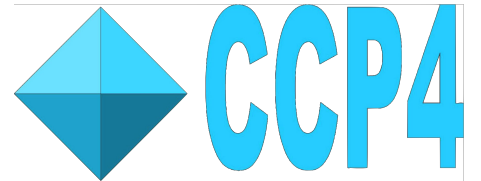


Moorhen ("Coot on the web")

Filomeno Sanchez
CCP-EM Lecture - October 2023



UNIVERSITY
of York



Motivation

- Offer coot users the ability to use coot in any device at any time.
- Facilitate access to crystallographic tools and model building to potential new users with little previous knowledge

Idea

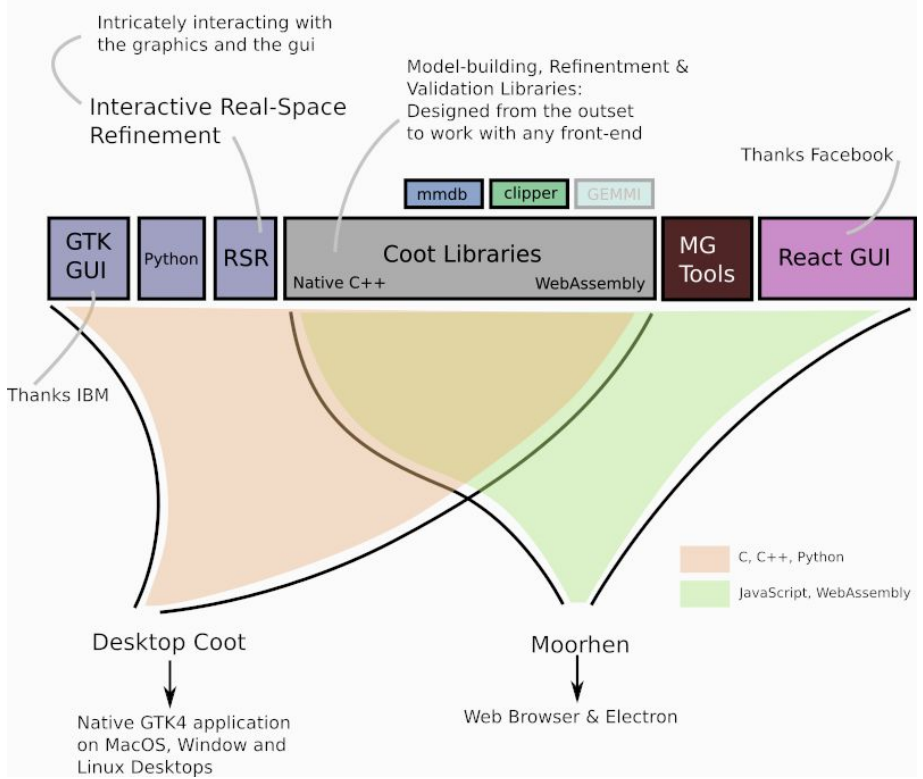
- Bring the coot experience into the browser: Moorhen.

Timeline

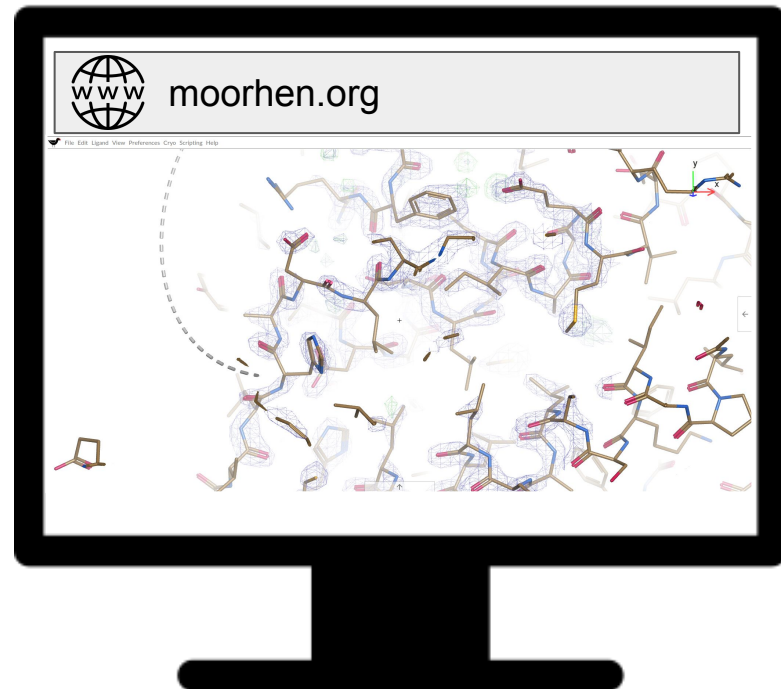
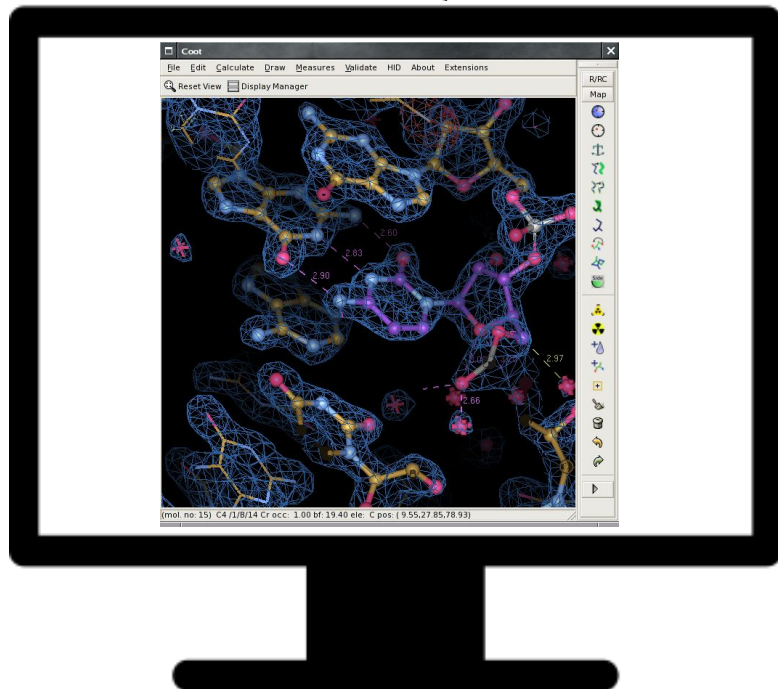
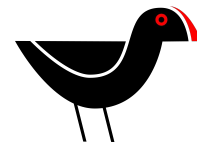
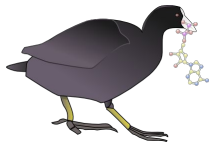


→ Moorhen is still under development... And we like feedback!

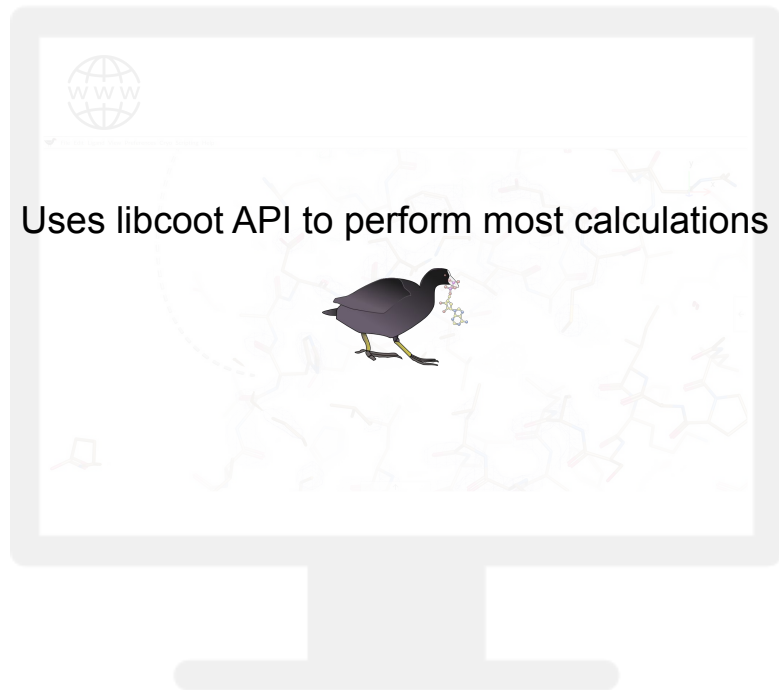
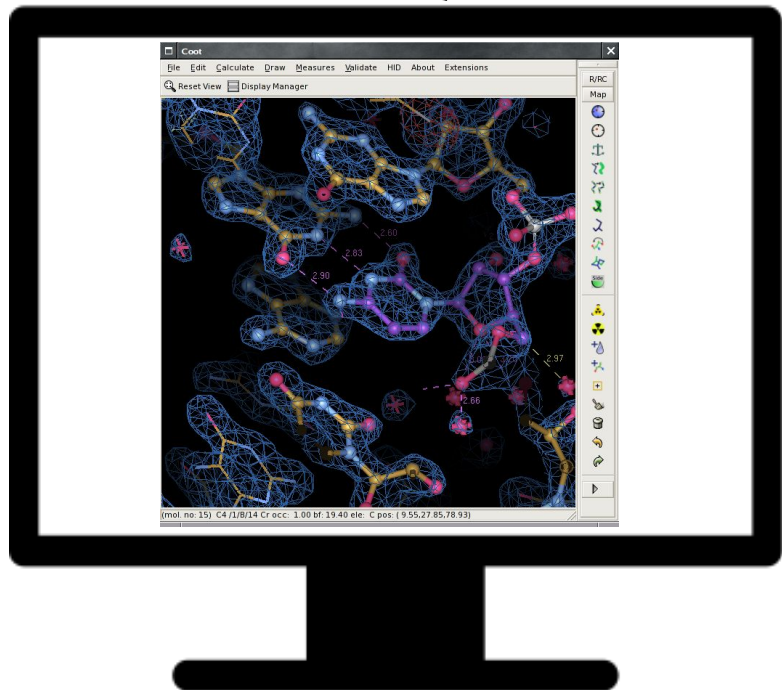
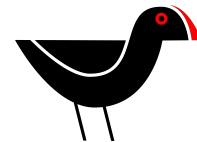
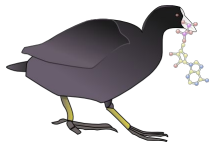
Coot vs. Moorhen



How does it compare to coot?



How does it compare to coot?



How does it compare to coot?

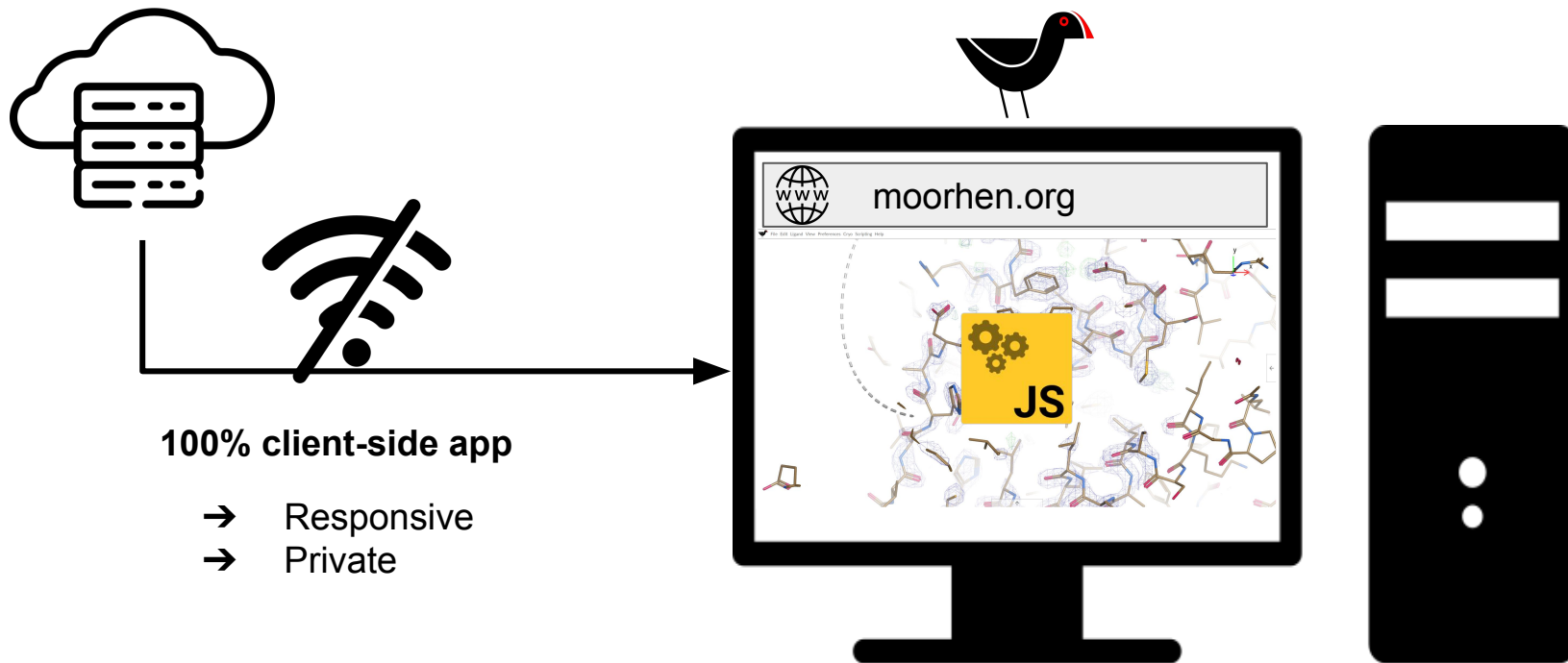
This is
a coot



This is a
moorhen



How does it work?



What can moorhen do?

Ligands

Fit ligand here

Get monomer

Validation tools

Ramachandran plot

Difference map peaks

MMRCC plot

Validation plots

Fill partial residues

Flip peptides

Edit tools

Cis / Trans

Rotate / Translate

Mutate

Real space refine

Add residue

Rotamers

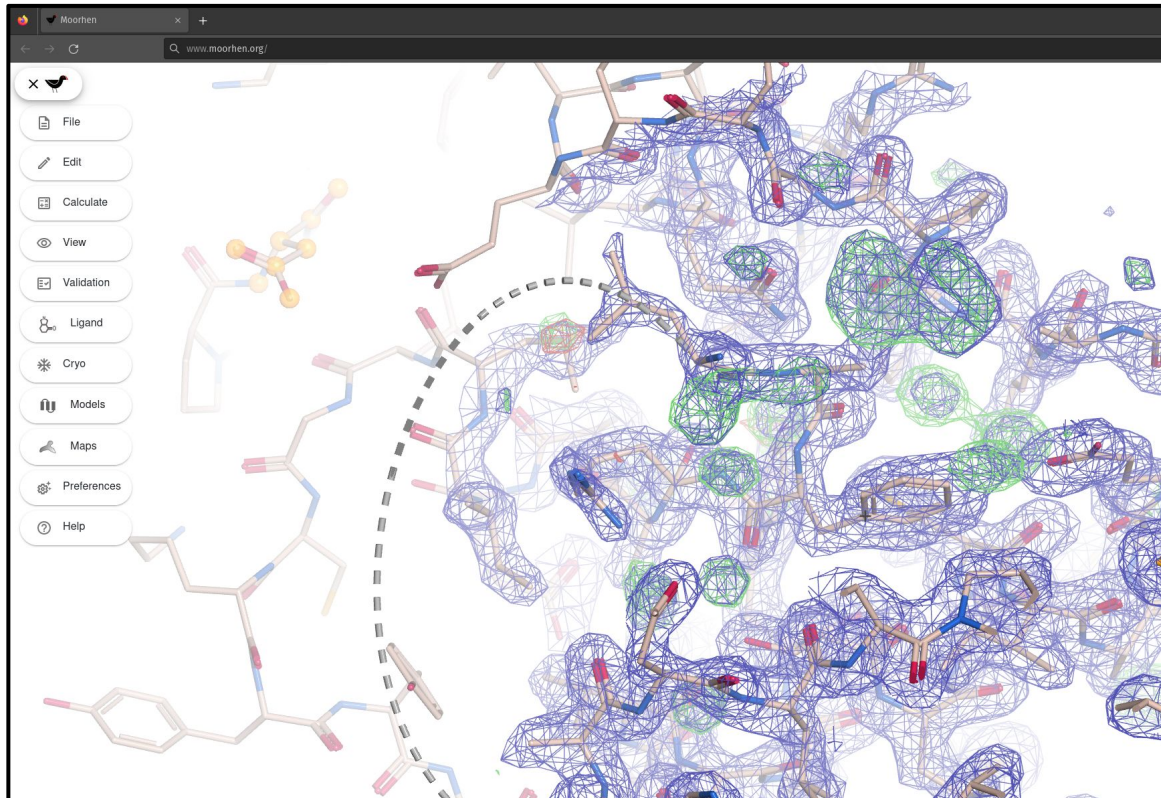
Updating maps, save state, AFDB fetch, symmetry, sequence selection, map masking, map blurring... and more!

Coot functions difficult to convert

- Carbohydrate Builder
- RCrane
- Pyrogen
- Gemmi-based Python
- **Lidia & FLEV**
- Coot-identify-protein
- Interactive Real Space Refinement
- RSR Morphing
- (Interactive) Sharpen/Blur

Where is it available?

www.moorhen.org



Where is it available?



CCP4 Cloud

A screenshot of the CCP4 Cloud web interface. The interface is titled "Gamma" and shows a list of tasks. The main task, "[0123] ccp4build - running", is expanded to show a list of sub-tasks under the heading "Coot (1)". The sub-tasks are: "Model Building with Coot" (with a red stop sign icon), "Edit Coordinates with Coot" (with a red stop sign icon), and "Model Building with WebCoot/Moorhen" (with a yellow checkmark icon). Below the task list is a graph showing "Cycle No." on the x-axis (0.5 to 3.5) and a y-axis (0.25 to 0.26). A "Print" button is located below the graph. At the bottom of the interface, there is a status bar with "Powered by CCP4 v8.0.010", logos for CCP4, iris, and CCP4 Cloud v1.7.11 [10.03.2023]. In the background, a 3D molecular model is visible in a window titled "[0123] CCP4Build current structure", showing a blue mesh structure with a stick model overlaid. A tooltip for the model shows "molecule/1/A/117(SER)/CA" and "Cycle 3: N_{res}=123 (100.0%), R/R_{free}=0.2685/0.3142".

Where is it available?

Coming soon...



The screenshot displays the CCP-EM web interface. At the top, a dark green header shows "Project: ~/ccpem-project" with a gear icon and a pencil icon. Below the header, there are four tabs: "PROJECT", "JOBS", "NODES", and "NEW JOB". The "JOBS" tab is active, showing a search bar "Filter jobs by type or alias" and a list of jobs:

- 7 - Fetch - coot-em-tutorial (with a green checkmark and a vertical ellipsis menu)
- 6 - Fetch - occupy-16890 (with a green checkmark and a vertical ellipsis menu)

Below the jobs list, there are four tabs: "RESULTS", "LOGS", "I/O", and "PARAMS". The "I/O" tab is active, showing "Open with:" options: "PDF VIEWER", "TEXT EDITOR", "UGLYMOL", "MOL*", "MOORHEN", and "TERMINAL". An arrow points to the "MOORHEN" button. Below this, it says "Inputs to this job: no inputs" and "Outputs from this job:" followed by two output entries:

- Fetch/job007/emd_32143.mrc (with a green checkmark, a "DensityMap" label, and "from_emdb")
- Fetch/job007/pdb7vvl.pdb (with a green checkmark, an "AtomCoords" label, and "from_pdb")

How does it look like?

Acknowledgements

Stuart McNicholas



Paul Emsley



Kevin Cowtan

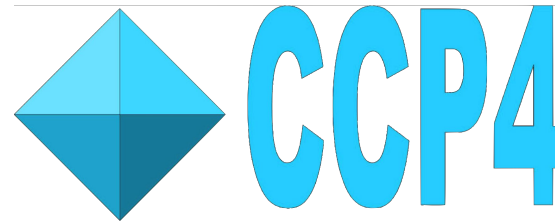


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Eugene Krissinel



Martin Noble



* **Special thanks to George Coldstream for integrating Moorhen into Doppio!**