

MSE 614 Course Schedule

#	DATE	TOPIC	HOMEWORK
1	1/23/2024	Introduction, Capabilities of Four Modeling Scales	
2	1/25/2024	Practical Introduction to ISAAC	
3	1/30/2024	Capabilities of Four Modeling Scales	
4	2/1/2024	A Working Person's Guide to MD I	Homework 1 Assign
5	2/6/2024	Guest Lecture: intramolecular degrees of freedom	
6	2/8/2024	A Working Person's Guide to MD II	
7	2/13/2024	Introduction to LAMMPS	
8	2/15/2024	LAMMPS input files	
9	2/20/2024	conservation of momentum and energy/Hamiltonian	Homework 1 Due
10	2/22/2024	thermostats and barostats and ensembles	Homework 2 Assign
11	2/27/2024	initial configurations	
12	2/29/2024	structural relaxation and energy minimization	
13	3/5/2024	visualization	
14	3/7/2024	time integrators: r-ReSPA	Homework 2 Due
15	3/12/2024	SPRING BREAK - NO CLASS	
16	3/14/2024	SPRING BREAK - NO CLASS	
17	3/19/2024	POSTER PRESENTATIONS OF FIRST PROJECT	Project 1: Poster, Report, Webpage Due
18	3/21/2024	multicomponent systems & potentials	
19	3/26/2024	nonpairwise (embedded atom method) potentials	Homework 3 Assign
20	3/28/2024	"NO CLASS DAY at UTK"	
21	4/2/2024	good statistical averaging, block averaging	
22	4/4/2024	thermodynamic properties	
23	4/9/2024	auto correlation functions	
24	4/11/2024	rigid constraints – molecules	Homework 3 Due
25	4/16/2024	transport properties	Homework 4 Assign
26	4/18/2024	structural properties (RDFs)	
27	4/23/2024	density distributions	
28	4/25/2024	Two-Phase Simulations	
29	4/30/2024	Guest Lecture: Dr. Michael Ohl: MD & Energy Storage	Homework 4 Due
30	5/2/2024	Reactive MD Simulation	
31	5/7/2024	POSTER PRESENTATIONS OF FINAL PROJECT	Project 2: Poster, Report, Webpage Due