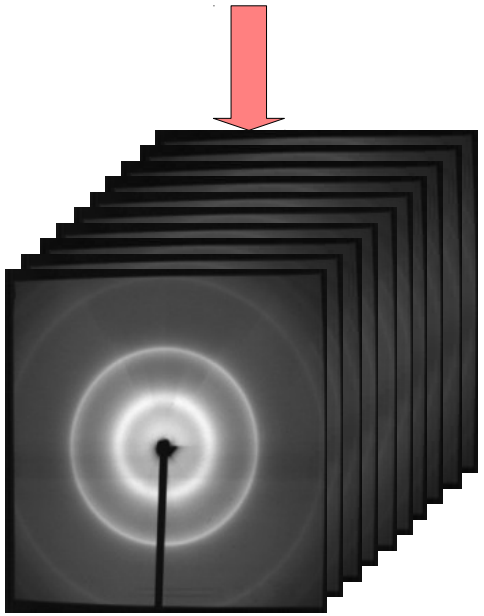
10-15h beamtime required/tomo scan
100 Go data generated/tomo scan

Slide from Pierre Bleuet

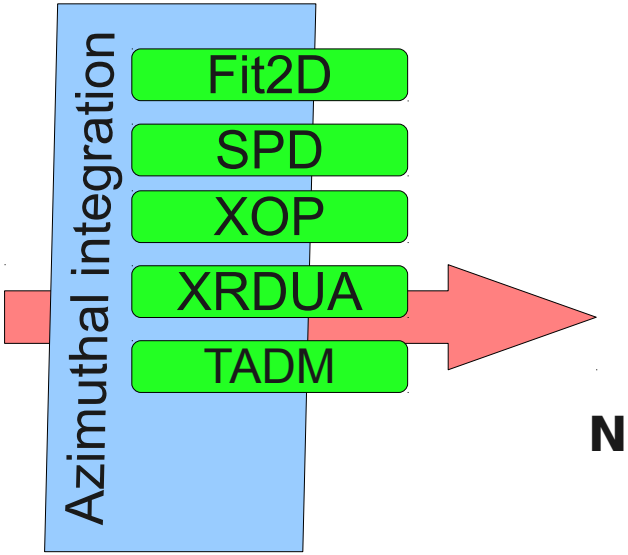
Online data Analysis for NINA

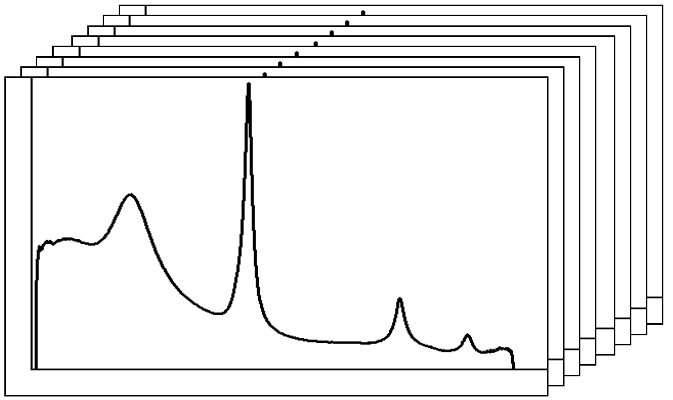
- Focus on most CPU demanding application: DiffractionCT

FReLoN2k
(EDF, 16bit UInt, LittleEndian)



N x **ω** 2D Diffraction Images

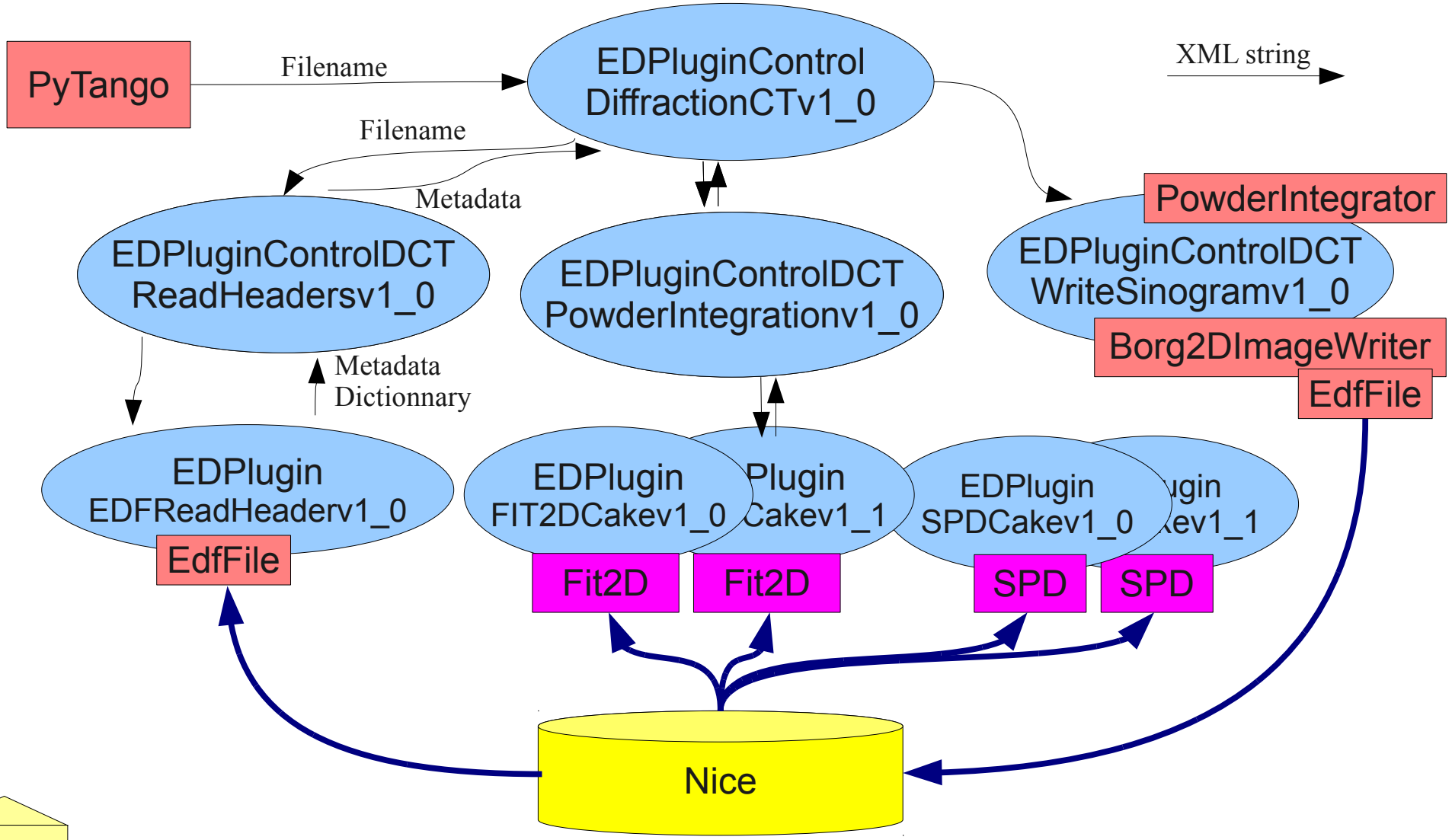




N x **ω** 1D diffraction patterns

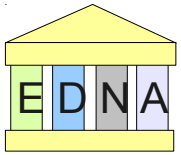
Integration of many tools
Need plugin gestion

Diffraction CT implementation in EDNA



Current development status

- Execution plugins:
  - MxExecPlugins: 24 exec plugins
  - Exec plugins: 21 exec plugins
  - Saxs(4), SPD (4), FIT2D (2), EDF (2), HDF5 (2), thumbnail, video, …
- Control plugins:
  - MX v1 26 control plugins, 7 exec plugins
  - MX v2 3 control plugins
  - DiffractionCT v1 6 control plugins
  - BioSaxs 5 control plugins
- Other projects (CCP4, Dimple, Darc ...):
  - Managed mainly by Diamond and CCP4
  - 27 plugins: 8 control plugins & 19 execution plugins
- Total: 119 – 71 Execution plugins, 48 control plugins



EDNA Testing Framework

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

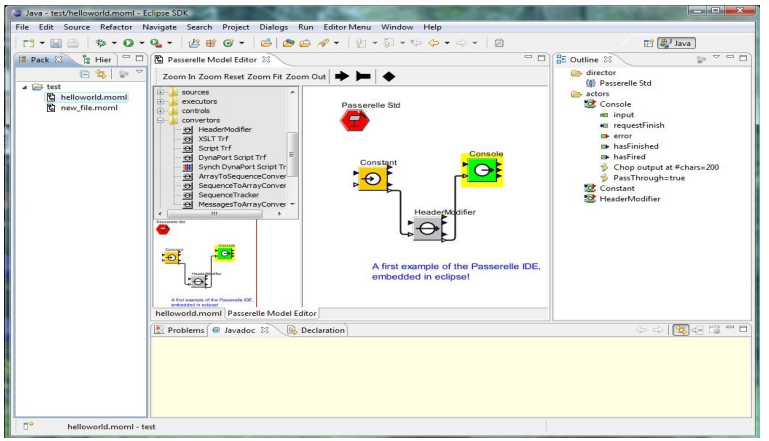
- Example of EDNA Plugin Execution tests result:

```
[UnitTest]: ###################################################################
[UnitTest]: Result for EDTestSuiteAll : SUCCES
[UnitTest]:
[UnitTest]:  Number of executed test suites in this test suite : 2
[UnitTest]:
[UnitTest]:
[UnitTest]:   Total number of test cases executed with SUCCESS : 175
[UnitTest]:   Total number of test cases executed with FAILURE : 0
[UnitTest]:
[UnitTest]: Total number of test methods executed with SUCCESS : 273
[UnitTest]: Total number of test methods executed with FAILURE : 0
[UnitTest]:
[UnitTest]:                                              Runtime : 630.138 [s]
[UnitTest]: ###################################################################
```

- Automatic testing every night + builds

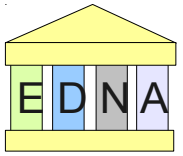
Future challenges for the EDNA framework

- 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



Upcoming events

- EDNA Full Meeting on Thursday September 23rd at the ESRF:
  - Overview of status of EDNA projects
  - MXv1 → MXv2 transition
  - Updated Memorandum of Understanding (MoU), separate kernel, MX and other MoUs
- Introduction to EDNA plugin development at the ESRF (not yet scheduled)
- Code camp / kernel developments (not yet scheduled)

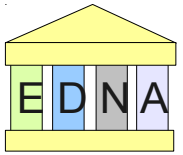


Conclusions

- The experiences of MX automated crystal characterisation (DNA) were used as the foundations for the EDNA collaboration

- The EDNA framework allow rapid and robust scientific application developments thanks to built-in support for four “pillars” of software engineering techniques:
  - Data modelling
  - Multi-threaded module/plugin development
  - Workflow developmet
  - Testing framework

- EDNA is now used for applications in MX and non-MX scientific data analysis developments



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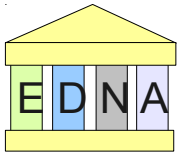


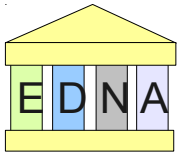
EDNA Data Model Framework

- 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.

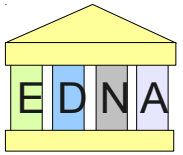
  Communication and precision are the two key benefits that make a data model important to applications that use and exchange data.

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



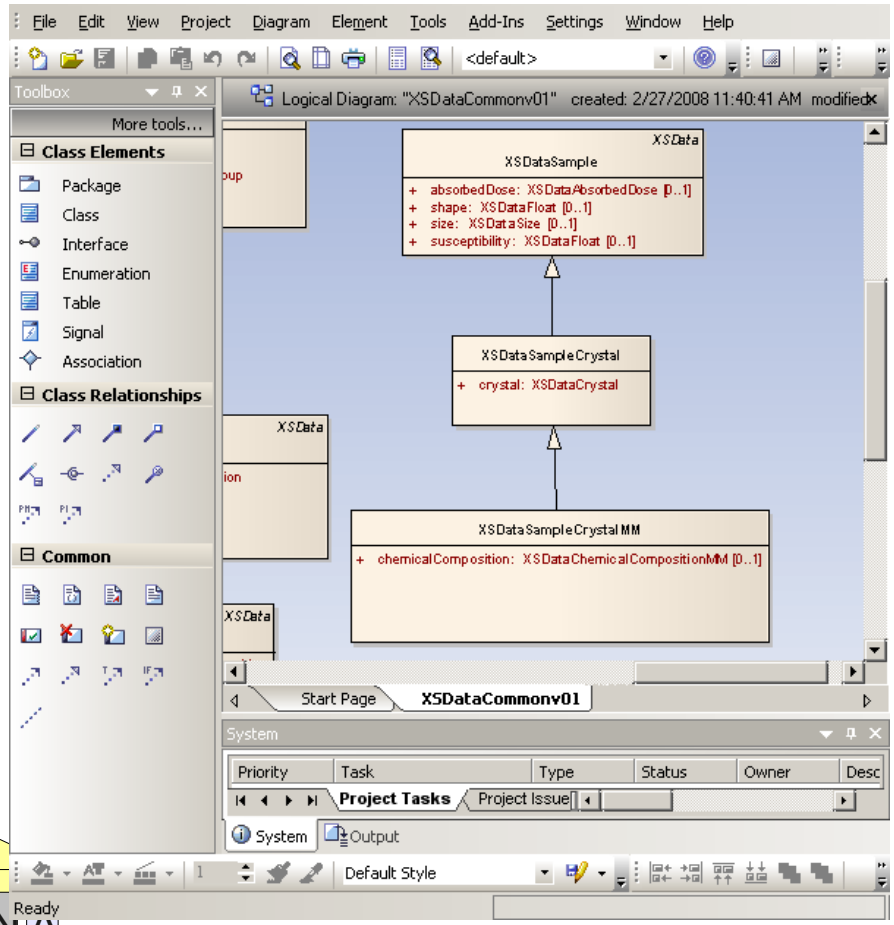
How are Data Models used in EDNA?

- 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) :




```
<xs:element name="XSDataSample" type="XSDataSample
<xs:complexType name="XSDataSample">
     <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="susceptibili
               </xs:sequence>
          </xs:extension>
     </xs:complexContent>
</xs:complexType>
```

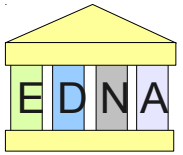
Why do we want modules / plugins ?

- Again from wikipedia:

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

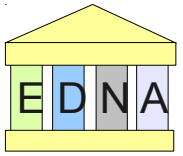
  Applications support plug-ins for many reasons. Some of the main reasons include:

  - *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.*



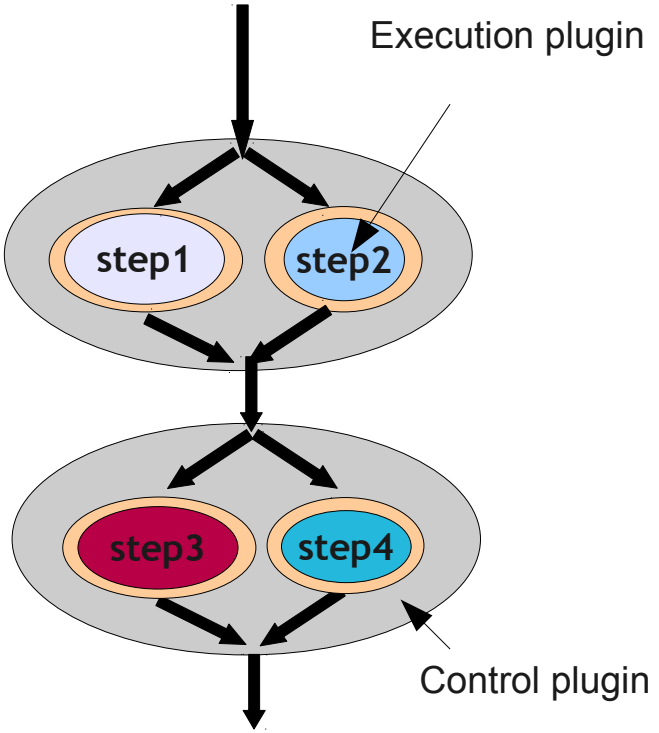
EDNA Plugins Features :

- 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)
- Multi-threaded plugin execution and synchronisation (threadsafe)
- Plugin configuration
- Persistence of data in XML using data bindings



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



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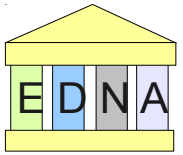

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