

MSE 614 Course Schedule

#	DATE	TOPIC	HOMEWORK
1	1/25/2022	Introduction, Capabilities of Four Modeling Scales	
2	1/27/2022	Practical Introduction to ISAAC	
3	2/1/2022	Capabilities of Four Modeling Scales	
4	2/3/2022	A Working Person's Guide to MD I	
5	2/8/2022	A Working Person's Guide to MD II	Homework 1 Assign
6	2/10/2022	Introduction to LAMMPS	
7	2/15/2022	LAMMPS input files	
8	2/17/2022	conservation of momentum and energy/Hamiltonian	
9	2/22/2022	thermostats and barostats and ensembles	Homework 1 Due
10	2/24/2022	initial configurations	Homework 2 Assign
11	3/1/2022	structural relaxation and energy minimization	
12	3/3/2022	visualization	
13	3/8/2022	time integrators: r-ReSPA	
14	3/10/2022	multicomponent systems & potentials	Homework 2 Due
15	3/15/2022	SPRING BREAK - NO CLASS	
16	3/17/2022	SPRING BREAK - NO CLASS	Collect HW 4/Assign HW 5
17	3/22/2022	POSTER PRESENTATIONS OF FIRST PROJECT	Project 1: Poster, Report, Webpage Due
18	3/24/2022	intramolecular degrees of freedom	
19	3/29/2022	nonpairwise (embedded atom method) potentials	Homework 3 Assign
20	3/31/2022	good statistical averaging, block averaging	
21	4/5/2022	thermodynamic properties	
22	4/7/2022	auto correlation functions	
23	4/12/2022	rigid constraints – molecules	
24	4/14/2022	"NO CLASS DAY at UTK"	Homework 3 Due
25	4/19/2022	transport properties	Homework 4 Assign
26	4/21/2022	structural properties (RDFs)	
27	4/26/2022	density distributions	
28	4/28/2022	Two-Phase Simulations	
29	5/3/2022	Reactive MD	Homework 4 Due
30	5/5/2022	Monte Carlo	
31	5/10/2022	POSTER PRESENTATIONS OF FINAL PROJECT	Project 2: Poster, Report, Webpage Due