24-623 2015 HM1

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1 Problem 1

1.1 (i)

$$2x^6 - 3x^4 + 4x^2 - 3$$

For efficient calculations we can use the following,

$$x^2 = x * x$$

$$x^4 = x^2 * x^2$$

$$x^6 = x^4 * x^2$$

This will minimize the number of FLOPS as well as any temporary variables created during the process.

1.2 (ii)

Prime number is only divisible by one and itself. Hence we iterate and find any numbers that factor the variable there by tagging it as composite. Algorithm to find if a number is prime is performed by using a common **primality** algorithm :

1. The given number is tested if it is PERFECT SQUARE or not (the code for this is already provided). This information is used in the subsequent steps to search.
2. A set of numbers check if a given number is a factor.
3. If the number has a PERFECT SQUARE, we iterate all the numbers starting from 2 till the square of that number because the factors will be repeated anyway.
4. If the number is NOT a PERFECT SQUARE, we iterate all the number starting from 2 till the (number-1).
5. NOTE : We start iterations from 2 and only iterate odd numbers as the even numbers can already divided by 2.

The output of the program is piped to `5output.txt`

2 Problem 2

2.1 Paper 1: (Application) Rapid transport of gases in carbon nanotubes

This paper is chosen based on the following reasons mostly focused on the applications,

1. The paper is interesting owing to the usage of molecular dynamics (MD) and monte-carlo (MC) techniques at various segments of the calculation.

2. MC technique has been used for sampling the phase space for equilibration and MD is used for the production calculations.

3. Usage of various concepts like equilibration, averaging techniques, usage of ensembles, etc have been made and it would be a good overview in applying to a practical system.

4. System under consideration is of enormous importance on which atomic simulations are performed to compute both the self- and transport diffusivities of light gases like CH_4 and H_2 in single walled carbon nanotubes (SWNTs) and also in zeolites with comparable pore sizes.

5. CH_4 and H_2 are treated as rigid spheres with pairwise lennard-jones interaction between species.

6. It would be of great interest to study the transport properties of the gases through the material so that better molecular sieves, membranes can be designed from the data obtained from atomistic simulations.

7. Defect-free nanotubes are considered for the calculations. The presence of defects in the nanotubes (heteroatoms, holes, etc.) will have an impact on molecular diffusion. The simplicity of the system would make it reproduce the calculations.

8. The results states that the rapid transport of adsorbed gasees in the SWNTs is not strongly dependent on the details of the adsorbate gas-nanotube interaction potentails becuase of the lack of corrugations in the PES. This would be an interesting observation to quantify.

2.2 Paper 2: (Theory) Application of Ewald summations to long-range dispersion forces

This paper is chosen from a theortical stand-point,

1. Effect of using explict summation terms for the r^{-6} dispersion term on the interfacial properties of a Lennard-Jones fluid and SPC/E water is discussed in this paper.

2. At large distances r, the effect of repulsive term drops in the LJ potential term.

$$u_{ij}(r) = 4\epsilon_{ij}\left[\cancel{\left(\frac{\sigma_{ij}}{r}\right)^{12}} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right]$$

3. Ewald summation technique is employed to perform summation of the pair-wise potential terms governing mostly dispersion at large-range distances and also ensuring convergence.

4. This has been widely reported in the LAMMPS and well documented which makes it interesting to study.

3 Problem 3

3.1 (a)

Assumption : Water at NPT conditions

Some mertics

1 mole = 6.023.1E+23 molecules, 1 lit = 1E+24 nm^3

diameter(nm)	Volume(nm^3)	moles	molecules	App. (molecules)
1	0.5238095	2.910052 (-23)	1.7527 (+01)	18
10	5.238095	2.910052 (-22)	1.7527 (+02)	180
100	52.38095	2.910052 (-21)	1.7527 (+03)	1800

3.2 (b)

The number of distinct interactions when treating water as a 3-body system with rigid bonds,

$$n = 3[3(N-1)] \implies 9(N-1)$$

where n is the number of distinct pairwise interactions and N is the number of molecules involved.

diameter(nm)	Molecules	Interactions
1	18	9(18-1) = 153
10	180	9(180-1) = 1611
100	1800	9(1800-1) = 16191

4 Problem 4

4.1 (a)

4.1.1 Equation 1 with two isolated atoms

$$u(r) = 4\epsilon\Big[\Big(\frac{\sigma}{r}\Big)^{12} - \Big(\frac{\sigma}{r}\Big)^{6}\Big] \tag{1}$$

Change of variables from r to r_{nn}.

$$U_i(r_{nn}) = \frac{1}{2}\sum_{j\neq i} u(r_{ij}) \tag{2}$$

Substitute (1) in (2),

$$U_i(r_{nn}) = 2\epsilon\Big[\Big(\frac{\sigma}{r_{nn}}\Big)^{12} - \Big(\frac{\sigma}{r_{nn}}\Big)^{6}\Big] \tag{3}$$

$$\boxed{\frac{U_i(r_{nn})}{\epsilon} = 2\Big[\Big(\frac{1}{r_{nn}/\sigma}\Big)^{12} - \Big(\frac{1}{r_{nn}/\sigma}\Big)^{6}\Big]} \tag{4}$$

4.1.2 Equation 3 with FCC

$$\frac{U_i(r_{nn})}{\epsilon} = 2\Big[A_{12}\Big(\frac{\sigma}{r_{nn}}\Big)^{12} - A_6\Big(\frac{\sigma}{r_{nn}}\Big)^{6}\Big] \tag{5}$$

$$\boxed{\frac{U_i(r_{nn})}{\epsilon} = 2\Big[A_{12}\Big(\frac{1}{r_{nn}/\sigma}\Big)^{12} - A_6\Big(\frac{1}{r_{nn}/\sigma}\Big)^{6}\Big]} \tag{6}$$

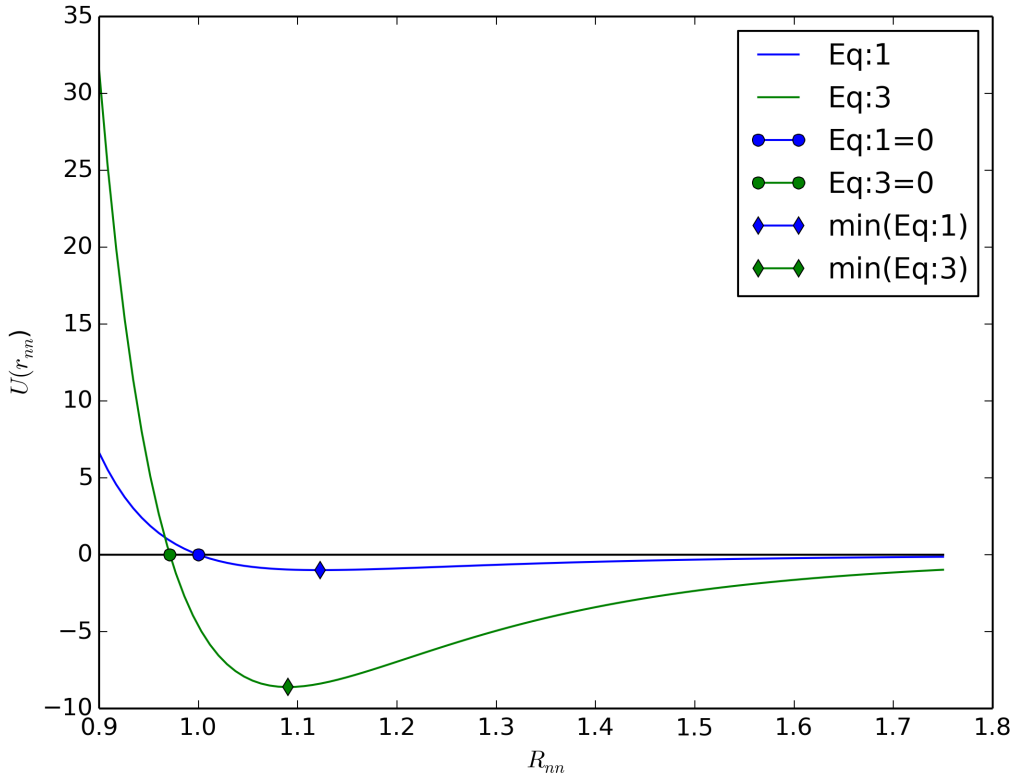

Figure 1: The figure shows the plot for LJ potential without environment (blue) and with environment in FCC (green). The potential is zero at larger distance for both the cases and it is zero at the positions shown in colored circle. The minima for the potential is also shown in filled diamonds.

The decay of the expression is faster for the (4) when compared to (6).

4.2 (b)

$$\boxed{u(r) = 4\epsilon\Big[\big(\frac{\sigma}{r}\big)^{12} - \big(\frac{\sigma}{r}\big)^{6}\Big]} \tag{7}$$

Setting u(r) = 0 in (7)

$$\implies 0 = 4\epsilon\Big[\big(\frac{\sigma}{r}\big)^{12} - \big(\frac{\sigma}{r}\big)^{6}\Big]$$

$$\implies \big(\frac{\sigma}{r}\big)^{6}\Big[\big(\frac{\sigma}{r}\big)^{6} - 1\Big] = 0) \tag{8}$$

Roots of the (8), $\underline{r = \infty}$ and $\underline{r = \sigma}$, at which $u(r) = 0$.
For finding minimum for (7), set $\frac{du(r)}{dr} = 0$

$$\frac{du(r)}{dr} = 4\epsilon\Big[\frac{-12\sigma^{12}}{r^{13}} + \frac{6\sigma^{6}}{r^{7}}\Big] \tag{9}$$

$$\implies 4\epsilon\sigma^{6}\Big[\frac{-12\sigma^{6}}{r^{13}} + \frac{6}{r^{7}}\Big] = 0 \tag{10}$$

$$\implies \frac{1}{r^{7}}\Big[\frac{2\sigma^{6}}{r^{6}} - 1\Big] = 0$$

Root of (10), $r = \infty$ and $r = \quad \sigma\sqrt[6]{2} \quad$ at which $u(r)$ is at minimum.

$$\boxed{U_i(r_{nn}) = 2\epsilon\Big[A_{12}\Big(\frac{\sigma}{r_{nn}}\Big)^{12} - A_6\Big(\frac{\sigma}{r_{nn}}\Big)^{6}\Big]} \tag{11}$$

Setting $U_i(r_{nn}) = 0$ in (12)

$$\implies 0 = 2\epsilon\Big[A_{12}\Big(\frac{\sigma}{r_{nn}}\Big)^{12} - A_6\Big(\frac{\sigma}{r_{nn}}\Big)^{6}\Big]$$

$$\implies 2\epsilon\Big(\frac{\sigma^6}{r_{nn}}\Big)\Big[A_{12}\Big(\frac{\sigma}{r_{nn}}\Big)^{6} - A_6\Big] = 0 \tag{12}$$

Roots of the (14), $r_{nn} = \infty$ and $r_{nn} = \quad \sigma\sqrt[6]{\frac{A_{12}}{A_6}} \quad$ at which $U(r_{nn}) = 0$.
For finding minimum for (12), set $\frac{dU_i(r_{nn})}{dr_{nn}} = 0$

$$\frac{dU_i(r_{nn})}{dr_{nn}} = 2\epsilon\Big[A_{12}\frac{-12\sigma^{12}}{r_{nn}^{13}} + A_6\frac{6\sigma^6}{r_{nn}^{7}}\Big] \tag{13}$$

$$\implies -12\frac{\epsilon\sigma^6}{r_{nn}^{7}}\Big[A_{12}\frac{\sigma^6}{r_{nn}^{6}} - A_6\Big] = 0$$

$$\implies \frac{1}{r_{nn}^{7}}\Big[A_{12}\frac{\sigma^6}{r_{nn}^{6}} - A_6\Big] = 0 \tag{14}$$

Root of (14), $r_{nn} = \infty$ and $r_{nn} = \quad \sigma\sqrt[6]{\frac{2A_{12}}{A_6}} \quad$ at which $U_i(r_{nn})$ is at minimum.
The plot of these singularity and minima is shown in the Figure.1

4.3 (c)

k_{LJ} is dimnesionless LJ thermal conductivity,

$$\boxed{k_{LJ} = \frac{k_B}{\sigma^2}\sqrt{\frac{\epsilon}{m}}}$$

4.4 (d)

dimensionless temperature (T^*),

$$T = T^*\Big(\frac{\epsilon}{k_B}\Big) \implies T^* = \frac{T}{\epsilon/k_B}$$

dimensionless thermal conductivity (k^*),

$$k = k^*\Big(\frac{k_B}{\sigma^2}\sqrt{\frac{\epsilon}{m}}\Big) \implies k^* = \frac{k}{\Big(\frac{k_B}{\sigma^2}\sqrt{\frac{\epsilon}{m}}\Big)}$$

Argon

4.4.1 Dimensionless Temperature

$$T^* = \frac{20K}{\frac{1.67.1E-21J}{1.3806.1E^{-23}J/K}}$$

$$\boxed{T^*_{Argon} = 0.1653}$$

4.4.2 Dimensionless thermal conductivity

$$k^* = \frac{1.4W/m - K}{\left(\frac{1.3806.1E{-}23J/K}{(3.4.1E{-}10m)^2}\sqrt{\frac{1.67.1E{-}21J}{6.63.1E{-}26kg}}\right)}$$

$$\boxed{k^*_{Argon} = 0.018955}$$

Krypton

4.4.3 Corresponding Temperature

$$T_{krypton} = T^*_{Argon}\Big(\epsilon/k_B\Big)$$

$$T = 0.1653K\Big(\frac{1.67.1E{-}21J}{1.3806.1E{-}23J/K}\Big)$$

$$\boxed{T_{krypton} = 26.82K}$$

4.4.4 Corresponding Thermal conductivity

$$k_{krypton} = k^*_{argon}\Big(\frac{k_B}{\sigma^2}\sqrt{\frac{\epsilon}{m}}\Big)$$

$$k = 0.018955\Big(\frac{1.3806.1E-23J/K}{(3.65.1E-10m)^2}\sqrt{\frac{2.24.1E-21J}{13.9.1E-26kg}}\Big)$$

$$\boxed{k_{krypton} = 2.4935.1E-4W/m-K}$$

References