

Distributed Computing for Crystallography: Experiences and Opportunities

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Distributed computing is one term that can be used to describe the notion of spreading discrete, computationally intensive jobs across a number of discrete compute resources. Such a notion is quite distinct from that of dedicated compute clusters such as Beowulf clusters and is one that can be easily identified with projects such as 'SETI@home' and the 'Anthrax Research Project' that have captured the public's imagination.

At the ISIS Facility, we have been investigating the use of distributed computing at the departmental level for some time, initially with the DCGrid system and more recently with GridMP. Our experience has, in general, been a very positive one, and we have 'grid-enabled' a wide range of applications, many of which have a direct impact upon problems of crystallographic interest. This presentation will focus on such applications (including structure determination from powder diffraction data, use of the Hybrid Monte-Carlo search method, molecular dynamics simulations, protein‑ligand docking and neutron instrument simulation) and will show how distributed computing has transformed the way in which we think about the scale of many crystallographic problems.

I will describe the steps involved in 'grid-enabling' a typical application, what constitutes a good application for the grid and will also discuss some of the problems that we have encountered in deploying the GridMP system and in running it.