GRADnet SEPnet Modelling Workshop 2015
Old Thorns Manor Hotel, Longmoor Rd, Griggs Green, Liphook, Hampshire GU30 7PE
Sunday 13th December 2015 – Tuesday 15th December 2015

Timetable

Sunday 13th December

1730 – 1830  Guest speaker – materials simulation
1830 – 1900  Dinner

Monday 14th December

Day 1 is devoted to first-principles quantum mechanical simulation of electrons and nuclei. The focus is on the package CASTEP, a full-featured materials modelling code using a plane-wave basis set and pseudopotentials.

0900 – 1000  First-principles materials simulation  Keith Refson
1000 – 1100  Introduction to plane waves and pseudopotentials
1100 – 1130  Refreshments
1130 – 1230  Using CASTEP – the practicalities
1230 – 1400  Lunch
1400 – 1530  Workshop 1 – using CASTEP  Keith Refson
1530 – 1600  Refreshments
1600 – 1700  Workshop 2 - using CASTEP
1730 – 1830  Guest speaker – application of modelling methods in industry

Tuesday 15th December

Day 2 is devoted to molecular dynamics (MD) and Monte Carlo (MC) simulation methods. Students will have the opportunity to tackle one or more simple MC simulation problems in the morning workshop and be introduced to the MD package DLPOLY in the afternoon.

0900 – 1030  Introduction to Monte Carlo methods  David Faux
1030 – 1100  Refreshments
1100 – 1230  Workshop 3 (MC)
1230 – 1400  Lunch
1400 – 1500  Introduction to Molecular Dynamics  Kostya Trachenko
1500 – 1530  Refreshments
1530 – 1700  Using DLPOLY – the practicalities and real examples