Format for delivery of report and programs

The format of the project is that of a printed file or hand-written report. The programs should also be included with the report. Write **only your candidate number** on the first page of the report and state clearly that this is your report for project 5 of FYS3150/FYS4150, fall 2013. There will be a box marked 'FYS3150/FYS4150' at the reception of the Department of Physics (room FV128).

Project 5, Diffusion in one and two dimensions, deadline Monday December 9, 12pm (noon)

This project consists of two parts. The first part is a continuation of project 4, but solves the diffusion equation in one dimension using Markov processes. The second part deals with the diffusion equation in two dimensions and the development of both an explicit and an implicit scheme for solving the equations.

We repeat here parts of the motivation for project 4. The dominant way of transporting signals between neurons (nerve cells) in the brain is by means of diffusion of particular signal molecules called *neurotransmitters* across the synaptic cleft separating the cell membranes of the two cells. A drawing of a synapse is given in Fig. 1.

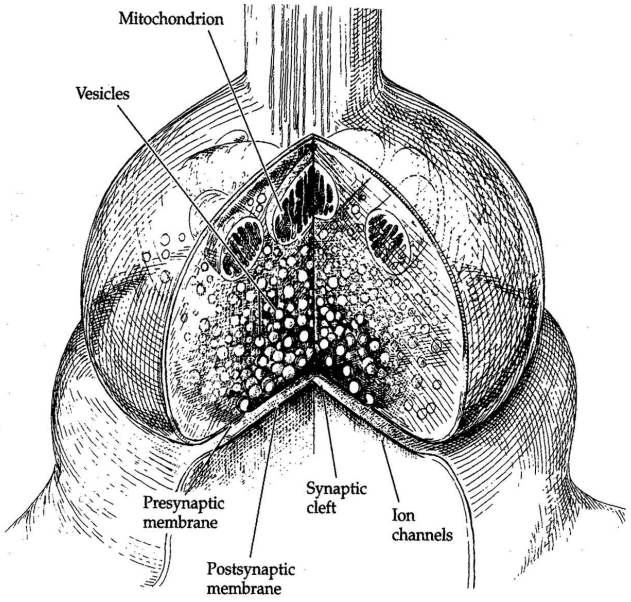

Figure 1: Drawing of a synapse. The axon terminal is the knoblike structure and the spine of the receiving neuron is the bottom one. The synaptic cleft is the small space between the presynaptic (axon) and postsynaptic (dendritic spine) membrane. (From Thompson: "The Brain", Worth Publ., 2000)

Following the arrival of an action potential in the axon terminal a process is initiated in which (i) vesicles inside the axon terminal (filled with neurotransmitter molecules) merge with the presynaptic (axon) membrane and (ii) release neurotransmitters into the synaptic cleft. These neurotransmitters diffuse across the synaptic cleft to receptors on the postsynaptic side which "receives" the signal. A schematic illustration of this process is shown in Fig. 2(left). Since the transport process in the synaptic cleft is governed by diffusion, we can describe it mathematically by

$$\frac{\partial u}{\partial t} = D\nabla^2 u, \tag{1}$$

where u is the concentration of the particular neurotransmitter, and D is the diffusion coefficient of the neurotransmitter in this particular environment (solvent in synaptic cleft).

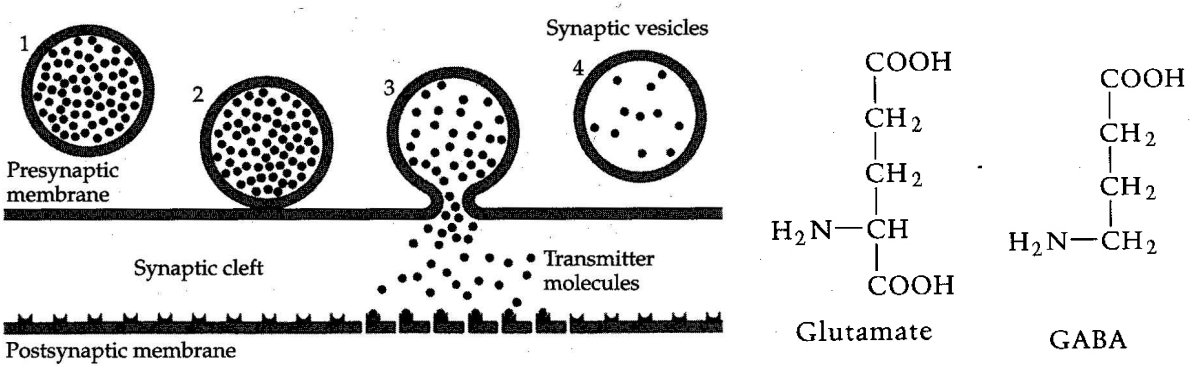

Figure 2: Left: Schematic drawing of the process of vesicle release from the axon terminal and release of transmitter molecules into the synaptic cleft. (From Thompson: "The Brain", Worth Publ., 2000). Right: Molecular structure of the two important neurotransmitters *glutamate* and *GABA*.

If we assume (i) that the neurotransmitter is released roughly equally on the "presynaptic" side of the synaptic cleft, and (ii) that the synaptic cleft is roughly equally wide across the whole synaptic terminal, we can, given the large area of the synaptic cleft compared to its width, assume that the neurotransmitter concentration only varies in the direction across the synaptic cleft (from presynaptic to postsynaptic side). We choose this direction to be the x-direction (see Fig. 3). In this case $u(\mathbf{r}) = u(x)$, the diffusion equation reduces to

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}. \tag{2}$$

Immediately after the release of a neurotransmitter into the synaptic cleft ($t = 0$) the concentration profile in the x-direction is given by

$$u(x, t = 0) = N\,\delta(x), \tag{3}$$

where N is the number of particle released into the synaptic cleft per area of membrane.

To get an idea over the time-dependence of the neurotransmitter concentration at the postsynaptic side ($x = d$), we can look at the solution of a "free" random walk (i.e., no obstacles or particle absorbers in either direction). The solution of Eq. (2) with the initial condition in Eq. (3) is given by (see Nelson: *Biological Physics*, p. 143 or Lectures notes chapter 12.3)

$$u(x, t) = \frac{N}{\sqrt{4\pi D t}} e^{-x^2/4Dt} \quad . \tag{4}$$

The concentration at the postsynaptic side $u(d, t)$ approaches 0 in the limit $t \to 0$ and $t \to \infty$.

The above assumption regarding the neurotransmitter molecules undergoing a "free" random walk, is obviously a simplification. In the true diffusion process in the synaptic cleft the neurotransmitter molecules

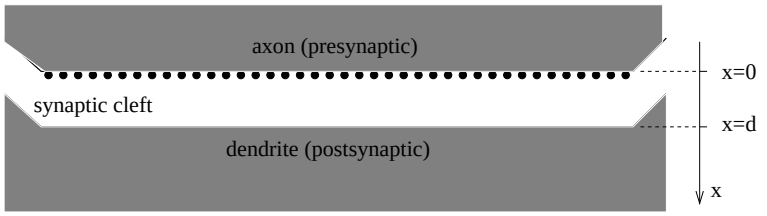

Figure 3: Schematic drawing of the synaptic cleft in our model. The black dots represent neurotransmitter molecules, and the situation shown corresponds to the situation immediately after neurotransmitter release into the synaptic cleft.

will, for example, occasionally bump into the presynaptic membrane they came from. Also at the postsynaptic side the neurotransmitters are absorbed by receptors located on the postsynaptic cell membrane and are thus (temporally) removed from the solution.

To approach this situation in our mathematical model we can impose the following boundary and initial conditions with $x \in [0, d]$

$$u(x = 0, t > 0) = u_0, \quad u(x = d, \text{all } t) = 0, \quad u(0 < x < d, t < 0) = 0 \ . \tag{5}$$

Hereafter we set $d = 1$. This corresponds to that (i) for $t < 0$ there are no neurotransmitters in the synaptic cleft, (ii) for $t > 0$ the concentration of neurotransmitters at the presynaptic boundary of the synaptic cleft ($x = 0$) is kept *fixed* at $u = u_0 = 1$ in our case, and (iii) that the postsynaptic receptors immediately absorb nearby neurotransmitters so that $u = 0$ on the postsynaptic side of the cleft ($x = d = 1$).

We are thus looking at a one-dimensional problem

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t}, t > 0, x \in [0, d]$$

or

$$u_{xx} = u_t,$$

with initial conditions, i.e., the conditions at $t = 0$,

$$u(x, 0) = 0 \qquad 0 < x < d$$

with $d = 1$ the length of the x-region of interest. The boundary conditions are

$$u(0, t) = 1 \qquad t > 0,$$

and

$$u(d, t) = 0 \qquad t > 0.$$

The full solution of the diffusion equation with boundary/initial conditions in Eq. (5) can be found in a closed form. In project 4 you solved this equation using three finite difference methods and compared the numerical solution with the closed-form solution.

You will need these results here as well. We will now solve the equations using Monte Carlo methods.

a) The above problem can be solved using Monte Carlo methods and random walks. We follow here Farnell and Gibson in Journal of Computational Physics, volume **208**, pages 253-265 (2005). Choose a constant step length $l_0 = \sqrt{2D\Delta t}$ and equal probability for jumping left and right. Set up an algorithm for solving the above diffusion problem using a random walk model and write a code to do it. Compare your results with those from the partial differential equation solution and comment the results.

b) Change the above stepsize by using a Gaussian distribution with mean value 0 and standard deviation $1/\sqrt{2}$. The step length of the random walker is now $l_0 = \sqrt{2D\Delta t}\xi$, where ξ is random number chosen from the above Gaussian distribution. Implement this stepsize to the program from f) and compare the results and comment. You can include the results from project 4 in your discussions here.

c) Extend the code you have developed here to two dimensions. It means that we deal with a $2 + 1$ dimensional problem. Our differential equation becomes

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} = \frac{\partial u(x,y,t)}{\partial t}, t > 0, x, y \in [0, 1],$$

where we now have made a model with a square lattice for x and y. How would you extend the boundary conditions from one dimension to two dimensions? And can you find a closed form solution here as well? It is left to you to decide upon what kind of boundary conditions you deem appropriate.

The next part deals with the development of an explicit and an implicit finite difference scheme for solving the diffusion equation in two dimensions. We will stay with the same problem as in c), that is we employ the same boundary and initial conditions as those you defined in c).

d) In this exercise you are asked to set up an explicit scheme for solving the above equation. You should also discuss convergence criteria and the numerical stability of the explicit scheme. Outline the algorithm for solving the two-dimensional diffusion equation and implement the explicit scheme as function of Δx (assuming $\Delta x = \Delta y$) and Δt. Solve the equations numerically and give a critical discussion of your results. Compare your results with the closed-form answer.

e) This part is optional and gives you an additional score of 30%. Implement the implicit scheme discussed in chapter 10 of the lecture notes using Jacobi's method as the iterative method. Outline the algorithm for solving the two-dimensional diffusion equation and implement the implicit scheme as function of Δx (assuming $\Delta x = \Delta y$) and Δt. Solve the equations numerically and give a critical discussion of your results. Compare your results with the closed-form answer and the explicit scheme from the previous exercise. Discuss the stability of the solution as function of different values of Δx and Δt.

References

[1] Farnell and Gibson, Journal of Computational Physics, volume **208**, pages 253-265 (2005).