CCP4i: activities and plans

Peter Briggs
• Current version

• Developments since last March

• Plans

• Future directions for CCP4i
Prologue: recap of interesting stuff in CCP4 6.0

- Also: CCP4 6.0.2 added Windows “spaces in filenames” fix (Francois)
- See CCP4 newsletters #42 and #44 for more info

28th March 2007
CCP4 Developers Meeting
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 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
  - ...

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“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 26\textsuperscript{th} June & 23\textsuperscript{rd} 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
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