Solving Macromolecular Structures Online with CCP4

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For over 40 years, the Collaborative Computational Project Number 4 in Protein Crystallography (CCP4) has maintained, developed, and provided an integrated Suite [1] of world-class software that allows researchers to determine macromolecular structures by X-ray crystallography and other biophysical techniques.

Traditionally, the Suite is operated via CCP4i(2) graphical user interface, available for all major desktop platforms. More recent developments include interfaces that offer users the convenience of crystallographic computing on mobile devices and access to cloud-based resources. There are several good reasons for exploiting the distributed computing paradigm in crystallography.

First, cloud-based solutions have become particularly appealing given recent advances in automated structure solution methods. Such methods are demanding for both computing power and various databases, making them less convenient for offline setups.

Second, the cloud model of operations relieves researchers from the burden of maintaining software locally, providing 24/7 access to always ready, tested, and updated software setup.

Third, cloud computing streamlines data management and logistics. Collected data may be put in cloud-based projects directly from synchrotrons, bypassing offload to user devices. Cloud projects can be shared in real-time between a team of researchers working from various geographic locations. This aspect has been particularly helpful at the virtual CCP4 workshops during the pandemic.

CCP4 currently provides two interfaces for online work [2]. CCP4 Online, started from automatic Molecular Replacement service "BALBES" in 2008, is a web portal allowing users to run in the cloud the molecular replacement and experimental phasing pipelines in the CCP4 suite. In 2020, CCP4 released an advanced online platform, CCP4 Cloud, featuring a full desktop experience online. CCP4 Cloud includes an HTML5 interface for most crystallographic tasks and allows to develop and maintain structure solution projects completely online using common web browsers on any modern platform, including mobile devices.

We will discuss the latest developments, achieved results, and future directions. Providing a global computing infrastructure for protein crystallography is now a feasible task; are we ready to accept it in practice?

[1] M. D. Winn et al. Acta. Cryst. D67, 235-242 (2011)

[2] E. Krissinel, V. Uski, A. Lebedev, M. D. Winn, C. Ballard. Acta Cryst. D74: 143-151 (2018)

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