

# Homework 3

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**Problem 1** (A) I created an Euler simulation of a ball of 0.5kg being thrown straight up at an initial speed of 15m/s and 11m above the ground. Acceleration was simply  $F_g/m = mg/m = g$ . Velocity was then the line with an intercept of 15 and a slope of -g. I used Euler's method to compute position at each point.

(B) I implemented RK4 to compute the same thing. For both (A) and (B), I found the analytic solution to position,  $p = 11 + 15t - gt^2$  and used the true values of position to compute the residuals (true position - predicted position) to see the amount of error with each method. RK4 was more accurate.

(C) I modified my code from part (B) to have an acceleration of  $a(t) = g + 0.01 * (v(t) + h(t)) + 0.3 * t^2$  and plotted my result using RK4. The ball went up and then came down while acceleration was negative but concave up.

(D) I implemented a simulation of a ball falling from 400m with a radius of 0.05m, a mass of 0.5kg, and a coefficient of air friction of -0.65. Initially the ball built up speed, until the force of friction and the force of gravity balanced out, to create a constant speed and constant rate of descent.

(E) From (A) to (B), I implemented a method for RK4 and changed the code in my loop to run the RK4 function. From (B) to (C) I merely changed my acceleration function and removed my code to calculate residual (since I didn't have an analytic solution). From (C) to (D), I added code to calculate the force of friction and used this to modify my acceleration function. I also made some trivial changes to graphs on each of these exercises. My code is maximally similar because I didn't need to change anything other than the changes in the problems themselves, e.g. acceleration function, and was able to keep my simulation loop and approximation code the same.

**Problem 2** (A) I created a simulation of a neuron action potential using the Hodgkin-Huxley model, i.e.  $\frac{dV}{dt} = (T_{ext} - I_K - I_{Na} - I_L)/C_M$  with the same values for all parameters from the textbook (except those changed in the table in the homework instructions). My plots matches the plots from the book pretty well, but the top of my voltage graph is a bit flatter and my sodium and potassium graphs intersect whereas the book's do not.

(B) Implemented the sodium-potassium pump created a strange bump in my plot, during hyperpolarization, most likely due to the potassium channel closing.

(C) I modified my Na-K pump so that it was not always on and started tracking concentrations of sodium and potassium. I tried to figure out the concentration of each but was unsuccessful despite my diligent unit analysis (I found a volume that was much too small). My plot was very similar to the one I made in (B) but the beginning (during equilibrium) was flat instead of rising as the leakage and Na-K pumps balanced each other out.

$$nA \cdot ms = A \cdot s \cdot 10^{-12} = C \cdot 10^{-12}.$$

A coulomb is equal to  $1.036 \cdot 10^5$  mol of protons.

$$1.036 \cdot 10^5 \cdot 10^{-12} = 1.036 \cdot 10^{-17} \text{ protons.}$$

**Voltage to Number of Positive Ions** Voltage is the difference in electrical potential between two points. Since the initial voltage in our system is -65 mV with respect to the outside of the cell, we know that there are more positive ions inside the cell than outside. But, how many is that?

Approximating the charge given by the excess positive ions inside the cell as a point charge, we can use the following formula for electrical potential.

$$V_E = \frac{Q}{4\pi\epsilon_0 r}$$

$Q$  is the charge,  $\epsilon_0$  is permittivity of vacuum, and  $r$  is the distance. A mammalian lipid bilayer is between 5.5 and 7.1 nm thick according to Wikipedia, so we can use the average of these two numbers, 6.3nm as our distance since the size and distance of the positive ions from the membrane is negligible.

Hence, we can solve for the number of positive ions inside our membrane based on our initial voltage.

$$Q = (V_E)(4\pi\epsilon_0 r)$$

We have voltage in mV, permittivity of vacuum in F/m, and distance in nm, so we will need to use some unit analysis to understand what unit conversions are necessary.

$$\begin{aligned}(mV)(Fm^{-1} \cdot nm) &= (10^{-3}V)(10^{-9}F) \\ &= V \cdot 10^{-12}F \\ &= 10^{-12}C \\ &= \frac{1.602176620898 \cdot 10^{19}q}{C}(10^{-12}C) \\ &= 1.602176620898 \cdot 10^7 q\end{aligned}$$

So, we are able to find the number of protons that correspond to this voltage. Since each positive ion (potassium or sodium) has a +1 charge, this is simply the number of additional positive ions within the membrane with respect to those outside of the membrane. We can then divide our result by Avogadro's constant,  $N_A$ , to get the number of moles of positive ions.  $\frac{1.602176620898 \cdot 10^7 q}{N_A}$ .

Since we have the initial concentration of positive ions inside of the cell, we can calculate the volume inside the cell for the modeled area by dividing the moles of positive ions by the moles per volume, which in this case is in units of mM/L. Once we've done this calculation, we have a volume which we can use to calculate changes in concentration from changes in number of positive ions. We don't have enough information to calculate the volume relevant to the outside of the cell or how much concentration changes, so using this same volume for the outside is a reasonable approximation for order of magnitude.

**Current to Change in Concentration** We have the leakage current, the current from the sodium-potassium pump, the sodium channel current, and the potassium channel current. Current is simply charge over time, so with a small enough timestep, it is reasonable to multiply our currents by our timestep (using the property of local linearity) to approximate changes in charge. Once we find the change in charge, we can convert to numbers of positive ions since the charge on these ions is +1. We can then convert to milli moles and divide by the volume we found earlier to yield change in concentration for each quantity.

$$I \cdot \Delta t = Q$$

We will also do some unit analysis to understand what conversion factors to use.

$$\begin{aligned}(nA)(ms) &= 10^{-12}A \cdot s \\ &= 10^{-12}C\end{aligned}$$

We found the conversion factor before to convert from  $10^{-12}$  C to elementary charge, so we can use the same factor again in the code.

Initially when I did this calculation, I arrived at a volume much too small. I realized this once I saw how large the changes in concentration were, corresponding to each change in number of ions, that this calculation didn't work for my purposes and reverted to the volume-less approximation for concentration (simply using number of atoms).

(D) I did not see any change.

(E) I did not see any major change in my graph in my graph from (B) and would need to investigate this hypothesis more, although I did not see any evidence to support it yet.

(F) Getting the action potential to a higher value could simply be achieved by raising the point at which the sodium channel switched off with the potassium channel.