

Minutes EDNA Prototype Demonstration meeting

June 26th – June 27th 2008

Presents :

Alun Ashton (Diamond, UK), Gleb Bourenkov (EMBL Hamburg, Germany), Sandor Brockhauser (EMBL Grenoble, France), Mirek Gilski (Center for Biocrystallographic Research, Poznan, Poland), Elspeth Gordon (ESRF, France), Marie-Françoise Incardona (ESRF, France), Andrew Leslie (MRC LMB, UK), Karl Levik (Diamond, UK), Andrew McCarthy (EMBL Grenoble, France), Sean McSweeney (ESRF, France), Harry Powell (MRC LMB, UK), Olof Svensson (ESRF, France), Takashi Tomizaki (SLS, Switzerland), Johan Unge (MAX lab, Sweden)

Partly presents :

Romeu Pieritz (ESRF, France), Sasha Popov (ESRF, France), Darren Spruce (ESRF, France)

Agenda :

Thursday June 26th :

14:00 - 18:00 : Prototype demonstration and discussion

- Demonstration
- Data model
- Implementation
- Configuration

18:00 - : Executive committee meeting with project manager

Friday June 27th :

9:00 – 12:00 : Future developments

- Improvements within the scope of the prototype
⇒ final requirements for the prototype, deadline end of July
- Generic data model + XDS
- Deploying EDNA on beamlines : MOSFLM post refinement, POINTLESS, MTZUTILS and SCALA plugins
- HTML pages
- Project agreement, licence, distribution
- Next meeting (December 2008?)
- Longer term developments (if time allows) : KAPPA (through STAC), GRID, MAD / SAD data collection strategy optimisation

1. Overview of the meeting

Olof opened the meeting with a short presentation describing the meeting agenda and the goals with the meeting. He then made a short demonstration of the prototype by running it on different sets of input images, illustrating successful runs with single or multiple images, including parallel indexing of several images, and explaining the organisation of the generated output files. This will be remembered as a very hot event due to broken air conditioning and the unusually hot weather in Grenoble that day...

After coffee the meeting moved to a new meeting room with air conditioning. Various aspects of the prototype were discussed (data model, logs, error handling etc). We started on Thursday to discuss as well the future of the project, and the meeting was closed by noon on Friday after having agreed on the points outlined in the following sections.

2. Prototype requirements (Deadline end of July)

We agreed on the following set of items that should be implemented in the prototype :

- **Add default RADDPOSE structure** : If no structure information is available, then EDNA should use a default structure (Gleb will provide one).
- **Generation of prediction images** : demonstrated but not fully implemented, should be a part of the final prototype.
- **Executive summary** : The prototype should give the essential results in the form of an executive summary. Elspeth will provide help on what should be present in this summary.
- **Integration I / sigma** : The integrated intensity I and I/sigma as function of resolution should be a part of the integration result.
- **Missing items in data model** : The following parameters were missing in the data model presented and should be part of the final prototype data model :
 - Ranking resolution, ring current
 - Diffraction plan: Resolution, I/sigma, multiplicity and completeness as input to strategy
 - Max phi speed, min exposure time, min osc width (should also be part of configuration)
- **Prototype report** :
 - Add why new development (from spike report)
 - Deployment / installation instructions
 - Annotate the UML diagrams
- **Licence** : It was suggested to release the prototype under LGPL3 with the same modifications that were introduced for the CCP4 licence to make it valid under British law..

3. After the prototype (August - October)

- **Tests of the prototype on beamlines** : Sandor and Alun agreed to make sure that the prototype will be tested on ESRF and Diamond beamlines respectively and would coordinate feedback.
- **Small XDS plugin meeting in September** : As Gleb and Sandor would like to help developing the XDS plugin, it was suggested that a small meeting is organised at the ESRF in the period mid-September till the end of September. The developers documentation (see below) will not be ready for this meeting.
- **Developers' documentation** : It was agreed that before developing any new functionality in EDNA, Marie-Françoise and Olof should write up developers' documentation, in particular :
 - “How to write an EDNA plugin” documentation
 - Data model implementation and development
 - Plugin hierarchy etc.
 - Coding convention, development tools etc.
- **Plugin Workshop by mid October** : Limited to max 10 people who are expected to be contributing to EDNA.
 - How to develop MOSFLM post refinement, LABELIT (ask Brookhaven to do this plugin), POINTLESS, SCALA, ISPyB (it was suggested that Karl could do this) and DENZO (Mirek).
 - As the BioXHIT funding has stopped travel money must be taken from individual institutes budgets.

4. New plugin submission / development procedure

We discussed briefly a work flow for submitting a new plugin for EDNA :

- Specifications – related Use Case
 - ⇒ Validation
- Coding including tests
 - ⇒ Code review

5. Next meeting – Soleil

We agreed to suggest to Andrew Thompson if Soleil could organise the next full EDNA meeting.

Possible dates (in December):

- 8th 14:00 -> 9th 12:00 or
- 15th 14:00 -> 16th 12:00