CCP4 Cloud

for macromolecular structure determination online

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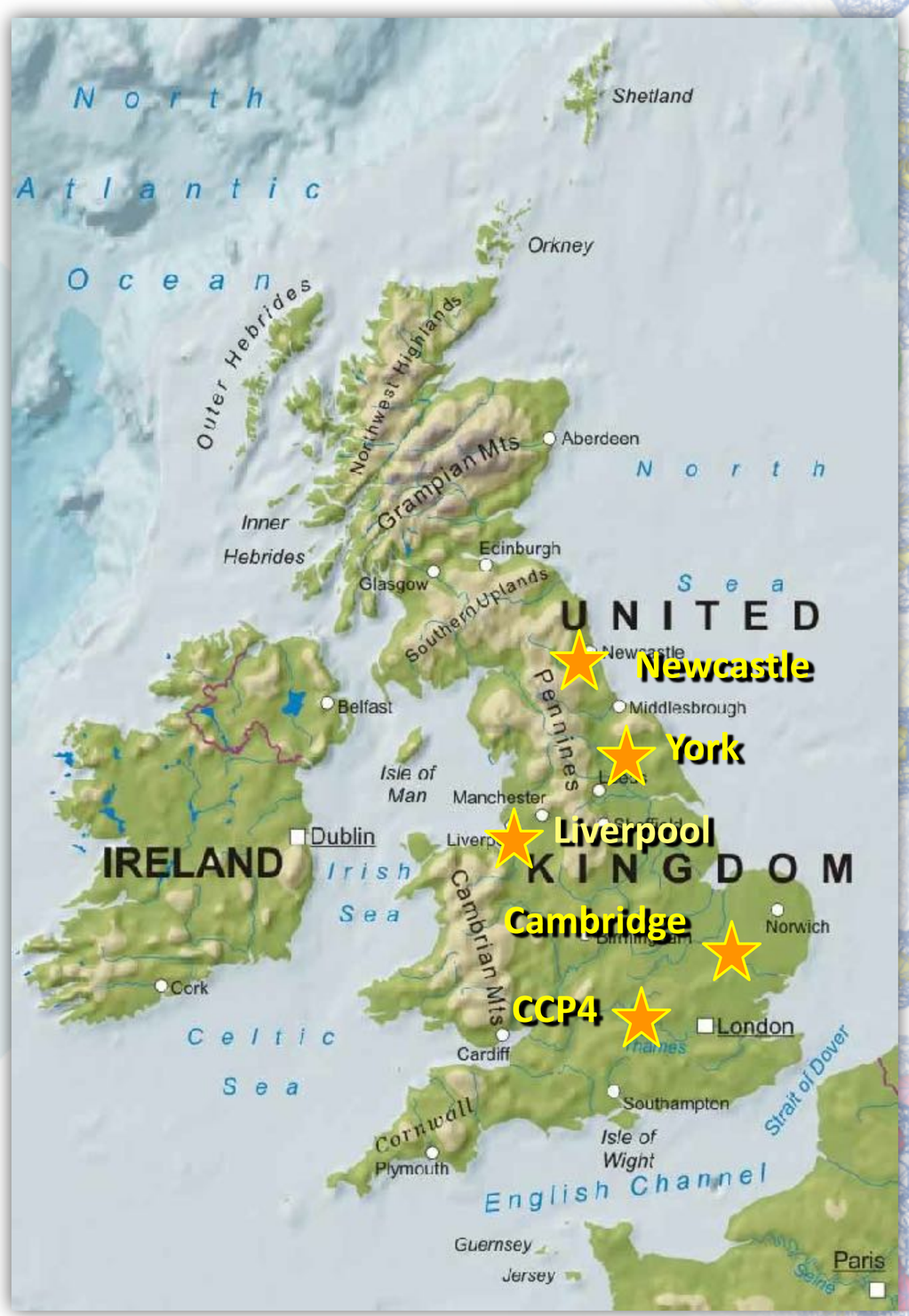
What we are

- CCP4 stands for **"Collaborative Computational Project No. 4 in Protein Crystallography"**
- One of several CCPs set up in the UK to advance and support scientific software developments
- 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 the Scientific Computing Department of STFC UK

Who we are

- Core Group @ RAL/Harwell (**Oxford**)
  - maintain and support software suite
  - application and infrastructural software developments
  - collaborate with Diamond on beam line deployment of CCP4 software and joint developments
  - educational outreach
  - maintain CCP4 resources such as the CCP4 bulletin board
- MRC/LMB (**Cambridge**)
  - data processing software (Mosflm, Aimless)
  - refinement software (Refmac)
  - model building (Coot)
- Phaser group (University of **Cambridge**)
- University of **York, Newcastle** University
  - Software developments (CCP4mg, Modelcraft, Privateer)
  - CCP4 GUI-2 developments
- Associated projects
  - Experimental Phasing from **Leiden** (Crank-2)
  - Arcimboldo MR Software (**Barcelona**)
  - Ab-initio and automatic MR, University of **Liverpool** (AMPLE)
  - Arp/wArp (EMBL-**Hamburg**)
  - SHELX (**Goettingen** and **Barcelona**)
  - PDB-Redo (NKI, the **Netherlands**)



Where we are

Science & Technology Facilities Council

Research Complex at Harwell

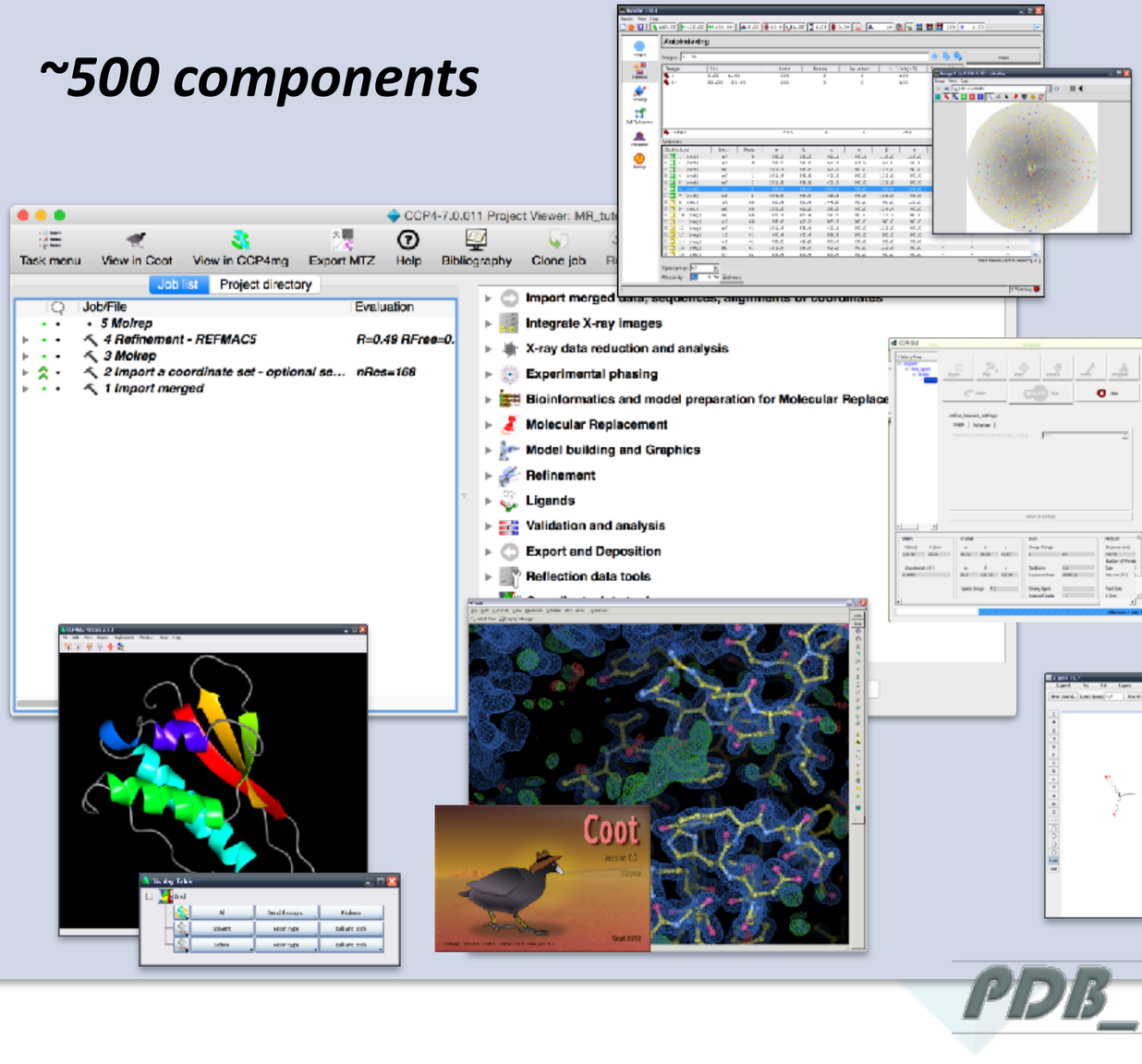
CCP4 Scope

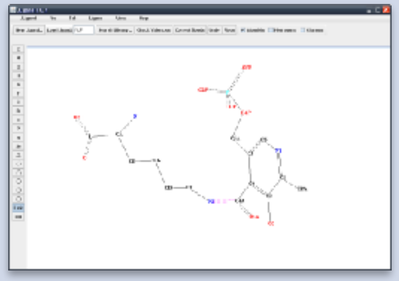
Science & Technology Facilities Council

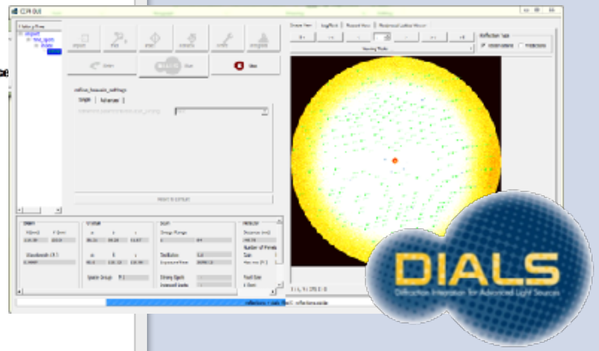
Research Complex at Harwell

Probably the largest MX Suite

~500 components







PDB_REDO

Crystallisation

Data Collection

Data Processing and Reduction

Experimental Phasing

Molecular Replacement

Density Modification

Model Building

Refinement

Structure Analysis

Deposition

SHELX

ARP wARP 7.3

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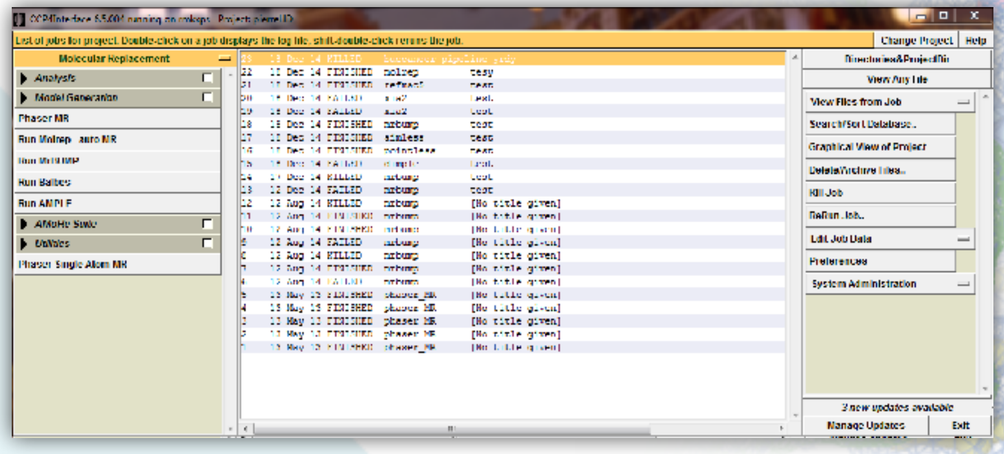
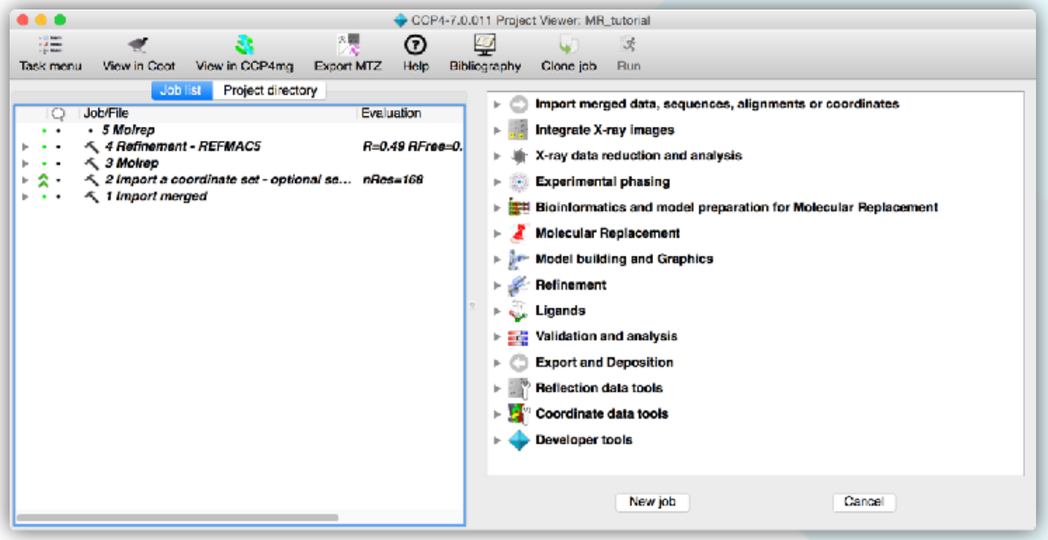
Three interfaces to the CCP4 Software Suite

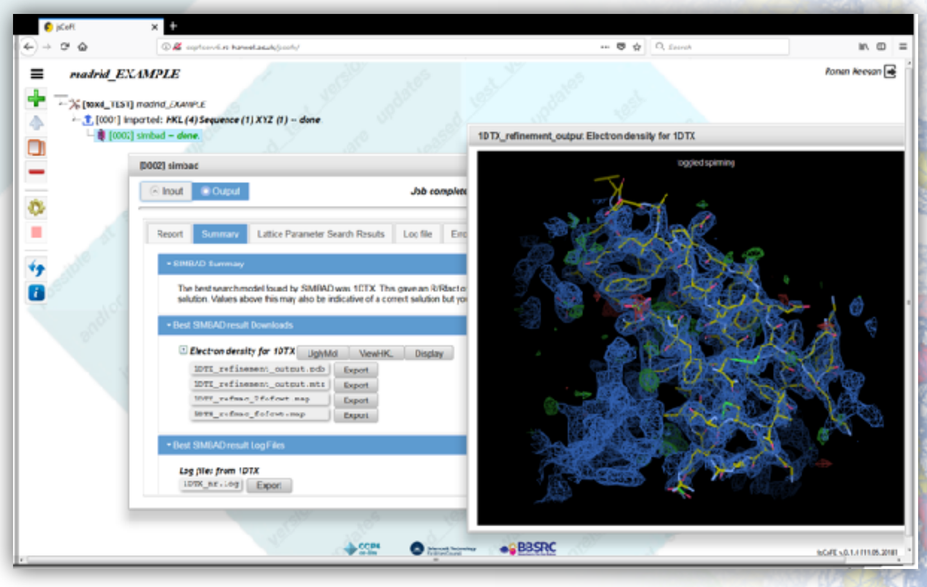
1. **CCP4i** – original interface developed around 2000 - ***discontinued***





2. **CCP4i2** – new graphical desktop interface (2016)

3. **CCP4 Cloud**, browser based (2019)



Why Cloud?

Growing software complexity

- *Supporting wide variety of computing platforms is difficult*
- *Full installation with 3rd party databases and software is difficult*

Growing software demands

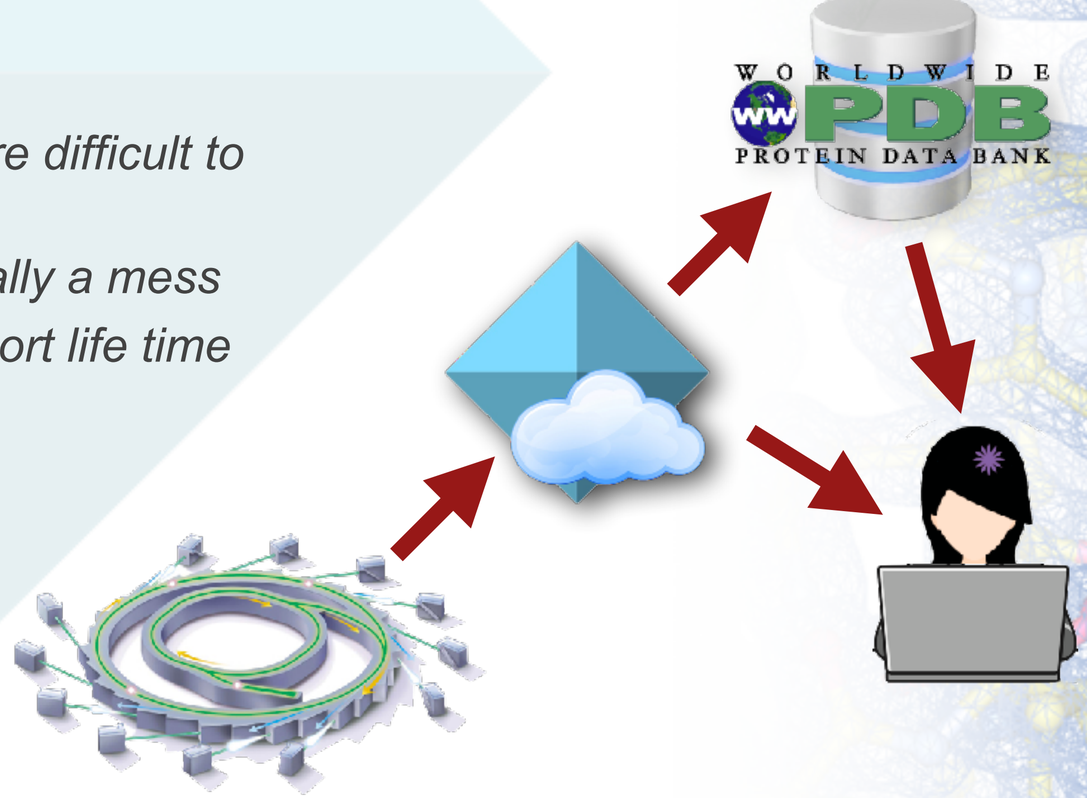
- *Modern automatic methods require more CPU and memory than most local setups can afford*

Data logistics and team working

- *Growing volumes of data from modern sources are difficult to handle locally*
- *File exchange in distributed collaborations is usually a mess*
- *Local data and project archives have usually a short life time*

Security

- *Increasingly more difficult to distribute for modern systems and corporate environments*
- *Cloud solutions are safer, getting preferential in industry*



What is CCP4 Cloud

A system for solving X-ray structures online using common web-browsers

Main features

- *Software, resources and data as a **service:** go-and-use*
- ***Cross-platform**: can be used on all Windows, Linux, Mac OSX, tablets and smartphones*
- *Rich **project development** functionality*
- ***All stages** of structures solution: from image processing to PDB deposition*
- *Integrates access to **web-resources** such as PDB and AFDB*
- *Facilitate **team work** by sharing projects in real time*
- *Can be run **locally***
- *Can be installed in a **lab, institute or firm***
- *Highly configurable and adaptable to using **mixed distributed computational resources***
- *Integrated documentation and tutorials*

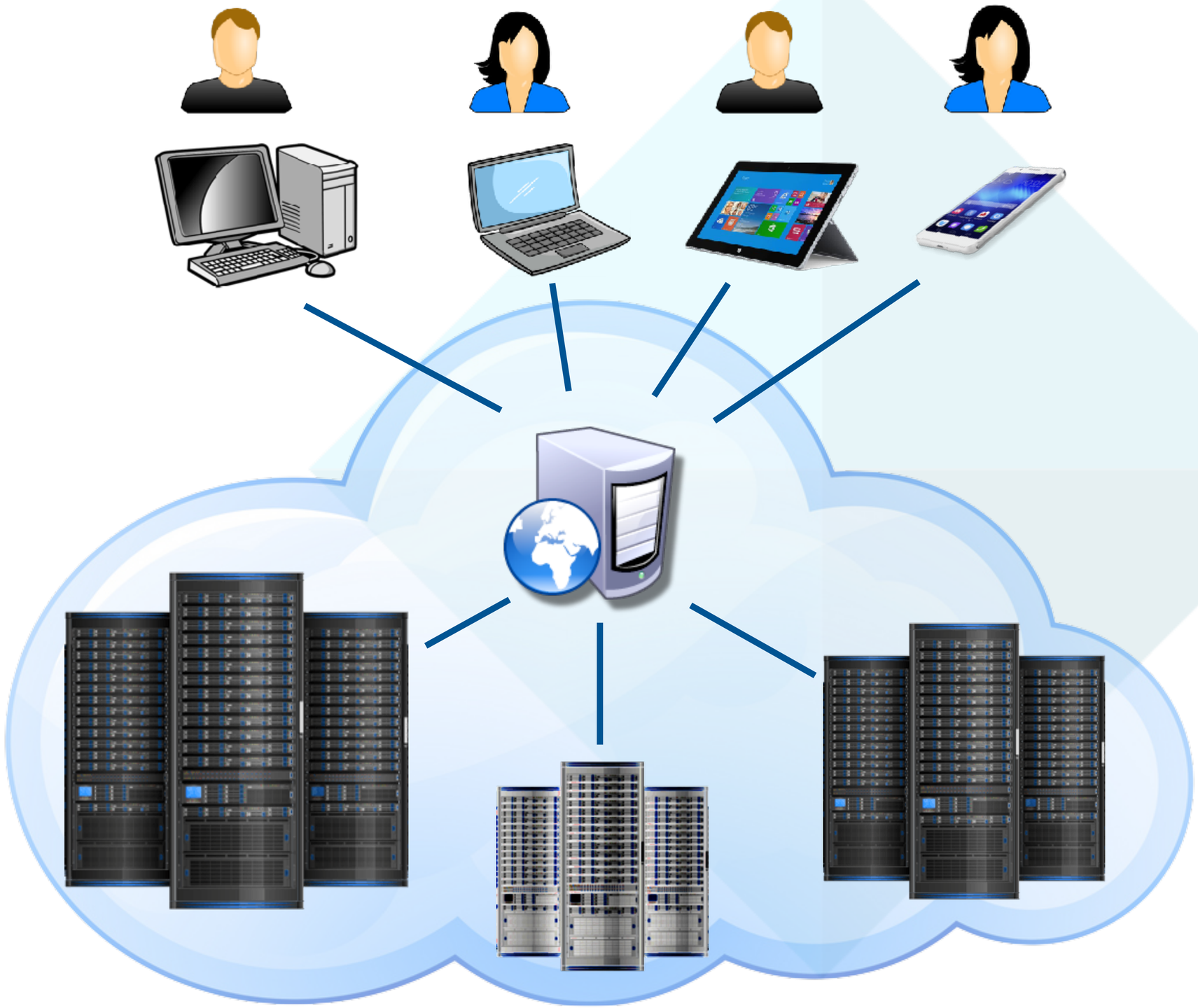
Current limitation

- *Local installation of CCP4 is required for using Coot and some other desktop applications*

Availability

- *Publicly available at https://cloud.ccp4.ac.uk*
- *Part of standard CCP4 distribution package starting from 7.1 release series (since June 2020)*

The Grand Idea



work anywhere

with anything

get power from the Cloud

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Look around CCP4 Cloud

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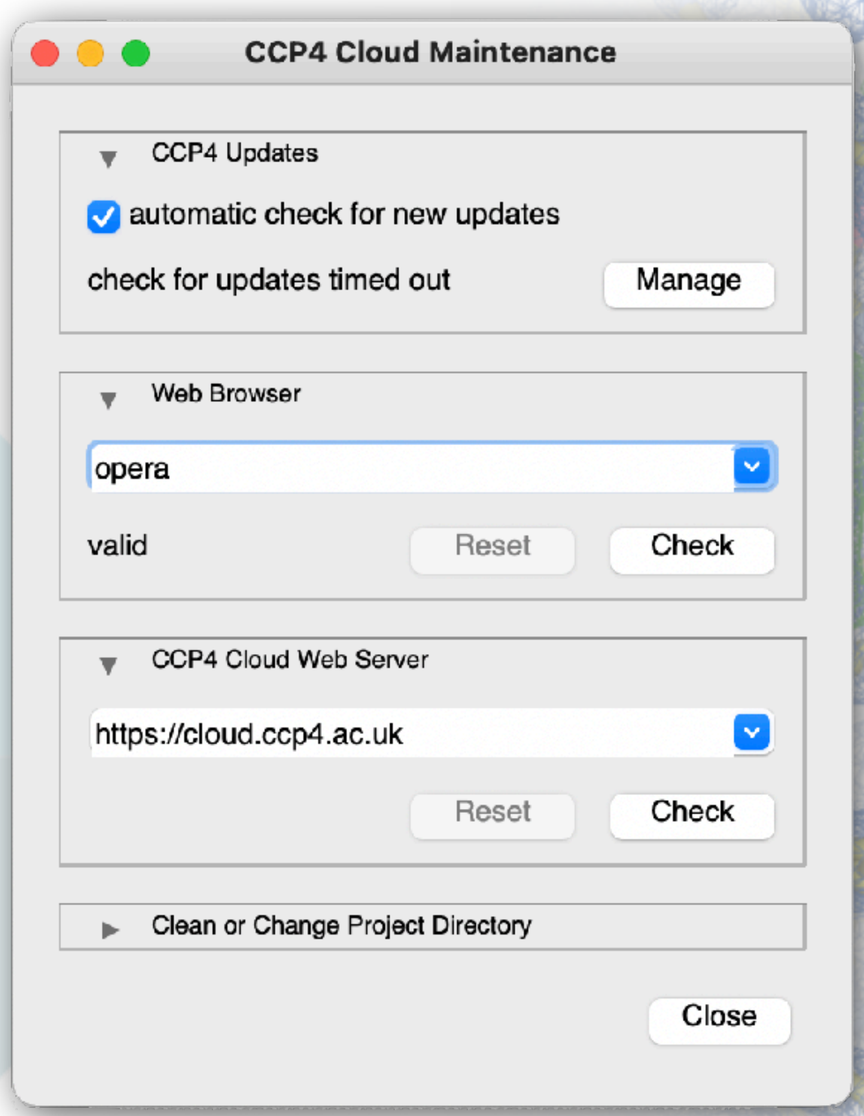
Start right!

CCP4 Cloud icons in CCP4 7.1+ setup

CCP4 Cloud
on your machine
(no internet)

CCP4 Cloud
on remote servers

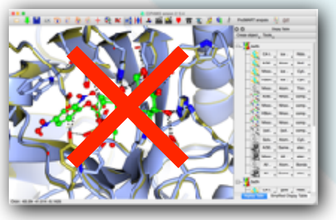
CCP4 Cloud
configurator/
maintainer



If started from direct URL *https://cloud.ccp4.ac.uk*:

No Coot

No DUI



No CCP4mg

Only direct URL
(no local CCP4)

CCP4 Cloud

localhost:51253

CCP4 Cloud Login

CCP4-Harwell

https://cloud.ccp4.ac.uk/

Login name: sbgrid-demo

Password: •••••

Login

Forgotten password

Registration

Check CCP4 Cloud roadmap for new users

Privacy Statement

Did you know? Crashed Coot task does not mean that your work is lost! Read here.

CCP4 Cloud

localhost:51253

My Projects

0% 0%:0% SBGrid Demo

Open | Add | Rename | Delete | Export | Import | Join | Tutorials | Help

ID	Name	R_{free}	Disk (MBytes)	CPU (hours)	Date Created	Last Opened

Your List of Projects is currently empty.

Use "Add" button to create a new Project;
"Import" button for importing a project exported from CCP4 Cloud;
"Join" button for joining project shared with you by another user;
or "Tutorials" button for loading tutorial/demo projects.

CCP4 Cloud

localhost:51253

My Projects

0% 0%:0% SBGrid Demo

My Account

Toggle fullscreen

Log out

Add | Rename | Delete | Export | Import | Join | Tutorials | Help

	R_{free}	Disk (MBytes)	CPU (hours)	Date Created	Last Opened

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CCP4 Cloud

localhost:51253

0% 0%:0% SBGrid Demo

My Account

CCP4-Harwell

https://cloud.ccp4.ac.uk/

User name:	SBGrid Demo
E-mail:	eugene.krissinel@stfc.ac.uk
Login name:	sbgrid-demo
Password:	password (old or new)
Retype password:	confirm password
Licence agreement:	academic
Feedback agreement:	accepted (1)
Software authorisations:	manage

Save changes

Delete my account

Preferences*

On login, go to: list of projects

Initial size (% of browser window):

	width	height
Job dialogs:	125	85
Viewers:	140	97

- [ ] Use project name as default file prefix
- [x] Guide through data import
- [x] Send end-of-job notifications

for jobs taking longer than 24 hours

* Save changes for Preferences to take an effect

CCP4 Cloud

localhost:51253

0% 0%:0% SBGrid Demo

My Account

CCP4-Harwell

https://cloud.ccp4.ac.uk/

User name:	SBGrid Demo
E-mail:	eugene.krissinel@stfc.ac.uk
Login name:	sbgrid-demo
Password:	password (old or new)
Retype password:	confirm password
Licence agreement:	academic
Feedback agreement:	accepted (1)
Software authorisations:	manage

Save changes

Delete my account

Preferences*

Software Authorisations

Software Authorisations

CCP4 Cloud provides access to 3rd party software, not covered by CCP4 license. In order to use this software, a user needs to be authorised by the corresponding software provider. This page gives a summary of your authorisations and allows you to send authorisation requests. Note that authorisation request will redirect you to the provider's web-site. Any data requested by software provider will be processed at provider's end and will not be stored in CCP4 Cloud.

Software:	GΦL	Global Phasing Ltd. Software Suite
Provider:	GΦL	Global Phasing Ltd.
Authorisation:	***not authorised***	request authorisation

Close

0% 0%:0% SBGrid Demo

Resource	Used	Quota	%%
Storage (MBytes)	0	5000	0%
CPU 24h (hours)	0	24	0%
CPU 30d (hours)	0	240	0%

User stats:

Total storage used (MBytes)	*0*
Total jobs run	*0*
CPU lifetime used (hours)	*0*

My Account

CCP4-Harwell

https://cloud.ccp4.ac.uk/

User name:	*SBGrid Demo*
E-mail:	*eugene.krissinel@stfc.ac.uk*
Login name:	*sbgrid-demo*
Password:	*password (old or new)*
Retype password:	*confirm password*
Licence agreement:	academic
Feedback agreement:	accepted (1)
Software authorisations:	manage

Save changes

Delete my account

*Preferences**

On login, go to: list of projects

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for jobs taking longer than 24 *hours*

* *Save changes for Preferences to take an effect*

CCP4 Cloud

localhost:51253

My Projects

0% 0%:0% SBGrid Demo

Open | Add | Rename | Delete | Export | Import | Join | Tutorials | Help

ID	Name	R_{free}	Disk (MBytes)	CPU (hours)	Date Created	Last Opened

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CCP4 Cloud

localhost:51253

My Projects

0% 0%:0% SBGrid Demo

Open | Add | Rename | Delete | Export | Import | Join | Tutorials | Help

ID	Name	R_{free}	Disk (MBytes)	CPU (hours)	Date Created	Last Opened

Add New Project

ID *mdm2*

Name *MDM2 Protein with bound Nutlin Molecule*

Initialisation mode

- **Autostart** — *Simplified mode for starting with one of automatic workflows featuring structure solution scenarios in CCP4 Cloud, and optimised list of essential tasks for structure completion (can be switched to the full list).*
- **Standard** — *Standard mode for operating all CCP4 Cloud tasks manually, with access to the full list of tasks by default.*
- **Hop on** — *Quick start from phased (possibly partially built and refined) structure or heavy-atom substructure, for further refinement and model building, with the optimised list of essential tasks for structure completion (can be switched to the full list).*

Add Project | Cancel

Demo Drive:

Automatic Structure Solution

Why Automate?

Avoid the routine

- *Similar targets → similar data → similar actions*

Save personal time

- *"Start-and-forget"*

Mitigate incompetence

- *Decision making in complex projects and workflows (**strategy**)*
- *Choose the right tool for the task (**tactics**)*
- *Cope with multiple options (**ambiguity**)*
- *Choose right parameters (**expertise**)*

The result

- *Works in standard cases (no crystal pathologies, good diffraction, close templates)*
- *May give further ideas even if fails*

Automation Level 1: Pipelines (super-scripts)

Image Processing

Xia-2

Experimental Phasing

Crank-2

Molecular Replacement

BALBES

MoRDa

MrBump

Simbad

Slicendice

Arcimboldo

Model Building

Buccaneer

Arp/wArp

CCP4Build

Nautilus

Modelcraft

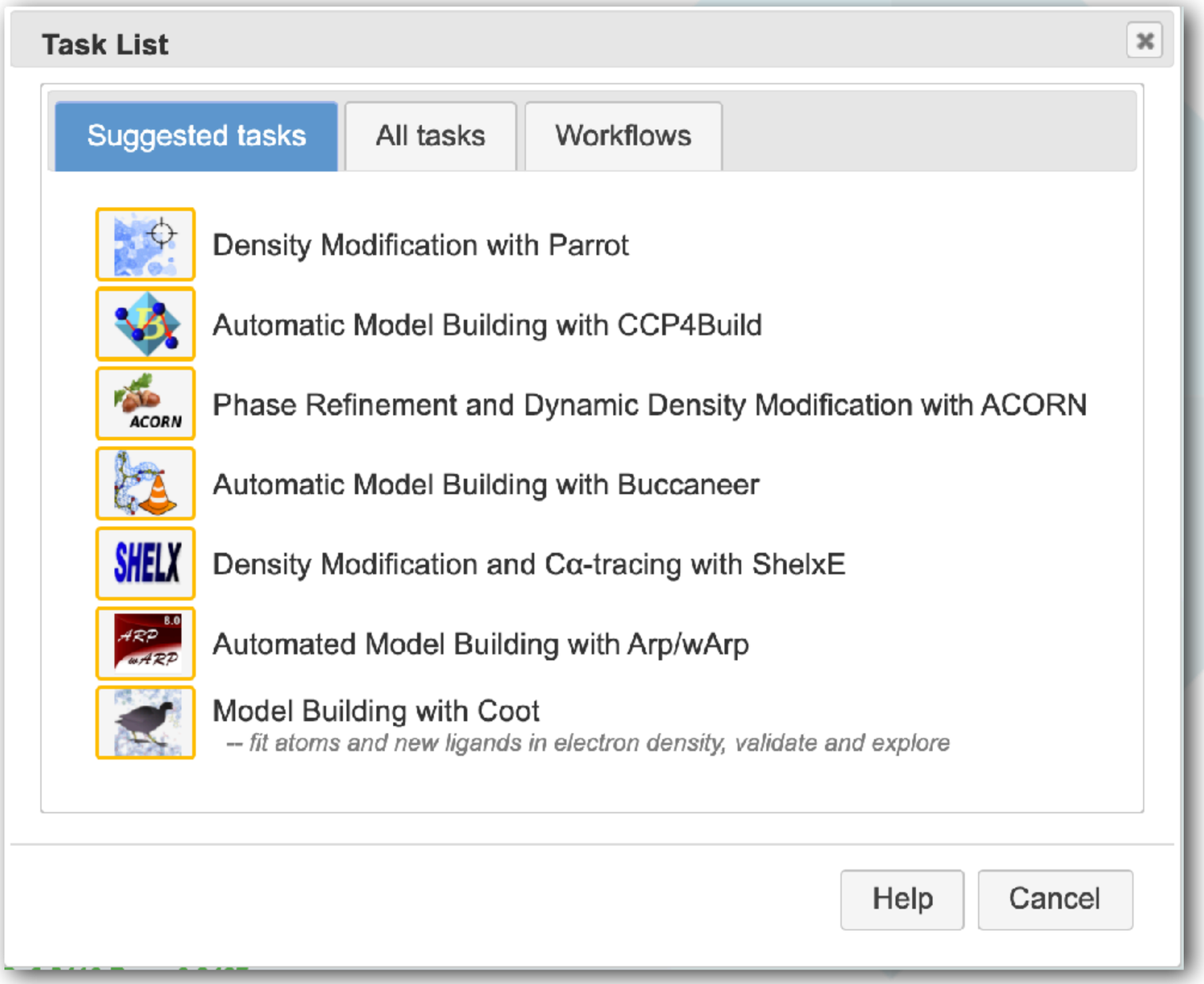
Refinement and Validation

LORESTR

DIMPLE

Zanuda

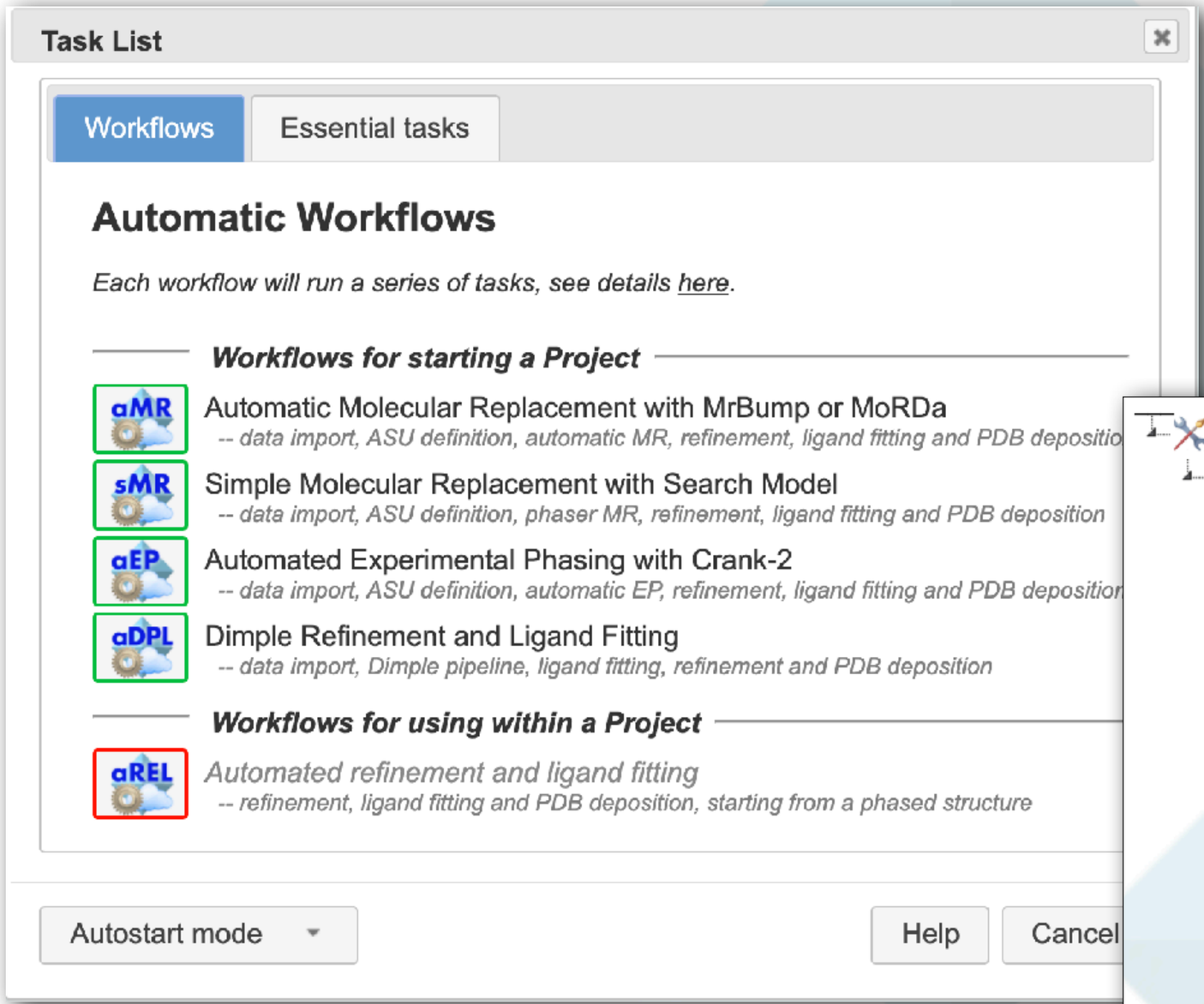
Automation Level 2: Project Navigation

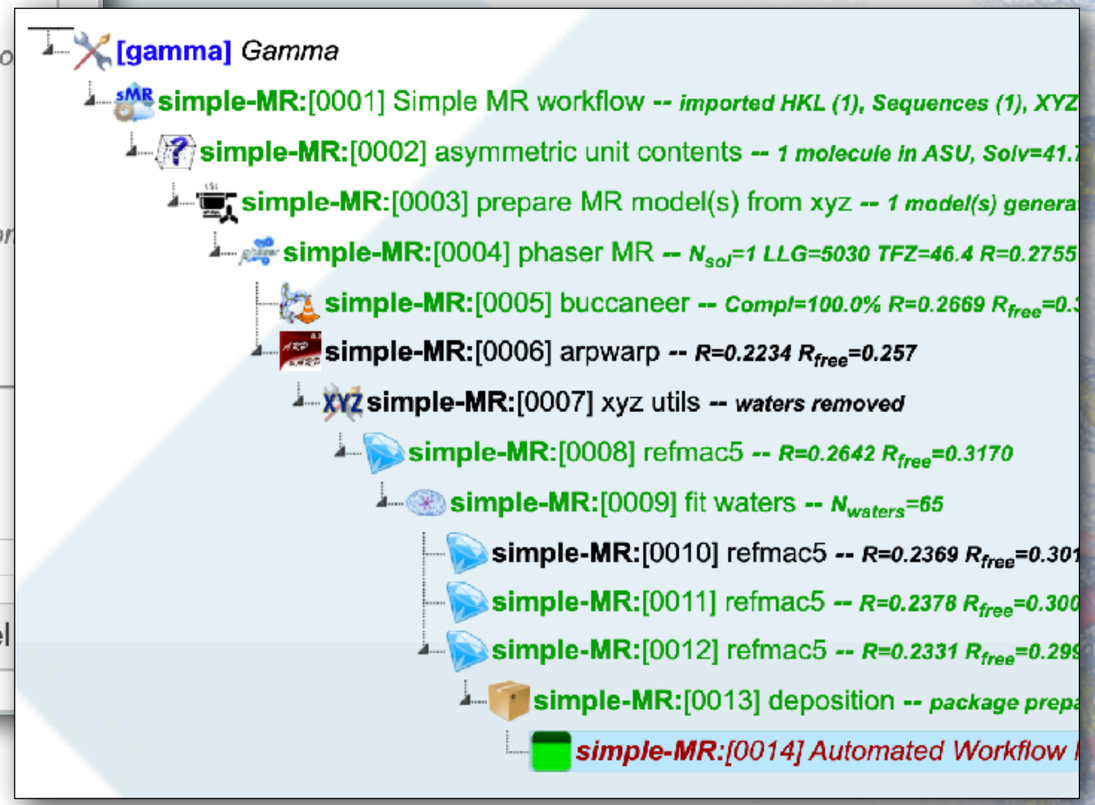


Intelligent next step suggestions based on in-built logics of project development and analysis of user actions

CCP4 Cloud learns your habits as you go …

Automation Level 3: Project Development





Automatic development of structure solution projects based on available data and their properties

CCP4 Cloud

localhost:51253

My Projects

0% 5%:1% SBGrid Demo

Open | Add | Rename | Delete | Export | Import | Join | Tutorials | Help

ID	Name	R_{free}	Disk (MBytes)	CPU (hours)	Date Created	Last Opened

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Introduction in CCP4 Cloud Projects

CCP4 Cloud

localhost:51253

MDM2 Protein bound to Nutlin 3A

4% 5%:1% SBGrid Demo

Add new job

Clone selected job

Delete selected job

Collapse long branch in folder

Add remark

Highlight current branch

Toggle multiple job selection

Open job

Stop job

Reload project

Help

Structure solution roadmap

Data transfer

Branching

2 Protein bound to Nutlin 3A

] Simple MR workflow -- *Imported Unmerged, Sequences (1), XYZ (1), Ligands (1); workflow started*

002] aimless -- *Compl=75.8% $CC_{1/2}$=0.998 R_{meas_all}=0.070 R_{meas_ano}=0.068 Res=1.25-61.93 SpG=P 61 2 2*

0003] asymmetric unit contents -- *1 molecule in ASU, Solv=64.7%*

:[0004] prepare MR model(s) from xyz -- *1 model(s) generated (molrep protocol)*

] phaser MR -- *N_{sol}=1 LLG=411 TFZ=22.0 R=0.5050 R_{free}=0.5027 SpG=P 65 2 2*

simple-MR:[0006] refmac5 -- *R=0.3880 R_{free}=0.4058*

simple-MR:[0007] buccaneer -- *Compl=100.0% R=0.3253 R_{free}=0.3478*

***simple-MR:**[0008] Large parts of the structure are likely missing as Rfree is only 0.406 (click for more comments)*

ple-MR:[0009] arpwarp -- *R=0.2742 R_{free}=0.288*

e-MR:[0010] xyz utils -- *waters removed*

nple-MR:[0011] refmac5 -- *R=0.3141 R_{free}=0.3331*

simple-MR:[0012] refmac5 -- *R=0.3141 R_{free}=0.3333*

simple-MR:[0013] refmac5 -- *R=0.3116 R_{free}=0.3325*

simple-MR:[0014] make ligand -- *ligand "00E" prepared*

simple-MR:[0015] fit ligand -- *N_{fitted}=1*

simple-MR:[0016] refmac5 -- *R=0.2801 R_{free}=0.3041*

simple-MR:[0017] fit waters -- *N_{waters}=62*

simple-MR:[0018] refmac5 -- *R=0.2501 R_{free}=0.2775*

simple-MR:[0019] refmac5 -- *R=0.2508 R_{free}=0.2777*

simple-MR:[0020] refmac5 -- *R=0.2517 R_{free}=0.2776*

simple-MR:[0021] deposition -- *package prepared, pdb report obtained*

***simple-MR:**[0022] Automated Workflow has finished succesfully (look inside for comments)*

MDM2 Protein bound to Nutlin 3A

- **[mdm2]** *MDM2 Protein bound to Nutlin 3A*
  - **simple-MR:**[0001] Simple MR workflow -- *imported Unmerged, Sequences (1), XYZ (1), Ligands (1); workflow started*
    - **simple-MR:**[0002] aimless -- *Compl=75.8% $CC_{1/2}$=0.998 R_{meas_all}=0.070 R_{meas_ano}=0.068 Res=1.25-61.93 SpG=P 61 2 2*
      - **simple-MR:**[0003] asymmetric unit contents -- *1 molecule in ASU, Solv=64.7%*
        - **simple-MR:**[0004] prepare MR model(s) from xyz -- *1 model(s) generated (molrep protocol)*
          - **simple-MR:**[0005] phaser MR -- *N_{sol}=1 LLG=411 TFZ=22.0 R=0.5050 R_{free}=0.5027 SpG=P 65 2 2*
            - **simple-MR:**[0006] refmac5 -- *R=0.3880 R_{free}=0.4058*
              - **simple-MR:**[0007] buccaneer -- *Compl=100.0% R=0.3253 R_{free}=0.3478*
              - ***simple-MR:****[0008] Large parts of the structure are likely missing as Rfree is only 0.406 (click for more comments)*
              - **simple-MR:**[0009] arpwarp -- *R=0.2742 R_{free}=0.288*
                - **simple-MR:**[0010] xyz utils -- *waters removed*
                  - **simple-MR:**[0011] refmac5 -- *R=0.3141 R_{free}=0.3331*
                    - **simple-MR:**[0012] refmac5 -- *R=0.3141 R_{free}=0.3333*
                      - **simple-MR:**[0013] refmac5 -- *R=0.3116 R_{free}=0.3325*
                        - **simple-MR:**[0014] make ligand -- *ligand "00E" prepared*
                          - **simple-MR:**[0015] fit ligand -- *N_{fitted}=1*
                            - **simple-MR:**[0016] refmac5 -- *R=0.2801 R_{free}=0.3041*
                              - **simple-MR:**[0017] fit waters -- *N_{waters}=62*
                                - **simple-MR:**[0018] refmac5 -- *R=0.2501 R_{free}=0.2775*
                                - **simple-MR:**[0019] refmac5 -- *R=0.2508 R_{free}=0.2777*
                                - **simple-MR:**[0020] refmac5 -- *R=0.2517 R_{free}=0.2776*
                                  - **simple-MR:**[0021] deposition -- *package prepared, pdb report obtained*
                                    - ***simple-MR:****[0022] Automated Workflow has finished succesfully (look inside for comments)*

MDM2 Protein bound to Nutlin 3A

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                                - **simple-MR:**[0018] refmac5 -- *R=0.2501 R_{free}=0.2775*
                                - **simple-MR:**[0019] refmac5 -- *R=0.2508 R_{free}=0.2777*
                                - **simple-MR:**[0020] refmac5 -- *R=0.2517 R_{free}=0.2776*
                                  - **simple-MR:**[0021] deposition -- *package prepared, pdb report obtained*
                                    - ***simple-MR:**[0022] Automated Workflow has finished succesfully (look inside for comments)*
                                  - [0024] coot (model building) -- *model saved*
                                    - [0025] refmac5 -- *R=0.2484 R_{free}=0.2742*

MDM2 Protein bound to Nutlin 3A

- **simple-MR:**[0017] fit waters -- N_{waters}=62
  - **simple-MR:**[0018] refmac5 -- R=0.2501 R_{free}=0.2775
  - **simple-MR:**[0019] refmac5 -- R=0.2508 R_{free}=0.2777
  - **simple-MR:**[0020] refmac5 -- R=0.2517 R_{free}=0.2776
    - **simple-MR:**[0021] deposition -- *package prepared, pdb report obtained*
      - ***simple-MR:****[0022] Automated Workflow has finished succesfully (look inside for comments)*
    - [0024] coot (model building) -- *model saved*
      - [0025] refmac5 -- R=0.2484 R_{free}=0.2742
- **simple-MR:**[0026] aimless -- *Compl=99.0% $CC_{1/2}$=0.998 R_{meas_all}=0.057 R_{meas_ano}=0.058 Res=1.5-61.92 SpG=P 61 2 2*
  - **simple-MR:**[0027] asymmetric unit contents -- *1 molecule in ASU, Solv=64.6%*
    - **simple-MR:**[0028] prepare MR model(s) from xyz -- *1 model(s) generated (molrep protocol)*
      - **simple-MR:**[0029] phaser MR -- N_{sol}=1 *LLG=400 TFZ=21.8 R=0.5036 R_{free}=0.5580 SpG=P 65 2 2*
        - **simple-MR:**[0030] refmac5 -- R=0.3906 R_{free}=0.4272
          - **simple-MR:**[0031] buccaneer -- *Compl=100.0% R=0.3261 R_{free}=0.3604*
            - ***simple-MR:****[0032] Large parts of the structure are likely missing as Rfree is only 0.427 (click for more comments)*
            - **simple-MR:**[0033] arpwarp -- R=0.2623 R_{free}=0.289
              - **simple-MR:**[0034] xyz utils -- *waters removed*
                - **simple-MR:**[0035] refmac5 -- R=0.3047 R_{free}=0.3261
                - **simple-MR:**[0036] refmac5 -- R=0.3049 R_{free}=0.3274
                - **simple-MR:**[0037] make ligand -- *ligand "00E" prepared*
                - **simple-MR:**[0038] fit ligand -- N_{fitted}=1
                - **simple-MR:**[0039] refmac5 -- R=0.2692 R_{free}=0.2850
                - **simple-MR:**[0040] fit waters -- N_{waters}=67
                - **simple-MR:**[0041] refmac5 -- R=0.2351 R_{free}=0.2622
                - **simple-MR:**[0042] refmac5 -- R=0.2034 R_{free}=0.2560
                - **simple-MR:**[0043] refmac5 -- R=0.2047 R_{free}=0.2556
                - **simple-MR:**[0044] refmac5 -- R=0.2068 R_{free}=0.2571
                - **simple-MR:**[0045] deposition -- *package prepared, pdb report obtained*
                - ***simple-MR:****[0046] Automated Workflow has finished succesfully (look inside for comments)*

CCP4 Cloud

localhost:51253

My Projects

8% 0%:2% SBGrid Demo

Open | Add | Rename | Delete | Export | Import | Join | Tutorials | Help

ID	Name	R_{free}	Disk (MBytes)	CPU (hours)	Date Created	Last Opened
mdm2	MDM2 Protein bound to Nutlin 3A	0.2556	380.4	2.4482	2022-01-21	2022-01-25

- Open
- Rename
- Delete
- Export
- Share

Share Project

Share Project "mdm2"

The following users:

login1,login2,...

can join this project and work on it simultaneously.

** Full (comma-separated) list of users with access to the project must be given. In order to unshare project with a user, remove their login name from the list.*

Apply | Cancel

My Projects

Open | Add | Rename | Delete | Export | Import | Join | Tutorials | Help

ID	Name	R_{free}	Disk (MBytes)	CPU (hours)	Date Created	Last Opened
mdm2-1	MDM2	0.287	114.7	0.1252	2022-01-15	2022-01-24
cd44	CD44: Auto-EP with Crank-2		0	0	2022-01-12	2022-01-12
[*sw-2022*]:gamma-af	Solving Gamma protein with alphafold models		*125.5*	*1.7625*	2022-01-06	2022-01-19
[*paul.bond*]:bugs	Testing for bugs			*0.2239*	2021-12-10	2022-01-04
[*maximeoef*]:project_Jari	JW05			*74.912*	2021-12-09	2021-12-13
rnase-script	DIMPLE from script			0.3548	2021-11-24	2021-11-26
gamma	Gamma			0.9806	2021-11-18	2022-01-20
docs	Documentation			0	2021-11-16	2021-11-16
T2_001	Creating Molecular Replacement			0.0005	2021-11-01	2022-01-12
[*fabi.sm*]:hGST	hGST			*33.7089*	2021-09-28	2021-10-13
[*Karthi*]:006	ROQ_112			*6.783*	2021-09-27	2021-11-12
CatV-PCI3-1	CatV-PCI3 Rescued			0.0381	2021-09-23	2021-09-24
[*ed.lowe*]:cd44-rec	CD44 recovery project			*0.1015*	2021-09-09	2022-01-12
MR-prac	Molecular Replacement Practical			0.0043	2021-08-20	2021-10-03
test	Installation Test			13.8841	2021-08-16	2022-01-18
[*nicholls*]:HemeTest	HemeTest			*0.0761*	2021-08-10	2022-01-21
[*Afshan*]:MBRWT	2.37_AUTOSELECT	0.1984	*9639.9*	*16.2544*	2021-08-10	2022-01-12
bl	Beta-lactamase		127.8	0.295	2021-07-28	2021-08-24
gdemo	Gamma demo to check parallel workflowing	0.2452	711.5	6.2086	2021-07-13	2021-11-15
[*bwithd*]:Demo	Demo	0.241	*570.2*	*2.8235*	2021-07-11	2021-12-16
[*andrey_aps*]:mdm2-2	mdm2	0.2915	*296*	*1.4473*	2021-07-02	2021-09-22
masha	Masha's data	0.5164	3432.7	164.3537	2021-06-24	2021-07-24
pisa	PISA		64.6	0.0062	2021-06-24	2021-06-24
SodM_Fraglites_060521	SodM_Fraglites_060521 initiated by script		10.9	0.0006	2021-06-01	2022-01-11

Join Shared Project

Join Shared Project

Select a project to join:

sbgrid-demo:[mdm2] "MDM2 Protein bound to Nutlin 3A"

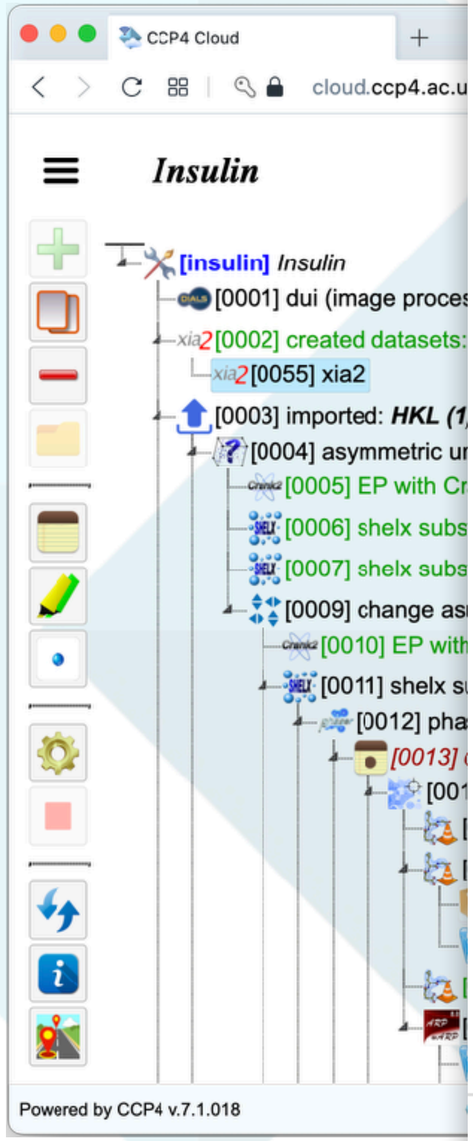
Join

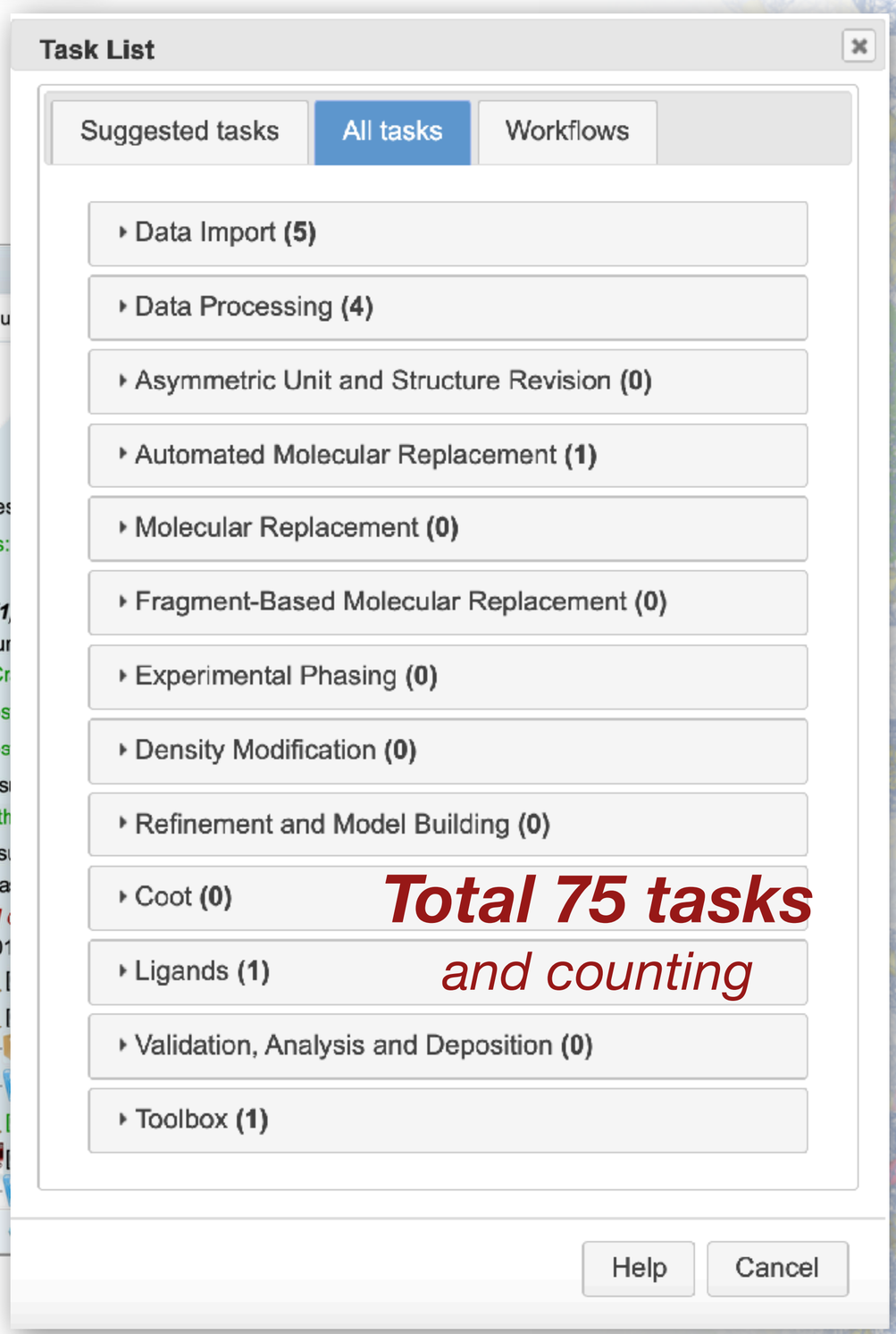
Cancel

Final Remarks

Scope of Tasks

- ✓ Image Processing
- ✓ Data Scaling and Merging
- ✓ Molecular Replacement
- ✓ Experimental Phasing
- ✓ Density Modification
- ✓ Model Building
- ✓ Ligand fitting
- ✓ Refinement
- ✓ Validation
- ✓ PDB Deposition





Development is largely finished, but not completed ...

- new tasks are being added on demand
- most of functionality is developed as addition to existing tasks, *e.g.*,
  - *no task for Patterson maps - they are calculated as part of data import*
  - *no task for peak finding - done automatically at every refinement*
- the overall scope is equivalent to desktop solutions

~

Documentation

Online Help

11.1. REFMAC5

Early stages (e.g. straight after MR)

- Run many cycles (up to 200 with jelly body restraints) of refinement

Medium stages – during model building

- 10-20 cycles
- Optimise additional parameters like NCS, TLS, etc
- Once your Rfree is lower than 40%, turn on twinning if twinned

Warning

DON'T USE TWIN REFINEMENT IF YOUR Rfree IS HIGHER THAN 40%!

- Play with geometry weight parameter

Final stages of refinement

Back | Forward | Return | Detach | Close

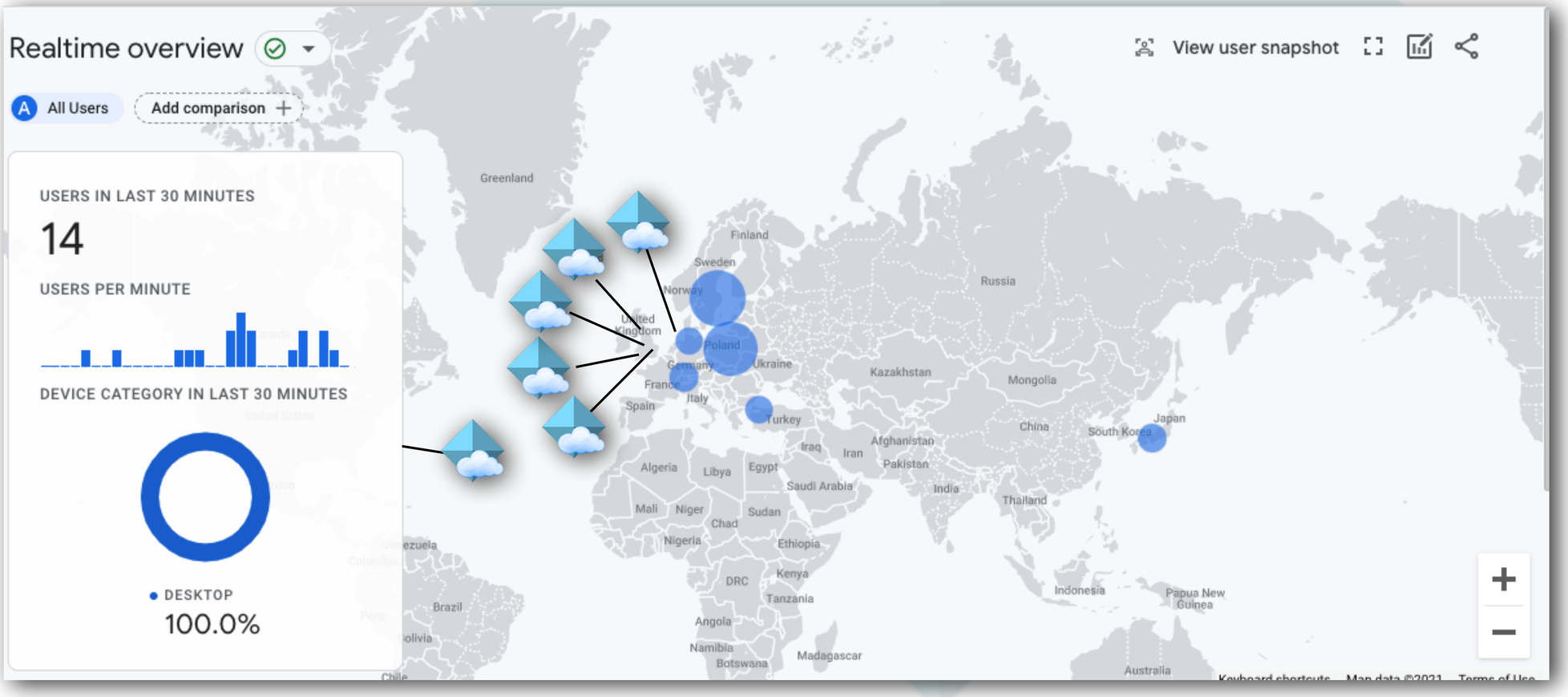
- Task Reference and User's Guide
- Integrated
- Cross-linked
- Demo projects and data
- Tutorials
- Designed for self-learning and using at Schools, Workshops and Courses
- Open for additions and corrections

GitLab

Contribution by Maria Fando

CCP4 Clouds are many

- Main CCP4 Cloud instance at CCP4-Harwell from 2018:
  - *Over 3,000 user accounts*
  - *Over 70,000 jobs/year*
- 5 CCP4 Cloud instances at partner sites, including industrial sector



RAL-Harwell

EMBL-Hamburg

Crick-London

Uni Newcastle

Uni Exeter

Pharma USA

To Cloud or Not To Cloud?

Why to Cloud? Easy:

Megaflops, Gigabytes, nothing to setup (go-and-use),
no maintenance, data backup,
24/7 from any device and anywhere! Forever!

** and **free** for you (CCP4 Cloud only)*

** and it is **green** (save our environment!)*

Today, it is trickier to say why not …

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~300 test users *Worldwide* — *Trial use and feedback on development versions of CCP4 Cloud*

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Grzegorz Chojnowski *EMBL-Hamburg*
Arnaud Basle *Newcastle University*
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— *Setup and maintenance of CCP4 Cloud instances in their home labs*

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