



Introduction to the course

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What is CCP4?

- CCP4 = "Collaborative Computational Project Number 4"
- One of several "CCP" projects set up in the UK to support scientific software development
- CCP4 was set up in the late 1970's to bring together the leading developers of software in the field of macromolecular X-ray crystallography in the UK

CCP4 activities

- Supports software developers at several universities in the UK and further afield
- Collaborates with a wider range of software developers
- Provides education and training through workshop and conference activities around the world



CCP4 Workshops arranged each year in the UK and various locations around the world

- Intensive week long courses with lectures and hands on problems solving sessions

CCP4 Study Weekend takes place each January

- Features a different topic each year



CCP4 today

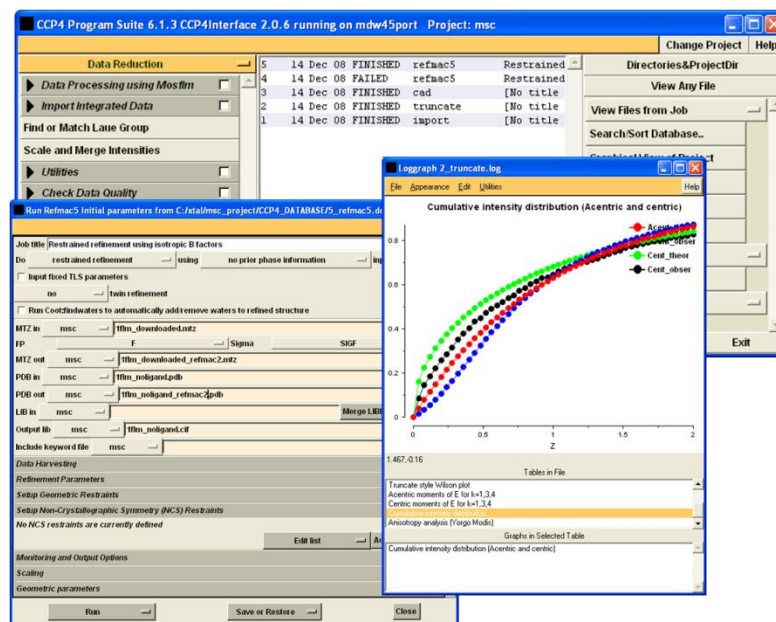
- Funded by the Biotechnology and Biological Sciences Research Council (**BBSRC**), the Medical Research Council (**MRC**) and industry.
- Coordinated by the Science and Technology Facilities Council (**STFC**)
- Core group based at the Research Complex at Harwell (**RCaH**) next door to the Diamond synchrotron in Oxfordshire.



The CCP4 suite of software

- The CCP4 suite is a comprehensive suite of software for macromolecular crystallography
- Includes many independently-developed programs
- Covers all areas from data processing right through to deposition and molecular graphics

- New versions of the suite are released about every 18 months
- Revisions to the major release are made available about every 6 months



Version 6.1.x series

- Current revision is 6.1.13
- Binaries are made available for Linux, Macs and Windows
- Emphasis put on automating some of the standard processes of structure solution
 - Xia2, Crank, BALBES, MrBUMP, Buccaneer
- Version 6.2 to be released soon
 - we will use a pre-release version in the tutorials



The screenshot displays the CCP4 Downloads Page in a web browser. The page header includes the CCP4 logo and navigation links: Home, About CCP4, CCP4 Projects, Downloads, Documentation, Courses, Developers, and CCP4 people. The main heading is "Downloading CCP4". Below this, there is a "Licensing" section with a link to the "Licensing Page" and a note about the current version, CCP4 6.1.13, released on 1st June 2010. A "Download site" section lists links for automated downloads, Daresbury links, precompiled binaries, and download instructions. The "Prerelease Software" section is also visible. The main content area is titled "Mac OSX" and lists four packages available for Macintosh:

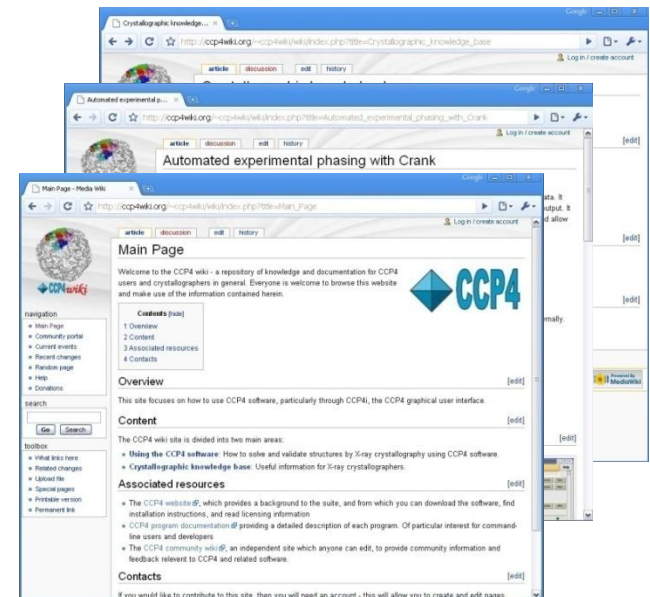
Package	Download Link	Size
CCP4 Crystallographic programs suite v6.1.13 (28/05/10)	[ppc.dmg installer]	480.0 MB
	[intel.dmg installer]	480.0 MB
	[source code tarball]	240.0 MB
Balbes DB (required for balbes)	[dmg installer]	585.0 MB
	[data tarball]	585.0 MB
COOT v0.6.1 (23/03/10)	[10.4+ universal.dmg installer]	208.9 MB
CCP4 Molecular Graphics v2.4.1 (26/06/10)	[QTMG intel installer]	208.0 MB
phaser 2.1.4 with cctbx (25/11/08)	[source code tarball]	21.0 MB
CHOOCH v0.02	[source code tarball]	2.9 MB

<http://www.ccp4.ac.uk/download.php>



Online Documentation

- CCP4 Website: <http://www.ccp4.ac.uk>
 - Download software
 - Online documentation and problems pages
 - Register for CCP4BB email list
- CCP4Wiki:
<http://ccp4wiki.org>
- Documentation of programs and detailed guides on how to use the software to solve structures

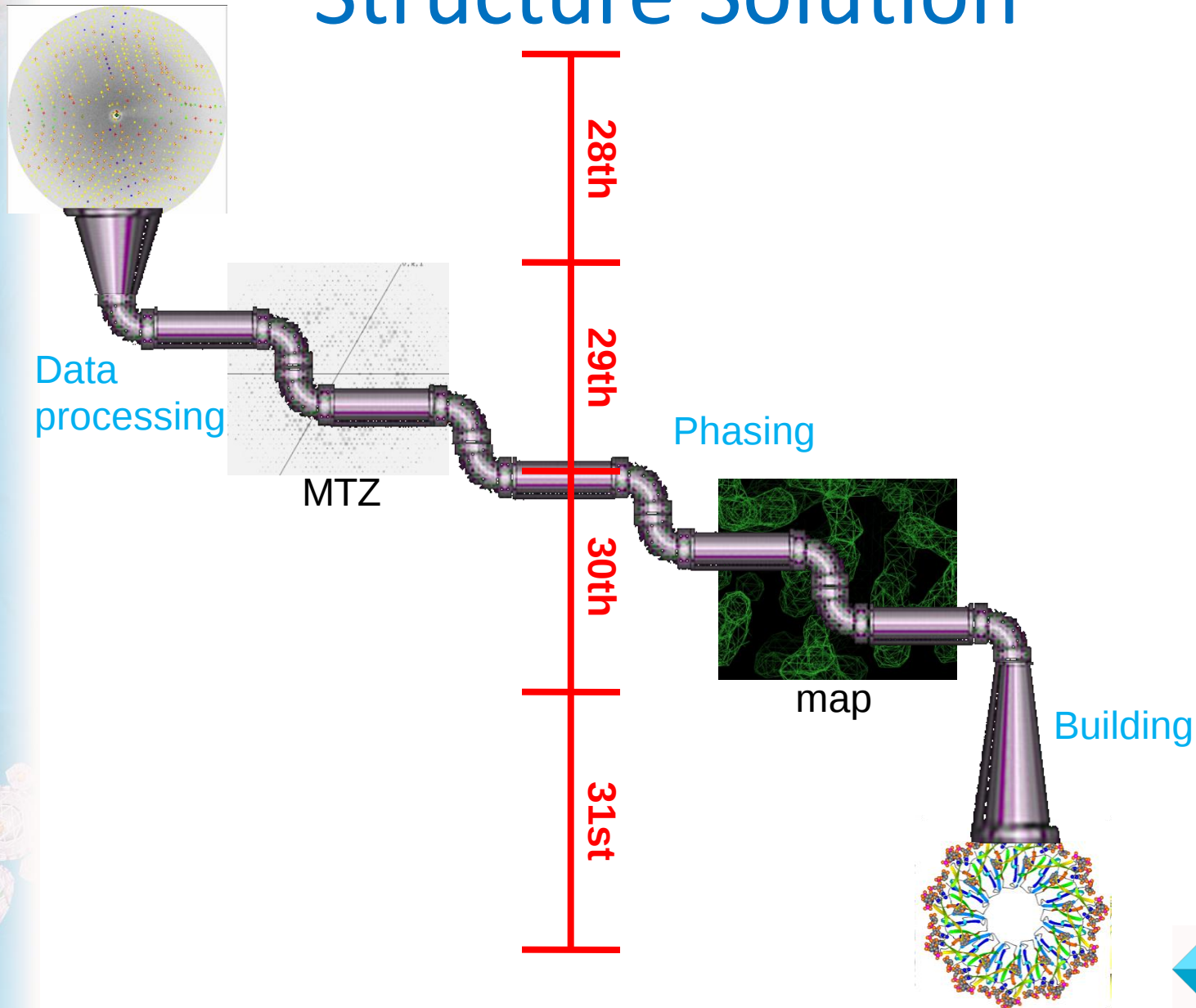




CCP4 Workshop - SSRF, March 2011

- Aim to cover all aspects of Macromolecular Crystallography using CCP4
- Morning - lectures
- Afternoon/evening - computer practicals
- Focus on using the software to solve structures
- Can also discuss theory / programming

Structure Solution



Tutors



Hai-fu Fan
CAS



Martyn Winn
Daresbury



Garib Murshudov
York



Paul Emsley
Oxford



Judit Debreczeni
AstraZeneca



Raj Pannu
Leiden



Bernhard Lohkamp
Stockholm



Melanie Vollmar
Oxford

Please ask us questions!