York Projects Using White Rose Grid

Introduction

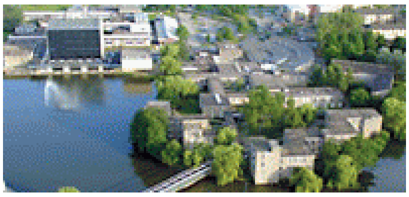
This handout briefly outlines some of the projects using the White Rose Grid from researchers based in York.

Further information can be obtained from the individual contributors.

BROADEN

Research under Prof. Jim Austin, Computer Science.

This project seeks to commercialise the DAME (Distributed Aircraft Maintenance Environment, an e-Science pilot project) tools for providing diagnostic information on high volumes of data from flight data recording from aero engines. The funding is from DTI within the IEC Technology Programme. Rolls-Royce is one of the lead partners in the £4 million project, along with its IT provider, EDS.



BROADEN's objectives are: to build an internal pilot grid; provide the academic partners with the opportunity to scale the core 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 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.

See Figure 1.

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

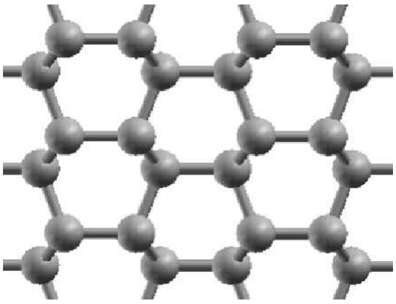


Figure 1: The structure of Lonsdaleite, an allotrope of carbon, looking down the [110] direction.

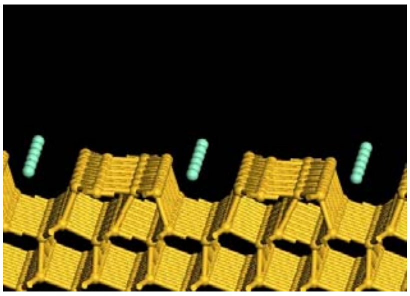


Figure 2: A surface formed by depositing Samarium on the Si(111) face.

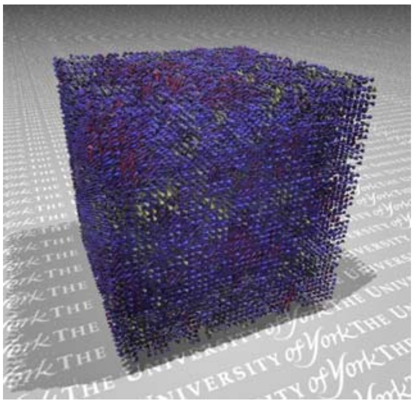


Figure 3: A snap shot of an equilibrium state of a magnetic media which contains 80x80x80 individual spins at room temperature. Every cone represents 2x2x2 spins. The blue/green cone colour represents the cones which are aligned parallel to the easy axes.

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.

See Figure 2.

Structure and Spectroscopy of Dyes

Laurence Abbot, Chemistry

In order to design new high-performance dyes that are resistant to fading due to light it is important to understand what processes are occurring on the molecular level during photo-fading.

Azo dyes can exist as a mixture of two structures which are in equilibrium: the azo and hydrazone conformers. 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 which allows thermodynamic properties to be calculated enabling an estimation of an equilibrium constant for a particular dye. 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 allow 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.

Simulation of Semiconductor Optical Amplifiers

Xibin Song

Parameter searches to optimise, realize reshape optical amplifiers with real-time output pulses in long distance transmission. This modelling includes bulk, vertical laser, and quantum dot semiconductor optical amplifiers to compensate for loss and reshape the phase of transmitted light.

Discovery of Patterns in Biological Sequence Data

M. A. Lones and A. M. Tyrrel, Electronics

The current focus is on finding regulatory motifs in DNA promoter regions, for which we have recently developed a population clustering evolutionary algorithm capable of finding multiple strong and weak signals within relatively long promoter sequences. We are also looking at the use of co-evolution to improve search and characterise the structure of regulatory regions.

See: M. A. Lones and A. M. Tyrrell, “A Co-Evolutionary Framework for Regulatory Motif Discovery”, Proc. IEEE Congress on Evolutionary Computation, to appear, September 2007.

Modelling Magneto-Crystalline Behaviours for Recording Media

Denise Hinzke

Due to its large value of magneto-crystalline anisotropy energy, FePt is an ideal candidate for recording media for storage densities of 1Tbit/in and beyond. In this context, a possible application is the so-called heat-assisted magnetic recording. We are interested in the investigation of thermal properties as well as the dynamic behaviour at elevated temperatures of FePt.

Bulk FePt in the chemically ordered phase using an effective, classical spin Hamiltonian is modelled. Atomistic as well as micromagnetic simulations as used, solved using the Landau-Lifshitz-Gilbert as well as the Landau-Lifshitz-Bloch equation numerically.

See Figure 3.

Time Series Modelling

Jianhua Gang

Semi non-parametric modelling of conditional mean and variance of time series.

Further Information

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