Differential Evolution Optimization of Diffraction Pattern Models with Clones[1] VICKIE LYNCH, Oak Ridge National Laboratory, HANS-BEAT BUERGI, University of Bern/University of Zurich, JUERG HAUSER, University of Bern, CHRISTINA HOFFMANN, Oak Ridge National Laboratory, TARA MICHELS-CLARK, University of Tennessee, STEVE MILLER, Oak Ridge National Laboratory
— With the TOPAZ single crystal diffractometer at the Spallation Neutron Source in operation, new computational methods are needed for analyzing the three-dimensional diffraction patterns recorded from disordered crystals. One such method uses a combination of differential evolution and Monte Carlo techniques to model the disorder and analyze the diffuse scattering. Software implementing this method originally developed at the University of Bern has been modified to use TeraGrid high performance computers. Since different model crystals produced from a given set of disorder parameters differ, the error of the fit to the data of such clones differs too. The performance of the differential evolution optimization in improving the fit of the model is being tested by using a variable number of clones for each individual gene set in a generation of differential evolution. A reference dataset with minimal noise has been generated for this purpose. Results of tests varying the number of clones will be presented.

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