Poster

Introducing the next major release of CCP4: What's new?

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CCP4 released version 9.0 of the CCP4 [1] software suite this summer. It delivers an infrastructural upgrade to Python 3.9 and new features in the graphical user interface, ccp4i2. Other highlights of this release include DIALS 3.18+ [2] with its graphical user interface, DUI2, which now supports multitasking and remote control. The release brings deeper integration with Coot scripting [3] and introduces Moorhen, also known as 'WebCoot' [4]. More PDB-REDO [5] tools have been incorporated in the suite. The suite provides automated pipelines and tools for the macromolecular structure solution process, such as Xia2 for data-processing, MrBUMP, MorDA [6] and ARCIMBOLDO for molecular replacement, CRANK2 for experimental phasing, ModelCraft for model building and others (cf. [1]). There is continued development of tools to use predicted models in phasing (MRParse, SliceNDice), model building and validation (Conkit). Monthly updates bring new developments to the suite.

The upgraded CCP4 Cloud [7] delivers the full model building functionality online through integrated Moorhen. It can be linked with data producing facilities to provide a one-stop shop for the structure solution. It now has a Data Fetch feature which uses the new DataLink service, allowing users to fetch diffraction image data from external repositories such as SBGrid, XRDa, IRRMC, as well as Globus endpoints. A highly requested feature has been a dark theme, which has now been implemented. The Molecular Replacement task in CCP4 Cloud now benefits from using predicted models imported from the AlphaFold database (AFDB) or generated from the given sequence by running AlphaFold2 directly in CCP4 Cloud.

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