



Introduction to Computer Simulation of Alloys

May 3–8th 2010

National e-Science Centre, Edinburgh
15 South College St.

This workshop provides an introduction to the theory and methodologies applied to engineering materials and the atomistic and nanoscale.

Monday May 3rd. Electron day

- 9:00 Assemble, registration
- 9:30 Welcome (Ackland, Callaghan)
- 9:40 Brief overview of MaMiNa (Siemers)
- 9:50 Quantum Mechanics, Density Functional Theory and their practical application to alloys (Clark)
- 11:00 Coffee break
- 11:30 Density functional codes, practical issues (Refson)

12:30 Lunch (eSI)
2:00 Demonstration of Castep
2:30–5:30 Hands on exercises with CASTEP
5:30 Reception at eSI

Tuesday May 4th. Continuum day

9:00 Phase diagrams, thermodynamics. (Perry)
10:00 Microstructure: elasticity and plasticity
(Ackland)
10:45 Coffee
11:00 Continuum introduction (Roy)
12:00 Group project description Compute your own alloy
properties.
12:30 Lunch
1:30 Student groups formed, materials challenges
presented
2:30 Student groups work on challenge project and
presentation.

Wednesday May 5th. Atom day

9:00 Linking Quantum and Atomistics: Interatomic
potentials (GJA)
9:30 Molecular Dynamics (Ackland)
10:00 Atomistic level effects in deformation and
fracture (Bacon)
11:00 Coffee
11:30 Commercial and Academic Codes: Capability and
Limitations
12:30 Sandwich Lunch, suggested activity: mountain
climb to Arthur's Seat
3:00 Demonstration of Moldy (Uhrin)
3:30–6:00 Hands on exercises with Moldy and BallViewer
(Uhrin, Ackland)

6:00 Avalanche Fracture, for atomic to geoscale .
(Invited seminar by Zaiser)
7:00 Conference dinner

Thursday May 6th FEM day

9:00 Introduction to Finite Elements (Baeker)
10:15 Linking atomistic and continuum (Ackland)
10:45 Coffee
11:15 Non-linear Finite Element Problems (Baeker)
12:30 Lunch, suggested activity: visit to Edinburgh
Castle
2:30 Student groups to review one rival proposal
3:00–3:30 Abaqus and other Simula products (Max Leadley-
Brown)
3:30–6:00 Hands on exercises with AbaqUS (Baeker, Roy)
6:00 Studying materials at high pressure. (Invited
seminar by McMahon)
7:00 Whisky tasting (McMahon).

Friday May 7th. Presentation day

9:00 Student group reconvene to consider grant
reviews, final revision to presentations.
9:30 Kevin Stratford (EPCC) Simulation on parallel
computers past and present
10:00 Miriam Marques. Potassium and sodium under pressure:
ionic compounds.
10:30 Coffee
11:00 Jamie Cole. Do atoms in metals have charges?
11:30 Ben Leimkuhler. Thermostats in molecular dynamics.
12:30 Lunch
2:00 Student group presentations

Group Projects.

Students will be broken into groups of 4-5, wherever possible of different nationalities and backgrounds. Each group will be given a materials challenge (e.g. turbine blades, nuclear reactor parts, airframe, stent, spectacles, dental fillings etc). They have to identify the problems, the types of materials to be investigated, main industrial players, possible academic partners. On Friday, they will present proposals to a mock funding panel, which will assess and rate each proposal.