The Role of *e*-Science in Service Crystallography: The UK National Crystallography Service on the Grid

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The The EPSRC funded UK National Crystallography Service (NCS) facility has been exploring the use of Web/Grid services in e-Science applications. The NCS approach[1,2] combines aspects of software and instrument automation to produce a service that increases user interaction and provides sample submission and data acquisition, processing and analysis services on the Grid.

A prospective user of the NCS applies for an allocation by filling in an electronic form and uploading a case for support, initiating the metadata capture process. Following successful peer review, the user and is provided with digital keys that enable secure access to the NCS Grid Facility. The user may now submit samples to the NCS through an electronic interface, which gathers all the chemical metadata concerning the sample, e.g. synthetic pathway, proposed formula 2D structure, sensitivity, COSHH safety information, etc.

A sample status database is used to monitor the progress of sample(s) in the queuing system. When a sample is scheduled for examination the user may initiate a secure, Web services based, interactive experiment from the sample status database. The crystal is mounted on the diffractometer by the sample changing robot or by a service operator. The user is then involved in a series of decision making stages, either automatically or with the service operator, which control the outcome of the unit cell determination and data collection procedures. At the conclusion of the experiment the data is automatically processed and made available to the user for download.

[1] S.J. Coles, J.G. Frey, M.B. Hursthouse, M.E. Light, K.E. Meacham, D.J. Marvin & M. Surridge. *J. Appl. Cryst., Submitted* [2] Coles S.J., Frey J.G, Hursthouse M.B., Light M.E., Surridge M., Meacham K.E., Marvin D.J., De Roure D.C. , Mills H.R., (2002). In Hopgood, F.R.A., Matthews, B. and Wilson, M.D. (eds.), British Computer Society. (http://eprints.soton.ac.uk/346/)

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