

'Pushing the Boundaries' of Differential Evolution in SDPD

Samantha Y. Chong, Maryjane Tremayne, *School of Chemistry, University of Birmingham, Edgbaston, Birmingham B15 2TT*. E-mail: spc715@bham.ac.uk

The development of direct space structure solution techniques is an important factor in the increasing number of crystal structures determined using PXRD [1]. Direct space methods involve assigning R factors to trial structures by comparison of the calculated powder profile to the experimental pattern. A global optimisation algorithm, such as Monte Carlo or evolutionary algorithms is applied to locate the correct crystal structure.

Differential Evolution (DE) is an evolutionary algorithm, which is simple to implement and offers robust searching of minima [2,3]. A population of trial structures is generated, characterised by parameters describing position, orientation of the molecule and any variable torsion angles. Associated with each parameter is a minimum and maximum boundary. The population is mated and mutated in a single step to produce successive generations until the structure with the lowest R factor is found.

This presentation describes a modification of the DE algorithm which enables the boundaries to be updated during a structure solution calculation, using information previously gained within the search. We examine the effect of restricting the search to regions where low R factor has been found on the efficiency of the DE optimisation.

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