Poster Presentations

[MS04-P07] CCP4 web services. Ville Uski, Charles Ballard, Ronan Keegan, Eugene Krissinel, Andrey Lebedev, David Waterman, Marcin Wojdyr

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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 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. There is ongoing work to include a new pipeline, AMPLE [4], as a web service. 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*. D67, 235-242 (2011)
[2] F. Long *et al. Acta. Cryst.* D64, 125-132 (2008)
[3] R. M. Keegan and M. D. Winn. *Acta. Cryst.* D64, 119-124 (2008)
[4] D. J. Rigden et al. Acta. Cryst. D64, 1288-1291 (2008)