

# **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?

### Core Staff

- Martyn Winn
- Peter Briggs
- Charles Ballard
- François Remacle
- Maeri Howard

### CCP4 Automation

- Norman Stein
- Daniel Rolfe

### PIMS

- Chris Morris
- A.N. Other

### BIOXHIT

- Wanjuan (Wendy) Yang



## 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

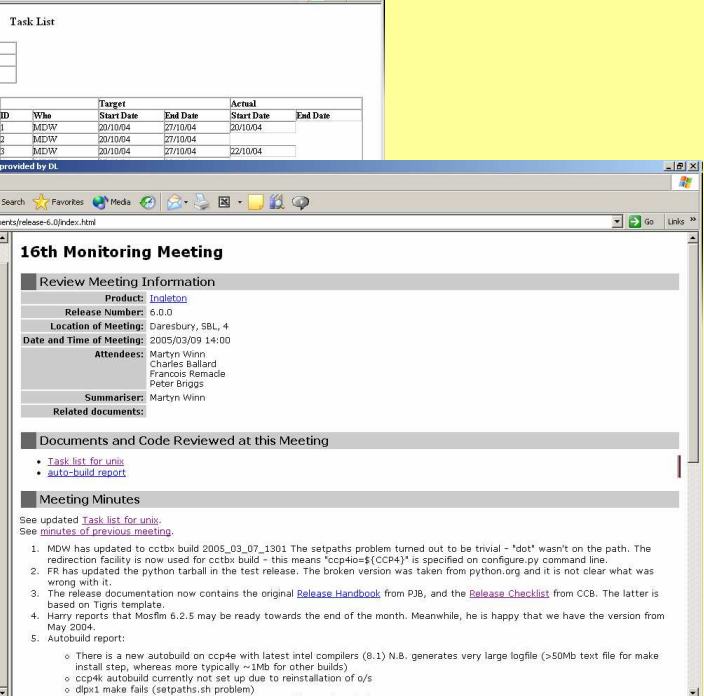
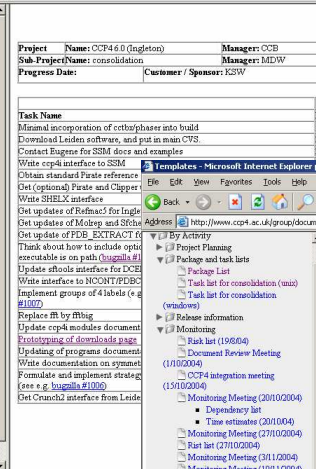
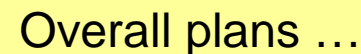
## Planning and coordination

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



## Task list ...

## Monitoring meetings

## 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
- **CHOOCH**: 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**
- **FFTBIG** 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

## New download pages

Prototype being developed by François with input from other staff

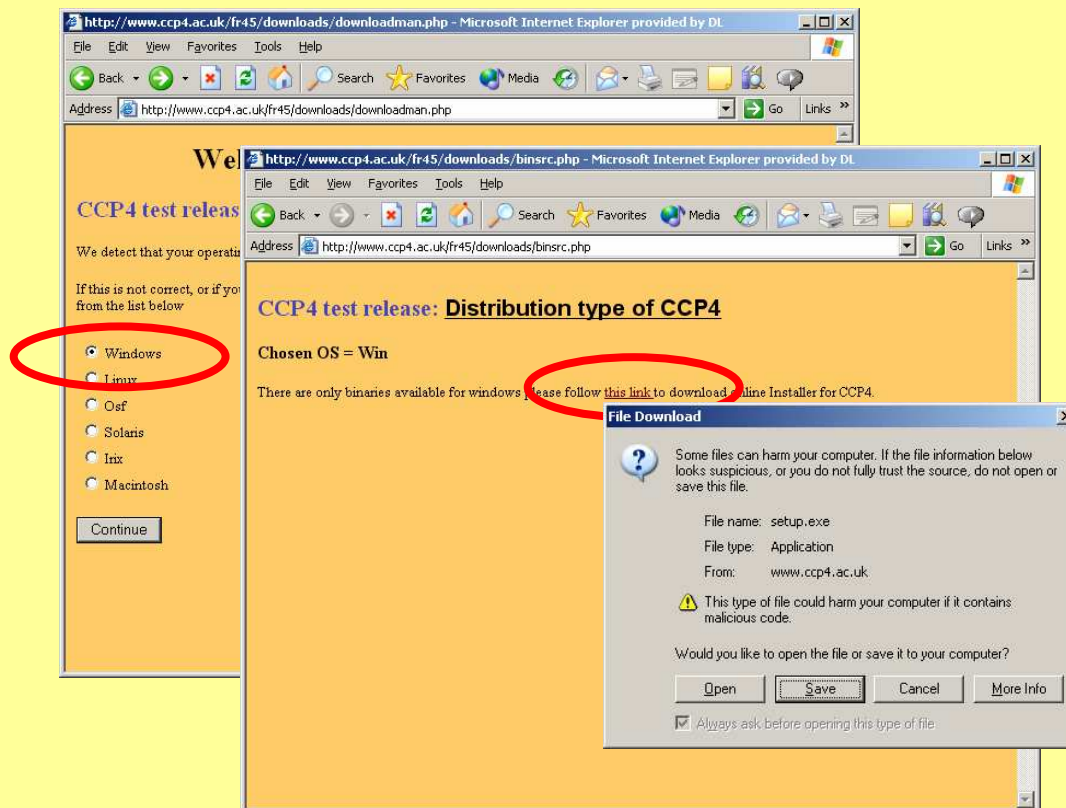
- User can select required packages from those that are available for their system and download a single file
- Warns about dependencies
- Includes external packages (**Tcl/Tk/BLT** and **python**)
- Guides the user to what they need to download

### Other changes

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



## Example 1: Windows binaries

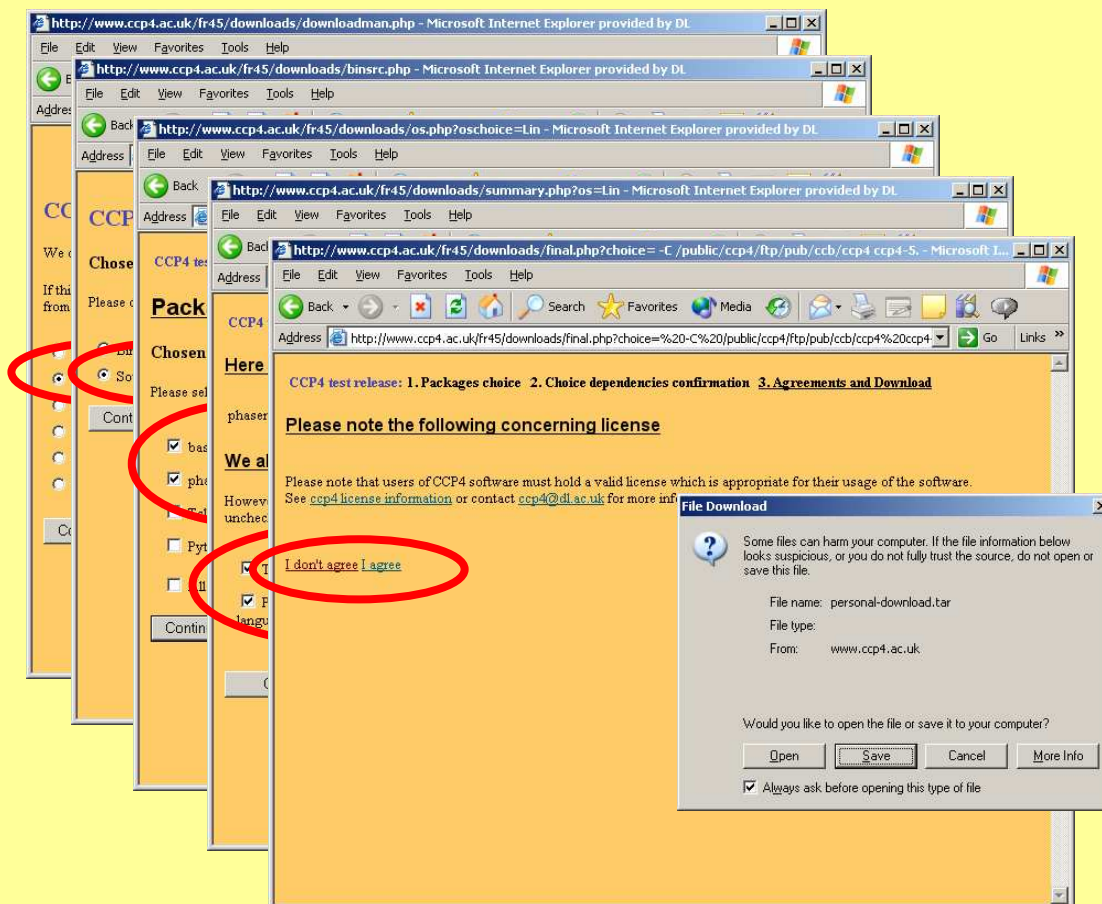


1. Select "Windows"

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<sup>st</sup> February: CCP4 5.99.0 to 17 test sites
  - 28<sup>th</sup> February: CCP4 5.99.1 to 19 test sites
  - 17<sup>th</sup> March: 5.99.1b to 10 sites (included Linux & Windows binaries)
  - **Disappointing feedback so far**
- Made available via prototype download page:
  - <http://www.ccp4.ac.uk/fr45/downloads/downloadman.php>
- Next test release after remaining outstanding tasks have been completed
- Full public release scheduled for “RSN” ☺