Introduction to the course

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Research Complex at Harwell

BBSRC bioscience for the future

MRC Medical Research Council

Science & Technology Facilities Council

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.

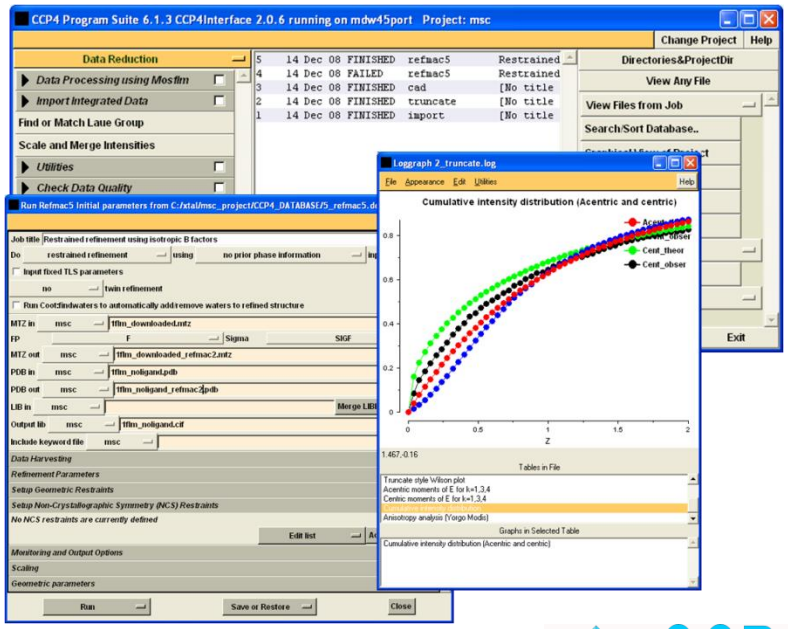
diamond

Research Complex at Harwell

CCP4

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 ever 6 months

Version 6.1.x series

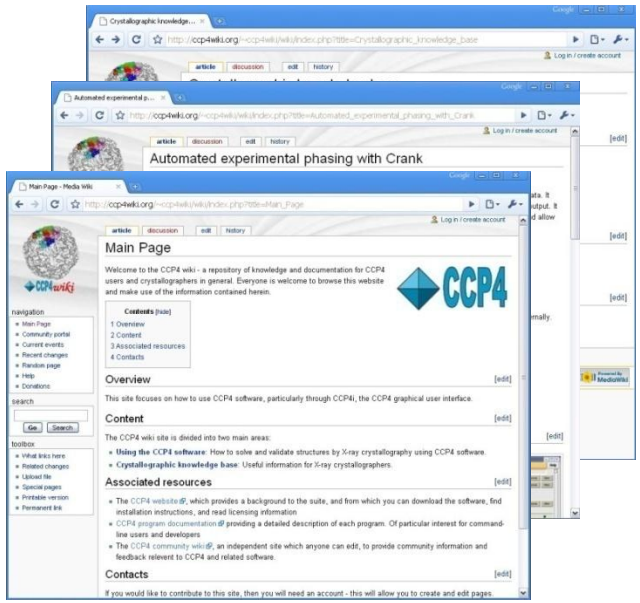
- Current revision is 6.1.13
- Binaries are made available for Linux, Macs and Windows
- Emphasis put on automating some of the standard processes of structure solution
  - Xia2, Crank, BALBES, MrBUMP, Buccaneer
- Version 6.2 to be released soon
  - we will use a pre-release version in the tutorials

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:

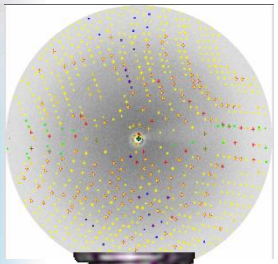
  http://ccp4wiki.org
- Documentation of programs and detailed guides on how to use the software to solve structures



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



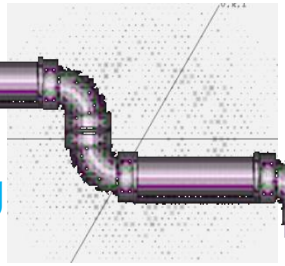
28th

29th

30th

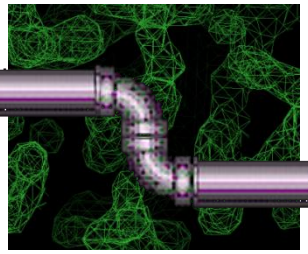
31st

Data processing



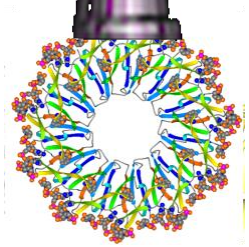
MTZ

Phasing



map

Building



CCP4

Tutors

Hai-fu Fan
CAS

Martyn Winn
Daresbury

Garib Murshudov
York

Paul Emsley
Oxford

Judit Debreczeni
AstraZeneca

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Bernhard Lohkamp
Stockholm

Melanie Vollmar
Oxford

Please ask us questions!

CCP4