



The EDNA initiative

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on behalf of Olof Svensson EDNA project Manager



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What is EDNA?

- Developed on the foundations of the project automated collection of data (“DNA”, www.dna.ac.uk).
- A new generation environment for automation of the collection of X-ray diffraction data from macromolecular crystals
- Based on a modular architecture able 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.



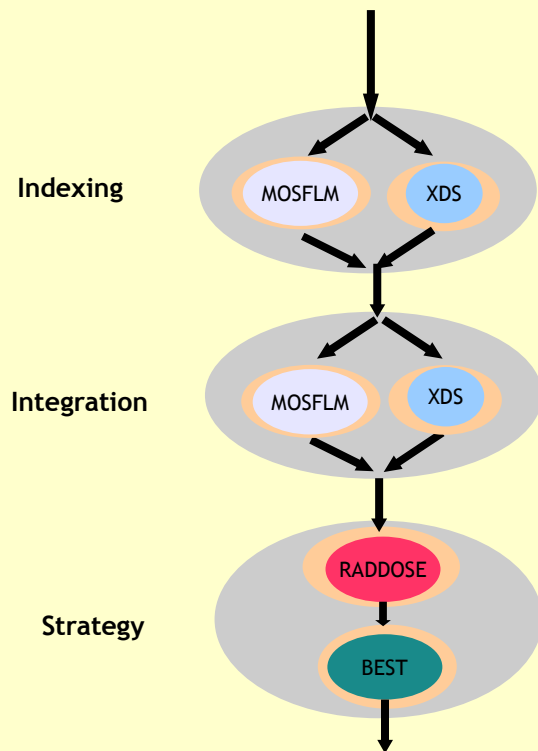
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Enhancements compared with DNA:

- Name:
 - “EDNA”: Enhanced automated collection of data
 - > no more potential ambiguity with the name of a macromolecule
- Architecture:
 - Modular and configurable system
- Initial features:
 - Radiation damage estimation
 - Multi-subwedges data collection strategies
 - Possibility to launch one or several parallel 3rd party software (i.e MOSFLM and/or XDS for the indexing step)
- Development process:
 - Test-driven development process
 - Code reviews



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The main scientific 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 (RADDPOSE)
Data collection strategy (BEST)



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Progress on the scientific level:

- Implementation of an indexing plugin:
 - › indexes a list of reference images (typically 2) by invoking the 3rd party software MOSFLM
 - › analyzes the MOSFLM output and returns the result in an XML format
- Implementation of a radiation damage estimation plugin:
 - › estimates the absorbed dose by a sample given its chemical composition by invoking the 3rd party software RADDPOSE
 - › analyzes the RADDPOSE output and returns the result in an XML format



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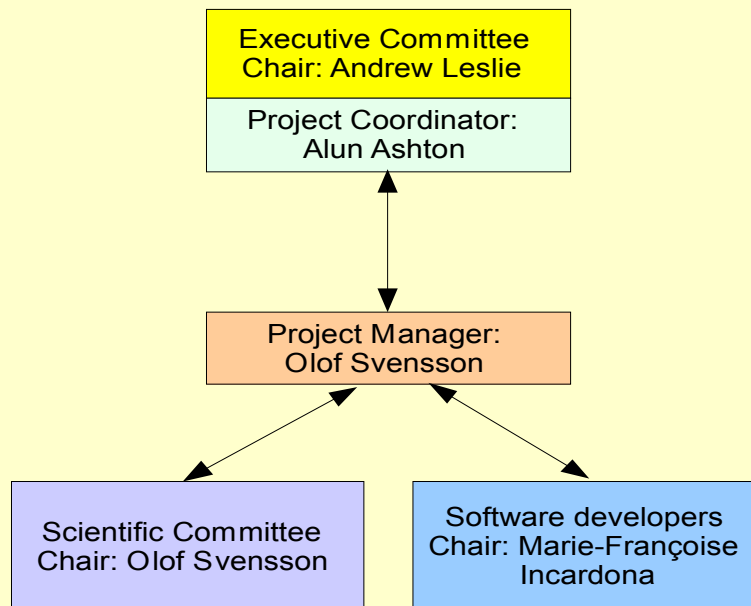
Progress on the project and technical levels:

- Communication (internal and external):
 - www.edna-site.org
 - Wikipedia, discussion forum, VC tool: Marratech
- Tools & Development framework:
 - IDE: Eclipse - Data Modeling: Enterprise Architect
 - Source and Bugs managements: Subversion, Bugzilla
 - Dedicated server: dedibox
 - Programming language: Python/Jython to allow also Java plugin development
 - Modular and multi-thread system (AALib)
 - Data classes code generation from UML (XSD data binding)
 - Main EDNA plugins hierarchy and configuration facility classes developed
 - EDNA Test Framework developed (framework, unit and validation Tests)



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EDNA project structure:



Executive Committee:

Alun Ashton : Diamond Light Source, UK
Gérard Bricogne: Global Phasing, Cambridge, UK
Andrew Leslie: MRC LMB, Cambridge, UK
Andrew McCarthy: EMBL-Grenoble, France
Sean McSweeney: ESRF, Grenoble, France
Thomas Schneider: EMBL-Hamburg, Germany
Andrew Thompson: Synchrotron Soleil, France

Scientific committee & Developers Team:

Not clearly defined yet



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Main EDNA Events during this year:

- EDNA full meetings

- 22nd February 2007: Diamond, UK
- 5th - 7th June 2007: ESRF-Grenoble, France

- EDNA developers meetings

- 20th - 21st November 2007: 1st EDNA developers workshop, EMBL-Grenoble, France
- 18th - 19th February 2008: Synchrotron Soleil-Paris, France



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Short and medium terms plans:

- Development of a prototype that will implement the whole chain (from indexing to strategy without parallelism using MOSFLM, RADDPOSE, BEST)
- Development of the application that will take into account parallel steps
- Implementation of a generic data model: possibility to invoke different 3rd party software for a given step (i.e: MOSFLM and XDS for the indexing step)
- Improvement and development of plugins regarding scientific use case requirements
- Documentation: user guide on the EDNA development framework
- ...



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- AALib support: Romeu Pieritz
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- MOSFLM inputs: Andrew Leslie, Harry Powell
- RADDOSE inputs: Gleb Bourenkov, Elspeth Garman, Elspeth Gordon, Peter Keller, Andrew Leslie, Alexander Popov
- XDS plugin start: Sandor Brockhauser, Pierre Legrand
- Management support: Alun Ashton, Gérard Bricogne, Andrew Leslie, Andrew McCarthy, Sean McSweeney, Andrew Thompson, Thomas Schneider
- BIOXHIT foundation



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- EDNA project members:

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Thank you !