This homework is designed to get you comfortable with Greens functions (in particular looking up and implementing the appropriate Greens functions, mostly from Polyanin's book) as well as to start to understand the role and influence of boundary conditions, which we did not explore explicitly in class, but are important in many real life situations. Note that formally the Greens function on finite domains is written as an infinite sum, which typically you have to truncate - take a large enough number such that the solution converges. This number is not fixed and for smaller time you usually need more terms, but looking at the solution you should have a sense if it is converged or not. Note in particular that if you do not include enough terms you may get funny oscillations in your solutions (these are called Gibbs phenomena and should be avoided as much as possible).
The final two problems are meant to get you comfortable with the finite difference and random walk methods that we explored in class and how these compare with the fully analytical solutions given by the Greens function method. You may use the codes provided from class and modify them, but make sure you study them carefully and know what they are doing.

Problem 1. Greens Functions on a Finite Domain

Consider the following problem

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2} \qquad 0 < x < 20$$

$$C(x, t = 0) = \delta(x - 10) \qquad \frac{\partial C}{\partial x}|_{x=0} = \frac{\partial C}{\partial x}|_{x=20} = 0 \tag{1}$$

This set of equations describes a problem where you have a pulse of unit mass centered at $x = 10$ that diffuses in a finite domain where $0 < x < 20$. At the edges of the domain none of the solute can enter of leave the domain (so called no flux boundary conditions - recall from Fick's law that a diffusive flux is proportional to $\frac{\partial C}{\partial x}$). Can you think of a system this might represent?

(i) Based solely on your physical intuition what do you expect the long term behavior of this system to look like (i.e. what is the solution to this problem as $t \to \infty$ and after what characteristic timescale τ do you expect the system to reach this asymptotic solution? In estimating τ think about the dimensions of constraints that you have in this system (i.e. the size of the domain L and the diffusion coefficient D and anything else that might exist).

(ii) Now implement the solution(s) as written in Polyanin and plot them for several times $t = 0.001\tau$, $t = 0.01\tau$, $t = 0.1\tau$, $t = \tau$ and $t = 10\tau$ where τ is the timescale you estimated in (i). Describe the resulting solutions and in particular discuss the role of the boundaries relative to the infinite domain problem that we studied in class.

(iii) Now implement the solution for different initial condition $C(x, t = 0) = \delta(x - 15)$, that is a pulse located at $x = 15$, which is no longer centered and plot the solutions again, in particular describing similarities and differences with solutions from (ii).

Problem 2. Greens Functions on a Semi-infinite Domain

Consider the following problem

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad 0 < x < \infty$$

$$C(x, t = 0) = 0 \qquad C(x = 0, t) = C_0; \tag{1}$$

This set of equations describes a problem where you have a semi-infinite domain and you are imposing a constant concentration at the *inlet* boundary. Can you think of a system this might represent?

(i) Look up the Greens function for this type of problem and write down the solution for this particular setup. Now look at the structure of the Greens function and compare it to that of the infinite domain - what are the similarities and differences? In particular compare this to the solution we derived in class where for the infinite domain with initial condition $C(x, t = 0) = H(-x)$. What physically are the similarities and differences in these setups?

(ii) Calculate the total mass in the domain as a function of time, i.e. $M(t) = \int_0^\infty C(x, t)$ and describe how it depends on the diffusion coefficient D, which is the only thing that allows transport in the system. Does the amount of mass always increase in time? does it always increase at the same rate, speed up or slow down? Does this make sense to you (think about why it might change with time based on the fact that the diffusive flux into the domain, that is the thing that is adding mass into the system, is proportional to $\frac{\partial C}{\partial x}|_{x=0}$ and how this might be changing in time).

(iii) Now specifically, set $D = 1$ and calculate the concentration distribution in the domain at $t = 10$. Now double D - how much more or less mass is in the domain? Does the result make sense to you?

Note: Throughout if you try to do the definite integrals with Mathematica, it may get angry with you (because of some odd singularities) so do the indefinite integrals and then evaluate the boundary terms by hand if this is the case. You can use use Mathematica or Wolfram online Integrator for this - http://integrals.wolfram.com.

Problem 3. Finite Differences

Change the finite difference code we used in class to solve the following problem

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2} \qquad 0 < x < 15$$

$$C(x, t = 0) = 0 \qquad C(x = 0, t) = 1; \qquad \frac{\partial C}{\partial x}|_{x=15,t} = 0; \tag{1}$$

(i) What is the steady state solution to this problem? (do it by hand) Show that at large times the finite difference solution gives this. Estimate the time it takes to reach this steady state - again use physical reasoning or the maths to guide you? What is the biggest difference with the case studied in class where C at the right boundary is 0 (i.e. a Dirichlet vs Neuman boundary condition)? Plot the solution at various times to help you in your discussion. Again, pick the times that you plot results at various times based on your chosen physical/asymptotic time scale (similar to the previous problem). What do differences and similarities between the two different right boundary conditions represent physically?

(ii) **Bonus - if you have time**: Change the Greens function solution to the appropriate one and show that it matches the finite-difference solution.

Problem 4. Random Walks and Greens Functions

Go back to problem 1 and implement a random walk code to solve the same problem. In particular use 10^3, 10^5 and 10^6 particles to solve the problem.

You may use the code that was presented in class and is available online. Note however that that in order to implement the no flux boundary conditions you have to bounce particles that have exited the domain back into the domain assuming an elastic collision (e.g. if a particle jumps to $x = -1$ bounce it back to 1 or if a particle jumps to $x = 22.5$ bounce it back to $x = 17.5$). You have to do this at the end of each time step before moving on to the next one. You may do so by any number of means - my preference is to use the Matlab function 'find' to search for particles that have exited the domain and then update just those positions.

i.e. apple=find($x > 2$) returns the elements in the vector x that are greater than 2. Then you only have to update x(apple)=x(apple)+ whatever. You have to figure out what 'whatever' is.

Compare results from the random walk to the results obtained from problem 1 and in particular discuss the influence of using more particles, both in terms of the solution obtained and the amount of computational time required. To measure computational time you can either use a feature in Matlab called 'profiler' or type 'tic' in the first line of your code and 'toc' in the very last one - when your code is finished running Matlab will tell you this will tell you the amount of time that has elapsed.