Midterm Study Questions

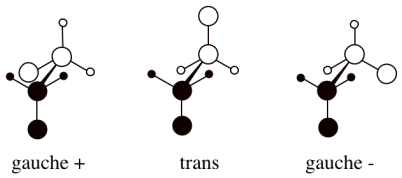
Ank: Explain why all atoms have an attractive force between them.

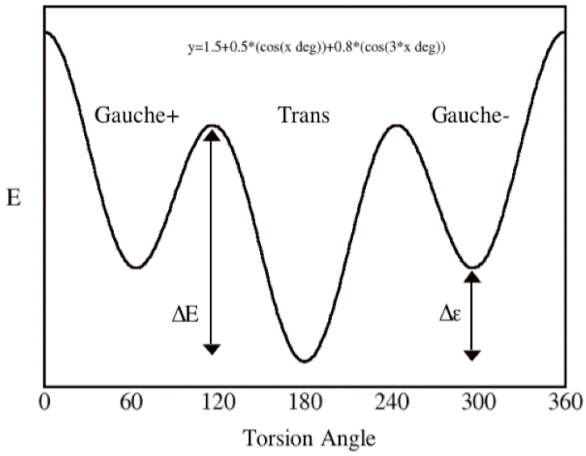
Lauryn (on board): Describe how the Lennard-Jones potential function models different components of atomic interaction.

Felipe: Reduced units are frequently used in molecular simulations.

a. What molecular mechanics model parameter defines the unit of length in reduced units in your Argon simulations?
b. What is the advantage of using reduced units in a computer simulation of molecules?

Christine: Consider a population of a hypothetical molecule with the following conformations that are observed to any significant extent.





These three conformations are predominant because only certain angles of rotation about the central bond are relatively energetically favored as shown in the following figure (figure is not to scale).

Using the information above explain the difference between **dynamic flexibility** and **static flexibility**.

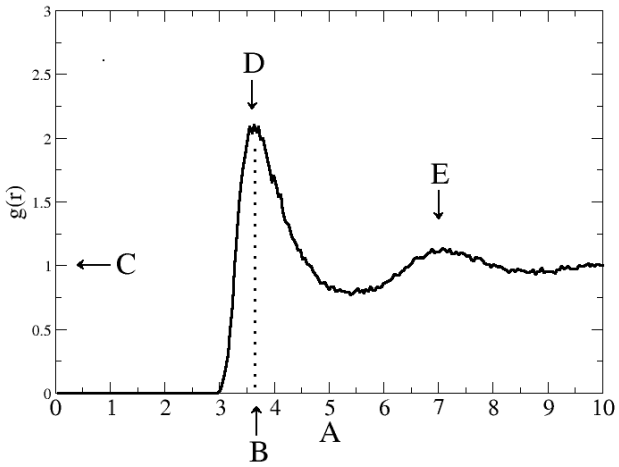
Bobby: All atoms have an interatomic attractive force.

a. Explain what causes this universal attractive force.
b. Explain why this attractive force falls off with a $1/r^6$ dependence on the interatomic distance.

Josh: (at the board): Answer both parts (a) and (b) below.

a. Write a form of the Metropolis criterion using temperature (T) in the expression appropriate to molecular simulations. (Use short answer or pseudo-code).
b. Applying the Metropolis criterion repetitively in a Monte Carlo molecular simulation generates a Boltzmann probability distribution of states. What assumption specific to MC must be true in order to achieve a Boltzmann distribution using the Monte Carlo procedure and provide a short description for of this assumption (words or equations)?

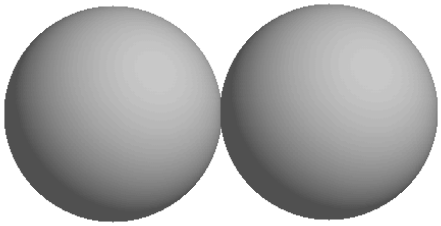
Below is a plot of the average structure of an argon system.



Provide answers for the following (A – F).

A. (Thea) What scalar parameter of the system is represented by the x axis?
B. (June) What atomic system parameter is represented by the x axis value at B? (Common name).
C. (Maru) What does g(r) = 1.0 on the y axis at C represent? (I.e. this is a normaliaed value for what characteristic of the system?)
D. (Vivian) What molecular system spatial characteristic is represented by the peak at D?
E. (Jacob) What molecular system spatial characteristic is represented by the peak at E?
F. (Young-wook) What is this 2D plot usually called?

Sanjay: The following molecular graphics image shows two single atom molecules at their **equilibrium** distance for the controlling Lennard-Jones energy function.



a. Is the hard shell radius or the van der Waals radius depicted in the image? [
b. Explain the difference between these two types of radii in terms of the Lennard-Jones potential function.

Arman: Both Monte Carlo and molecular dynamics simulations have the same initial purpose.

a. What is that common purpose?
b. Describe at two analytical comparisons one could do in the lab to demonstrate that both methods give comparable results?

Ash: What is a typical good cut off distance for LJ potential calculation and why is such a cut off used? What value was used in your argon simulations?

Lance (at the board): Explain how T plays a role in MC versus how T determines velocity distribution in MD? (Use pseudo-code, equations or words).

David Li: Below are extracts from a PDB file showing the ATOM lines for two different isoleucine residues in the same polypeptide chain. The structure of this polypeptide was determined by X-ray crystallography.

```
ATOM     36  N   ILE     5      15.428   6.674 -10.737  1.00  9.15
ATOM     37  CA  ILE     5      14.361   5.721 -10.503  1.00  6.28
ATOM     38  C   ILE     5      14.926   4.428  -9.933  1.00  7.56
ATOM     39  O   ILE     5      15.892   3.898 -10.465  1.00 10.20
ATOM     40  CB  ILE     5      13.534   5.480 -11.801  1.00 11.90
ATOM     41  CG1 ILE     5      12.772   6.790 -12.289  1.00 18.26
ATOM     42  CG2 ILE     5      12.598   4.256 -11.549  1.00 11.20
ATOM     43  CD1 ILE     5      13.324   7.109 -13.674  1.00 26.31

ATOM    116  N   ILE    17      17.099   0.203   1.744  1.00  5.29
ATOM    117  CA  ILE    17      16.291   1.102   2.563  1.00  7.88
ATOM    118  C   ILE    17      17.166   2.091   3.361  1.00  6.17
ATOM    119  O   ILE    17      16.906   3.321   3.488  1.00  7.20
ATOM    120  CB  ILE    17      15.390   0.280   3.534  1.00  8.14
ATOM    121  CG1 ILE    17      14.287  -0.431   2.668  1.00  9.31
ATOM    122  CG2 ILE    17      14.707   1.195   4.570  1.00  9.84
ATOM    123  CD1 ILE    17      13.569  -1.563   3.529  1.00  8.69
```

a. Which residue is most likely to be buried in the core of the protein?
b. What column in the PDB file allowed you to make your decision?
c. Why would the numbers in this column be different?

(I will display code below on screen): Below is Python code for a function that was included in the programs used in the lab.

Write an explanatory comment appropriate for each # symbol in the code, i.e. what is being done by each section of code following the comment symbol? (Comments (2 – 5) below).

```
def run(Data,X,Y,Z,En,Vir,Attemp,Nacc,Dr):
```

Alexis `# (1) Overall purpose of function`

```
    from math import exp
    from random import random

    Npart = int(Data['NPART'])
    Rho = float(Data['RHO'])
    Box = (Npart/Rho)**(1.0/3.0)
    Beta = 1.0/float(Data['TEMP'])

    Attemp = Attemp + 1
    Jb = 0
```

Kevin `# (2)`

```
    o = int(Npart*random())

    # Calculate energy of old configuration
    xo = X[o]
    yo = Y[o]
    zo = Z[o]
    Eno,Viro = eneri(Data,X,Y,Z,xo,yo,zo,o,Jb)
```

Chichi `# (3)`

```
    xn = X[o] + (random()-0.5)*Dr
    yn = Y[o] + (random()-0.5)*Dr
    zn = Z[o] + (random()-0.5)*Dr

    # calculate energy new configuration
    Enn,Virn = eneri(Data,X,Y,Z,xn,yn,zn,o,Jb)
```

Andrew `# (4)`

```
    if random() < exp(-Beta*(Enn-Eno)):
        Nacc = Nacc + 1
        En = En + (Enn-Eno)
        Vir = Vir + (Virn-Viro)
```

David Ramirez-Chavez `# (5)`

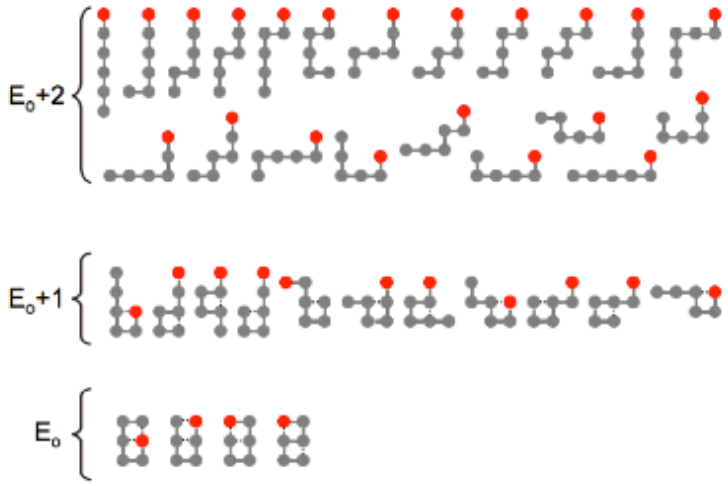
```
        if xn < 0.0:
            xn = xn + Box
        if xn > Box:
            xn = xn - Box
        if yn < 0.0:
            yn = yn + Box
        if yn > Box:
            yn = yn - Box
        if zn < 0.0:
            zn = zn + Box
        if zn > Box:
            zn = zn - Box
        X[o] = xn
        Y[o] = yn
        Z[o] = zn

    return X,Y,Z,En,Vir,Attemp,Nacc
```

Jessica: Either an MC or an MD simulation may be used to calculate average properties of a molecular system. But in order for these calculations to be valid two conditions or

assumptions must be met by the simulation. What are these two conditions and explain what they refer to. (Note: These assumptions apply to BOTH types of simulations).

Michael (on board): The figure below depicts available microstates for a hypothetical 2-dimensional polymer containing six monomers. These are distinguishable microstates as indicated by the position of the red monomer. The conformations of this polymer may be stabilized by non-covalent interactions, each noncovalent interaction (black dashed line). Write an expression for the molecular Boltzmann energy partition function (Z) for a system containing this polymer. You do not have to calculate a numerical value, just give the complete expression with all relevant terms. (Hint: Use the convention that the lowest energy state $E_o = 0$. Molecular in this case means use k instead of R).



Jonah: For both the MC and MD simulations of Argon the distance or time steps are very small. Larger distance or time moves would allow faster exploration of conformational space. Why can't one increase the distance (MC) or time (MD) moves in a molecular simulation?

Amy (on board): Assume that a hypothetical peptide has multiple (>> 2) conformations. However, it is known that the peptide has only two different internal enthalpies, A and B. Write an expression defining the difference in free energy (ΔG) between the two conformations in terms of their respective internal enthalpies (H_A, H_B) and number of conformations (g_A, g_B).