Unit 16 - Week 11

Assignment 11

The due date for submitting this assignment has passed.
As per our records you have not submitted this assignment.

Due on 2020-04-15, 23:59 IST.

1) Which command specifies the pairwise force field coefficients for one or more pairs of atom types? *2 points*

- pair_modify command
- pair_style command
- pair_write command
- pair_coeff command

No, the answer is incorrect.
Score: 0
Accepted Answers:
pair_coeff command

2) What is the expression for Diffusion Coefficient in 3-dimensions? *2 points*

- $D = 6N \lim_{t\to\infty} \frac{d}{dt} \left\langle \sum_i^N (r_i(t) - r_i(0))^2 \right\rangle$
- $D = \frac{1}{6N} \lim_{t\to\infty} \frac{d}{dt} \left\langle \sum_i^N (r_i(t) - r_i(0))^2 \right\rangle$
- $D = 6N \lim_{t\to 0} \frac{d}{dt} \left\langle \sum_i^N (r_i(t) - r_i(0))^2 \right\rangle$
- $D = \frac{1}{6N} \lim_{t\to 0} \frac{d}{dt} \left\langle \sum_i^N (r_i(t) - r_i(0))^2 \right\rangle$

No, the answer is incorrect.
Score: 0
Accepted Answers:
$D = \frac{1}{6N} \lim_{t\to\infty} \frac{d}{dt} \left\langle \sum_i^N (r_i(t) - r_i(0))^2 \right\rangle$

3) _____ command deletes all atoms, restores all settings to their default values, and frees all memory allocated by LAMMPS. *2 points*

- next
- quit
- run
- clear

No, the answer is incorrect.
Score: 0
Accepted Answers:
clear

4) _____ command assigns the next value to the variable from the list of values defined for that variable by the variable command. *2 points*

- dump
- echo
- variable
- next

No, the answer is incorrect.
Score: 0
Accepted Answers:
next

5) The "#" wild card is used to indicate that the interactions spans all atom types in the pair_coeff command *2 points*

- True
- False

No, the answer is incorrect.
Score: 0
Accepted Answers:
False

6) Stillinger-Weber potential is NOT a 3 body potential *2 points*

- True
- False

No, the answer is incorrect.
Score: 0
Accepted Answers:
False

7) Embedded atom potential is a cluster functional *2 points*

- True
- False

No, the answer is incorrect.
Score: 0
Accepted Answers:
False

8) _____ command defines a computation in LAMMPS that calculates the mean-squared displacement (MSD) of the group of atoms. *2 points*

- compute ti
- compute hma
- compute msd/chunk
- compute msd

No, the answer is incorrect.
Score: 0
Accepted Answers:
compute msd

9) _____ command closes the current input script file, opens the file with the specified name, and begins reading LAMMPS commands from that file. *2 points*

- clear
- info
- echo
- jump

No, the answer is incorrect.
Score: 0
Accepted Answers:
jump

10) Which command set the style and content for printing thermodynamic data to the screen and log file? *2 points*

- thermo_modify command
- fix_modify command
- thermo command
- thermo_style command

No, the answer is incorrect.
Score: 0
Accepted Answers:
thermo_style command

11) It is sufficient to initialize the velocities once using the following command to have the system at equilibrium at a temperature of 300K. *2 points*

Note: velocity all create 300 102939 dist gaussian mom yes rot yes

- True
- False

No, the answer is incorrect.
Score: 0
Accepted Answers:
False

12) In the following LAMMPS command the number 102939 represents *2 points*

Note: velocity all create 300 102939 dist gaussian mom yes rot yes

- the pressure
- the energy
- a random number
- the atom id with the highest velocity of the atom

No, the answer is incorrect.
Score: 0
Accepted Answers:
a random number