BIOXHIT/CCP4(i) Database

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Outline of the presentation

- Talk (Peter)
  - Background
  - Components
  - Plans
  - Availability

- Demonstration (Wendy)
Background

CCP4 contribution to BIOXHIT project

Aims

• Make CCP4i job db accessible to non-CCP4i applications
• Expand scope of CCP4i job db for tracking
• Provide visualisation tools
• Store crystallographic data (“knowledge database”)

Staff

• Wendy Yang: principal programmer (100%)
• Peter Briggs: project lead & programming (50%)
Additional information

- CCP4 Newsletter #45 (Winter 2007)
- www.ccp4.ac.uk/projects/bioxhit_public/

Acknowledgements

- Graeme Winter, Charles Ballard
- EC for funding via BIOXHIT project
- CCP4 and CCLRC
Core components

- dbccp4i – database handler

- client APIs
  - libraries for programs to interact with dbccp4i
  - Python and Tcl

- dbviewer – visualiser for project history data

- knowledge base
  - will store crystallographic data
  - under development
System Architecture

- **dbccp4i**
  - database handler
  - Tcl Client API
  - CCP4i db

- **StarKey**
  - XML generator
  - Python Client API

- **XIA**
  - Python Client API

- **dbviewer**
  - visualiser
  - Tcl Client API

- **CCP4i 1.4**
  - current version

- **CCP4i projects**
  - database.def files

- **CCP4i 2.0**
  - Tcl Client API

- SQL knowledge database

...other client applications (e.g. consoles,...)
Using the Python Client API: examples

```python
import dbClientAPI
...
# start and connect to handler
dbClientAPI.DbStartHandler()
conn = dbClientAPI.handlerconnection()
conn.DbRegister(user, 'dummy', True)
...
# list projects
projects = conn.ListProjects()
...
# create a new project
newproject_result = conn.CreateDatabase('NEWPROJECT', '/home/wy45/projects/newproject')
...
# open an existing project
project = conn.OpenDatabase('OLDPROJECT', '/home/wy45/projects/oldproject')
...
# get/set data
status = conn.GetData('oldproject', 1, 'STATUS')[1]
conn.SetData('oldproject', 1, 'TITLE', 'Run of scala')
...
# create a new job
newjob_result = conn.NewRecord('oldproject')
jobid = newjob_result[1]
...
# add input file
conn.AddInputFile('myproject', jobid, 'toxd.mtz', 'TOXD')
```
Knowledge Base

• Next major development phase
• Will store crystallographic data
• Complements CCP4i job database

• Technical details:
  • Will be defined in SQL
  • Implemented using SQLite

• Content:
  • To be decided via consultation
  • Needs input from potential end users
Availability of current version

• dbccp4i 0.1 available from:
  ftp://ftp.ccp4.ac.uk/bioxhit/dbccp4i-0.1.tar.gz

Installation

• Minimal: unpack & set 2 environment variables

Dependencies

• Minimal: CCP4 and Python (2.4)
• dbviewer: also needs Tcl/Tk and Graphviz
• SQLite and pySQLite (not currently required)
• Producing a bundle of the dependencies
Future Plans

• Develop CCP4i job database scope for tracking and improve client APIs
  • Encourage developers to use it and feed back

• Extend the dbviewer and add new functionality
  • Encourage users to try it and feed back

• Develop the knowledge database
  • Feedback from all!

Please let us know if you might be interested in contributing to any of these areas
Now for the demonstration...
What to demo

• Dbviewer
• Dbviewer and dbconsole
• Dbviewer and CCP4i
We need your help!

We’re looking for:

- Developers interested in using the client APIs to store data in the job db
- Users to try the dbviewer and give feedback on improvements
- Anyone to give us input into the contents of the crystallographic knowledge database

Download dbccp4i version 0.1 via http://www.ccp4.ac.uk/projects/bioxhit_public/

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