EDNA at Diamond

diamond

Why is Diamond developing software

- To help users maximise their beamtime by helping users get as much from their data and samples.
- Because of this:
  - Software must be fast to allow feedback within a reasonable timescale.
  - Software must be as automated as possible as users are otherwise occupied (or at best tired ☹!).
  - Data collection is only a part of the process so the scientific software presented to the users at Diamond must be all encompassing.
- ‘Remote’ beamtime.

EDNA activities (Active/deployed)

- EDNA Kernel
- EDNA MX Characterisation V1, (Alun session 2)
  - Deployed and investigating best way to use it
- DArc – EDNA Archiving pipeline
  - Actively developed, prone to system failures
- EDNA Tomography Pipeline, (Mark)
  - Used but bespoke
- DIMPLE, EDNA Difference Map Pipeline, (Ronan)
  - Non EDNA prototype available to users
- SAXS – automated ab initio low resolution shape determination (GNOM/DAMMIN)
  - Early stages

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Future (not started) EDNA applications

- Spectroscopy
- Further SAS pipelines
- Data reduction manager
  - (we run many data reduction packages and the tasks need managing)
- XIA2
- MX structure Solution

Current resources

- Out of a scientific software team of 8 developers supporting all diamond science beamlines, 6 are capable of developing/have developed EDNA applications, 5 are actively developing a range of applications.

- ~2.5 FTE developing EDNA Kernel, MXCharaterisation, DIMPLE, DArc, Tomography and SAXS.

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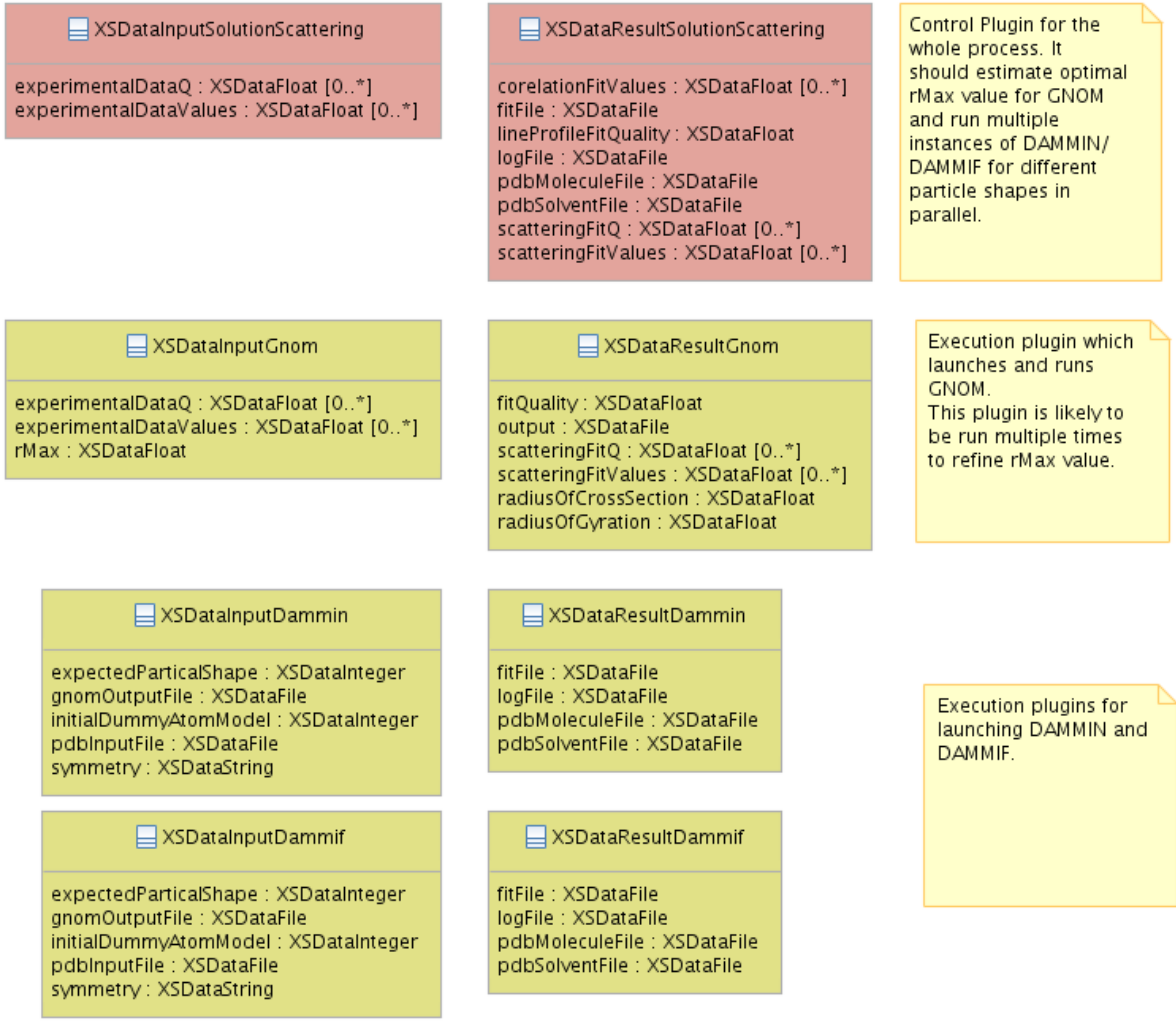
Automated ab initio low resolution shape determination



SolutionScattering control plugin will automate small angle scattering data processing by running GNOM and DAMMIN/DAMMIF programs for optimal reconstruction of the shape of the sample.

Control plugin will iterate GNOM runs to obtain optimal value for rMax parameter and run several instances of DAMMIN/DAMMIF with different particle shapes in parallel.

SolutionScattering plugin: Current status

- Execution tests for all plugins are implemented using Lysosyme test data supplied with GNOM/DAMMIN/DAMMIF.
- Input/Output data is referenced in the corresponding .xml configuration files.
- Execution plugin tests can be run independently.
- Pipeline test makes single run of GNOM with the default rMax value (50). The output data is processed using DAMMIF with the spherical particle model.