BIOENG 455 Test 3

1) List the 7 common elements in the anatomy of all Newtonian-like simulation techniques. (3 points)

System
State
Boundary conditions
Initial conditions
Interactions
Equations of motion
Observables

2) What are the two major classes of error in the Newtonian simulation techniques we have considered? Give two examples of each type. (2 points)

Systematic errors
Initial state
Finite system size
Approximations in forces
Truncation error (missing terms in Taylor series) Round-off error (machine precision, sqrt, order of calculations)
Random number generator isn't
Bugs in the code

Statistical errors
Too few samples
Samples too close together
Correlations
Stuck in metastable state

3) Coarse-graining atomistic molecular dynamics into a technique like DPD typically requires two approximations (or transformations). What are they? And how do they achieve the speedup associated with coarse-grained simulations? Also give two advantages of coarse-grained simulations over atomistic MD (do not include "they're faster" that one is given). (4 points)

1) Combine several atoms into a single particle thereby reducing the number of degrees of freedom to integrate.

2) Softer forces between particles allow larger integration time step because there is no hard-core repulsion.

Advantages of CG simulations: they reveal motions much larger than the atomic; they don't require detailed knowledge of atomic / chemical interactions; much cheaper computationally to get insight into dynamics; less likely to get stuck in metastable states

4) Typical cell membranes contain thousands of distinct types of phospholipid; what are four material properties of the membrane that might be modulated by the local lipid composition? (4 points)

Membrane thickness, bending stiffness, area stretch modulus, fluidity (lipid diffusivity), local composition, area per molecule

5) What four structural or functional properties do lipid membranes provide to a cell? (2 points)

Stable structure separating inside / outside

Self-healing due to hydrophobic effect

Controlled permeation allowing material in and out

Provide an environment for membrane proteins to function

6) Would DPD would be a good simulation technique for each of the following problems (answer with yes or no) (2 points):

a) measure the surface tension of a lipid bilayer 100 nm in linear size. Yes

b) measure the diffusion of a lipid vesicle 50 nm in diameter in a complex polymeric solvent (e.g., water plus PEG) . Yes

c) predict the binding energy of a glutamate molecule to an AMPA receptor. No

d) measure the diffusion rate of sodium ions through a membrane protein channel. No

7) State the Equipartition theorem (making clear the key assumptions) (3 points)

Each additive, quadratic degree of freedom in the Hamiltonian of a system in equilibrium contributes 1/2 $k_B T$ to its internal energy. The energy is shared among all accessible degrees of freedom of the system: if the temperature is such that some degrees of freedom cannot be excited they do not contribute to the internal energy.