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

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

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

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

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

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

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

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

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

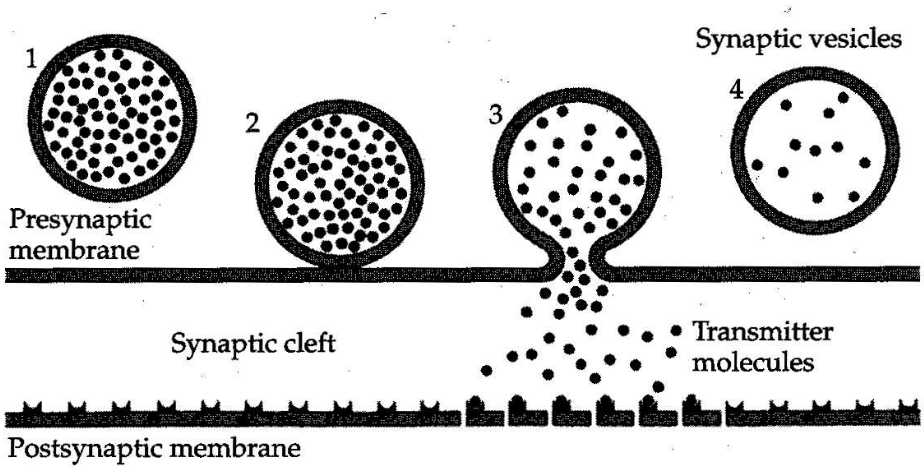

Figure 1.1: *Left: Schematic drawing of the process of vesicle release from the axon terminal and release of transmitter molecules into the synaptic cleft. (From Thompson: "The Brain", Worth Publ., 2000). Right: Molecular structure of the two important neurotransmitters glutamate and GABA.*

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 $w_2 < x_2 \le w$. However the Uniqueness theorem does not exclude other boundary conditions to result in a unique solution, so we make another ansatz to separate the concentration $u\left(\{x_i\}_{i=1}^2, t\right)$ into two functions $u_1(x_2, t)$ and $u_2\left(\{x_i\}_{i=1}^2, t\right)$ as follows

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

Putting this into the heat equation (1) we get

$$u_2\left(\{x_i\}_{i=1}^2, t\right) \frac{\partial u_1(x_2, t)}{\partial t} + u_1(x_2, t) \frac{\partial u_2\left(\{x_i\}_{i=1}^2, t\right)}{\partial t} = D\left(u_1(x_2, t) \sum_{j=1}^{2} \frac{\partial^2 u_2\left(\{x_i\}_{i=1}^2, t\right)}{\partial {x_j}^2} + u_2\left(\{x_i\}_{i=1}^2, t\right) \frac{\partial^2 u_1(x_2, t)}{\partial {x_2}^2}\right),$$

which can be written as a heat equation in one dimension

$$\frac{\partial u_1(x_2, t)}{\partial t} = D \frac{\partial^2 u_1(x_2, t)}{\partial {x_2}^2} \tag{4}$$

with the boundary condition that must satisfy $u(0, x_2, t)$ and initial condition that must satisfy $u(0, x_2, 0)$

$$\forall t \in \mathbb{R}_0 \left(: u_1(0,t) = u_1(w,t) = 0 \wedge \forall x_2 \in \mathbb{R}_{w_1}^{w_2} : u_1(x_2,t) = u_0 \right) \wedge \forall x_2 \in \mathbb{R}_0^{w} \setminus \mathbb{R}_{w_1}^{w_2} : u_1(x_2,0) = 0\,; \tag{5}$$

and a heat equation in two dimensions

$$\frac{\partial u_2\left(\{x_i\}_{i=1}^2, t\right)}{\partial t} = D \sum_{j=1}^{2} \frac{\partial^2 u_2\left(\{x_i\}_{i=1}^2, t\right)}{\partial {x_j}^2} \tag{6}$$

with the boundary condition that must satisfy $u_1(x_2,t)$, $u(0,x_2,t)$, $u(d,x_2,t)$, $u(x_1,0,t)$ and $u(x_1,w,t)$, and initial condition that must satisfy $u(x_1,x_2,0)$

$$\forall t \in \mathbb{R}_0 \left(\forall x_2 \in \mathbb{R}_{0+}^{w-} : u_2(0,x_2,t) = 1 \wedge u_2(d,x_2,t) = 0 \wedge \forall x_1 \in \mathbb{R}_0^{d} : u_2(x_1,0,t) = u_2(x_1,w,t) = 0 \right). \tag{7}$$

The boundary condition in both (5) and (7) have specified values on all their boundaries, which means that we have the Dirichlet boundary condition on both (4) and (6), and through the the Uniqueness theorem for the Poisson's equation we have shown that u_1 and u_2 have a unique solution, which again means that u has a unique solution.

The analytical solution to one dimensional heat equation (4) we found in project 4, and it's derivation is the same as the following steps for two dimensional case, only simpler. Therefore I will skip it's derivation here and give the solution directly

$$u_1(x_2,t) = u_0 \begin{cases} \frac{x_2}{w_1} - \sum_{n=1} \frac{2}{n\pi} \sin\left(n\pi\left(1-\frac{x_2}{w_1}\right)\right) \exp\left(-D\left(\frac{n\pi}{d}\right)^2 t\right) & : x_2 \in \mathbb{R}_0^{w_1-} \\ 1 & : x_2 \in \mathbb{R}_{w_1}^{w_2} \\ \frac{x_2-w}{w_1-w} - \sum_{n=1} \frac{2}{n\pi} \sin\left(n\pi \frac{w_1-x_2}{w_1-w}\right) \exp\left(-D\left(\frac{n\pi}{d}\right)^2 t\right) & : x_2 \in \mathbb{R}_{w_2+}^{w}\,, \end{cases} \tag{8}$$

which is the result of boundary and initial condition in (5). To solve the heat equation in (6) with the boundary and initial condition in (7) I make another ansatz that we can separate $u_2\left(\{x_i\}_{i=1}^2, t\right)$ into two functions $u_3(x_1)$ and $u_4\left(\{x_i\}_{i=1}^2, t\right)$ as follows

$$u_2\left(\{x_i\}_{i=1}^2, t\right) = u_3(x_1) + u_4\left(\{x_i\}_{i=1}^2, t\right), \tag{9}$$

such that u_4 satisfies

$$\frac{\partial u_4\left(\{x_i\}_{i=1}^2, t\right)}{\partial t} = D \sum_{j=1}^{2} \frac{\partial^2 u_4\left(\{x_i\}_{i=1}^2, t\right)}{\partial {x_j}^2} \tag{10}$$

with the 0th Dirichlet boundary condition (all boundary values are zero). For u_4 to be determined by the heat equation as well, u_3 must be on the form

$$u_3(x_1) = a_0 + a_1 x_1\,, \tag{11}$$

because then u_3 vanishes from (6) when we have put (9) into it. Now lets try to impose the 0th Dirichlet boundary condition on u_4

$$u_4(0, x_2, t) = u_4(d, x_2, t) = u_4(x_1, 0, t) = u_4(x_1, w, t) = 0\,. \tag{12}$$

When put into (9) and using the boundary condition (7) we have the following equations that u_1 must satisfied

$$\begin{aligned} u_2(0, x_2, t) &= u_3(0) + u_4(0, x_2, t) = u_3(0) = 1 \\ u_2(d, x_2, t) &= u_3(d) + u_4(d, x_2, t) = u_3(d) = 0\,, \end{aligned}$$

which means that (11) is given by

$$u_3(x_1) = 1 - \frac{x_1}{d}\,. \tag{13}$$

Since the heat equation for u_4 in (10) satisfies the 0th Dirichlet boundary condition we can do the final ansatz to find the solution by separating $u_4\left(\{x_i\}_{i=1}^2\,, t\right)$ is separable into $u_5\left(\{x_i\}_{i=1}^2\right)$ and $u_6(t)$ as follows

$$u_4\left(\{x_i\}_{i=1}^2\,, t\right) = u_5\left(\{x_i\}_{i=1}^2\right) u_6(t)\ , \tag{14}$$

where the 0th Dirichlet boundary condition for u_4 impose the following condition onto of u_5

$$u_5(0, x_2) = u_5(d, x_2) = u_5(x_1, 0) = u_5(x_1, w) = 0.$$

Now putting (14) into (10) yields

$$u_5\left(\{x_i\}_{i=1}^2\right) \frac{\partial u_6(t)}{\partial t} = D u_6(t) \sum_{j=1}^{2} \frac{\partial^2 u_5\left(\{x_i\}_{i=1}^2\right)}{\partial {x_j}^2}\,.$$

and separating the variables

$$\frac{1}{D u_6(t)} \frac{\partial u_6(t)}{\partial t} = \frac{1}{u_5\left(\{x_i\}_{i=1}^2\right)} \sum_{j=1}^{2} \frac{\partial^2 u_5\left(\{x_i\}_{i=1}^2\right)}{\partial {x_j}^2} = -\lambda^2\,, \tag{15}$$

where λ is a constant, because t and x_i can vary independently. These two equations have the following solutions

$$\begin{aligned} u_5\left(\{x_i\}_{i=1}^2\right) &= \sum_{i=1}^{2} \sum_{j=i}^{2} \prod_{k=i}^{j} A_{ijk} \sin\left(\lambda_{ijk} x_k + \varphi_{ijk}\right) \qquad \text{and} \\ u_6(t) &= C e^{-D\lambda^2 t}\,. \end{aligned}$$

The boundary condition $u_5(0, x_2) = u_5(x_1, 0) = 0$ gives $A_{111} = A_{222} = \varphi_{121} = \varphi_{122} = 0$, and $u_5(d, x_2) = u_5(x_1, w) = 0$ gives

$$\lambda_{121} = \frac{n_1\pi}{d} \qquad \text{and} \qquad \lambda_{122} = \frac{n_2\pi}{w} \qquad \text{for } \{n_i\}_{i=1}^{2} \in \mathbb{N}/\{0\},$$

where I let $\mathbb{N} = \mathbb{N}_{-\infty}^{\infty}$ represent all positive and negative integers including zero. These λ's must satisfy

$$\lambda^2 = {\lambda_{121}}^2 + {\lambda_{122}}^2$$

for (15) to hold. Hence

$$u_4\left(\{x_i\}_{i=1}^{2}, t\right) = \sum_{n_1,n_2=1} A_{n_1n_2} \sin\left(n_1\pi\frac{x_1}{d}\right)\sin\left(n_2\pi\frac{x_2}{w}\right)\exp\left(-D\pi^2\left(\left(\frac{n_1}{d}\right)^2 + \left(\frac{n_2}{w}\right)^2\right)t\right), \tag{16}$$

where the negative values of n_1 and n_2 are absorbed into the coefficient $A_{n_1n_2}$. Applying the initial condition from (7) on the concentration in (9) with (13) and (16) we must satisfy the following equation

$$u_2\left(\{x_i\}_{i=1}^{2}, 0\right) = 1 - \frac{x_1}{d} + \sum_{n_1,n_2=1} A_{n_1n_2} \sin\left(n_1\pi\frac{x_1}{d}\right)\sin\left(n_2\pi\frac{x_2}{w}\right) = 0. \tag{17}$$

We need to determine the coefficients $A_{n_1n_2}$, and the trick is to do something with the equation above such that we isolate the $A_{n_1n_2}$ coefficients. To achieve this we use the fact that $\sin\left(n\pi\frac{x}{d}\right)$ is orthogonal with $\sin\left(m\pi\frac{x}{d}\right)$ under integration

$$\int \sin\left(m\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right)\mathrm{d}x = -\frac{d}{m\pi}\cos\left(m\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right) + \frac{n}{m}\int \cos\left(m\pi\frac{x}{d}\right)\cos\left(n\pi\frac{x}{d}\right)\mathrm{d}x$$
$$= -\frac{d}{m\pi}\cos\left(m\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right) + \frac{n}{m}\left(\frac{d}{\pi m}\sin\left(m\pi\frac{x}{d}\right)\cos\left(n\pi\frac{x}{d}\right) + \frac{n}{m}\int \sin\left(m\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right)\mathrm{d}x\right),$$

where I have used integration by parts $\int u\dot{v} = uv - \int \dot{u}v$. Solving this equation with regard to the integral we get

$$\int \sin\left(m\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right)\mathrm{d}x = \frac{d}{\pi\left(n^2 - m^2\right)}\left(n\sin\left(m\pi\frac{x}{d}\right)\cos\left(n\pi\frac{x}{d}\right) - m\cos\left(m\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right)\right).$$

We want to make the result of this integral zero for $n \neq m$, which is the result if $x = \frac{kd}{2}$ and $x = \frac{\ell d}{2}$ where $k, \ell \in \mathbb{N}$ (for zero,negative and positive integers), because then $\sin()\cos()$ parts above becomes zero. This means that we need to integrate from $x = \frac{kd}{2}$ and $x = \frac{\ell d}{2}$. However the result above is not defined for $n = m$ because we get $\frac{0}{0}$. So we redo the integration for $n = m$;

$$\int_{\frac{kd}{2}}^{\frac{\ell d}{2}} \sin^2\left(n\pi\frac{x}{d}\right)\mathrm{d}x = -\left[\frac{d}{\pi n}\cos\left(n\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right)\right]_{\frac{kd}{2}}^{\frac{\ell d}{2}} + \int_{\frac{kd}{2}}^{\frac{\ell d}{2}} \cos^2\left(n\pi\frac{x}{d}\right)\mathrm{d}x = \int_{\frac{kd}{2}}^{\frac{\ell d}{2}} \cos^2\left(n\pi\frac{x}{d}\right)\mathrm{d}x$$
$$= \int_{\frac{kd}{2}}^{\frac{\ell d}{2}} \left(1 - \sin^2\left(n\pi\frac{x}{d}\right)\right)\mathrm{d}x = [x]_{\frac{kd}{2}}^{\frac{\ell d}{2}} - \int_{\frac{kd}{2}}^{\frac{\ell d}{2}} \sin^2\left(n\pi\frac{x}{d}\right)\mathrm{d}x = \frac{d}{2}(\ell - k) - \int_{\frac{kd}{2}}^{\frac{\ell d}{2}} \sin^2\left(n\pi\frac{x}{d}\right)\mathrm{d}x = \frac{d}{4}(\ell - k),$$

where I solve the equation with regard to in $\int \frac{d}{2}(\ell - k)\sin^2\left(n\pi\frac{x}{d}\right)\,\mathrm{d}x$ in the last step. I have also used integration by parts $\int u\dot{v} = uv - \int \dot{u}v$ and the Pythagoras trigonometric relation $\sin^2 x + \cos^2 x = 1$. So the solution of the following integral is

$$\int_{\frac{kd}{2}}^{\frac{\ell d}{2}} \sin\left(m\pi\frac{x}{d}\right)\sin\left(n\pi\frac{x}{d}\right)\,\mathrm{d}x = \frac{d}{4}(\ell - k)\,\delta_{mn}\,,$$

where δ_{mn} is the Kronecker delta, and hence I have showed the orthogonality of the above integral. Applying this to (17);

$$\begin{aligned}
&\int_{\frac{k_1 d}{2}}^{\frac{\ell_1 d}{2}}\int_{\frac{k_2 w}{2}}^{\frac{\ell_2 w}{2}} \sum_{n_1,n_2=1} A_{n_1n_2}\sin\left(n_1\pi\frac{x_1}{d}\right)\sin\left(n_2\pi\frac{x_2}{w}\right)\sin\left(m_1\pi\frac{x_1}{d}\right)\sin\left(m_2\pi\frac{x_2}{w}\right)\mathrm{d}x_2\mathrm{d}x_1\\
&= \int_{\frac{k_1 d}{2}}^{\frac{\ell_1 d}{2}}\int_{\frac{k_2 w}{2}}^{\frac{\ell_2 w}{2}}\left(\frac{x_1}{d}-1\right)\sin\left(m_1\pi\frac{x_1}{d}\right)\sin\left(m_2\pi\frac{x_2}{w}\right)\mathrm{d}x_2\mathrm{d}x_1\,,
\end{aligned}$$

we can isolate $A_{n_1n_2}$ at $n_i = m_i$ because of the Kronecker deltas $\delta_{n_im_i}$;

$$A_{n_1n_2} = \frac{16}{dw\prod_{i=1}^{2}(\ell_i - k_i)}\int_{\frac{k_1 d}{2}}^{\frac{\ell_1 d}{2}}\int_{\frac{k_2 w}{2}}^{\frac{\ell_2 w}{2}}\left(\frac{x_1}{d}-1\right)\sin\left(n_1\pi\frac{x_1}{d}\right)\sin\left(n_2\pi\frac{x_2}{w}\right)\mathrm{d}x_2\mathrm{d}x_1\,.$$

Since $x_1 \in \mathbb{R}_0^d$ and $x_2 \in \mathbb{R}_0^w$ leads to $k_i, \ell_i \in \{0, 2\}$ and $k_i \neq \ell_i$ for $A_{n_1n_2}$ to apply to the whole interval of x_1 and x_2, which is independent of each other.

$$\begin{aligned}
A_{n_1n_2} &= \frac{4}{dw}\int_0^d\left(\frac{x_1}{d}-1\right)\sin\left(n_1\pi\frac{x_1}{d}\right)\int_0^w \sin\left(n_2\pi\frac{x_2}{w}\right)\mathrm{d}x_2\mathrm{d}x_1\\
&= -\frac{4}{d\pi n_2}\int_0^d\left(\frac{x_1}{d}-1\right)\sin\left(n_1\pi\frac{x_1}{d}\right)\left[\cos\left(n_2\pi\frac{x_2}{w}\right)\right]_0^w\mathrm{d}x_1 = \frac{8}{d\pi n_2}\int_0^d\left(\frac{x_1}{d}-1\right)\sin\left(n_1\pi\frac{x_1}{d}\right)\mathrm{d}x_1\\
&= -\frac{8}{\pi^2 n_1 n_2}\left(\left[\left(\frac{x_1}{d}-1\right)\cos\left(n_1\pi\frac{x_1}{d}\right)\right]_0^d - \frac{1}{d}\int_0^d\cos\left(n_1\pi\frac{x_1}{d}\right)\mathrm{d}x_1\right)\\
&= -\frac{8}{\pi^2 n_1 n_2}\left(1 - \frac{1}{\pi n_1}\left[\sin\left(n_1\pi\frac{x_1}{d}\right)\right]_0^d\right) = -\frac{8}{n_1 n_2\pi^2}\,,
\end{aligned}\tag{18}$$

where I have used integration by parts $\int u\dot{v} = uv - \int \dot{u}v$. To summarize we now have the analytical solution by putting (8), (9), (13), (14) and (18) into (8)

$$\begin{aligned}
&\forall x_1 \in \mathbb{R}_0^d \forall x_2 \in \mathbb{R}_0^w \forall t \in \mathbb{R}_0 : u\left(\{x_i\}_{i=1}^2, t\right)\\
&= u_0\left(1 - \frac{x_1}{d} - \sum_{n_1,n_2=1}\frac{8}{n_1n_2\pi^2}\sin\left(n_1\pi\frac{x_1}{d}\right)\sin\left(n_2\pi\frac{x_2}{w}\right)\exp\left(-D\pi^2\left(\left(\frac{n_1}{d}\right)^2+\left(\frac{n_2}{w}\right)^2\right)t\right)\right)\\
&\cdot\begin{cases}
\frac{x_2}{w_1} - \sum_{n=1}\frac{2}{n\pi}\sin\left(n\pi\left(1-\frac{x_2}{w_1}\right)\right)\exp\left(-D\left(\frac{n\pi}{d}\right)^2 t\right) & : x_2 \in \mathbb{R}_0^{w_1-}\\
1 & : x_2 \in \mathbb{R}_{w_1}^{w_2}\\
\frac{x_2-w}{w_1-w} - \sum_{n=1}\frac{2}{n\pi}\sin\left(n\pi\frac{w_1-x_2}{w_1-w}\right)\exp\left(-D\left(\frac{n\pi}{d}\right)^2 t\right) & : x_2 \in \mathbb{R}_{w_2+}^{w}\,.
\end{cases}
\end{aligned}\tag{19}$$

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

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[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

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