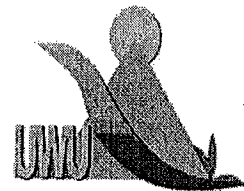


Uva Wellassa University, Sri Lanka
End Semester Examination - March 2012



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 Hartree and Hartree Fock methods.
(20 marks)
- (b). Derive the HF equation of an electron in N electron system
(40 marks)
- (c). Derive the Roothaan 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)