Physics 347 Problem Set 1 due: Sept. 24

1. Heat balance of the earth: the one-layer atmosphere.
In tutorial I showed you how to estimate the heat balance of the earth, first in the simplest model and then including the effects of the albedo (a) and the atmospheric absorption of outgoing IR.
Show for the "one-layer atmosphere model discussed in class that the surface temperature T_s of the earth satisfies $\sigma T_s^4 = \frac{(1-a)f}{2(1+\alpha)}$, where f=1350 W/m^2 is the solar flux and $\sigma = 5.67 \times 10^{-8}$ W/m^2 K^4. Is called the Stephan-Boltzmann constant. Evaluate T_s for

(a) The simple case $a = 0; \alpha = 1$ (no albedo, no atmosphere)
(b) The case $a = 0.39; \alpha = 1$ (realistic albedo, IR-transparent atmosphere).
(c) The case $a = 0; \alpha = 0$ (no albedo, fully absorbing atmosphere).
(d) The approximately realistic case $a = 0.39; \alpha = 0$. (I find 292 K, an excellent estimate, although, perhaps, a bi fortuitous, considering the various complications discussing in tutorial.

Comment: The mean surface temperature of the earth is about 288 K (15 C). Note the sensitive balance between the albedo and the atomspheric IR absorption. That's what is at issue in global warming.

I did most of this for you in class (see Tutorial 1):
The solar energy in less the reflected light out (due to the earth's albedo) is $(1-a)f\pi R_e^2$.
This must be balanced by terrestrial radiation output. This has two parts:
(i) The direct radiation from the earth's surface: $\sigma T_s^4 \times 4\pi R_e^2 \times \alpha$
(ii) The energy reradiated upwards from the atmosphere: $\sigma T_s^4 \times 4\pi R_e^2 \times (1-\alpha) \times \frac{1}{2}$
Equating input and output (notice that the common factors πR_e^2 cancel out) gives:
$(1-a)f = 4\alpha\sigma T_s^4 + 2(1-\alpha)\sigma T_s^4 = 2(1+\alpha)\sigma T_s^4$ from which the formula follows.

The rest is just putting in numbers. I find:
(a) T=278 K (accidentally close to the measured value of 288 K)
(b) T=245 K (much too cold for comfort)
(c) T=330 K (much too hot for comfort)
(d) T=292 K (remarkably good estimate)

2. Human rates of heating and cooling. **2**

Your normal body temperature is regulated to be at or near 37 C. Body temperatures 5 C above or below this figure can have serious—even fatal—consequences.

(a) If your body has no way of dissipating metabolic heat, your body temperature must increase. Suppose you are surrounded by perfect insulation (no heat in or out). Assuming a basal metabolic rate of 100 W, estimate how long will it take your body temperature to rise 5 C?

(b) In summer the surface waters of the Georgia Strait can be as warm as 17 C. Assuming that all heat transport is by conduction, estimate how long a swimmer (or a capsized boater, for that matter) can be in the water before body temperature drops 5 C. Assume the basal metabolic rate.

Notes:

(i) You will need two figures for these calculations:

Thermal conductivity (estimate, water) $\kappa_T = 0.6 \dfrac{W}{m \cdot {}^{o}C}$

Specific heat (estimate, water) $C = 4.2 \times 10^{3} \dfrac{J}{kg \cdot {}^{o}C}$

(ii) The estimate which you reach will turn out to be broadly reasonable. Actual survival time can be longer or shorter than your estimate for many reasons:

- Long before you die of hypothermia, you become severely incapacitated from the cold, so without a PFD you are likely to drown.
- In the calculation, we have used the basal metabolic rate. Your body can for a while run at a rate several times higher than this, at least until you run out of sources of metabolic energy.
- A wet suit or even clothing will decrease the rate of conductive loss, thus increasing survival times. These coverings have insulating properties themselves (i..e., they change the effective thermal conductivity) but, also, they trap water, which can then warm up increasing the "thickness" factor d.
- I have assumed a thickness d of 1 cm, based on the distance from your surface blood vessels and the surface of your body. When you are sufficiently cold, your surface vessels constrict, thus decreasing blood flow to the surface and increasing the thickness d over which the temperature decreases from your core temperature (37 C) to that of the surrounding water (17 C). This is a natural (evolutionary?) physiological response to protect you from hypothermia.

(a) The metabolic energy $\Gamma_0 t$ increases your body temperature. Thus, **3**
$\Gamma_0 t = CM\Delta T$ where C is the specific heat, M is the mass, and ΔT is the temperature rise. Putting in numbers:

$$t = \frac{CM\Delta T}{\Gamma_0} = \frac{\left(4.2\times10^3\right)80(5)}{100} = 16.8\times10^3\ s = \boxed{4.7\ hr}$$

(b) The conductive energy loss is $\kappa_T \frac{S}{d}\Delta T_{body-water}\cdot t$.

The sources of energy are now two:

First the metabolic energy $\Gamma_0 t$, just as in part (a) .

Second the energy $CM\Delta T$ that comes out of body tissues in cooling

Note: I will assume for simplicity that the temperature difference $\Delta T_{body-water}$ is always 20 C. Of course, this is not quite true. Your body is getting colder, so the temperature difference gets smaller as you get colder and the energy loss rate decreases. This is a small effect.

It follows that $\Gamma_0 t + CM\Delta T = \kappa_T \frac{S}{d}\Delta T_{body-water} t$. Solve for the time T:

$$t = \frac{CM\Delta T}{\left(\kappa_T \frac{S}{d}\Delta T_{body-water} - \Gamma_0\right)} = \frac{\left(4.2\times10^3\right)80(5)}{\left(0.6\frac{2}{0.01}(20) - 100\right)} = 730\ s = \boxed{12\ \text{min}}\ ,$$

where I have used S=2 m^2 and d=1 cm, as in class.

Note: Standard survival tables give a survival times of 2—3 hours with proper PFD (personal floatation device). This number is obviously a bit too small. Although it probably does represent accurately the speed of your initial cooling. There are two issues: (a) the warmer-water layer around your body (e.g., water tapped by clothes) and (b) As your skin cools, the surface layer d over which the temperature gradient occurs gets thicker. The cooling rate is very sensitive to this depth. For example, by increasing d to 4 cm, the time t increases to 56 minutes.

Comment:

One person put in a radiation term. It is not wrong but it is a relatively small correction to the effects included here.

3. Allometric scaling for walking speed.

You will see on Ahlborn's table that normal walking speed V is found empirically to scale with body mass as $V = 0.5M^{1/6}$, i.e., as $V = aM^{\alpha}$ with a=0.5 and α=1/6. I want you to derive this relation from simple physical principles, including an estimate of the amplitude a.

(a) Estimate the amplitude a using the fact that an 80 kg adult walks naturally at about 5 km/hr. (Do not be upset if your estimate comes out a little larger than Ahlborn's number!)

Now, treat the leg as a simple pendulum and estimate a walking speed as the frequency of the pendulum times the step length.

(b) Show that the walking speed scales as $V \sim M^{1/6}$.

(c) Estimate the amplitude a as well as you can from this simple physical picture.

(a) **4**

$$V = \frac{5000}{60^2}(m/s) = a(80)^{1/6}$$

$$a = \frac{5000}{60^2 \cdot (80)^{1/6}} = \boxed{0.67}$$

Note: The units of a are $\left[\frac{m}{s(kg)^{1/6}}\right]$.

(b)

Walking speed is the product of a frequency times a step length L. For normal walking (as opposed to running) the frequency is simply the natural frequency of your leg swinging as a simple pendulum. For a point mass at the end of a string, that frequency is given by $f = \frac{1}{2\pi}\sqrt{\frac{g}{\ell}}$, where $g = 9.8\,\frac{m}{s^2}$ and ℓ is the length of the string. But, each step is only half a cycle, so $\boxed{V = 2fL = \frac{L}{\pi}\sqrt{\frac{g}{\ell}}}$.

To get the scaling relation, it is only necessary to note that both L and ℓ scale with the basic ("spherical cow") body dimension $R \sim M^{1/3}$; hence, $V \sim \frac{M^{1/3}}{\sqrt{M^{1/3}}} \sim \boxed{M^{1/6}}$.

(c)

To derive the amplitude, all we need to know(or estimate) are the (dimensionless) numerical factors connecting L and ℓ with R.

Recall that $R = \left(\frac{3}{4\pi}\right)^{1/3}\left(\frac{1}{\rho}\right)^{1/3} M^{1/3} = 0.062\,M^{1/3}$, which gives R=0.129 m for an 80 kg adult. Now, my leg is about 90 cm long, so I am inclined to estimate, $\ell = C_\ell R$ with $C_\ell \approx 7$, i.e., $\ell \approx 3\cdot(0.062)M^{1/3}$. My step length for a normal walking pace is perhaps 50 cm, so $L \approx C_L R$ with $C_L \approx 4$, i.e., $L \approx 2\cdot(0.062)M^{1/3}$.

It follows that $V = \frac{L}{\pi}\sqrt{\frac{g}{\ell}} \approx \frac{4(0.062)}{\pi}\sqrt{\frac{9.8}{7(0.062)}}M^{1/6} = 0.38M^{1/6}$, i.e., $\boxed{a \approx 0.38.}$

Note: The agreement between (a) and (c) is not very good. The main reason for this is I have treated the leg as if all the mass were concentrated in the foot.

Treating the leg as a uniform solid rod gives and extra factor of $\sqrt{\frac{3}{2}}$, so that the amplitude increases $0.38 \rightarrow 0.38\sqrt{\frac{3}{2}} = 0.47 = a$. But, even this is not a very good approximation, since the thigh is appreciably heavier than the calf. In fact, if you examine your walk, you will see that most of the motion is of the lower leg. **5** This has a length of about $\ell/2$ instead of ℓ, which increases V by another factor of $\sqrt{2}$ (why?) with $a \rightarrow 0.38\sqrt{2} = 0.53$ or $0.47\sqrt{2} = 0.66$. These—especially the latter—are quite close to the empirical value. This is not surprising, since we have modeled both (a) and (c) on human parameters.
Comment: Two people tried to connect this problem to the calculations for flying objects. There is no connection.

For the following two problems, you will need to learn how to manipulate molecular-structure files in order to be able to examine visually some molecules of biological importance and to measure their sizes. These files, some of which are available from the textbook website at
http://www.garlandscience.com/textbooks/0815341636/resources/,
usually (but not always) have the suffix .pdb. For convenience, I have posted these files with the problem set at the course website. (They are text files and you should try opening one or two in any text editor to see what they contain.) They can be read and manipulated with software available for download free from the web. I suggest using "VMD 1.8.7.app" which can be downloaded to your computer from
http://www.ks.uiuc.edu/Research/vmd/
along with a pdf Users Guide and some protein structure files. There is also an on-line tutorial. Structure files are also available on the web. One of the main sites for proteins in the "Protein Data Bank" at
http://www.pdb.org/pdb/browse/browse.do?t=4&useMenu=no
from which many protein structure files can be downloaded. Each file has its own unique four-part code, consisting of a number followed by three letters. Thus, 1MBO is a particular myoglobin molecule along with surrounding water molecules.

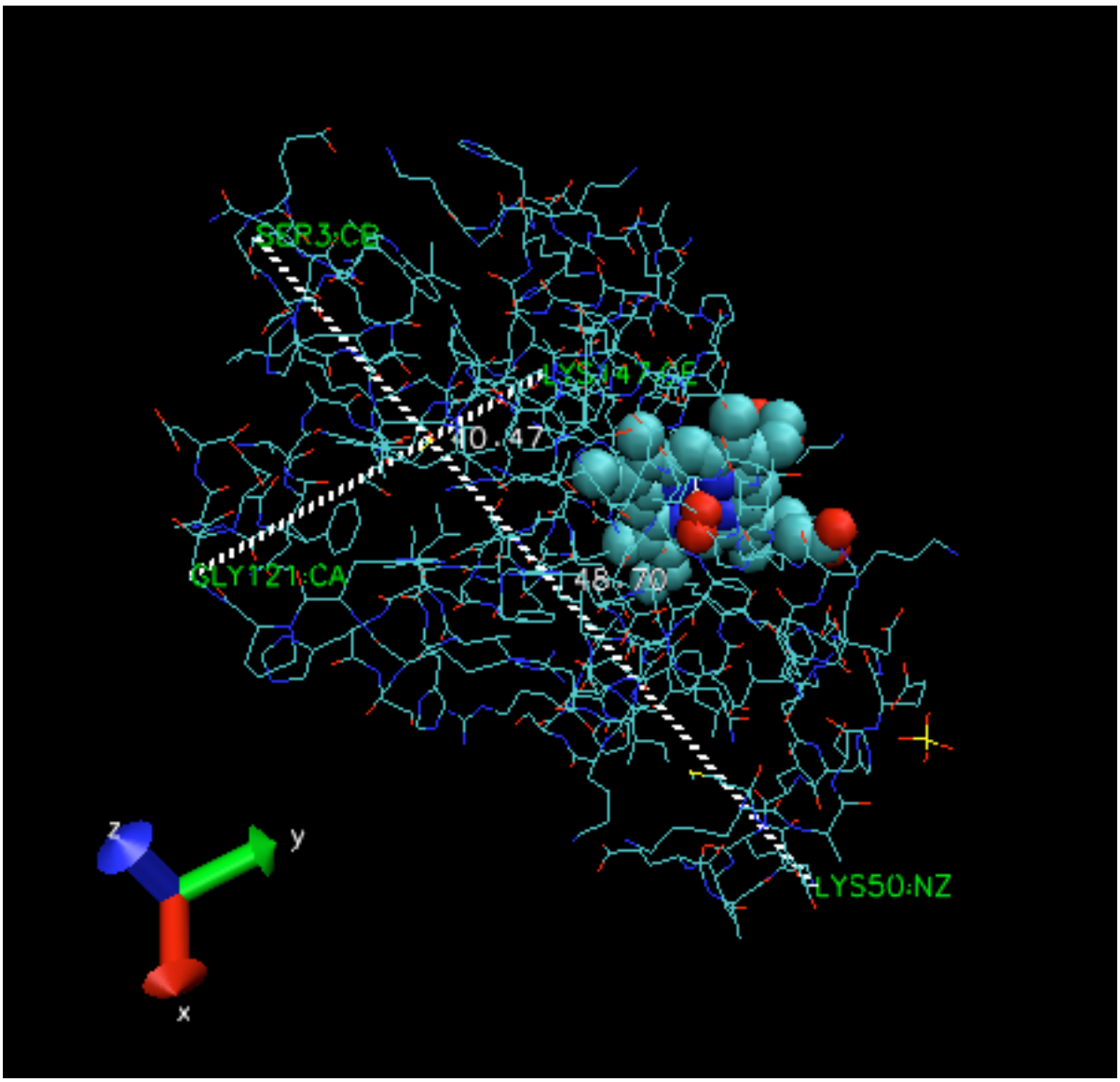
Once you have learned how to load these files into VMD and to display the molecular structure in various forms, a method for "measuring" molecular size is: In the "line" representation (see the "Graphics" menu in the VMD Main window), go to the "Mouse" menu and select Label>Bonds. Now, when you click on two atoms in the "Display" window, a line will appear between them labeled with the distance in Angstroms (10^{-10} m). Once you have established the scale of each representation, you can just use your ruler on the screen. To get an impression of the size of the atoms, it is often useful to use the van der Waals sphere representation (VDW).

4. PKT Problem 2.4 (p. 72)
Notes:
(a) and (b): These two parts are just getting you set up with the data files and the visualization software, as described above. Just to give you a specific objective here, I am asking you to load the sperm-whale myoglobin file 1mbo.pdb and
(i) show the entire molecule in the "line" representation with the waters deleted (command "not water") but
(ii) select the heme group and display it in the VDW representation, and:
(iii) use the label>bond in the mouse menu to draw the longest molecular diameter you can find. (I find one at 48.7 Angstroms but there may be some longer ones.) **6**
Finally, render the resulting image and save it as a pdf file to turn in for this part of your homework assignment.
(c) The file provided by the book is "stearoyl-oleyl-phosphacholine.pdb", which is defective. Instead of doing a lipid, load the file bdna.pdb, which shows the structure of the DNA double helix. Measure from this:

(i) the diameter of the double helix and
(ii) the axial distance ℓ_{bp} between base pairs,
(iii) the axial distance for a full turn of the double helix, then
(iv) calculate from (i) and (ii) the DNA volume per base pair V_{bp}. Finally,
(v) Compare your results with those given in PKT, Table 1.1 (p. 26)

(d) Examples of glucose and phosphoglycerate kinase are provided on the website.

(a) and (b)



(c)

(i) I find 19—20 Angstroms = 1.9—2.0 nm.

(ii) I find numbers in the range of 3.5 Angstroms=0.35 nm.

(iii) I find 32—35 Angstroms = 3.2—3.5 nm.

(iv) The volume of the (roughly cylindrical) double helix associated with one bp is

$$V = \pi R^2 L = \pi(10)^2(3.5) = 1.1\times10^3 \left(\frac{o}{A}\right)^3 = 1.1\, nm^3$$

(d) I find diameters of 6-7 Angstroms for the glucose and 65-70 Angstrom for the phosphoglycerate kinase.

Comment: Several of you quoted results with what seem to me to be an unrealistic number of significant digits. I don't want to be a stickler on such issues; but, it is bad form to do this.

5. PKT Problem 2.2 (p. 7) **8**

Notes:

(a) Do this first by calculating the molecular weight of each amino acid (from its chemical formula) and then calculating the volume by assuming it has the (generic) density of water. Then, check your results by looking at the VMD images of a selected few of the amino acids and estimating the volume geometrically from molecular dimensions (you will find it best for this to use the van der Waals (VDW) representation). It will help to make a table (excel spreadsheet?), listing each amino acid, with columns for mass, estimated volume (from mass), estimated volume from dimensions. This problem is also designed so that you can become a little more familiar with the 20 amino acids, so take a few moments to look at the structure of each one.

(c) There are several versions of the listed molecules and I have found it not always easy to get MW data and number of amino acid residues for the same version. Just so we are all on the same page, use the following data:

	MW (kDa)	number residues
Myosin	520	3500
G-actin	42	375
Hemoglobin (human)	64	574
Hexokinase (yeast)	102	972

(a)

My spreadsheet is given below.

You will note that the precision of the volume "measurement" is poor and the agreement with the estimate via the density is variable. But, there is certainly a broad agreement.

Comments:

1. Most of you used the molecular weights of the "free" form of the amino acids. This is OK, I suppose, in part (a); however, in parts (b) and (c) the animo acids are linked into proteins. For each carboxyl bond one water is lost in the condensation process. Thus, as they appear in proteins, the average molecular weight of each amino-acid residue is actually 18 less than you will have calculated. This is not an enormous correction but it is significant. In my solution, I have used the lower MW's throughout.

2. No one got anything like good agreement between the amino-acid volumes based on the density and those based on the geometry. I am not sure why this is; my agreements were OK. But, my guess is that you used dimensions measured from atomic centres and not the full van der Waals radii. This makes a significant difference. You have to measure a atom-to-atom bond to get the scale; but, then you can go to the van der Waals representation and get realistic dimensions.

3. This is not a big deal. However, it did surprise me that no one commented on the bad agreement of the two methods.

(b)
I've calculated on the spreadsheet the average MW of all 20 of the amino acids (119). Comparing with the four suggested ones (Gly, Pro, Arg, and Trp). Two are below the typical (average) figure and two above. The average of these four is 124, which is pretty close to the average of all 20 amino acids.
(c) The rule would be:

$$\#\,residues = \frac{10^3 (MW\ kDa)}{119}$$, so, adding an extra column to the table I find:

	MW (kDa)	number residues	estimate
Myosin	520	3500	4400
G-actin	42	375	353
Hemoglobin (human)	64	574	538
Hexokinase (yeast)	102	972	857

The estimates are not great but the order of magnitude is OK.

Amino acids					
1 letter	3 letter	formula	MW	vol=M/ρ	vol(pdb)
A	Ala	C_3H_5ON	71	0.118	0.12
R	Arg	$C_6H_{12}ON_4$	156	0.259	
N	Asn	$C_4H_6O_2N_2$	114	0.189	
D	Asp	$C_4H_5O_3N$	115	0.191	
C	Cys	C_3H_5ONS	103	0.171	
E	Glu	$C_5H_7O_3N$	129	0.214	
Q	Gln	$C_5H_8O_2N_2$	128	0.212	
G	Gly	C_2H_3ON	57	0.095	
H	His	$C_6H_7ON_3$	137	0.227	
I	Ile	$C_6H_{11}ON$	113	0.188	
L	Leu	$C_6H_{11}ON$	113	0.188	0.16
K	Lys	$C_6H_{12}ON_2$	128	0.212	0.22
M	Met	C_5H_9ONS	131	0.217	
F	Phe	C_9H_9ON	147	0.244	
P	Pro	C_5H_7ON	97	0.161	
S	Ser	$C_3H_5O_2N$	87	0.144	
T	Thr	$C_4H_7O_2N$	101	0.168	
W	Trp	$C_{11}H_{10}ON_2$	186	0.309	0.36
Y	Tyr	$C_9H_9O_2N$	163	0.271	
V	Val	C_5H_9ON	99	0.164	
		ave=	118.75		
		ave 4	124		