

W0317

The Integration of Data Collection, Data Reduction and Structure Solution - From Diffraction Images to an Initial Model in Minutes. W. Minor¹, M. Cymborowski¹, K. Lazarski², M. Chruszcz¹, Z. Otwinowski³, A. Joachimiak², Z. Dauter⁴, ¹Univ. of Virginia, Charlottesville, VA 22908, ³UT Southwestern Medical Center at Dallas, TX 75390, ²Argonne National Laboratory, Argonne, IL 60439, ⁴National Cancer Inst., Argonne Station, Argonne, IL 60439.

A new approach that integrates data collection, data reduction, phasing and model building significantly accelerates the process of structure determination and, on average, minimizes the number of data sets and synchrotron time required for a structure solution. The initial testing of the system with 50+ of novel structure determinations proved its high value for MAD/SAD experiments. The heuristics of choosing the best computational strategy for different data resolution limits of phasing signal and crystal diffraction are being optimized. Typical end result is interpretable electron density map with partially built structure and in some cases even almost complete, refined model. The current development is oriented towards a very fast structure solution, in order to provide feedback during the diffraction experiment. Work is also proceeding towards improving the quality of phasing calculation and model building.