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A NOTE ON NUMERICAL APPROACHES FOR HEAT-DIFFUSION EQUATION WITH HETEROGENEOUS MEDIA AND ITS APPLICATIONS

Sat byul Seo

Abstract. In this paper, we introduce a numerical approach to solve heat-diffusion equation with discontinuous diffusion coefficients in the three dimensional rectangular domain. First, we study the support operator method and suggest a new method, the continuous velocity method. Further, we apply both methods to a diffusion process for neurotransmitter release in an individual synapse and compare their results.

1. Introduction

The heat-diffusion equation is defined by

$$\frac{\partial u}{\partial t} - \nabla \cdot (\beta \nabla u) = f(\mathbf{x}, t), \quad t \geq 0, \quad \mathbf{x} = (x, y, z) \in \Omega, \tag{1}$$

in a cubic shaped domain $\Omega = (a, b) \times (a, b) \times (c, d)$ in $\mathbb{R}^3$. Within the region, suppose diffusion coefficient β is piecewise continuous. Heat-diffusion with discontinuous coefficients arises when heat transfer occurs at an interface of two different materials. We define two sub-regions Ω^+, Ω^- separated by an interface Γ. Define $\Omega^+ = \{(a_1, b_1) \times (a_1, b_1) \times (c, d)\}$, with $a < a_1 < b_1 < b$, and $\Omega^- = \Omega \setminus (\Omega^+ \cup \Gamma)$.

Let β be a piecewise constant function in Ω is defined as

$$\beta(x, y, z) = \begin{cases} \beta^+, & \mathbf{x} \in \Omega^+, \\ \beta^-, & \mathbf{x} \in \Omega^-. \end{cases}$$

We assume homegeneous Neumann boundary conditions

$$\left.\frac{\partial u}{\partial \mathbf{n}}\right|_{\partial\Omega} = 0, \tag{2}$$

the initial condition at $t = 0$ is smooth and the boundary conditions on $\partial\Omega$ are known, the solution is uniquely determined in $W^{1,1}(\Omega)$ [1].

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Identification of the mechanism and structure in a single synapse has been challenging in neuroscience. The only heat-diffusion equation is mentioned as a model of the release process in synapse[2]. Heterogeneous media in the cleft, for example, a protein guide surrounding around release site can be represented as different values of diffusion coefficients in two regions in cleft. Thus, the main goal of this paper is to approximate the solution of heat-diffusion model with different diffusion coefficients in different regions. Several finite difference algorithms with discontinuous coefficients for parabolic equations and elliptic equations have been seen in the literature[3, 4, 5, 6, 11, 12]. Shashkov and Steinberg showed a new finite difference algorithm named support-operator methods to approximate a numerical solution of diffusion problems in heterogeneous and nonisotropic media[9, 11]. Li and Shen provided a numerical method which allows different values of coefficients for each sub-region in two dimensions and proved its second order accuracy[5]. We construct a model for glutamate molecules release process in synapse clefts using the numerical methods[9, 5]. The main goal of this paper is to approximate the solution of heat-diffusion model with piecewise continuous coefficients.

2. Preliminaries

2.1. Conservation Law

Let Ω is a finite region, then

$$\frac{d}{dt}\int_{\Omega} u\ dV = \int_{\Omega} f dV - \int_{\partial\Omega} \mathbf{J}\cdot\mathbf{n}\ dA, \tag{3}$$

where $\partial\Omega$ is the boundary of Ω and $\mathbf{n}$ is the outward unit normal to the boundary of Ω, f is the local production of u per unit volume, and $\mathbf{J}$ represents the flux of u. If $\mathbf{J}$ is sufficiently smooth, we have this equation by the divergence theorem,

$$\int_{\partial\Omega} \mathbf{J}\cdot\mathbf{n}\ dA = \int_{\Omega} \nabla\cdot\mathbf{J} dV. \tag{4}$$

From the conservation law (3), we obtain

$$\frac{d}{dt}\int_{\Omega} u\ dV = \int_{\Omega} f - \nabla\cdot\mathbf{J} dV. \tag{5}$$

Then we derive the following from 5

$$\frac{du}{dt} = f - \nabla\cdot\mathbf{J}. \tag{6}$$

2.2. Fick's Law

We introduce the simplest description the flux of one chemical species called Fick's law. The flux $\mathbf{J}$ is proportional to the gradient ∇u, but points in the opposite direction since the flow is from space of higher to lower concentration.

$$\mathbf{J} = -\beta\nabla u. \tag{7}$$

The scalar β is the diffusion coefficient, and u represent the heat content of the volume. When Fick's law applies into the Eq.(6), then we obtain the following equation:

$$\frac{du}{dt} = \nabla \cdot (\beta \nabla u) + f. \tag{8}$$

Concentration u is continuous across the interfaces Γ, and the normal flux is continuous across the interface Γ [4, 9].

$$[u]_\Gamma = 0, \tag{9}$$

$$\left[\beta \frac{\partial u}{\partial \mathbf{n}}\right]_\Gamma = 0, \tag{10}$$

where, $[u]_\Gamma = (u|_{\Omega^+})_\Gamma - (u|_{\Omega^-})_\Gamma$. However, the tangential flux may or may not be continuous across Γ.

2.3. Support Operator Method

An approach for a numerical solution of the heat-diffusion solution in heterogeneous media is derived using the support operator method, which constructs discretization of divergence and flux operator [9]. The flux vector $\mathbf{J}$ whose form of diffusion equation is commonly used in the case of discontinuous β. The Eq.(1) can be written as a first-order system:

$$\frac{\partial u}{\partial t} = -\nabla \mathbf{J}, \quad \mathbf{J} = -\beta \nabla u. \tag{11}$$

Lemma 2.1. *The discretization of $\nabla \cdot \beta \nabla u$ from Eq.(1) for three dimensional is as following :*

$$\frac{\beta\xi_{(i+1,j,k)} \frac{u_{(i+1,j,k)} - u_{(i,j,k)}}{\Delta x} - \beta\xi_{(i,j,k)} \frac{u_{(i,j,k)} - u_{(i-1,j,k)}}{\Delta x}}{\Delta x}$$

$$+ \frac{\beta\eta_{(i,j+1,k)} \frac{u_{(i,j+1,k)} - u_{(i,j,k)}}{\Delta y} - \beta\eta_{(i,j,k)} \frac{u_{(i,j,k)} - u_{(i,j-1,k)}}{\Delta y}}{\Delta y}$$

$$+ \frac{\beta\zeta_{(i,j,k+1)} \frac{u_{(i,j,k+1)} - u_{(i,j,k)}}{\Delta z} - \beta\zeta_{(i,j,k)} \frac{u_{(i,j,k)} - u_{(i,j,k-1)}}{\Delta z}}{\Delta z}.$$

Proof. The heat-diffusion equation is semi-discretized implicitly as following:

$$\frac{u^{n+1} - u^n}{\Delta t} = \nabla \cdot \beta \nabla u^{n+1}, \tag{12}$$

where $t_n = n\Delta t$ and $u^n = u(t_n, x, y, z)$.
The flux form of the Eq.(11) can be discretized in time as following.

$$\mathbf{J}^{n+1} = -\beta \nabla u^{n+1}, \quad \frac{(u^{n+1} - u^n)}{\Delta t} + \nabla \cdot \mathbf{J}^{n+1} = 0. \tag{13}$$

We induce the discretization of $\nabla \cdot \beta \nabla u$ using the form of the support-operators approaches, which leads to the well-known harmonic average the diffusion coefficients β on the interfaces[7, 9].

$$\begin{aligned}
\beta\xi_{(i,j,k)} &= \frac{2\beta_{(i-1,j,k)}\beta_{(i,j,k)}}{\beta_{(i-1,j,k)} + \beta_{(i,j,k)}}, \\
\beta\eta_{(i,j,k)} &= \frac{2\beta_{(i,j-1,k)}\beta_{(i,j,k)}}{\beta_{(i,j-1,k)} + \beta_{(i,j,k)}}, \\
\beta\zeta_{(i,j,k)} &= \frac{2\beta_{(i,j,k-1)}\beta_{((i,j,k)}}{\beta_{(i,j,k-1)} + \beta_{(i,j,k)}}.
\end{aligned}$$

Denote $u = u(x_i, y_j, z_k, t_n) \equiv u_{(i,j,k)}(t)$, then the discretization of $\nabla \cdot \beta \nabla u$ is as desired. □

Theorem 2.2. *The discretization of operators $\nabla \cdot \beta \nabla u$ for discontinuous diffusion coefficients are equivalent to the harmonic averaging procedure and the truncation error is $O(h^2)$.*

Proof. The scheme is second-order accurate in truncation errors for the numerical solution of diffusion problems in heterogeneous and nonisotropic materials constructed in rectangular grids[9]. □

In this model, the number of molecules is assumed to be infinite. It may or may not be a difference for velocity of concentrations between two different materials. However, this existing model may or may not perfectly match with our problem because the number of molecules is limited in our study.

3. Main Results

3.1. Continuous Velocity Method

We introduce a new method, called continuous velocity method, which is possibly suitable for limited amount of molecules. 4000 glutamate molecules diffuse out from a single vesicle pore, and it will take a few moments (approximating $10ms$) for molecules to be cleared out of the cleft. The particle velocity may also be continuous within the time flushing out even if there are different materials in the cleft. We assume the derivative is continuous at the interface Γ to reflect the scenario of fewer particles moving in a porous medium. Because the velocity is continuous on the interface, there is no jump of the first derivative in normal direction. Thus, we do not treat a point on the interface as a grid point, but the point is located in between two grids points. Li and Shen provided a numerical method which allows different values of coefficients for each sub-region in two dimensions and proved its second order accuracy[5]. We expand the numerical method in three dimensional rectangular grids.

Definition 1. Eq.(1) can be rewritten in the three dimensional rectangular grids with piecewise continuous diffusion coefficients β as following.

$$u_t = (\beta u_x)_x + (\beta u_y)_y + (\beta u_z)_z \tag{14}$$

Definition 2. Define $\Omega = (a,b)\times(a,b)\times(c,d)$ in $\mathbb{R}^3$. $\Omega^+ = \{(a_1,b_1)\times(a_1,b_1)\times(c,d)\}$, with $a < a_1 < b_1 < b$, and $\Omega^- = \Omega\backslash(\Omega^+\cup\Gamma)$. P_{reg} be *regular grids points* if $P_{reg} = \{(x_i,y_j,z_k) \in \Omega^{sign} : (x_{i_0},y_{j_0},z_{k_0}) \in \Omega^{sign}, i_0 = i-1 \text{ or } i+1, j_0 = j-1 \text{ or } j+1, k_0 = k-1 \text{ or } k+1\}$.

Definition 3. Let $u_{i,j,k}$ be a numerical solution discretized in the x-direction, y-direction, and z-direction with a mesh of size h as following:

$$u_{xx} \approx \frac{1}{h^2}(u_{i-1,j,k} - 2u_{i,j,k} + u_{i+1,j,k}) \equiv \delta_x u_{i,j,k}, \tag{15}$$

$$u_{yy} \approx \frac{1}{h^2}(u_{i,j-1,k} - 2u_{i,j,k} + u_{i,j+1,k}) \equiv \delta_y u_{i,j,k}, \tag{16}$$

$$u_{zz} \approx \frac{1}{h^2}(u_{i,j,k-1} - 2u_{i,j,k} + u_{i,j,k+1}) \equiv \delta_z u_{i,j,k}. \tag{17}$$

Theorem 3.1. *For a regular grid point (x,y,z) in Ω, The local truncation error of (15), (16), and (17) from $(\beta u_x)_x + (\beta u_y)_y + (\beta u_z)_z$ is $O(h^2)$.*

Proof. Assume the exact solution $u(x,y,z)$ is smooth then, by Taylor expansions, $\delta_x G_{i,j,k}$ can be denoted by

$$\delta_x u_{i,j,k} = \left[u_{xx}(x_i,y_j,z_k) + \frac{1}{12}h^2 u^{(4)}(x_i,y_j,z_k) + O(h^4)\right]. \tag{18}$$

Therefore,

$$\tau_x = u_{xx} - \delta_x u_{i,j,k} = -\frac{1}{12}h^2 u^{(4)}(x_i,y_j,z_k) + O(h^4). \tag{19}$$

Also $u_{yy} - \delta_y u_{i,j,k}$, $u_{zz} - \delta_z u_{i,j,k}$ are similar. □

Definition 4. Define $\Omega = (a,b)\times(a,b)\times(c,d)$ in $\mathbb{R}^3$. $\Omega^+ = \{(a_1,b_1)\times(a_1,b_1)\times(c,d)\}$, with $a < a_1 < b_1 < b$, and $\Omega^- = \Omega \setminus (\Omega^+ \cup \Gamma)$. P_{irr} be *irregular grids points* if $P_{irr} = \{(x_i,y_j,z_k) \in \Omega^+ : (x_{i_0},y_{j_0},z_{k_0}) \in \Omega^-, i_0 = i-1 \text{ or } i+1, j_0 = j-1 \text{ or } j+1, k_0 = k-1 \text{ or } k+1\} \cup \{(x_i,y_j,z_k) \in \Omega^- : (x_{i_0},y_{j_0},z_{k_0}) \in \Omega^+, i_0 = i-1 \text{ or } i+1, j_0 = j-1 \text{ or } j+1, k_0 = k-1 \text{ or } k+1\}$.

Remark 1. The interface $\Gamma = \partial\Omega^+$ is a cubic shape and consists of all points on surfaces, edges, and corners of a cubic domain.

Remark 2. Let $[u]$ denote the difference of the limits of C cross the discontinuity from exterior(Ω^+) to interior(Ω^-) along the normal direction.

$$[u] \equiv (u|_{\Omega^+})_\Gamma - (u|_{\Omega^-})_\Gamma = 0, \tag{20}$$

$$[u_n] \equiv \left(\frac{\partial u}{\partial \mathbf{n}}\bigg|_{\Omega^+}\right)_\Gamma - \left(\frac{\partial u}{\partial \mathbf{n}}\bigg|_{\Omega^-}\right)_\Gamma = 0. \tag{21}$$

Theorem 3.2. *For a irregular grid point (x, y, z) in Ω, The local truncation error of (15), (16), and (17) from $(\beta u_x)_x + (\beta u_y)_y + (\beta u_z)_z$ is $O(h)$.*

Proof. Let (x_i, y_j, z_k) be an irregular point. Then we obtain

$$[u_{xx}] = [u_{yy}] = [u_{zz}] = \left[\frac{u_t}{\beta}\right]. \tag{22}$$

We use correction terms in three directions, x-direction, y-direction, and z-direction. Let (x^*, y^*, z^*) be the actual corner. Then we have

$$\begin{aligned}(u_{i,j,k})_t =& \beta(\delta_x u_{i,j,k} + \delta_y u_{i,j,k} + \delta_z u_{i,j,k}) + \beta\left[\frac{u_t}{\beta}\right]\frac{\tau_{x_0}(x_{i_0} - x^*)^2}{2h^2} \\ &+ \beta\left[\frac{u_t}{\beta}\right]\frac{\tau_{y_0}(y_{j_0} - y^*)^2}{2h^2} + \beta\left[\frac{u_t}{\beta}\right]\frac{\tau_{z_0}(z_{k_0} - z^*)^2}{2h^2} + O(h),\end{aligned}$$

where $i_0 = i - 1$ or $i + 1$, $j_0 = j - 1$ or $j + 1$, $k_0 = k - 1$ or $k + 1$, and τ_{x_0}, τ_{y_0}, $\tau_{z_0} = 1$ or -1.
Now, we have

$$\left[\frac{u_t}{\beta}\right] = u_t^-\left[\frac{1}{\beta}\right] + \frac{[u_t]}{\beta^+} = u_t^+\left[\frac{1}{\beta}\right] + \frac{[u_t]}{\beta^-}.$$

This implies

$$\left[\frac{u_t}{\beta}\right] = u_t\left[\frac{1}{\beta}\right] + \frac{[u_t]}{\hat{\beta}} + O(h), \tag{23}$$

where $\hat{\beta} = \beta^-$ if $\beta = \beta^+$, $\hat{\beta} = \beta^+$ if $\beta = \beta^-$. Using (23), we have the following system of ordinary differential equations

$$(u_{i,j,k})_t = F(u_{i-1,j,k}, u_{i,j-1,k}, u_{i,j,k-1}, u_{i,j,k}, u_{i+1,j,k}, u_{i,j+1,k}, u_{i,j,k+1}),$$

where F is equal to

$$\frac{\beta(\delta_x u_{i,j,k} + \delta_y u_{i,j,k} + \delta_z u_{i,j,k} + \frac{[u_t]}{\hat{\beta}}\, T_{i,j,k})}{1 - \beta[\frac{1}{\beta}]\, T_{i,j,k}}, \tag{24}$$

for

$$T_{i,j,k} = \frac{\tau_{x_0}(x_{i_0} - x^*)^2}{2h^2} + \frac{\tau_{y_0}(y_{j_0} - y^*)^2}{2h^2} + \frac{\tau_{z_0}(z_{k_0} - z^*)^2}{2h^2}. \tag{25}$$

□

Proposition 3.3. *The local truncation error for discretizing on t is $O(\Delta t)$.*

$$\begin{aligned}u_{i,j,k}^{n+1} =& u_{i,j,k}^n \\ &+ \Delta t \cdot F(u_{i-1,j,k}^n, u_{i,j-1,k}^n, u_{i,j,k-1}^n, u_{i,j,k}^n, u_{i+1,j,k}^n, u_{i,j+1,k}^n, u_{i,j,k+1}^n).\end{aligned}$$

We discretize time t by choosing $\Delta t = C \cdot h^2$ for CFL condition where C is a constant[8]. The local truncation error from the discretization of time is $O(\Delta t) = O(h^2)$.

Theorem 3.4. *Let F be defined as Eq.(24). At any point (x_i, y_j, z_k) in Ω, the numerical solution has global error to be $O(h^2)$.*

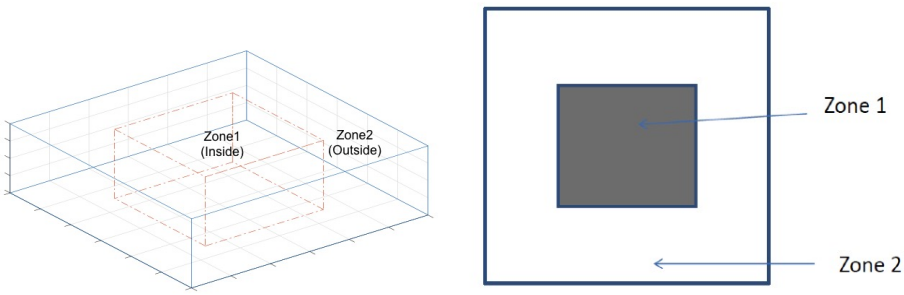
Proof: Since the interface is one dimension lower than the solution domain, we will need the local truncation error at irregular grid points to be $O(h)$ to obtain second order accuracy globally[3, 5]. From Theorem 3.1, the local truncation error is $O(h^2)$ for a regular grid point. At an irregular grid point, the local truncation error is $O(h)$ by Theorem 3.2. Therefore, All these imply that the numerical solution has global error $O(h^2)$.

4. Applications

In this section, we simulate the process of neurotransmitters release through a single synapse. In other to solve the heat diffusion equation numerically to achieve glutamate molecules concentration in the synaptic cleft, we use on explicit finite difference method that is implemented in MATLAB codes[8].

$$\begin{aligned} u_{i,j,k}^{n+1} &= u_{i,j,k}^{n} + \alpha[S_{i+1,j,k}u_{i+1,j,k}^{n} + S_{i-1j,k}u_{i-1j,k}^{n} + S_{i,j+1,k}u_{i,j+1,k}^{n} \\ &+ S_{i,j-1,k}u_{i,j-1,k}^{n} + S_{i,j,k-1}u_{i,k,j,k-1}^{n} - (S_{i,j,k}u_{i,j,k}^{n} + S_{i-1,j,k}u_{i,j,k}^{n} \\ &+ S_{i,j+1,k}u_{i,j,k}^{n} + S_{i,j-1,k}u_{i,j,k}^{n} + S_{i,j,k+1}u_{i,j,k}^{n} + S_{i,j,k-1}u_{i,j,k}^{n})], \end{aligned}$$

where $u_{i,j,k}^{n} = u(x_i, y_j, z_k, t_n)$ and $\alpha = \beta_{glut}\frac{\Delta t}{(\Delta x)^2}$. For our simulation, we satisfy a condition of $\alpha < (1/2)^3$ known as CFL condition to ensure the scheme is numerically stable. We take the space step $\Delta x = 0.01\mu m$ and the time step $\Delta t = C \cdot (\Delta x)^2$, where C is a constant.



(A) Synaptic Cleft in 3-D (B) Top View of Synaptic Cleft

FIGURE 1. (A) The synaptic cleft is divided into two zones. Diffusion coefficients were taken different values in two regions(inside and outside), which represent slow and fast motion of neurotransmitters released due to different compositions in the synaptic cleft. (B) Top view of synaptic cleft dividing into two parts.

We simulate three different models for releasing glutamates. In the base model, we take $\beta = 0.4$ uniformly. In high affinity center, we take $\beta^{+} = 0.1$ in

β^+ and $\beta^- = 0.4$ in Ω^-. Also in high affinity edge model, $\beta^+ = 0.4$ in Ω^+ and $\beta^- = 0.1$ in Ω^- are taken.

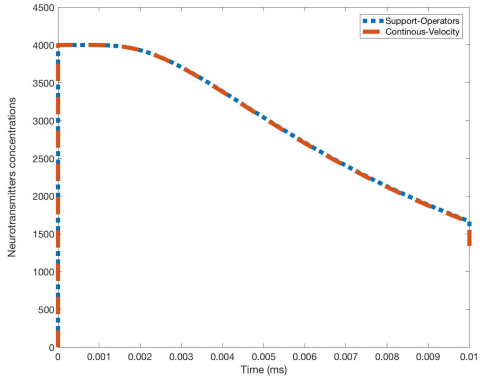


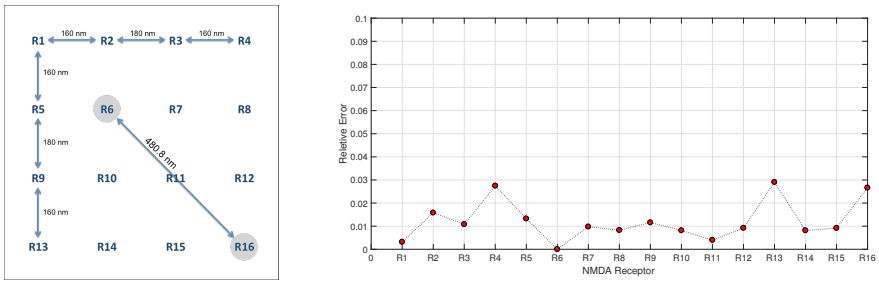
FIGURE 2. Total concentration of glutamate molecules as time spends.

4.1. Comparison of Two Models

We compare our model(continuous velocity model) with the support operator model. The relative discrepency for the total concentration is 0.2% as shown in Figure 2, which indicates that there is no significantly difference between two models for total concentration. However, two models are taken different modelings on the interfaces, thus we expect that concentrations depending upon locations might be different. We track glutamate concentrations at the specific locations beyond 16 NMDA receptors (R1-R16) and estimate the relative errors between two models as shown in Figure 3b.

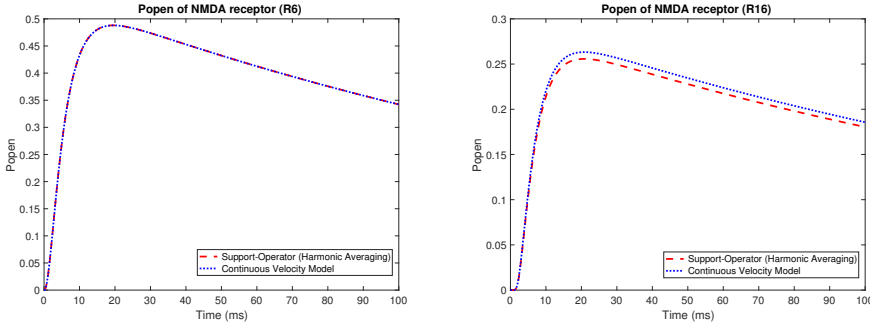
We simulate the glutamate release around R6 (Figure 3a), then the glutamate molecules diffuse out and cross the interface to flush out of the cleft. R4, R13, and R16 produce the errors large than others. Nevertheless, the maximum relative error of 16 location is 2.9×10^{-2}, which is not significant for our problem as we are interested in relative ratio of opening probability. Figure 3b presents the comparative discrepancy of two models.

As shown in Figure 4, when glutamate molecules release near the center, then the maximum opening probability of NMDA receptor (R6) is 0.4880. The range of maximum opening probability of NMDA receptor (R16) near edge is 0.2557-0.2632. For errors of opening probabilities between two methods do not make any significantly different outcomes, thus we will use only our new model(continuous velocity model) for following steps.



(A) (B)

FIGURE 3. (A) 16 NMDA receptors are evenly distributed on the postsynaptic terminal surface (B) Relative discrepancy between Support-Operator and Continuous Velocity models of glutamate concentration over 16 NMDA receptors.



(A) Release from Center (B) Release From Edge

FIGURE 4. NMDA receptor opening probability

5. Conclusion and Discussion

Identification of the mechanism and structure in a single synapse has been challenging and still remains a lot more questions. Many mathematical and computational neuroscientists have been developing for sophisticating model to solve the questions. We suggested a new method to be applicable for neurotransmission procedures. Our future research would be to validate our theoretical results with experimental results and estimate errors to be consistent.

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Sat byul Seo
Department of Mathematics Education
Kyungnam University
Changwon, Gyeongnam 51767, South Korea
E-mail address: sbseo@kyungnam.ac.kr