

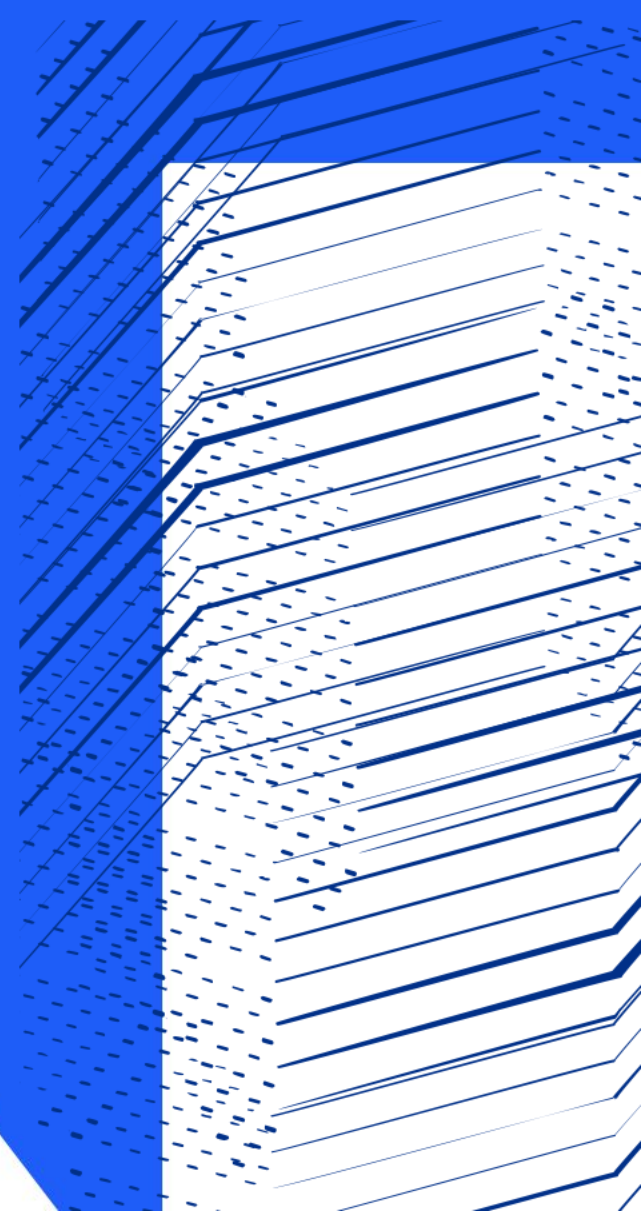


Science and
Technology
Facilities Council



Working Group 1 2025

CCP-EM Group
1 May 2025
Online



CCP-EM WG1: Agenda

1. Welcome to new members
2. Election of Chair and Deputy Chair
3. Overview of CCP-EM software
4. Training
5. Spring Symposia 2025 / 2026
6. Grant renewal update
7. AOB



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Medical
Research
Council



Research Complex
at Harwell



University of
Pittsburgh

Department for
Science, Innovation
& Technology

GΦL
Global Phasing Limited

ada lovelace centre

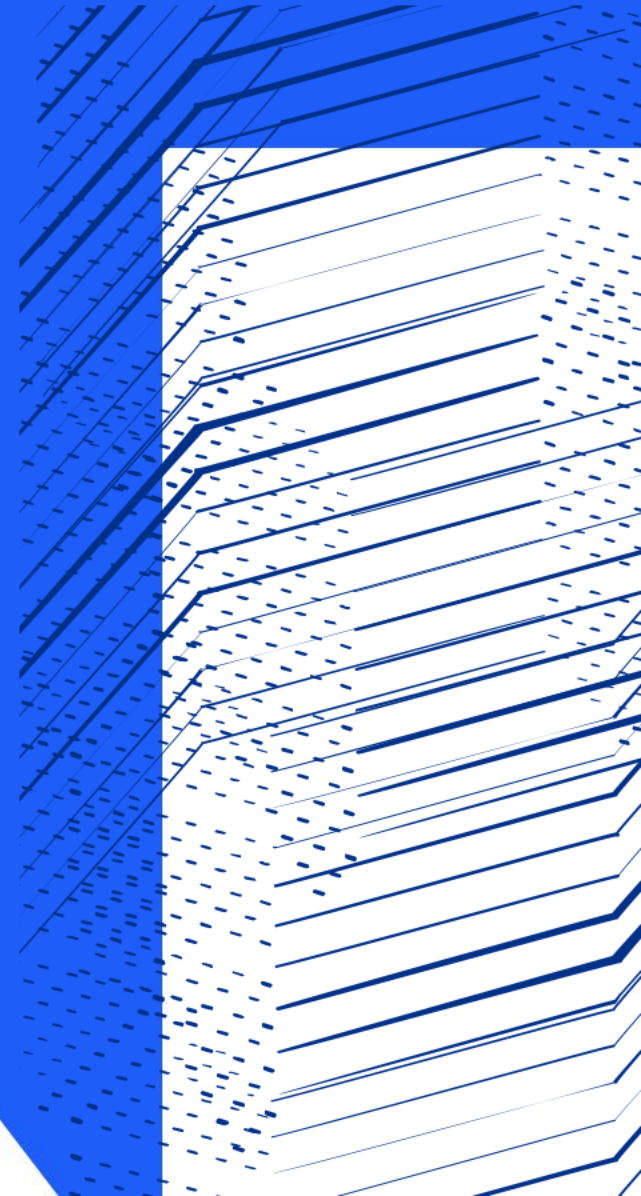
CoSec



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Welcome to new members



Welcome to new members

Executive Group



Provides day-to-day management, sets policies, and approves new collaborations or software.

Chair and Deputy



Provide leadership and represent the project to external stakeholders

Working Group 1



Provide community oversight for the project and helps to set priorities

www.ccpem.ac.uk/about/working-groups

Welcome to new members

National Laboratories



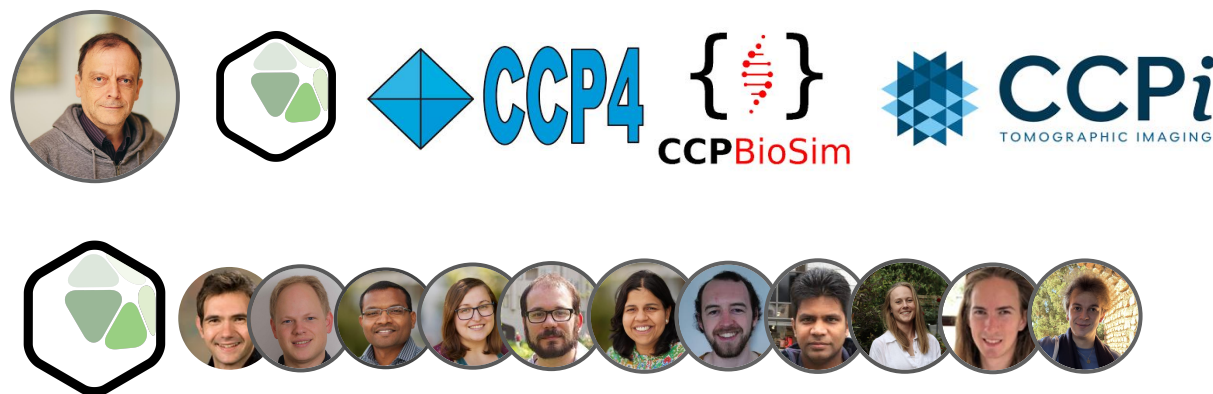
Scientific Computing



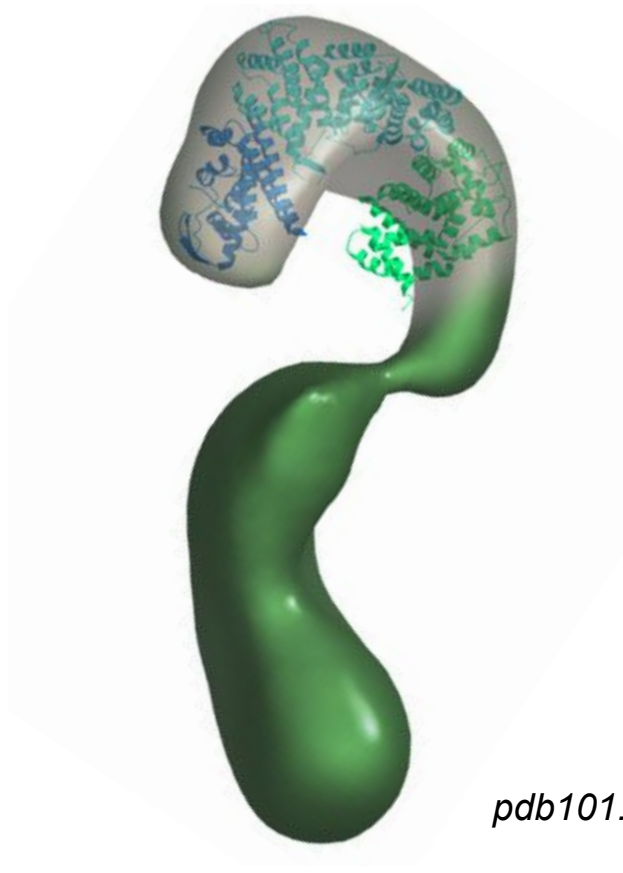
Computational Biology Theme



Electron Microscopy Group



New member questions?



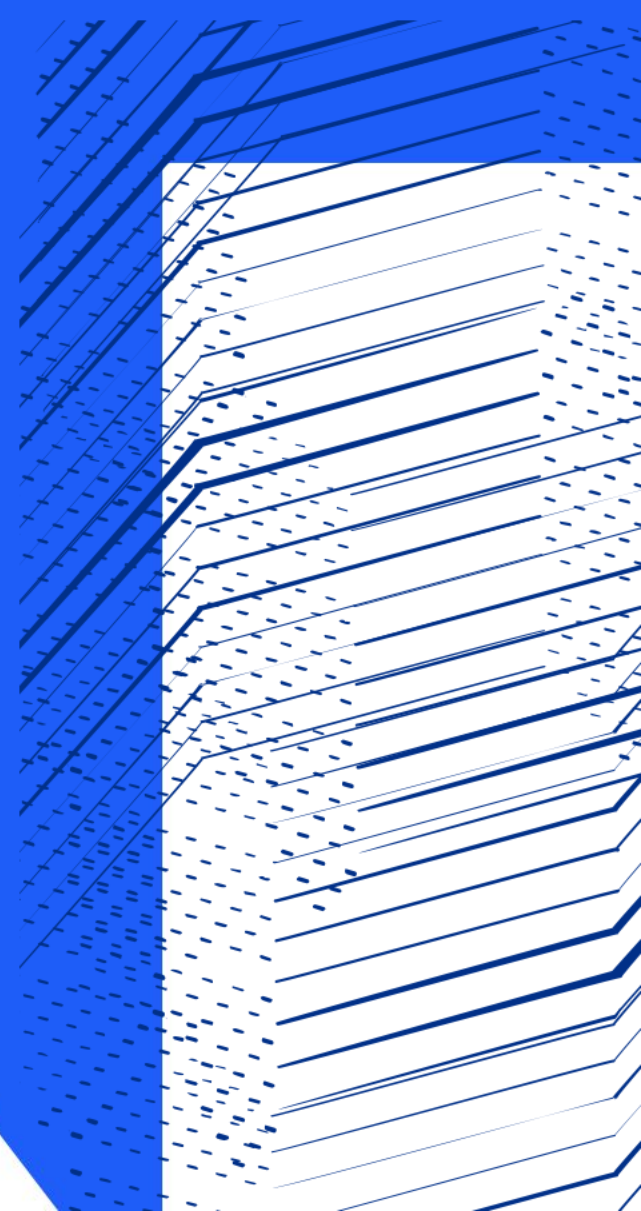
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***Election of new Chair and
Deputy Chair***



Election of Chair and Deputy Chair

Founding



Peter Rosenthal &
Neil Ranson

Current



Neil Ranson & Maya
Topf

Proposed



Maya Topf &
Giulia Zanetti

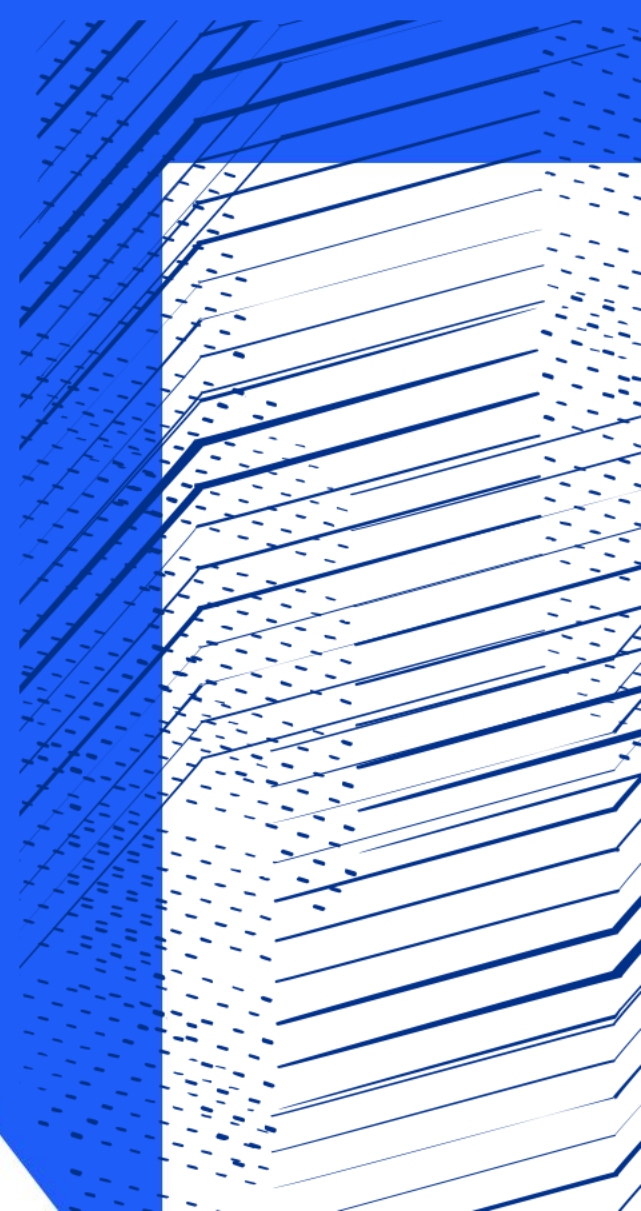
Chair & Deputy



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Overview of CCP-EM software



Overview of CCP-EM software

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Scientific Computing



What's new in CCP-EM?

Colin Palmer and Rangana Warshamanage

22 April 2025

CCP-EM Spring Symposium, Nottingham



CCP-EM Software Suite: *Doppio*

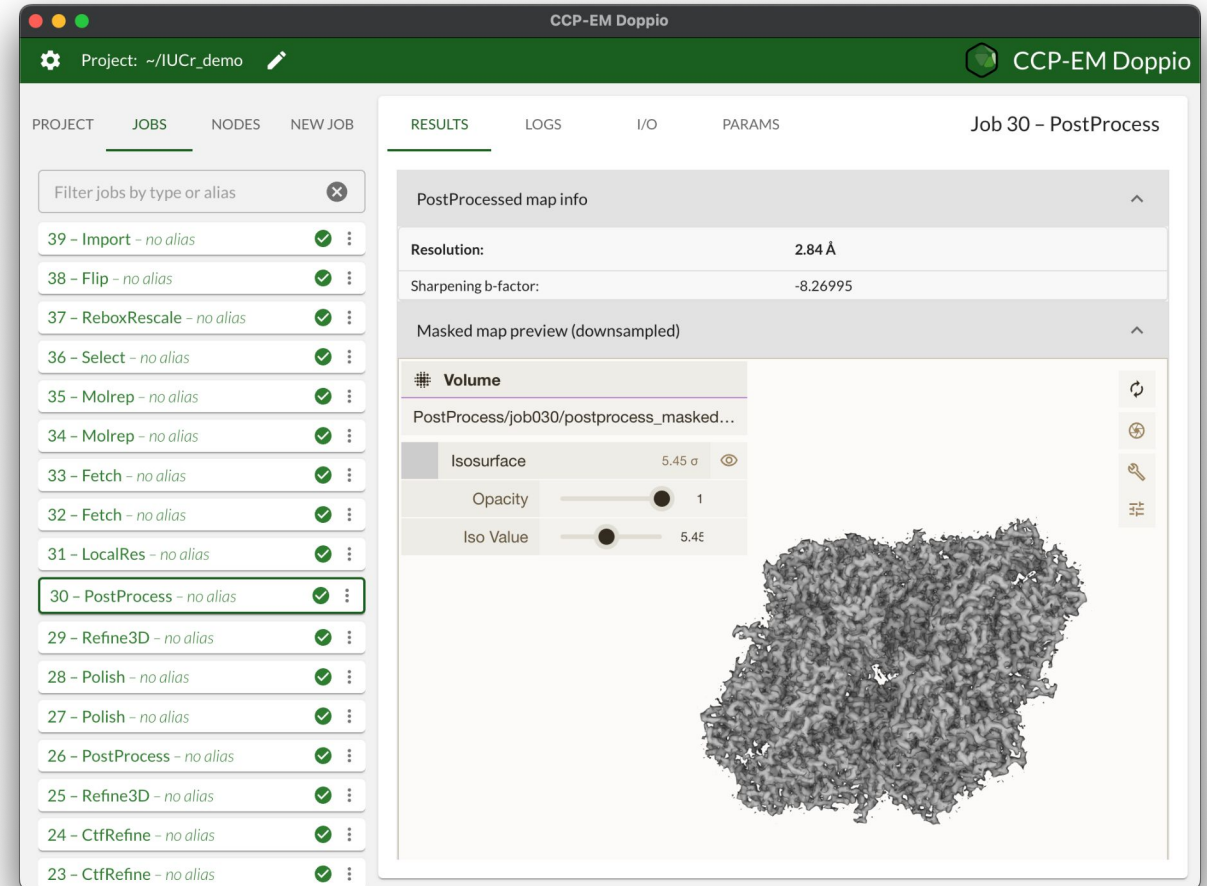
Supports SPA, STA and model building

Local / Remote modes

Linux and Mac

CCP-EM licence, free for academic use, fee for commercial use

Supports: Relion, CCP4, Chimera/x



The screenshot displays the CCP-EM Doppio software interface. The top bar shows the project name as ~/IUCr_demo and the software version as CCP-EM Doppio. The main window is divided into several sections:

- PROJECT**: A list of jobs with a filter box. The jobs listed are: 39 - Import - no alias, 38 - Flip - no alias, 37 - ReboxRescale - no alias, 36 - Select - no alias, 35 - Molrep - no alias, 34 - Molrep - no alias, 33 - Fetch - no alias, 32 - Fetch - no alias, 31 - LocalRes - no alias, 30 - PostProcess - no alias (highlighted), 29 - Refine3D - no alias, 28 - Polish - no alias, 27 - Polish - no alias, 26 - PostProcess - no alias, 25 - Refine3D - no alias, 24 - CtfRefine - no alias, and 23 - CtfRefine - no alias. Each job has a green checkmark and a menu icon.
- RESULTS**: A section for job 30 - PostProcess. It displays "PostProcessed map info" with a resolution of 2.84 Å and a sharpening b-factor of -8.26995. Below this is a "Masked map preview (downsampled)" section showing a 3D volume map of a protein complex. The map is rendered as a grey isosurface. The interface includes controls for "Volume" (PostProcess/job030/postprocess_masked...), "Isosurface" (5.45 σ), "Opacity" (1), and "Iso Value" (5.45).
- LOGS**, **I/O**, and **PARAMS**: Additional tabs for viewing logs, input/output, and parameters.

CCP-EM software overview

GUI



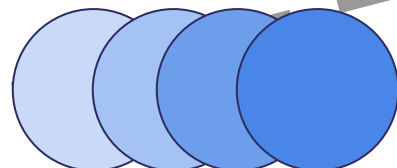
CCP-EM Doppio

Manager



CCP-EM Pipeliner

Jobs



D

PL

RR

LS

FE

DE

RS

MV

Relion Refine

LocScale

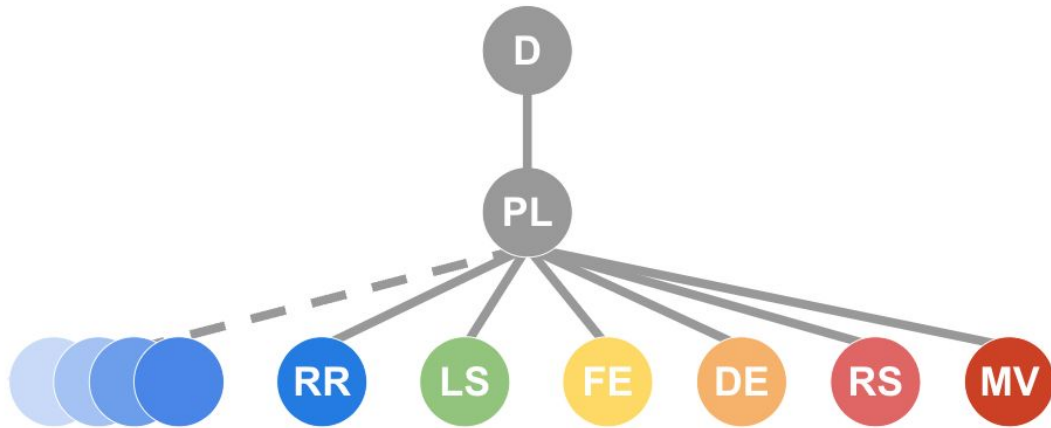
Flex-EM

DockEM

Refmac
Servalcat

Model
Validation

CCP-EM software overview



Doppio

- GUI layer
- JavaScript – web browser or standalone desktop app
- STFC licence, free for academic use

Pipeliner

- Project and job management layer
- Written in Python
- Project graph structure, fully compatible with RELION 4 & 5
- Open Source MPL 2.0 licence

Pipeliner jobs

- Python modules that call other software
- Plug-in architecture

CCP-EM Doppio 1.3

Last year: Doppio 1.0 release

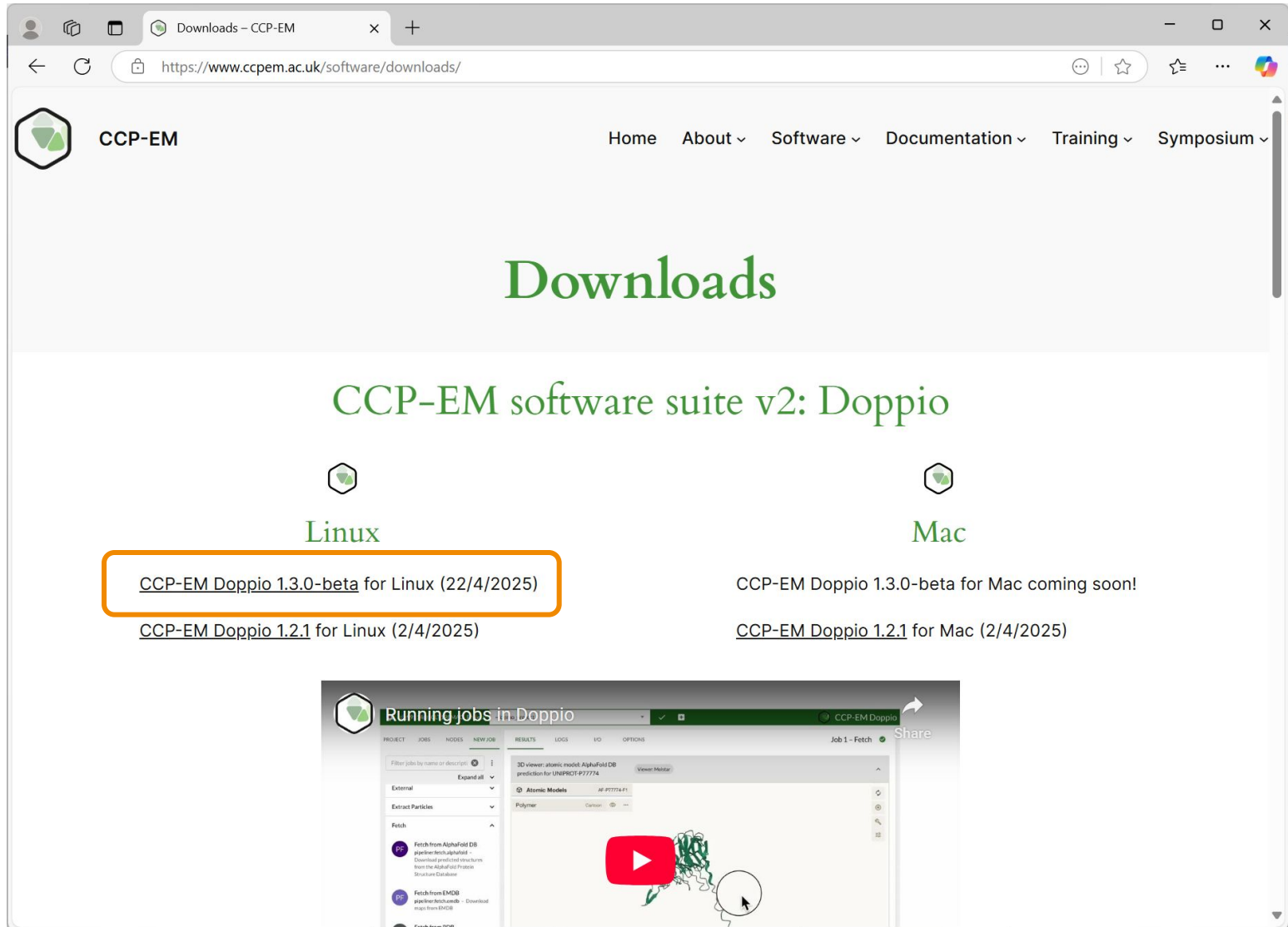
Now: Doppio 1.3 (beta version)

Major GUI developments:

- Conda packaging
- Class selection tool
- Image viewer

Main aims:

- Make Doppio easier to use
- Reduce need to step out and use other tools



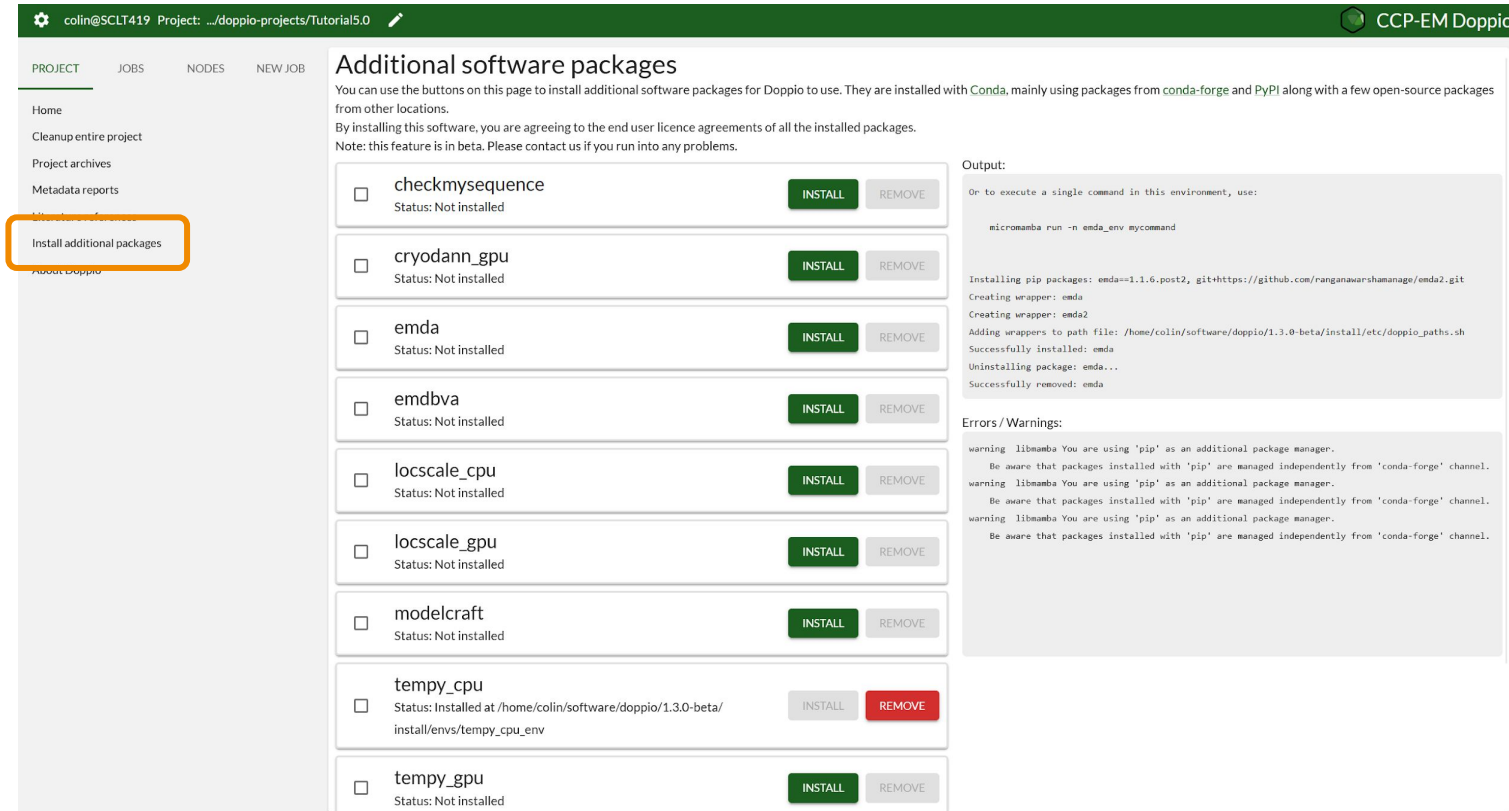
The screenshot shows the CCP-EM Downloads page. The main heading is "Downloads" in green. Below it, the text "CCP-EM software suite v2: Doppio" is displayed. There are two columns for "Linux" and "Mac". The Linux column has two links: "CCP-EM Doppio 1.3.0-beta for Linux (22/4/2025)" which is highlighted with an orange box, and "CCP-EM Doppio 1.2.1 for Linux (2/4/2025)". The Mac column has two links: "CCP-EM Doppio 1.3.0-beta for Mac coming soon!" and "CCP-EM Doppio 1.2.1 for Mac (2/4/2025)". At the bottom, there is a thumbnail for a video titled "Running jobs in Doppio" showing a 3D molecular model.

Doppio: installing additional packages

- One-click installation of new packages
- Each in its own Conda environment
- Not exclusive, can still use separately installed packages too

Future plans:

- More, clearer information
 - Which jobs need which packages?
 - If multiple copies found, which one will be used?
- Add packages for RELION 5, cryoDRGN and more



colin@SCLT419 Project: .../doppio-projects/Tutorial5.0 CCP-EM Doppio

PROJECT JOBS NODES NEW JOB

Home
Cleanup entire project
Project archives
Metadata reports
Install additional packages
About Doppio

Additional software packages

You can use the buttons on this page to install additional software packages for Doppio to use. They are installed with Conda, mainly using packages from conda-forge and PyPI along with a few open-source packages from other locations.
By installing this software, you are agreeing to the end user licence agreements of all the installed packages.
Note: this feature is in beta. Please contact us if you run into any problems.

<input type="checkbox"/>	checkmysequence Status: Not installed	INSTALL REMOVE
<input type="checkbox"/>	cryodann_gpu Status: Not installed	INSTALL REMOVE
<input type="checkbox"/>	emda Status: Not installed	INSTALL REMOVE
<input type="checkbox"/>	emdbva Status: Not installed	INSTALL REMOVE
<input type="checkbox"/>	locscale_cpu Status: Not installed	INSTALL REMOVE
<input type="checkbox"/>	locscale_gpu Status: Not installed	INSTALL REMOVE
<input type="checkbox"/>	modelcraft Status: Not installed	INSTALL REMOVE
<input type="checkbox"/>	tempy_cpu Status: Installed at /home/colin/software/doppio/1.3.0-beta/ install/envs/tempy_cpu_env	INSTALL REMOVE
<input type="checkbox"/>	tempy_gpu Status: Not installed	INSTALL REMOVE

Output:

Or to execute a single command in this environment, use:

```
micromamba run -n emda_env mycommand
```

Installing pip packages: emda==1.1.6.post2, git=https://github.com/ranganawarshamanage/emda2.git
Creating wrapper: emda
Creating wrapper: emda2
Adding wrappers to path file: /home/colin/software/doppio/1.3.0-beta/install/etc/doppio_paths.sh
Successfully installed: emda
Uninstalling package: emda...
Successfully removed: emda

Errors / Warnings:

```
warning libmamba You are using 'pip' as an additional package manager.  
Be aware that packages installed with 'pip' are managed independently from 'conda-forge' channel.  
warning libmamba You are using 'pip' as an additional package manager.  
Be aware that packages installed with 'pip' are managed independently from 'conda-forge' channel.  
warning libmamba You are using 'pip' as an additional package manager.  
Be aware that packages installed with 'pip' are managed independently from 'conda-forge' channel.
```

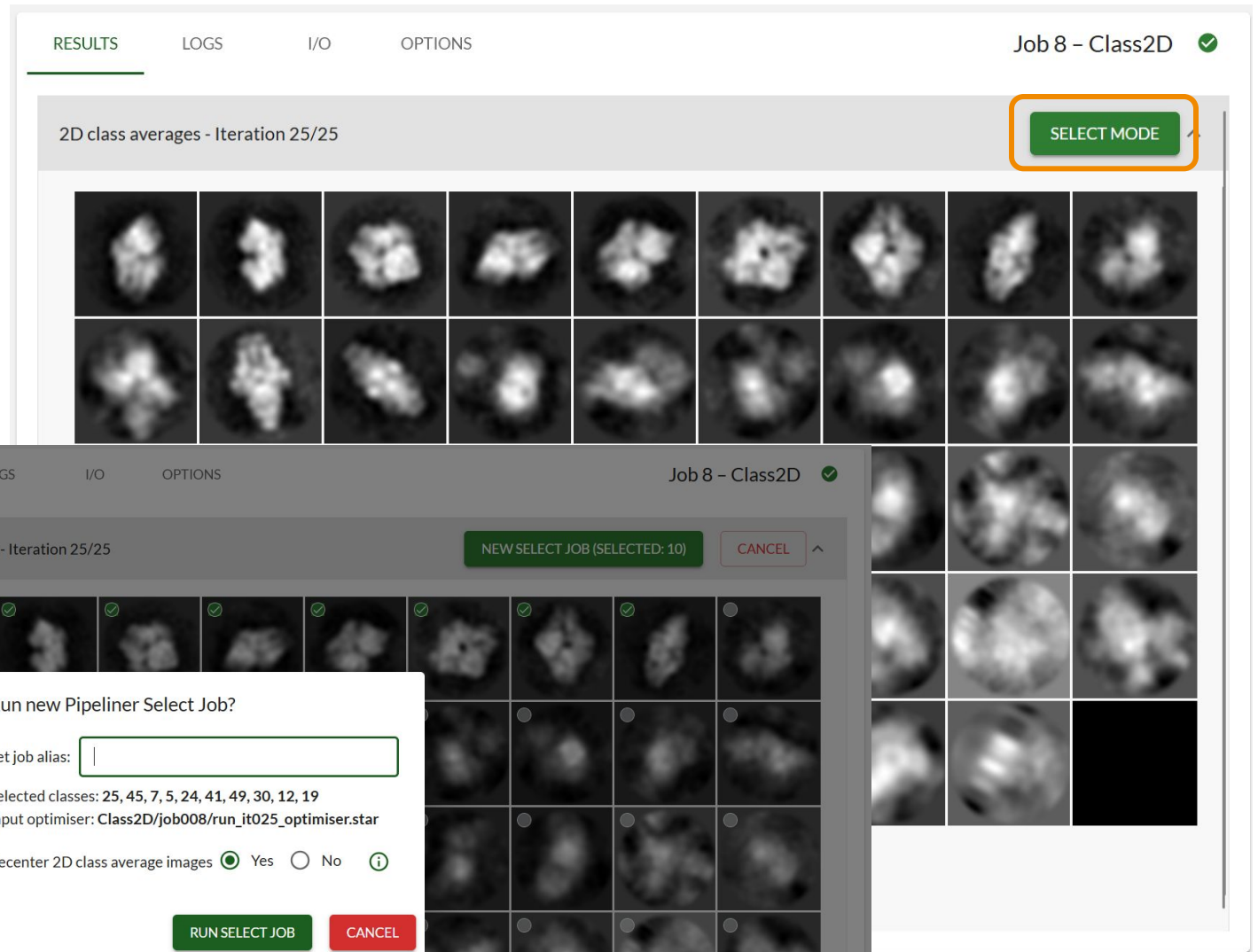


Class selection tool

Interactive class selection

Directly available from
Class2D and Class3D results

Save choices into a new
Select job



RESULTS LOGS I/O OPTIONS Job 8 - Class2D ✓

2D class averages - Iteration 25/25 SELECT MODE

RESULTS LOGS I/O OPTIONS Job 8 - Class2D ✓

2D class averages - Iteration 25/25 NEW SELECT JOB (SELECTED: 10) CANCEL

Run new Pipeliner Select Job?

Set job alias:

Selected classes: 25, 45, 7, 5, 24, 41, 49, 30, 12, 19

Input optimiser: Class2D/job008/run_it025_optimiser.star

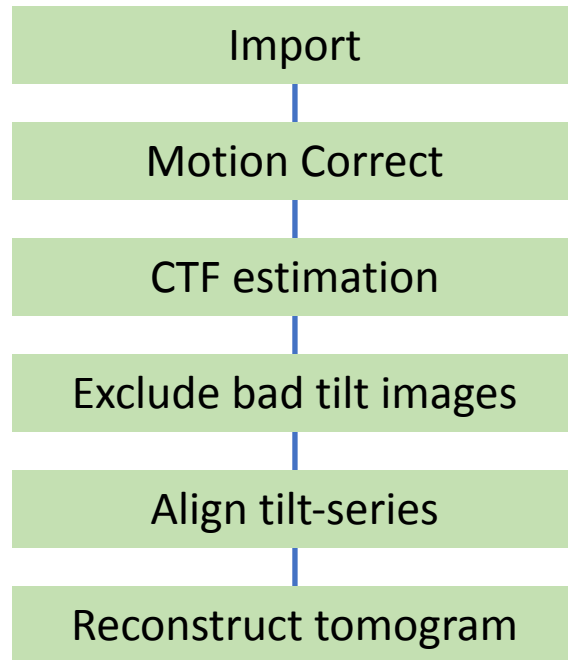
Recenter 2D class average images Yes No ⓘ

RUN SELECT JOB CANCEL

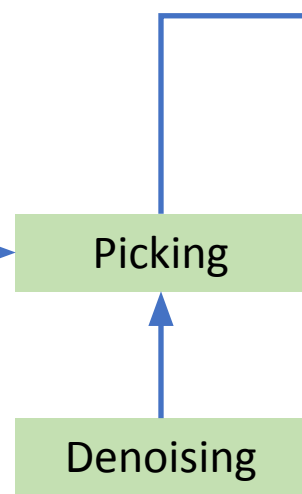
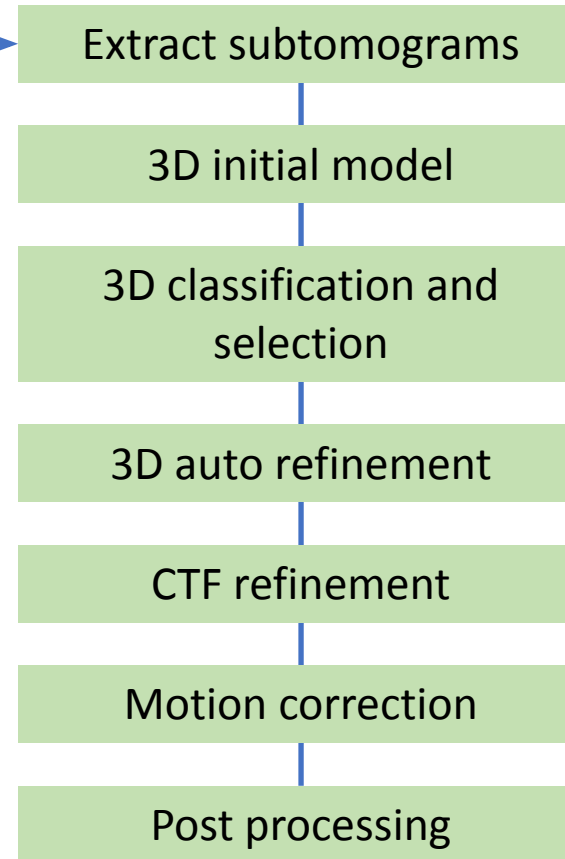
Overview of CCP-EM Tomography Pipeline



(1) Tomogram generation



(2) Subtomogram averaging

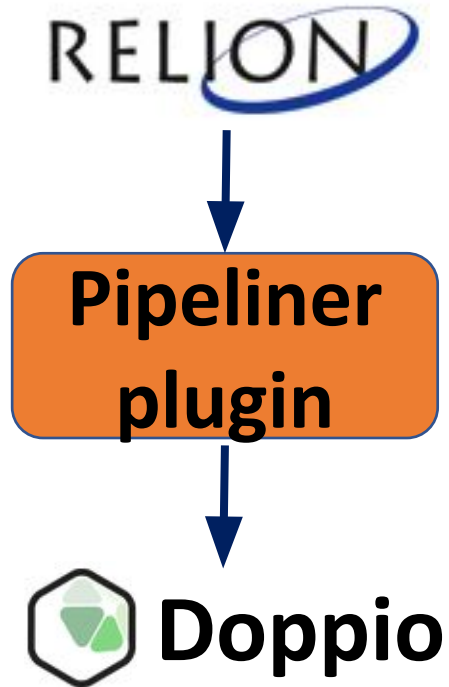
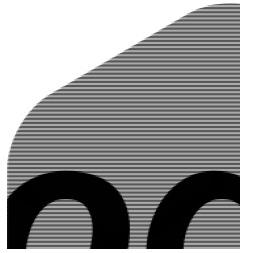


Metadata flows through all stages (centralized handling)

Remote-friendly: Port forwarding



Pipeline Plugins for Relion Tomography

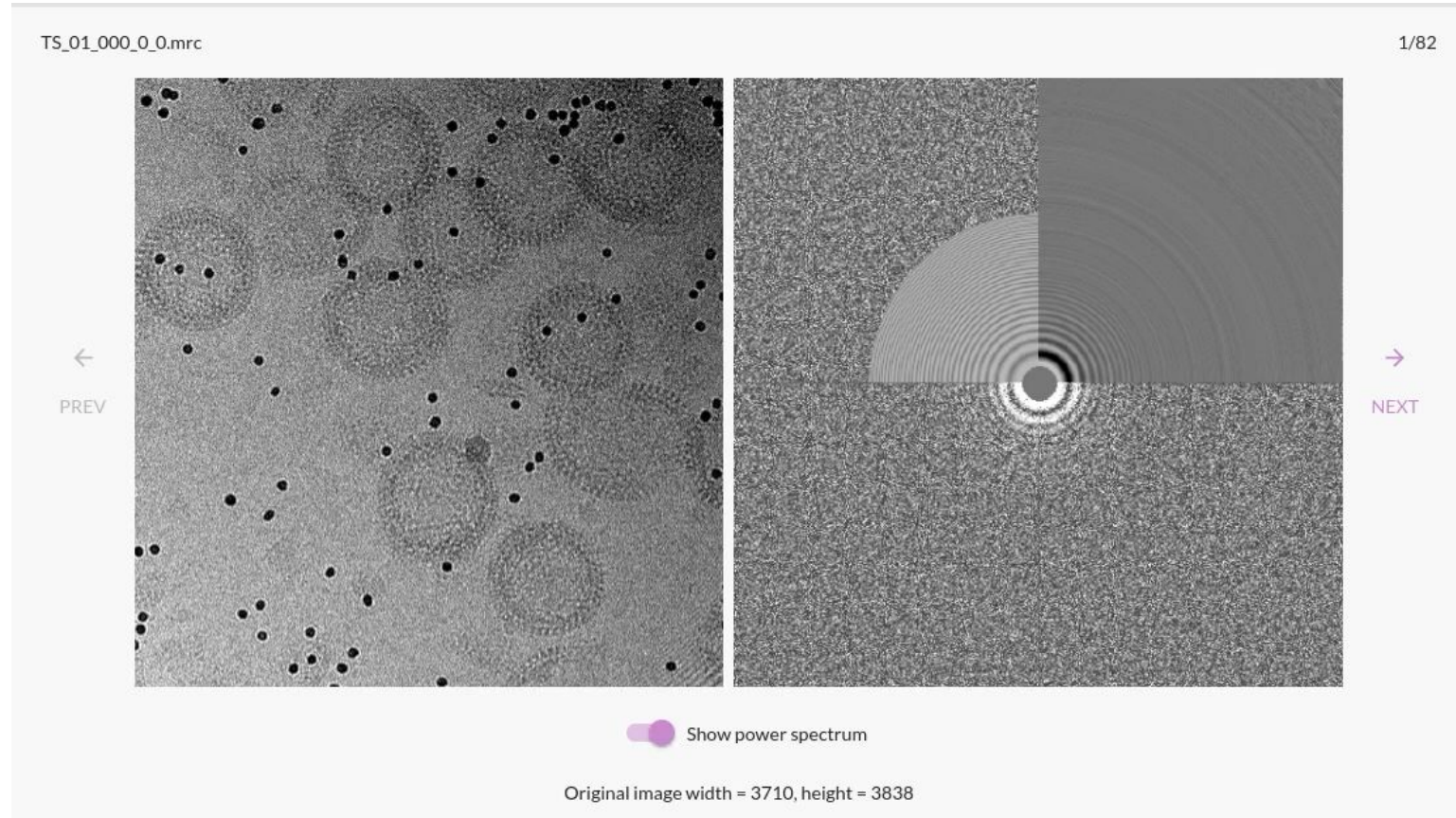
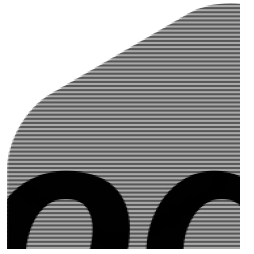


- Parameters & metadata flow automatically between steps
- Easy to plug into broader CCP-EM workflows
- Reproducible & transparent workflows

relion_tomo_reconstruct_tomogram

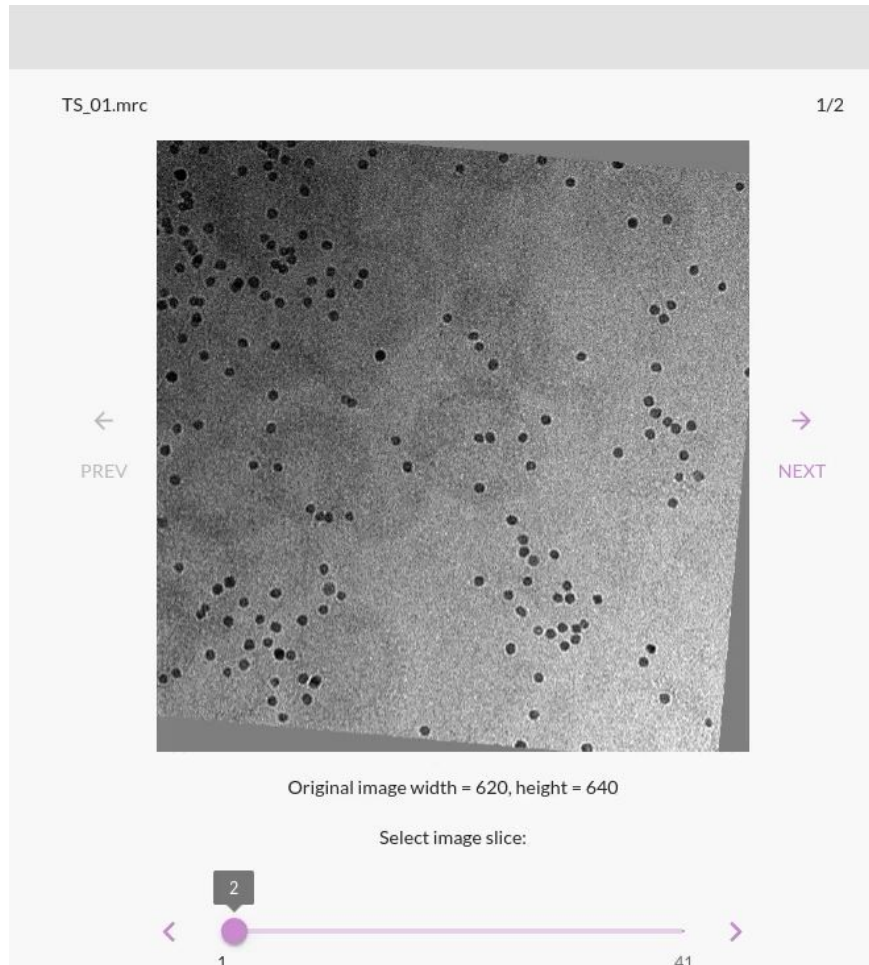


Pipeline Plugins for Relion Tomography



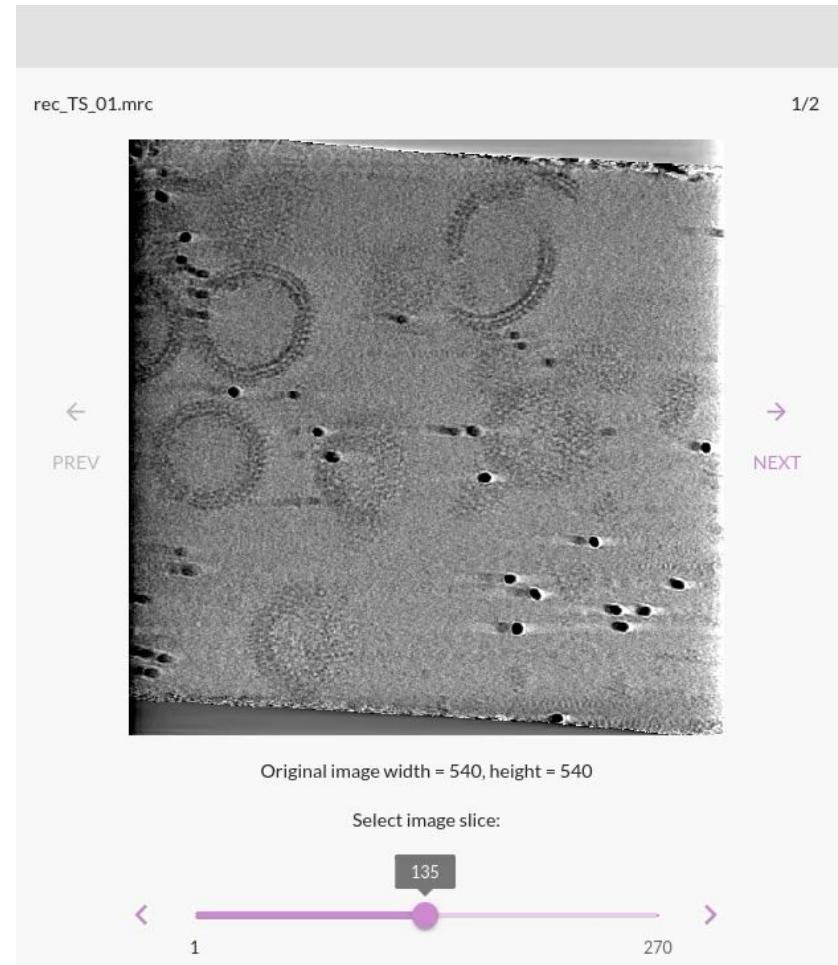
CTF Estimation





Alignment

Inspect shifts, angles, and quality of tilt series alignment



Tomogram Inspection

Evaluate reconstruction quality and look for artifacts

Overview of CCP-EM software

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What's new in CCP-EM?

Colin Palmer and Rangana Warshamanage

22 April 2025

CCP-EM Spring Symposium, Nottingham



Software feedback?

Is there any key functionality missing in Doppio?

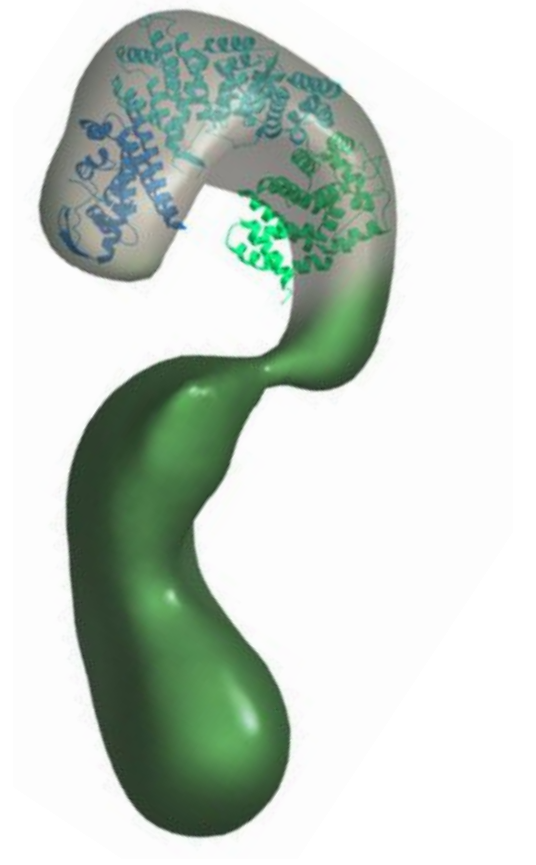
What new tools (from you or others) should be included in the CCP-EM suite?

What would help users in your group/facility adopt Doppio for SPA/STA/modelling?

What should be our main focus(es):

- New scientific functionality
- Ease of use
- Ease of install/setup
- Documentation
- Improvements to scripting

If you/your group haven't used Doppio - why and what can we do to help?

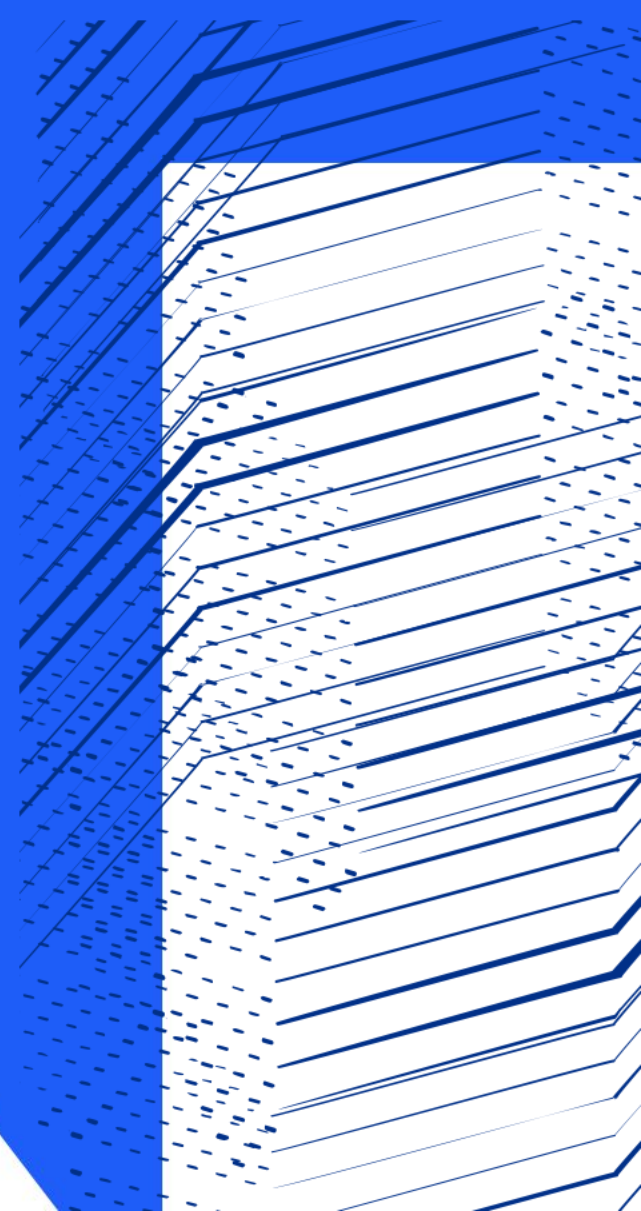




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Overview of CCP-EM training



CCP-EM Workshops 2024-25

- Since 2013 we have led or co-led 42 workshops, teaching over 1,300 researchers
- Icknield workshop, RAL, Nov 2024
- Dutch cryoEM school, Leiden/Delft, June 2024
- CERN Inverted School Of Computing, March 2025
- Leeds Doppio Workshop, Sept 2024
- EMBO Cryo-EM image processing, EMBL Heidelberg, Aug 2024
- EMBO Integrative structural biology, EMBL Hamburg, Nov 2024
- Czech Society for Structural Biology, March 2025

- Various Doppio road shows around UK
- New website for more efficient dissemination of materials



Training using STFC DAaaS & SCD Cloud

Doppio and example data installed on STFC Data Analysis as a Service (DAaaS) training system

Runs on STFC Cloud VM (with or without GPU)

User access managed through DAaaS training website and proxy

Doppio app runs in user's local browser – much faster than a remote desktop

Very good way of running training courses

The screenshot shows the DAaaS Training website interface. The browser address bar displays <https://training.analysis.stfc.ac.uk/workspaces/>. The page title is "DAaaS Training" and there is a "LOGOUT" button in the top right corner. On the left side, there is a navigation menu with "Workspaces" and "Data" options. The main content area features a "New Workspace" button with a right-pointing arrow and a descriptive text: "Workspaces provide you with course materials, software and compute resources to partake in your training course". Below this, the section "Your Workspaces" displays a workspace named "CCP4 developers meeting" owned by "Colin Palmer". A preview window shows the "Doppio" application interface, which includes a terminal window with code and a "Project" configuration form. The form fields include "Project Name" (New project), "Description" (A new CCP 4M pipeliner project), "Project directory" (analysis-training/home/step462/01space/project), "Created" (2023-10-19 15:00:58), and "Last modified" (2023-10-20 16:04:10). At the bottom left of the interface, there is a "Terms of Use" link.

CCP-EM Upcoming Events

- EM Facilities Meeting, Warwick, 2-3 June 2025
- Integrative structural biology, Padua, Italy, July 2025
- India model building workshop, Bangalore, India, 28 July – 2 August 2025
- EMBO cryo-EM image processing, Birkbeck, London, Sept 2025
- CCP-EM Icknield model building workshop, RAL, Oxford, Oct 2025

See our mailing list for more info!

If you would like us to visit your institute as part of the Doppio roadshow or host cryoEM workshop please get in touch



Training Questions

Should we focus on?

SPA

Tomography

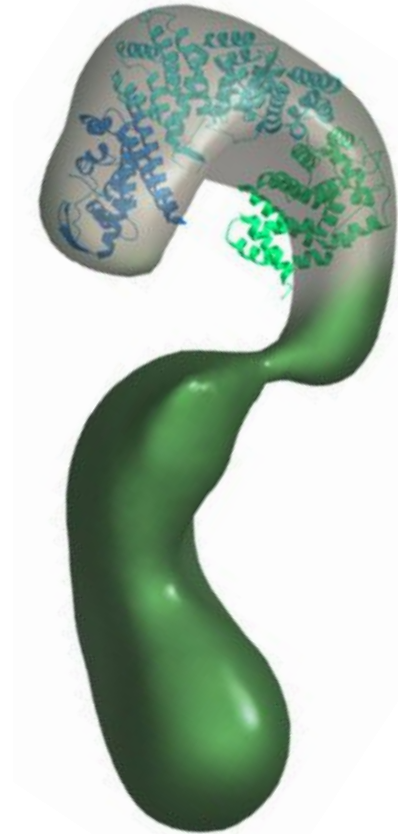
Model building

Software development

What's correct balance of online vs in-person?

Are you aware of other training resources we disseminate?

If you would like us to run a course at your institute please get in touch!

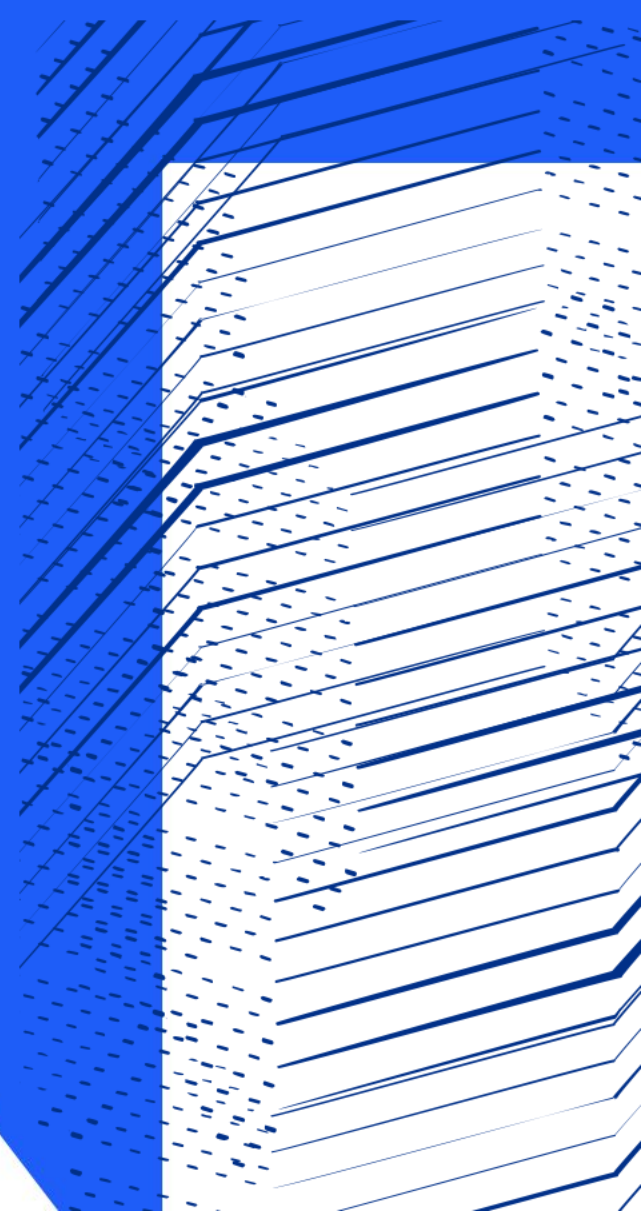




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*Overview of CCP-EM Spring
Symposium conference*



Spring Symposia 2025 / 2026

2025: 11th Ed. EMCC, Nottingham (23-25 April)

Includes Diamond **Biological Cryo-Imaging meeting (BCI)**

CCP-EM Scientific Organisers **Laura Spagnolo & Rene Frank**

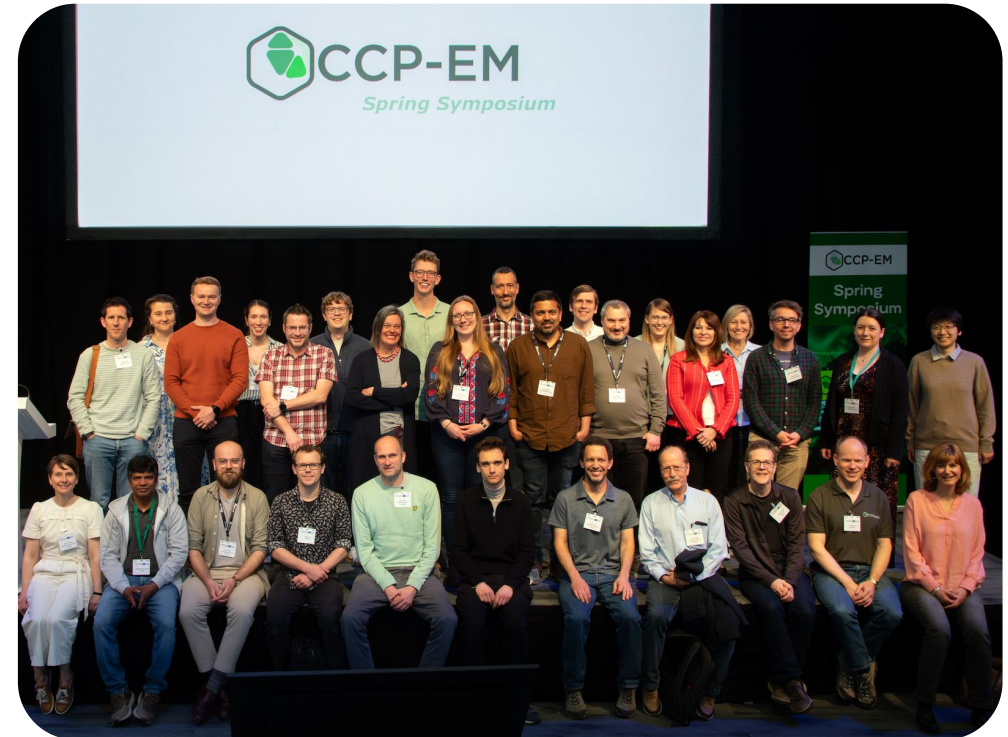
376 In-person delegates (20 countries, 4 continents)

613 virtual delegates (unique Zoom views, 29 cont., 6 conti.)

£21k sponsorship - 32 bursaries (registration & accomodation)

Raw recordings now available online

Previous years talks on YouTube





Spring Symposium

Edition	Venue	Year	In person	Virtual (unique views)
10	Nottingham EMCC	2024	366	833
9	Nottingham EMCC	2023	257	680
8	Nottingham EMCC	2022	150	917
7	Virtual	2021	-	900
6	Virtual	2020	-	2439
5	Nottingham Jubilee	2019	286	?
4	Keele	2018	180	?
3	RAL	2017	215	?
2	RAL	2016	159	?
1	RAL	2015	100	?



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Spring Symposia 2025 / 2026

2026: EMCC, Nottingham (21-24 April)

Karen Davies Memorial Symposium, 21 April

Diamond Biological Cryo-Imaging meeting (BCI), 22 April

CCP-EM Spring Symposium, 23-24 April

Continue in-person / virtual hybrid format



Karen Davies

Spring Symposia Questions

*For specific logistic & scientific feedback
please use the feedback form sent to delegates
yesterday*



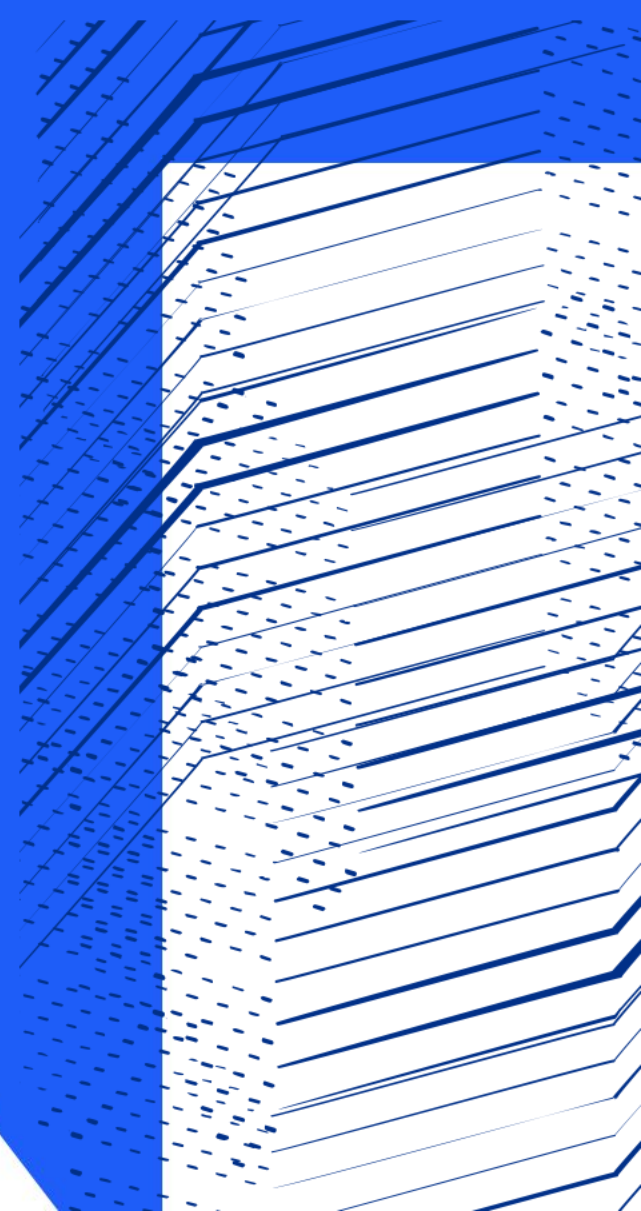
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*Overview of CCP-EM core grant
renewal*



Grant renewal update



MRC Partnership CCP-EM Core Grant: *“Collaborative Computational Project for cryo electron microscopy (CCP-EM): expanding the reach of cryoEM”*

Investigators:

Tom Burnley (STFC, PI), Martyn Winn (STFC), Maya Topf (LIV/CSSB), Giulia Zanetti (Birkbeck), Sjors Scheres (MRC-LMB), Kyle Morris (EMBL-EBI), Peijun Zhang (Oxford/Diamond), Peter Rosenthal (Crick) and Paula da Fonseca (Glasgow)

Project Partners:

Randy Read (Cambridge), Zach Freyberg (Pittsburgh), Arjen Jakobi (Delft), Ivo Tews (Southampton/CCP4), Geerten Vuister (Leicester/CCPN), Sarah Harris (Sheffield/CCPBioSim), Paul Verkade (Bristol), Dan Rigden (Liverpool), Keitaro Yamashita (Tokyo), Ellen Zhong (Princeton), Dari Kimanius (CZII), Mark Basham (RFI)



Grant renewal update



Science themes:

- ***In situ* cryo electron tomography**, for the determination of macromolecular structures in their native environment and their role in medically important pathways;
- **High resolution cryoEM with ligand** identification and validation, contributing to rational drug design;
- **Heterogeneous reconstruction** to identify conformational and/or compositional variability;
- **Data/metadata management** to handle the increasing data volumes, and ensure that database entries are well annotated and FAIR.

Funding period: March 2026 - February 2031

Fund: Agnel Joseph & Colin Palmer, 0.5 Matt Iadanza, 0.3 Lauren Giles

Activities: Spring Symposium, CCP-EM workshops (SPA/STA/model building), developer meetings, software development and maintenance

Submitted January 2025



Any other business?

CZII tomography metadata working group and TomoBabel library (w/ CZII, EMBL-EBI & CNB-CSIC Madrid)

Carbon Cost of cryoEM: Working Group

Community Initiative: Heterogeneity Challenge

...



CCP-EM Core Team

CCP4 Core Team

STFC Business & Innovation

CCP-EM Commercial License Holders

CCP-EM Collaborators

CCP-EM Users

Website & Downloads: www.ccpem.ac.uk

Mailing list: www.jiscmail.ac.uk/ccpem

Bluesky: ccpem.bsky.social

Email: ccpem@stfc.ac.uk

