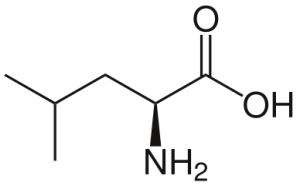
CBB 752 2016 Spring Final Quiz - 4/29/2016
NAME:

Total: 40 points (Please answer 4 questions out of 6)

1. (10 points)



<Leucine>

(a) How many side-chain dihedral angles does the amino acid Leu possess?

2

(b) If a polypeptide consists of seven Cα atoms, how many unique backbone dihedral and bond angles does it possess?

DA=4 BA=6

2. (10 points)
(a) What is the densest packing fraction for monodisperse hard spheres?

phi = 0.74

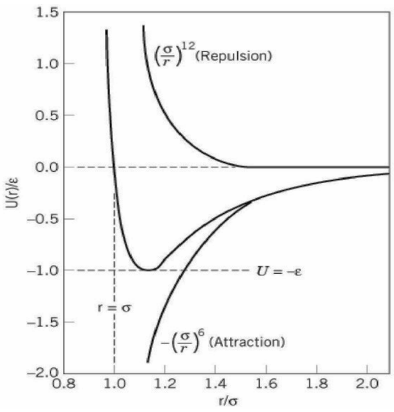
(b) What is the densest packing fraction for disordered collections of monodisperse hard spheres?

phi = 0.64

(c) What is the packing fraction of all-atom hard-sphere representations of residues in protein cores?

phi = 0.56

3. (10 points) Plot the purely repulsive Lennard-Jones interatomic potential V(r_ij) as a function of the separation between atoms r_ij.



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4. (10 points)
(a) What is the difference between a deterministic and stochastic model?

No randomness is involved in a deterministic model. Given model structure, parameter values, and initial conditions, there is no variation in output. In stochastic models, the next state of is not fully determined by the previous state – probability is involved.

(b) Which term applies to Ordinary Differential Equation (ODE) models?

Deterministic

5. (10 points) In the context of mathematical modeling, what is an F test used for?

The F test can be used to determine whether a parameter (or variable) should be added or deleted from a model. For example, it is used as part of a forward selection or backward elimination strategy.

6. (10 points) The SIR model can be used to predict the course of an epidemic in a large population. In the model equations given below, describe the meaning of each state variable (S, I and R) and each parameter (β and μ):

$$\frac{dS}{dt} = -\beta SI$$

$$\frac{dI}{dt} = \beta SI - \mu I$$

$$\frac{dR}{dt} = \mu I$$

S is the population of susceptible individuals
I is the population of infectious individuals
R is the population of individuals who were infected, but have now recovered
β is the infection rate
μ is the recovery rate