

# **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/](http://www.ccp4.ac.uk/projects/bioxhit_public/)

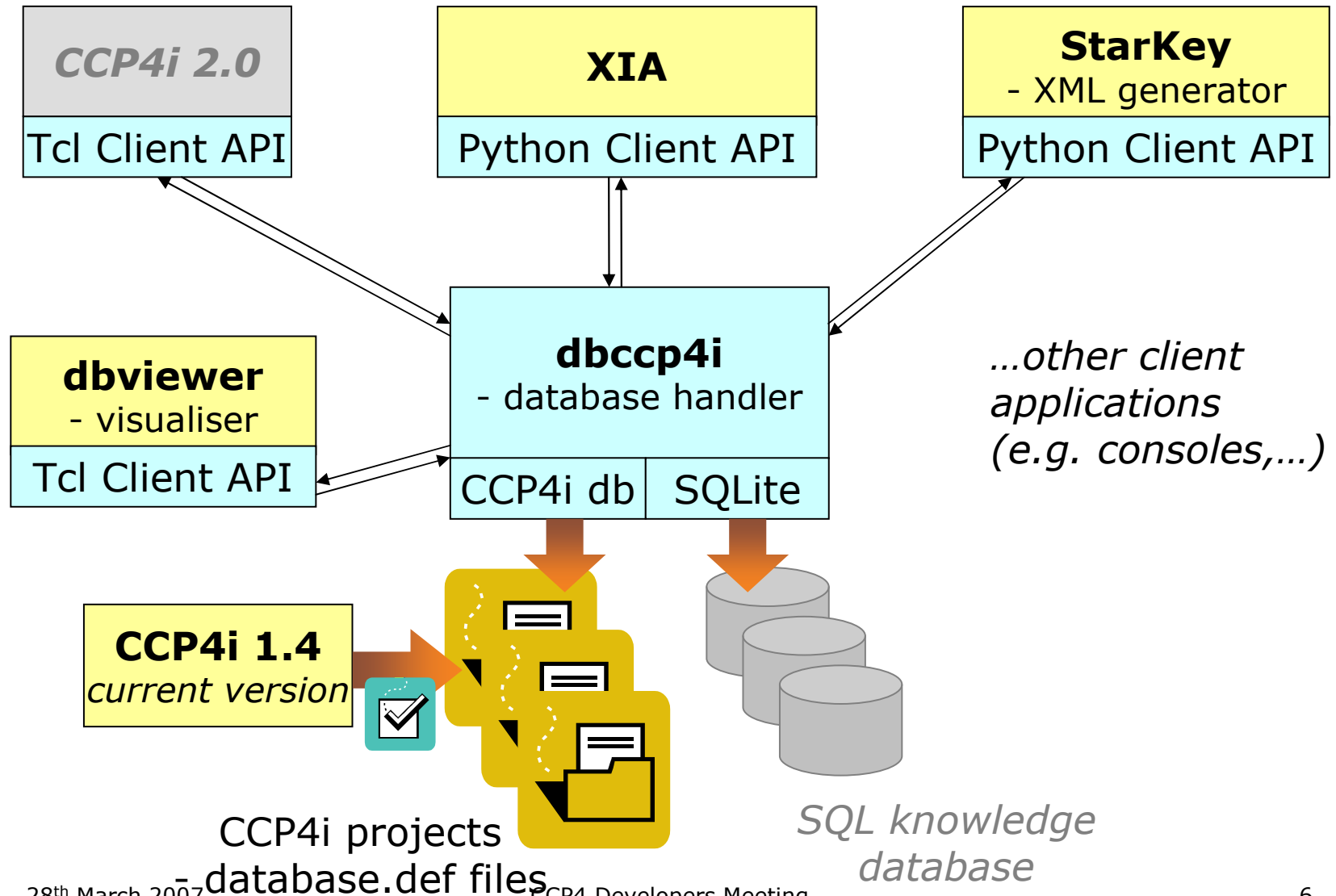
## **Acknowledgements**

- Graeme Winter, Charles Ballard
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- 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



# Using the Python Client API: examples

```
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, 'tox.d.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/](http://www.ccp4.ac.uk/projects/bioxhit_public/)**

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