POWders and ‘peER-PRESSure’: Pitfalls AND PROGRESS

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An important factor in the increasing number of crystal structures determined by PXRD is the development of direct space structure solution techniques [1], in which a range of predicted structural models are compared with the experimental powder data using a global optimisation technique to locate the best crystal structure solution. A number of optimisation algorithms have been applied to this problem, but our work has focussed recently on the development of the Cultural Differential Evolution (CDE) technique, which combines the traditional biological dictates of mating, mutation and natural selection in the Differential Evolution algorithm (DE) [2,3] with an approach that models human social behaviour or cultural selection.

We will present our implementation of the CDE algorithm in which ‘cultural’ behaviour or ‘peer pressure’ – in this case, the distribution in values of structural parameters in each generation – is used to guide and enhance the DE process. This approach uses social factors to guide and speed-up evolution but natural biological selection to drive the optimisation process. Our results show an average 40% improvement in efficiency of a structure solution calculation in all test cases, over the DE method alone, demonstrating a simple ‘real-world’ implementation of a combined cultural and biological evolutionary approach that has potential applications in many other optimisation problems in materials science. [4].

Although the main focus of this presentation will be on the progress that we have made in development of the CDE approach, potential pitfalls in the structure solution process will also be discussed. Examples will include the effects of preferred orientation on the location of the global structure solution and refinement minima [5], and limitations that should be considered when defining a structural model.