

# EDNA at 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

# 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, MXCharacterisation, DIMPLE, DArc, Tomography and SAXS.

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  - **Early stages**

# Automated ab initio low resolution shape determination

## XSDatInputSolutionScattering

experimentalDataQ : XSDataFloat [0..\*]  
experimentalDataValues : XSDataFloat [0..\*]

## XSDataResultSolutionScattering

corelationFitValues : XSDataFloat [0..\*]  
fitFile : XSDataFile  
lineProfileFitQuality : XSDataFloat  
logFile : XSDataFile  
pdbMoleculeFile : XSDataFile  
pdbSolventFile : XSDataFile  
scatteringFitQ : XSDataFloat [0..\*]  
scatteringFitValues : XSDataFloat [0..\*]

Control Plugin for the whole process. It should estimate optimal rMax value for GNOM and run multiple instances of DAMMIN/DAMMIF for different particle shapes in parallel.

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.

## XSDatInputGnom

experimentalDataQ : XSDataFloat [0..\*]  
experimentalDataValues : XSDataFloat [0..\*]  
rMax : XSDataFloat

## XSDataResultGnom

fitQuality : XSDataFloat  
output : XSDataFile  
scatteringFitQ : XSDataFloat [0..\*]  
scatteringFitValues : XSDataFloat [0..\*]  
radiusOfCrossSection : XSDataFloat  
radiusOfGyration : XSDataFloat

Execution plugin which launches and runs GNOM. This plugin is likely to be run multiple times to refine rMax value.

## XSDatInputDammin

expectedPartialShape : XSDataInteger  
gnomOutputFile : XSDataFile  
initialDummyAtomModel : XSDataInteger  
pdbInputFile : XSDataFile  
symmetry : XSDataString

## XSDataResultDammin

fitFile : XSDataFile  
logFile : XSDataFile  
pdbMoleculeFile : XSDataFile  
pdbSolventFile : XSDataFile

Execution plugins for launching DAMMIN and DAMMIF.

## XSDatInputDammif

expectedPartialShape : XSDataInteger  
gnomOutputFile : XSDataFile  
initialDummyAtomModel : XSDataInteger  
pdbInputFile : XSDataFile  
symmetry : XSDataString

## XSDataResultDammif

fitFile : XSDataFile  
logFile : XSDataFile  
pdbMoleculeFile : XSDataFile  
pdbSolventFile : XSDataFile

# 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.