CCP4 and BIOXHIT

Data Management and Project Tracking in Structure Solution

Peter Briggs, CCP4
Outline

- Background
- Staff involved in CCP4 effort
- Aims and Deliverables
- Current Status
- Links to other projects
- Next steps

23rd March 2005

CCP4 Annual Developers' Meeting
Background: the BIOXHIT Project

• BIOXHIT
  • Bioxtallography on a Highly Integrated Technology Platform for European Structural Genomics
  • EU Framework Programme 6 “Integrated Project”
  • 20+ partner institutions

• Aim
  • “To provide platform for high-throughput structure determination from crystallisation to structure solution”

• Timeframe
  • started 1st January 2004 for 4 years
  • problems with recruitment meant late start for CCP4

• Website
  • http://www.bioxhit.org
WP 5.2: Data Management & Project Tracking in Structure Solution:

- “To fill the need for project tracking within the BIOXHIT structure solution software pipeline”
- Pipeline covers software components post-data processing (scaling and merging, phasing, model building, refinement)
- Complementary to PIMS and DNA

Staff for CCP4 effort at Daresbury:

- Peter Briggs
  - project coordinator for CCP4
- Wanjuan (Wendy) Yang
  - full time programmer
The need for data tracking

Manual structure determination can generate large quantities of data rapidly:

For automated systems this is likely to be even more of a problem.
Aims

• Implement system for both manual and automated structure determination
  • Use CCP4i as a starting point
  • Accommodate non-CCP4(i) applications

• Implement multiple database backends
  • Don’t force user to have mySQL

• Gather as much information as possible automatically
  • using this system gives you tracking “for free”

• Recognise that structure determination will most likely not be performed exclusively within a single software package and that data will most likely not be stored in a single database
  • exchange of data between systems requires standards for transfer e.g. standards developed in BIOXHIT WP 5.1
Project Deliverables

Project Database Handler
- broker application to mediate interactions between database and client applications
- hides implementation of backend
- aim to provide client APIs to handler from different languages
- deal with multiple users/clients within/outside CCP4 system

Database for Project Tracking
- project history (steps in the determination process)
- project data ("knowledge base") & data history
- "operational" data
- aim to provide database schema and multiple implementations

Visualisation Tools
- provide views of data to facilitate review and analysis
Prototype architecture and database

Prototype client-server architecture

Prototype basic database schema
Current Status/Work so far

- Currently prototyping to gather requirements
  - working with Graeme Winter
  - key criterion: “needs” rather than “would like”

- Wendy has produced prototypes for:
  - basic database schema implemented in mySQL
  - database handler and client API for Python
  - visualiser ("project data explorer")

- Principal outcomes:
  - define requirements & build a list of issues to be resolved in full implementation
Project Data Explorer

23rd March 2005

CCP4 Annual Developers’ Meeting
Links to other projects

Current collaborators:

- **e-HTPX**: Graeme Winter & **XIA** (ongoing)
- **CCP4i**: obviously

*Other relevant projects:*

- **CCP4 Automation**: requirements still largely to be determined
- **PIMS**: requirement to able to exchange data

- Other projects interfacing with CCP4(i):
  - **CCP4MG & Coot**
  - **CRANK** (Steven Ness/Leiden)
  - **MOSFLM** (transferring data from processing)
Next steps

Immediate plans:

- Work with Graeme to use prototype in XIA code
- Prototype implementation of CCP4i-compatible backend
  - *integrate original handler prototype into CCP4i?*
- Develop prototype visualiser for project tracking in CCP4i
- Talk to other projects for possible links/requirements