

A decorative background consisting of numerous light blue circles of varying sizes, arranged in a pattern that resembles a light scattering or diffraction pattern.

EDNA

Quick status of the project

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Why do we need EDNA?

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

What is EDNA?

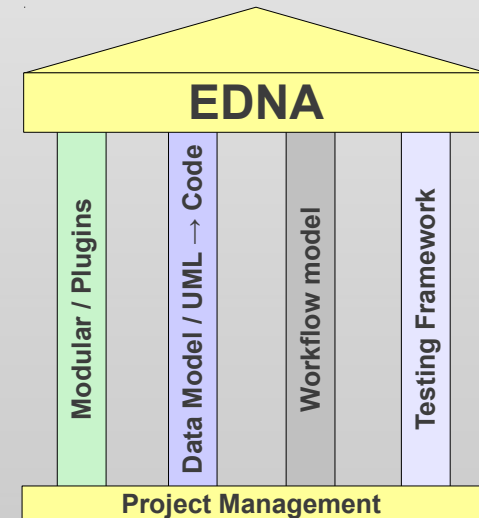
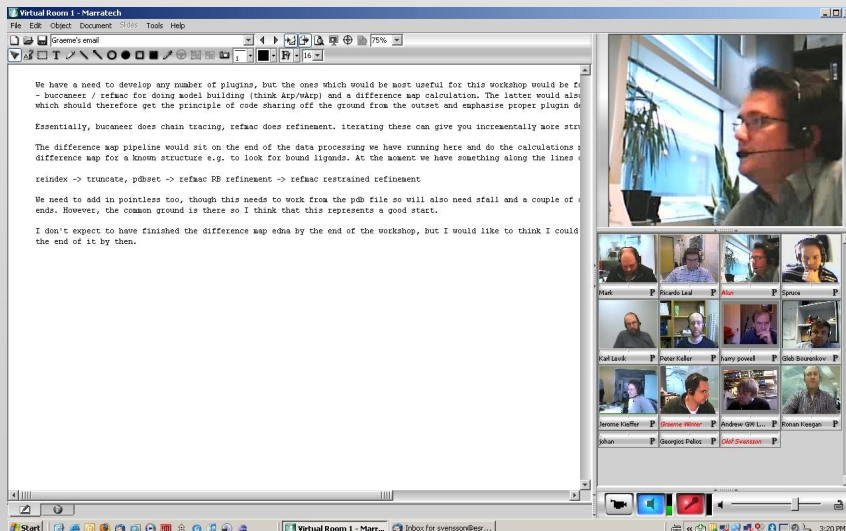


EDNA is about collaboration:

- 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

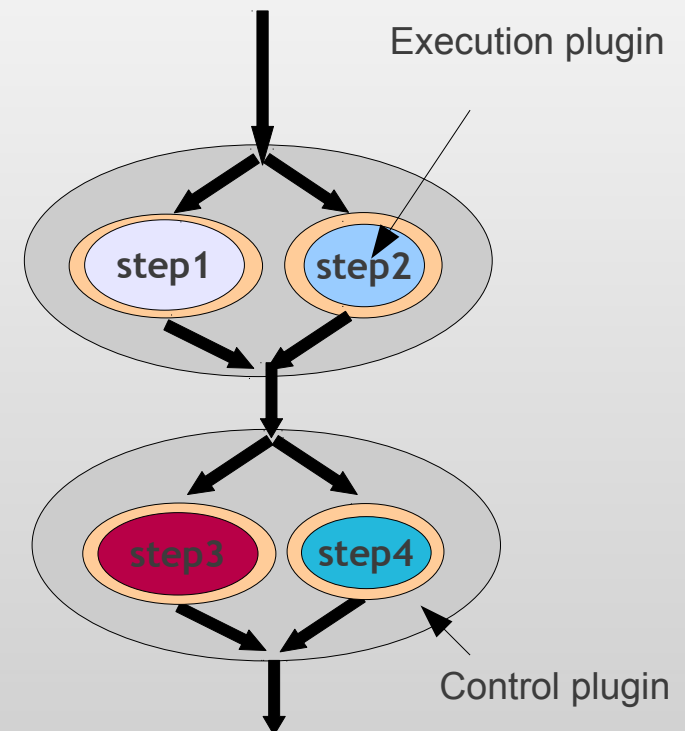
EDNA is a framework:

- “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



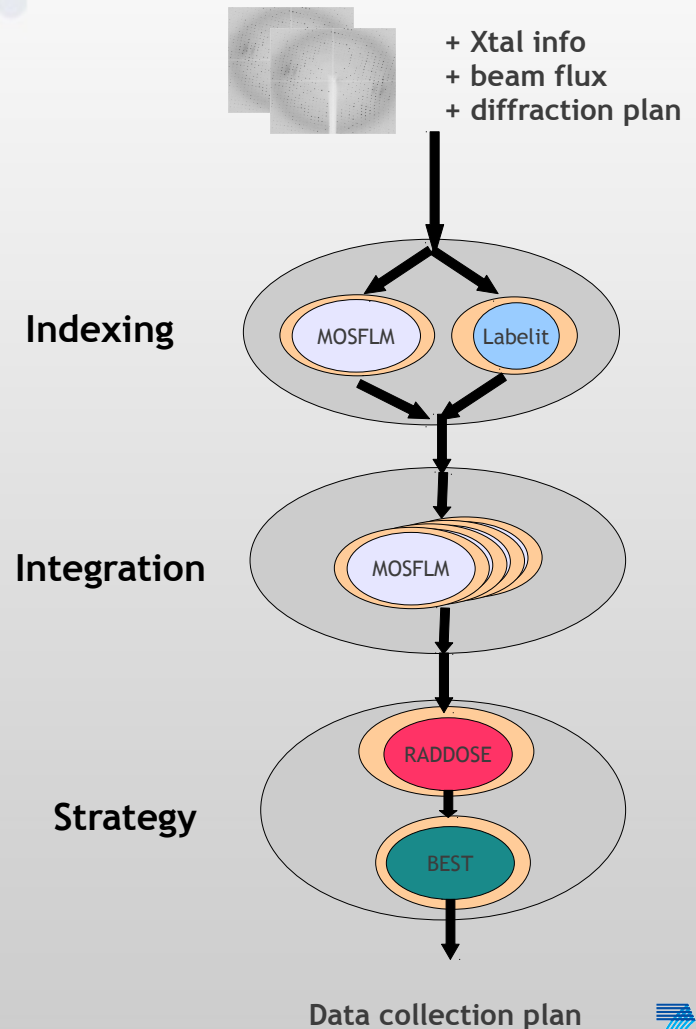
EDNA Modularity : Plugins and their hierarchy

- 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



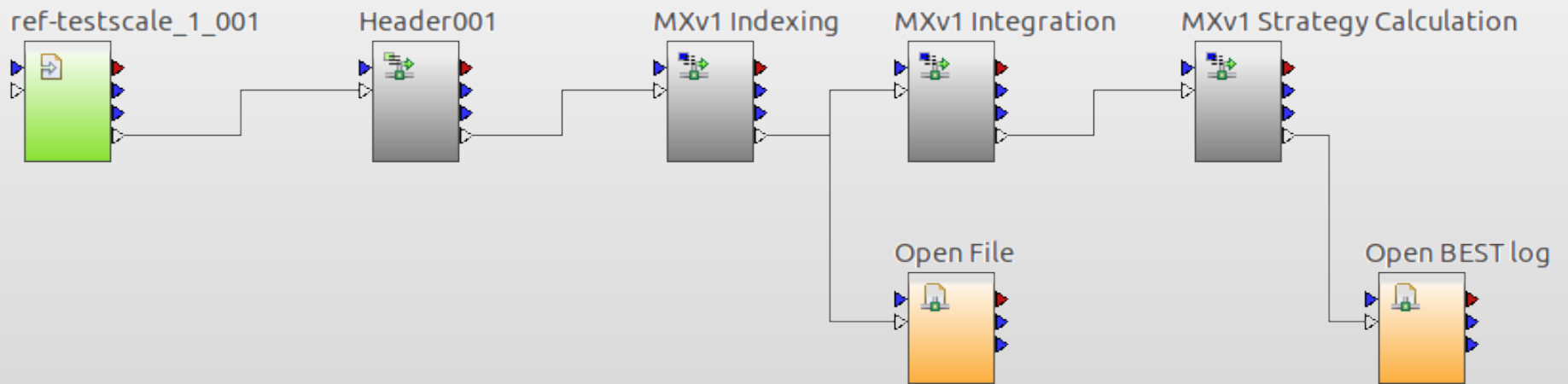
MXv1 Characterisation v1.1

- 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
- BEST strategy calculation
 - taking into account radiation damage
 - multi-subwedge data collection strategies

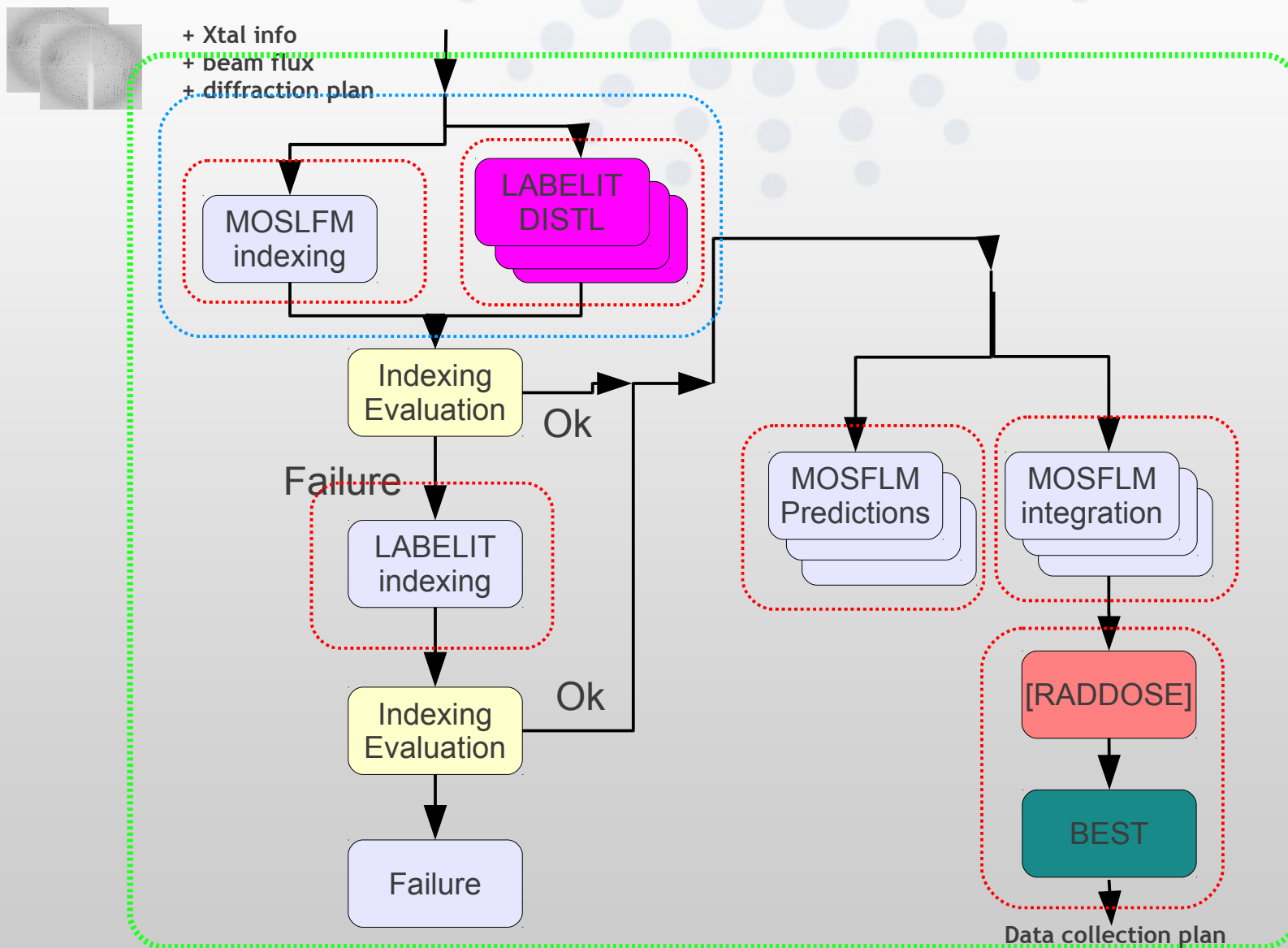


EDNA / Passerelle Characterisation Workflow

Director



MXv1 Characterisation v1.2



Existing scientific EDNA workflows

- Macromolecular crystallography:
 - Characterisation taking into account radiation damage (MOSFLM, Labelit, RADDPOSE, BEST)
 - Connection with experiment data base (ISPyB)
 - Parallel execution of characterisation (GRID data processing)
 - Parallel creation of image thumbnails
- Diffraction Computed Tomography
 - SPD: Image correction, fast azimuthal integration
 - Sinograms saved in HDF5 format
- Small Angle Scattering
 - Image correction and fast azimuthal integration
- Full Field XAS
 - Image correction (dark, flat)
 - Image alignment (offset measurements by FFT)
 - HDF5 output

How EDNA will evolve in the future

- Common EDNA developments (Kernel):
 - Improvements of the data model framework (in progress)
 - Improvements of logging (in progress)
 - Full support of Windows and MacOS (in progress)
 - Enhanced support of grid engines / job schedulers
 - Improved documentation (plugin use cases)
 - Graphical workflow editor (Data Analysis Workbench)
- Scientific developments:
 - MX further enhancements of characterisation (kappa, XDS etc)
 - MX auto processing wrappers
 - Biosaxs data analysis (EMBL Hamburg software suite)
 - Tomography
 - More to come...