

Rachel B. Getman Contact: rgetman@g.clemson.edu, http://computationalcatalysis.sites.clemson.edu **Example Assignment #1: WebMO/Quantum Chemical Calculations/Intermolecular Forces** • Illustrate how intermolecular interactions are quantum in nature. ojectives: • Illustrate physical bonding and the use of the Lennard-Jones potential for modeling physical bonding. Improve students' understanding about how pairs of molecules orient during intermolecular interactions • Determine correlations between physical bond strength, Lennard-Jones parameters, and physical properties Improve students' perceptions of quantum chemistry software OK Apply Cancel La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Users select computational Cancel A carbon atom. Clicking "clean" Users can specify distances and other parameters from a list. They can view Users can "copy and paste" Periodic table tool converts it to a CH₄ molecule. geometrical parameters the actual input file if desired. udents place two CH₄ molecules in proximity and then "drag" them apart, calculating the energy of interaction at each point they correlate to properties such as molecular weight - CHE - F... 💿 nsf.gov - CBET -... 🥱 CoES Proposal De... 🔇 FERPA::Summation 🔗 Factsheets : AFOS... 🔇 Factsheets : AFOS... 🄇 Defense Advance... 资 PRF: Doctoral Ne... 🔇 The Alfred P. Sloa... 🔇 Camille Drayh • Each pair of students works on a different pair of molecules File Edit Tools Adjust Cleanup Calculate Lookup Help Inter mol) gy of | //L/ • Students also list the types of intermolecular forces that are present in the interaction • While completing the assignment, students use the "pilot/navigator" approach to problem solving

Illustrating Molecular-Level Phenomena and Molecular Simulation Techniques with Commonly Used Software Department of Chemical and Biomolecular Engineering, Clemson University

 Many grand challenges facing chemical engineers today invol molecular-level chemistry 	
	ve
 Having an appreciation for molecular-level phenomena we better prepare chemical engineers to handle problems in energy water, food, catalysis, advanced materials, and other fields 	vill gy,
 A major impediment to teaching and learning about molecula level phenomena is the learning curve associated with molecul simulation software 	ar- lar
 The goal of this work is to demonstrate molecular phenome and simulation techniques using straightforward graphical us interfaces and familiar software 	na ser
 Specifically, we focus on conceptual aspects of molecular-levelocity chemical engineering, including students' abilities to connection molecular-level phenomena with observable properties 	vel ect
All assignments (and more!) are	
available for public use on	
Canvas Commons. Search for	
"chemical engineering".	
Image: State of the state	•
COURSE BY APPLE EDUCATION	•
Image: Course BY APPLE EDUCATION Image: Course BY Designers FOR LEARNING App Development with Swift Meaningful Inclusion I Special Olympics 9 - Undergraduate 9 - 12	•

Example Assignment #3: MATLAB/Monte Carlo/Temperature Swing Adsorption

Objectives:

- Practice using Monte Carlo for molecular applications, including practicing operating the most important simulation parameters (intermolecular potential, temperature, number of moves, ratio of translate to replace moves) Demonstrate how the simulation parameters influence the number of moves required to achieve equilibrium
- Introduce the concepts of temperature swing adsorption and adsorptive separations. Learn how to tune operating conditions to achieve optimal performance for these two applications. • Demonstrate how molecules with different interaction strengths exhibit different adsorptive properties.
- Develop an appreciation for how results obtained in a molecular simulation can be transposed to experimental or real world operation (e.g., trends rather than exact values) • Improve students' perceptions of and confidence in installing and using MATLAB Students change simulation parameters in a pre-written code. The goal is to identify the "storage" and '

•••	MATLAB R2018b - academic use				Figure 1
HOME PLOTS APPS EDI	TOR PUBLISH VIEW	🗟 🔁 🕐 💿 🔍 QSearch Docu	mentation 🛕 Rachel 👻	File Edit View Insert Tools	Deskton Window Help
🕒 🛌 🖃 🗔 Find Files 😒 😒	Insert 🔜 🗴 🔚 👻 🕞 🔀 🚬				
La Compare ▼ 🖓 Go To ▼ Com	mment % ½ %				_ <u>=</u>
New Open Save	Indent 🛐 👰 🜠 🗸 war a kun ang 🔯 Advance kun ang 🔤 Advance kun ang 🔤 Advance kun ang kun				
FILE NAVIGATE	EDIT BREAKPOINTS RUN		<u> </u>		
< 🔶 🔁 🔀 💭 🔚 / 🕨 Users 🕨 rgetman 🕨 C	:LEMSON → classes → 190109_ChE4450_6450 → assignments → MC1		- ₽		Positions During Monte Carlo Simulation
Current Folder 💿	Z Editor - /Users/rgetman/CLEMSON/classes/190109_ChE4450_6450/assignments/MC1/runMC.m 💿 🗴	Workspace	•		
Name ▲	runMC.m × +	Name A	Value		
alc_pairwise_energy.m	1 %%%%% enter in the following:%%%%%%%%%%%	acceptance_rate	'/Users/rgetman	100 —	
check_positions.m	3 - N molecules = 30; % how many molecules to simulate.	avg_CN	4000x1 double		
Create_positions.m Addetermine_coordination_number_m	4 - LJ_sigma = 3.7; % Enter the Lennard-Jones sigma value of your molecule in units of Angstroms.	avg_CN_initial	0		
dist.m	5 - LJ_epsilon = 155; % Enter the Lennard-Jones epsilon value of your molecule in units of Kelvin.	Conc	0.0409	90 —	
place_molecules.m	7 - Temperature = 100: % Enter the temperature in units of Kelvin.	Delta_E	0.8658		
i replace_molecules.m	8 %	dist_to_floor	35.1993		
translate molecules m	9 - N_MC_steps=4000; % enter the number of Monte Carlo steps to take	E_after_move	-3.2337	80 —	
	10 - frac_translate=0.8; % enter the fraction of steps that you wish to be of the type "translate". Th	E target	-4.0994		
	11 * *********************************	Einit	-0.7241		
	13 %	energyif	-2.6340e-05	70 —	
	14 % There are three options pertaining to how to define your box size.	floor area	-5.2762e-07		
	15 % 16 % OPTION 1: Concentration is ~ that of an ideal gas at STP:	frac_translate	0.8000		
	17 - box_length=(((1/0.0409)*(1/(6.0221409e23))*N_molecules*(1/1000))^(1/3))*(10^10); %	h h	30x30 double	60	
	18 %		4000	00	• • •
	19 % OPTION 2: Concentration is ~ that of a liquid. 20 % liquid density = 556, so enter in the density of the liquid of choice in units of k_0/m^{2}	LI epsilon	155		$\bigcirc \bigcirc \land \land \land \bigcirc$
	20 % induce on the state of the density of the trade of induce in this of the state of the stat	LJ_epsilon_floor	10000	50	
	22 %	LJ_sigma	3.7000	50 —	•
	23 % OPTION 3: You can define your own box length. If you want to define your own box	moves accepted	4 3633		
	24 % length, uncomment this line: 25 % how length = 20 : % The how is a cube. How big should a leg be? Units = Angstroms.	N_MC_steps	4000		
	26 % This code does a "sanity check" on the system setup:	N_molecules	30	40	
	27 %	number_adsorbed	4000x1 double		
	28 - disp('checking the reasonableness of the system setup.') 29 - Vsphere (4/3)-pris(1) simp(2)/324 malecules: * subjc Apastrons	p	0.3390		
	30 - Vfractsphere(tox)tenth(3); % unitless	R	0.0083	30 —	
		sigma_mix	6		•
	Command Window	target molecule	7		
	New to MATLAB? See resources for Getting Started.	× H Temperature	100	20 —	
	Checking the reasonableness of the system setup	- Vfrac	6.5325e-04		
	Creating initial positions of molecules. This may go through many tries and take some time.	Vsphere	795.6555 30x1 double		
Details 🗸 🗸	Initial configuration was generated successfully.	x_new	31.5176	10 —	
	Determining average coordination number of initial configuration.	x_plot	21x21 double		
	Determining coverage of initial configuration.	± xsph	21x21 double		
	The initial coverage is 0 molecules adsorbed per 1.140507e+04 square Angstrom.	y new	45.3694	0	
Select a file to view details	Calculating energy of initial configuration.	y_plot	21x21 double		
	Ine energy of the initial configuration is -/.241261e-01 kJ/mol. Running the Monte Carlo algorithm.	📥 ysph	21x21 double	100 90 80	70 60 50 40 30 20 10 00 10 20
	The Monte Carlo algorithm has finished. I am now making your plots. There will be 4 total. Please wait.	Z new	5 8022		
	$h \gg$		21x21 double	enh	eres adsorbing to t
					cies ausorbing to t

C-C distance (Å)

jectives:

st (click = select; double-click = select all; right-click = popup men

- Ilustrate how process variables influence process outcomes
- ntroduce or re-enforce reaction runaway and chemical reactor safety
- Practice chemical engineering design,
- particularly the balance between safety and naximizing production rate
- ntroduce the method of Monte Carlo using amiliar software

Example Assignment #2: Excel/Monte Carlo/Safety and Risk

Students use the random number generator a





This work was funded by the National Science Foundation Under grant number CBET-1554385. We thank Prof. Karen High (Clemson Engineering and Science Education Department) for assisting with assessment. Travel support from CACHE is gratefully acknowledged.

• After completing the assignment, 2-3 pairs of students are combined into a bigger group to compare results. • Examples of larger groups: Ne-Ne, H_2S-H_2S , H_2O-H_2O ; CH_4-CH_4 , CCI_4-CCI_4 , $C_2H_6-C_2H_6$; HCI-HCI, HCI-Ar, HCI-H_2O • The larger groups are asked to write a paragraph describing the differences in the results in the context of the different intermolecular forces

🗧 🕘 💿 AutoSave 🗨 📭 🏠 🕤 🗸 🦉 🖛	Ja 1	170802_SafetyAndRisk		Q v Search Sheet	💿 🕒 🔵 Auto	Save 🗨 🖬 🏠 🕤 🗸 🕻	5 =			💼 170802_Safety	AndRisk				Q~ Search
Home Insert Draw Page Layout Formulas Data	Review View			년 Share 🗘 Comments	Home Insert	Draw Page Layout	Formulas Data Revi	w View							B
Cut Calibri (Borbi) x 12 x A A	E =	Normal Bad	Σ	AutoSum v Asy AutoSum v Asy	Cut	0.0.10.10.11	10 A1 A1 = -	- ab				Namal		- Σ A	utoSum v Ar
Copy v		A Conditional Format		Fill V Z V V Z	LO Č Copy	v Calibri (Body) v		= = •/• • ²⁰ m	rap lext v Ger	nerai 🗸	■ * ■ *	Good Neutral	_, 🕮 * 🏎	T 🔜 T 🔂 Fill	, Z∖
Veste S Format B I U V V A V A V	= = = •= •= •= •= Merge & Center • \$ • %	Formatting as Table	insert Delete Pormat X	Clear Y Filter Select	Paste 🗳 Forma	nt B I U v ⊞ v	<u> </u>	= = <u>=</u> = = ⊞ M	erge & Center 👻 💲	× % 9 58 -38	Formatting as Table	Good Neutral	Insert Deleti	Format X Cle	lear v Filt
H4 $\stackrel{*}{\bullet}$ \times \checkmark f_x =A4*2-1				Ŧ	F3 🗍 🔆 🗙	✓ fx =F2/(MAX(A3:A300)	00)*MAX(calculations!A22:A3	001))							
A B C D	E F G	L I H	K L M	N O	А	В	C D	E	F G	н	1 1	к	L M	N	0
1 random numbe	c	random numbers be	tween -1 and 1		1										
2 ndot PO-in ndot MeOH-in ndot W-in frac con	PO T feed mdot-H2O-cool	ndot PO-in ndot MeOH-in ndot W-in fr	ac conv PO T feed mdot-H2O-r	200	2 run #	# above tolerance	sum of colu	mn B =	4161						
3 0.601781346 0.80401626 0.476425 0.55982	3388 0.216735514 0.08921599	0.203562692 0.608032521 -0.0471505 0	119656777 -0.566529 -0.82156	802	3 1	177	What is the	failure rate? 0.	.16644						
4 0.958250896 0.141163618 0.051791 0.05258	3739 0.925141413 0.365353137	0.916501793 -0.717672763 -0.8964178 -0	.894832522 0.85028283 -0.269293	727	4 2	164									
5 0.290417218 0.029804217 0.432959 0.51869	3202 0.917558393 0.75799441	-0.41916556 -0.940391566 -0.1340818 0	0.037386403 0.83511679 0.51598	882	5 3	174									
6 0.292347235 0.226463776 0.592314 0.02630	0169 0.0053344 0.705719129	-0.41530553 -0.547072449 0.18462747 -0	.947381662 -0.9893312 0.411438	258	6 4	149									
7 0.607496135 0.564695023 0.848137 0.76582	7382 0.066005658 0.078835006	0.21499227 0.129390047 0.69627425 0	.531654765 -0.8679887 -0.842329	987	7 5	143									
8 0.794726316 0.485658439 0.103784 0.84398	0.289340774 0.591935584	0.589452633 -0.028683121 -0.7924319 0	.687979404 -0.4213185 0.183871	169	8 6	160									
9 0.084439549 0.658363856 0.000383 0.04005	851 0.209949373 0.806787716	-0.8311209 0.316727712 -0.9992343 -0	.919882297 -0.5801013 0.613575	431	9 7	153									
10 0.437340992 0.812370714 0.250509 0.09752	073 0.875768449 0.814645295	-0.12531802 0.624741428 -0.4989819 -0	.804955854 0.7515369 0.629290	591	10 8	176									
11 0.172392981 0.606428315 0.335925 0.74136	0.276529379	-0.65521404 0.212856629 -0.3281499 0	.482726454 0.69142372 -0.446941	242	11 9	1/9									
12 0.86190304 0.858797161 0.730693 0.71014	6687 0.285286498 0.581484685	0.723806081 0.717594323 0.46138545 0	.420293375 -0.429427 0.16296	937	12 10	1/8									
13 0.963975599 0.272135117 0.895237 0.99762	144 0.067549883 0.367603147	0.927951198 -0.455729766 0.79047354 0	.995248288 -0.8649002 -0.264793	706	14 12	186									
14 0.194788035 0.444022087 0.646231 0.83306	2878 0.55143249 0.276179939	-0.61042393 -0.111955825 0.29246161 0	0.666125756 0.10286498 -0.447640	122	15 13	145									
15 0.61815146 0.652452588 0.122566 0.85502	2996 0.484632418 0.83486148	0.236302921 0.304905176 -0.7548679 0	0.710045992 -0.0307352 0.66972	296	16 14	164									
16 0.133925666 0.611104616 0.485986 0.05645	1442 0.400326976 0.489404032	-0.73214867 0.222209231 -0.0280288 -0	0.887091117 -0.199346 -0.021191	936	17 15	155									
17 0.606637904 0.9103787 0.078919 0.46241	3804 0.255432114 0.105047841	0.213275809 0.820757401 -0.8421623 -0	0.075162392 -0.4891358 -0.789904	318	18 16	161									
	0.050499438	0.988560575 -0.770452068 -0.5411822 0	0.078331767 0.72936018 -0.899001	124	19 17	186									
	0.26649956	-0.24792604 -0.33626116 0.96010852 -0	0.25399555 -0.467000	474	20 18	155									
		0.1501/004 -0.354/14232 0.04589419 -0	0.727650864 -0.7410347 0.13029	164	21 19	187									
22 0.418725458 0.05581525 0.018808 0.51025	1219 0 271140736 0 584182703	-0.44467108 -0.661179435 -0.8208613 -0	A31871561 -0.4577185 0.168365	406	22 20	183									
22 0.277004438 0.103410282 0.083509 0.28400	019 0.077161427 0.920288482	0 251338814 0 985828944 -0 793386 0		965	23 21	162									
24 0 133737439 0 934634029 0 226153 0 42302	8235 0.513926642 0.057326231	-0.73252512 0.869268058 -0.5476949 -	0 15394353 0 02785328 -0 885347	538	24 22	166									
25 0.189331247 0.736693941 0.093206 0.60479	2903 0.411032725 0.349851422	-0.62133751 0.473387882 -0.8135875 0	.209585806 -0.1779345 -0.300297	156	25 23	168									
26 0.625569409 0.802322926 0.199523 0.22100	3791 0.364564225 0.050702868	0.251138818 0.604645851 -0.600954 -0	.557982419 -0.2708716 -0.898594	263	26 24	1/2									
27 0.261965781 0.552588324 0.288384 0.14107	0.507147585 0.680273726	-0.47606844 0.105176648 -0.4232327 -0	0.717854565 0.01429517 0.360547	452	27 23	138									
28 0.40921074 0.421020322 0.049249 0.4747	0159 0.644659875 0.897614528	-0.18157852 -0.157959356 -0.9015018 -0	0.050416819 0.28931975 0.795229	056	29										
29 0.315611786 0.854172408 0.678561 0.0053	8863 0.524754659 0.911568667	-0.36877643 0.708344816 0.35712118 -0	.989322739 0.04950932 0.823137	333	30										
30 0 925880247 0 915533855 0 771678 0 87165	986 0 385959712 0 455552864	0.851760493 0.83106771 0.54335523 0	743303972 -0 2280806 -0 088894	273	21										

Students use WebMO to find the transition state for HCN isomerization to CNH • Demonstrates transition state theory, transition state structures, reaction coordinates, use of quantum chemical calculations, vibrational modes Students use WebMO to calculate the energy levels of a 3d metal atom

- Demonstrates

ope College. Anyone in the world can run WebMO with just an Internet connection

Before completing the exercise, students complete a module that describes how Monte Carlo is used for various applications from sports to molecular adsorption

- During the exercise, students calculate the number of "failures" for a base case Failure occurs when the reactor
- temperature exceeds a certain value Students then change different process variables until they achieve a failure rate of 0.

Other Available Assignments

• Demonstrates quantized (versus continuous) energy levels, quantum chemical calculations, deciding how to choose basis sets and methods of electron correlation, solutions to the Schrödinger equation

Students use WebMO to calculate electronic, vibrational, translational, rotational contributions to the energy, and free energy for H, O, and H₂O

• Demonstrates statistical mechanics, different contributions to the energy and entropy as functions of temperature, quantum chemical calculations, deciding how to choose basis sets and methods of electron correlation Students use a Monte Carlo algorithm in MATLAB to predict the outcomes of the March Madness (basketball bracket)

configurational disorder, configurational entropy, ensembles, and intentional biasing ... AND promotes women's basketball!

Coming soon: All MATLAB assignments will be converted to Python to promote Open Educational Resources