



THE WHITE ROSE GRID e-Science Centre

Sample e-Science Projects at York

Introduction

This handout briefly outlines some of the projects using the White Rose Grid from researchers based in York.

Business Resource Optimisation for Aftermarket and Design on Engineering Networks (BROADEN)

This is the follow-up to the successful e-Science DAME (Distributed Aircraft Maintenance Environment) pilot project. The DAME concepts are maturing into commercial realisation through DTI funding within the IEC Technology Programme. Rolls-Royce is one of the lead partners in the £35 million project, along with its IT provider, EDS.

DAME was designed to provide diagnostic information on high volumes of data from flight data recording from aero engines.

BROADEN's objectives are: to build an internal pilot grid and to provide the academic partners with the opportunity to scale the core research technologies developed in DAME into production level systems; to extend the framework to include tools for design optimisation, large-scale agent-based modelling of aftermarket business processes, logistics and the supply chain; develop a strategy to transfer this technology to production networks.

York's contribution is focused on high volume pattern matching technology, which must now be scaled to a production level.

For further details please contact Professor Jim Austin (austin@cs.york.ac.uk) or Dr Tom Jackson (tom.jackson@cs.york.ac.uk)

Quantum Computing

Research under Professor Sam Braunstein, Computer Science

This research is aimed at constructing Bell inequalities based on error correcting codes.

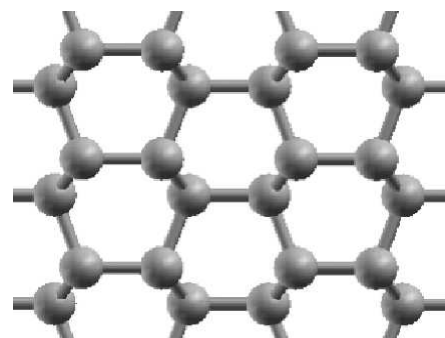
Testing the inequalities requires ensuring that the locally realistic bounds are within the bounds under quantum mechanics. To do this a brute force search over all possible configurations was performed (almost 1010 such configurations were required). Using a single machine to calculate this bound would require many months, but using a cluster it can be reduced to just a few days.

Other research involves running a differential evolution algorithm for the design of more efficient optical interferometers for quantum error correction. So far no lab has performed more than a partial demonstration of quantum error correction. With a more simple design it is hoped that the team can be the first to achieve this goal.

<http://www-users.cs.york.ac.uk/~schmuel/>
Crystal Structure Solution

Luke Abraham, Physics

This research involves using Genetic Algorithms to search for the minimum energy configurations of crystal structures, and also to search for polymorphs of different materials. This work is performed using the CASTEP code and requires a large number of parallel processors to be available for the calculation. The facilities that the White Rose Grid offers have been indispensable during the course of this research.



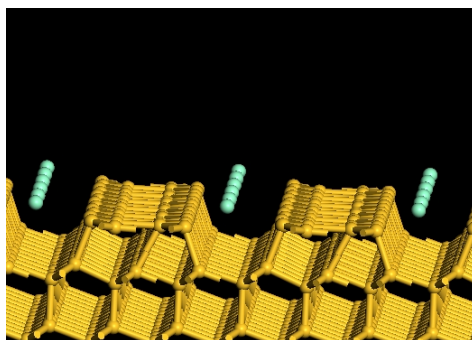
The structure of Lonsdaleite, an allotrope of carbon, looking down the [110] direction.



Nanomaterials

Chris Eames, Physics.

This research involves making novel surface structures and nanomaterials using the Rare Earth metals deposited onto semiconductor surfaces. This uses the FORTRAN-based CASTEP program on White Rose Grid to find the lowest energy atomic arrangement of nanostructures and to then determine the electronic properties. This is used as a suggestion for the structure of the surface as prepared in the laboratory. Such calculations are invaluable in ruling out structurally unstable models and for comparing the energies of any plausible candidate models.



A surface formed by depositing Samarium on the Si(111) face.

Structure and Spectroscopy of Dyes

Laurence Abbot, Chemistry

There is a vast literature on dyes but the majority of the literature is qualitative in nature, with relatively little information on the molecular level. Some dyes are very susceptible to fading by light whereas others are more resistant. In order to design new high-performance dyes it is important to understand what processes are occurring on the molecular level during photo-fading.

One class of dyes, azo dyes, can exist as a mixture of two structures which are in equilibrium: the azo and hydrazone conformers. The ratio of these two species depends both on the structure of the dye and also on the molecular environment such as the solvent or substrate. Some fading mechanisms have been proposed to involve one or other of these forms and, thus, it is important to characterise the azo-hydrazone equilibria of these dyes.

Experimentally, these equilibria are difficult to study because both conformers will be present simultaneously. Using quantum chemistry high level density functional theory calculations the azo and hydrazone tautomers can be studied individually. Thermodynamic properties can be calculated which can then be used to estimate an equilibrium constant for a particular dye. Furthermore, calculations on the transition-state structure between the conformers allow the rate constants for the inter-conversion to be estimated. The computing facilities offered by the White Rose Grid allows these calculations on large, real dyes rather than smaller model dyes, and it also allows calculations to be performed on molecules in a solvent field environment.

Reinforcement Learning

Matthew Grounds, Computer Science

This is focused on using parallel hardware for machine learning, in particular reinforcement learning problems. In reinforcement learning, an agent is situated in an environment. The agent can take a series of actions which affect the state of the environment. At each discrete time step, the agent receives a numerical reward to indicate the desirability of the current state of the environment. A reinforcement learning agent gradually learns to maximise the cumulative reward received over time.

Standard RL algorithms are highly sequential, and offer no natural route to parallelization. However, in the special case where the environment can be simulated, it is possible to replicate the simulation on each node of a workstation cluster, and have learning agents on each. If the agents are also able to exchange intermediate results over an interconnection network, it is possible to find near-optimal solutions much more quickly using the cluster. The implementation of the algorithms was based on the MPICH message passing library.

Further Information

Contact:

Aaron Turner, aaron@cs.york.ac.uk

The Project Web site:

<http://www.wrg.york.ac.uk>