Using Evolutionary Algorithms for the Investigation of Disordered Materials, Thomas Weber, *Lab. of Crystallography, ETH Zurich, Switzerland*. E-mail: thomas.weber@mat.ethz.ch

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In the last decade the availability of new experimental tools like third generation synchrotron sources and powerful area detectors was accompanied by a significant increase of computing power. This combination opened the possibility of simulating disordered structures based on high quality diffuse scattering data. The introduction of Monte Carlo (MC) methods as modelling techniques was an important step, because it allowed describing even complicated disorder phenomena by only a few parameters. Initially, MC simulations were used as a qualitative tool only, *i.e*. simulated diffraction patterns were visually compared to the experimental diffraction patterns. Later, least-squares methods were used to optimize the underlying model parameters and to minimize the differences between experimental and simulated intensities [1]. An intrinsic problem of least-squares methods is, however, that they require starting values close to the final values before this technique can successfully be used. Otherwise, this procedure is prone to get stuck in a local minimum. On the other hand, searching for good start values by trial-and-error is a very time consuming procedure, which also requires some expertise. A major part of this work can be left to the computer, if the parameter space is searched by evolutionary algorithms [2]. In this contribution the principles of evolutionary techniques and their application to crystallographic disorder problems are outlined. Based on several examples, potential and practical problems of this technique will be discussed.

[1] Welberry, T. R., Proffen, T. & Bown, M.: Analysis of single-crystal diffuse X-ray scattering via automatic refinement of a Monte Carlo model. Acta Cryst. A**54**(1998) 661-674.

[2] Weber, T. & Burgi, H. B.: Determination and refinement of disordered crystal structures using evolutionary algorithms in combination with Monte Carlo methods. Acta Cryst. A**58**(2002) 526-540.