Uva Wellassa University, Sri Lanka
End Semester Examination - March 2012

SCT 433-1 Multi-scale Modeling Methods in Materials Science

Time: One (01) hour

Total 03 questions
Answer all questions
All symbols carry standard meanings
Use of standard symbols without a definition

01). (a). Define following terms (mathematical relationships are adequate)
(i). Phase space (ii). Autonomous system (iii). Radial distribution function

(20 marks)

(b). Determine the family of trajectories of simple harmonic oscillator (SHO)?

(40 marks)

(c). How the trajectories drawn in Section (b) differ when the sign of the applied potential field is reversed?

(40 marks)

(d).State mathematical relationships to derive pressure, temperature, entropy and chemical potential of a system in terms of $\Omega(E, V, N)$.

(20 marks)

02).

(a). State a key difference between Hatree and Hartree Fock methods.

(20 marks)

(b). Derive the HF equation of an electron in N electron system

(40 marks)

(c). Derive the Roothan Hall equation for N-electron system

(40 marks)

(d). State Hornberg and Kohn theorems of DFT.

(20 marks)

03).

(a) State the four steps included in a typical MD computational experiment.

(20 marks)

(b). What do you mean by Lyapunov instability in MD simulations?

(20 marks)

(c). What do you mean by ergodicity

(20 marks)

(d). Prove that the Verlet algorithm is fourth order accurate (hint: use Taylor series expansion of a given function)

(20 marks)

(e). State the equi-partition theorem.

(20 marks)