

CCP4 web services

Ville Uski

CCP4, Research Complex at Harwell, Rutherford Appleton Laboratory, Didcot OX11 0FA, UK

Software as a service has become a popular software-delivery model with the advent of cloud computing. In this model, the software and the related data are centrally hosted on the cloud (network of remote computers), instead of installed on each user's personal computer, and they are typically accessed by using a thin client via a web browser, the so-called web application. Some of the benefits of the web applications as opposed to desktop applications include the lower cost of software maintenance and easier scalability of resources. Moreover, the ubiquity of ultra-portable devices has put forward the idea of having super-computing facilities available via the internet on the go.

Web services have recently stirred interest among macromolecular crystallographers, due to the increasing rate and volume of data collected in the experiments, and the complexity of computational setups, posing difficulties for small to medium size laboratories with limited access to full-scale IT support. There are already various web services hosted by facilities such as Diamond, which provides automatic data analysis and long-term data storage solutions with web access, and EMBL-Hamburg with its [ARP/wARP model-building web service](#). CCP4 has recently incorporated in its strategy a focus on cloud computing. The plans include collaborations with Diamond and the new CCP4 GUI, which would include access to CCP4 web services through RESTful APIs.

CCP4 has provided [some utility programs](#) as a web service for almost 10 years now. The idea was originally to expand the service as an alternative way to run such utilities without needing to install the whole CCP4 software suite. While this service has not been actively maintained for some time now, there have still been some users. More recently, the Balbes webserver has migrated from the York Structural Biology Laboratory to the Research Complex at Harwell, and was taken over by the CCP4 core team. [This webserver](#) provides the Balbes molecular replacement pipeline (Long et al, 2008) as a web service (see figure 1). Using the web service has perhaps been the most common way to run the pipeline, and there have been many users.

CCP4 Collaborative Computational Project No. 4 Software for Macromolecular X-Ray Crystallography

Home

Welcome to BALBES Web Server

Any problems? - please contact flong@mrc-lmb.cam.ac.uk

Runnable Programs
[Login](#) to run Balbes
Other Options - [Register](#), [Forgotten Password](#), [Change Password](#)

Downloads
Click on the links below to download and access documentation for other CCP4 programs:

Balbes	an automated molecular replacement (MR) pipeline
Molrep	an automated program for molecular replacement
Refmac	a macromolecular refinement program
Jligand	a Java interface which allows links descriptions to be created
Sfcheck	assessment of X-ray data and/or agreement between atomic model and X-ray data
CCP4	general CCP4 page with links to downloads
CCP4mg	an easy way to create beautiful publication quality images and movies

wellcome trust
MRC Medical Research Council
BBSRC
MRC

Figure 1: Web front-end of the Balbes molecular replacement pipeline.

Under the hood, as it were, the Balbes webserver is a Java servlet application, implementing the model-view-controller software architecture pattern. It runs in the Tomcat servlet container. Its development started over 10 years ago by Paul Young, was further developed by Fei Long, and recently modified by the CCP4 core team. The new webserver under development is also written in Java and implements the same architecture. However, it makes use of some of the modern Java frameworks, such as Tapestry, Hibernate and Shiro, and will implement APIs following the [RESTful](#) design model. Using the frameworks improves the scalability, security and the ease of maintenance of the web services, and makes it relatively easy to improve the user experience with the help of [Ajax](#) features.

Molecular replacement (MR) is an excellent candidate for a web service, as it requires large databases and can involve large-scale computations. MR pipelines implement computationally intensive tasks that can greatly benefit from parallelisation. The Balbes webservice is a front-end for Balbes, which runs in our Linux cluster. This pipeline has not yet been parallelised, but we are currently in the process of setting up a web service for MrBUMP (Keegan and Winn, 2008), which has been parallelised. The webservice will have a new front-end, including both Balbes and MrBUMP. Yet another computationally intensive MR pipeline, AMPLE (Bibby et al, 2012), will be included next.

There are several other CCP4 applications that are tentatively planned to become web services. These include various automatic pipelines for data processing, experimental phasing, model building and validation. Other ideas include web interfaces to CCP4's structure solution components and useful utilities.

References

- Long F., Vagin A., Young P. and Murshudov G.N. "BALBES: a Molecular Replacement Pipeline" (2008). Acta Cryst. section D64, 125-132.
- Keegan, R.M. and Winn, M.D. "MrBUMP: an automated pipeline for molecular replacement" (2008) Acta Cryst. D64, 119-124
- Bibby J., Keegan R. M., Mayans O., Winn M. D. and Rigden D. J. "AMPLE: a cluster-and-truncate approach to solve the crystal structures of small proteins using rapidly computed ab initio models" (2012) Acta. Cryst. D68, 1622-1631