Nested sampling: a black-box method for statistical mechanics

Dr. Robert Baldock,
Theory of Condensed Matter Group, Department of Physics
University of Cambridge

Wednesday Sept 2, 14:00, Room MXC 320

Abstract: Nested sampling is an algorithm for calculating the integrated density of states for a material, in a highly automated fashion. From the integrated density of states, one can calculate the partition function as an explicit function of temperature, and thus do statistical mechanics from first principles. The only inputs required are the interatomic potential energy function and the desired pressure and temperature ranges.

In this talk I shall describe the nested sampling algorithm, and explain how it can be used to simulate materials under periodic boundary and constant pressure conditions. With applications to Lennard-Jonesium and an embedded atom model for aluminium, I will show how complete pressure-temperature phase diagrams can be determined by examining the heat capacity. In particular solid-solid phase transitions are recovered without any *a priori* knowledge about the structure of the solid phases. I will also demonstrate how free energy landscapes can be calculated retrospectively and as a function of temperature, from the output of nested sampling.