Data Analysis in Real Time with RAPDv2.0

Frank V. Murphy[a], Jon P. Schuermann[b], Kay Perry[c], David B. Neau[d], Kanagalaghatta Rajashankar[e].

Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853. NE-CAT, APS Sector 24, 9700 S. Cass Ave., Lemont, IL 60439.
[a] fmurphy@anl.gov
[b] schuerjp@anl.gov
[c] kperry@anl.gov
[d] dneau@anl.gov
[e] rajashankar@aps.anl.gov

RAPD is a modular package of programs written for the automated processing of macromolecular crystallographic data at the NE-CAT beamlines. It watches for collected data, processes snapshots to create strategies for data collection, integrates runs of data in real time for structure solution, and can then solve the structure using molecular replacement or single-wavelength anomalous diffraction. Importantly, all results are presented to users in an HTML-based interface that is accessible over the Internet for remote collaboration. RAPD is written primarily in Python and can be modified to suit different environments, or extended to add functionality. Here we present the secopnd release of RAPD, describe its design, and showcase its current capabilities.