with data to 2.5 Å or better.

Xsolve, a Java Message Service (JMS) based control system, can run on a Linux cluster different processing strategies in parallel, e.g. the data can be processed in several different space groups or MAD/SAD structure determination can be attempted using various wavelength combinations.

Xsolve supports a wide range of crystallography software programs, which can be used in parallel: data reduction with Mosflm, Denzo/HKL2000, XDS and Scala; heavy atom solution and phase determination with Solve, SHELXD/E and Sharp; phase improvement with Resolve and model building with Resolve and ARP/wARP.

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Keywords: automatic structure solution, MAD, software

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Iterative Model Building and Evaluation with Statistical Density Modification

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Automated model-building beginning with an FFT-based search for helices and sheets and followed by chain extension using tripeptide fragments from high-resolution structures and pattern-based probabilistic identification of side chains has been successful in automated model building for maps with resolution as low as 3 A. Model-building can be combined with refinement and statistical density modification to improve the quality and completeness of atomic models of macromolecules and to evaluate the quality of atomic models. A useful tool in removing model bias is prime-and-switch phasing. In this technique a substantially correct model containing some atoms in incorrect positions is used to estimate ("prime" initial phases, and a second source of phase information such as a flat solvent region is used without reference to the original phase probabilities in density modification. After prime-and-switch phasing the density at incorrect atomic positions is often considerably decreased compared to that at correct positions. This technique has been incorporated as an integral part of iterative model-building and refinement in the PHENIX software (http:www.phenix-online.org).

Keywords: model building, PHENIX, atomic models

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Automated Operation of Protein Crystallography Beamlines at the SPring-8

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RIKEN Structural Genomics Beamlines (BL26B1&B2) at the SPring-8 have been constructed for high throughput protein crystallography. The beamline operation is automated cooperating with the sample changer robot named SPACE (SPring-8 Precise Automatic Cryo-sample Exchanger) [1].

Since April 2004, BL26B2 has been continuously operated with the sample changer. More than twenty-five crystals a day have been constantly delivered by sample-tray to the beamline. The crystal screening at the beamline can be finished within ten minutes per a sample. For qualified crystals, unattended data collections have been perpetually performed. The sample-tray is portable with a Dewar and experimental conditions are uploaded to the web site, which have been developed considering the mail-in data collection.

The operation software BSS (Beamline Scheduling Software) provides the intuitive GUI and unified control of beamline instruments with the networked client-server architecture. The software structure has flexibility to be implemented at other protein crystallography beamlines. Other than BL26B1 and B2, three other beamlines have already adopted BSS. Further application to other beamlines is progressing to achieve the unified and user-friendly environment among all beamlines at the SPring-8.

[1] Ueno G., Hirose R., Ida K., Kumasaka T., Yamamoto M., *J. Appl. Cryst*.,2004, **37**, 867-873.

Keywords: automated data collection, high-throughput protein crystallography, mail-in data collection

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Automated Protein Structure Determination with *BnP*

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BnP[1] is a protein structure determination package with a graphical user interface suitable for both manual and automated operation. *BnP*'s main function is to couple the direct-methods program *SnB*, used to determine heavy atom/anomalous scatterer substructures, with the protein-phasing package *PHASES*, used for heavy atom refinement, protein phasing, density modification, and skeletonization. It also creates data and scripts for external programs required for automated chain tracing, graphical visualization, and refinement. In addition to seamlessly interfacing the various packages, near total automation is implemented such that one needs only to specify a few parameters, and the entire phasing process starting with diffraction data and resulting in interpretable electron-density maps is carried out by clicking a single button. With a couple of additional button clicks external programs for automated chain tracing or chain tracing/refinement can then be launched. The overall strategies and methodology employed will be described, with emphasis on those aspects required to facilitate automation and recent developments simplifying user input. Extensive test results verify the package's effectiveness. This work was supported by NIH grant EB002057.

[1] C. M. Weeks et. al., *Z. Kristallogr*., 2002, **217**, 686-693.

Keywords: automated structure determination, high-throughput, phasing methods

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MS42 COMPLEMENTARITIES OF NEUTRON AND X-RAYS METHODS IN MATERIAL SCIENCE

Chairpersons: Andreas Schreyer, Mark R. Daymond

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Integrated Use of Synchrotron and Neutron Diffraction to Monitor Residual Stress Evolution in Welded Aerospace Structures

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The factors controlling fatigue initiation and crack growth in welds are reasonably well understood and the importance of residual stress, HAZ hardness and microstructure is well known. However, previous access to reliable, spatially accurate residual stress field data has been limited. Recent advances in neutron and synchrotron diffraction allow a far more detailed picture of weld residual stress fields to be obtained which permits the development and use of predictive models that can be used for accurate design against fatigue in aircraft structures. This paper describes a fully integrated study of the 3D residual stress distribution accompanying state-of-the-art fusion welds in 2024 and 7150 aluminium aerospace alloys, and how they are affected by subsequent machining and service loading. A particular feature of this work has been the development of integrated neutron and synchrotron techniques allowing the non-destructive evaluation of the residual stress field in the full range of specimens used to provide the design data required for welded aircraft structures. This has included small bend specimens used to study initiation and short fatigue crack growth, centre-cracked panels used to study long fatigue crack growth, and large integral welded double stringer/skin mock-ups used to investigate the likely failure mode of welded wing-