Powders, Prediction and Epitaxy: Applications of Differential Evolution

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Differential evolution (DE) is a robust and efficient global optimization algorithm based on evolutionary principles, which has been applied to a wide range of problems [1]. It shares the attractive features of other evolutionary algorithms but has a simpler implementation and fewer user defined control parameters enabling a greater insight into the control of the optimization process to be achieved.

Direct space methods of structure determination from powder diffraction is a field of rapid growth due to a number of computational and experimental developments [2, 3]. DE has been successfully applied to the determination of a number of organic and inorganic molecular structures from laboratory powder data.

The DE algorithm has also been applied to the prediction of crystal structures and epitaxial interfaces of organic crystals. In both cases, the lattice energy of the trial packing is calculated by an appropriate force field and then minimized by the DE algorithm. Utilization of a Beowulf cluster enables optimization of the DE algorithm control parameter to be performed in parallel.

In this talk, I will discuss these applications of DE with particular attention to the optimization of the performance of the algorithm, while highlighting areas of potential improvement and future developments.

[1] Price K.V., Storn R.M., Lampinen J.A., *Differential Evolution: A Practical Approach to Global Optimization*, Springer-Verlag, London, 2005. [2] Harris K.D.M., Tremayne M., Kariuki B.M., *Agnew. Chem. Int. Ed.,* 2001, **40**, 1626. [3] David W.I.F., Shankland K., McCusker L., Baerlocher C. (Eds.), *Structure Determination from Powder Diffraction Data*, Oxford University Press, Oxford, UK, 2002.

Keywords: optimization algorithms, ab-initio powder structure determination, epitaxy