

DNA Developers Meeting Minutes Day 2: General

Those attending:

SRS

Steve Kinder

Karen Ackroyd

Graeme Winter

ESRF

Olof Svensson

Darren Spruce

Diamond

Richard Wooliscroft

Gwyndaf Evans

EMBL Hamburg

Venkat Parthasarathy

Probably others!

Agenda

BEST

Licenses

Posters/Web Pages & PR

Version 1.0 Release Features

LIMS

Documentation & User Support

Testing

Reference Images

Spacegroup determination through Scaling

Scoring

e-HTPX input & output

Scheduler update

The discussion of including BEST was postponed to the third day of the meeting, since it was critical that Harry was there.

Licenses

Martyn Winn described the situation regarding the CCP4 license in some detail. It was felt that a license was important, since we're planning to make a release of DNA (version 1.0) public in the not to distant future. The possibility of charging (industrial users) for either the software or support for the software was also considered, but no conclusions were drawn at this stage. However, most parties agreed that having a license in place would simplify charging in the future.

Poster & Web Pages

Many of the DNA developers have been and will be presenting DNA at conferences. It was felt that having a single “repository” for diagrams, logos and descriptions would save a great deal of effort duplication, and also make it look like everyone was singing from the same song sheet. However, no specific actions from this were defined.

Version 1.0

This was a substantial part of the day – defining the features which should be implemented for the DNA 1.0 release. Since this is scheduled to occur before the next full DNA meeting (early July) the time was limited, so some items were postponed for version 2.0.

DNA 1.0

1. Single wavelength data – not MAD
2. Automatic screening & ranking
3. Determine optimum exposure time – BEST
4. Spacegroup determination
5. Automatically integrate & scale data – but displaying the output on the DNA gui may have to wait.
6. Run offline
7. Run at home – Linux only

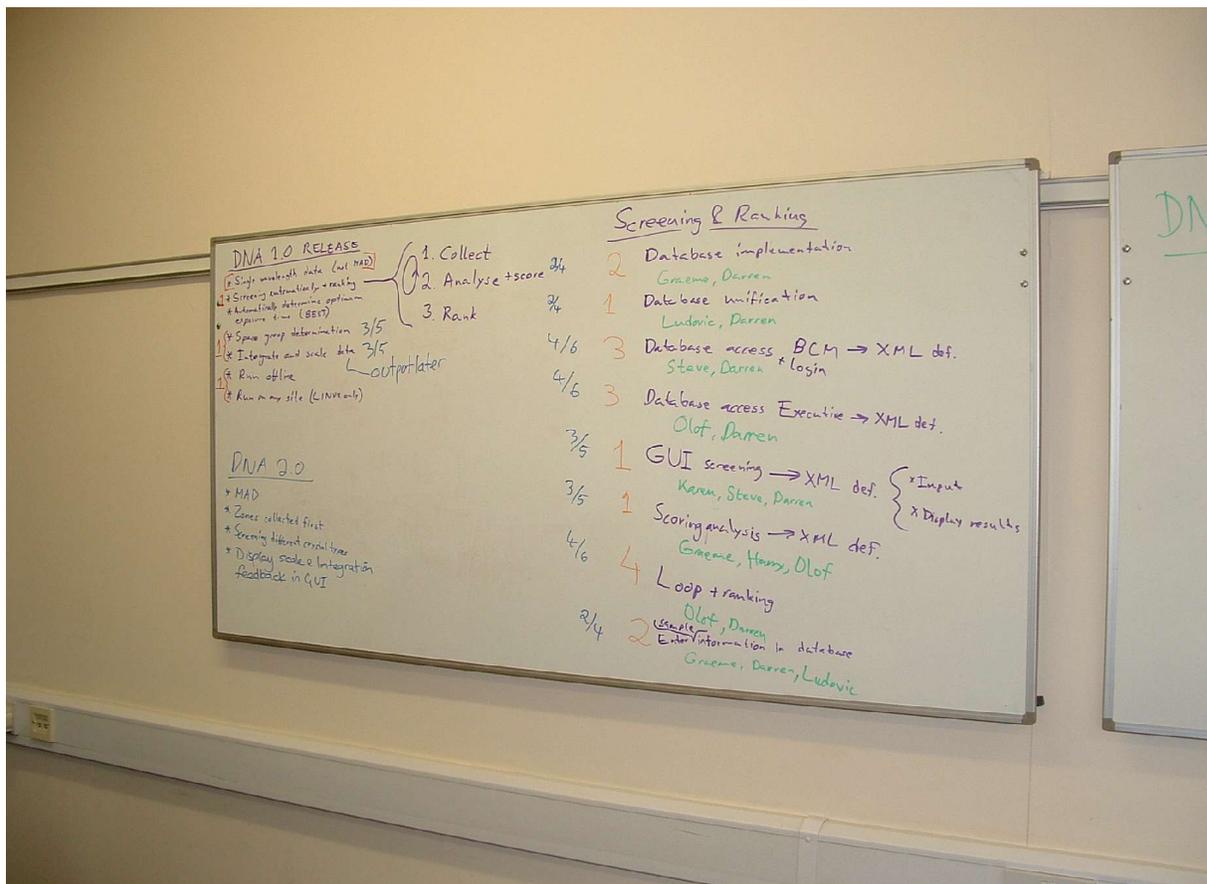
DNA 2.0 (speculative)

1. MAD
2. Collect interesting zones first
3. Screening different crystal types
4. Display scaling & integration results in GUI

Each of the tasks for version 1.0 was prioritised, deadlines determined and someone to actually do the work proposed. This was:

Date	Priority	Action	People
02/04/04	2	Database implementation	Darren, Graeme
02/04/04	1	Database unification	Darren, Ludovic
04/06/04	3	Database access	Darren, Steve
04/06/04	3	Database Access from Executive	Darren, Olof
03/05/04	1	GUI screening – require XML definition	Karen, Steve, Darren
03/05/04	1	Scoring analysis	Graeme, Hary, Olof
04/06/04	4	Loop structure for ranking	Olof, Darren
02/04/04	1	Enter sample information into database	Graeme, Darren, Ludovic

I have a digital photograph of the whiteboard on which we decided this – so I'll put that on the web.



Release 1.0 Discussion

Clearly the considerations for the 1.0 release are non trivial – in particular the changes which are required for making the system run offline efficiently....

The GUI will need a facility to browse around the files, so that a user can pick up the appropriate files. We'll also have to put a change into DNA so that the beam centre in the image header is respected.

The LIMS Situation

There is no beamline database or LIMS at the SRS, while at the ESRF there will shortly be two. Darren Spruce has been developing (with much help from others) PXWeb, which is in use at the ESRF. Ludovic Launer, as part of e-HTPX, is developing a new lims, which aims to be more generic. At the meeting Ludovic and Darren agreed to unify their data models, to make a items consistant. Darren also agreed to come to the SRS to help deploy PXWeb, to give the SRS users some experience with a beamline database, and also provide a database for DNA to use.

Documentation & User Support

The requirements for documentation and user support were described, with particular reference to the 1.0

release. It was decided that we should have a dna-support@esrf.fr mailing list, which would send messages to

Harry
Graeme
Olof
Steve
Karen
Darren

So that the appropriate person could respond. In addition, I think we thought about deploying something like bugzilla for tracking problems and assigning people to fix them... as well as a FAQ, which could be placed on the web – Graeme was actioned to do the FAQ.

An associated problem is that there is currently no method to globally “switch on” debugging – which would be very useful. This global log could be included with the 'mail to dna-support.

Some elements of the documentation are missing, in particular:

1. Overall scheme of how dna works
2. GUI UML diagram
3. Scheduler documentation
4. Documenting the components of DNA
5. Class diagrams for Executive & Scheduler
6. Features list – what we have, want and are working on

Basically I think that some work will be required on most components of DNA, but more for developers than for users.

Testing

It was decided that we should have a built in test which comes with DNA, so check to see if it's OK, something like

```
> ./isMyDNAHappy.sh  
yes  
>
```

Also, we agreed that it was about time we had another beta release – there are a lot of people who'd like to have a go with this.