PHY00016H

UNIVERSITY OF YORK

DEPARTMENT OF PHYSICS

Third Year Examinations 2016

MOLECULAR SIMULATION

THEORETICAL PHYSICS STUDENTS ONLY

Issued at:12:00 25 February 2016

Submission deadline:16:00 Thursday 28 April 2016

Feedback by: Thursday 26 May 2016

Please identify yourself by your examination number and not your name on each sheet of paper you use.

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Turn over

Molecular Simulation - PHY000016H

1 Using the molecular dynamics program with which you have been provided, generate trajectories for the Lennard-Jones fluid with density $\rho^* = 0.7$, using $N = 256$ particles over a range of initial temperatures, T^*, from 1.0 to 2.5. A time-step $\Delta t^* \simeq 0.004$ should be satisfactory for these simulations. (All quantities are quoted in MD units). Hence:

(a) Using the method of block averages, estimate the errors in the simulated values of internal configuration energy$\langle U^* \rangle$ and temperature $\langle T^* \rangle$. Ensure that you have used sufficient steps in your trajectories to give one standard deviation from the mean of U^* which is less than 0.002.

(b) Plot $\langle U^* \rangle$ v. $\langle T^* \rangle$ and obtain the best fit cubic polynomial relating these quantities. Hence find an expression for the constant volume thermal capacity, C_v^* as a function of temperature.

(c) For each trajectory find C_v^* from the fluctuation formula:

$$C_v^* = \frac{3}{2}\left[1 - \frac{2}{3NT^{*2}}\langle(\delta E_k^*)^2\rangle\right]^{-1}$$

Where total kinetic energy $E_K^* = \frac{3}{2}NT^*$ and

$$\langle(\delta E_k^*)^2\rangle = \langle(E_k^*)^2\rangle - \langle E_k^*\rangle^2 \ .$$

Estimate the error in each of these measurements.

(d) Plot your estimates of C_v^* from the fluctuation formula and the polynomial expression on a graph.

Present your work in the form of a Laboratory Formal Report. Your report should be no more than 10 sides of A4, using 12 point font, including figures, tables and references. In addition to this you should include a listing of your own code (not the molecular dynamics code unless modified by you) in an appendix.

End of paper