

Karbowski model in 2-D

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1. Introduction

This is a working document starting from the model described in Eqs. 2 and 4 in “Model of the Early Development of Thalamo-Cortical Connections and Area Patterning via Signaling Molecules”, Karbowski & Ermentrout, 2004 [2]. I then consider extending this model into two dimensions.

2. One dimensional system

Equations 1-4 of [2] is the full set of differential equations describing their system:

$$\frac{\partial c_i(x, t)}{\partial t} = -\alpha_i c_i(x, t) + \beta_i n(x, t) [a_i(x, t)]^k \quad (1)$$

$$\frac{\partial a_i(x, t)}{\partial t} = \frac{\partial J_i(x, t)}{\partial x} + \alpha_i c_i(x, t) - \beta_i n(x, t) [a_i(x, t)]^k \quad (2)$$

$$n(x, t) + \sum_{i=1}^N c_i(x, t) = 1 \quad (3)$$

with the flux current

$$J_i(x, t) = D \frac{\partial a_i(x, t)}{\partial x} - a_i \left(\gamma_{Ai} \frac{\partial \rho_A(x)}{\partial x} + \gamma_{Bi} \frac{\partial \rho_B(x)}{\partial x} + \gamma_{Ci} \frac{\partial \rho_C(x)}{\partial x} \right) \quad (4)$$

Note that (unlike in the original paper) I have been explicit about the space and time dependence of the state variables a_i , c_i , J_i , n , ρ_A , ρ_B and ρ_C . Note also that i *always* refers to the thalamo-cortical connection type; there is one equation system for each connection type. Keep this in mind when reading the sums in the maths below. Note finally that I’ve not defined all the terms in this working document, but I’ve used the same variable names as in the paper [2].

3. Two dimensional system

Extending the system above to two spatial dimensions changes x into a two-dimensional \mathbf{x} and changes the flux term, $J_i(x)$ as follows:

$$\frac{\partial c_i(\mathbf{x}, t)}{\partial t} = -\alpha_i c_i(\mathbf{x}, t) + \beta_i n(\mathbf{x}, t) [a_i(\mathbf{x}, t)]^k \quad (5)$$

$$\frac{\partial a_i(\mathbf{x}, t)}{\partial t} = \nabla \cdot \mathbf{J}_i(\mathbf{x}, t) + \alpha_i c_i(\mathbf{x}, t) - \beta_i n(\mathbf{x}, t) [a_i(\mathbf{x}, t)]^k \quad (6)$$

$$n(\mathbf{x}, t) + \sum_{i=1}^N c_i(\mathbf{x}, t) = 1 \quad (7)$$

with the flux current

$$\mathbf{J}_i(\mathbf{x}, t) = D \nabla a_i(\mathbf{x}, t) - a_i (\gamma_{Ai} \nabla \rho_A(\mathbf{x}) + \gamma_{Bi} \nabla \rho_B(\mathbf{x}) + \gamma_{Ci} \nabla \rho_C(\mathbf{x})) \quad (8)$$

The boundary condition that I’d like to apply to these equations is:

$$\mathbf{J}_i(\mathbf{x}, t) \Big|_{\text{boundary}} = 0 \quad (9)$$

to agree with the boundary condition applied in the paper for the 1D system.

3.1. Computing div J: approach 1

In order to compute $\nabla \cdot \mathbf{J}_i(\mathbf{x}, t)$, I need to do a little work. First, I point out that

$$\mathbf{g}(\mathbf{x}) \equiv (\gamma_{Ai} \nabla \rho_A(\mathbf{x}) + \gamma_{Bi} \nabla \rho_B(\mathbf{x}) + \gamma_{Ci} \nabla \rho_C(\mathbf{x})) \quad (10)$$

is a static vector field; once computed at the start of the simulation, it is time-invariant. \mathbf{J}_i is thus:

$$\mathbf{J}_i(\mathbf{x}, t) = D \nabla a_i(\mathbf{x}, t) - a_i \mathbf{g}(\mathbf{x}) \quad (11)$$

Taking the divergence of Eq. 11:

$$\nabla \cdot \mathbf{J}_i(\mathbf{x}, t) = \nabla \cdot (D \nabla a_i(\mathbf{x}, t) - a_i \mathbf{g}(\mathbf{x})) \quad (12)$$

Now simply multiply the current values of a_i and \mathbf{g} and compute an approximation to ∇a_i , resulting in a vector field which is \mathbf{J} . The boundary condition can be forced by setting this to 0 for boundary hexes (ugly, and quite possibly completely fallacious). Finally, compute $\nabla \cdot \mathbf{J}_i(\mathbf{x}, t)$ using the result that divergences can be simplified by means of Gauss's Theorem. This states that (in a two-dimensional system) the area integral of the divergence of a vector field \mathbf{f} is equal to the integral around the boundary of the field dotted with the normal to the boundary:

$$\iint_A \nabla \cdot \mathbf{f} \, dxdy = \oint_c \mathbf{f} \cdot d\hat{\mathbf{n}} \quad (13)$$

See, for example [1], Sect. 1.11, p 58.

This can be used to find the average value of the divergence of \mathbf{f} over the area of a hexagon; \mathbf{f}_0 is the average value of the vector field at the centre of the hexagon; \mathbf{f}_1 – \mathbf{f}_6 are the average values of the field in the 6 neighbouring hexagons. The contour integral can be discretized for this hexagonal region, which has area Ω and a side length v :

$$\begin{aligned} \frac{1}{\Omega} \oint_c \mathbf{f} \cdot d\hat{\mathbf{n}} &\approx \frac{1}{\Omega} \sum_{j=1}^6 \frac{\mathbf{f}_j + \mathbf{f}_0}{2} \cdot \hat{\mathbf{n}} \, v \\ &= \frac{1}{\Omega} \sum_{j=1}^6 \frac{\mathbf{f}_j^x + \mathbf{f}_0^x}{2} \cdot \hat{\mathbf{n}} \, v + \sum_{j=1}^6 \frac{\mathbf{f}_j^y + \mathbf{f}_0^y}{2} \cdot \hat{\mathbf{n}} \, v \\ &= \frac{1}{\Omega} \sum_{j=1}^6 \frac{\mathbf{f}_j^x + \mathbf{f}_0^x}{2} \cos(60 \times (j-1)) \, v + \frac{1}{\Omega} \sum_{j=1}^6 \frac{\mathbf{f}_j^y + \mathbf{f}_0^y}{2} \sin(60 \times (j-1)) \, v \end{aligned} \quad (14)$$

An advantage to using this approach is that if it is required that the *divergence* be 0 across the boundary then for those edges of the hex that lie on the boundary \mathbf{f}_j can be set equal to \mathbf{f}_0 (this is the ghost cell method), satisfying this boundary condition, whilst permitting flow through the hex parallel to the boundary. However, it is not so easy to choose a ghost cell with properties that will force the *value* of \mathbf{f}_0 to 0.

3.2. Computing div J: approach 2

An alternative approach is to apply some vector calculus identities to work out the divergence of $\mathbf{J}_i(\mathbf{x})$. Because the divergence operator is distributive, Eq. 12 can be expanded:

$$\nabla \cdot \mathbf{J}_i(\mathbf{x}) = \nabla \cdot (D \nabla a_i(\mathbf{x}, t)) - \nabla \cdot (a_i \mathbf{g}(\mathbf{x})) \quad (15)$$

D is a constant and applying the vector calculus product rule identity to $\nabla \cdot (a_i \mathbf{g}(\mathbf{x}))$:

$$\nabla \cdot \mathbf{J}_i(\mathbf{x}) = D \nabla \cdot \nabla a_i(\mathbf{x}, t) - (a_i(\mathbf{x}, t) \nabla \cdot \mathbf{g}(\mathbf{x}) + \mathbf{g}(\mathbf{x}) \cdot \nabla a_i(\mathbf{x}, t)) \quad (16)$$

(to prove $\nabla \cdot D \nabla a = D \nabla \cdot \nabla a$, apply the product rule and note that $\nabla D = 0$ for constant D). Expanding the brackets we have:

$$\nabla \cdot \mathbf{J}_i(\mathbf{x}) = D \nabla \cdot \nabla a_i(\mathbf{x}, t) - a_i(\mathbf{x}, t) \nabla \cdot \mathbf{g}(\mathbf{x}) - \mathbf{g}(\mathbf{x}) \cdot \nabla a_i(\mathbf{x}, t) \quad (17)$$

which has three elements to compute: the Laplacian of $a_i(\mathbf{x}, t)$; a time-independent modulator of $a_i(\mathbf{x}, t)$ [because $\nabla \cdot \mathbf{g}(\mathbf{x})$ is a time-independent static field]; and the dot product of the static vector field $\mathbf{g}(\mathbf{x})$ and the gradient of $a_i(\mathbf{x}, t)$.

Each of the divergences can be simplified by means of Gauss's Theorem. Reference [3] presents an application of Gauss's Theorem to the solution of Poisson's equation, which contains a Laplacian term, on an hexagonal grid. The computation of the mean value of our Laplacian, $D \nabla \cdot \nabla a_i(\mathbf{x}, t)$, across the area of one hexagon located at position \mathbf{p}_0 , with neighbours at positions \mathbf{p}_1 – \mathbf{p}_6 is:

$$D \nabla \cdot \nabla a_i(\mathbf{p}_0, t) = D \frac{2}{3d^2} \sum_{j=1}^6 (a_i(\mathbf{p}_j) - a_i(\mathbf{p}_0)) \quad (18)$$

where d is the centre-to-centre distance between hexes in the grid. Let's work it through. In the following, v is the length of each of the 6 edges of the hexagon's perimeter and $v = d/\sqrt{3}$. $d\gamma$ is an infinitesimally small distance along the perimeter of the hexagon. The area of each hexagon in the lattice is $\frac{\sqrt{3}}{2}d^2$.

$$\begin{aligned} \frac{1}{\Omega} \iint_A \nabla \cdot \nabla a_i(\mathbf{x}) dx dy &= \frac{1}{\Omega} \oint_c \frac{\partial a_i}{\partial \hat{\mathbf{n}}} d\gamma \\ &\approx \frac{1}{\Omega} \sum_{j=1}^6 \left. \frac{\partial a_i(\mathbf{p}_j)}{\partial \hat{\mathbf{n}}} \right|_{mid} v \\ &= \frac{2}{\sqrt{3}d^2} \sum_{j=1}^6 \frac{a_i(\mathbf{p}_j) - a_i(\mathbf{p}_0)}{d} \frac{d}{\sqrt{3}} \\ &= \frac{2}{3d^2} \sum_{j=1}^6 (a_i(\mathbf{p}_j) - a_i(\mathbf{p}_0)) \end{aligned} \quad (19)$$

Applying Gauss's Theorem to the second term, the computation of $a_i(\mathbf{p}_0, t) \nabla \cdot \mathbf{g}(\mathbf{p}_0)$ can be written out in a similar way:

$$\begin{aligned} \frac{1}{\Omega} \iint_A a_i \nabla \cdot \mathbf{g} dx dy &= \frac{a_i(\mathbf{p}_0)}{\Omega} \oint_c \mathbf{g} \cdot d\hat{\mathbf{n}} \\ &\approx \frac{a_i(\mathbf{p}_0, t)}{\Omega} \sum_{j=1}^6 \frac{\mathbf{g}_j + \mathbf{g}_0}{2} \cdot \hat{\mathbf{n}} v \\ &= \frac{2a_i(\mathbf{p}_0, t)v}{\sqrt{3}d^2} \left(\sum_{j=1}^6 \frac{\mathbf{g}_j^x + \mathbf{g}_0^x}{2} \cdot \hat{\mathbf{n}} + \frac{1}{\Omega} \sum_{j=1}^6 \frac{\mathbf{g}_j^y + \mathbf{g}_0^y}{2} \cdot \hat{\mathbf{n}} \right) \\ &= \frac{2a_i(\mathbf{p}_0, t)d}{\sqrt{3}d^2\sqrt{3}} \left(\sum_{j=1}^6 \frac{\mathbf{g}_j^x + \mathbf{g}_0^x}{2} \cdot \hat{\mathbf{n}} + \frac{1}{\Omega} \sum_{j=1}^6 \frac{\mathbf{g}_j^y + \mathbf{g}_0^y}{2} \cdot \hat{\mathbf{n}} \right) \\ &= \frac{a_i(\mathbf{p}_0, t)}{3d} \left(\sum_{j=1}^6 (\mathbf{g}_j^x + \mathbf{g}_0^x) \cos(60 \times (j-1)) + \sum_{j=1}^6 (\mathbf{g}_j^y + \mathbf{g}_0^y) \sin(60 \times (j-1)) \right) \end{aligned} \quad (20)$$

The final expression is suitable for a numerical computation. Lastly, the final term in Eq. 17 is the scalar product of two vector fields which I'll carry out simply with Cartesian x and y components - so I'll re-use my `spacegrad2D` function to find ∇a_i .

I think that the advantage of separating this computation out is that I can ensure that \mathbf{J} resulting from the first term remains 0, by the ghost cell method, then I can tailor $\mathbf{g}(\mathbf{x})$ so that it, and its normal derivative go to 0 at the boundary, ensuring that the second and third terms also contribute nothing to \mathbf{J} at the boundary. To do this, I'll apply a fairly sharp logistic function based on distance to the boundary to $\mathbf{g}(\mathbf{x})$.

References

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3. D. Lee, H. Tien, C. Luo, et al. *International Journal of Computer Mathematics*, 91(9):1986–2009, Sept. 2014.