

MS41 Automation in data collection and processing

MS41-01

Supporting high-quality experiments through better use of sample optical images

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Abstract

This work is about sample optical images and how they can aid in better experiment design. Specifically we ask the following: Can we build an artificial system that recognizes, localizes and segments out a sample? Can it further tell apart pin from stem, stem from loop and crystal from either of them? Can it do it at arbitrary scale, orientation and varying lighting conditions? Can all of that be done in real time?

The main thesis of the present work is that answer to all of the questions above is yes.

If that is indeed true the following becomes possible: Upon sample mount we can instantly zoom in on sample areas that are most likely to contain interesting objects and dedicate costlier evaluation methods e.g. X-ray based raster to relatively small areas. By performing sample optical segmentation at multiple orientations we can gain information sufficient for reconstruction of a 3d model of the sample which can be then used as a natural reference for any automatically or manually defined point, line, area or a higher dimensional object. The great advantage of this natural reference is its invariance with respect to arbitrary reorientation particularly in a multiaxis goniometer setting. We believe this last point is of great importance in supporting wider use of experiment design benefiting from sample probing at multiple orientation by solving a problem of achieving submicron precision when reorienting samples with goniometers of much lesser expected precision, alleviating necessity of costly and unreliable manual re-alignments.

The main contributions of the present work are the following: I. Pixel annotated dataset of ~1200 high resolution sample images II. An artificial network network [1] based program capable to segment out a sample image in real time (including discussion of finer points of how it was trained) III. A program for rapid 3d sample shape reconstruction and registration at arbitrary orientation.

A practical demonstration of how a system based on those contribution can serve in day to day operation on an MX beamline concludes the talk.

References

[1] S. Jégou, M. Drozdal and D. Vazquez, A. Romero and Y. Bengio, The One Hundred Layers Tiramisu: Fully Convolutional DenseNets for Semantic Segmentation, <https://doi.org/10.48550/arxiv.1611.09326>