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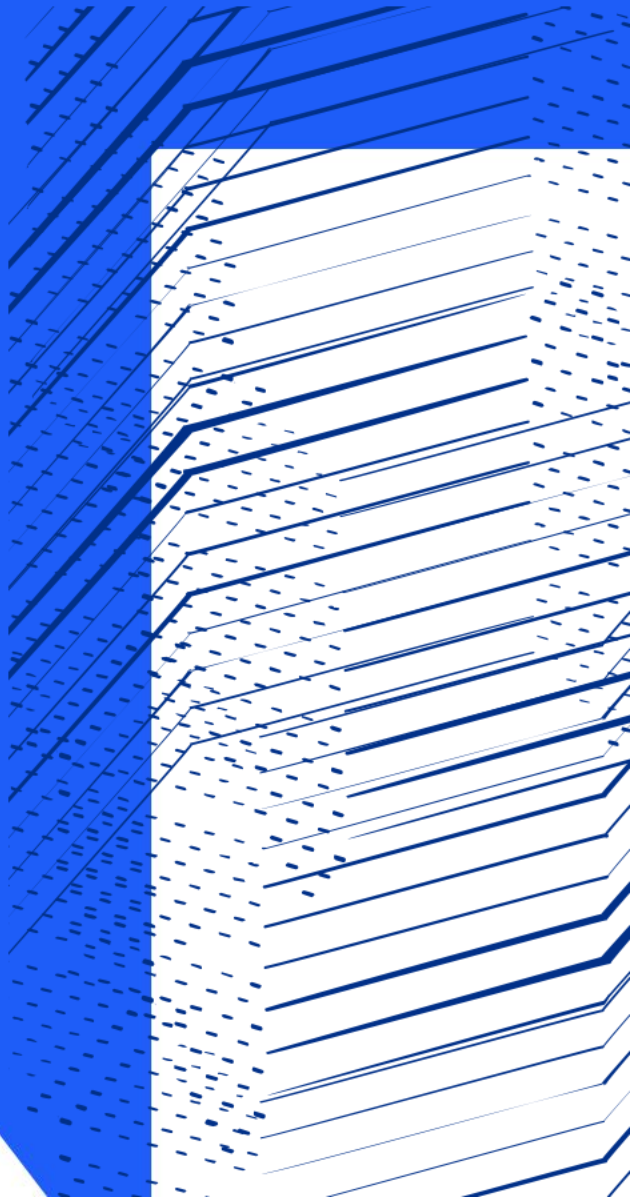
CCP-EM
8th Icknield Workshop

Tom Burnley CCP-EM/STFC

4th November 2024

RAL/DLS



What is CCP-EM?

CCP-EM

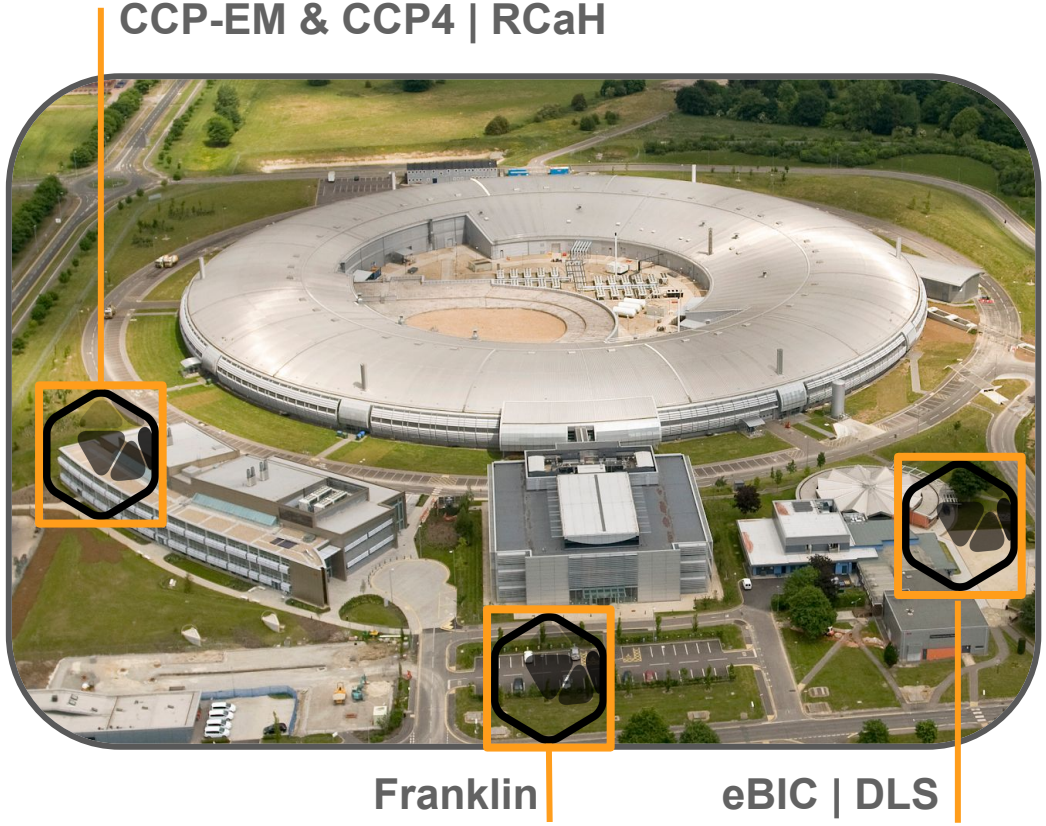
Support users and developers in computational aspects of biological EM

Based at STFC RAL national laboratory

CCP-EM software suite

- EM community (>3.5K subscribers)
- Software users (>1200 downloads, >30 industrial licences)
- Support developers (>10 external groups)

Core funding from MRC since 2012



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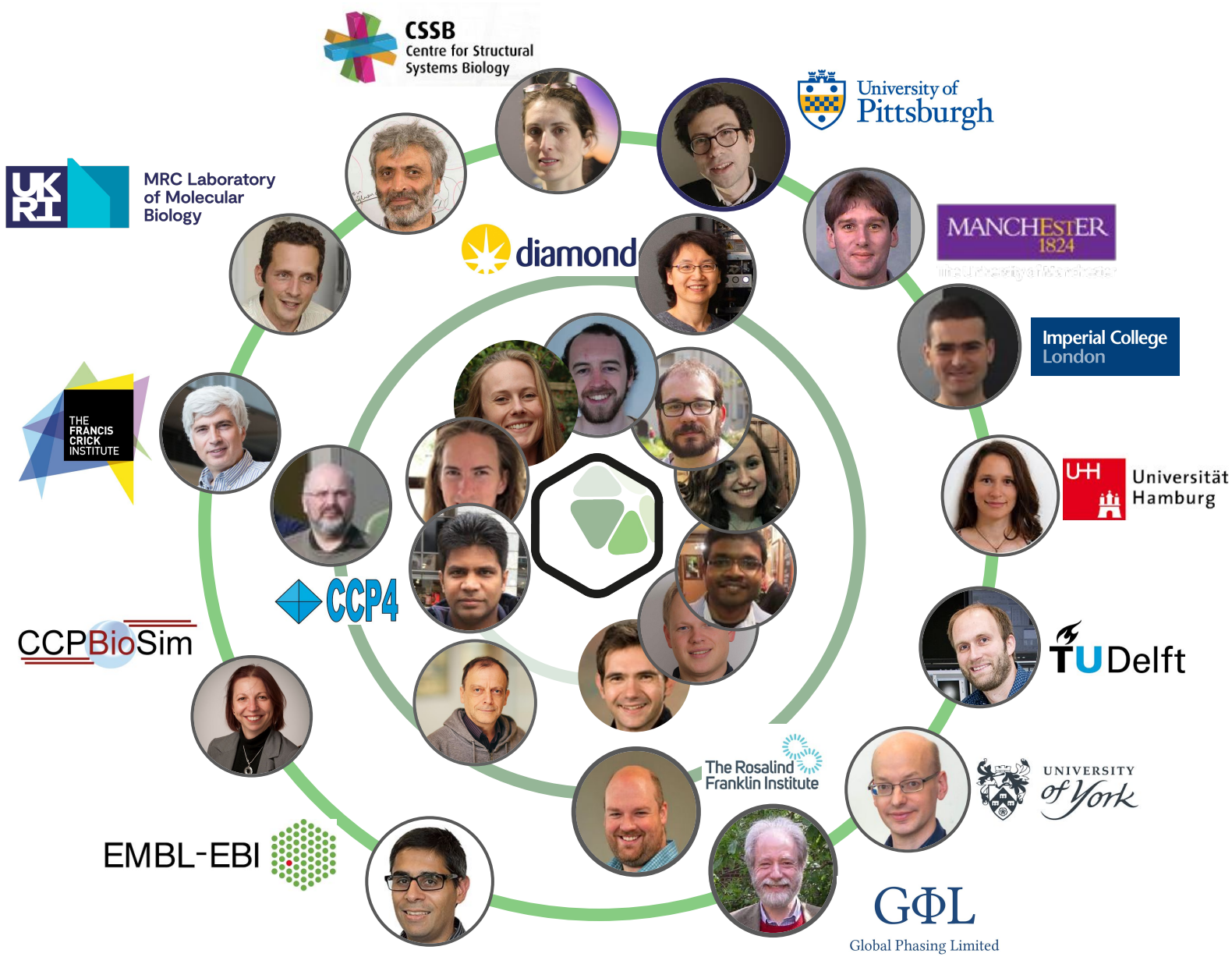
Medical Research Council

Research Complex at Harwell

CCP-EM

Collaborative Computational Project



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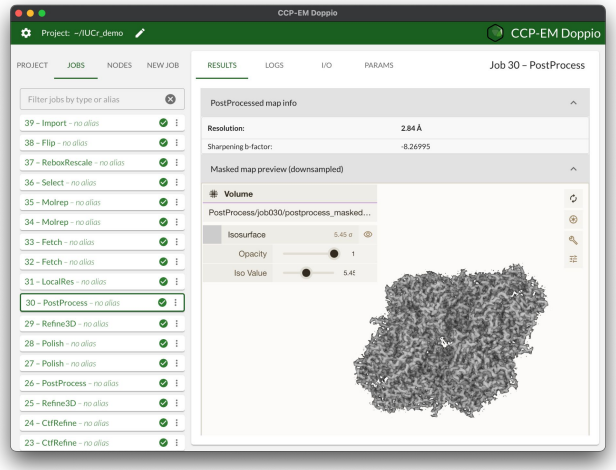
Collaborative Computational Project



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Tom Burnley

George Coldstream

Joel Greer

Lauren Giles

Matt Iadanza

Agnel Joseph

Sony Malhotra

Jola Mirecka

Colin Palmer

Rangana Warshamanage

Martyn Winn

CCP-EM

Collaborative Computational Project


Yuriy Chaban


Lorna Malone


Karen Davies


Dan Hatton


Stephen Riggs

diamond

UKRI Science and Technology Facilities Council

CCP-EM software suite

30+ tasks in a common Python framework

Raw micrographs to validated atomic model

Uses some CCP4 programs

Download from ccpem.ac.uk

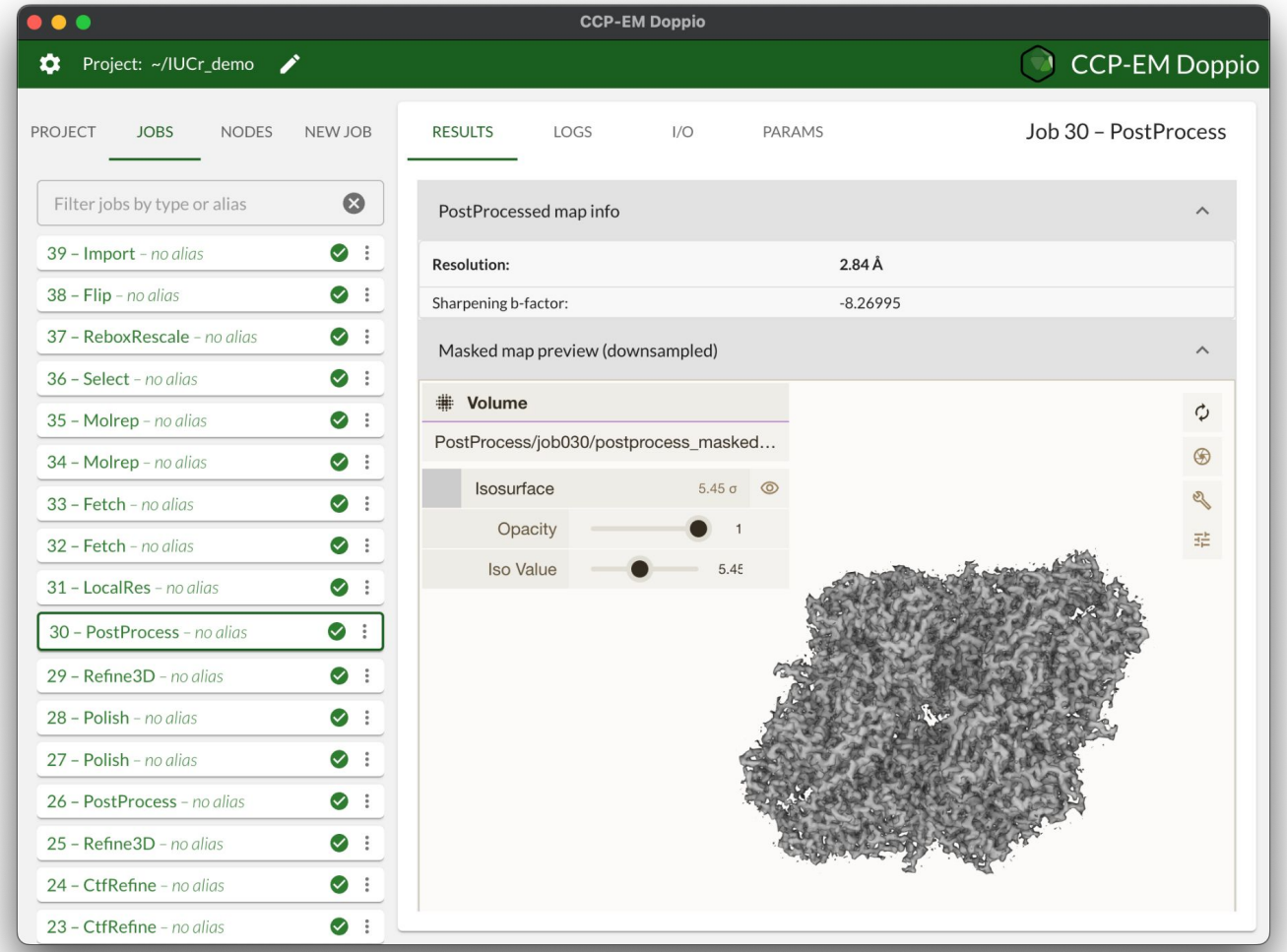
Linux & Mac

Free for academic use, fee for commercial

Bugs & requests:

ccpem@stfc.ac.uk

Recommend using latest nightly



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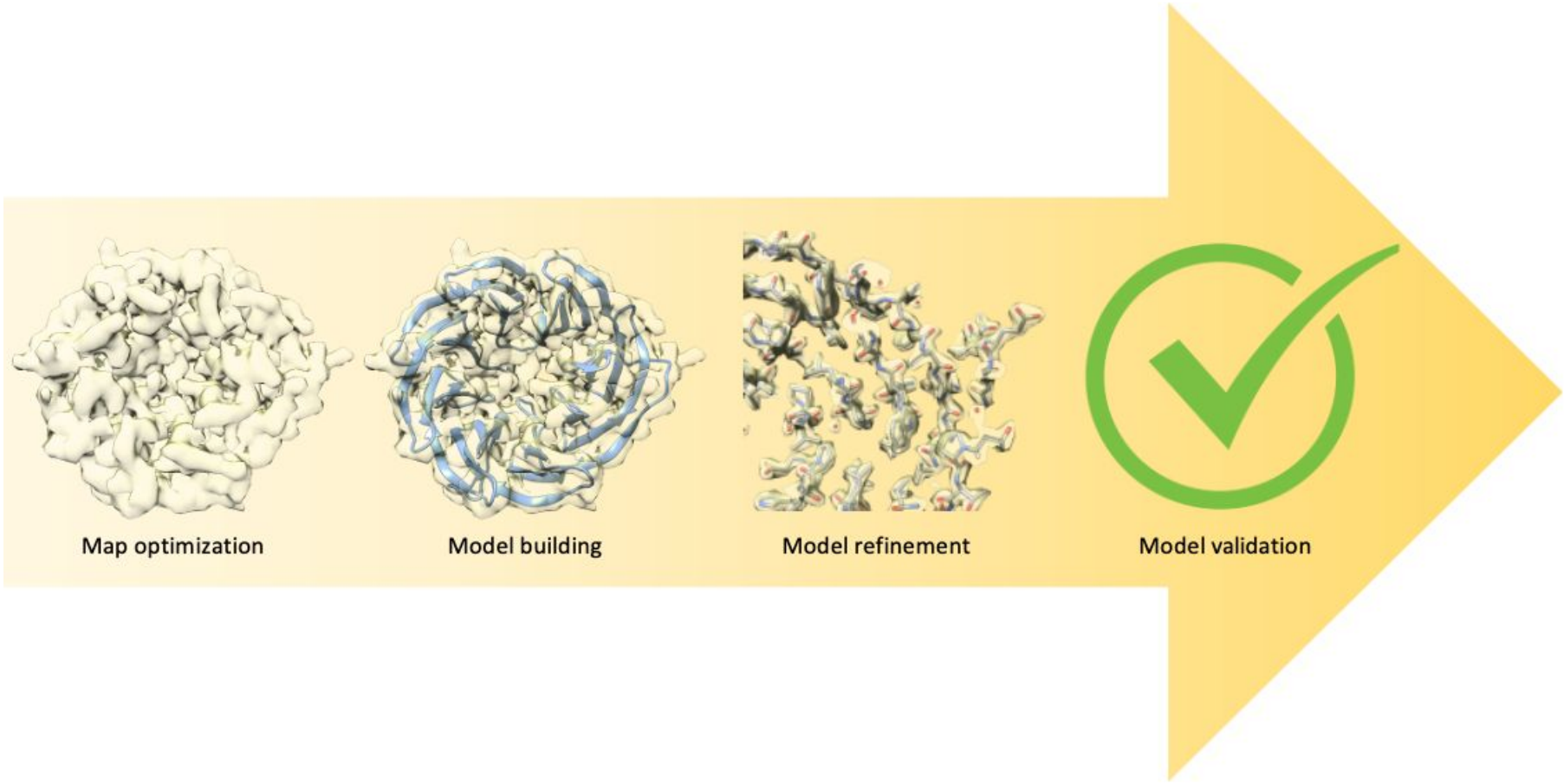
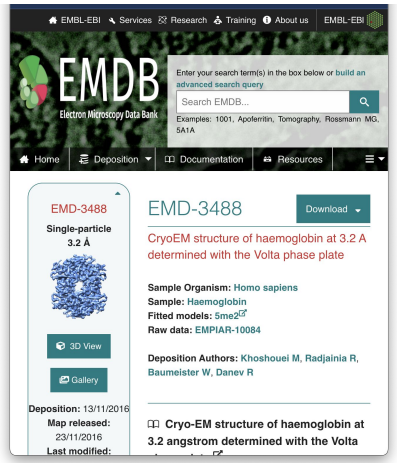
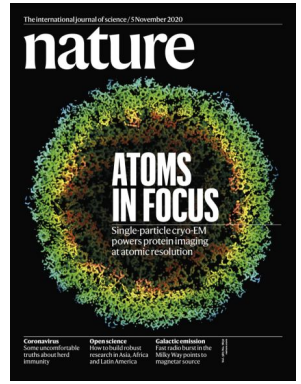
CCP-EM workflow at Icknield

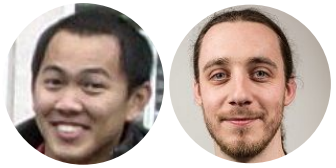
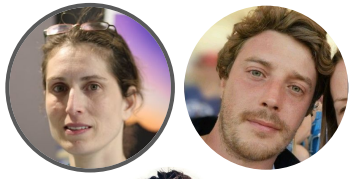
Map Optimisation | **Model Building** | **Model Docking** | **Automated Refinement** | **Interactive Refinement** | **Map/Model Validation** | **Deposition**







CCP-EM workflow at Icknield

Map Optimisation	Model Building	Model Docking	Automated Refinement	Interactive Refinement	Map/Model Validation	Deposition
LocScale	ModelCraft	EM_placement	Refmac Servalvat	Coot Moorhen	CCP-EM Validation	EMDB
						
	Model Angelo		TEMPy -REFF	ChimeraX/ ISODLE	Find/Check MySeq	AF-DB & 3DBeacons
						
					Privateer	

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sharpen... build... refine... validate... repeat...

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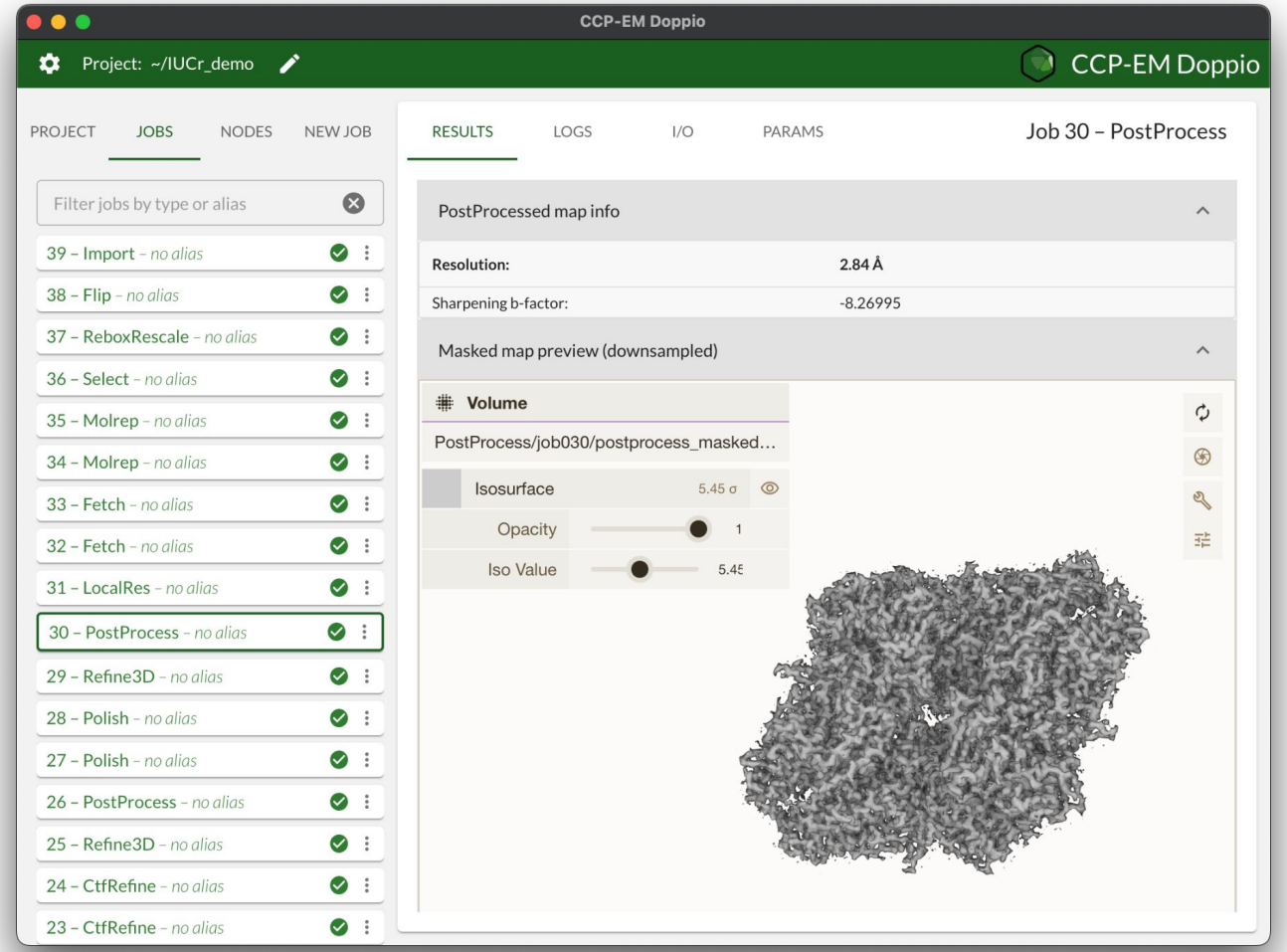
CCP-EM 2.0: pipeliner & Doppio



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CCP-EM version 1.x

CCP-EM

- Map post processing
- Atomic modelling
- PyQt5 GUI
- No data model
- Basic project management

RELION

- Single particle reconstruction
- FLTK GUI
- Data model
- DAG project management

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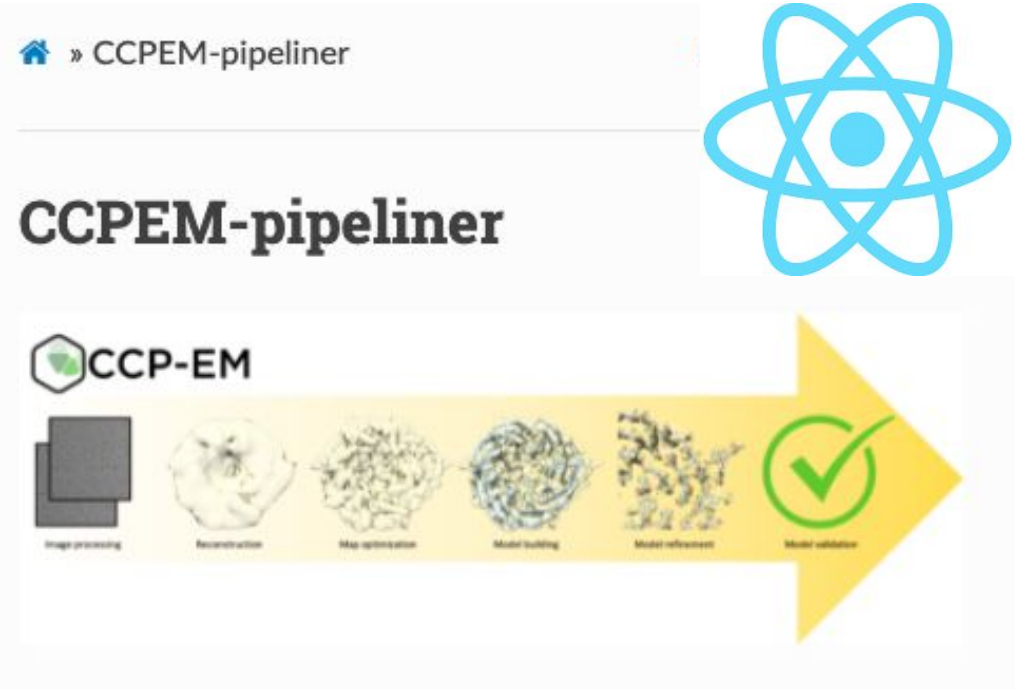
CCP-EM version 2.x



Images to structures

- Python pipeliner python API
- JS react GUI

- Updated data model
- Project management

- Single particle
- Atomic modelling
- Tomography (coming soon)

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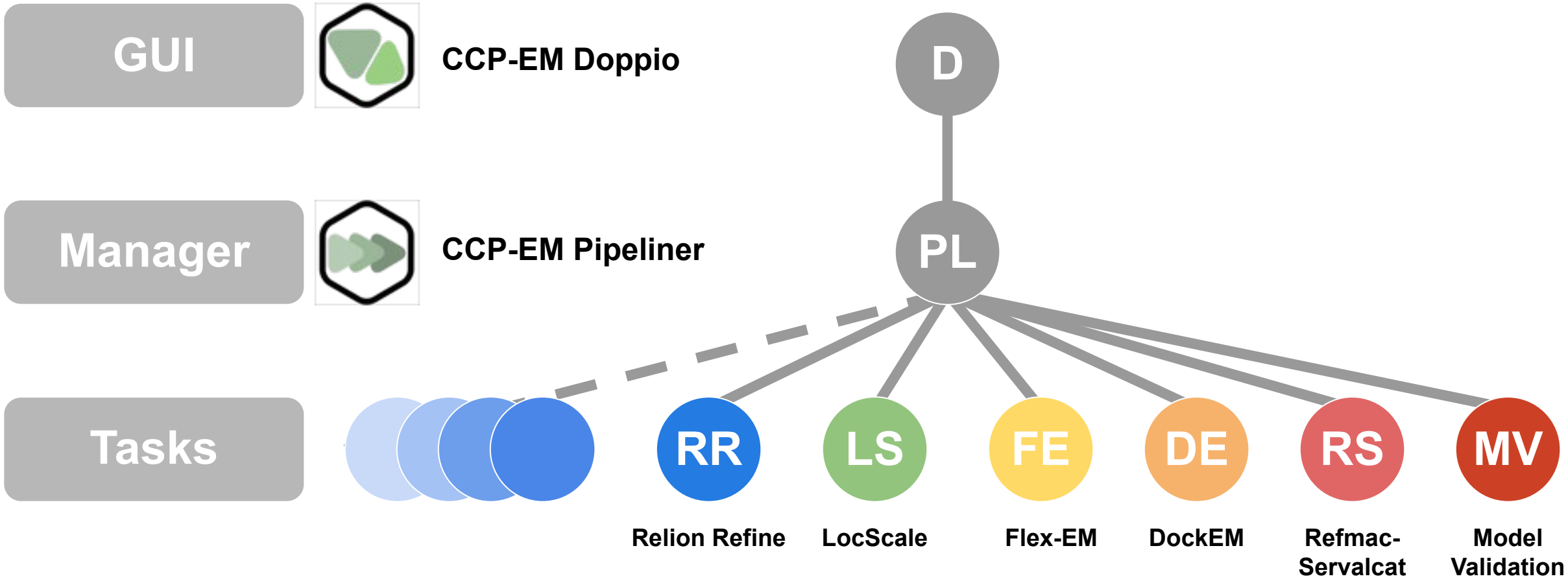
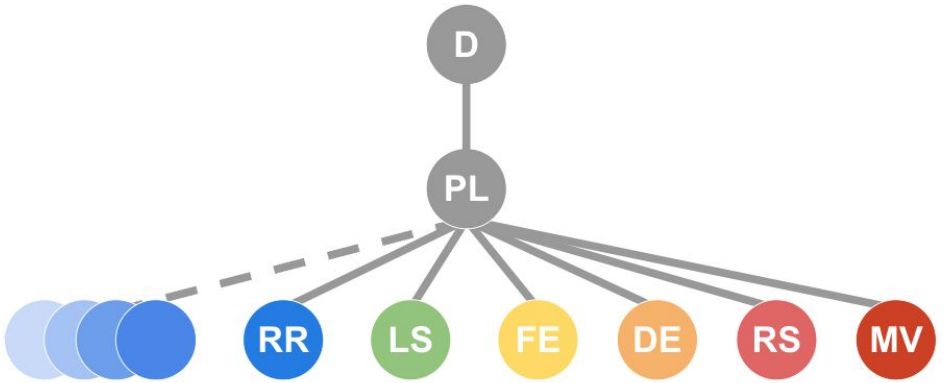
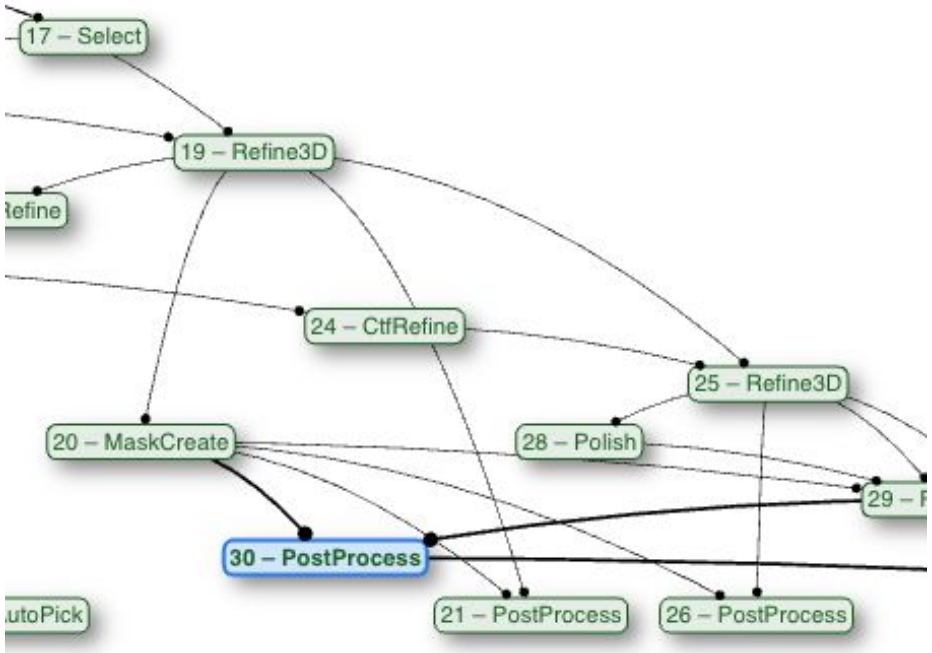
CCP-EM software plan



ccpem-pipeliner

- ***Business logic layer decoupled from tasks and UI***
- Python 3
- MPL 2.0 license
- https://gitlab.com/ccpem/ccpem-pipeliner
- Directly Acyclic Graph dataflow
  - Metadata tracking
  - Archiving
  - Jobs have input/output nodes





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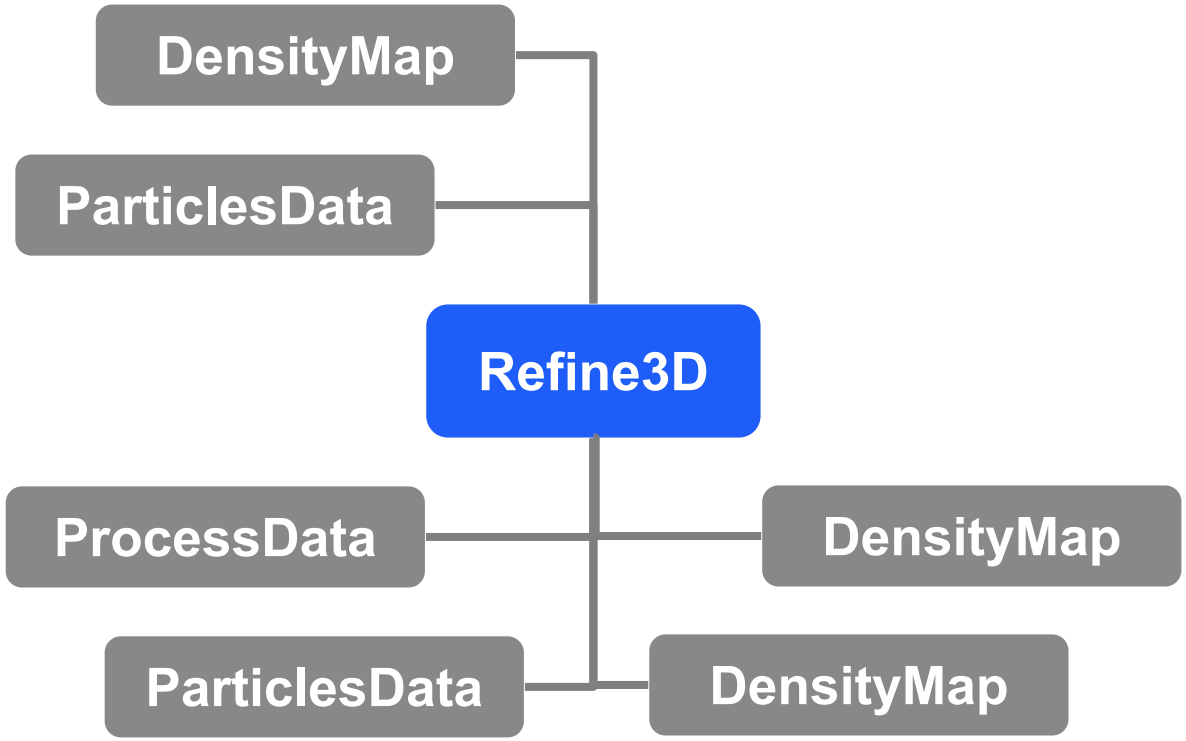
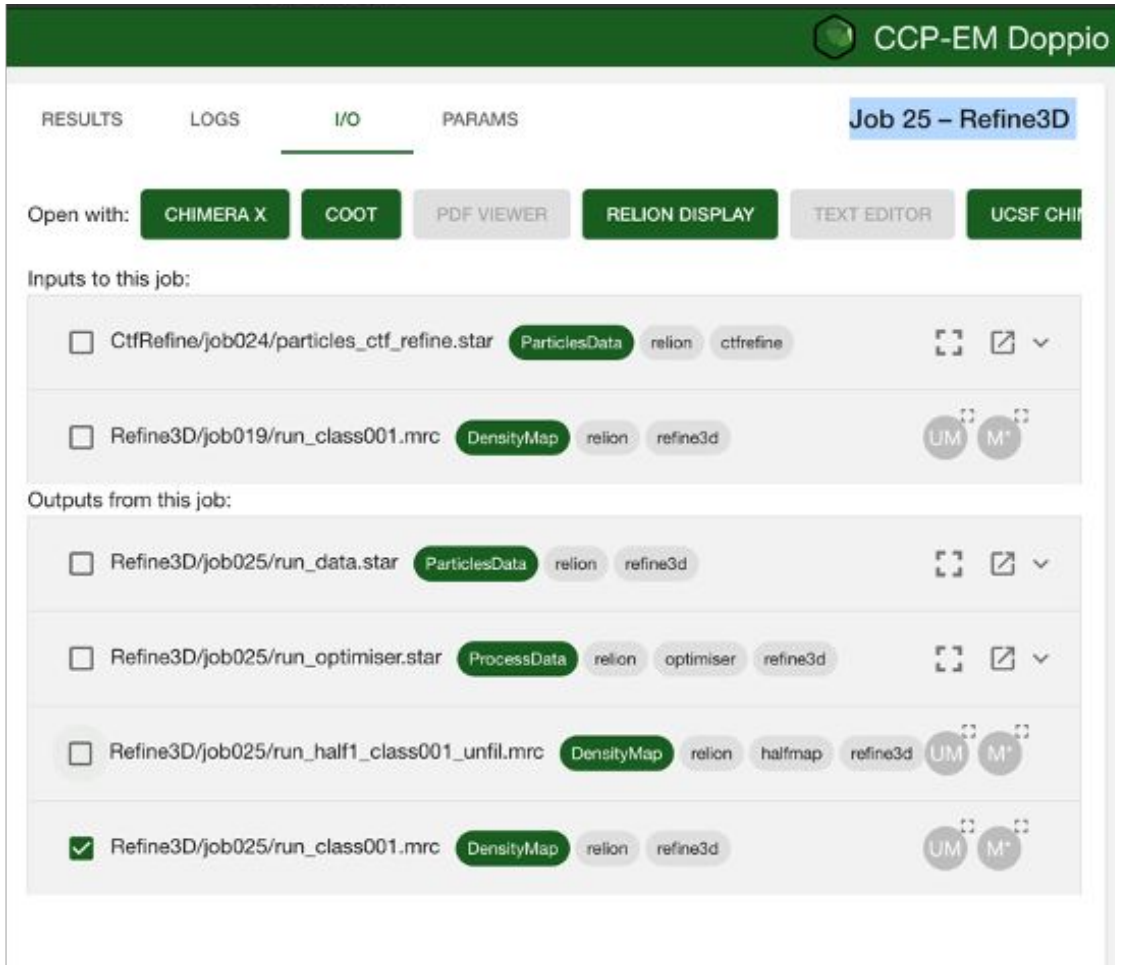
Job Nodes

Each job has input and output nodes & nodes are specific data types





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Job Nodes

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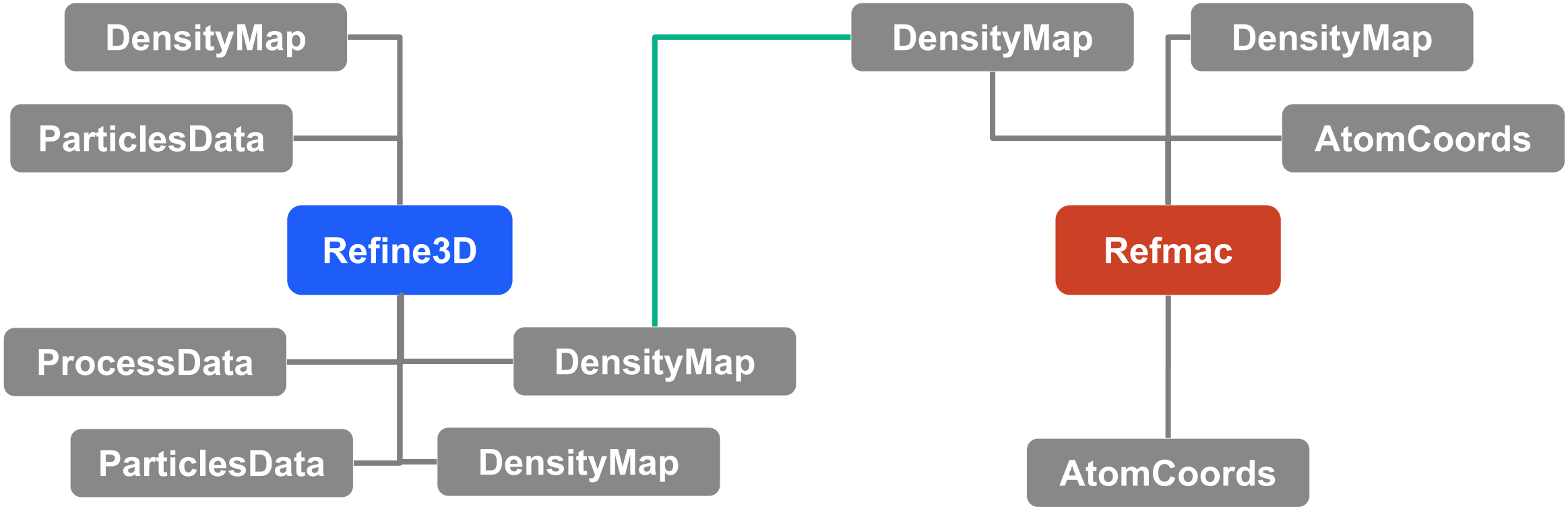

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Automating complex workflows

- ***CLI***

```
#!/user/bin/bash
pipeliner --start_new_project
pipeliner --schedule_job Import_job.star
pipeliner --schedule_job MotionCorr_job.star
pipeliner --schedule_job CtfFind_job.star

pipeliner --run_schedule --name Schedule1 --jobs Import/job001/ job002 CtfFind/new_alias --min_between 15
    --nr_repeats 3 --min_wait_before 2 -sec_wait_after 15

pipeliner --metadata_report job003
```

- ***Python API***

```
from pipeliner.api.manage_project import PipelinerProject

my_project = PipelinerProject()

my_project.schedule_job("Import_job.star")                  # adds Import/job001/ to the pipeline
my_project.schedule_job("MotionCorr_job.star")              # adds MotionCorr/job002/ to the pipeline
my_project.schedule_job("CtfFind_job.star")                 # adds AutoPick/job003/ to the pipeline

my_project.run_schedule(
          name="Schedule1",
          job_ids=["Import/job001/", "MotionCorr/job002/", "CtfFind/job003/"],
          nr_repeat=3,
          minutes_wait=15,
          minutes_wait_before=2,
          seconds_wait_after=15,
          )
my_project.get_network_metadata("CtfFind/job003/", "my_metadata.json")          # returns metadata
                                                                                # and all upstream jobs
```

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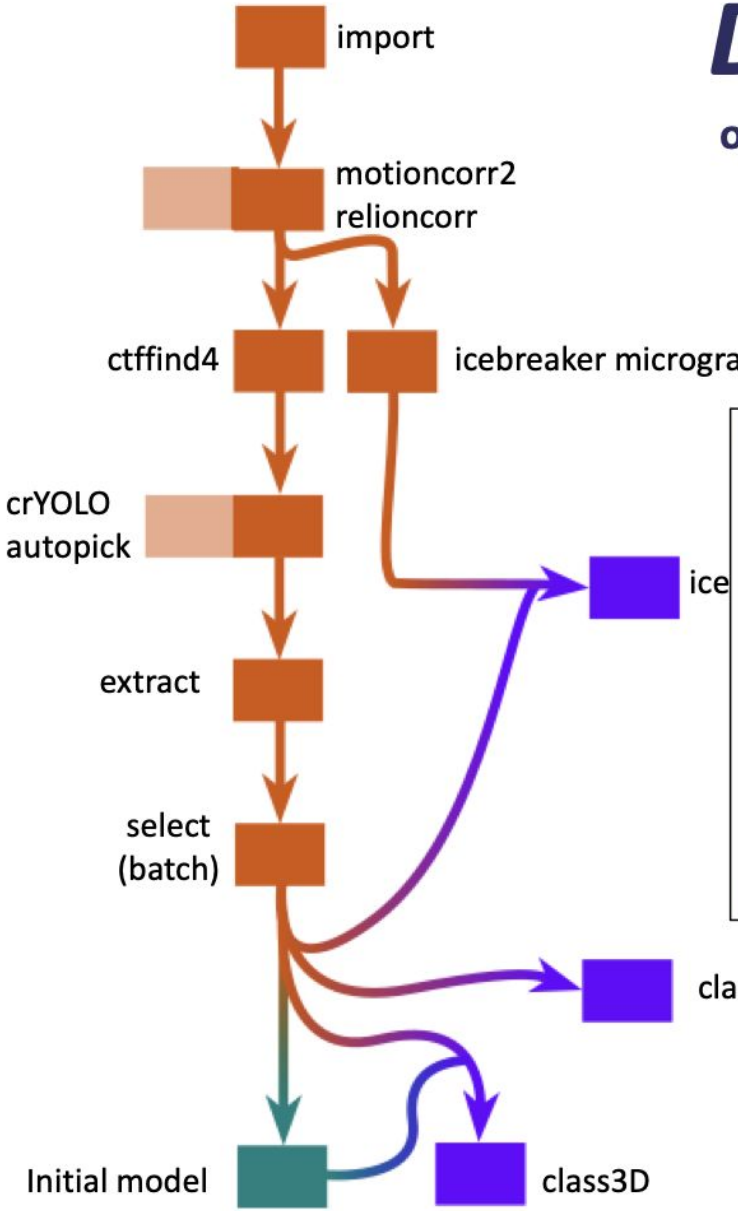
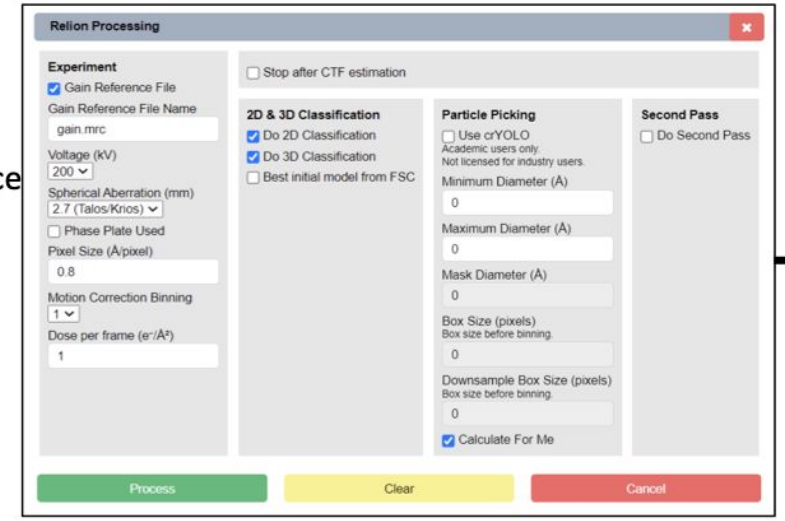
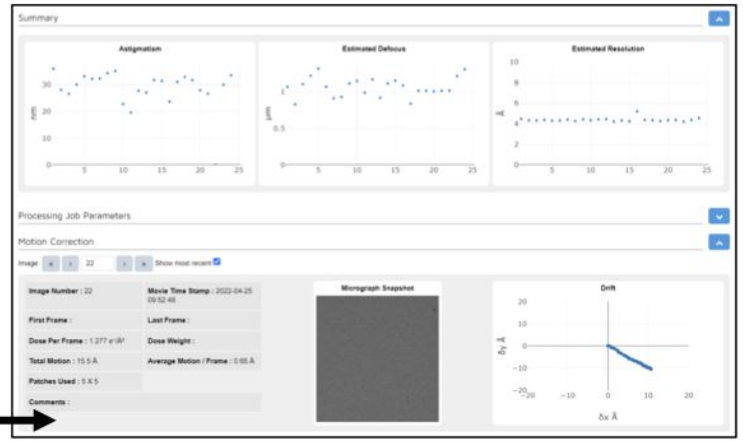
DLS/eBIC Processing

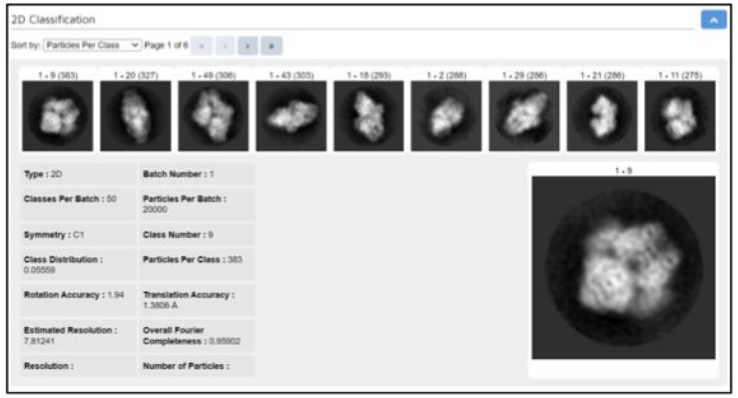
on-the-fly batched preprocessing and evaluation





ISPyB

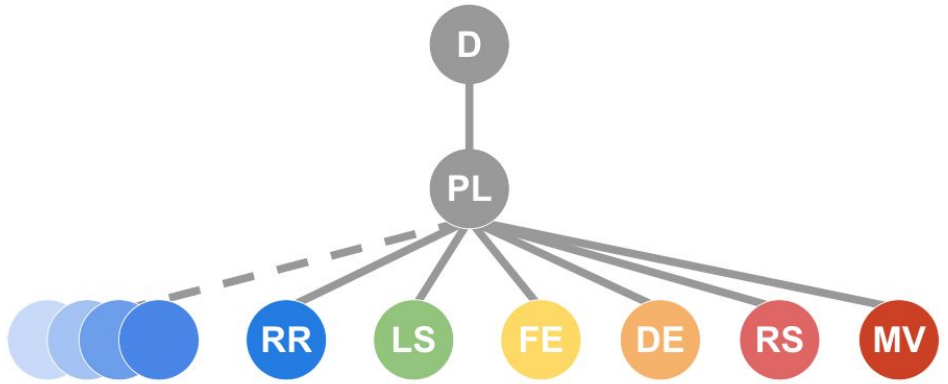


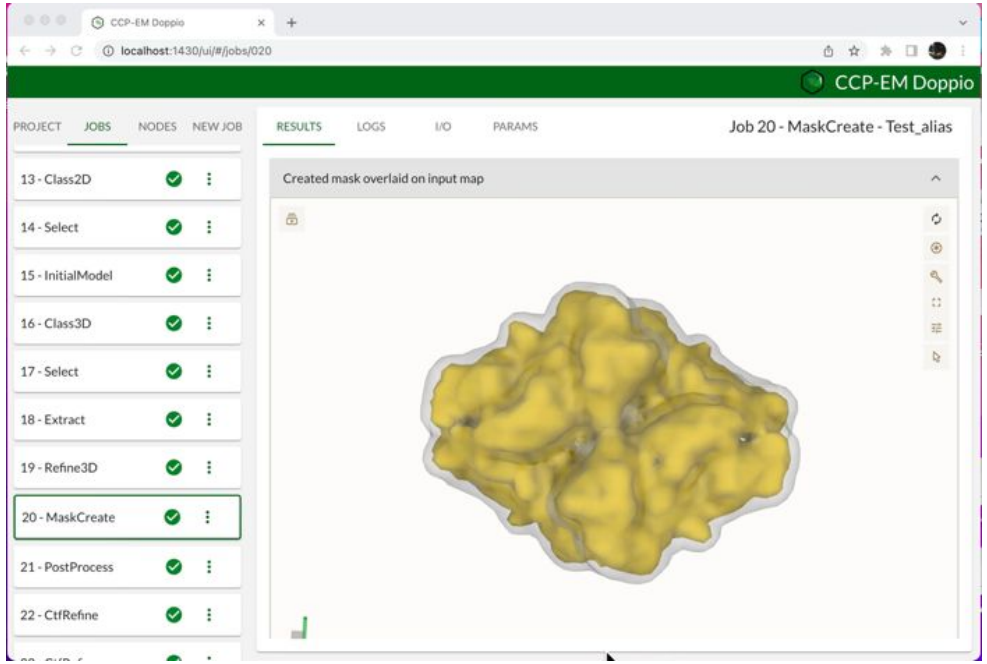


Dan Hatton Diamond Light Source

CCP-EM *Doppio*

- ***JavaScript UI***
- React.js / FastAPI / Material UI
- Remote browser app or local Electron app
- Task UIs auto generated from Python plugins
- Full support for ***Image Processing*** through to ***Model Validation***
- https://gitlab.com/ccpem/doppio
- STFC dual license
- Funding: BEIS / STFC BID / CCP-EM





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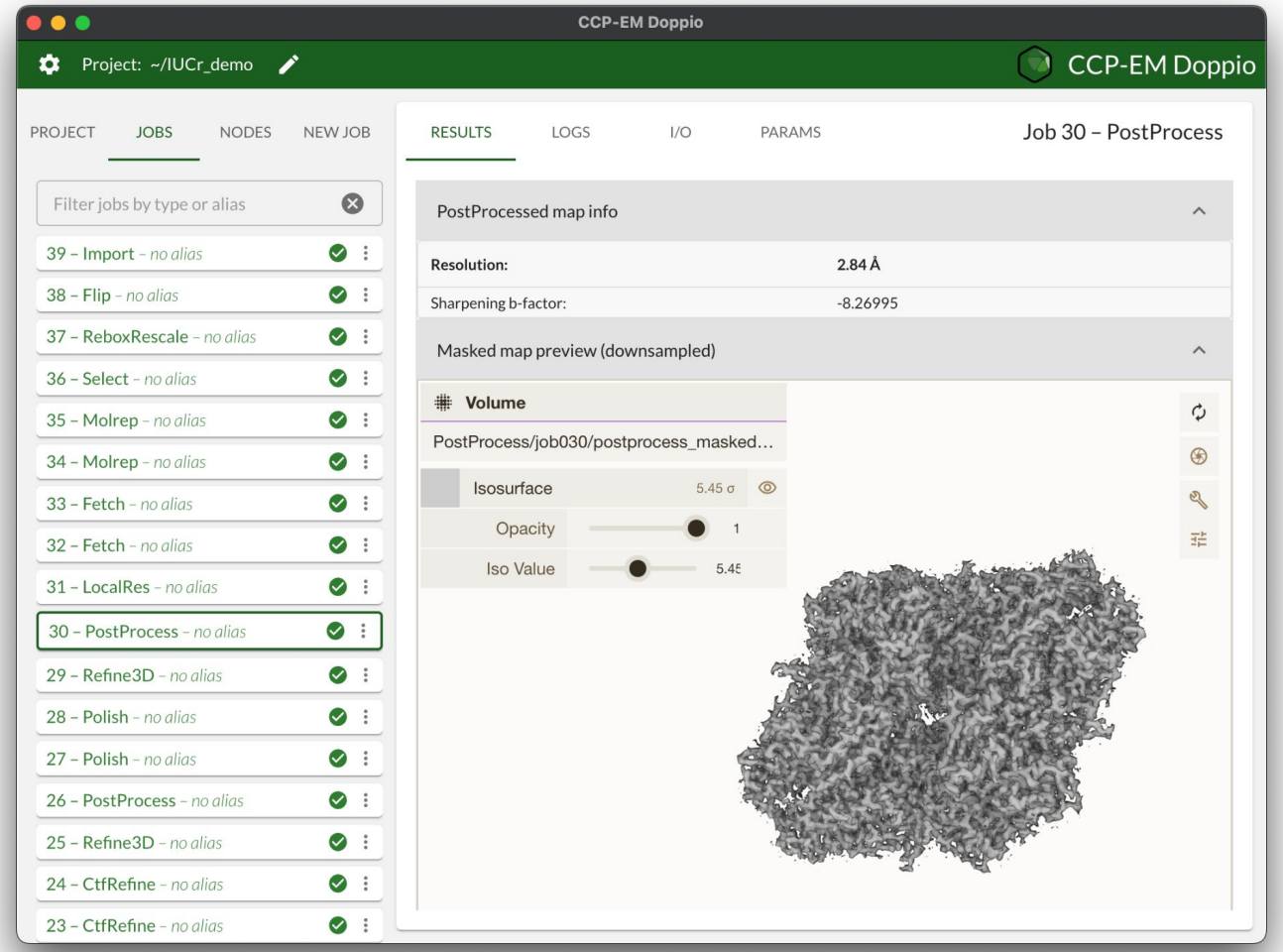
Doppio demo



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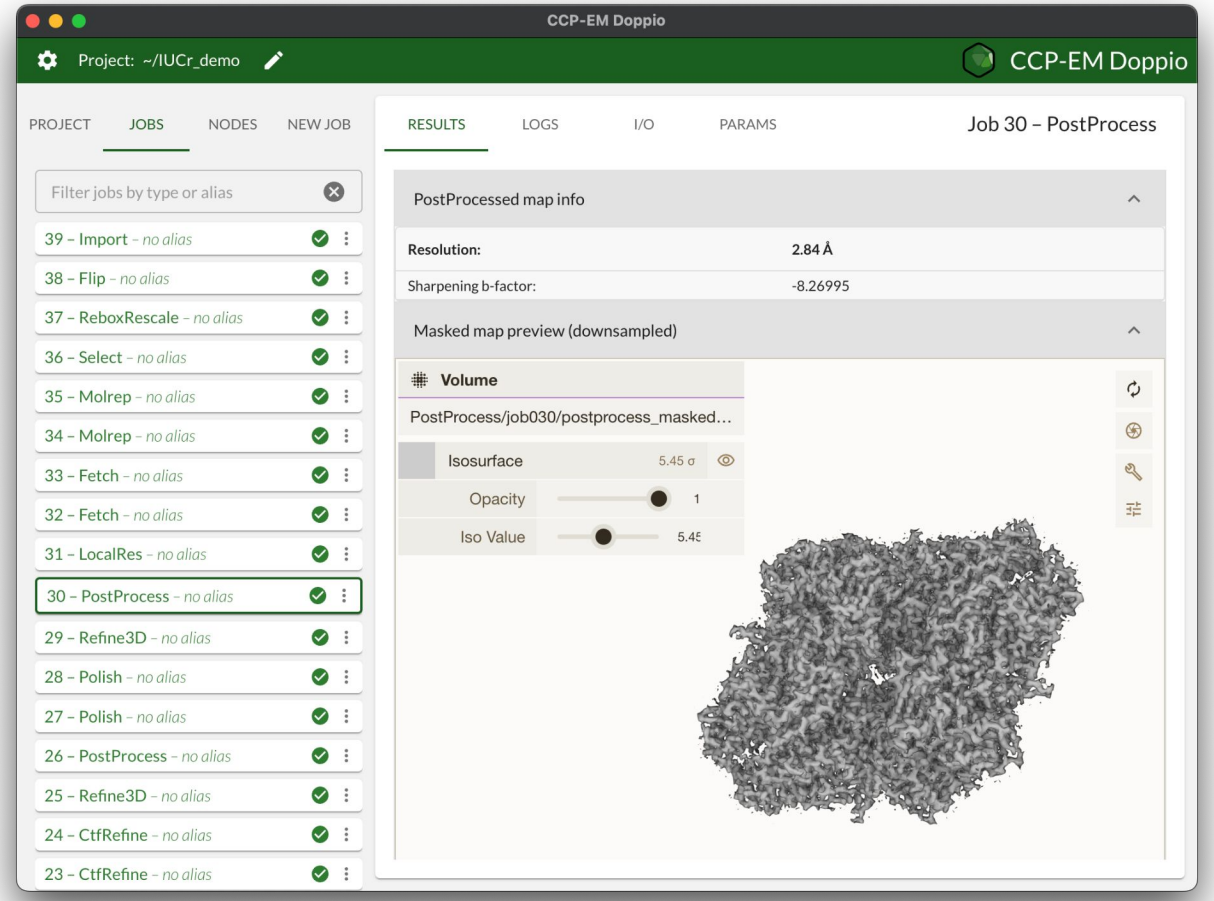
CCP-EM Doppio

- **Doppio 1.1.0**
  - Linux and Mac
  - Requires CCP-EM 1.x
  - Optionally CCP4 9.x & Relion 5.0

- **Future plans:**
  - Tomography STA Relion 5 pipeline
  - Conda based installation
  - Automated metadata deposition



www.ccpem.ac.uk/download.php

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Kaizen

Kaizen (Japanese: 改善, "improvement") is a concept referring to business activities that continuously improve all functions and involve all employees.

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CCP-EM Core Team

CCP4 Core Team

STFC Business & Innovation

CCP-EM Commercial License Holders

CCP-EM Collaborators

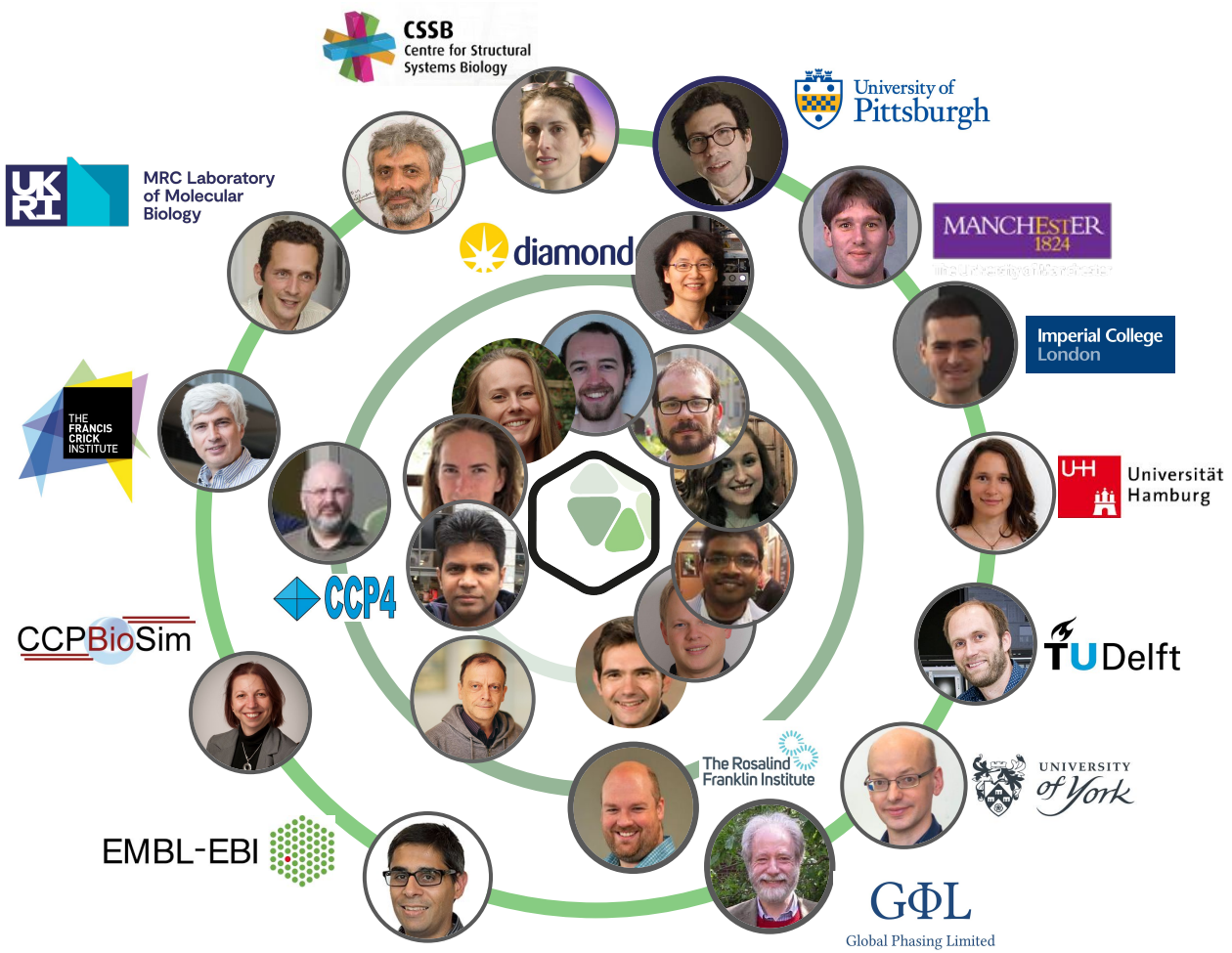
CCP-EM Users

Website: www.ccpem.ac.uk

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

Twitter: @ccp_em

Email: ccpem@stfc.ac.uk



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Research Complex at Harwell

Medical Research Council

wellcome

Department for Business, Energy & Industrial Strategy

GΦL Global Phasing Limited