Microsymposium

MS51.O05

CCP4 web services

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The CCP4 software suite [1] provides a comprehensive set of tools for use in the macromolecule structure solution process by X-ray crystallography. Traditionally, these tools have been run through the graphical interface or the command line on each user's personal workstation. Recently, some of the tools, including the molecular replacement pipelines Balbes [2] and MrBUMP [3] have been provided as web services in the Research Complex at Harwell. These pipelines can be especially useful in cases where there is low sequence identity between the target-structure sequence and that of its set of possible homologues. These services can be accessed through a web client, allowing one to submit molecular replacement jobs to our Linux cluster and view the results from these jobs. The molecular replacement pipelines are ideal candidates for web services, as they require installation and maintenance of large databases and benefit from parallel computing resources, provided by the cluster. Further plans for web services will be discussed. With ever-increasing mobility of scientific setups and the ubiquity of ultra-portable devices, there is a demand for a consistent framework of remote crystallographic computations and data maintenance. This framework is planned to include an interface for synchronising data with the facilities of Diamond Light Source, as well as with local CCP4 GUI-2 setups.

[1] *M. D. Winn et al., Acta. Cryst., 2011, D67, 235-242,* **[2]** *F. Long et al., Acta. Cryst., 2008, D64, 125-132,* **[3]** *R. M. Keegan et al. Acta. Cryst., 2011, D67, 313-323*

Keywords: biological macromolecular X-ray crystallography, software for crystallography, crystal structure determination