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SGXPRO: A Versatile Structure Solving Engine for Structural Biology/Genomics. Bi-Cheng Wang[1], Zheng-Qing (Albert) Fu[1], Yunzhou Wu[1], Dongsheng Che[2], Jizhen Zhao[2], Haijin Yan[2], John P. Rose[1], SECSG, Depts. of [1]Biochemistry & Molecular Biology, [2]Computer Sciences, Univ. of Georgia, Athens, GA 30602, USA.

SGXPRO, a versatile workflow engine designed for the automation of data processing/structure determination process will be reported. SGXPRO complements our laboratory's high-throughput structure determination pipelines, SCA2STRUCTUREpipe and AMOREpipe that have been reported by Praissman et al. (Abs. 01.07.07, ACA meeting, July 2003). While the current software suite has the capability to perform high-throughput operations, considerable flexibility has been built into the system that allows users to seamlessly navigate through the structure determination process. It also allows the user to tackle problem structures using a variety of methods and gives the user the ability to pay closer attention to the data in hand.

The SGXPRO uses a pseudo-parallel algorithm to automatically manage communication among different steps, search algorithms/programs and parameter space to generate the best possible results for a given data set. SGXPRO runs under both Linux and Windows and has been developed to run on both single and multi-processor systems including large Linux clusters.

The work was supported in part by NIGMS Grant GM62407, University of Georgia Research Foundation and Georgia Research Alliance.