



CCP4i: activities and plans

Peter Briggs



- Current version
- Developments since last March
- Plans
- Future directions for CCP4i

Major developments since last meeting



- **March 2006:** GUI WP proposed w/ PJB as chair
 - Never instituted or met, instead...
- **April:** prototyped improved modules/tasklist w/ Charlie Bond
- **June:** STAB proposed 2 parallel threads:
 - *CCP4i-classic* – enhancements of existing GUI
 - *CCP4i-auto* – “designed for greater automation of crystallography”
- **December:** looked at “plugins” for CCP4i to launch external apps (MG, Coot, others...?)
- **March 2007:** “process manager” (Liz Potterton)
- ... & database work ongoing through all this



Plans for “CCP4i classic”

Three areas of development:

1. Reorganisation of modules and tasklist (work started with Charlie Bond)
2. Reorganisation of the database (work being done by Wendy)
3. Feedback mechanism between database, CCP4i and non-CCP4i applications (plugins/process manager)

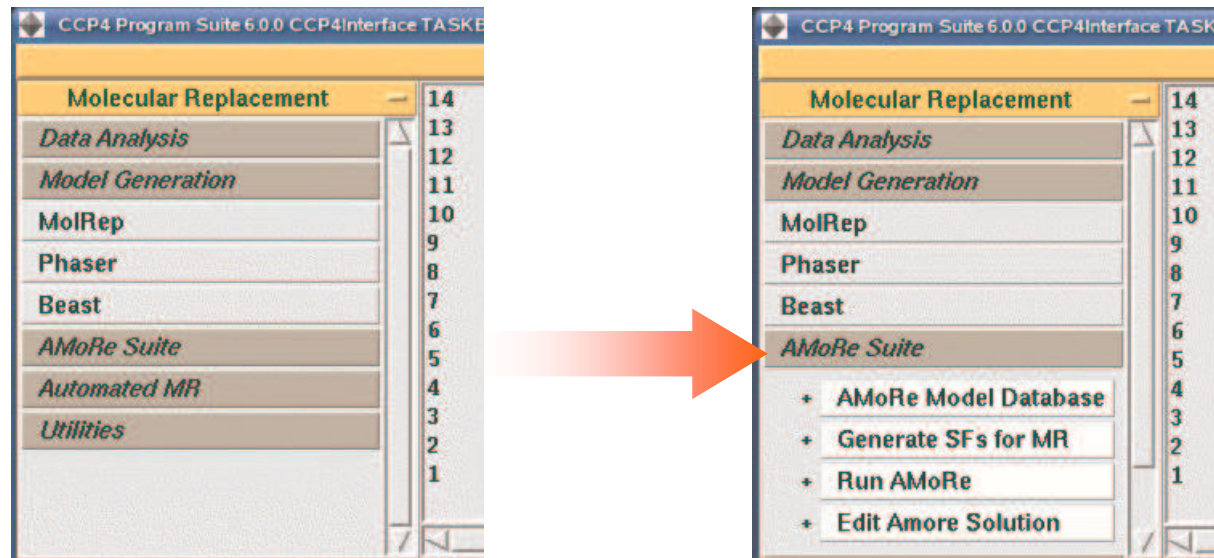
Quoting from STAB minutes:

- *“The completion of these developments should mark the end of development work on CCP4i, except for maintenance work”*

CCP4i-classic: Reorganising the modules and tasklists

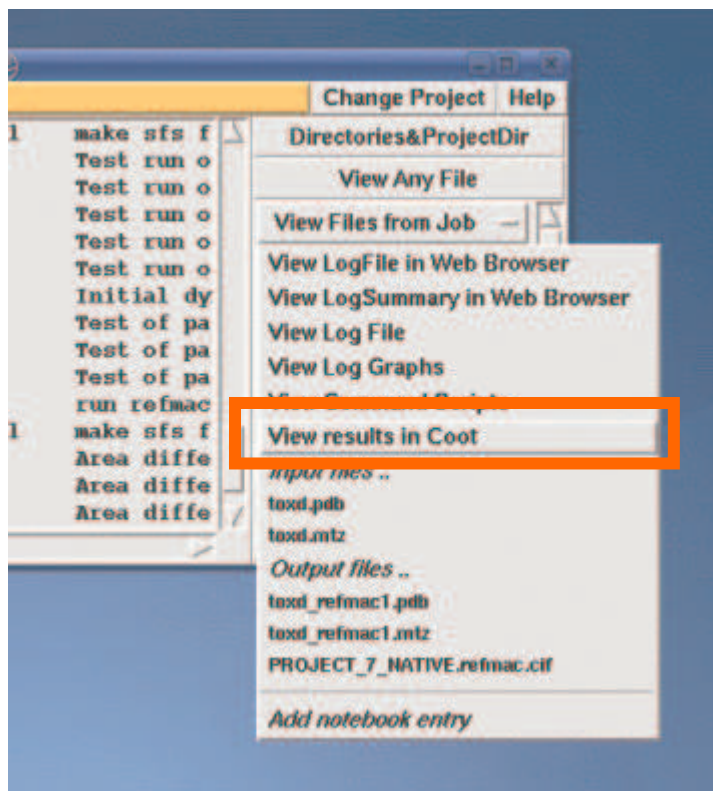


Prototype version exists:



- Will give more structure to the lists
- Needs input on how best to re-organise tasks
 - Workshop will be organised to discuss this

CCP4i-classic: Plugins



- Launch Coot, CCP4mg (others?) from CCP4i
 - e.g. via "View Files from Job" menu
- Not clear how best to implement this:
 - Generic mechanism for defining "plugins"
 - Best way to to present options to the user



Database and Process Manager

- Database "dbccp4i"
 - see next talk
 - needs to be integrated fully in CCP4i
- "Process manager"
 - Provide a way for programs to communicate
 - Speculative development
 - Liz Potterton planning to look at reusing Wendy's database handler code for this



Short term plans for CCP4i-classic

- Implement the code changes for modules/tasklist improvements
- Workshop to update tasklists and fix annoyances
- Plans document outlining medium-term fixes:
 - Fixing annoyances, minor functionality improvements, ...

Longer term

- Plugins
- Integrate database handler into CCP4i
- Develop “process manager”

Other planned developments (CCP4 6.1)

- Improvements to “View Files from Job” for tasks with large numbers of output files
 - e.g. MrBUMP, BALBES...
- Re-installer for installed tasks e.g. ARP/wARP
- New and updated interfaces, e.g.
 - POINTLESS
 - RAMPAGE (in “sfcheck and procheck”) interface
 - ACORN
 - ...

“CCP4i auto”



- STAB's vision of the next generation of interface
 - not clear how this will come about?
- From June 26th STAB minutes:
 - *"... several different models will probably need to be taken forward for user trials..."*
 - *"... important that the Executive consider what resources should be allocated to this project as soon as possible"*
- End of session discussion could focus on CCP4i-auto?



Further Reading/Links

STAB minutes:

- CCP4 website: <http://www.ccp4.ac.uk/wg/>
- Teleconferences 26th June & 23rd Nov 2006

CCP4i tasklist reorganisation:

- http://www.ccp4.ac.uk/peter/ccp4/ccp4i_tasklist_changes.html
- http://www.ccp4.ac.uk/peter/ccp4/ccp4i_modules.html

Plugins:

- http://www.ccp4.ac.uk/peter/ccp4/ccp4i_plugins.html
- Contact me (**p.j.briggs@dl.ac.uk**) if you're interested in the planning document being developed



Acknowledgements

- Liz Potterton (original developer of CCP4i)
- Daresbury staff: Francois Remacle, Charles Ballard, Ronan Keegan, Norman Stein, Martyn Winn, Wendy Yang
- CCP4 STAB
- All users and developers who have contributed ideas, bug reports, fixes and new code