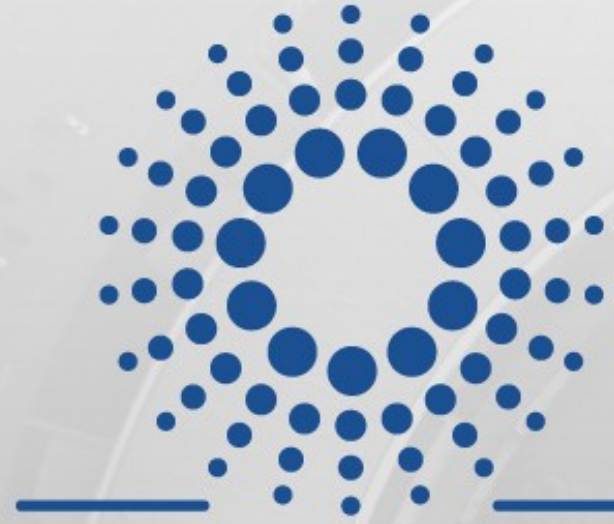
A Light for Science



ESRF

European Synchrotron Radiation Facility

Data Analysis Workbench

- Project started in June 2010
- 'Workbench for online data analyis'
- Based on and contributing to existing products
- Delivered using RCP
- ESRF management tracking project using Jira, http://jira:8080/browse/DAWB

  (Internal to ESRF)

Project Goals

1. Ability to view various file formats:
   - srs, dat, png, jpg, jpeg, tif, tiff, cbf, img, ciff, mccd, edf, pgm, cor, bruker, h5, nxs, pdb, (gz, bz2, zip)
   - Others?
2. Ability to visualize and run workflow pipelines.
3. Ability to interact with data and plotting using CPython.
4. Ability to configure data analysis in 'DAD' XML based system at ESRF.
5. Provide a workbench which can run other analysis tools.

Project Running

- Collabortations / APIs where possible, for example:
  - GDA/SDA, Passerelle, Fable, Eclipse/RCP, jmol etc. Other small APIs
- Supported on Windows, Mac and Linux
- Packaged to work 'out of the box'
- Unit tests, regression tests and nightly builds
- Agile project management

Why RCP?

- It uses SWT and JFace an MVC layer for SWT
- Programming at a higher level
- Reusable components available on web
  - CSV editor, GEF, XY Graphing
- Modular plugins and parts increase productivity
- Growing and large user community with significant inward investment.

Current Visualization Status

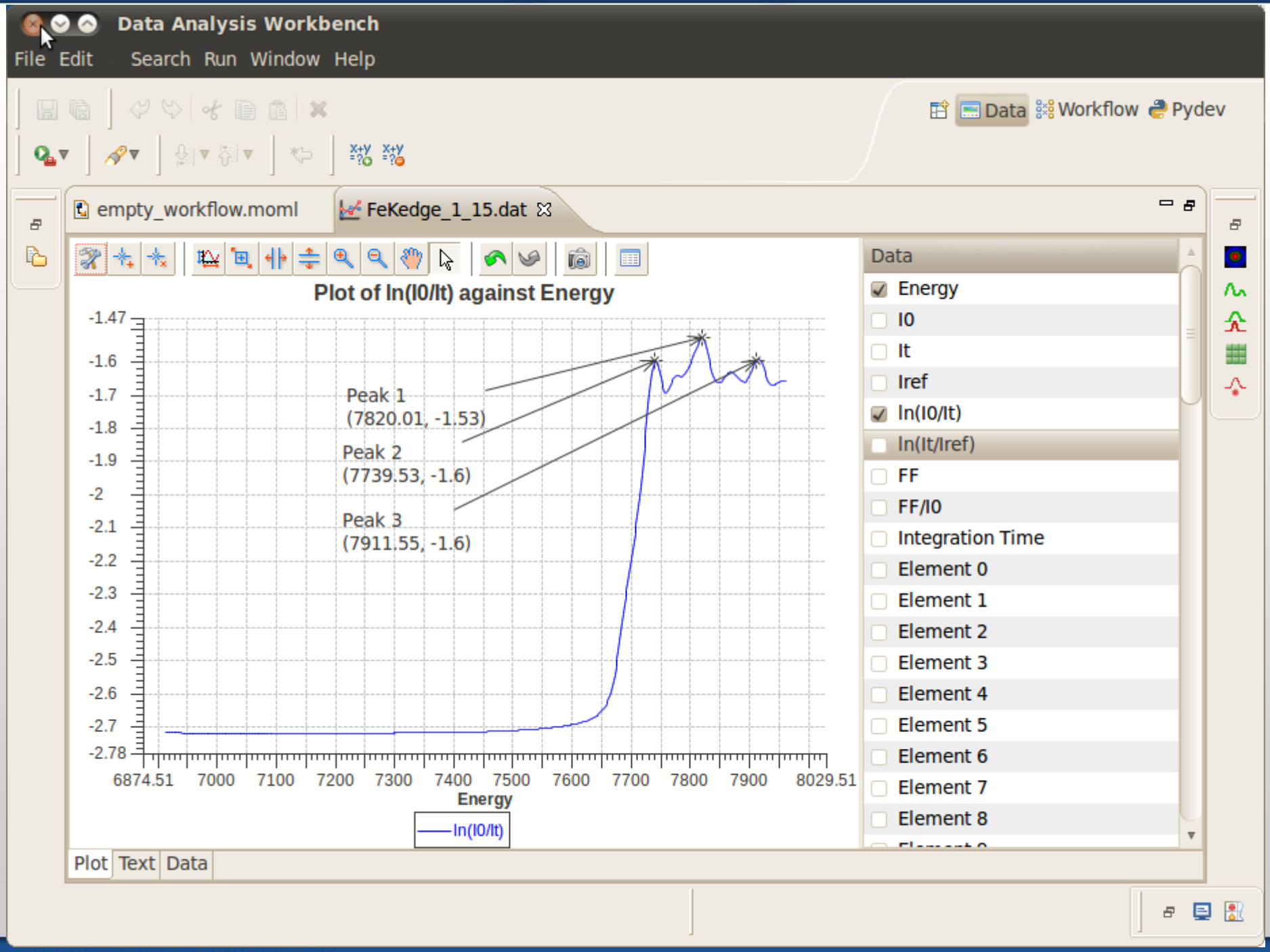
- Diamond SDA plotting
  - + Hardware acclerated, Same interface for 1D, 2D and 3D
  - - Specific OS and hardware requirements. Does not integrate to RCP properly. Crashes. Does not pass through remote desktop properly at ESRF.
  - > Does not work well at ESRF but is available in workbench just in case
- JLPlotting used by Fable for 1D
  - + Easy to use and used widely at ESRF
  - - Uses swing so not really an option
  - > Being phased out of fable 1D views
- Fable Image Viewer
  - + Works well on any system as uses raw SWT layer. Clean integration with RCP.
  - - Only supports images
  - > Chosen as the default image viewer in the workbench
- SWT XY Graph
  - + Works well on any system as useds raw SWT layer. Based on GEF.
  - - Only supports X/Y graphs
  - > Chosen as the defalut XY graph
- **Conclusion: SWT based graphics are the best choice for 1D and 2D**

Current HDF5 Status

- Nexus plugin from Diamond
  - Poor stability in multi-treaded environment
  - Synchronization used to combat this.
  - Does not support most of old h5 files at ESRF
- HD5 plugin
  - Supports multi-threaded reading
  - Does not cause JVM exit with same tests as nexus
  - No need to set LD_LIBRARY_PATH
  - Works with larger files better based on testing at ESRF.
- Conclusion
  - Use raw hdf5 for reading files at ESRF.

Other SDA Experiences

- Complex dependency tree, highly coupled.
- Abscence of clean and reusable API's.
- Side plot system poor RCP design.
- Plotting causing OS crash, application hanging and application exits when tested at ESRF.
- Design principles such as single use objects, DRY and design patterns not currently used.
- Poor unit testing and low quality.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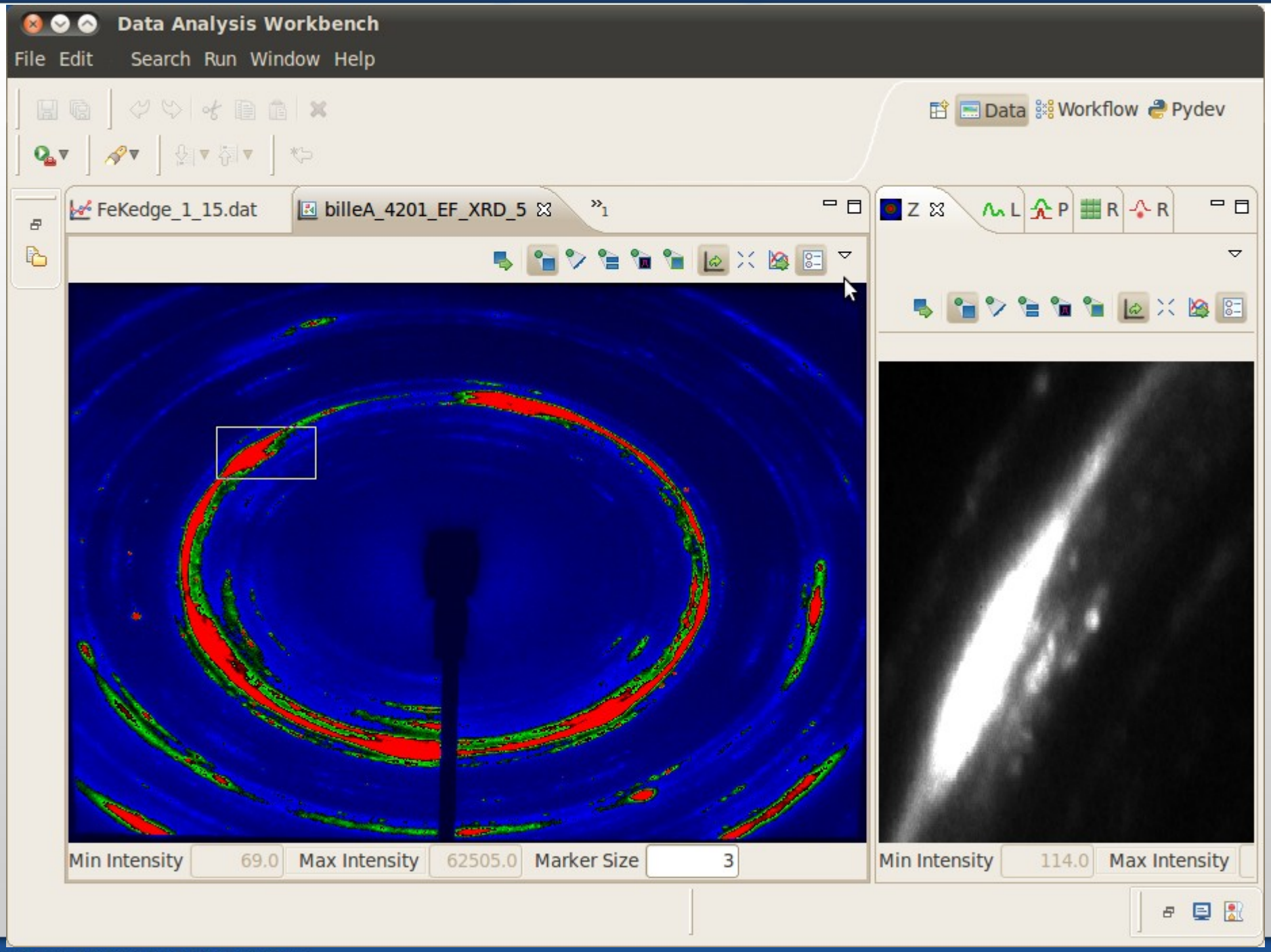
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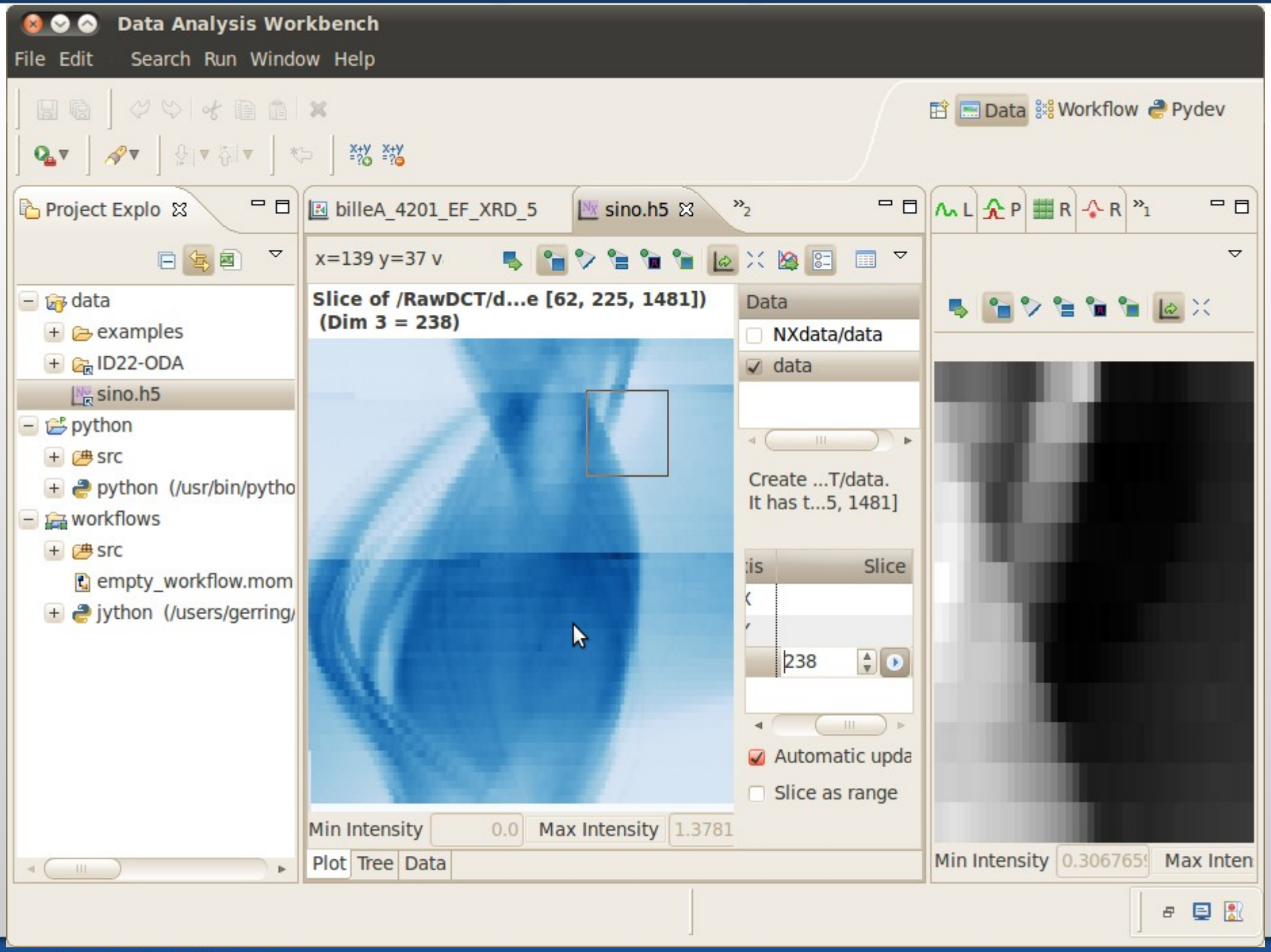
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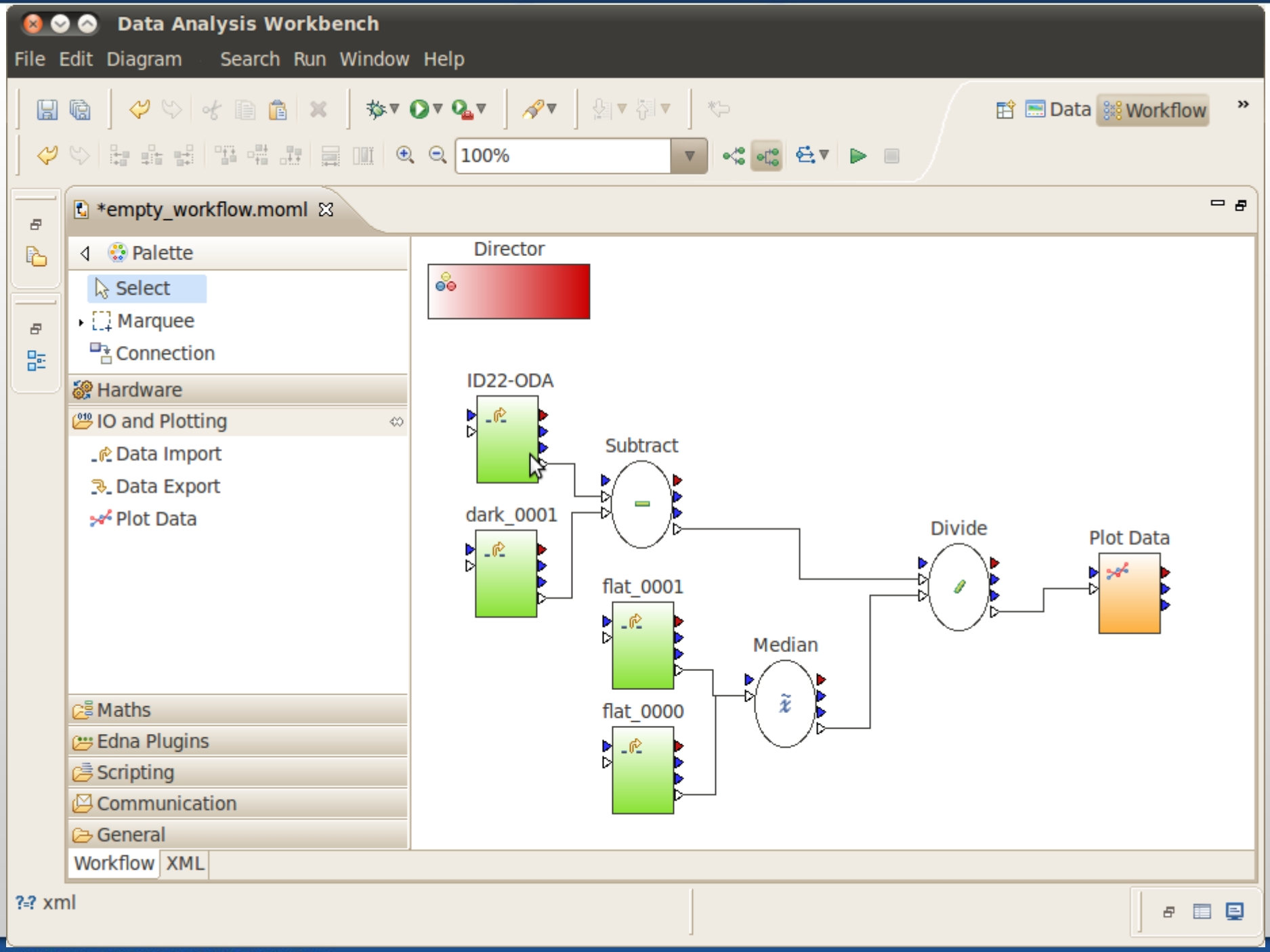
Workflow for Results Analysis

- 'Simple to use subset of Python'
- A pipeline which runs as a service
- Workbench can author and deploy pipeline
- Workbench connects to and starts / stops pipeline
- Able to run nodes from:
  - CPython projects, KNIME extension points, SDA data analysis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CPython in Workflow Integration

- Support of Numpy nodes.
- Support of EDNA nodes.
- Support of Fable diffraction nodes.
- Interfaces to transform data to and from workflow.
- Interfaces to support plotting.
- Expectation to use same memory space as Java process.

Extensions

- Connection of Data Collection and Data Analysis in integrated system.
- More Fable tools
- Bioclipse views/editors
- Domain Specific Language (DSL) for SPEC
- Beamline control with Passerelle

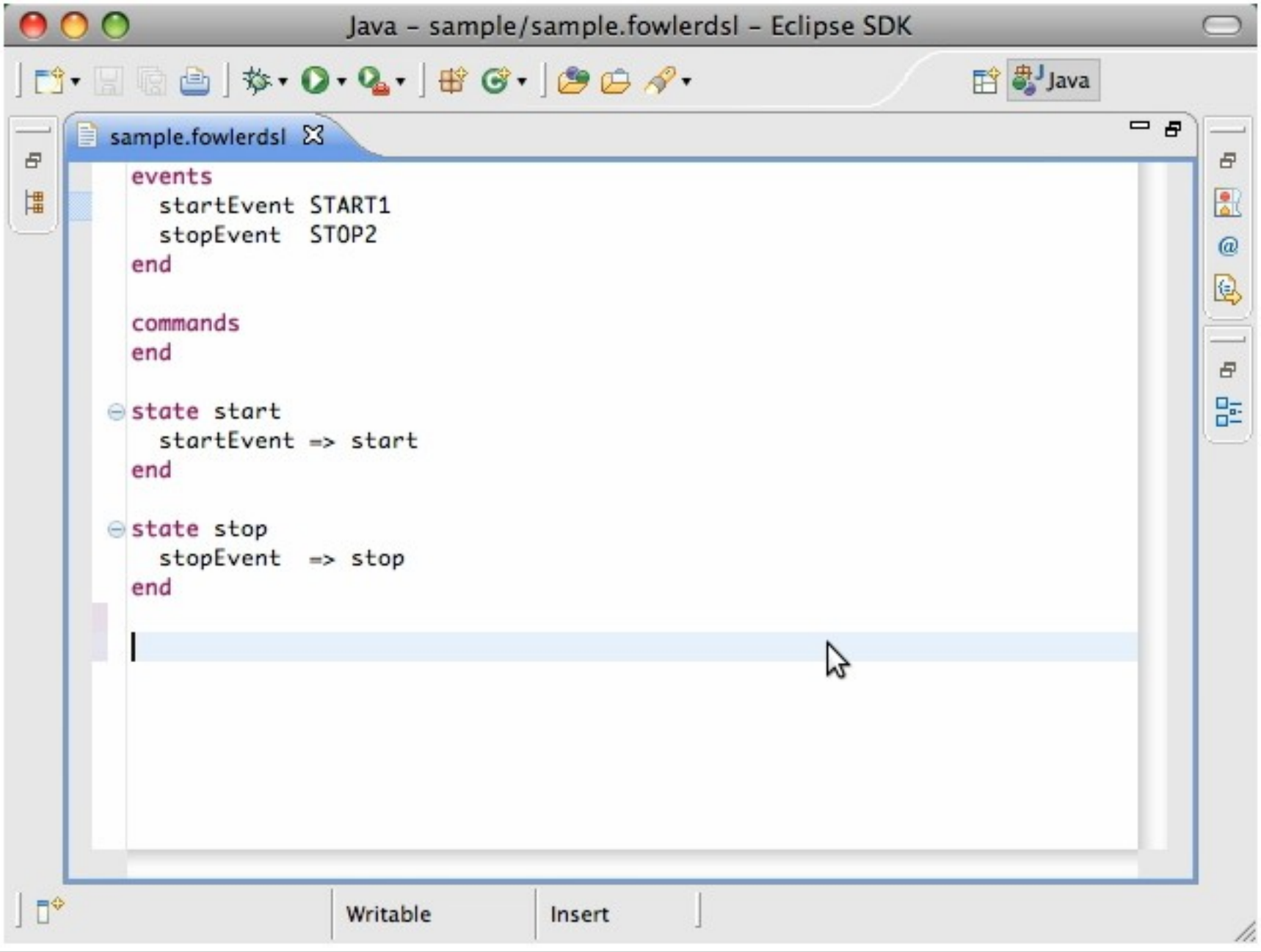
Fable Tools

- Some Fable tools being packaged with project.
- Being moved incrementally.
- Packaged in standard distribution.
- Heavy use of CPython in Fable a challenge.
- Diffraction tools most likely candiate to be moved next.

SPEC DSL

- Syntax checking, highlighting, search, refactoring of SPEC scripts.
- Scripts orgnanised into projects.
- Better integration with plotting and other UI operations.
- Ability to upgrade beamlines incrementally as SPEC is supported.
- Better ability to analysis and visualize script structure.
- Better sharing between beamlines.
- SPEC console integrated to rest of GUI.

http://www.eclipse.org/Xtext/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startEvent => start
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state stop
stopEvent => stop
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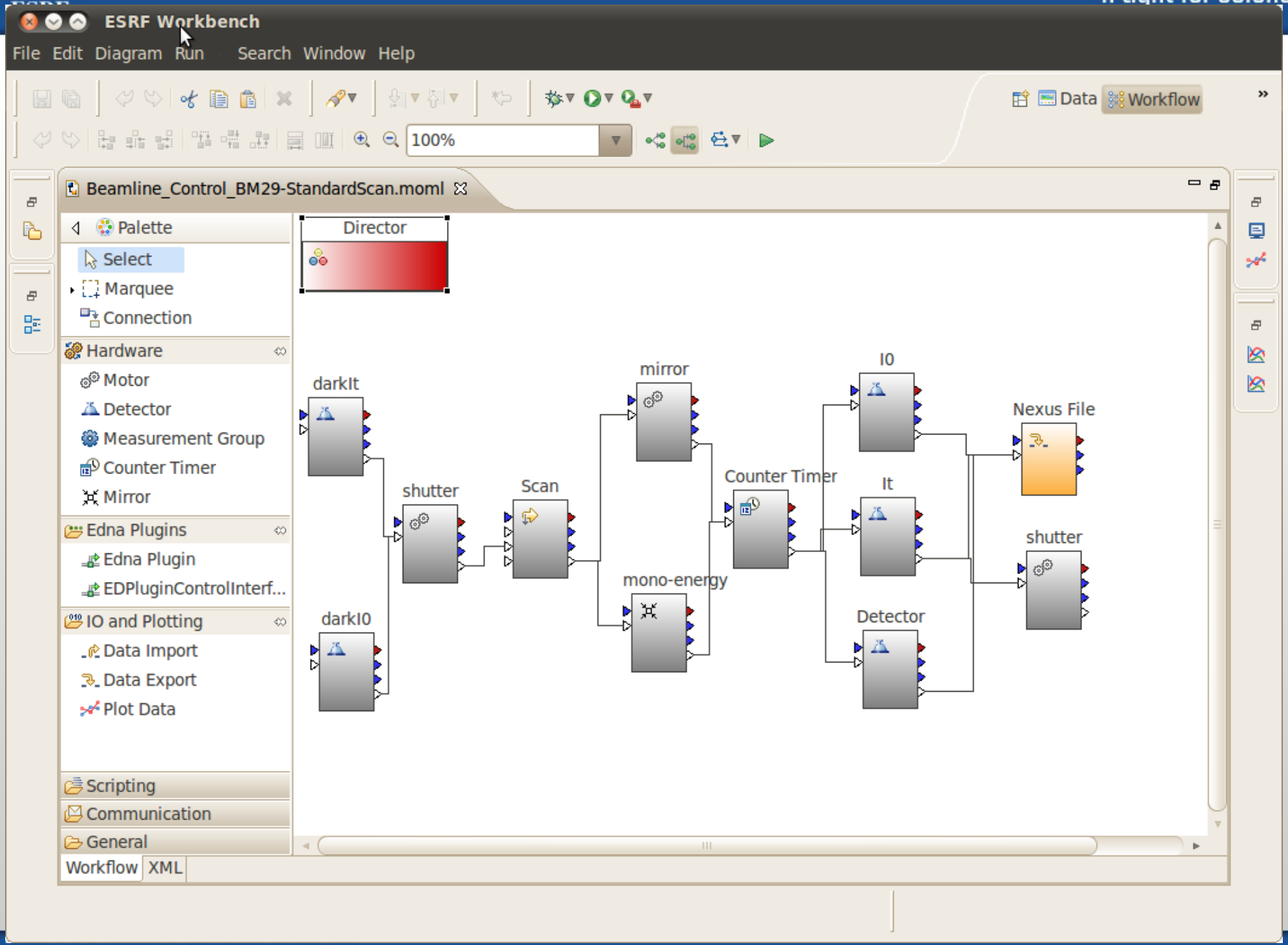
Beamline Control using Passerelle Workflows

- Ability to easily change experiment.
- Ability to add in new hardware and have it tighly coupled to the data collection.
- Ability to run the data analysis pipeline automatically within the data collection scheme.
- Hardware integrated to collection algorithm off site, allowing testing and setup before the visit
- Increase user throughput as experiment is run in simulation before visit.
- Supports SPEC, Tango, EPICS, GDA etc. As experiment configuration better abstracted from hardware.
- Multi-threading issues reduced.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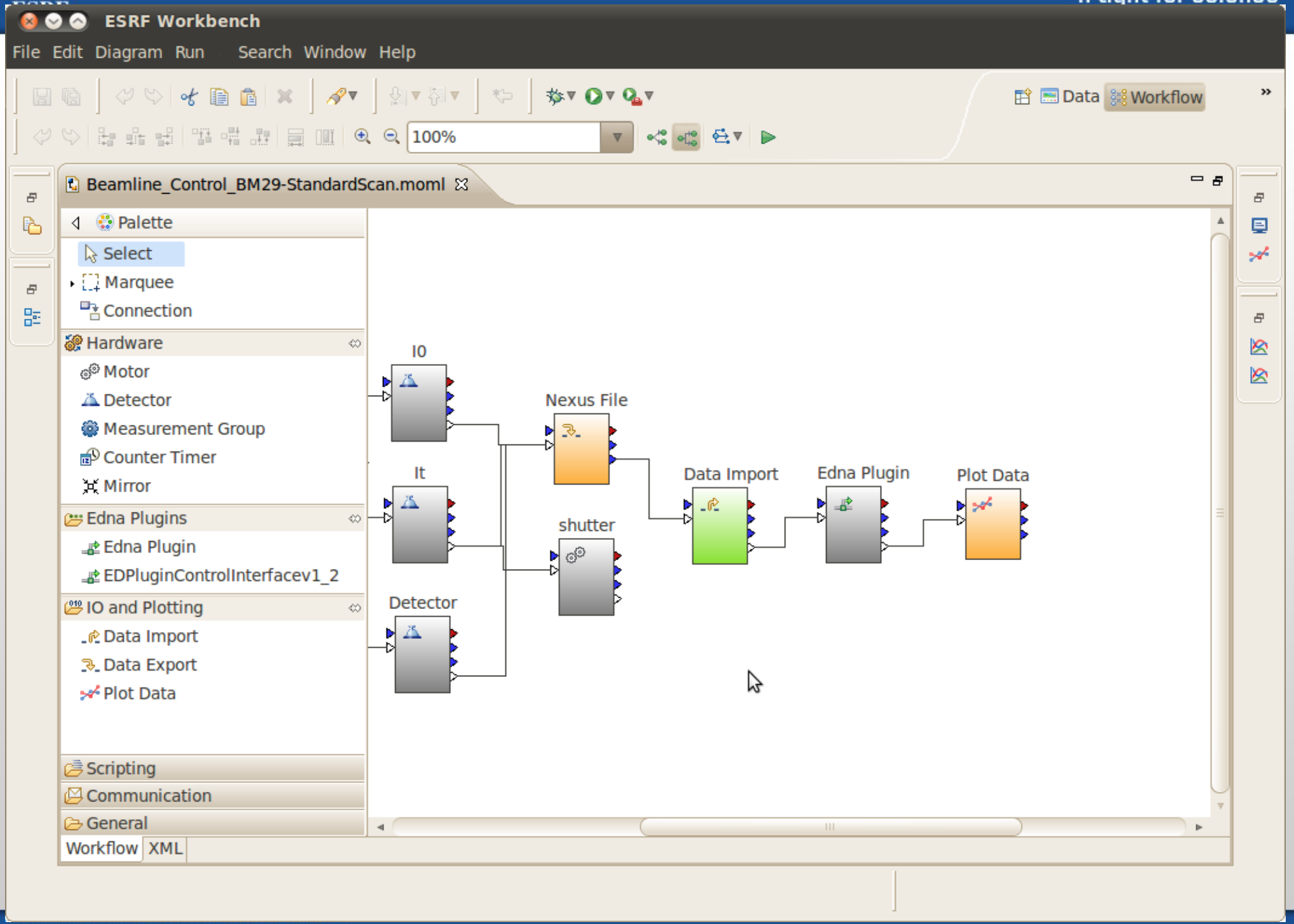
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Conclusions

- Collaborations are good and should continue.
- Testing is required of code written in collaboration.
- Developers in collaboration need to develop resuable decoupled code.
- Collaborations need to consider all users and code should be created as reusable APIs.
- Eclipse/RCP is ideal platform for this.