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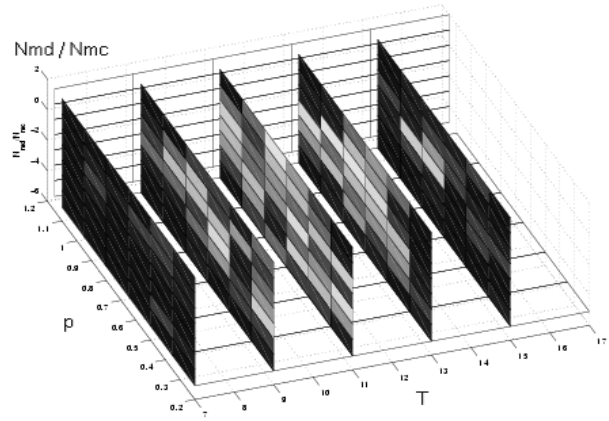
GRID-enabled Structure Determination from Powder Diffraction Data. A.J. Markvardsen, K. Shankland, W.I.F. David, ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX11 0QX,UK.

'The GRID' is a term used to describe a system for the sharing, selection and aggregation of computing resources spread over a number of sites. Whilst of 'distributed' computing is nothing new, the GRID will provide a stable framework that match resources to tasks on a massive scale.

Our interest in the GRID has arisen from the intrinsic parallelism of some 'structure determination by global optimisation' methodolgies. We have used the Entropia DCGRID [1] system to implement a small test grid of 19 non-dedicated Windows clients (ranging in CPU speeds from 350MHz to 2400MHz) and have used this to parameterise a hybrid Monte-Carlo (HMC) method of structure determination from powder diffraction data [2]. Calculations that would normally take 6 months on the fastest machine are completed in less than 2 weeks on the GRID. The figure below shows the results of 4200 individual HMC runs on the crystal structure of capsaicin as a function of the parameters which affect the performance of the HMC algorithm: T, number of MD (Molecular Dynamics) steps, number of MC (Monte Carlo) steps and p(accept). Light areas indicate regions where the structure determination success rate is high.



Our understanding of the HMC algorithm has been greatly enhanced by the results of these calculations, which would be extremely difficult to carry out in any other way. We are currently investigating other GRID systems for applications including molecular dynamics and neutron instrument simulation.

[1] http://www.entropia.com
[2] ISIS 2003 Science Highlight "Optimising a hybrid Monte-Carlo search
process using distributed computing".