

DNA “Scheduler” Meeting

8th-9th March 2005

DLS

axes.grind()

or

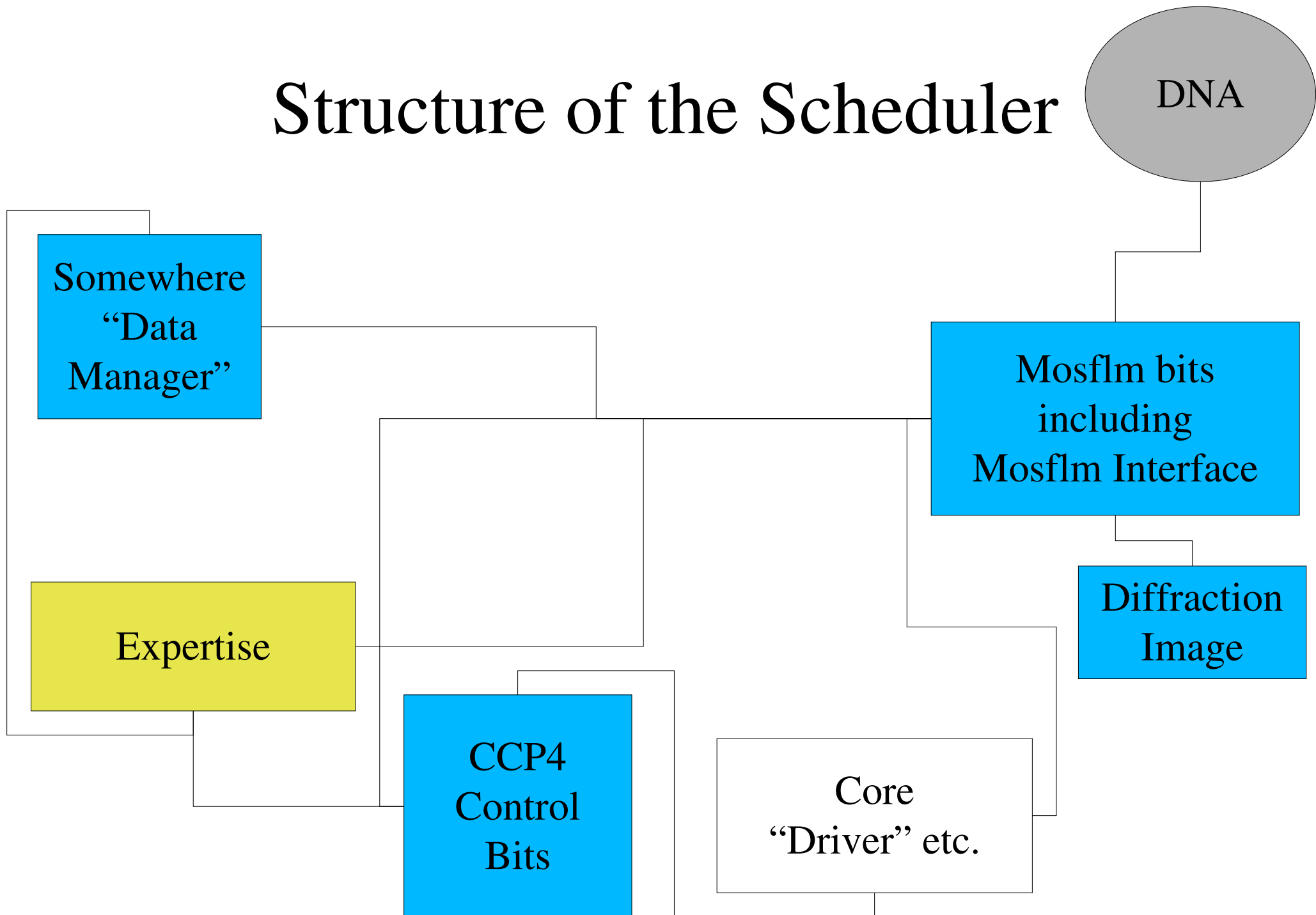
progress.make()

?

Outline

- Structure of the Scheduler
- What's going on in there at the moment
- What's going on in XIA
- What needs to be done ... IMHO
- What must not happen
- Testing of implementations

Structure of the Scheduler



What's going on in there?

- Provides DNA “services”:
 - Screening
 - Indexing
 - Strategy
 - Cell Refinement
 - Integration
- Provides automatic processing services

What's going on in XIA?

- Scheduler ++
- Includes and extends Scheduler functions to:
 - Point group determination
 - Space group determination
 - Anomalous atom phasing
 - Format transformation
- Provides forum for interaction from others
 - BMP
 - HAPhaser/XIA “Images2Structure” application

What needs to be done

- Testing by non-developers or at least non-Graeme
- Code review/QA analysis
- Investigation of data management
- Scoping for future developments
- Provision of framework to allow BOTH stabilization of infrastructure AND research and development
- Bus proofing :o)

What must not happen...

- Repeat of “DiffractionImage” branch
- Repeat of “graeme” branch
- Stopping development altogether
- Flaky/not-at-all documented development
- Clashing of requirements
- Rewriting of existing code instead of merging

Testing

- Offline versions of all of the code are available
- “graeme” branch includes useful functionality which should/will end up in DNA
- Includes some scientific additions which need to be tested and evaluated
- Some “white box” testing also needed – more eyes need to look at the scheduler code – volunteers?