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Parallel Workflow Engine to Optimize the Program and Parameter Space Searching for Protein Structure Determination. Zheng-Qing Fu, John Rose, Bi-Cheng Wang, Southeast Collaboratory for Structural Genomics, Dept. of Biochemistry & Molecular Biology, Univ. of Georgia, Athens, GA 30602..

Our concept of automation includes not only the automatic execution of a series of popular crystallographic programs, but also automatic searching of best combination of programs and input parameters that bring out the best performance of individual programs and thus, maximize the success of structure solution from a given crystal. This automated process is carried out by a parallel workflow engine (Fu et al., to be published) designed for the automation of the whole process from protein crystal data collection, data reduction, to structure determination. Current version of the program includes the signal-based data collection protocols using: (1) the Ras index (Fu, *et al.*, Acta Cryst. D60:499-506, 2004) to monitor the signal/noise ratio during data acquisition; (2) new software for more efficiently correcting experimental errors in diffraction data; (3) parallel workflow engine with a library of crystallographic computer programs plugged-in for optimization of structure-solving process.

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