

# The Collaborative Computational Project Number 4 (CCP4)

towards new challenges in crystallographic computing

Eugene Krissinel

CCP4, STFC Research Complex at Harwell  
Didcot, United Kingdom

*eugene.krissinel@stfc.ac.uk*

NIH/NCBI, 27 June 2013, Bethesda, MD



*Research Complex at Harwell*

# What is CCP4?

- It is the Collaborative Computational Project No. 4 in Protein Crystallography
- CCP4 is not a single group in RCaH-Rutherford but a world-wide collaboration of developers and users
- CCP4 was formally set up in **1979** to support collaboration between researchers working on MX software in the UK, and to assemble a comprehensive collection of software to satisfy the computational requirements of the relevant UK groups
- CCP4 was originally supported by the UK Science and Engineering Research Council (SERC), and is now supported by the Biotechnology and Biological Sciences Research Council (BBSRC).
- The project is coordinated at Computational Science and Engineering Department of STFC



Research Complex at Harwell



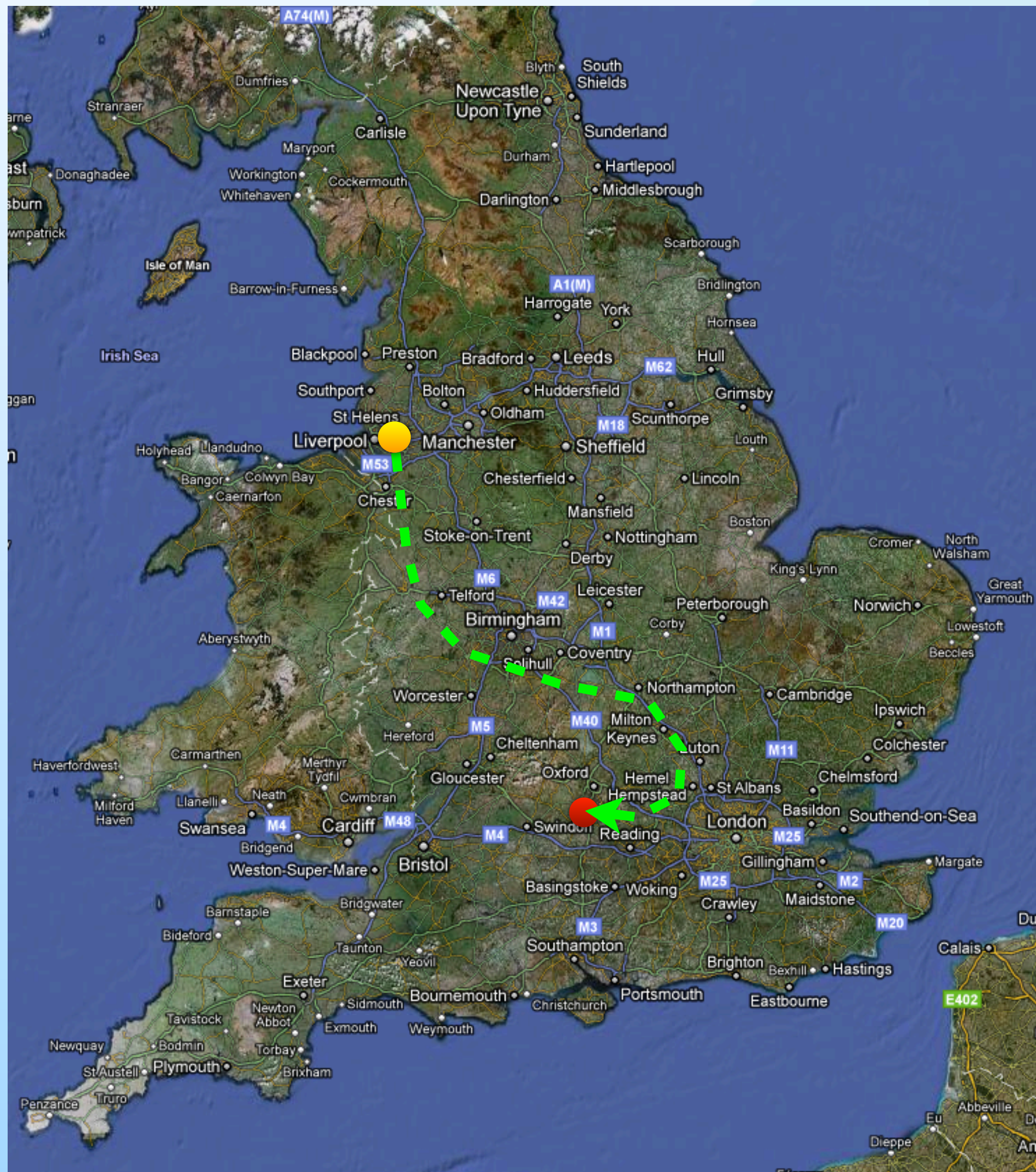
# Long Happy Years in Daresbury, UK (1982-2009)



Research Complex at Harwell



# We have moved!



New address:

CCP4, Building R92  
STFC Research Complex at Harwell  
Rutherford Appleton Laboratory  
Harwell Science and Innovation Campus  
Didcot  
Oxon  
OX11 0FA  
United Kingdom

Tel: +44 (0) 1235 56 7725

Fax: +44 (0) 1235 56 7720

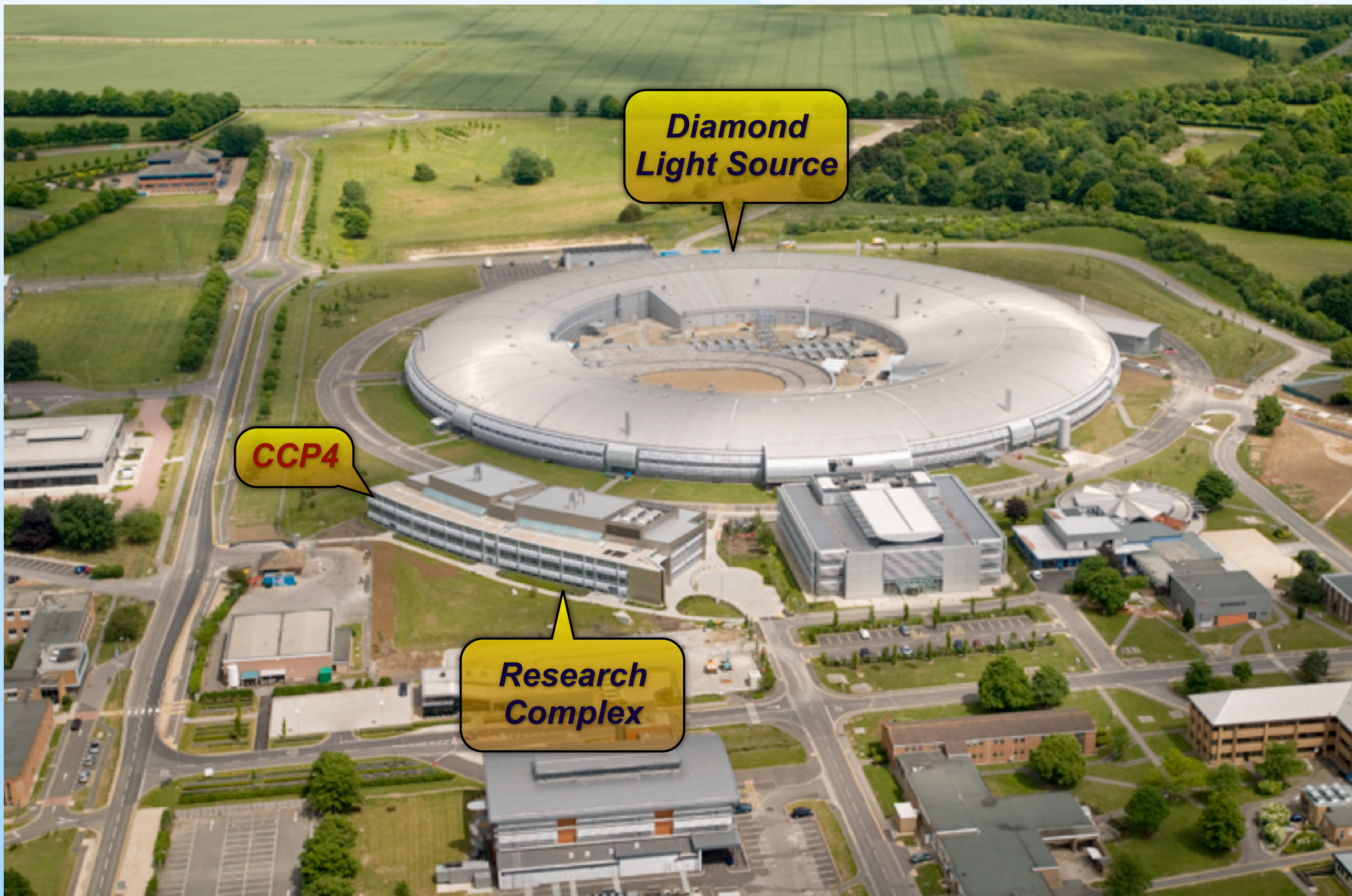
Web: <http://www.ccp4.ac.uk>



Research Complex at Harwell

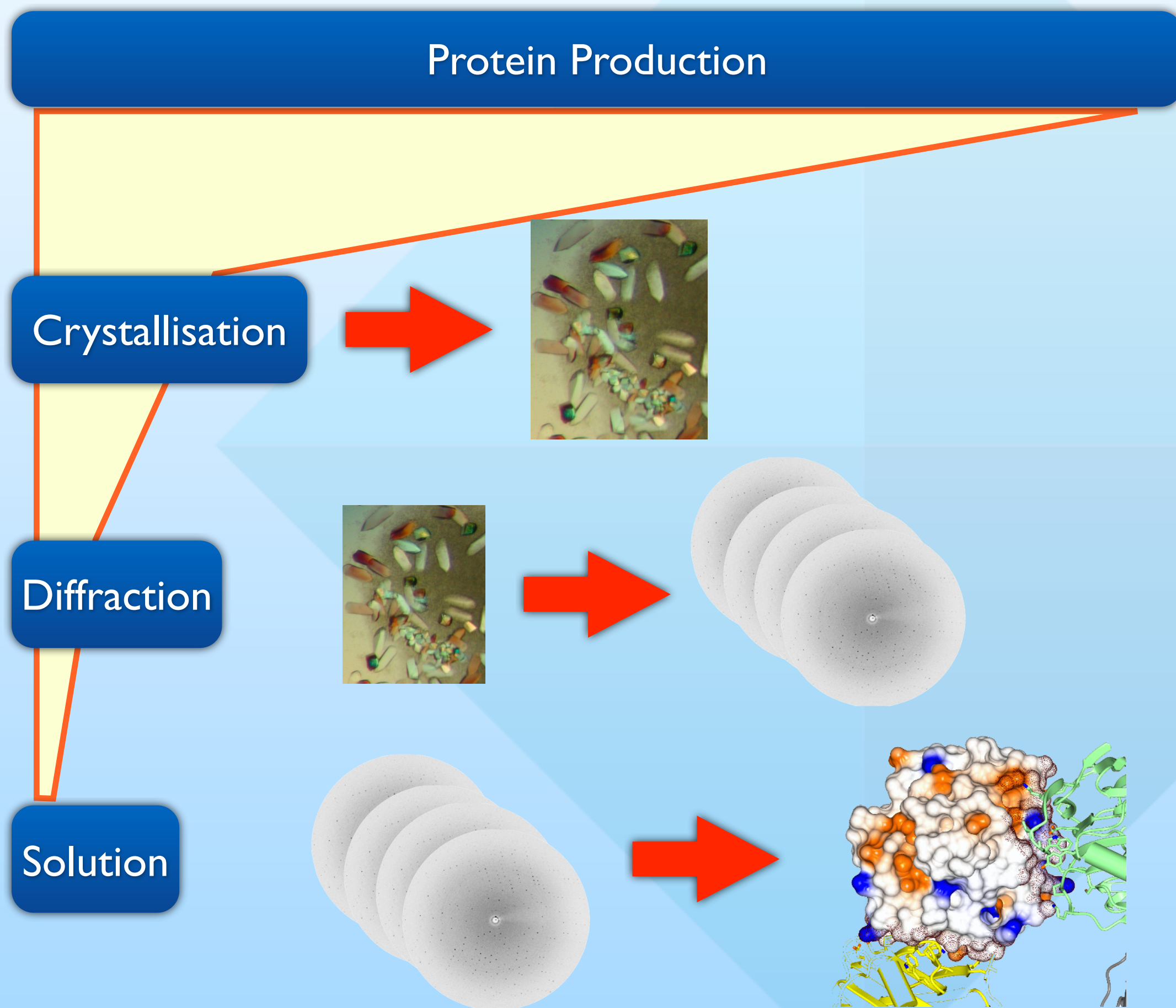


# Home, New Home ... @ RAL



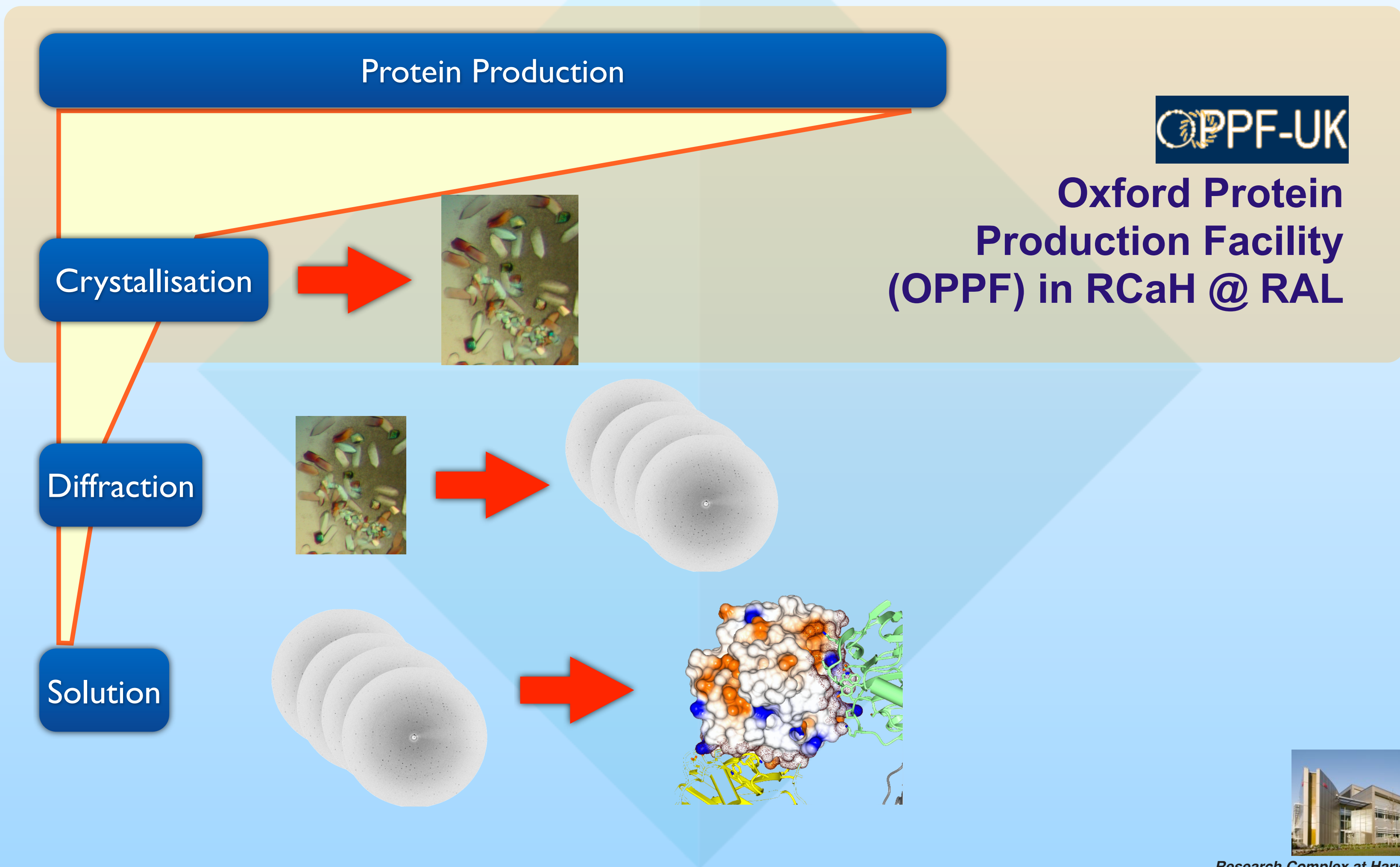


# Complete MX Cycle @ RAL



*Research Complex at Harwell*

# Complete MX Cycle @ RAL





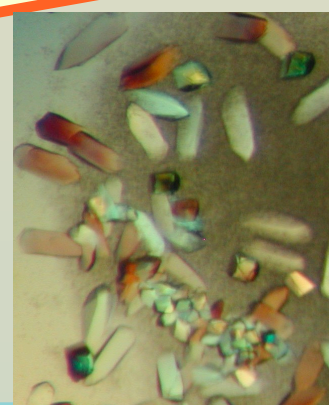
# Complete MX Cycle @ RAL

Protein Production

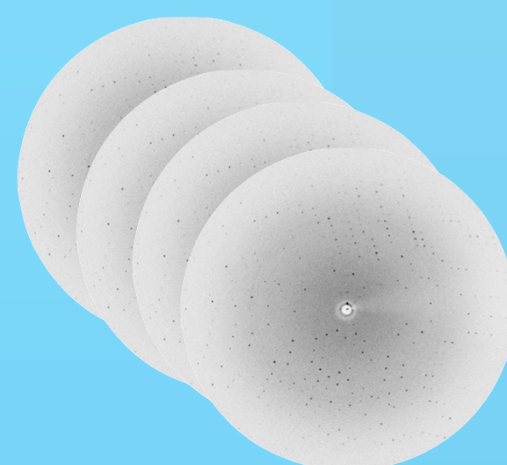
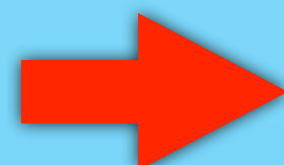
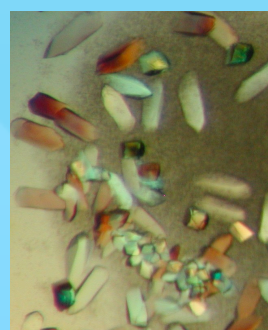


**Oxford Protein  
Production Facility  
(OPPF) in RCaH @ RAL**

Crystallisation

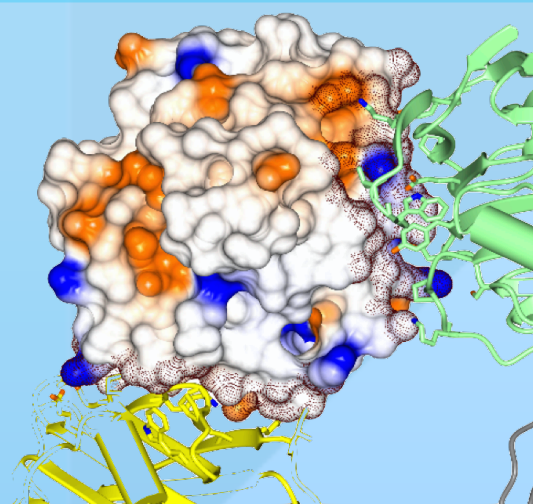
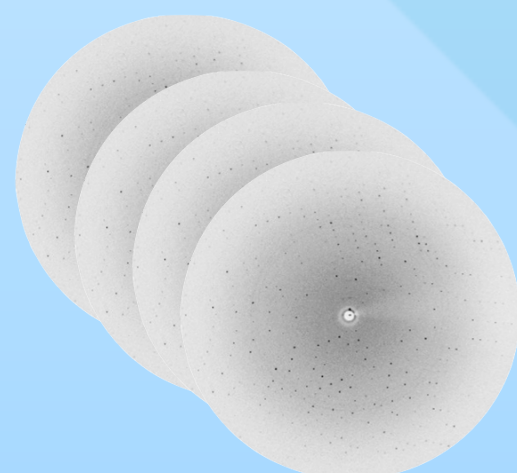


Diffraction



**Diamond Light  
Source @ RAL**

Solution



Research Complex at Harwell

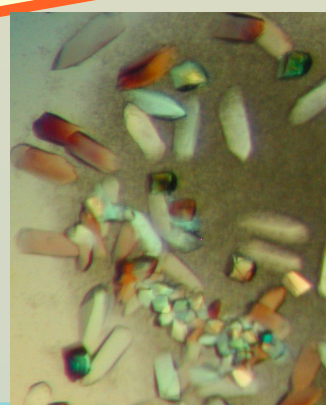
# Complete MX Cycle @ RAL

Protein Production

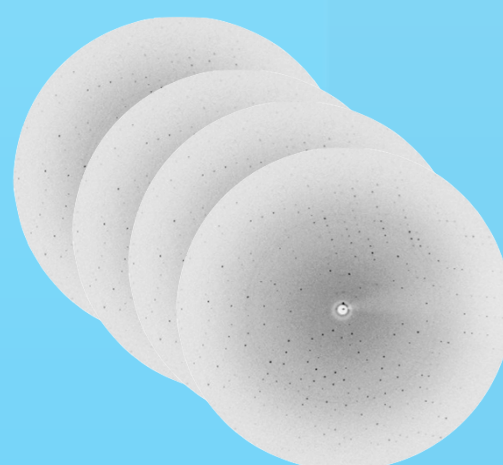
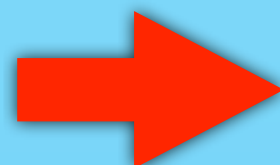
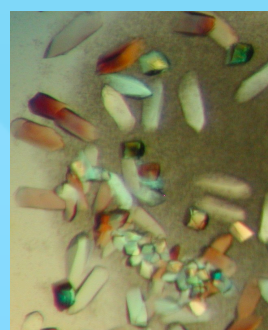


**Oxford Protein  
Production Facility  
(OPPF) in RCaH @ RAL**

Crystallisation

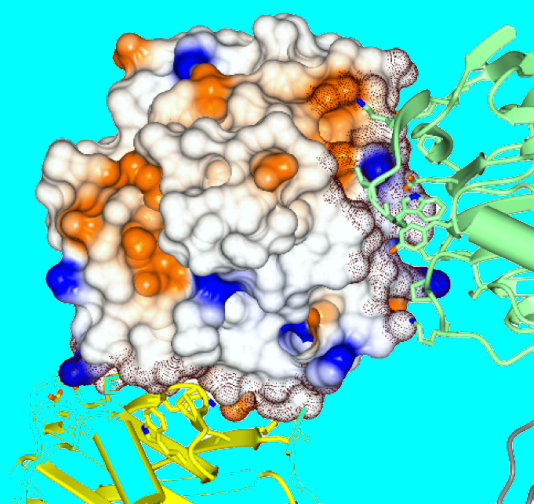
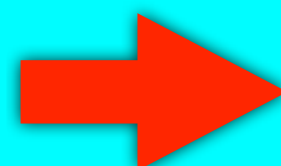
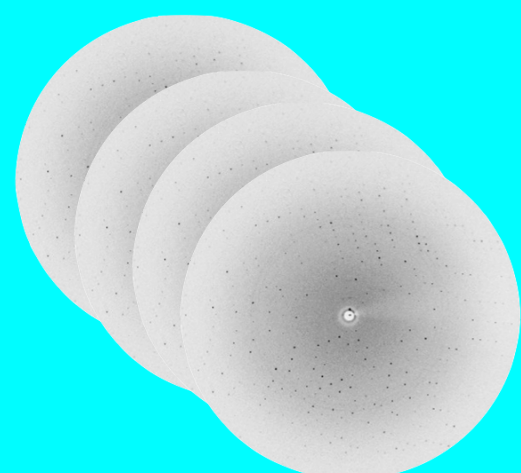


Diffraction

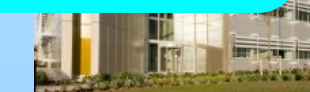


**Diamond Light  
Source @ RAL**

Solution

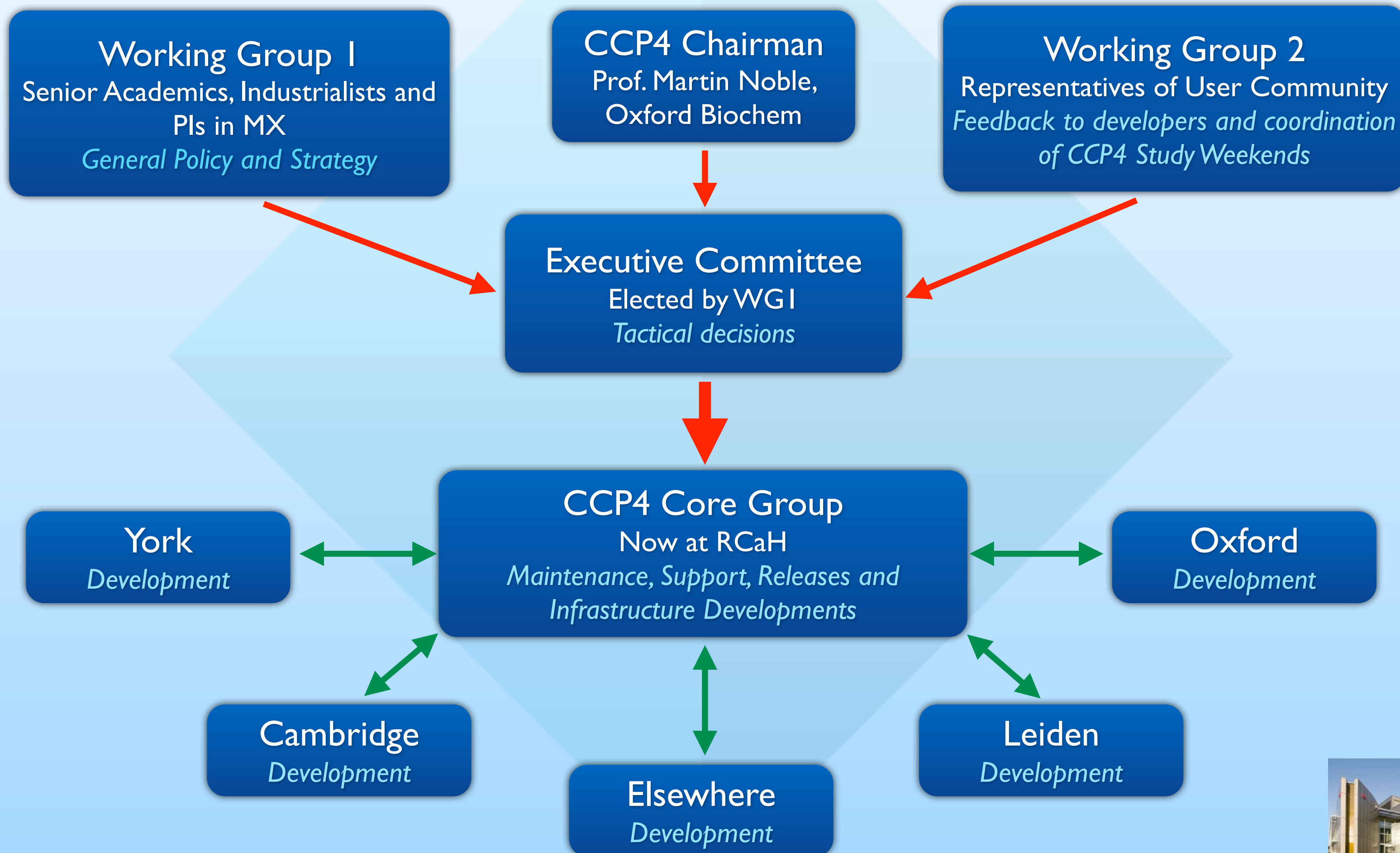


**now in RCaH  
@ RAL**





# Structure of CCP4 Collaboratory



Research Complex at Harwell

# CCP4 Software Suite

- Unlike many other software packages, CCP4 is a set of separate programs, communicating through standard files, rather than all operations integrated into one big program.

## *Advantages:*

- easy to add, update and upgrade
- extreme flexibility of use

## *Disadvantages:*

- decision-making relies on user expertise
- may not be easy to use by complete novices

## *This is changing:*

- CCP4 builds automatic pipelines that involve many components and make intelligent choice of actions and parameters

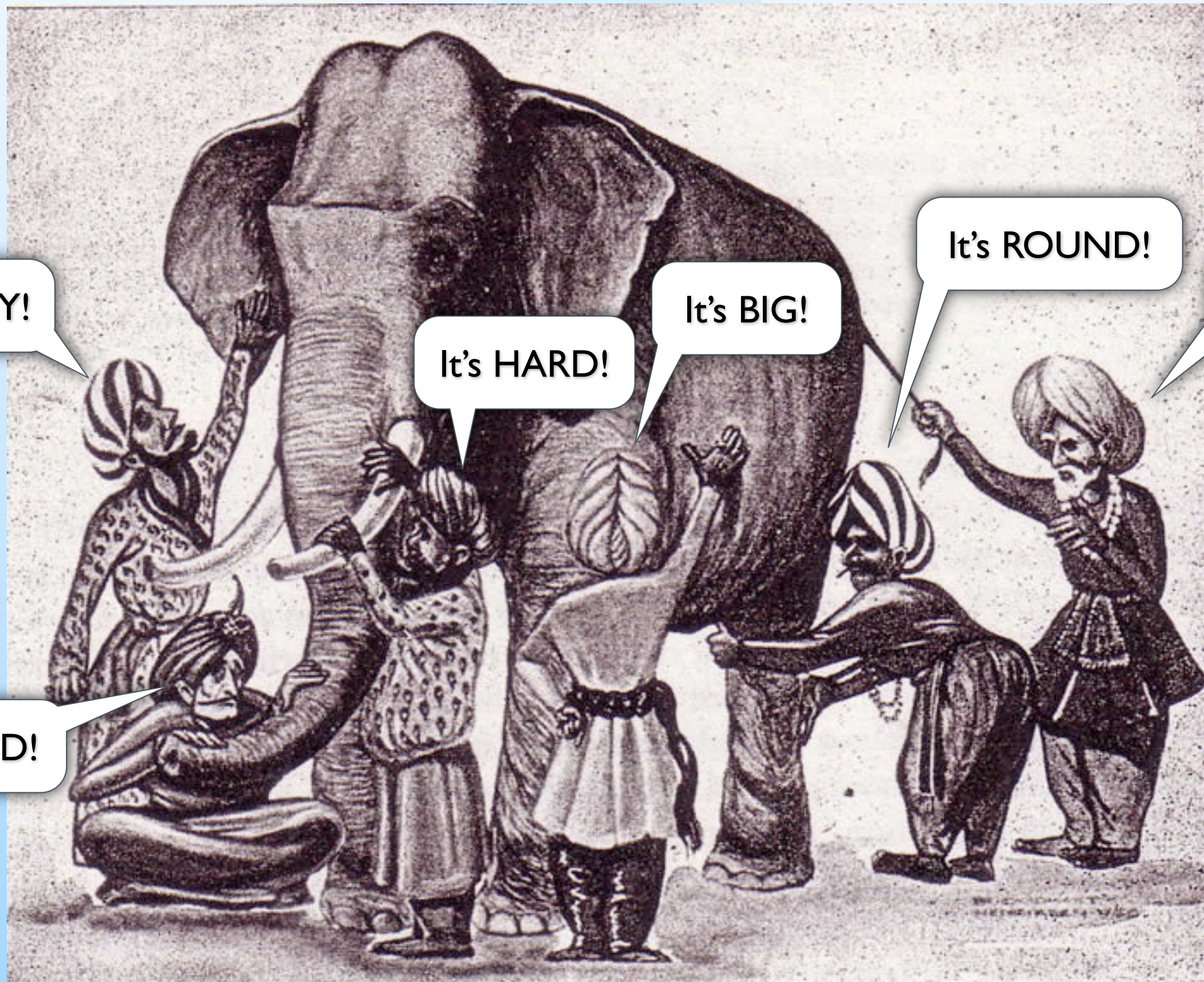
- CCP4 Software is free for academic and not-for-profit use.
- CCP4 Software undergoes a regular update and release cycle, usually once or twice an year.
- CCP4 provides technical user support through its Helpdesk.



Research Complex at Harwell




# What is CCP4 Software?



Research Complex at Harwell




# CCP4 is a Structure Solution Suite

-  CCP4 contains about 250 program components



*Research Complex at Harwell*

# CCP4 is a Structure Solution Suite

 CCP4 contains about 250 program components


 ~30% components directly related to structure solution

*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.



*Research Complex at Harwell*

# CCP4 is a Structure Solution Suite

 CCP4 contains about 250 program components

 ~30% components directly related to structure solution


*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.

It's **HARD!**



*Research Complex at Harwell*

# CCP4 is a Structure Solution Suite

 CCP4 contains about 250 program components

- ~30% components directly related to structure solution

*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.

It's HARD!


- ~45% components assisting structure solution

*CHAINSAW, HGEN, WATERTIDY, CTRUNCATE, PROFESS, LIBCHECK, SFALL, SKETCHER, JLIGAND, ECALC, RFCORR, DETWIN, SAPI, WATPEAK, SEQWT* etc.



Research Complex at Harwell

# CCP4 is a Structure Solution Suite

 CCP4 contains about 250 program components

- ~30% components directly related to structure solution

*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.

It's **HARD!**

- ~45% components assisting structure solution

*CHAINSAW, HGEN, WATERTIDY, CTRUNCATE, PROFESS, LIBCHECK, SFALL, SKETCHER, JLIGAND, ECALC, RFCORR, DETWIN, SAPI, WATPEAK, SEQWT* etc.


It's **BIG!**



*Research Complex at Harwell*



# CCP4 is a Structure Solution Suite

 CCP4 contains about 250 program components

- ~30% components directly related to structure solution

*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.

It's **HARD!**

- ~45% components assisting structure solution

*CHAINSAW, HGEN, WATERTIDY, CTRUNCATE, PROFESS, LIBCHECK, SFALL, SKETCHER, JLIGAND, ECALC, RFCORR, DETWIN, SAPI, WATPEAK, SEQWT* etc.

It's **BIG!**


- ~20% related to file transforms and various jiffies

*COORD\_FORMAT, PDBSET, PDBCUR, PDB2TO3, COORDCONV, GENSYM, SYMCONV, PHISTATS, STEREO, MTZDUMP, PDB\_EXTRACT, F2MTZ, MTZ2CIF, MTZ2VARIOUS, MTZUTILS, SORTMTZ* etc.



Research Complex at Harwell

# CCP4 is a Structure Solution Suite

 CCP4 contains about 250 program components

- ~30% components directly related to structure solution

*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.

It's **HARD!**

- ~45% components assisting structure solution

*CHAINSAW, HGEN, WATERTIDY, CTRUNCATE, PROFESS, LIBCHECK, SFALL, SKETCHER, JLIGAND, ECALC, RFCORR, DETWIN, SAPI, WATPEAK, SEQWT* etc.

It's **BIG!**

- ~20% related to file transforms and various jiffies

*COORD\_FORMAT, PDBSET, PDBCUR, PDB2TO3, COORDCONV, GENSYM, SYMCONV, PHISTATS, STEREO, MTZDUMP, PDB\_EXTRACT, F2MTZ, MTZ2CIF, MTZ2VARIOUS, MTZUTILS, SORTMTZ* etc.

It's **ROUND!**



Research Complex at Harwell

# CCP4 is a Structure Solution Suite

## CCP4 contains about 250 program components

- ~30% components directly related to structure solution

*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.

It's HARD!

- ~45% components assisting structure solution

*CHAINSAW, HGEN, WATERTIDY, CTRUNCATE, PROFESS, LIBCHECK, SFALL, SKETCHER, JLIGAND, ECALC, RFCORR, DETWIN, SAPI, WATPEAK, SEQWT* etc.

It's BIG!

- ~20% related to file transforms and various jiffies

*COORD\_FORMAT, PDBSET, PDBCUR, PDB2TO3, COORDCONV, GENSYM, SYMCONV, PHISTATS, STEREO, MTZDUMP, PDB\_EXTRACT, F2MTZ, MTZ2CIF, MTZ2VARIOUS, MTZUTILS, SORTMTZ* etc.

It's ROUND!

- ~5% post-structure solution analysis


*A relatively small subset of the Suite that may be used by structural biologists to aid their research when they have their structure solved or otherwise obtained*



Research Complex at Harwell



# CCP4 is a Structure Solution Suite

 CCP4 contains about 250 program components

- ~30% components directly related to structure solution

*MOSFLM, XIA2, POINTLESS, SCALA, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, PHASER, COOT* etc.

It's **HARD!**

- ~45% components assisting structure solution

*CHAINSAW, HGEN, WATERTIDY, CTRUNCATE, PROFESS, LIBCHECK, SFALL, SKETCHER, JLIGAND, ECALC, RFCORR, DETWIN, SAPI, WATPEAK, SEQWT* etc.

It's **BIG!**

- ~20% related to file transforms and various jiffies

*COORD\_FORMAT, PDBSET, PDBCUR, PDB2TO3, COORDCONV, GENSYM, SYMCONV, PHISTATS, STEREO, MTZDUMP, PDB\_EXTRACT, F2MTZ, MTZ2CIF, MTZ2VARIOUS, MTZUTILS, SORTMTZ* etc.

It's **ROUND!**

- ~5% post-structure solution analysis

*A relatively small subset of the Suite that may be used by structural biologists to aid their research when they have their structure solved or otherwise obtained*

It's **FLOPPY!**



Research Complex at Harwell

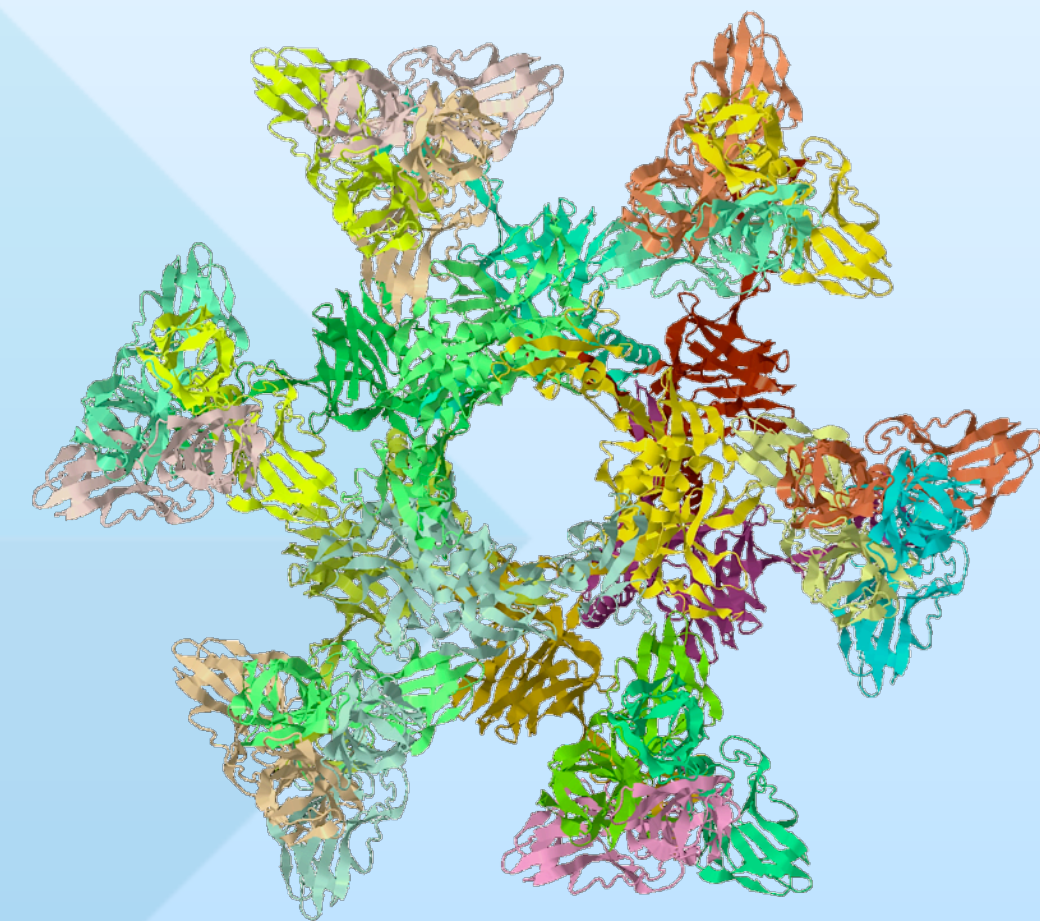
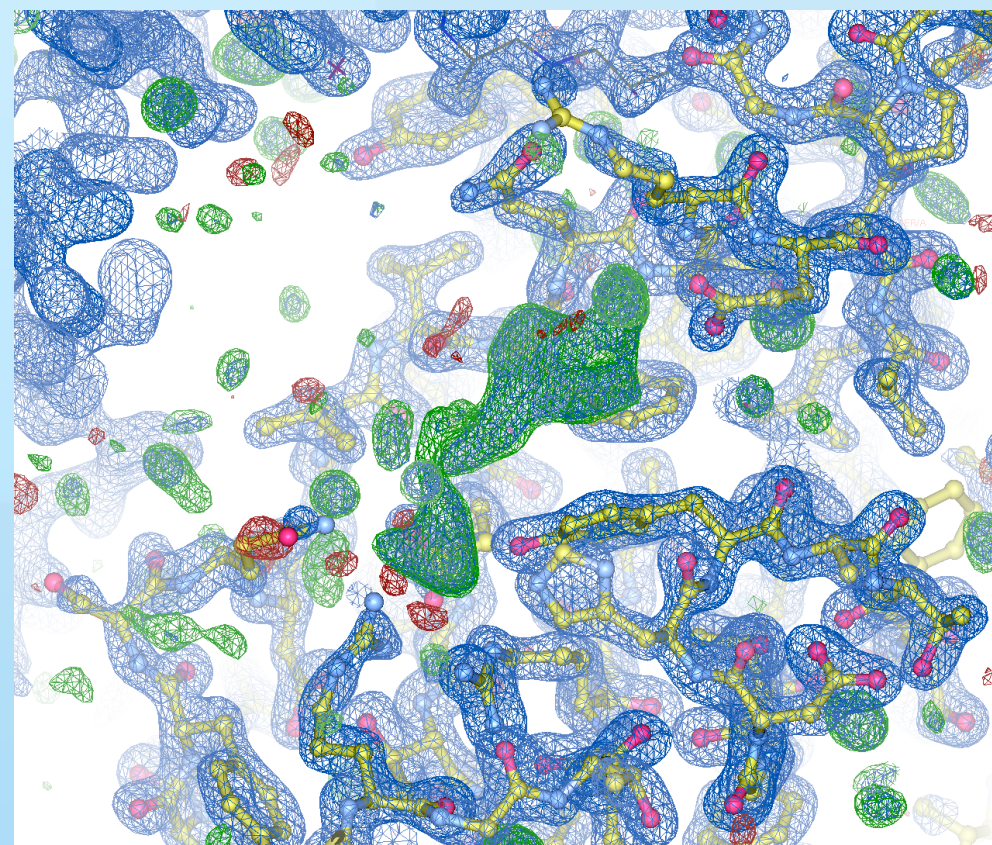
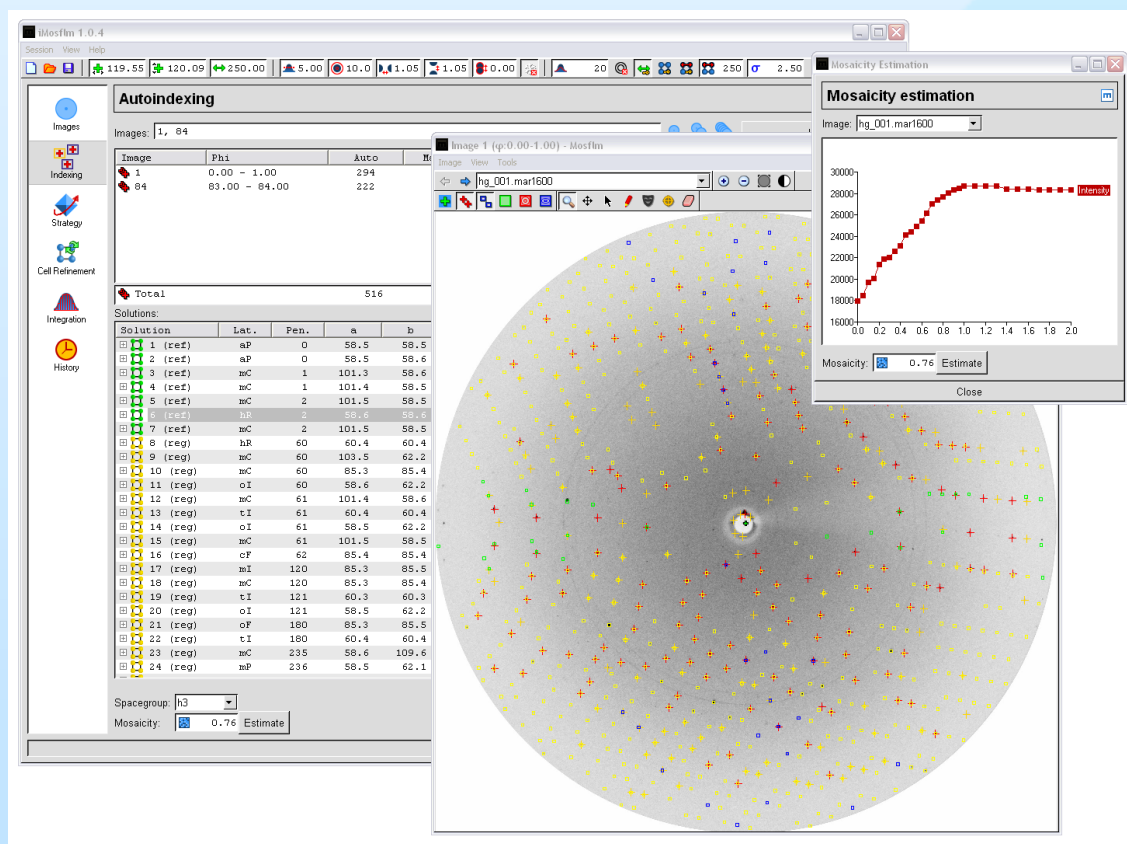


# CCP4 is a Comprehensive Structure Solution Suite



CCP4 Software Suite remains to be the most comprehensive one in MX

*Over 250 programs to take you from raw data processing and reduction to structure solution, validation and analysis*



## Data Processing and Reduction

**Automatic pipeline:** XIA2

**Major programs:** Mosflm, Scala, Pointless, Aimless

## Structure Solution

**Automatic pipelines:** MrBump, Balbes, Crank, Buccaneer

**Major programs:** Refmac, Phaser, DM, Pirate, Parrot, Molrep, Amore, Coot

## Validation and Analysis

Watertidy, Superpose, PISA, Act, Areaimol, ProCheck, Rotamer, Contact, SFCheck and many more



Research Complex at Harwell



# CCP4 Software Suite: Challenges



## The Suite is more than 30 years old

- many components are written in obsolete technical frameworks and are difficult to maintain
- the Suite is big and periodically requires revision and trimming
- considerable maintenance and testing effort
- most components remain command-prompt applications, a bit odd for 21st century
- the Suite's functionality is quite fragmented, which makes it more difficult for novices



*Research Complex at Harwell*

# CCP4 Software Suite: Challenges



## The Suite is more than 30 years old

- many components are written in obsolete technical frameworks and are difficult to maintain
- the Suite is big and periodically requires revision and trimming
- considerable maintenance and testing effort
- most components remain command-prompt applications, a bit odd for 21st century
- the Suite's functionality is quite fragmented, which makes it more difficult for novices



## The new user

- the Suite originated in times when crystallographers were a few, highly experienced and coding mostly for themselves
- for many years, the Suite was created and used by people focused on crystallography as a subject
- today's user is, on average, much less experienced, with little programming skills and focused on application aspects rather than methods
- today's expectations of the Suite are more as of a professional user-oriented software



Research Complex at Harwell

# CCP4 Software Suite: Challenges



## The Suite is more than 30 years old

- many components are written in obsolete technical frameworks and are difficult to maintain
- the Suite is big and periodically requires revision and trimming
- considerable maintenance and testing effort
- most components remain command-prompt applications, a bit odd for 21st century
- the Suite's functionality is quite fragmented, which makes it more difficult for novices



## The new user

- the Suite originated in times when crystallographers were a few, highly experienced and coding mostly for themselves
- for many years, the Suite was created and used by people focused on crystallography as a subject
- today's user is, on average, much less experienced, with little programming skills and focused on application aspects rather than methods
- today's expectations of the Suite are more as of a professional user-oriented software



## New data

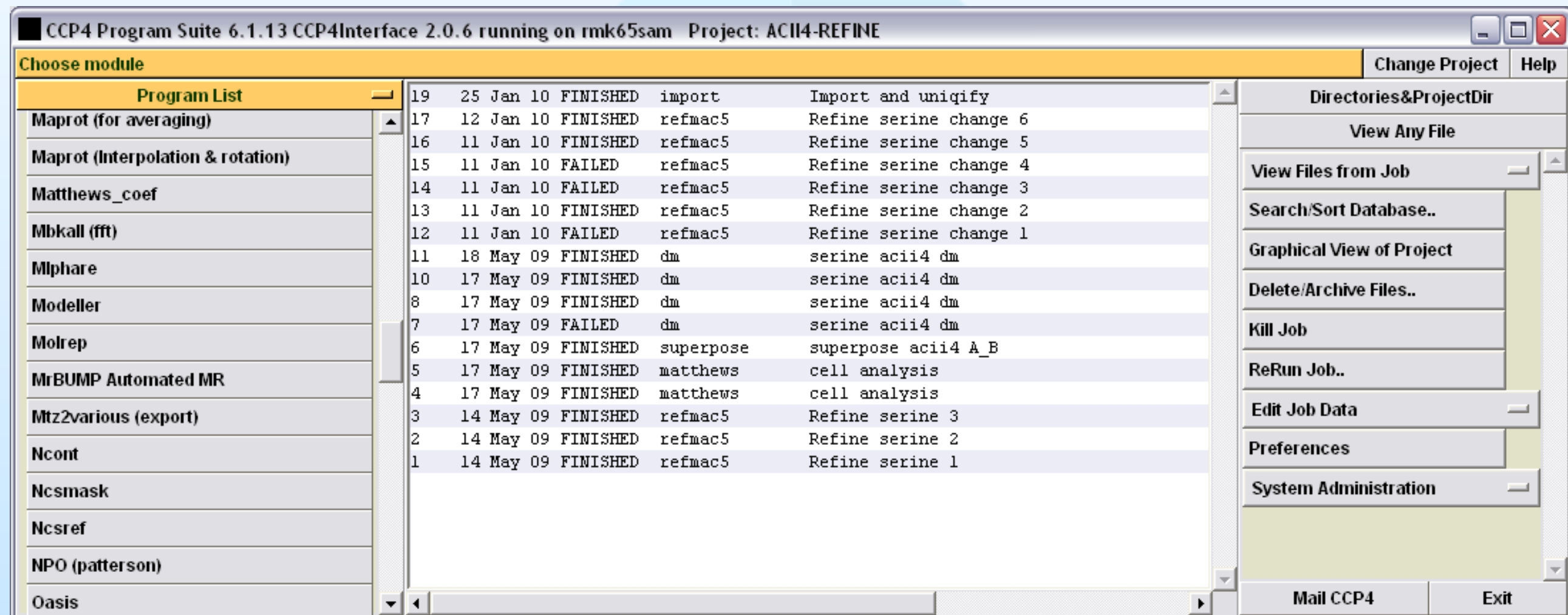
- all the might of modern experimental techniques does not seem to translate into data quality
  - all easy cases solved already?
  - as software advances, researches are more prepared to take on difficult cases?
- relevant CCP4 components are in constant development for being able to cope with low resolution data, higher mosaicity, twinning etc.



Research Complex at Harwell



## CCP4 GUI (CCP4i)

Liz  
Potterton

- The work began in 1998, released in 2001
- Tcl/Tk based, extendable
- Fairly advanced for its time
- Includes graphical interfaces - launchers for most CCP4 components
- Provides a developed project-related functionality:
  - project data organisation and maintenance
  - book-keeping structure solution process in database
  - essential multi-project capabilities and parallelism
  - data exchange between projects



Research Complex at Harwell

# CCP4 GUI-2

## Why:

- Technological change wanted (PyQt vs tcl/tk)
- Enhanced project management wanted
- New, better, look and design wanted
- Workflow configure wanted

## What and how:

- PyQt framework
- Python plugins for components
- Customisable interfaces
- Qt's html capabilities for custom output
- Signalling between processes
- Hierarchy of users
- Hierarchy of projects
- Essentially multi-user interface
- A formal database platform

## The new look? Sorry, not at this time.



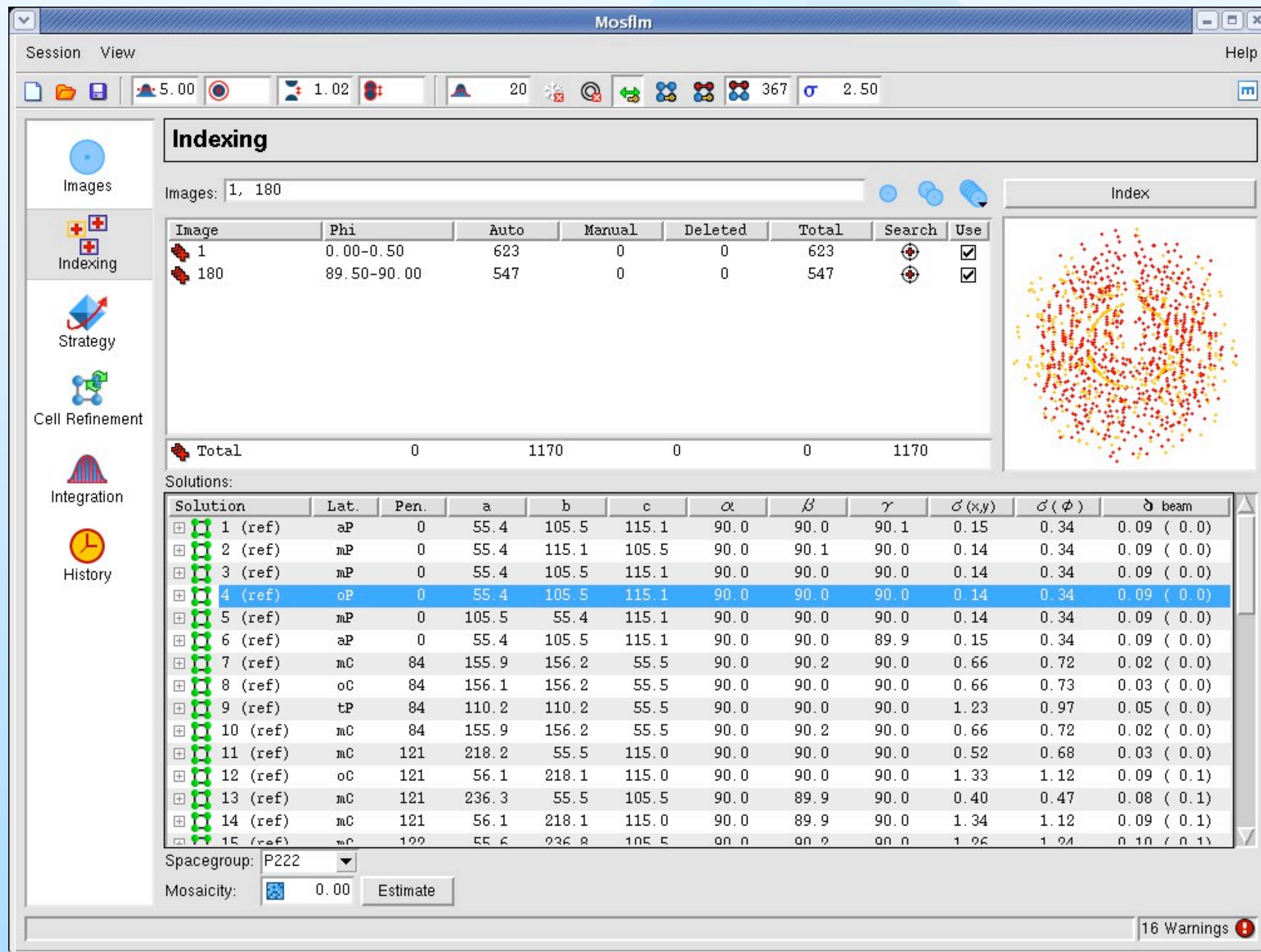
Liz  
Potterton



Research Complex at Harwell



# Interactive Data Processing



Andrew  
Leslie



Harry  
Powell



Luke  
Kontogiannis



Geoff  
Battye



Owen  
Johnson



## iMosflm GUI:

- Tcl-based
- provides access to all aspects of image processing with Mosflm
- modern look-n-feel
- available for all platforms



Research Complex at Harwell



# DIALS: New Data Processing Software

- 🔧 Stands for **D**iffraction **I**ntegration for **A**dvanced **L**ight **S**ources
- 🔧 Part of new pan-European Biostruct-X Initiative
  - CCP4 is a contributing partner
  - development is mostly done at CCP4, Diamond and Phenix (Berkeley)
- 🔧 Objectives:
  - to develop a data analysis suite that is forward compatible and can keep pace with the changes in the way we measure and analyse diffraction data, such as
    - new pixel array detectors (both counting and integrating)
    - very high speeds
    - very high mosaicity
    - overlapping diffraction spots and patterns
  - to attempt to unify, wherever possible, the analysis of synchrotron and FEL data
    - present a unified view of MX analysis to structural biologists
    - e.g., handling of coherence effects, crystal modelling
  - develop tools to manage and handle very large numbers of diffraction images
    - pre-classification and mining tools



David  
Waterman



Phil  
Evans



Andrew  
Leslie



Gwyndaf  
Evans



Graeme  
Winter



Nicholas  
Sauter

Luis Fuentes-Montero (DLS)  
James Parkhurst (DLS)  
Johan Hattne (LBL)  
Gleb Bourenkov (EMBL)

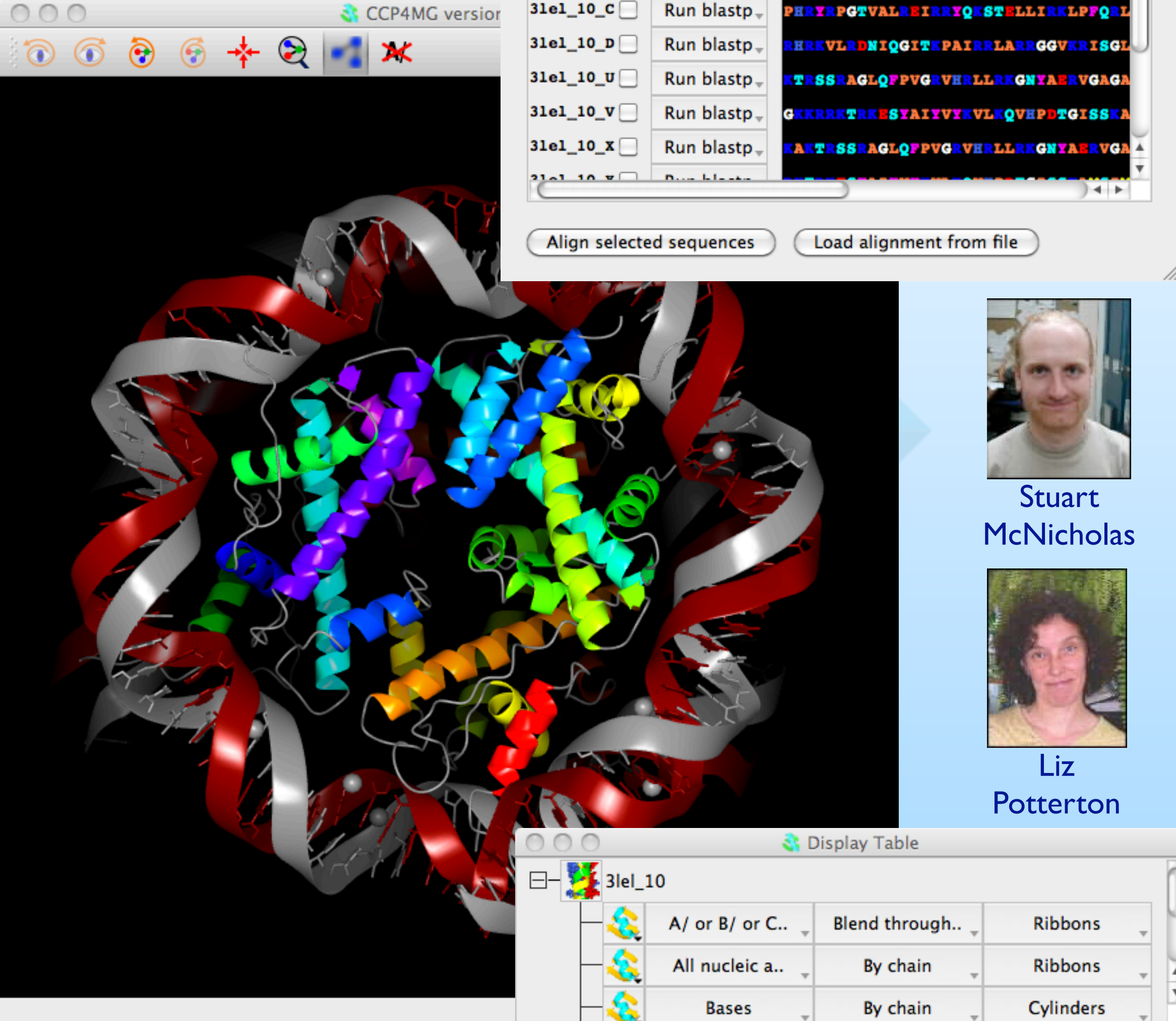


# CCP4 Molecular Graphics



## Version 2.7.3: High-spec MX imaging:

- fast and (almost) stable
- highest publication-quality rendering
- flexible image composition
- rich set of tools and options
- developed selection capabilities
- integrated with other CCP4 components, such as SSM and PISA
- connected to external web-services from NIH, PDB, Uppsala and EBI
- stereo capabilities
- integrated structure analysis
- integrated sequence and structure alignment
- normal mode analysis
- movies
- advanced Picture Wizard
- open architecture with PyQt framework



The screenshot displays the CCP4MG version 2.7.3 interface. The main window shows a 3D ribbon diagram of a protein structure, with various chains highlighted in different colors (red, blue, green, yellow, orange, purple). The top toolbar contains icons for file operations, viewing, and analysis. A 'Sequence Viewer' window is open on the right, showing a list of sequences (31el\_10\_A through 31el\_10\_Y) and a corresponding sequence alignment. Below the list are buttons for 'Run blastp', 'Align selected sequences', and 'Load alignment from file'. A 'Display Table' window is also visible at the bottom right, showing a table with columns for sequence selection, blending, and display style (Ribbons, Cylinders).



Stuart  
McNicholas



Liz  
Potterton



## Crystallographic Object-Oriented Toolkit

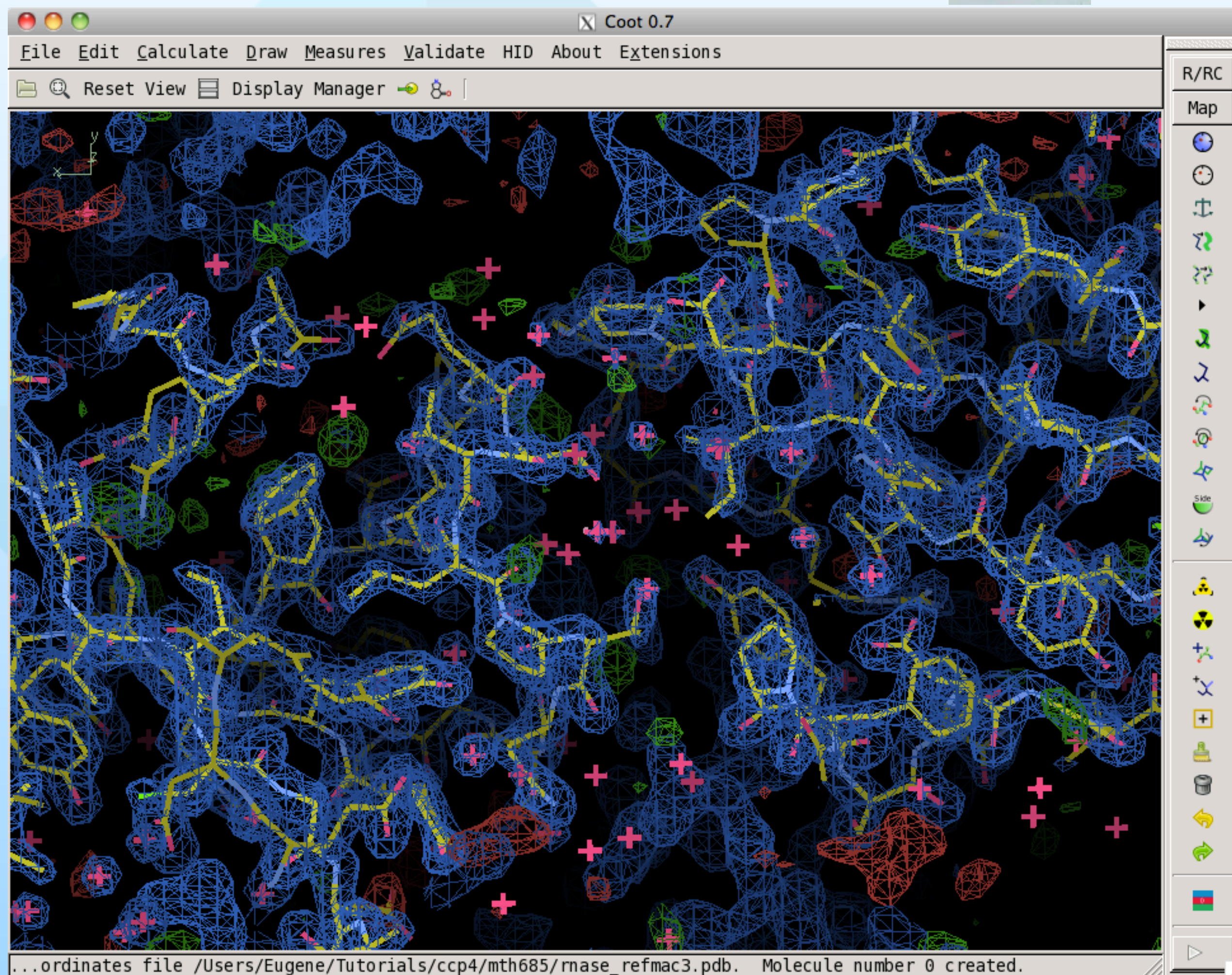
## Jewel of CCP4 model-building functionality:

- de-facto standard nowadays
- true interactivity in model building
- wealth of structure analysis and validation tools
- integrated with all relevant CCP4 components
- efficient graphical engine
- developed chemoinformatics support
- handles all major file formats
- architecture open for customization via a system of scripts
- available on all platforms

# Coot



Paul  
Emsley



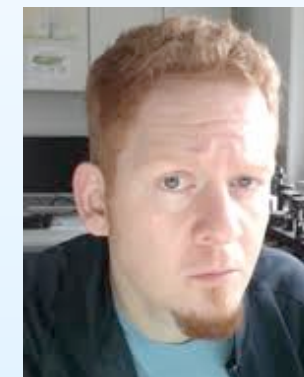


# CCP4 - Arp/wArp Union

- In 2011, CCP4 and Arp/wArp have agreed to synchronise their release cycles
- In 2012, Arp/wArp was included in CCP4 v6.3.0 as 3rd-party software



Victor  
Lamzin



Tim  
Wiegels



Philipp  
Heuser



Ciaran  
Carolan

EMBL



Ioan  
Vancea

- Starting from CCP4 v6.4.0, Arp/wArp will be included into CCP4 update mechanism



Research Complex at Harwell

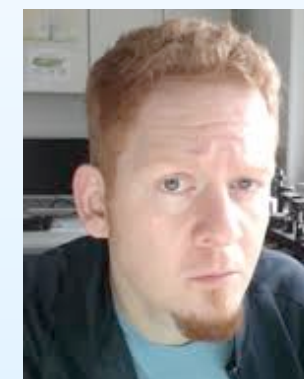


# CCP4 - Arp/wArp Union

- In 2011, CCP4 and Arp/wArp have agreed to synchronise their release cycles
- In 2012, Arp/wArp was included in CCP4 v6.3.0 as 3rd-party software



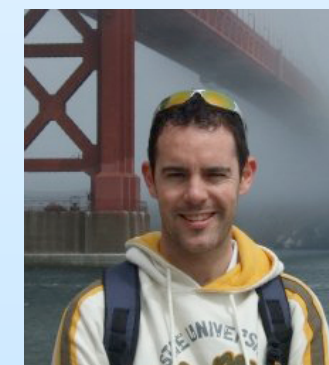
Victor  
Lamzin



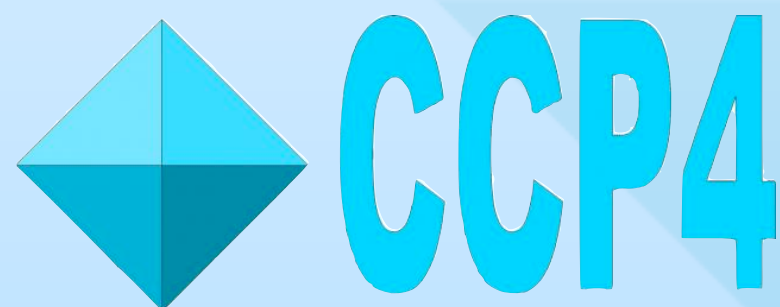
Tim  
Wiegels



Philipp  
Heuser



Ciaran  
Carolan



EMBL



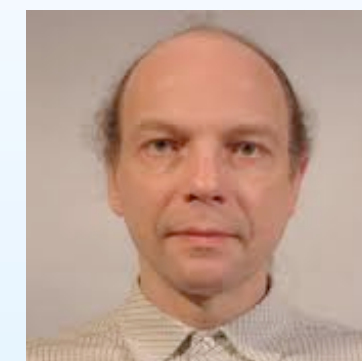
Ioan  
Vancea

- Starting from CCP4 v6.4.0, Arp/wArp will be included into CCP4 update mechanism



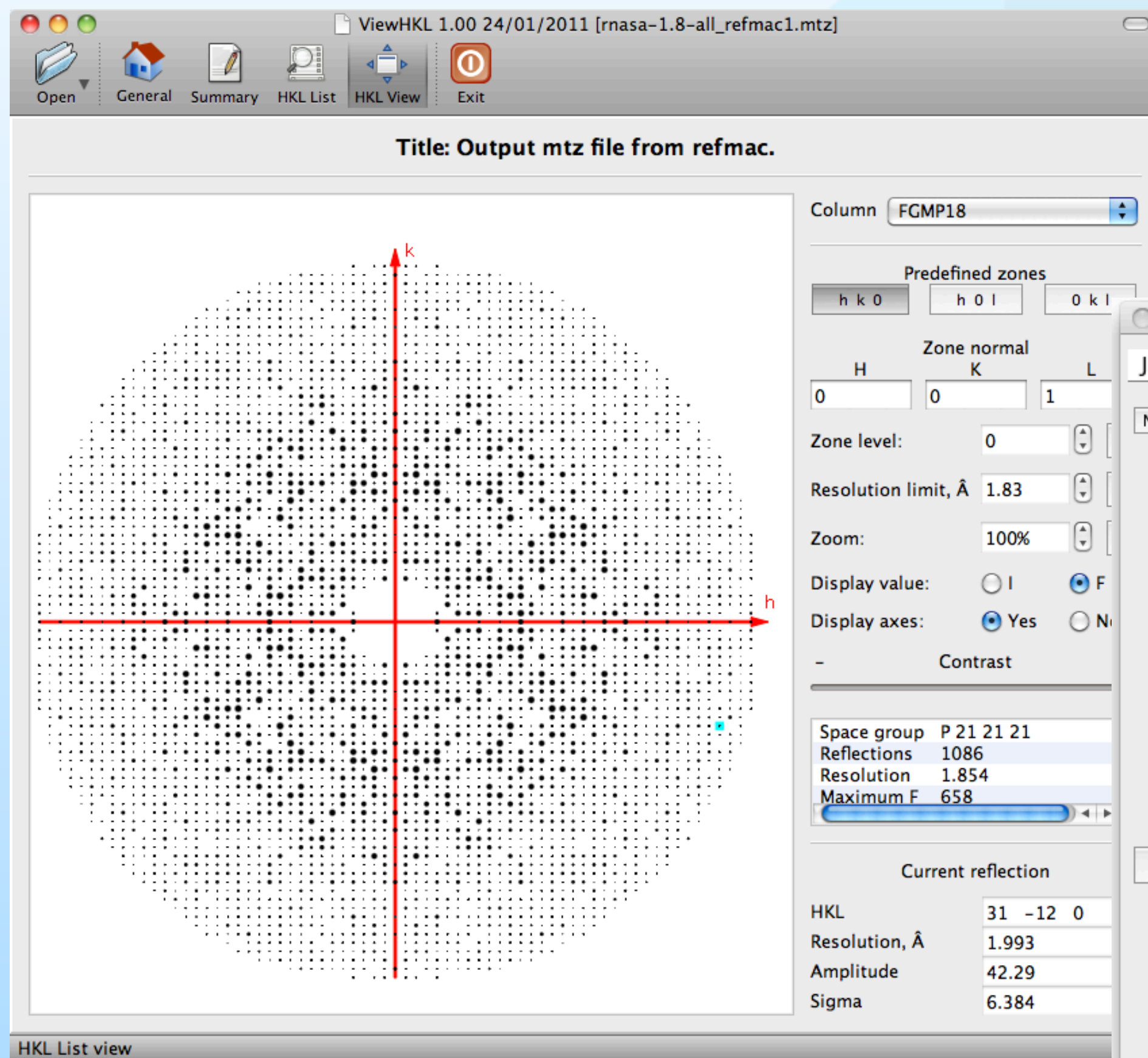
Research Complex at Harwell

# Remakes of Old Graphics

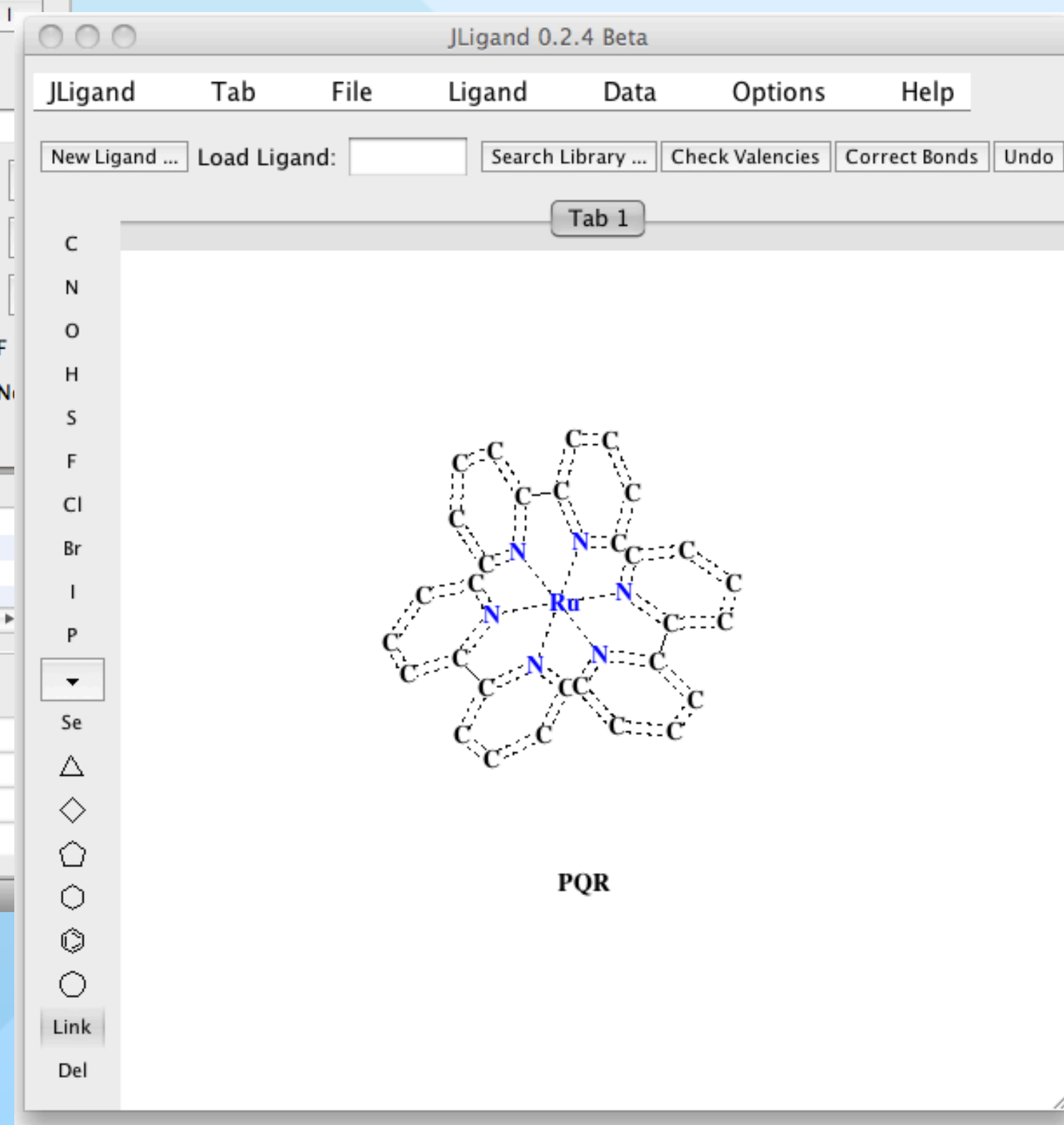


Andrey  
Lebedev

## New “Sketcher”

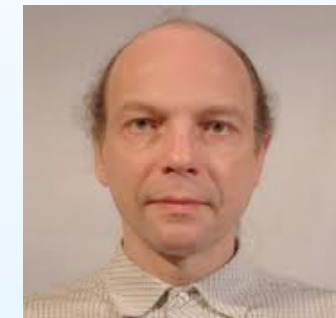


## New “HKLView”





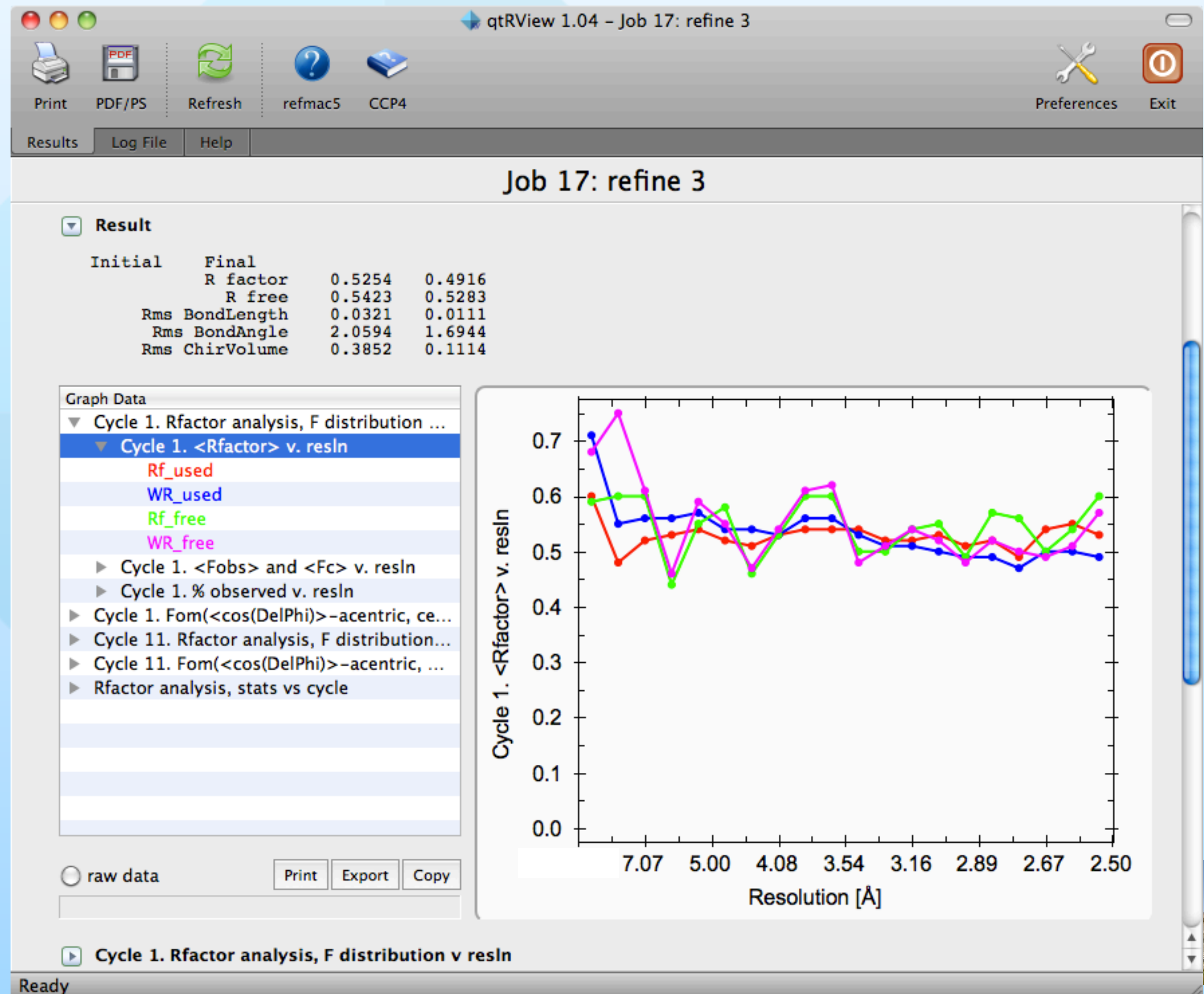
# Generic Result Viewer



Andrey  
Lebedev

## Advanced result presentation for old codes

- automatically greps log files
- makes output structured
- identifies graph data and presents it accordingly
- provide interactive launchers for other CCP4 components such as Coot
- provides dynamic output
- provides easy access to documentation and manuals
- search engine for log files
- printing and export in PDF and PNG



# Automation Projects



To provide a maximum possible aid to an innocent user

- most today's tasks are fairly standard and may be (and therefore should be) automated
- the ultimate goal is to relieve a user of decision-making chores



Automatic pipelines in CCP4:

- XIA2 (image processing, data reduction)
- MrBump, Balbes (molecular replacement)
- Crank (experimental phasing)
- Buccaneer (model building)



Graeme  
Winter



Raj  
Pannu



Ronan  
Keegan

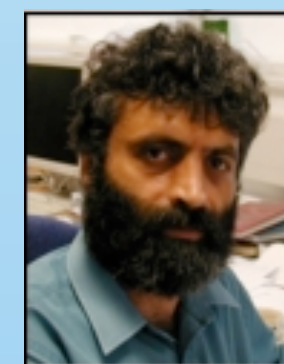


Kevin  
Cowtan



Nice-to-have:

- automatic ligand identification and fitting
- automatic model completion
- sweet dream: full one-button solution



Garib  
Murshudov



Alexei  
Vagin



Fei  
Long



Research Complex at Harwell



# Towards Complete Automation

## AMPLE - *ab initio* modelling for Molecular Replacement

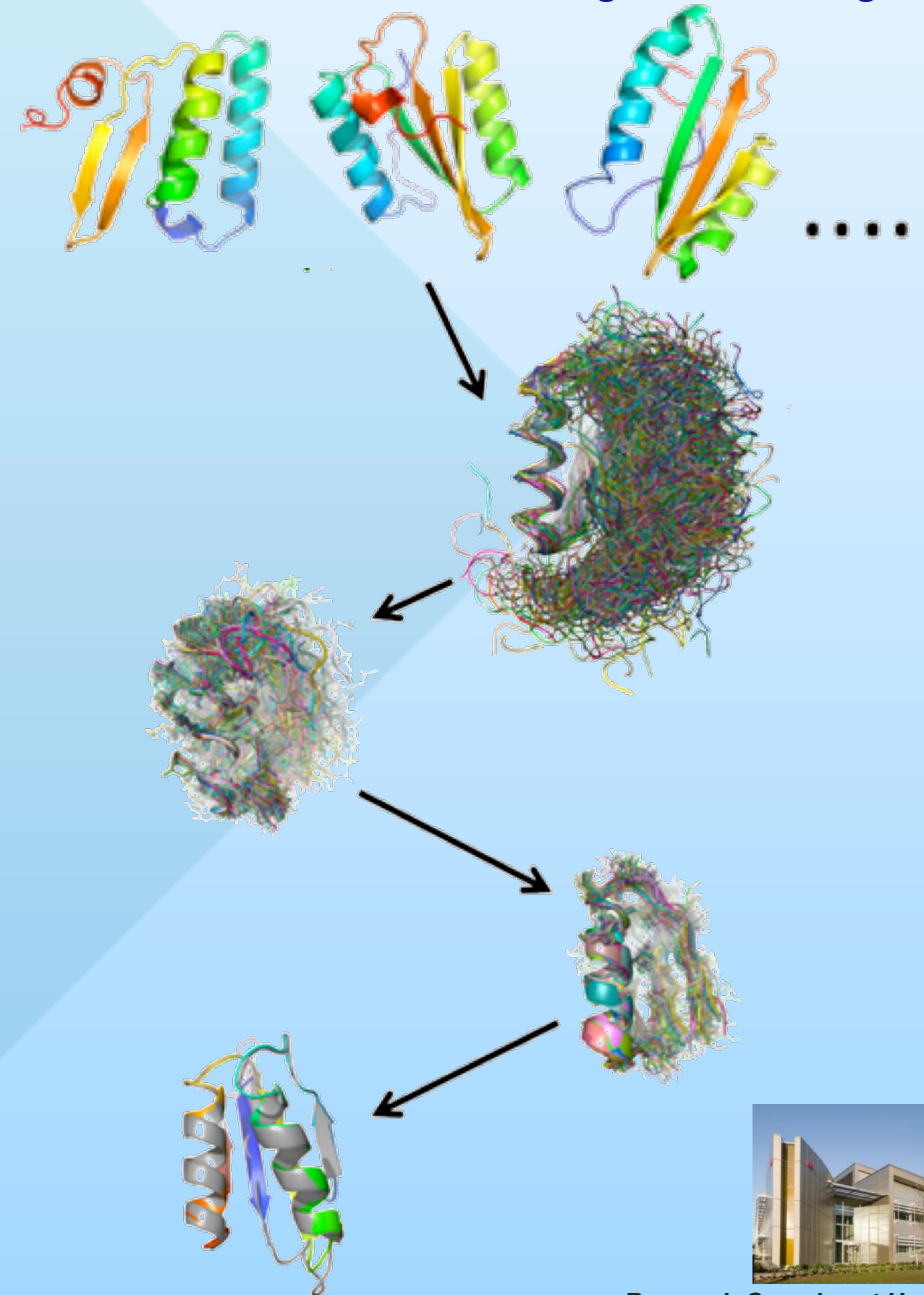
- makes use of improving techniques in *ab initio* modelling programs, such as Rosetta and Quark, to enhance the chances of success in difficult MR cases
- makes MR available to crystallographers who would normally have to rely on Experimental Phasing techniques
- testing on smaller proteins (< 130 residues) has shown that it can work in ~43% of test cases
- method can also be used to enhance the chances of success when using NMR models of distant homologues as MR search models



Daniel  
Rigden



Ronan  
Keegan



Research Complex at Harwell

# Towards Automated Structure Solution

## Challenges:

- Automatic but not a black box
- Automatic vs controllable
- Interactive vs silent
- Configurable vs predefined
- Targeted vs carpet bombing
- Decision making
- Quality assessment
- Resource management
- Persistent layer (the database)
- +1001 more



*Research Complex at Harwell*



# CCP4 Infrastructure Modernisation

- 📌 A software project of CCP4 scale is not manageable unless set up properly
- 📌 New CCP4 development kit
  - New BAZAAR-based repositories
  - Distributed development framework
  - Separation of development and release branches
  - New distributed JHBUILD-based CCP4 builder
  - *It is not possible to herd cats and academic software developers, however, we try it really hard*



Charles  
Ballard



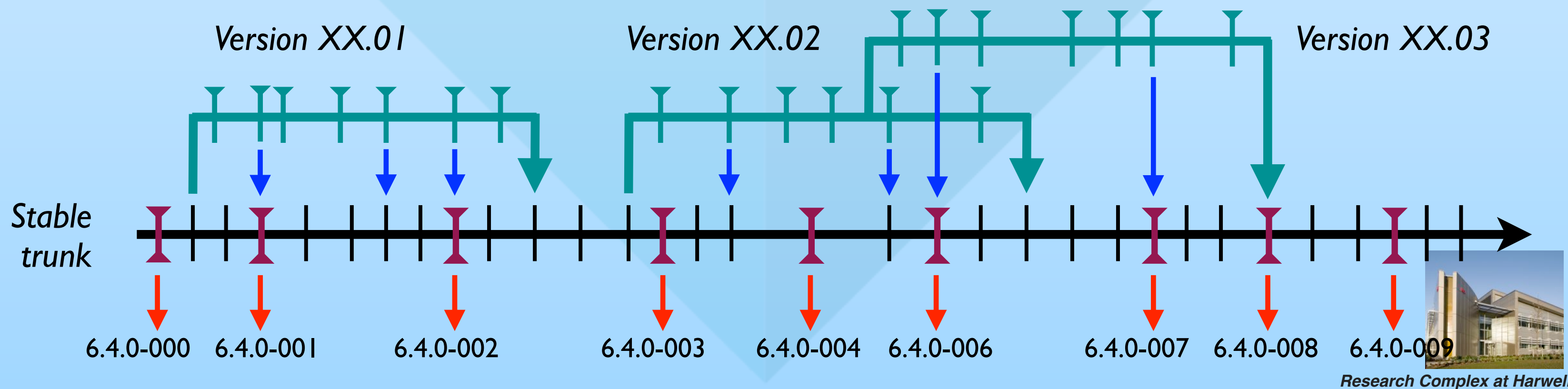
Ronan  
Keegan



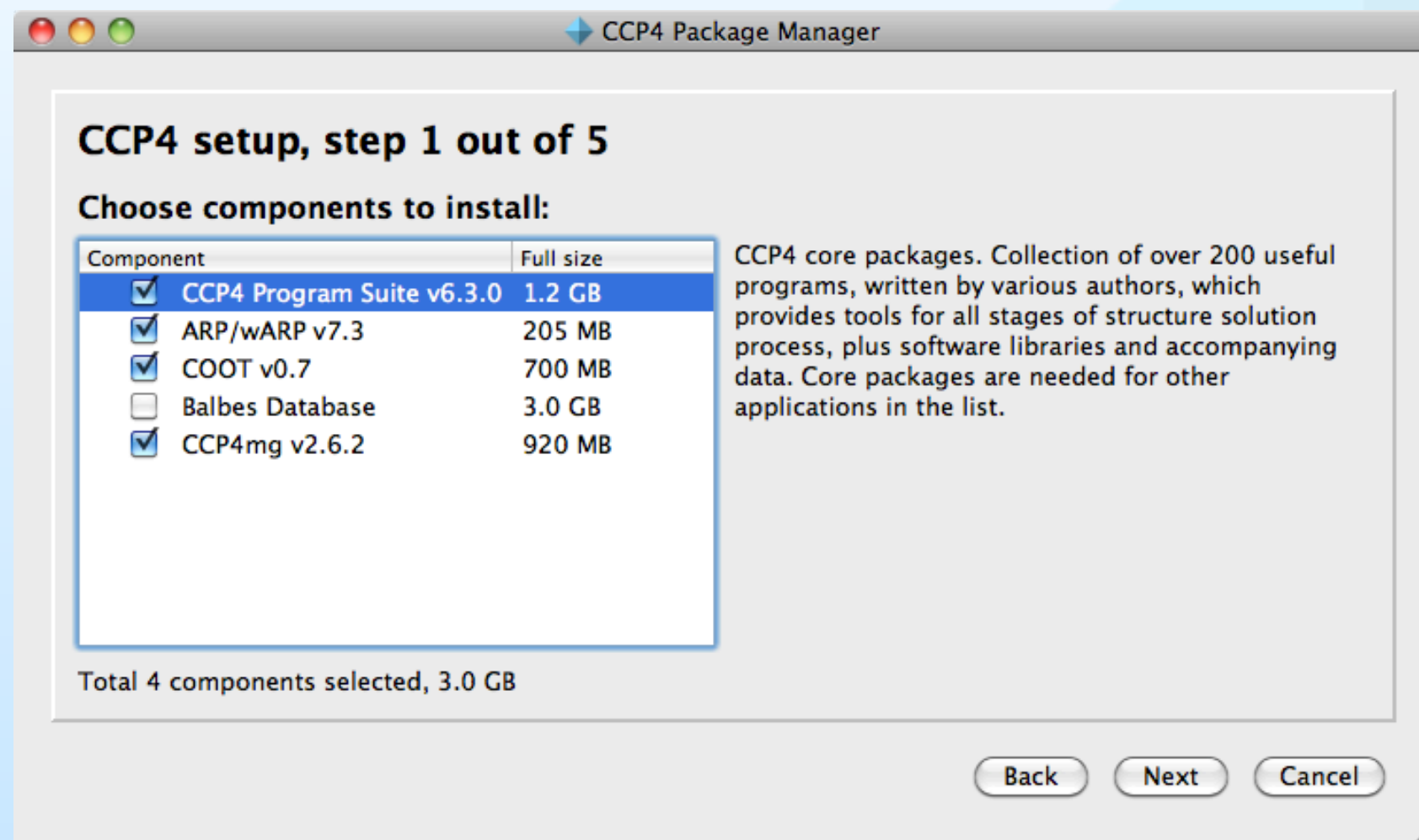
Ville  
Uski



Marcin  
Wojdyr

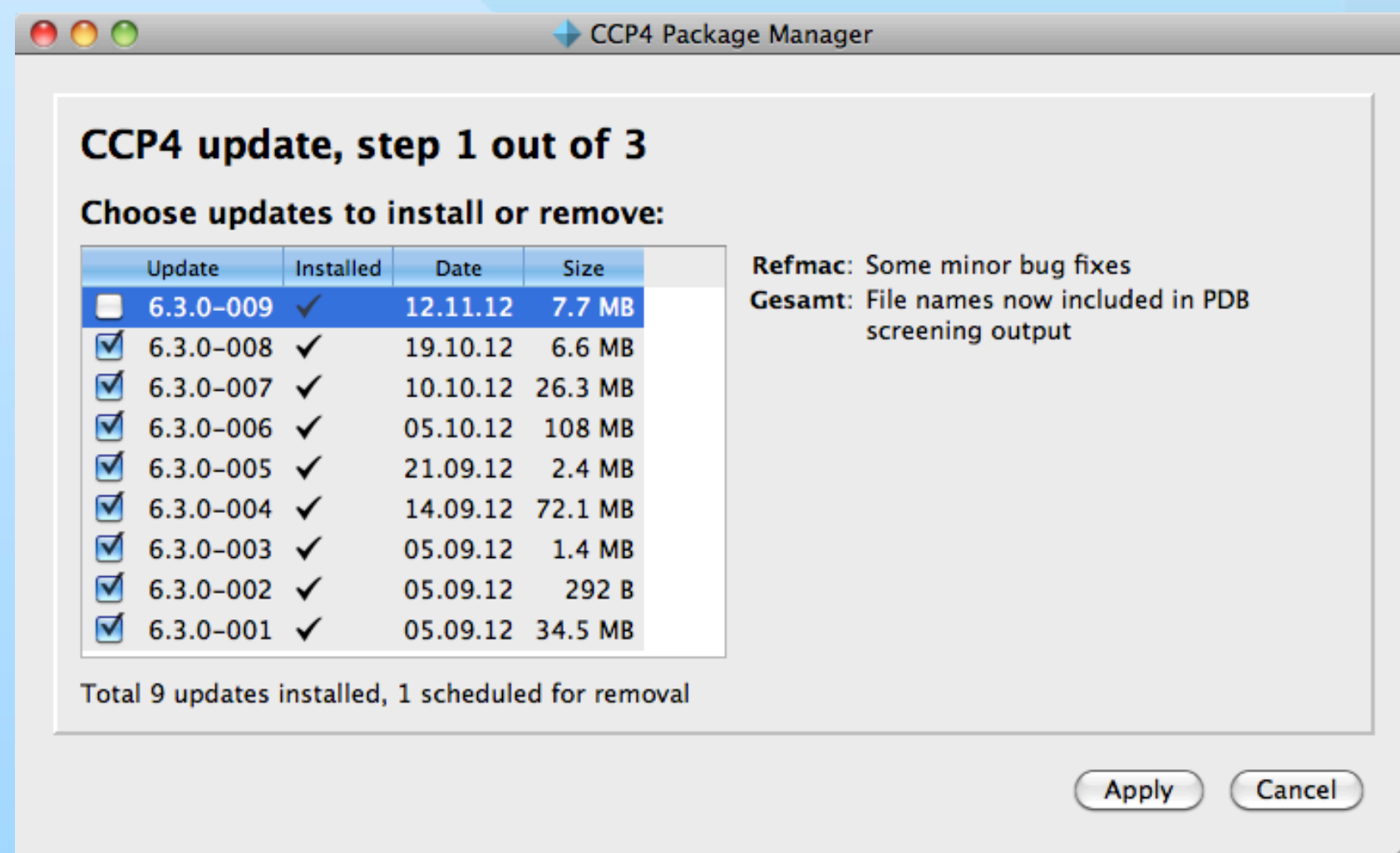


# CCP4 New Release and Update Mechanisms



## Graphical installer

- cross-platform
- custom configuration
- resumable downloads
- easy licensing
- auto-installation in 5 steps
- *easier installation - higher take-up*



## Graphical updater

- cross-platform, similar to Linux updates
- roll-back feature
- automatic notifications through CCP4 GUI
- “just works”
- 21 updates for last CCP4 release



Research Complex at Harwell



# CCP4 Dissemination and Publicity Programs

## CCP4 has a well-established outreach program

### Study Weekends

- big annual events (400-500 participants) in the beginning of January
- have approximate 5-year topic cycle (for PhD student + postdoc to capture all of it)
- lectures are given by leading scientists in the field
- not limited to CCP4 Software!



### International Workshops and Crystallography Schools

- 4-6 day events to get PhD students and postdocs familiar with CCP4 software
- includes both lectures and intensive practical courses
- either annual or bi-annual events
- a number of designated locations worldwide
- not limited to CCP4 Software!

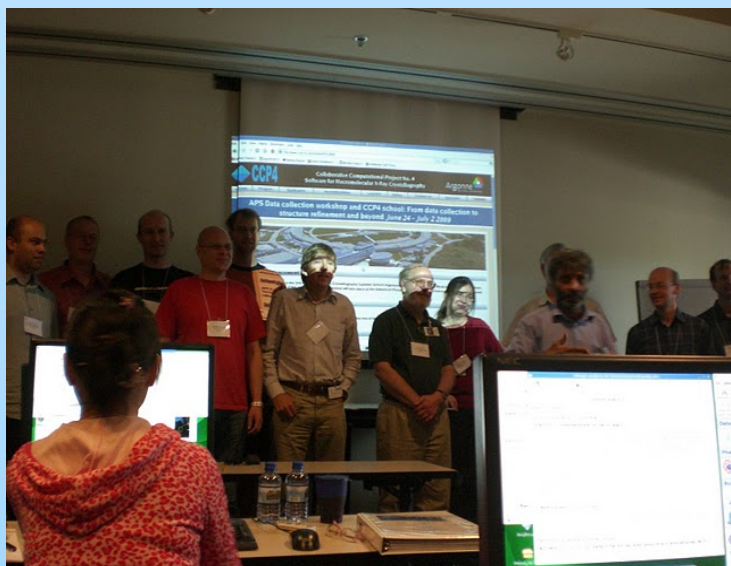


### Helpdesk

- problems resolved with the help of CCP4 core team and developers

### Bulletin Board

- many-year established place in WWW for crystallographers to share their experience, ideas, problems and get help



Research Complex at Harwell



CCP4: Software for Macromolecular Crystallography

http://www.ccp4.ac.uk/

Home RAL Mail SSC Oracle CCP4Forge CCP4 wiki Yahoo! Mail Google Mail STFC Google Google Maps Wikipedia Apple YouTube News Popular

 **Collaborative Computational Project No. 4**  
**Software for Macromolecular X-Ray Crystallography** 

Home About CCP4 CCP4 Projects Downloads Documentation Courses Developers CCP4 people

\*\*\* New [BALBES web service](#) \*\*\* New CCP4 documentation wiki available at <http://ccp4wiki.org/> \*\*\* CCP4 6.3.0 available, see [Downloads](#) \*\*\* CCP4MC

CCP4 exists to produce and support a world-leading, integrated suite of programs that allows researchers to determine macromolecular structures by X-ray crystallography, and other biophysical techniques. CCP4 aims to develop and support the development of cutting edge approaches to experimental determination and analysis of protein structure, and integrate these approaches into the suite. CCP4 is a community based resource that supports the widest possible researcher community, embracing academic, not for profit, and for profit research. CCP4 aims to play a key role in the education and training of scientists in experimental structural biology. It encourages the wide dissemination of new ideas, techniques and practice.

**Resources**

**Download CCP4 Software Suite**  
[\[Current Release\]](#) [\[Updates to Current Release\]](#)  
[\[Latest Prerelease Software\]](#)

**Installation and Usage**  
[\[Documentation\]](#) [\[Installation\]](#) [\[Referencing CCP4\]](#) [\[Licensing\]](#)  
[\[CCP4 Wiki\]](#) [\[Community Wiki\]](#)

**Help and Support**  
[\[Current known problems and fixes\]](#) [\[Non-version specific issues\]](#)  
[\[Report a Problem\]](#)

**Web Services**  
[BALBES web server](#)

**CCP4 Bulletin Boards**  
[\[CCP4bb Mailing List\]](#) [\[Developers List\]](#) [\[Archives\]](#)

**CCP4 Newsletter**  
[\[Current issue\]](#) [\[Back issues\]](#) [\[Contribute!\]](#)

**CCP4 Working Groups 1 & 2, and Exec**  
[\[How to join and meeting minutes\]](#)

**Study Weekend and Courses**

**Upcoming Courses and Events**

- [ICSG2013-SLS International Conference on Structural Genomics](#) 29/07/2013 to 20/07/2013
- [APS Data collection workshop and CCP4 school: From data collection to structure refinement and beyond, APS, Chicago, USA](#) 18/06/2013 to 26/06/2013
- [CCP4/OIST school, Okinawa, Japan](#) 04/11/2013 to 08/11/2013

[Browse all forthcoming and past courses and events](#)

**BALBES Automated Molecular Replacement Service**

 NEW! The BALBES automated molecular replacement service is now being hosted on the CCP4 site. To access the service please [click here](#). York University will continue to host their version of service but it may be taken down at some point.

**CCP4 Documentation Wiki**

 For up-to-date documentation on all of CCP4's software and lots of other useful information for X-ray crystallographers see the [CCP4 Wiki](#).

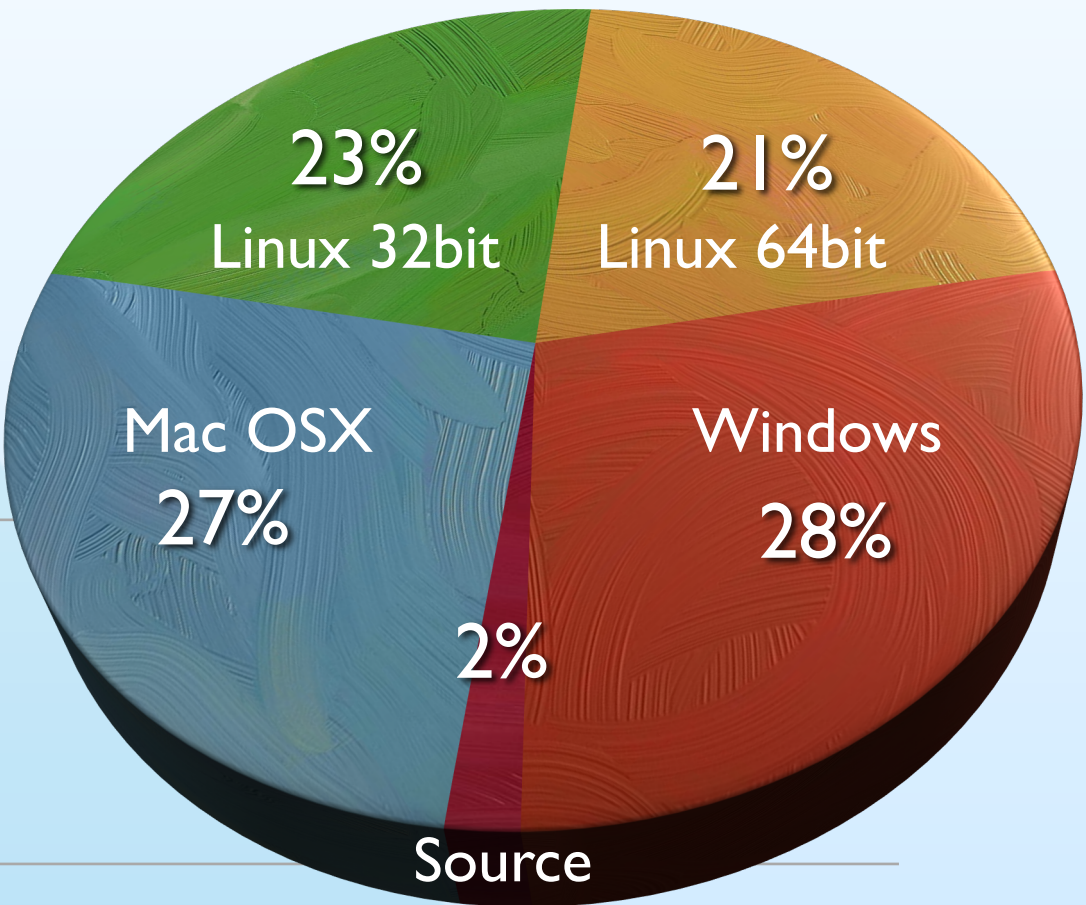
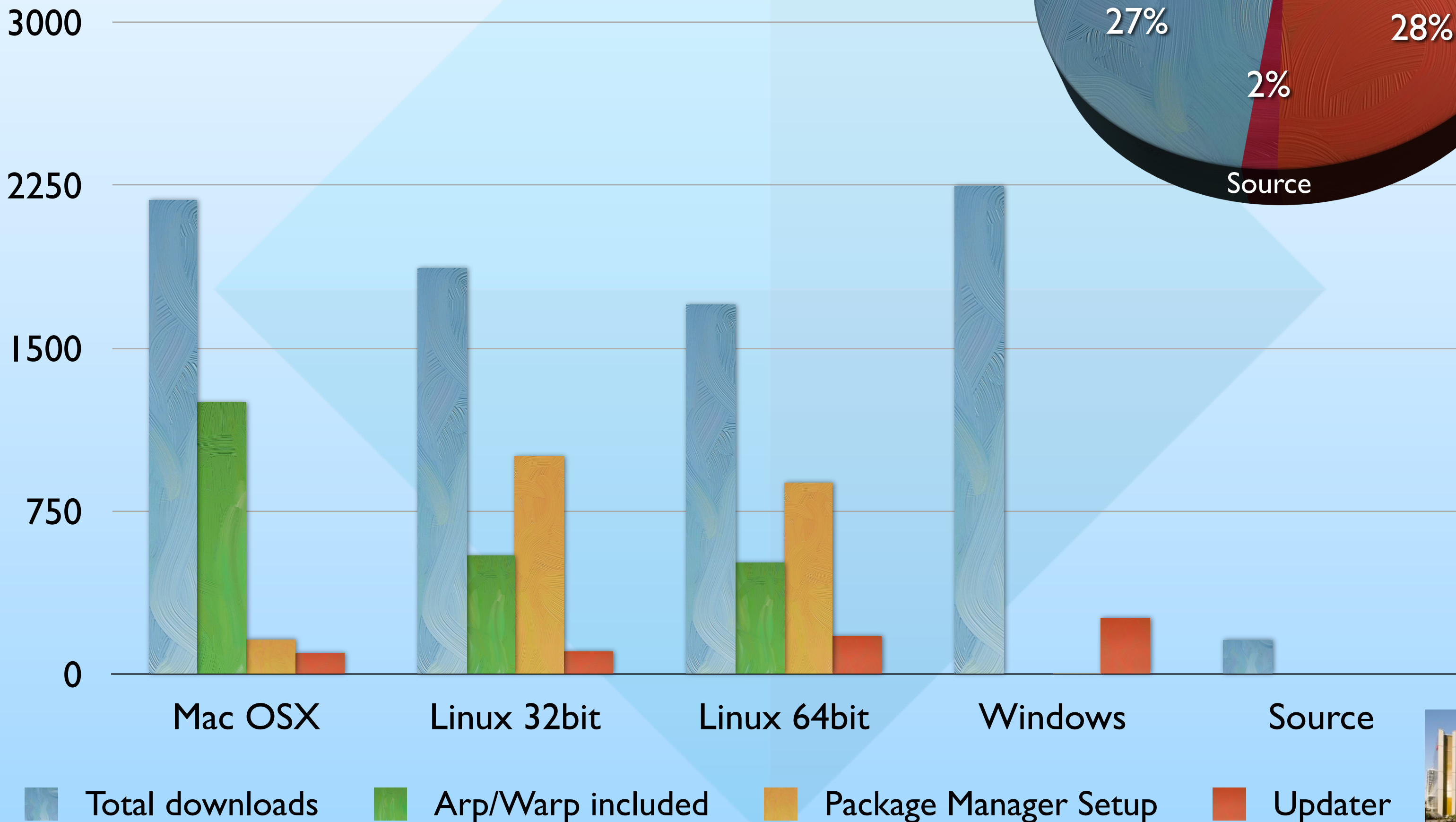
**Search the CCP4 Website**

Google  Search ☒ CCP4 website ☐ CCP4 Wiki



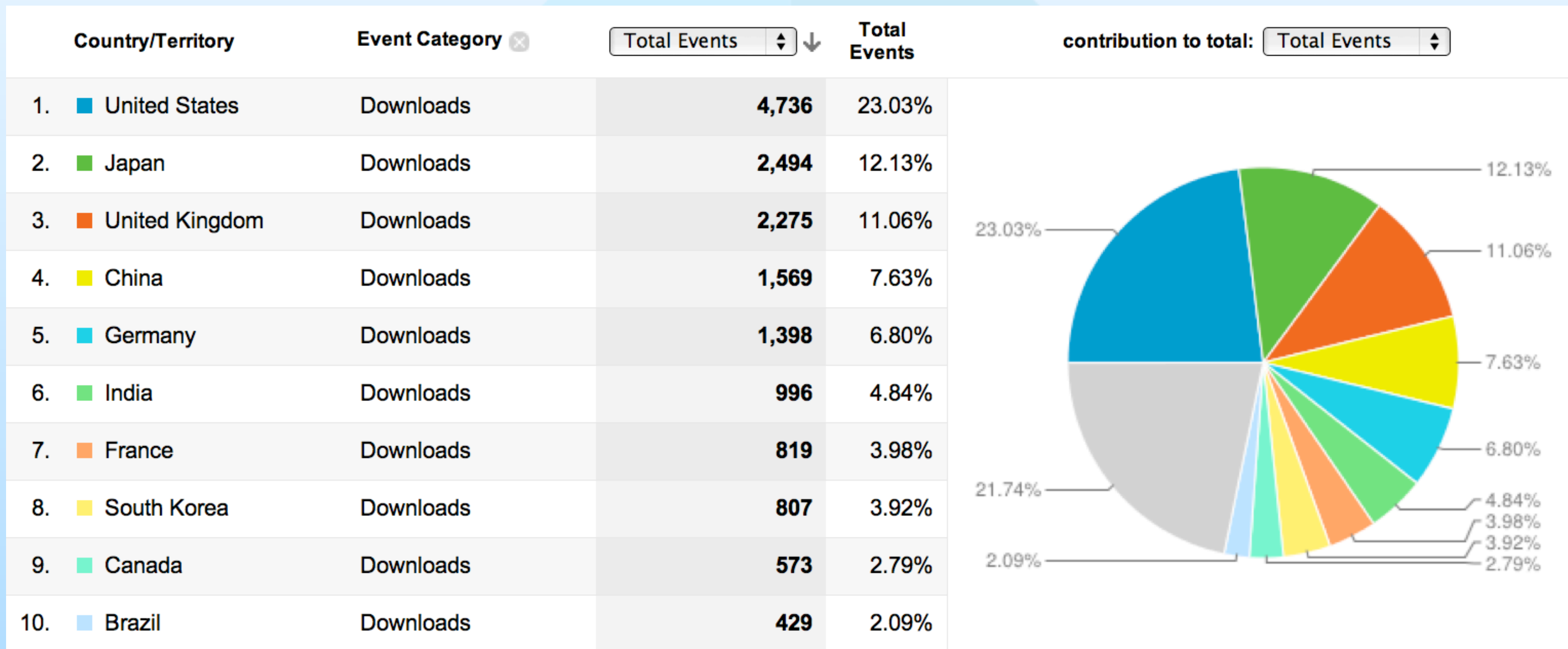
# CCP4 Download Statistics

Source: Google Analytics



Research Complex at Harwell

# CCP4 6.3.0 Download Geography (Mar 2013)



*Screenshot from Google Analytics*



*Research Complex at Harwell*



# CCP4 on Map



Research Complex at Harwell



# CCP4 People (core and associated developers)



Martyn  
Winn



Charles  
Ballard



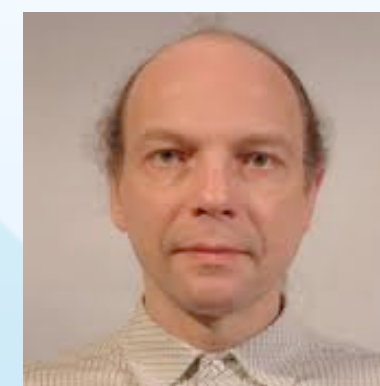
Eugene  
Krissinel



Ronan  
Keegan



David  
Waterman



Andrey  
Lebedev



Keith  
Wilson



Eleanor  
Dodson



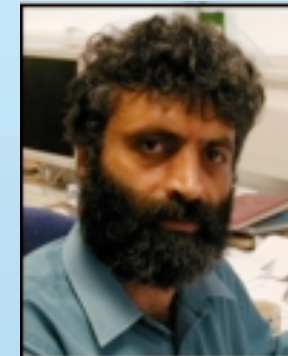
Liz  
Potterton



Stuart  
McNicholas



Kevin  
Cowtan



Garib  
Murshudov



Alexei  
Vagin



Fei  
Long



Phil  
Evans



Andrew  
Leslie



Harry  
Powell



Owen  
Johnson



Randy  
Reed



Martin  
Noble



Paul  
Emsley



Raj  
Pannu



Chris  
Morris



Graeme  
Winter











# 34 years of CCP4

