

FYS4150 - COMPUTATIONAL PHYSICS - PROJECT 5

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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

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

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

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

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

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

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

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

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

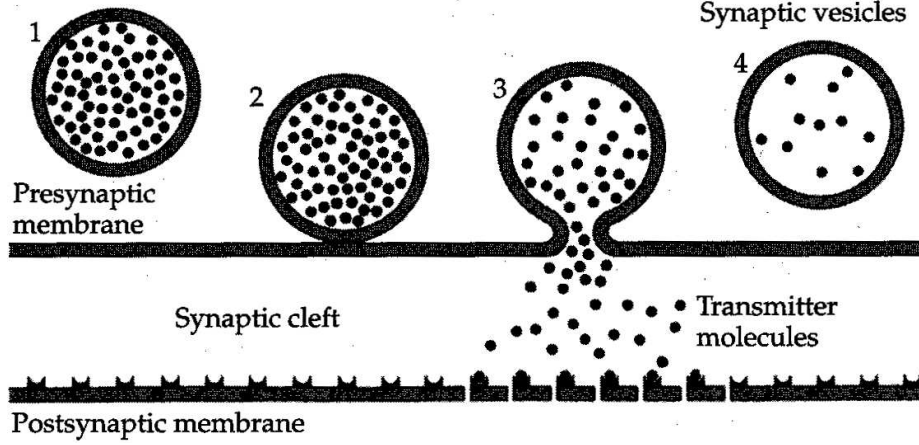


Figure 1.1: *Left: Schematic drawing of the process of vesicle release from the axon terminal and release of transmitter molecules into the synaptic cleft. (From Thompson: "The Brain", Worth Publ., 2000). Right: Molecular structure of the two important neurotransmitters glutamate and GABA.*

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

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 $x_1 = 0$, $0 \leq x_2 < w_1$ and $w_2 < x_2 \leq w$, 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

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

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

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

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

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

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

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

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 Numerical methods

2.1 The θ -rule

The Taylor expansion is given by

$$u(x) = \sum_{n=0} \frac{u^{(n)}(x_0)}{n!} (x - x_0)^n \quad (9)$$

where $u^{(n)} = \frac{d^n u}{dx^n}$ and x_0 is a initial value where we step from to x . If we now use the first order approximation

$$u(x) \approx u(x_0) + u^{(1)}(x_0)(x - x_0).$$

The first order differential equation $u^{(1)}(x) = f(x)$ is determined when we have the initial condition $u(x_0)$, however $u^{(1)}(x_0)$ is not an initial condition, and it depends on how we calculate it numerically from the initial condition. Now note that $u^{(1)}(x_0)$ is the same for different values of x in the approximation above and lets say that we calculate it as given from the approximation above;

$$u^{(1)}(x_0) \approx \frac{u(x) - u(x_0)}{x - x_0}. \quad (10)$$

So now use this in another point $x_\theta = \theta x + (1 - \theta) x_0$ which we also approximate to the first order, and if we use the expression above for $u^{(1)}(x_0)$ we get

$$\begin{aligned} u(x_\theta) &\approx u(x_0) + u^{(1)}(x_0)(x_\theta - x_0) = u(x_0) + \theta u^{(1)}(x_0)(x - x_0) \\ &\approx u(x_0) + \frac{u(x) - u(x_0)}{x - x_0} \theta (x - x_0) = \theta u(x) + (1 - \theta) u(x_0), \end{aligned} \quad (11)$$

this is known as the θ -rule. The θ -rule can be used to approximate the solution of the following first order differential equation

$$u^{(1)}(x) = f(u(x)), \quad (12)$$

where we use (10) to approximate the expression $u^{(1)}(x)$ and given an even better or worse approximation to the solution $u(x)$ by approximating $f(x) \approx f(x_\theta)$;

$$\frac{u(x) - u(x_0)}{x - x_0} \approx f(u(x_\theta)) = f(\theta u(x) + (1 - \theta) u(x_0)),$$

which discretize to

$$\frac{u_{i+1} - u_i}{x_{i+1} - x_i} = f(\theta u_{i+1} + (1 - \theta) u_i) \quad \text{where } i \in \mathbb{N}_0 \text{ and } u_0 \text{ is an initial condition.} \quad (13)$$

We can find the the next step in the numerical solution to (12) by solving this difference equation with regard to u_{i+1} . Note the above discretization is known as Forward Euler scheme (Explicit) when $\theta = 0$, Backward Euler scheme (Implicit) when $\theta = 1$ and Crank-Nicolson scheme when $\theta = \frac{1}{2}$.

The truncation error of the Forward and Backward Euler scheme can be found by an alternative derivation, where expand the Taylor series in (9) around the point $x_0 \pm \Delta x$ accordingly;

$$u(x_0 \pm \Delta x) = \sum_{n=0}^{\infty} \frac{u^{(n)}(x_0)}{n!} (\pm \Delta x)^n, \quad (14)$$

and solve it with regard to $u^{(1)}(x_0)$

$$u^{(1)}(x_0) = \frac{u(x_0 \pm \Delta x) - u(x_0)}{\Delta x} + O(\Delta x),$$

which means that we have a local truncation error of $O(\Delta x)$ with the Forward and Backward Euler scheme. However the Crank-Nicolson scheme can be found by subtraction the Taylor expansion above for the two points

$$u(x_0 + \Delta x) - u(x_0 - \Delta x) = 2 \sum_{n=1}^{\infty} \frac{u^{(2n-1)}(x_0)}{(2n-1)!} \Delta x^{2n-1},$$

and solve it with regard to $u^{(1)}(x_0)$

$$u^{(1)}(x_0) = \frac{u(x_0 + \Delta x) - u(x_0 - \Delta x)}{2\Delta x} + O(\Delta x^2),$$

which means that we have a local truncation error of $O(\Delta x^2)$. With the θ -rule we can get even better or worse truncation error, because we can change the θ value to change the approximation.

2.2 Second order derivative

We approximated the first order derivative in (10), but we need to approximate the second order derivative to be able to solve the diffusion in (1). We can achieve this by adding the two expansions in (14)

$$u(x_0 + \Delta x) + u(x_0 - \Delta x) = 2 \sum_{n=0}^{\infty} \frac{u^{(2n)}(x_0)}{(2n)!} \Delta x^{2n} = 2u(x_0) + u^{(2)}(x_0) \Delta x^2 + 2 \sum_{n=2}^{\infty} \frac{u^{(2n)}(x_0)}{(2n)!} \Delta x^{2n},$$

and solve it with

$$\begin{aligned} u^{(2)}(x_0) &= \frac{u(x_0 + \Delta x) - 2u(x_0) + u(x_0 - \Delta x)}{\Delta x^2} - 2 \sum_{n=2}^{\infty} \frac{u^{(2n)}(x_0)}{(2n)!} \Delta x^{2(n-1)} \\ &= \frac{u(x_0 + \Delta x) - 2u(x_0) + u(x_0 - \Delta x)}{\Delta x^2} + O(\Delta x^2), \end{aligned}$$

So the second order derivative can be approximated with

$$u^{(2)}(x_0) \approx \frac{u(x_0 + \Delta x) - 2u(x_0) + u(x_0 - \Delta x)}{\Delta x^2} \quad (15)$$

with the local truncation error $O(\Delta x^2)$.

2.3 The heat equation

We want to discretize the dimensionless heat equation from (1), where we use $D = 1$, $u_0 = 1$ and $d = 1$,

$$\frac{\partial u(\{x_i\}_{i=1}^2, t)}{\partial t} = \sum_{\ell=1}^2 \frac{\partial^2 u(\{x_i\}_{i=1}^2, t)}{\partial x_{\ell}^2},$$

to numerically solve diffusion of neurotransmitters. First we do the θ -rule discretization in (13)

$$\begin{aligned} \frac{u_{(i+1)\{j_k\}_{k=1}^2} - u_{i\{j_k\}_{k=1}^2}}{\Delta t} &= \sum_{\ell=1}^2 \frac{\partial^2 u_{(i+\theta)\{j_k\}_{k=1}^2}}{\partial x_{\ell}^2} = \sum_{\ell=1}^2 \frac{\partial^2 \left(\theta u_{(i+1)\{j_k\}_{k=1}^2} + (1-\theta) u_{i\{j_k\}_{k=1}^2} \right)}{\partial x_{\ell}^2} \\ &= \sum_{\ell=1}^2 \left(\theta \frac{\partial^2 u_{(i+1)\{j_k\}_{k=1}^2}}{\partial x_{\ell}^2} + (1-\theta) \frac{\partial^2 u_{i\{j_k\}_{k=1}^2}}{\partial x_{\ell}^2} \right) \end{aligned}$$

where index i is stepping of t and j_k are stepping of x_k . Note also that the following notation expand accordingly $u_{i\{j_k\}_{k=1}^2} = u_{ij_1j_2}$, which becomes a more elegant notation for larger n in $u_{i\{j_k\}_{k=1}^n} = u_{ij_1j_2\dots j_n}$. Now we implement the discretization of the second order in (15)

$$\begin{aligned} \frac{u_{(i+1)\{j_k\}_{k=1}^2} - u_{i\{j_k\}_{k=1}^2}}{\Delta t} &= \sum_{\ell=1}^2 \left(\frac{\theta}{\Delta x_\ell^2} \left(u_{(i+1)\{j_k+\delta_{k\ell}\}_{k=1}^2} - 2u_{(i+1)\{j_k\}_{k=1}^2} + u_{(i+1)\{j_k-\delta_{k\ell}\}_{k=1}^2} \right) \right. \\ &\quad \left. + \frac{1-\theta}{\Delta x_\ell^2} \left(u_{i\{j_k+\delta_{k\ell}\}_{k=1}^2} - 2u_{i\{j_k\}_{k=1}^2} + u_{i\{j_k-\delta_{k\ell}\}_{k=1}^2} \right) \right), \end{aligned} \quad (16)$$

where $\delta_{k\ell}$ is the Kronecker delta, and we now clearly see the elegance of the notation $u_{i\{j_k\}_{k=1}^n}$.

The dimensionless initial condition from (4) gives us

$$u_{0\{j_k\}_{k=1}^2} = \begin{cases} 1 & : j_1 = 0 \text{ and } x_{2j_2} \in \mathbb{R}_{w_1}^{w_2} \\ 0 & : \text{elsewhere,} \end{cases}$$

where $x_{2j_2} = x_{20} + \frac{j_2}{\Delta x_2}$. For the explicit scheme $\theta = 0$ we get

$$u_{(i+1)\{j_k\}_{k=1}^2} = u_{i\{j_k\}_{k=1}^2} + \sum_{\ell=1}^2 \alpha_\ell \left(u_{i\{j_k+\delta_{k\ell}\}_{k=1}^2} - 2u_{i\{j_k\}_{k=1}^2} + u_{i\{j_k-\delta_{k\ell}\}_{k=1}^2} \right) \quad (17)$$

where

$$\alpha_\ell = \frac{\Delta t}{\Delta x_\ell^2} \quad \text{and} \quad n_\ell = \frac{1}{\Delta x_\ell}.$$

3 Attachments

The source files developed are

4 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>
- [9] http://en.wikipedia.org/wiki/Kronecker_delta