Unit 15 - Week 10

Course outline

Assignment 10

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

Due on 2020-04-08, 23:59 IST.

1) One dump ID in a LAMMPS input script to be used twice, which of the following command should be used before using the second one? *2 points*

○ dump-modify
○ read-dump
○ undump
○ unfix

No, the answer is incorrect.
Score: 0

Accepted Answers:
undump

2) '10.0' in the following LAMMPS commands represents _____ ? *2 points*
fix 1 all npt iso 0.0 0.0 10.0 temp 150.0 300.0 0.01

○ Tdamp
○ Pdamp
○ Tstop
○ Pstop

No, the answer is incorrect.
Score: 0

Accepted Answers:
Pdamp

3) If a NVE simulation is done just after temperature initialization using *'velocity create'* command, then the temperature of the system at the end of NVE simulation generally reduces to its one fourth of initial value. *2 points*

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

4) The *'thermo'* command in LAMMPS is generally used to print the thermodynamic information of individual atoms. *2 points*

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

5) Both scalars and vectors input values can be used separately to perform *'fix ave/time'* command. *2 points*

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

6) *Compute*, *fix*, or *variable* command that produces a per-atom or local quantity can be used as inputs to perform *'fix ave/time'* command *2 points*

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
False

7) The rdf plot/data can be visualized by _____ modification operation in OVITO. *2 points*

○ Coordination analysis
○ Cluster analysis
○ Spatial correlation function
○ Voronoi analysis

No, the answer is incorrect.
Score: 0

Accepted Answers:
Coordination analysis

8) Radial distribution function is nothing but the relative density of atoms as function of radius. *2 points*

○ True
○ False

No, the answer is incorrect.
Score: 0

Accepted Answers:
True

9) Which of following is not true for radial distribution function (rdf)? *2 points*

○ Provides information about transport properties
○ Provides information about dynamical change of structure
○ Provides structural information
○ Considers only pairs of atoms

No, the answer is incorrect.
Score: 0

Accepted Answers:
Provides information about transport properties

10) The _____ helps us to computationally characterize a given structure as a solid,liquid or gas. *2 points*

○ Radial Distribution Function (RDF)
○ Mean squared displacement (MSD)
○ Radius of gyration function
○ Diffusion Coefficient function

No, the answer is incorrect.
Score: 0

Accepted Answers:
Radial Distribution Function (RDF)

11) The Radial distribution function can be used to obtain *2 points*

○ The temperature of a system
○ Radial distance up to which an interaction can be felt by an atom
○ Coordination number of atoms
○ Radius of atoms

No, the answer is incorrect.
Score: 0

Accepted Answers:
Coordination number of atoms

12) Which of the following commands will output information pertaining to each atom *2 points*

○ fix
○ thermo
○ dump
○ lattice

No, the answer is incorrect.
Score: 0

Accepted Answers:
dump