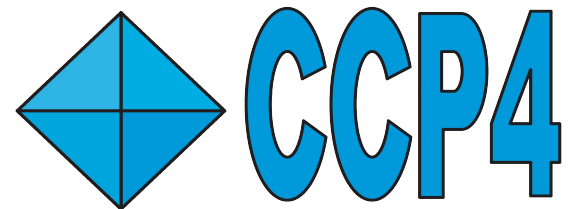




CCP4 Study Weekend 2018

What's new in CCP4?

Ville Uski, CCP4
Research Complex at Harwell



- ❖ “What’s new in CCP4”
 - Ville Uski (CCP4)
- ❖ “What’s new in PanDDA and XChemExplorer”
 - Nicholas Pierce (Utrecht University)
- ❖ “Using homology for model building and refinement: PDB-REDO redone”
 - Robbie Joosten (Netherlands Cancer Institute)
- ❖ “What’s new in Refinement with CCP4 programs”
 - Oleg Kovalevskiy (MRC Laboratory of Molecular Biology)

Lunchtime Bytes (Thu 13:30-14:15)



Room 1 ARCIMBOLDO - Andrey Lebedev

Room 2 CCPEM - Colin Palmer

Room 3 SIMBAD - Adam Simpkin

Room 4 Privateer - Jon Agirre

Room 5 CCP4mg - Stuart McNicholas

Room 6 CC based hierarchical clustering - Gianluca Santoni

Room 7 BLEND - David Waterman

Room 8 ARP/wARP - Sravya Kantamneni

Room 9 CCP4i2 - Kyle Stevenson

Room 10 Pointless and Aimless - Phil Evans

Room 11 REFMAC - Oleg Kovalevskiy

Lunchtime Bytes (Fri 13:45-14:30)



Room 1 ISPyB - Neil Smith

Room 2 jsCoFE - Eugene Krissinel

Room 3 AMPLE - Dan Rigden & Jens Thomas

Room 4 Buccaneer/Nautilus - Kevin Cowtan

Room 5 PDBe - John Berrisford

Room 6 CrystFEL - Thomas White

Room 7 ContaMiner - Stefan Arold

Room 8 PDB2INS + SHELXL - Tim Gruene & Anna Luebben

Room 9 CCP4i2 - Kyle Stevenson

Room 10 DIALS - James Parkhurst

Room 11 AceDRG - Fei Long

CCP4 7.0 (Gargrove)

Released in January 2016

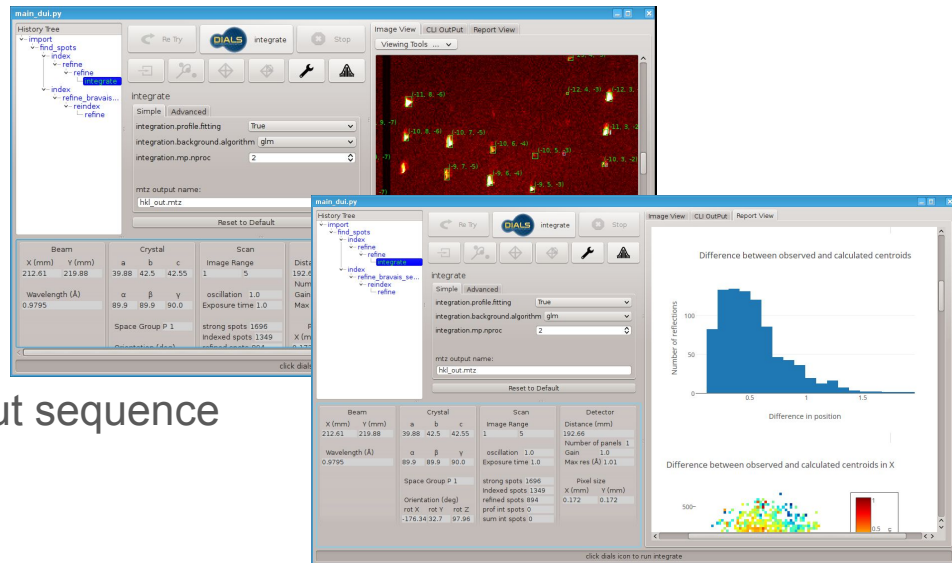
48 updates since then

Active development of

- Aimless (scaling and data analysis) (see lunchtime bytes)
- DIALS (diffraction integration) (see lunchtime bytes)
- CCP4i2 (graphical user interface) (see lunchtime bytes)
- Multi-dataset analysis (see the next talk)
- Many others (see the next talks and the lunchtime bytes)

Coming soon in CCP4

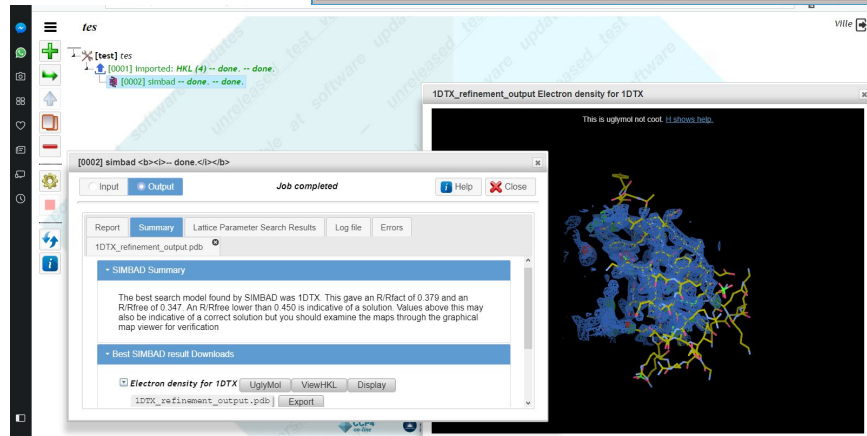
- SIMBAD - Molecular replacement without sequence
- DUI - DIALS User Interface
- jsCoFE - CCP4 on the Cloud



Check the lunchtime bytes!

Also soon(ish):

- CCP4 7.1

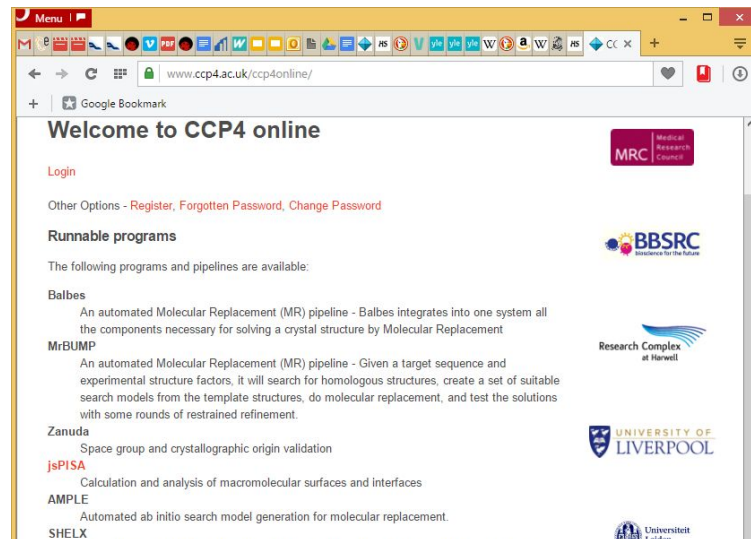


What's new in CCP4 Online?

www.ccp4.ac.uk/ccp4online

Pipelines to automated model
building with ARP/wARP

from molecular replacement
(MoRDa, MrBUMP, Balbes)



CCP4 on-line Collaborative Computational Project No. 4 Software for Macromolecular X-Ray Crystallography

Home (Logout) > Login > Programs > MoRDa > New MoRDa Run

New MoRDa Run

The file formats accepted for input are **mtz** and **cif** (structure factors) and should be pasted into the text box.

Job title (optional):
 Structure Factors:
 Target sequences:

Choose file | No file chosen
 Choose file | No file chosen
**Instead of entering a below:
 (Note that a comment sequence)**

Check alternative space groups: ☐
 Run ARP/wARP (on the MoRDa solution): ☐ Dissemination Level: World

CCP4 on-line Collaborative Computational Project No. 4 Software for Macromolecular X-Ray Crystallography

Home (Logout) > Login > Programs > MoRDa > View Results

MoRDa

Please cite the following paper, if you used a solution from MoRDa:
 A. Vagin, A. Lebedev, Acta Cryst. (2015) A71, s19

MoRDa homepage contains more details and instructions for local installation.

An ARP/wARP solution exists - click here to access your ARP/wARP results from the website in Hamburg

MoRDa has produced a solution with $Q = 0.856$.

Submit this solution to the PDB_REDO server for rebuilding and re-refinement (requires ARIA login / registration).

PROCESS 1640689083 HAS ENDED

Report | Prep | Details

- Job Details
- Input Data
- Best Solution

morda_input.png 5874409-dzone-rc-.pdf refmac_final_result_.pdb payara-micro

ARP/wARP Web Service

User: ville.uski@st

DWdLbrPocO (via Morda)
 Job-ID: 00652_99bcd6
 started: 7. Jul 2017 18:24:11 h

0.216 **0.000** **95%**
 Done R-Factor R-Free Completeness Model

FINAL RESULT	
Job started	7. Jul 2017 - 18:24:11
Job done	7. Jul 2017 - 18:39:31
Number of residues built	56
Number of chains built	1
Percent of expected residues built	94.92 %

DOWNLOADS

LOG

Logfile

PDB

Final Model

MTZ

MTZ with final phases

TAR

TAR with all files

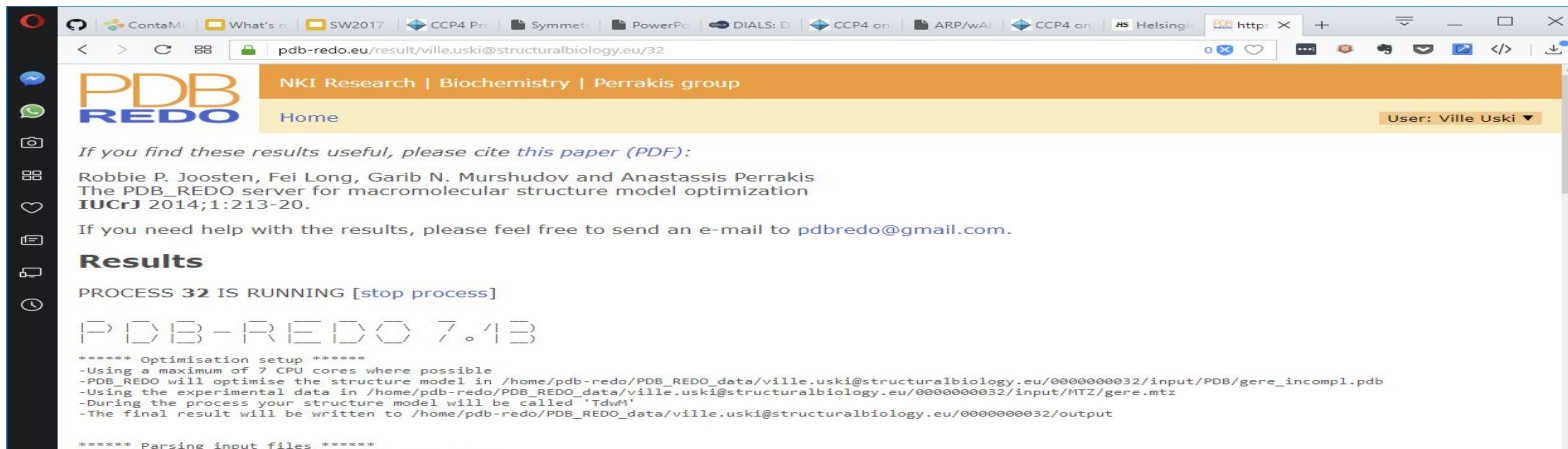
R-FACTOR VS. ITERATIONS

The R-Factor should decrease and at the end it should ideally be between 0.15 and 0.25.

Iteration	R-Factor
1	0.24
2	0.23
3	0.21
4	0.20
5	0.19
6	0.18
7	0.17
8	0.16
9	0.15
10	0.15
11	0.16
12	0.17
13	0.18
14	0.19
15	0.20
16	0.19
17	0.18
18	0.17
19	0.16
20	0.15
21	0.16
22	0.17
23	0.18
24	0.19
25	0.20
26	0.21
27	0.22
28	0.23
29	0.24
30	0.25

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- Coming very soon:
 - interface to ContaMiner (see Byte by Stefan Arold)
 - Pipeline to automated optimization with PDB_REDO



- Work in progress:
 - More computing power via European Grid Infrastructure
 - Virtual folder

CCP4 Schools/Workshops



<http://www.ccp4.ac.uk> – Courses & Events



We are pleased to announce the 1st CCP4/BGU Structure Solution Workshop, to be held at Ben-Gurion University of the Negev, in Beer-Sheba, Israel on 18-23 February 2018. The workshop program covers all aspects of structure determination such as data collection, phasing, model building, crystallographic refinement, validation, and structural analysis. Lectures and tutorials will be delivered by experts in the field, and participants will be able to work alongside world-leading scientists and methods developers on their own projects.

Full information and on-line application form found at:
<https://lifeserv.bgu.ac.il/wp/ccp4workshop/>



Coming crystallography schools

- 1st CCP4/BGU Workshop (Beer-Sheva, Israel) Feb 2018
- APS (Chicago, USA) June 2018
- São Carlos, Brazil, November 2018
- Diamond Workshop (Didcot, UK) Dec 2018

To be confirmed:

- Chandigarh, India, October 2018

Other Resources

- CCP4BB mailing list – bulletin board, news, expert help and advice
- CCP4 help desk – ccp4@ccp4.ac.uk – bug reports, problems with software
- CCP4 wiki – <http://ccp4wiki.org>
- CCP4i2 documentation and tutorials
- CCP4 web page – <http://www.ccp4.ac.uk>

Acknowledgements

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- **Leiden:** Raj Pannu, Pavol Skubak
- **Others:** Bernhard Lohkamp, Clemens Vornrhein, Ruslan Sanishvili, Frank Von Delft, Martin Noble, Jaclyn Bibby, Daniel Rigden, Jens Thomas, Alun Ashton, David Brown, Arwen Pearson, Tim Gruene, George Sheldrick, Isabel Usón, and many more..