CCP4 @ DL: Releases, Conferences and Other Activities

Peter Briggs, CCP4 Daresbury
Outline of the presentation

- Overview of CCP4 @ Daresbury Laboratory
- Release of CCP4 v6.0 (“Ingleton”)
- Future Release Plans
  - Martyn Winn
- Conference and Workshop Activities
  - Maeri Howard
Overview of CCP4 @ Daresbury Laboratory

• CCP4 core group
• Responsible for:
  – Maintaining & developing core suite
    • build system, libraries, CCP4i …
  – Making software releases
  – Providing technical support
  – Industrial liaison
  – Maintaining on-line resources
    • website, mailing lists …
  – Coordinating publicity activities:
    • Study Weekend, conference presence, workshops …
  – Other projects
    • CCP4 Automation, e-HTPX, BIOXHIT …
### Who are we?

<table>
<thead>
<tr>
<th>Core Staff</th>
<th>CCP4 Automation</th>
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<tr>
<td>• Martyn Winn</td>
<td>• Norman Stein</td>
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<td>• Peter Briggs</td>
<td>• Daniel Rolfe</td>
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<td>• Charles Ballard</td>
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<td>• François Remacle</td>
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<td>• Chris Morris</td>
<td>• Wanjuan (Wendy) Yang</td>
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<td>• A.N. Other</td>
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Projects at Daresbury

CCP4 Automation
  • Coordinated by Charles Ballard

e-HTPX
  • CCP4 activities coordinated by Martyn Winn

BIOXHIT
  • CCP4 activities coordinated by Peter Briggs

Links to DNA + PIMS
Release of CCP4 v6.0: “Ingleton”

Peter Briggs, CCP4 Daresbury
Outline of presentation

• Aims and ambitions for CCP4 v6.0

• Staff and resources

• Planning and coordination activities

• Contents and major changes
  • For users
  • For developers

• Delivery method

• QA activities

• Outstanding Issues

• Current status and planned release schedule
Aims and ambitions for CCP4 v6.0

Comes soon after major changes in CCP4 v5.0

Mission statement:

• “To make a high-impact release within a short timescale, to provide increased functionality including the CCP4MG and PHASER packages”

Aims:

• Consolidate major changes to the core libraries in 5.0

• Bring in major new developments and make them available to CCP4 users
Staff and resources

Core staff:

- Charles Ballard – release coordinator
- Martyn Winn – progress monitoring
- Peter Briggs – QA activities
- François Remacle – Windows build

- but all involved in coding/updating software/bug fixing etc

Resources:

- CVS – invaluable for managing files
- Bugzilla – for tracking bugs and feature requests
- Project planning documents (from tigris.org)
- Download pages
Planning and coordination

Release of v6.0 coordinated using more formal project management:

- Lists of packages to included and tasks to be performed
- Reviewed at weekly meetings
- Planning materials on internal webpages

Why adopt this approach?

- Dramatic growth in size and complexity of the suite
  - more packages, libraries, languages etc
- Outcome of the review of release 5.0
Overall plans ...

Package list ...

Task list ...

Monitoring meetings

23rd March 2005 CCP4 Annual Developers’ Meeting
Contents and Major Changes for Users

New packages:

- **CCP4MG**: CCP4 Molecular Graphics package
- **PHASER**: maximum-likelihood molecular replacement
- **Coot**: graphical model building tools
- **Pirate**: statistical phase improvement
- **Superpose**: secondary structure alignment
- **PMF, CRUNCH2, BP3**: heavy atom location/experimental phasing
- **CHOOC**: anomalous scattering factors from raw fluorescence spectra

**CCP4i:**

- **CRANK**: automated structure solution via SAD, SIR, SIRAS
- **SHELXC/D/E** interface
- **Clipper utilities** module: set of interfaces to Clipper programs
- **Database search and sort utility**
Contents and Major Changes for Users

Updated packages:

- New versions of REFMAC5, MOLREP, SFCHECK, SCALA, PDBEXTRACT
- Additional coordinate utilities using pdbcur, ncont, coord_format, pdb_merge
- FFTBICG replaces FFT

Other changes:

- For PHASER, SHELX etc: CCP4i task buttons are only active if the underlying programs are available
Contents and Major Changes for Developers

• No changes to the core CCP4 libraries

• *cctbx* library is included for *PHASER*

• *Clipper* and *FFTW* packages are built by default

• Some minor updates to CCP4i for developers:
  • *FindExecutable, taskname_prereq* ...
  • Includes updates for *CCP4MG*

• Support for building under Linux IBM compilers
Package arrangement and delivery method

CCP4 v6.0 sees addition of major new packages
  • Some are very large (e.g. cctbx)
  • Some are not available for all platforms (e.g. Coot)
  • Updated on faster timescales than CCP4 releases

Decision to divide the release into packages
  • Basic CCP4 (~ same as v5.0)
  • Phaser
  • CCTBX
  • CCP4mg
  • Coot
  • CHOOCH

Needs a flexible way of delivering release to the end users:
  • Build on automated binary download scripts from 5.0
  • Make it easy for users to know what is available for their system, and to download and install

23rd March 2005  CCP4 Annual Developers’ Meeting
New download pages

Prototype being developed by François with input from other staff

- User can select required packages from those that are available for their system and download a single file
- Warns about dependencies
- Includes external packages (Tcl/Tk/BLT and python)
- Guides the user to what they need to download

Other changes

- Unix/Linux binaries provided as a single download
- Possibly use InstallShield for Unix binaries as well as Windows
Example 1: Windows binaries

1. Select “Windows”

2. Binaries only for Windows

3. Download
Example 2: Linux source distribution

1. Select “Linux”
2. Select “source”
3. Select packages:
   - Basic CCP4
   - Phaser
4. Dependencies:
   - Tcl/Tk
   - Python
5. Licence agreement
6. Download
Quality Assurance – testing and bug tracking

CCP4 v6.0 has a QA plan

- Automated build testing from CVS on platforms at DL
  - IRIX, OSF1 V4.0, SunOS, Linux Fedora/SuSE/RedHat
- Use Bugzilla to track reported bugs
- Test releases for compatibility testing and user/developer feedback

Release conditional on

- All packages incorporated and tasks completed
- No outstanding MAJOR or CRITICAL bugs in Bugzilla
Outstanding Issues

Compatibility Testing
• If you use CCP4 in your own software then please try test versions and report problems asap

Communications
• Reports from test release that some components are out-of-date
• We rely on developers telling us when new versions of their software are available
• Please don’t assume that we’re omniscient! 😊

Licensing
• Not a release issue *per se* but obviously has a major impact

Patching post 6.0
• Still working on a patching mechanism
Current Status of CCP4 release 6.0

- Test releases:
  - 1\textsuperscript{st} February: CCP4 5.99.0 to 17 test sites
  - 28\textsuperscript{th} February: CCP4 5.99.1 to 19 test sites
  - 17\textsuperscript{th} March: 5.99.1b to 10 sites (included Linux & Windows binaries)
- Disappointing feedback so far

- Made available via prototype download page:

- Next test release after remaining outstanding tasks have been completed

- Full public release scheduled for “RSN” 😊