EDNA Full Meeting 23rd September 2010
ESRF Auditorium, Grenoble

Session 1 : Overview and status reports

09:00 - 09:10 Introduction to the full meeting (Andrew)

09:10 - 09:30 EDNA Usage at the ESRF / DLS (Olof + Alun)

09:30 - 09:45 EDNA for X-ray Imaging (Jerome)

09:45 - 10:00 EDNA for Tomography (Mark)

10:00 - 10:15 The joint DLS/CCP4 Difference Map Pipeline (Ronan)

10:15 - 10:30 A workflow tool for EDNA (Matthew)

10:30 - 11:00 Coffee Break

Session 2 : MXv1 to MXv2 transition
11:00 to 12:30

- Current status of MXv1 (Olof)
- Current status of MXv2 (Sandor)
- Suggested plan for migration MXv1 -> MXv2
- Agreement on roadmap

12:30 - 14:00 Lunch

Session 3 : Project agreement revision
14:00 to 15:30

- Kernel executive committee + project agreement
- MXv1 / MXv2 executive committee + project agreement
- BioSAXS
- Other developments / collaboration agreements

15:30 - 16:00 Coffee Break

Session 4 : Future perspectives of the EDNA collaboration
16:00 to 17:30

Kernel developments, data modelling tools open discussion:

- Involvement of new participants
- Fundings

List of participants:

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Session 1. Overview and Status reports

Andrew Leslie gave an introduction in which he thanked all developers for the progress made since the last full meeting in June 2009, and particularly Olof Svensson at ESRF for his role as project manager and Alun Ashton for coordinating activities at Diamond. He reported that EDNA now encompassed a range of different applications and that this had strengthened the project particularly the EDNA kernel. Crystal characterization with MXv1 was working well, but progress with MXv2 (to enable use of a kappa goniostat and alternative processing packages) had been much slower. One of the major goals of the meeting was to find a way to accelerate progress with MXv2 and preliminary discussions suggested that this would probably require a change in structure of the project.

Olof Svensson reported that the MASSIF project at ESRF depended heavily on both EDNA and ISPyB while the NINA upgrade project would also be using EDNA. Current challenges included replacement of Enterprise Architect with an Eclipse based model.

Alun Ashton described how the EDNA framework was being used for MX, an archiving pipeline, a tomography pipeline, DIMPLE (an difference map pipeline) and SAXS (at an early stage of development) within the DLS/CCP4 environment. It may be used in the future for spectroscopy, a data reduction manager and MX structure solution. Approximately 2.5 FTE were employed on these developments.

Usage of EDNA MX is not logged at DLS as it is run automatically when reference images are collected.

Four presentations followed on non-MX applications of EDNA[1]. Several speakers commented on the strengths of EDNA: robust, multithreaded, testing framework, many plugins available, many collaborators, good support. Identified weaknesses were an initial lack of documentation (now greatly improved), large overhead of UML modeling, and a steep learning curve. It was felt that a straightforward tutorial was very valuable and one for raw digital photography was being developed. A code camp is planned for the near future.

There was some discussion of whether non-MX applications should be deposited in the EDNA SVN. Some projects are currently represented while others are not. One of the difficulties was that some projects are difficult to distribute as they rely on multiple compilers.

Session 2 MXv1 to MXv2 transition

Olof gave a brief history of the EDNA project and its relationship to DNA. He explained the relationship between MXv1, which has a simplified data model and deals with crystal characterization using a single axis goniostat, and MXv2 which has more advanced (generalized) detector and goniostat descriptions, enabling it to deal with kappa goniostats and other processing packages. The data model for MXv2 is quite advanced, but is still missing some important features (eg transmission).

He explained that an MXv2 kappa strategy does exist today, in combination with MXv1 indexing and integration, so that it is possible to obtain a kappa strategy. This was achieved with minimal effort by reusing the MXv1 indexing and integration components and writing only a new MXv2 strategy component. Two routes were possible for moving towards MXv2:

1. Continue to develop MXv1 and slowly migrate to MXv2
2. Stop MXv1 development and make all new developments in MXv2.

A general discussion followed about the relative merits of these alternatives and indeed whether a transition to MXv2 is currently feasible. Several developers (Gleb, Sandor) felt that it was very important to advance to MXv2, reflecting that there was clear interest in the use of kappa goniostats from many synchrotrons including Petra III, BESSY, SLS, and Max Lab. Martin Walsh asked whether any statistics were available on the current usage of the kappa goniostat at ESRF, where it has been available for several years. No detailed statistics were available, although specific cases were known where use of kappa was essential to the success of a project. Alun Ashton reported that DLS are concentrating on MXv1 optimisation and are currently deciding about MXv2 and how much effort will be put into it by Diamond.

Sandor suggested that the least demanding route was to work further with the current implementation, using an MXv2 layer on top of MXv1. Sandor was the only person identified as being able to commit time to MXv2 developments.

The current outstanding goals for MXv1 were listed as:
i) Use of a sacrificial crystal for strategy determination (by BEST).
ii) Improved error messages
iii) Fine tuning of BEST strategies

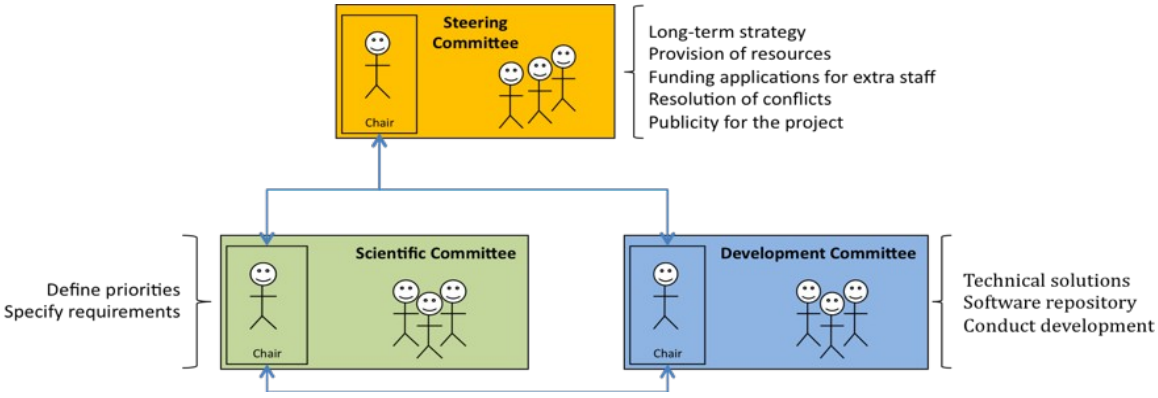
Sean recognized that MXv2 was well adapted for more challenging cases, but questioned the resources necessary to achieve the transition, and emphasized the importance of having a properly defined project plan. Without this he felt it was not possible to make any progress.

After lengthy discussion it was agreed that no decision could be taken at the meeting on the best way forward, and the meeting adjourned for lunch.

During the lunch break there was an ad hoc meeting of the executive members present.

Session 3 :Project agreement revision

Olof proposed a new MOU that involves a change in structure of the project (*see below*).



He feels his position is better described as Project coordinator than manager as there are currently no resources to manage. In addition, he felt that he is not the best person to coordinate the development of future EDNA MX scientific roadmaps, and that this would be better done by scientists, while his own role would be to coordinate development of the EDNA MX code (in addition to also coordinating the kernel developments).

In addition, with the increasing number of non-MX applications using the EDNA framework, he felt that there were advantages in setting up a new steering group for the EDNA kernel. This steering group would have an MX representative, to ensure that any changes proposed did not have any adverse effects on EDNA MX.

In the subsequent discussion, Sean asked if separation of the Kernel from MX was really necessary, and whether this would have a negative impact on the MX development that he felt was the most important. Thomas Schneider agreed that this was a concern. Olof suggested that this could be avoided by having an MX person on the steering committee.

Sean was also concerned that if a new steering committee was set up for MX, then would it be done for all the other interest groups ? He would prefer one grouping to cover all aspects of life sciences. There was no general agreement on this, however.

Alun pointed out that the risk of a fork in the kernel development was real if one scientific group were seen to be the only people in charge of a part of the project that was needed for all developments.

Again, it was concluded that no decision could be taken at this stage on splitting the kernel. Sean requested that Olof develop a formal proposal, spelling out:
i) why the split was necessary and how it would benefit the collaboration
ii) How the separation of the kernel will operate
iii) How this will link to other EDNA projects, processes etc.
iv) A mechanism for dealing with conflicts, prioritization etc.

There was general agreement with Olof's suggestion that further input from beamline scientists and users was required to help define future priorities. The following plan of action was proposed:

1. The executive member for each site should nominate a scientific representative to collect and coordinate input from beamline scientists, and if possible users, about their priorities for future EDNA MX developments.

2. These should be assembled as a single prioritized list for all sites. An estimate of the resource implications for each item on the list should be obtained from the developers.

3. This list of prioritized objectives, with resource implications, should be passed to the EDNA executive who will make the decision on what resources are actually available and provide a final prioritization.

Session 4: Future perspectives of the EDNA collaboration

This session started with the description of an application of EDNA to the BALBES pipeline from Fei Long. Some of the difficulties encountered Many generations of inheritance) were due to the use of Aalib, which was removed from the package during the summer. Other issues (data binding) will be addressed in the upcoming code camp. Jerome made the point that he wanted scientists to be able to use EDNA, which requires that the UML component is simpler.

There was further discussion of the need to include non MX developments into SVN so that they could be subjected to the nightly tests.

Finally the prospects of obtaining additional funding that might contribute to EDNA were discussed. Thomas Schneider suggested that he would look into the possibility of obtaining German funding for interdisciplinary projects. Sean mentioned the possibility of rearranging internal (ESRF) funding or an ANR (French) grant, but that the latter had failed in 2009. Otherwise there were no obvious sources of new funding.

Andrew drew the meeting to a close by concluding that additional scientific input was clearly required to determine the future course of the EDNA MX development, but that a consensus had at least been reached about a route to determine how this would be done.