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Structure Determination Online with CCP4 Cloud

CCP4 Cloud is a front-end for the CCP4 Software Suite, which represents a new approach to developing, organising and maintaining crystallographic projects and running CCP4 programs. It exploits the paradigm of remote computing, when all projects and data are kept online and tasks are executed on remote servers. CCP4 Cloud is designed for deployment at scientific centres and data-producing facilities (synchrotron beamlines). The system complements remotely driven, online experiments with online structure solution, starting from image processing to deposition in the PDB.

Obvious benefits of a fully online approach to structure determination are in the optimal use of resources, both experimental and computational, and systemic approach to data management, which includes retention of structure solution projects, the usually missing link between experimental data and their interpretation in form of solved structures.

CCP4 Cloud includes tasks for all stages of computational structure determination and provides integrated access to relevant web-resources (PDB, UniProt, AlphaFold, ESM etc.) and 3rd-party software (e.g., Buster from Global Phasing and PDB-REDO from NKI, Amsterdam). A set of automated tools are provided for image processing, phasing, model building, refinement, validation and preparation for deposition in the PDB. As a unique feature, CCP4 Cloud offers automatic development of structure solution projects, which can deliver a full solution, and allow for user intervention when a good-quality solution is not achieved. CCP4 Cloud projects can be initiated online in a web-browser or via background push of data from point of collection.

CCP4 Cloud facilitates teamwork by providing a shared access to structure solution projects, when several researchers can work simultaneously in real time on the same project. The projects can be also exchanged as zip files and stored locally in personal archives. Alternatively, projects can be archived in CCP4 Cloud and made accessible via stable web-links similar to DOI, a feature that can be used at publishing, refereeing, education and exchange within a wider collaboration.

CCP4 maintains a publicly available instance of CCP4 Cloud at https://cloud.ccp4.ac.uk, and several private instances have been deployed at other academic and industrial sites. CCP4 Cloud is included in standard CCP4 distribution and runs out-of-the-box on the user's machine. CCP4 encourages wider use of CCP4 Cloud, especially at data-producing facilities, in hope that it will grossly improve and streamline user experience in MX structure determination, data and project management.

Primary authors: Dr KRISSINEL, Eugene (CCP4); Dr LEBEDEV, Andrey (CCP4); Ms FANDO, Maria (CCP4); Dr BALLARD, Charles (CCP4); Dr USKI, Ville (CCP4); Dr KEEGAN, Ronan (CCP4)

Presenter: Dr KRISSINEL, Eugene (CCP4)