2 points

2 points

2 points

2 points

Unit 14 - Week 9

How does an NPTEL online

Course outline

MATLAB_SCRIPTS

LAMMPS_SCRIPTS

Installation_Procedure

course work?

MATLAB

Week 1

Week 2

Week 3

Week 4

Week 5

Week 6

Week 7

Week 8

Week 9

Week 10

Week 11

Week 12

Basic introduction to MD

Input script for LAMMPS 1

Input script for LAMMPS 2

Foundations of Computational

O Quiz: Assignment 9

Week 9 Feedback :

Materials Modelling

Additional Documents

Download videos

Text Transcripts

	this assignment has passed. not submitted this assignment. Due on 2020-04-01, 23	:59
1) True or False:		
In molecular dynamics, ins	tead of computing the time averages, we calculate the phase averages.	
True		
False		
No, the answer is incorrect. Score: 0 Accepted Answers: False		
For a commonly used exp	oression for the Lennard-Jones potential given by the equation	
$\phi(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right) \right]$	$\left[\frac{\sigma}{r}\right]^{Y}$	
\boldsymbol{X} , \boldsymbol{Y} are most likely		
12,6		
○ 6,12 ○		
X - Y = 5		
○ X - Y must always be 6		
No, the answer is incorrect. Score: 0		
Accepted Answers: 12,6		
	entain anapahata of atama and various per atam values and are written at a appoified frequency	
	ontain snapshots of atoms and various per-atom values and are written at a specified frequency.	
Dump files Restart files		
O Data files		
Input files		
No, the answer is incorrect. Score: 0		
Accepted Answers: Dump files		
Periodic boundary condit and make the system mo	ions (PBC) are used in molecular dynamics simulations to avoid problems with boundary effects caused by finite size, ore like an infinite one	
True		
False		
No, the answer is incorrect. Score: 0		
No, the answer is incorrect. Score: 0 Accepted Answers: True		
Score: 0 Accepted Answers: True	n each atom in the system is calculated by multiplying the mass of the atom by the acceleration of the atom	
Score: 0 Accepted Answers: True	n each atom in the system is calculated by multiplying the mass of the atom by the acceleration of the atom	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of	n each atom in the system is calculated by multiplying the mass of the atom by the acceleration of the atom	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of	n each atom in the system is calculated by multiplying the mass of the atom by the acceleration of the atom	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers:	n each atom in the system is calculated by multiplying the mass of the atom by the acceleration of the atom	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false		
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full	n each atom in the system is calculated by multiplying the mass of the atom by the acceleration of the atom	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false		
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Group functions Math functions		
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Interatomic potentials Group functions Math functions Atom functions		
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Interatomic potentials Group functions Math functions Atom functions No, the answer is incorrect. Score: 0		
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full full full full full full full fu		
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Interatomic potentials Group functions Math functions Atom functions No, the answer is incorrect. Score: 0 Accepted Answers: Interatomic potentials	unctions for calculating the potential energy of a system of atoms with given positions in space.	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Interatomic potentials Group functions Math functions Atom functions No, the answer is incorrect. Score: 0 Accepted Answers: Interatomic potentials 7) What is the expression for the second in the sec	unctions for calculating the potential energy of a system of atoms with given positions in space.	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Interatomic potentials Group functions Math functions Atom functions No, the answer is incorrect. Score: 0 Accepted Answers: Interatomic potentials 7) What is the expression for the second in the sec	unctions for calculating the potential energy of a system of atoms with given positions in space.	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Interatomic potentials Group functions Math functions Atom functions No, the answer is incorrect. Score: 0 Accepted Answers: Interatomic potentials 7) What is the expression for $\phi = -Ae^{Br} + \frac{-C}{r^6}$	unctions for calculating the potential energy of a system of atoms with given positions in space.	
Score: 0 Accepted Answers: True 5) In LAMMPS, the forces of True false No, the answer is incorrect. Score: 0 Accepted Answers: false 6) are mathematical full Interatomic potentials Group functions Math functions Atom functions No, the answer is incorrect. Score: 0 Accepted Answers: Interatomic potentials 7) What is the expression for the second in the sec	unctions for calculating the potential energy of a system of atoms with given positions in space.	

Accepted Answers: $\phi = Ae^{-Br} - \frac{C}{r^6}$

No, the answer is incorrect.

Score: 0

○ True

False No, the answer is incorrect.

Score: 0 Accepted Answers:

False

9) In LAMMPS input script file, _____ command creates a simulation box based on the specified region.

create_box region

obox

O fill_box No, the answer is incorrect.

Score: 0 Accepted Answers:

create_box

10) Which of the following commands is always needed for a LAMMPS input script to run successfully orun

No, the answer is incorrect.

units create box

dump

Score: 0 Accepted Answers: units

11) Which of the following commands will output information pertaining to the simulation box

fix dump

region No, the answer is incorrect.

○ thermo

Accepted Answers: thermo