DNA Scheduler Meeting
8/9th of March
G59, Diamond House, RAL

The purpose of the meeting is to decide how we manage, maintain and use the existing scheduler (e.g. developments with kappa, XDS) and a development route from here.

March 8th

Time	Agenda	
10.30	Coffee/Tea/biscuits	G59, 10 people
	Part 1	
11.00	Closed DNA core developers meeting. Agenda and invitations will be made separately.	
11.10	Everyone should make/prepare a (frank) statement of what they want from the scheduler and this meeting. Agenda may change as a result (e.g. to clear blood off carpet).	
11.30	How you could get other DNA projects to interact with the current scheduler. To get the ball rolling Graeme has offered to make a quick 15 min presentation on how he thinks this could currently be done.	Graeme Winter
11.45	How we are going to manage these interactions to make sure we maintain stability for any dependencies yet still allowing developments e.g. do we need a change control board? Can we identify and stabiles a scheduler core?	
12.30	Sandwich working lunch for core developers. Coffee/Tea/biscuits	G59, 10 people
12.45	Future developments for the scheduler.	
13.30	Using DNA/Scheduler for other techniques. What do people think?	
13.45	Set/formalise agenda for Part 2 and 3.	
	Part 2	
14.00	DNA-DEV meeting. To discuss what the requirements and	

	interactions developments such as Kappa, XDS (and the XSD extensions), MAD and crystal Ranking are with regards to the scheduler.		
	How you could get other DNA projects to interact with the current scheduler. Graeme Could we have <> 5min presentations by Sandor (thoughts on Kappa), Olof maybe on Crystal ranking and MAD. Update on UML'ing. Lorenzo?		
15.30	Tea/Coffee	G59, 12 people	
17.30	Close		
Eve	Accommodation in Wantage (see below)		

March 9th

	Part 3		
9.30	Tour of Diamond construction site.	Maybe!	
10.30	Coffee/Tea/biscuits	G59, 15 people	
11.00	Open scheduler meeting. To discuss how the scheduler fits in with or how other projects fit in with the scheduler. The two main projects in consideration here are CCP4-automation and BioXHIT. How you could get other projects to interact with the current scheduler. Graeme What do other projects want from DNA? Please think and prepare presentations accordingly. What can other projects contribute to the work? Please think and prepare presentations accordingly.		
12.30	Sandwich lunch (DH Atrium or ground floor) Coffee/Tea	DH, 20 people	
13.30	Continuation of Part 3		
15.30	Tea/Coffee/biscuits	G59, 15 people	

Attending

	Name	From	8th of March		9th of March
			Part 1	Part2	Part3
1	Alun Ashton	DLS	☑	☑	☑
2	Graeme Winter	DL	☑	☑↩	☑

3	Olof Svensson (virtually)	ESRF	☑	☑	☑
4	Sandor Brockhauser	EMBL		☑⤶	☑⤶
5	Raymond Revelli	EMBL		☑⤶	☑⤶
6	Lorenzo Milazzo	GlobalPhasing		☑⤶	☑
7	Steve Kinder	DL	☑	☑⤶	☑
8	Karen Ackroyd	DL	☑	☑	
9	Colin Nave	DL	☑	☑	
10	Andrew Leslie	MRC Cam	☑	☑	
11	Paul Emsley	Uni of York			☑
12	Ronan Keegan	DL			☑
13	Marc Malfois	DLS observer			☑
14	Fajin Yuan	DLS observer			☑
15	Jason Roche	DLS observer			☑
16	Bill Pulford	DLS observer			☑

⤶ Accommodation is at the Bear Hotel, Wantage Market Place, 01235 766366 booked in the name of Alun Ashton, B&B £65 Pounds a night, please settle your own account.

MINUTES
DNA Scheduler Meeting
8/9th of March
G59, Diamond House, RAL

Attending in Diamond
Graeme Winter (DL)
Karen Ackroyd (DL)
Steve Kinder (DL)
Colin Nave (DL)
Andrew Leslie (LMB-Cam)
Alun Ashton (DLS)

Lorenzo Milazzo (GlobalPhasing)
Katherine McAuley (DLS)

Richard Woolliscroft (DLS)
Sandor Brockhauser (EMBL-Grenoble)
Raymond Revelli (EMBL-Grenoble)

Paul Emsley (Uni of York)
Ronan Keegan (DL)
Marc Malfois (DLS observer)
Fajin Yuan (DLS observer)
Jason Roche (DLS observer)
Bill Pulford (DLS observer)

Attending at the ESRF
Olof Svenson
Darren Spruce
Romeu Pieritz

Attending at Soleil
Pierre Legrand
Andrew Thompson

Attending at Daresbury
Norman Stein

Part 1
Closed session for DNA core developers and available exec members.

At the start of the meeting it was felt appropriate that everyone attending
expressed what they would like from this meeting.
There was a general desire to understand more fully how the current
scheduler works, and what limitations (if any) its structure imposes on
current and future developments of DNA. Additional documentation at both
a scientific and programming level would be useful. The possible
applicability of DNA to other areas than MX was raised. Incorporation of
Graeme's branch remains an outstanding issue, and this includes developing
a procedure for deciding whether or not additional features are to be included
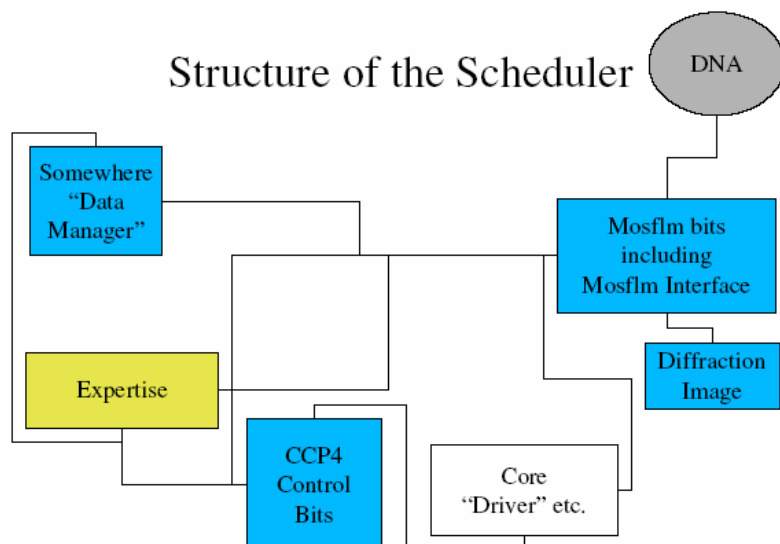in the main branch.

Following this Graeme made a presentation of his thoughts and overview of
his current ideas with regards to the relationship between the current
scheduler and the future within XIA.

Presentation available at:
http://www.dna.ac.uk/minutes/240105/graeme1.pdf

During this ensuing discussion Graeme outlined the problems and restraints currently imposed with the current scheduler structure below and outlined a proposal of how the future scheduler would be modularised:
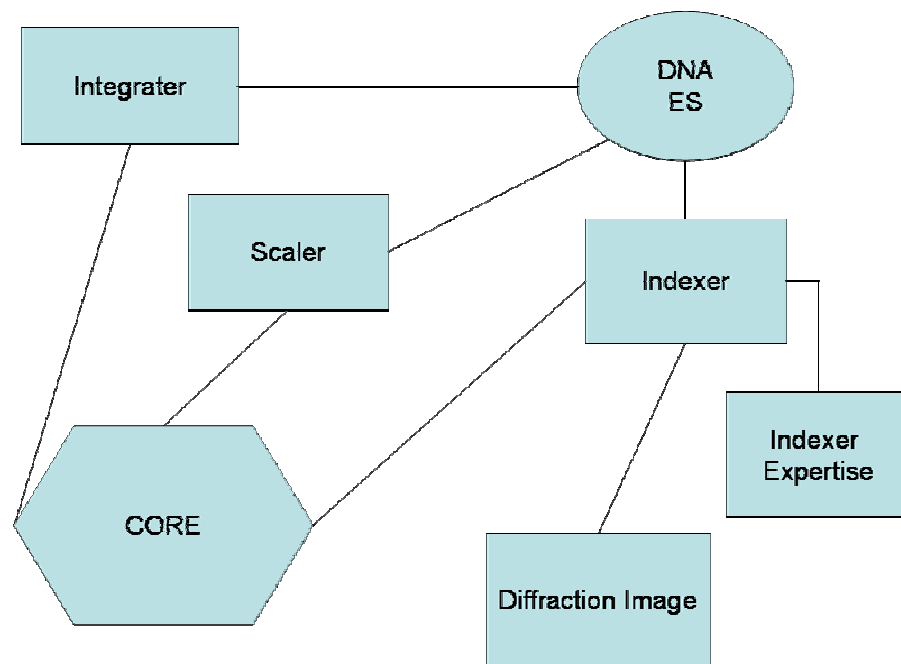
Current Scheduler (from Graeme's presentation):

The "Core-Driver" is responsible for running programs in a very generalised way, using specific input prepared by other modules and passing output back to appropriate modules (e.g. results of an "indexing" operation back to the "Expertise" module).

The major drawback of this structure is that the code is becoming unmanageable, particularly the module "Mosflm bits". Most of the bugs in the scheduler have been in this module. It is also "mosflm-centric", making incorporation of other data processing modules (eg XDS) very difficult. It is therefore desirable to break up this component into a number of specific tasks.

Graeme has started to do this within the XIA structure, which is also intended to allow the development of other aspects of automation which do not come under the remit of the DNA project (eg phasing and structure solution). However it should be noted that these other developments should not affect the stability of the basic scheduler as used by DNA. The scheduler within XIA started as exactly the same code as that within DNA, and there is nothing *radically* different between the structure of the scheduler within XIA and that within DNA.

Future Structure (reproduced from flip chart):

Integrater
DNA ES
Scaler
Indexer
Indexer Expertise
CORE
Diffraction Image

Realistically it is likely to take until the end of 2005 to achieve this new structure.

What needs to be done:

1) Testing by non-developers. Is the scheduler core OK ?

2) It is requested that developers start to look at the code as a code review exercise, and feedback to Graeme as much as possible. Although major changes to the structure design may be difficult it is not ruled out if there is justification and agreement.

3) Investigation of data management (crucial for ranking).

4) Scoping for future developments.

5) Provision of framework for both stability and development.

Ranking

Olof gave a report on the recent DNA pipeline test that occurred at the ESRF. A full report on this will be made available elsewhere.

Documentation

The issue of documentation was raised to Graeme as a problem for a number of developers. It was pointed out that low level documentation does exist as extracted from the code. A commitment to higher level documentation was made on the following basis:

Graeme will produce documentation based on replies to specific questions asked by 'anyone'. E.g. the following question was asked by SK:

"How do I add a new module?"

Questions of this kind should be emailed to Graeme whereupon he will produce documentation as an answer. The questions and answers will be distributed and made available on dna-dev and the DNA web site.

Testing
The issue of testing was raised. An initial comment was made that before a major upgrade to an area of DNA is deployed on the beamline/site it would be useful if the individual who made the changes could travel to the respective site to assist in the upgrade E.g. before major upgrades to the scheduler are tested or made on the ESRF beamlines Graeme should try and travel to the ESRF to help.

It was pointed out that the 'live' testing of DNA at the SRS should now be more thorough as Station 7.2 is now a dedicated test beamline.

Off line testing of modules such as Automation.py were considered useful but Graeme pointed out that a number of modules such as the DNA GUI and the ES would need changes to allow them to work fully as a DNA module.

ALL:
*** It is not clear to me from the above (or from my notes) how the issue of testing the current structure is going to be carried out. We really need to run entire datasets of various kinds to check the performance of the system from a scientific viewpoint (rather than a programming one). Graeme, do you have any suggestions how this should be done? I would like to carry such tests at LMB ***

Future developments for the Scheduler.

Graeme has already outlined the relationship between the scheduler and XIA. It was pointed out by Graeme that modules developed for the scheduler will work in XIA and this is a design requirement for backward compatibility with legacy modules.

It was pressed on Graeme that this was an important point and he has committed himself to support the backward compatibility for legacy modules.

A lively discussion was had on how best to achieve a reliable framework that would fit in with the need to develop and the need for a level of stability.

Scheduler/XIA Core.
An agreement was reached that a core for the Scheduler/XIA would be identified by Graeme. This core would be the stable framework upon which other modules were dependent. Changes to the core would be infrequent and controlled.

For control of the XIA core code a committee is to be formed outside the DNA executive which will review the impact and on agreement, implement changes as required. The DNA executive will only be consulted on major decisions where agreement cannot be reached.

The Committee will be formed from developers who have had experience of the scheduler/XIA code and would be able to implement and test any relevant changes. **Nominations are now requested.**

The timescale for identifying the core and nominating the core committee is by the 18ᵗʰ of March.

The committee will then be expected to report on the core and its stabilisation by the May Hamburg DNA-DEV meeting.

It was felt that incorporation of the new scheduler (as in XIA) into DNA was a reasonable target for DNA version 2.0

Making DNA available to other techniques.
The group felt that although in principle using DNA for other techniques should be encouraged, the only aspect of the DNA code which was possibly useful to techniques other than Protein Crystallography was the core of the DNA scheduler. Other aspects of the code were considered to be too specific towards PX.

Part 2

DNA-DEV meeting.
To discuss what the requirements and interactions developments such as Kappa, XDS (and the XSD extensions), MAD and crystal Ranking are with regards to the scheduler.

2.1 Graeme Introduction
See presentation http://www.dna.ac.uk/minutes/240105/graeme2.pdf

2.2 Kappa – Sandor

Sandor gave a comprehensive presentation on his thoughts on integrating Kappa work into DNA.

The presentation is available at
http://www.dna.ac.uk/minutes/240105/sandor.pdf

Most notable was the potential requirement to integrate the work with the whole of DNA and not just the scheduler/XIA. This could case many problems to ensure it works properly and DNA developers are asked to feedback their thoughts to Sandor as soon as possible so he can make a full presentation of the plans in the Hamburg DNA-DEV meeting. Sandor already has a mailing list for interested parties in the Kappa work and has been encouraged to setup a web page on the DNA web site.

2.3 MAD - Olof.

Olof outlined his current plans for integrating MAD experiments into DNA. The question was raised on whether or not the MAD module should call and interact with external programs directly or whether it should do this by interacting with the scheduler/XIA. It was agreed that this should be done through XIA and a test should be done with integrating CHOOCH into DNA. As the timescale for the MAD work is DNA V2.0 (End 2005)
It was also suggested that Olof sets up a MAD web page and uses (in the first instance) the DNA-DEV mailing list for discussions and information.

Action Olof and Graeme: Integrate Chooch into XIA.

2.4 Screening and Ranking - Olof

Screening and ranking was revisited with respect to its interactions with the Scheduler/XIA.

Olof commented that the main thing missing from the screening experiment was the diffraction plan.

It was thought prudent to revisit the changes that were made prior to the pipelining experiment with regards to the XSD and GUI changes required to make the experiment work.

Action: Karen volunteered to lead and to make sure the changes to the XSD and GUI reviewed. Please report back in the DNA-DEV Hamburg meeting.

With regards to the ranking of crystals it was suggested that this would require its own web area as with many of the other modules.

The issue of Data management was highlighted as one of the main barriers to enable Ranking. See Day 2 2.6

2.5 UML - Lorenzo.

Lorenzo gave a presentation on the UML generation for data management in the DNA structure.

Issues were raised with the UML diagrams in XXpackage nameXXX as they did not represent something??? Graeme?

Lorenzo's talk is available at XXXXXXXXXXXXXXX

There was much agreement that the representation of the work in UML was a useful exercise but currently the tools for the code auto generation would not be useful within DNA. XXX some DNA code already auto generated? Can someone remind me where this was? XXX

DAY 2

2.6 Data Management - General
Data management within DNA has been raised as a serious and urgent issue. It was recognised that ISpyB can be extended to hold the majority of the data required so circumventing the need for the scheduler 'bucket'. A bucket of sorts was deemed necessary to allow speed etc.

A discussion on data access resulted in an agreement that components requiring to communicate with the database could do so directly and this would not go through one central area.

Work on defining and building a data access / management layer is believed to be of a high priority.

2.7 XDS – Pierre
By Video conf Pierre was able to give us a presentation on the work required for XDS incorporation into DNA.

Most of the work hinges on a more comprehensive data management/access layer.

The presentation is available at
http://www.dna.ac.uk/minutes/240105/pierre.pdf

The timescales for incorporating XDS into DNA is by 2.0

Part 3

General discussion and demonstration.