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.
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 (RADDOSE)
- 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 RADDOSE
  ➢ analyzes the RADDOSE 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
Main EDNA Events during this year:

- **EDNA full meetings**
  - 22\textsuperscript{nd} February 2007: Diamond, UK
  - 5\textsuperscript{th} - 7\textsuperscript{th} June 2007: ESRF-Grenoble, France

- **EDNA developers meetings**
  - 20\textsuperscript{th} - 21\textsuperscript{st} November 2007: 1\textsuperscript{st} EDNA developers workshop, EMBL-Grenoble, France
  - 18\textsuperscript{th} - 19\textsuperscript{th} 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, RADDONE, 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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- BIOXHIT foundation
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- EDNA project members:

  Alun Ashton\(^{(d)}\)
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  Jose Gabadinho\(^{(c)}\)
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Thank you!