

## W0396

**A Generic Way to Combine Crystallographic Software.** Jeremy Praissman, Dawei Lin, Zhi-jie (James) Liu, Wolfram Tempel, John Rose, Bi-Cheng Wang, Southeast Collaboratory for Structural Genomics, Dept. of Biochemistry & Molecular Biology, Univ. of Georgia, Athens, GA 30602.

Software pipelines have proven useful in high-throughput crystal structure determination. They have increased structure determination success rate by enabling more extensive exploration of the crystallographic parameter space, especially when high performance computing resources are available (Praissman et al. Abs. 01.07.07, ACA meeting, July 2003). Although there are a number of frameworks available for constructing software pipelines, few offer generic solutions for connecting external programs together without significant programming efforts.

This has limited development of pipelines involving more complex analyses, such as screening rotation and translation solutions for molecular replacement.

We are attempting to solve these problems by keeping track of the types of inputs and outputs of programs involved in a pipeline. This “type” information can be used by the framework to automatically determine the order in which the programs must be run and the method for mapping the outputs from one stage of execution (one set of programs) to the inputs of another stage. This approach has been successfully used to build a molecular replacement pipeline based on Phaser.

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