FYS4150 - Computational Physics - Project 5

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19th November, 2014

Abstract

1 Diffusion of neurotransmitters

I will study diffusion as a transport process for neurotransmitters across synaptic cleft separating the cell membrane of two neurons, for more detail see [1]. The diffusion equation is the partial differential equation

$$\frac{\partial u\left(\mathbf{x},t\right)}{\partial t} = \nabla \cdot \left(D\left(\mathbf{x},t\right)\boldsymbol{\nabla} u\left(\mathbf{x},t\right)\right) ,$$

where u is the concentration of particular neurotransmitters at location $\mathbf{x}$ and time t with the diffusion coefficient D. In this study I consider the diffusion coefficient as constant, which simplify the diffusion equation to the heat equation

$$\frac{\partial u\left(\mathbf{x},t\right)}{\partial t} = D\nabla^2 u\left(\mathbf{x},t\right) .$$

I will look at the concentration of neurotransmitter u in two dimensions with x_1 parallel with the direction between the presynaptic to the postsynaptic across the synaptic cleft, and x_2 is parallel with both presynaptic to the postsynaptic. Hence we have the differential equation

$$\frac{\partial u\left(\{x_i\}_{i=1}^2, t\right)}{\partial t} = D\sum_{j=1}^{2}\frac{\partial^2 u\left(\{x_i\}_{i=1}^2, t\right)}{\partial {x_j}^2} , \tag{1}$$

where $\{x_i\}_{i=1}^2 = (x_1, x_2) = \mathbf{x}$. The boundary and initial condition that I'm going to study is

$$\begin{aligned}
\exists\{d,w\} \subseteq \mathbb{R}_{0+} \exists\{w_i\}_{i=1}^2 \subseteq \mathbb{R}_{0+}^{w-} &\left(\forall t \in \mathbb{R}_0 : \forall x_2 \in \mathbb{R}_{w_1}^{w_2} : u\left(0,x_2,t\right) = u_0\right. \\
&\wedge \forall t \in \mathbb{R}\left(\forall x_2 \in \mathbb{R}_{0+}^{w-} : u\left(d,x_2,t\right) = 0 \wedge \forall x_1 \in \mathbb{R}_0^d : \left(u\left(x_1,0,t\right) = 0 \wedge u\left(x_1,w,t\right) = 0\right)\right) \\
&\left.\wedge \forall x_1 \in \mathbb{R}_{0+}^{d-} \forall x_2 \in \mathbb{R}_{0+}^{w-} : u\left(\{x_i\}_{i=1}^2, 0\right) = 0 \wedge \forall x_2 \in \mathbb{R}_0^w \setminus \mathbb{R}_{w_1}^{w_2} : u\left(0,x_2,0\right) = 0\right)
\end{aligned} \tag{2}$$

where d is the distance between the presynaptic and the postsynaptic, and w is the width of the presynaptic and postsynaptic. Note that the notation $\forall x \in \mathbb{R}_{a+}^{b-} \Leftrightarrow a < x < b$, where as $\forall x \in \mathbb{R}_a^b \Leftrightarrow a \leq x \leq b$. Note also that these boundary conditions implies that the neurotransmitters are transmitted from presynaptic at $x_1 = 0$ and $w_1 \leq x_2 \leq w_2$ with constant concentration u_0; the neurotransmitters are immediately absorbed at the postsynaptic $x_1 = d$; there are no neurotransmitters at boundary width $x_2 = 0$ and $x_2 = w$ of the synaptic cleft; and we have the initial condition at $t = 0$ where there are no neurotransmitters between the pre- and postsynaptic as well on the side of the

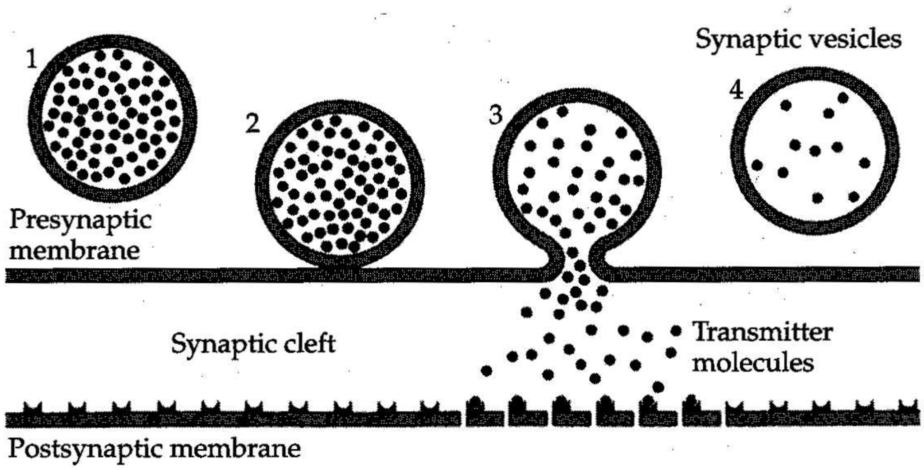

Figure 1.1: *Left: Schematic drawing of the process of vesicle release from the axon terminal and release of transmitter molecules into the synaptic cleft. (From Thompson: "The Brain", Worth Publ., 2000). Right: Molecular structure of the two important neurotransmitters glutamate and GABA.*

synaptic vesicles $x_1 = 0, 0 \le x_2 < w_1$ and $w_2 < x_2 \le w$.

To solve the differential equation (1) with the boundary and initial condition (2) we make an ansatz that the solution is unique, which is the case for a deterministic system. We recognize the heat equation as part of the class of partial differential equation spanned by the Poisson's equation for each time instance. The Uniqueness theorem for the Poisson's equation $\nabla^2 u = f$ [7] says that the Poisson's equation has a unique solution with the Dirichlet boundary condition, where Dirichlet boundary condition is here defined as a boundary that specifies the values the solution must have at the boundary.

Unfortunately the boundary condition in (2) is not a Dirichlet boundary, since the boundary is not specified on the side of the synaptic vesicles $x_1 = 0, 0 \le x_2 < w_1$ and $w_2 < x_2 \le w$, and closer investigation will show that the boundary condition in (2) does not provide a unique solution. So we need to add further condition to make the solution unique, and I make an assumption that the total concentration u in an infinitesimal area has uniform concentration per length u_1 and u_2 in each direction x_1 and x_2 accordingly. Hence $u = u_1 u_2$ at every point and therefore we can write

$$\forall x_1 \in \mathbb{R}_0^d \forall x_2 \in \mathbb{R}_0^w \forall t \in \mathbb{R}_0 : u\left(\{x_i\}_{i=1}^2, t\right) = u_1(x_1, t)\, u_2(x_2, t)\ . \tag{3}$$

Putting this into the heat equation (1) we get

$$u_2(x_2, t)\frac{\partial u_1(x_1, t)}{\partial t} + u_1(x_1, t)\frac{\partial u_2(x_2, t)}{\partial t} = D\left(u_2(x_2, t)\frac{\partial^2 u_1(x_1, t)}{\partial {x_1}^2} + u_1(x_1, t)\frac{\partial^2 u_2(x_2, t)}{\partial {x_2}^2}\right),$$

which can be written as two heat equations

$$\forall i \in \mathbb{N}_1^2 : \frac{\partial u_i(x_i, t)}{\partial t} = D\frac{\partial^2 u_i(x_i, t)}{\partial {x_i}^2}\ . \tag{4}$$

I make another assumption that the the boundary at $u(0, x_2, t)$ determined by $u_2(x_2, t)$ alone, and by satisfying initial condition $u(0, x_2, 0)$ for u_2

$$\forall t \in \mathbb{R}_0 \left(: u_2(0, t) = u_2(w, t) = 0 \land \forall x_2 \in \mathbb{R}_{w_1}^{w_2} : u_2(x_2, t) = u_0\right) \land \forall x_2 \in \mathbb{R}_0^w \setminus \mathbb{R}_{w_1}^{w_2} : u_2(x_2, 0) = 0 \tag{5}$$

we have now determined the values on all the boundaries have therefore Dirichlet boundary condition, and therefore a unique solution of u. We found the analytical solution to the heat equation in (4) for $i = 2$ with similar boundary and initial condition, and I will therefore not show the derivation here, but just state the solutions

$$u_2(x_2,t) = u_0 \begin{cases} \frac{x_2}{w_1} - \sum_{n=1} \frac{2}{n\pi} \sin\left(n\pi\left(1-\frac{x_2}{w_1}\right)\right) \exp\left(-D\left(\frac{n\pi}{w_1}\right)^2 t\right) & : x_2 \in \mathbb{R}_0^{w_1-} \\ 1 & : x_2 \in \mathbb{R}_{w_1}^{w_2} \\ \frac{w-x_2}{w-w_2} - \sum_{n=1} \frac{2}{n\pi} \sin\left(n\pi\frac{x_2-w_2}{w-w_2}\right) \exp\left(-D\left(\frac{n\pi}{w-w_2}\right)^2 t\right) & : x_2 \in \mathbb{R}_{w_2+}^{w} . \end{cases} \quad (6)$$

Since I have established that the boundary at $u(0,x_2,t)$ determined by $u_2(x_2,t)$ alone, means that u_1 has the following boundary and initial condition

$$\forall t \in \mathbb{R}_0 \left(: u_1(0,t) = 1 \land u_1(d,t) = 0\right) \land \forall x_1 \in \mathbb{R}_{0+}^{d-} : u_1(x_1,0) = 0 . \quad (7)$$

And using the analytical solution from project 4 to heat equation (4) for $i = 1$ with boundary and initial condition in (7), we have

$$u_1(x_1,t) = 1 - \frac{x_1}{d} - \sum_{n=1} \frac{2}{n\pi} \sin\left(n\pi\frac{x_1}{d}\right) \exp\left(-D\left(\frac{n\pi}{d}\right)^2 t\right) . \quad (8)$$

To summarize the solution to the concentration u is given by (3) with (6) and (8).

2 Attachments

The source files developed are

3 Resources

1. QT Creator 5.3.1 with C11
2. Eclipse Standard/SDK - Version: Luna Release (4.4.0) with PyDev for Python
3. Ubuntu 14.04.1 LTS
4. ThinkPad W540 P/N: 20BG0042MN with 32 GB RAM

References

[1] Morten Hjorth-Jensen, *FYS4150 - Project 5 - Diffusion in two dimensions*, University of Oslo, 2014

[2] Morten Hjorth-Jensen, *Computational Physics - Lecture Notes Fall 2014*, University of Oslo, 2014

[3] http://en.wikipedia.org/wiki/Diffusion_equation

[4] http://en.wikipedia.org/wiki/Heat_equation

[5] http://en.wikipedia.org/wiki/Dirichlet_boundary_condition

[6] http://en.wikipedia.org/wiki/Poisson%27s_equation

[7] http://en.wikipedia.org/wiki/Uniqueness_theorem_for_Poisson%27s_equation

[8] http://en.wikipedia.org/wiki/Ansatz