Data Analysis Sequencing - EDNA

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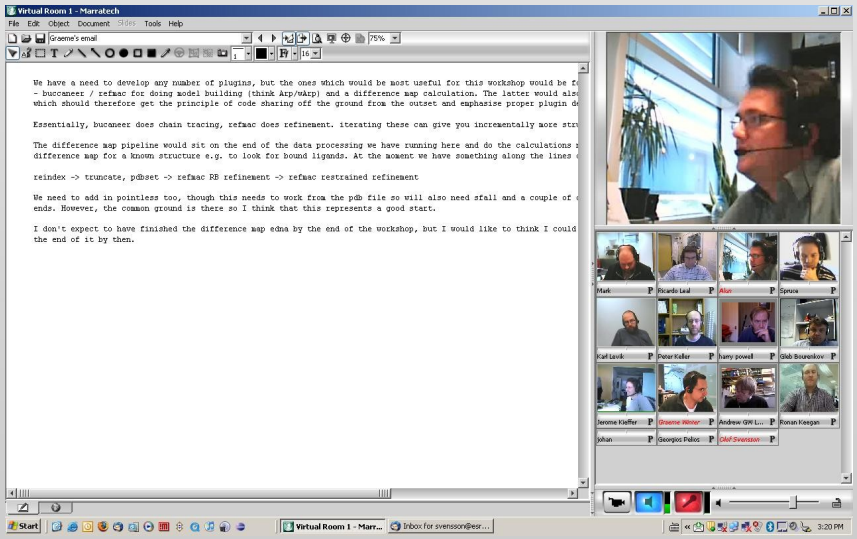
Why do we need EDNA?

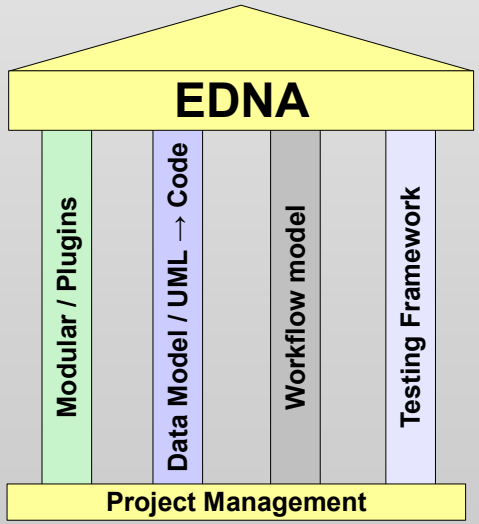
- EDNA is the best answer we (developers) have come up with so far for answering these questions :
  - How can we automate data analysis workflows?
    - “pipeline” existing scientific software for (online) data analysis workflows
    - abstract certain calculations to be “generic”, e.g. indexing of 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

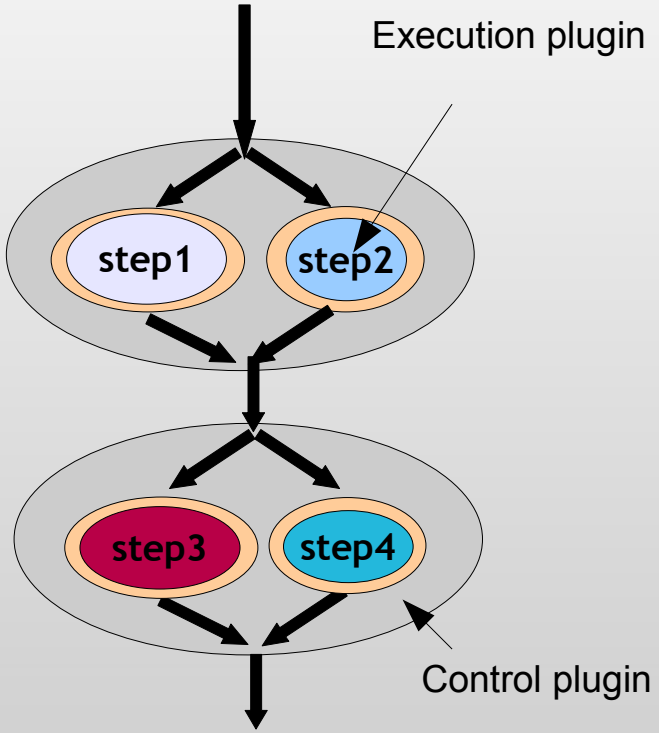
- EDNA is a framework:
  - "Generic" kernel
    - Data modelling framework
    - Support for multi-threaded modules (plugins) development
    - Support for workflow development
    - Testing framework
  - "Specific" applications (MXv1, bioSaxs etc.)
  - Automatic testing and nightly builds
  - Automatic API doc generation
  - No GUI





EDNA Modularity : Plugins and their hierarchy

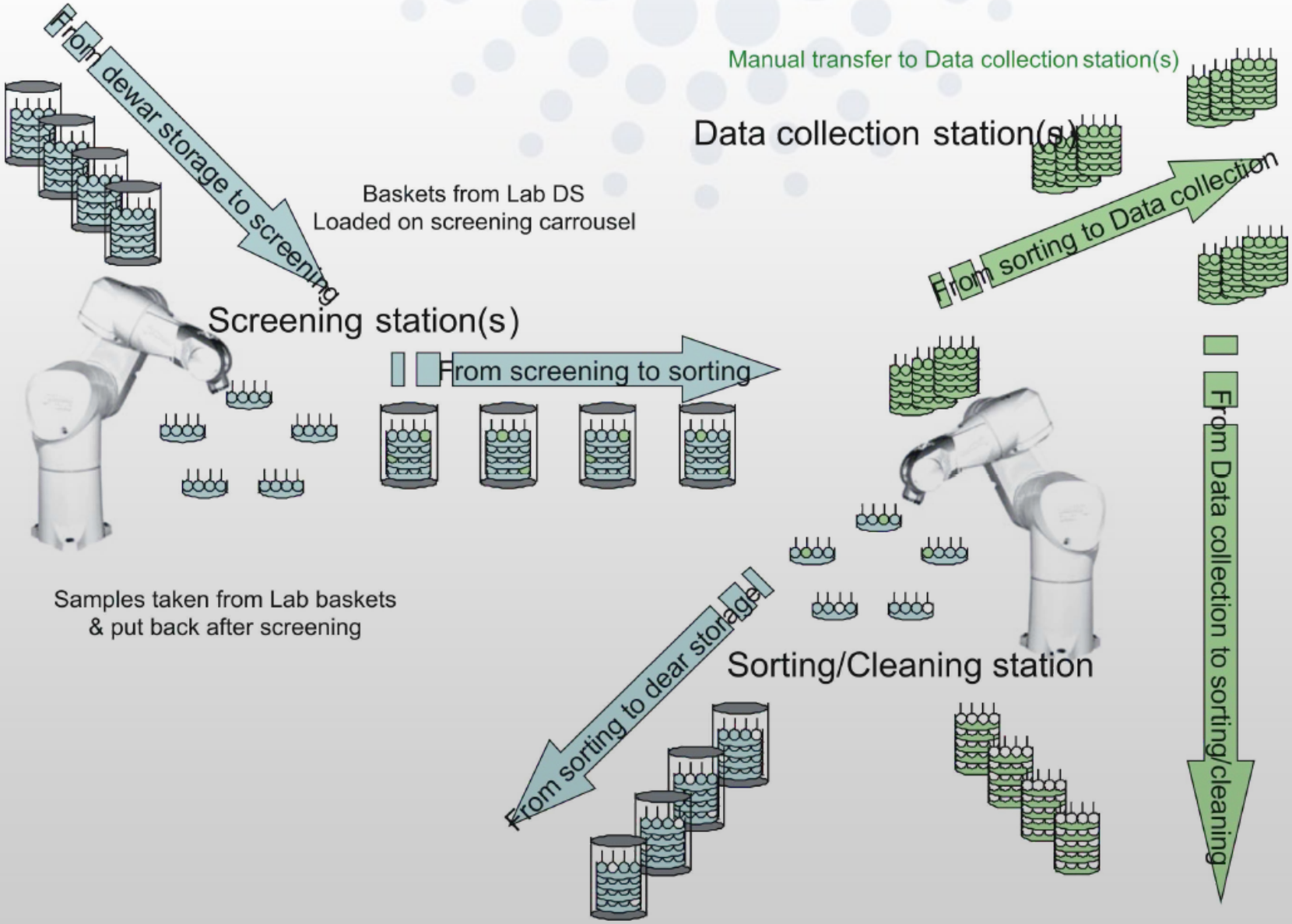
- Plugin base class :
  - Configuration, working directory, etc.
- Execution plugins :
  - Execution of external programs, e.g. (bash) scripts
- Controller plugins:
  - Control of execution plugins
  - Parallel execution
  - Synchronisation



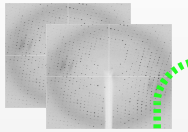
Existing scientific EDNA workflows

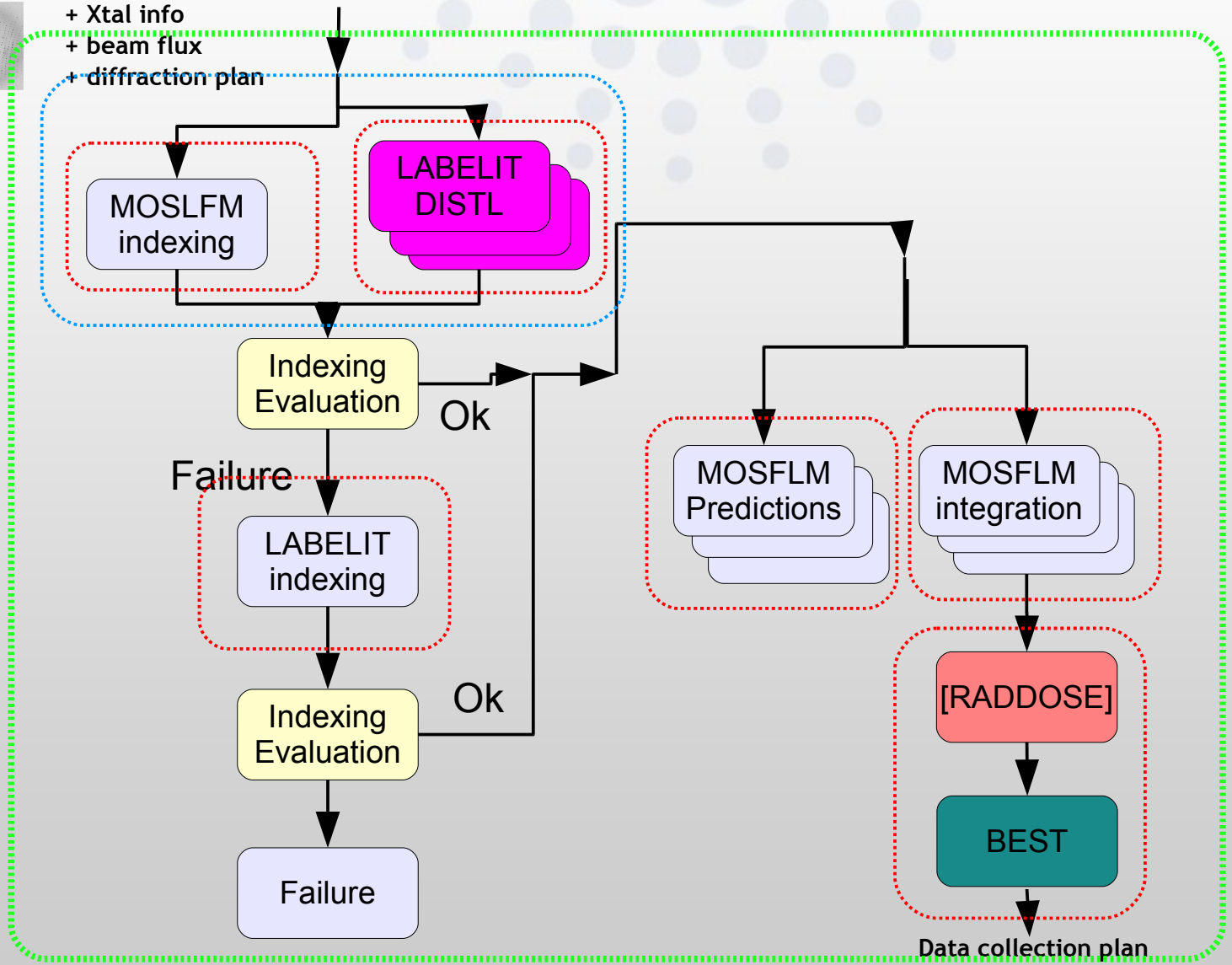
- Macromolecular crystallography:
  - Characterisation taking into account radiation damage (MOSFLM, Labelit, RADDOSE, BEST)
  - Connection with experiment data base (ISPyB)
  - Parallel execution of characterisation (GRID data processing)
  - Parallel creation of image thumbnails
- Diffraction Computed 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

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



MXv1 Characterisation v1.2





EDNA Testing Framework

```
[UnitTest]: ##########################################################################
[UnitTest]: Result for EDTestSuiteKernel : SUCCESS
[UnitTest]:
[UnitTest]:  Number of executed test suites in this test suite : 2
[UnitTest]:
[UnitTest]:
[UnitTest]:   Total number of test cases executed with SUCCESS : 14
[UnitTest]:   Total number of test cases executed with FAILURE : 0
[UnitTest]:
[UnitTest]: Total number of test methods executed with SUCCESS : 48
[UnitTest]: Total number of test methods executed with FAILURE : 0
[UnitTest]:
[UnitTest]:                                    Runtime : 25.847 [s]
[UnitTest]: ##########################################################################
```

EDNA Testing Framework

```
[UnitTest]: ##########################################################################
[UnitTest]: Result for EDTestSuitePluginUnitAll : SUCCESS
[UnitTest]:
[UnitTest]:  Number of executed test suites in this test suite : 5
[UnitTest]:
[UnitTest]:
[UnitTest]:   Total number of test cases executed with SUCCESS : 83
[UnitTest]:   Total number of test cases executed with FAILURE : 0
[UnitTest]:
[UnitTest]: Total number of test methods executed with SUCCESS : 202
[UnitTest]: Total number of test methods executed with FAILURE : 0
[UnitTest]:
[UnitTest]:                                    Runtime : 122.892 [s]
[UnitTest]: ##########################################################################
```

EDNA Testing Framework

```
[UnitTest]: ######################################################################
[UnitTest]: Result for EDTestSuitePluginExecuteAll : FAILURE
[UnitTest]:
[UnitTest]:  Number of executed test suites in this test suite : 5
[UnitTest]:
[UnitTest]:
[UnitTest]:   Total number of test cases executed with SUCCESS : 124
[UnitTest]:   Total number of test cases executed with FAILURE : 8
[UnitTest]:
[UnitTest]:
[UnitTest]: OBS! The following test methods ended with failure:
[UnitTest]:
[UnitTest]:   EDTestCasePluginExecuteControlCharForReorientationv2_0_noKAPPA_ :
[UnitTest]:     testExecute :
[UnitTest]:       Plugin failure assert: should be False, was True FAILURE: Expected different from obtained - identifier
/mntdirect/_scisoft/users/svensson/tmp/EDTestSuitePluginExecuteAll_20110114-093729/tmpPW7olu
[UnitTest]:
 ...
[UnitTest]:
[UnitTest]:
[UnitTest]: Total number of test methods executed with SUCCESS : 129
[UnitTest]: Total number of test methods executed with FAILURE : 8
[UnitTest]:
[UnitTest]:                                   Runtime : 1108.997 [s]
[UnitTest]: ######################################################################
```

EDNA Testing Framework

Checking out EDNA Repository... to revision 2758
Tests using the default python under linux: Python 2.6.5
Launching EDTestSuiteKernel with /usr/bin/python .....SUCCESS! 16.411 [s]
Making EDNA-kernel tarball distribution.....
Launching EDTestSuiteCCP4v0 with /usr/bin/python .....SUCCESS! 16.466 [s]
Making CCP4v0 tarball distribution.....
Launching EDTestSuitePluginExecPlugins with /usr/bin/python .....SUCCESS! 920.778 [s]
Making ExecPlugins tarball distribution.....
Launching EDTestSuiteBioSaxs with /usr/bin/python .....SUCCESS! 49.655 [s]
Making BioSaxsv1 tarball distribution.....
Launching EDTestSuitePluginUnitMXPluginExec with /usr/bin/python .....SUCCESS! 57.916 [s]
Launching EDTestSuitePluginExecuteMXPluginExec with /usr/bin/python .....SUCCESS! 365.850 [s]
Launching EDTestSuitePluginUnitMXv1 with /usr/bin/python .....SUCCESS! 73.398 [s]
Launching EDTestSuitePluginExecuteMXv1 with /usr/bin/python .....SUCCESS! 3040.207 [s]
Making MXv1 tarball distribution.....
Tests using jython under linux: Jython 2.5.2rc2
Launching EDTestSuiteKernel with /home/tester/bin/jython .....SUCCESS! 80.371 [s]
Tests using the default python under : WinePython 2.7.1
Launching EDTestSuiteKernel with /home/tester/bin/pythonw .....SUCCESS! 44.725 [s]

How EDNA will evolve in the future

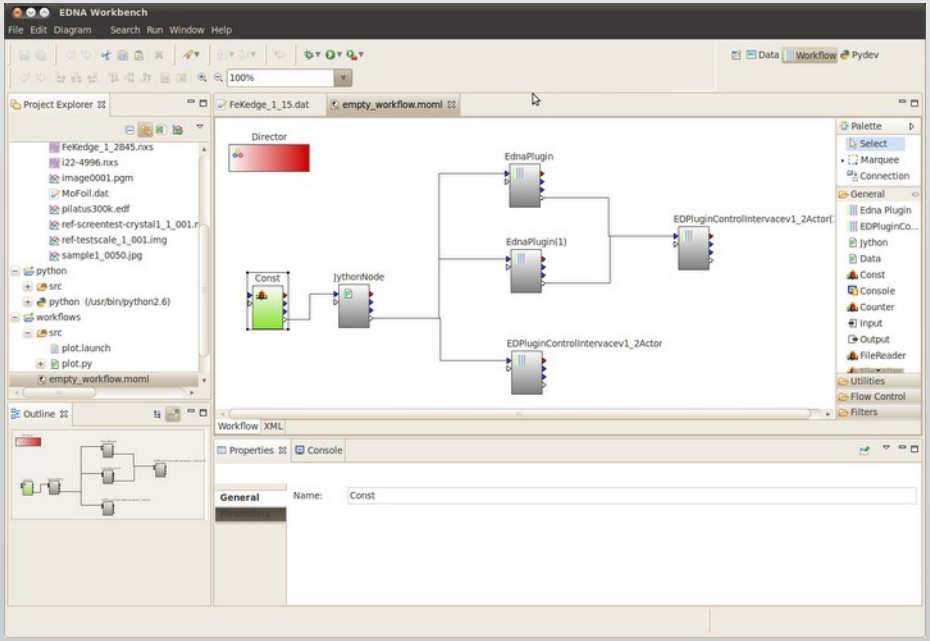
- Common EDNA developments (Kernel):
  - Improvements of the data model framework (in progress)
  - Improvements of logging (in progress)
  - Full support of Windows and MacOS (in progress)
  - Enhanced support of grid engines / job schedulers
  - Improved documentation (plugin use cases)
  - Graphical 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...

How to run EDNA on a cluster with a job scheduler

- EDNA is optimised for parallel execution of processes/plugins:
  - Thread safe parallel execution of plugins
  - Automatic synchronisation
  - Automatic workload limitation
- Implemented : EDNA TANGO server
  - No job scheduler → no load balancing
- Today the EDNA kernel provides a limited support for running workflows on a cluster with a job scheduler:
  - Works only if the program is started by EDNA in a script
  - Call to grid engine submission must be blocking (sun/oracle grid engine "-sync y")
- Future : support for any job scheduler (sun/oracle, torque, condor, pbs, oar etc)
  - Synchronisation through sockets?
  - Persistent EDNA plugin launchers?

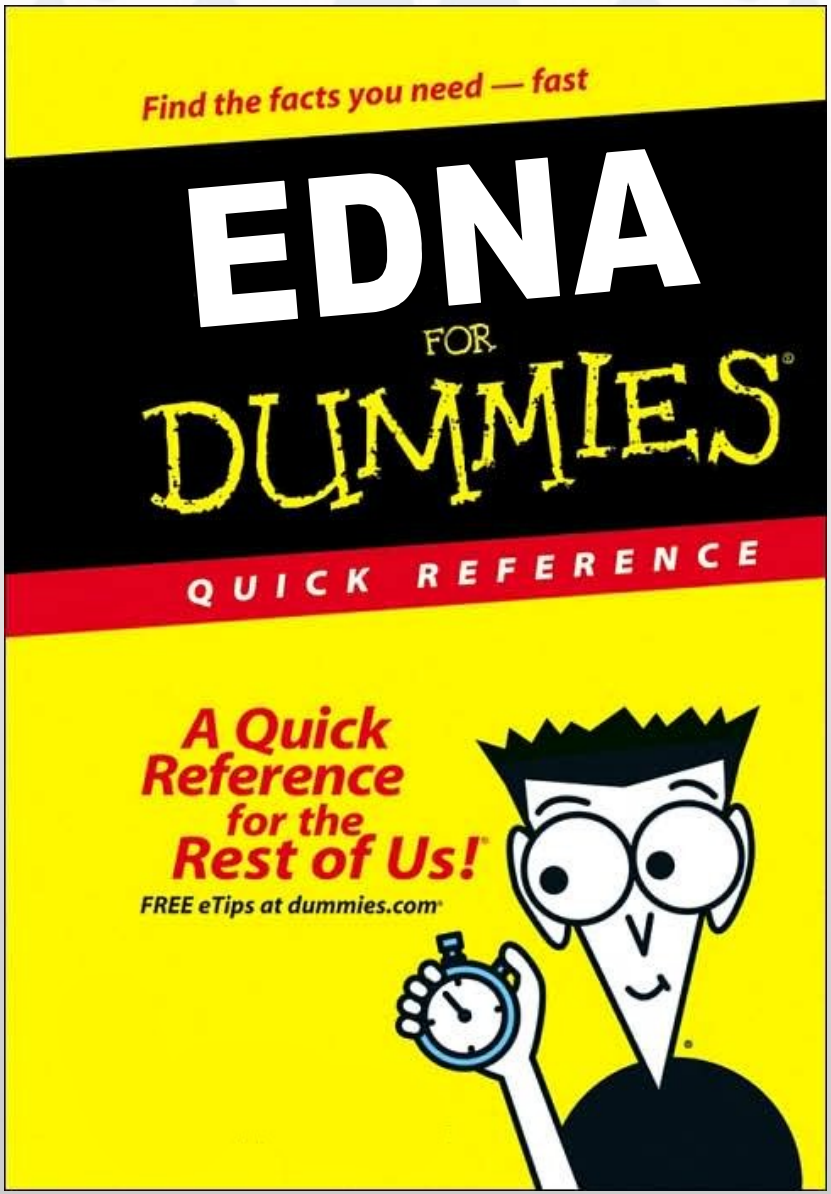
What the EDNA GUI could look like

- EDNA has no GUI framework
- All EDNA workflows must be executable on the command line
- Possible solution for a generic EDNA GUI:



- 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

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 Collaborators 2010

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Andrew Thompson(k)
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Clemens Vonrhein(f)
Darren Spruce(e)
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Gordon Leonard(e)
Graeme Winter(b)
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Executive committee