Technology Offer

Protein Cristallography (XDS)

Ref.-No.: 0105-1318-WT

X-ray Detector Software for processing single-crystal monochromatic diffraction data recorded by the rotation method.

XDS can process data images from CCD-, imaging-plate-, multiwire-, and pixel-detectors in a variety of formats. It also accepts images recorded by multi-segment detectors that are assembled from several rectangular components in arbitrary arrangement.

XDS runs under a Unix or Linux operating system controlling a cluster of independent servers of the same type. Each server may comprise several processors that share the same address space. The user can easily tailor XDS to the capabilities of the hardware (notebook or main frame) by specifying two input parameters. Alternatively, if unspecified, XDS automatically distributes balanced pieces of the work to up to 99 nodes of the cluster, each work piece for parallel execution by up to 99 threads.

Documentation and executable versions of the XDS package for widely used computer systems running under Linux or OSX can be obtained from the XDS homepage (http://xds.mpimf-heidelberg.mpg.de/) free of charge for use by academics for noncommercial applications. For commercial applications, please contact Max Planck Innovation (email: info@max-planck-innovation.de) to receive a license offer.

Publications

XDS
Wolfgang Kabsch
Acta Crystallographica Section D, Volume 66, Part 2, February 2010, Pages 125-132
https://doi.org/10.1107/S0907444909047337
 and references therein

Integration, scaling, space-group assignment and post-refinement
Wolfgang Kabsch
Acta Crystallographica Section D, Volume 66, Issue2, February 2010, Pages 133-144
https://doi.org/10.1107/S0907444909047374
and references therein

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