The BIOXHIT Project

EDNA

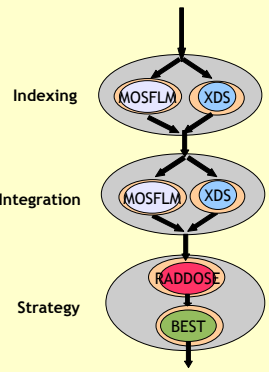
The new generation environment for diffraction data collection

Marie-Françoise Incardona[c], Romeu Pieritz[c] and Olof Svensson[c]

EDNA will be a new generation environment for automation of the collection of X-ray diffraction data from macromolecular crystals, developed on the foundations of the project automateD collectioN of datA ("DNA", www.dna.ac.uk). This new environment is based on a modular architecture capable to invoke the appropriate third party program in order to fully automate the crystal characterization (indexing and integration) and the generation of a realistic and appropriate data collection strategy that will take radiation damage into account.

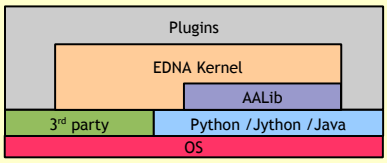
The Main Goal

The aim is to develop a configurable application able to launch sequentially the crystal characterization and the data collection strategy steps by executing one or several parallel external programs according to the user configuration :
Indexing (MOSFLM and/or XDS and/or other)
Integration (MOSFLM and/or XDS)
Radiation damage estimation (RADDOSE)
Data collection strategy (BEST)



Architecture

A modular system based on a plugins factory mechanism
and multi-thread management (AALib)
A programming language that allows the integration of EDNA with the python and Java worlds (Python/Jython)



Current status

Development framework:
- Main classes (plugins hierarchy, configuration facilities)
- Data classes code generation from UML (XSD data binding)
- Automated Tests Framework (Unit and validation Tests)
- IDE: Eclipse / Data Modeling: Enterprise Architect
- Source and Bugs Management: Subversion, Bugzilla

Implementation of scientific cases:
- Indexing plugin (MOSFLM)
- Radiation damage estimation plugin (RADDOSE)

Web Site:
- www.edna-site.org

EDNA Project Members :

A. Ashton[d]*, G. Bourenkov[b]*, G. Bricogne[e]**, S. Brockhauser[a]*, J. Gabadinho[c], E. Gordon[c]*, M.-F. Incardona[c], P. Keller[e]*, P. Legrand[j]*, G. Leonard[c], A. Leslie[f]**, K. Levik[d]*, K. McAuley[d], S. McSweeney[c]**, E. Panepucci[h], R. Pieritz[c], A. Popov[c]*, H. Powell[f]*, O. Roudenko[c], A. McCarthy[a]**, T. Schneider[b]**, C. Schulze[h], J. Skinner[g], D. Spruce[c], O. Svensson[c], R. Sweet[g], L. Roussier[i], T. Tomizaki[h], J. Turkenburg[k], P. Turner[i], C. Vonrhein[e], M. Wang[h], A. Thompson[f]**

(a) EMBL, Grenoble, France
(b) EMBL, Hamburg, Germany
(c) ESRF, Grenoble, France
(d) Diamond Light Source, UK
(e) Global Phasing, Cambridge, UK
(f) MRC LMB, Cambridge, UK
(g) NSLS, Brookhaven, U.S.
(h) SLS, Villigen, Switzeland
(i) Synchrotron Soleil, France
(j) University of Sydney, Australia
(k) University of York, UK

(*) are especially acknowledged for their inputs and effort
(**) executive committee members