Rapid Structure Solution using global Optimisation and distributed Computing

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The use of global optimisation methods has helped to increase the size and complexity of molecular organic structures that can be solved directly from powder diffraction data. These methods require many repeat runs to be performed in order to confirm the location of the global minimum in parameter space; this is particularly true of very complex structures, where success rates in locating the minimum may fall to only a few percent. Fortunately, these multiple runs can be performed independently of each other and as such, they are ideally suited to the notion of grid-type computing. We have recently adapted the DASH [1] program to run under the GridMP [2] distributed computing system; the current setup allows up to eighty DASH simulated annealing runs to be executed in parallel on *existing* desktop resources. Initial results show not only impressive performance gains but also indicate that new computational routes that were previously closed to us (due to their compute-intensive requirements) are now open. For example, full characterisation of a hybrid Monte Carlo (HMC) method of structure determination from powder diffraction data required many months of CPU time; the work was performed in a matter of days using a grid-adapted version of the HMC code [3].

[1] David W.I.F., Shankland K., Shankland N., *Chem. Commun*., 1998, 931-932. [2] http://www.ud.com [3] Markvardsen A.J., Shankland K., David W.I.F., Didlick G., *J. Appl. Cryst*., 2005, **38**, 107-111.

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