

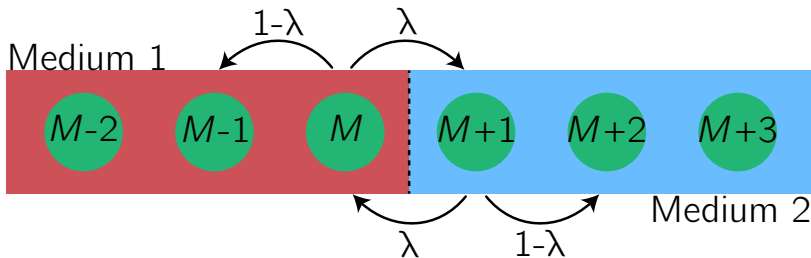
Semi-permeable membranes as domain walls

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Semi-permeable membranes as domain walls

- Consider a 1d lattice of spacing $a > 0$. The lattice is separated by placing a semi-permeable membrane between sites M and $M + 1^1$, which can be crossed with probability $\lambda < 1/2$
- On the left of the membrane consists of a media with temporal step size τ_l and on the right a media with step size τ_r – eventually amounting to varying diffusivities



The master equation

- Let $p_j(t)$ denote the probability of being at site j at time t and $\Delta = \frac{1}{2} - \lambda$. The (global) master equation for the system reads

$$\begin{aligned} \frac{\partial p_j(t)}{\partial t} = & \left[\frac{1}{2} p_{j+1} + \frac{1}{2} p_{j-1} - p_j \right] \left(\frac{1}{\tau_l} \sum_{k=-\infty}^M \delta_{j,k} + \frac{1}{\tau_r} \sum_{k=M+1}^{\infty} \delta_{j,k} \right) \\ & + \frac{\Delta}{\tau_l} p_M(t) \delta_{j,M-1} + \frac{\Delta}{\tau_r} p_{M+1}(t) \delta_{j,M+2} \\ & + \left(\frac{\lambda}{\tau_r} - \frac{1}{2\tau_l} \right) p_{M+1}(t) \delta_{j,M} + \left(\frac{\lambda}{\tau_l} - \frac{1}{2\tau_r} \right) p_M(t) \delta_{j,M+1} \quad (1) \end{aligned}$$

The continuum limit

- Consider the discrete-to-continuum mapping, $p_j(t) \rightarrow p(x, t)$, $M \rightarrow x_b$, $D_i = a^2/2\tau_i$ and $\delta_{j,k} \rightarrow a\delta(x - y)$

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- Keep terms to $\mathcal{O}(a^4)$ and let the **reluctivity** of the media, $\nu_i = \frac{4(2\lambda-1)\tau_i}{a}$, remain finite in the limit $a \rightarrow 0$,

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left[D(x) \frac{\partial p}{\partial x} \right] + (4\lambda - 1) (D_r - D_l) p(x_b, t) \delta'(x - x_b) - D_r^2 \nu_r \frac{\partial p(x_b, t)}{\partial x} \delta'(x - x_b), \quad (2)$$

where $D(x) = D_l \Theta(x_b - x) + D_r \Theta(x - x_b)$ is the state-dependent diffusivity

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- When $D_r = D_l$, diffusion becomes homogeneous across membrane and we recover Kay & Giuggioli (2022)²
- When $\lambda = 1/2$, $\nu_r \rightarrow 0$ and the third term on RHS vanishes

Replacing deltas with BCs

- We can write the right-hand side of Eq. (2) in terms of a generalized probability flux,

$$J(x, t) = -D(x)\partial_x p(x, t) - \chi(t)\delta(x - x_b), \quad (3)$$

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- Can then use the piecewise continuity of p to show that we can equivalently write Eq. (2) $\partial_t p = \partial_x (D(x)\partial_x p)$ with the boundary conditions (i) J is everywhere continuous and (ii) obeys the self-consistency condition

$$D(x_b)[p(x_b, t)] = (4\lambda - 1)(D_r - D_l)p(x_b, t) - D_r^2 \nu_r \frac{\partial p(x_b, t)}{\partial x}, \quad (4)$$

where $[p(x_b, t)] := p_r(x_b^+, t) - p_l(x_b^-, t)$

A FPE interpretation

- The Dirac delta is the distribution satisfying $\langle \delta_a, \varphi \rangle = \varphi(a)$ for a test function φ

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- Differential operator acts on distributions as

$\langle \delta'_a, \varphi \rangle = -\langle \delta_a, \varphi' \rangle = -\varphi'(a)$ so

$\delta'(x - a)f(a) = \delta(x - a)\partial_x f(x) + \delta'(x - a)f(x)$ leading to

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x} [\mu(x, t)p(x, t)] + \frac{\partial^2}{\partial x^2} [\sigma(x, t)p(x, t)] \quad (5)$$

for drift

$$\mu(x, t) = \frac{\partial D}{\partial x} + (4\lambda - 1)(D_r - D_l)\delta(x - x_b) - D_r^2 \nu_r \delta'(x - x_b)$$

and effective diffusivity

$$\sigma(x, t) = D(x) - D_r^2 \nu_r \delta(x - x_b)$$

The case of many domains

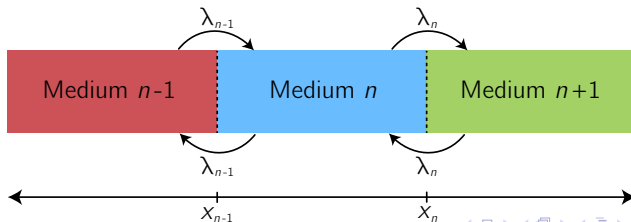
- Membranes are specified by 3-tuples $\{(x_i, \lambda_i, D_i)\}$, for $x_{i+1} > x_i$, containing their position, probability of crossing, and diffusivity in the domain between x_{i-1} and x_i , respectively – satisfying $x_0 = -\infty$, $x_{\max i} = +\infty$ and $\lambda_{\max i} = 0$:

$$\frac{\partial p(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[\sum_i D_i [\Theta(x - x_{i-1}) - \Theta(x - x_i)] \frac{\partial p(x, t)}{\partial x} \right] + \sum_i \left[(4\lambda_i - 1) (D_{i+1} - D_i) p(x_i, t) - D_{i+1}^2 \nu_{i+1} \frac{\partial p(x_b, t)}{\partial x} \right] \delta'(x - x_i),$$

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Are there distinct behaviours depending on values of ν_i ?
- ④ How many times, on average, does a particle cross a membrane at time t ?
- ⑤ How much time is spent “at” the membrane?

A probabilistic approach

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 - ② Given the reluctivity ν in a domain, diffusivity and domain size, $r_i = x_i - x_{i-1}$, are (conditionally) independent and PDFs depend on reluctivity as $p(\cdot | \nu) = f(\nu/\Lambda)$ for some function f
- The joint PDF can be written as

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- If $x(t)$ has (i) uncorrelated increments and (ii) $\langle x^2(t) \rangle \sim t^\beta$, then the process has non-stationary increments and shows weak ergodicity breaking³

References

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- [2] T. Kay and L. Giuggioli, Phys. Rev. Res. **4**, L032039 (2022).
- [3] P. Massignan, C. Manzo, J. A. Torreno-Pina, M. F. García-Parajo, M. Lewenstein, and G. J. Lapeyre, Phys. Rev. Lett. **112**, 150603 (2014).

The continuum limit I

$$\begin{aligned}\frac{\partial p(x, t)}{\partial t} = & [D_l \Theta(x_b - x) + D_r \Theta(x - x_b)] \frac{\partial^2 p(x, t)}{\partial x^2} \\ & + a \frac{\Delta}{\tau_l} p(x_b, t) \delta(x - (x_b - a)) + a \frac{\Delta}{\tau_r} p(x_b + a, t) \delta(x - (x_b + 2a)) \\ & + a \left(\frac{\lambda}{\tau_r} - \frac{1}{2\tau_l} \right) p(x_b + a, t) \delta(x - x_b) \\ & + a \left(\frac{\lambda}{\tau_l} - \frac{1}{2\tau_r} \right) p(x_b, t) \delta(x - (x_b + a)) \quad (6)\end{aligned}$$

The continuum limit II

$$\begin{aligned}\frac{\partial p(x, t)}{\partial t} = & [D_l \Theta(x_b - x) + D_r \Theta(x - x_b)] \frac{\partial^2 p(x, t)}{\partial x^2} \\ & + a^2 \left(2\lambda - \frac{1}{2} \right) p(x_b, t) \delta'(x - x_b) \left(\frac{1}{\tau_r} - \frac{1}{\tau_l} \right) \\ & + \frac{a^2}{2} \left(\frac{1}{\tau_r} - \frac{1}{\tau_l} \right) \frac{\partial p(x_b, t)}{\partial x} \delta(x - x_b) \\ & + \frac{a^3}{4} \left(\frac{1}{\tau_r} - \frac{1}{\tau_l} \right) \left[\frac{\partial p(x_b, t)}{\partial x} \delta(x - x_b) - p(x_b, t) \delta''(x - x_b) \right] \\ & - \frac{a^3}{\tau_r} (2\lambda - 1) \frac{\partial p(x_b, t)}{\partial x} \delta'(x - x_b) + \mathcal{O}(a^4) \quad (7)\end{aligned}$$

- The fourth term vanishes as $\tau \sim a^2$ and there is no additional coupling

On the unphysicality of the reluctivity

In defining a non-trivial membrane, we take

$$\nu = \lim_{\tau, a \rightarrow 0} \frac{4\tau(2\lambda - 1)}{a} = \lim_{a \rightarrow 0} \frac{2a}{D}(2\lambda - 1)$$

to remain finite, positive and non-zero unless $\lambda = 1/2$. If we constrain $\lambda \in [0, 1]$, this is clearly impossible, necessitating that we let

$$\lambda(a) = \frac{1}{2} + \frac{c}{a},$$

where c is defined such that the limit is ν . As the lattice spacing becomes vanishingly small, the necessity of the divergence of λ arises from the unphysical nature of the membrane: it only influences an infinitesimal volume, which can only have a finite effect if the local flow is infinite.

Moments

- The mean moments of the distribution can be found by integrating with respect to $p(x, t)$. Using Eq. (2), can determine the rate of change of these moments as

$$\frac{d \langle x^n(t) \rangle}{dt} = \int_{-\infty}^{\infty} x^n \frac{\partial p(x, t)}{\partial t} dx \quad (8)$$

- To first and second order, with $\varsigma = D_r - D_l$,

$$\frac{d \langle x(t) \rangle}{dt} = 2(1 - 2\lambda)\varsigma p(x_b, t) - D_r^2 \nu_r \frac{\partial p(x_b, t)}{\partial x} \quad (9a)$$

$$\frac{d \langle x^2(t) \rangle}{dt} = 2(D_l \mathbb{P}_t(x < x_b) + D_r \mathbb{P}_t(x > x_b)) + 2x_b \frac{d \langle x(t) \rangle}{dt} \quad (9b)$$

Deriving BCs I

Since the probability factors are evaluated at the boundary, we may take them to be constant so

$$p(x_b, t)\delta'(x - x_b) = \frac{\partial}{\partial x} [p(x_b, t)\delta(x - x_b)]$$

and hence may rewrite the equation as

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} D(x) \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[(4\lambda - 1) \varsigma p(x_b, t) - D_r^2 \nu_r \frac{\partial p(x_b, t)}{\partial x} \right] \delta(x - x_b),$$

where I have defined $D(x) = D_l \Theta(x_b - x) + D_r \Theta(x - x_b)$. The required form, Eq. (3), follows by subtracting the right-hand side from the left and rearranging

Deriving BCs II

Suppose that $p(x, t)$ is piecewise smooth and bounded so we may write

$$p(x, t) = p_l(x, t)\Theta(x_b - x) + p_r(x, t)\Theta(x - x_b). \quad (10)$$

Note that the derivative with respect to t reads

$$\partial_t p(x, t) = \partial_t p_l(x, t)\Theta(x_b - x) + \partial_t p_r(x, t)\Theta(x - x_b),$$

so is likewise smooth and bounded in the vicinity of x_b . Now consider integrating each side of the continuity equation near x_b ,

$$\int_{x_b - \varepsilon}^{x_b + \varepsilon} \partial_t p \, dx = - \int_{x_b - \varepsilon}^{x_b + \varepsilon} \partial_x J \, dx = J(x_b - \varepsilon, t) - J(x_b + \varepsilon, t)$$

Deriving BCs III

Since $\partial_t p$ is bounded near x_b , it follows that

$$\int_{x_b - \varepsilon}^{x_b + \varepsilon} \partial_t p \, dx \leq 2\varepsilon \sup_{|x - x_b| \leq \varepsilon} |\partial_t p(x, t)|,$$

and hence vanishes in the limit as $\varepsilon \rightarrow 0$ so we find that the (generalized) current itself is continuous across the boundaries, in the sense that $J(x_b^-, t) = J(x_b^+, t)$. If we are to consider instead the spatial derivatives of the piecewise probability, Eq. (10), we find

$$\partial_x^2 p = \partial_x^2 p_l \Theta(x_b - x) + \partial_x^2 p_r \Theta(x - x_b) + [\partial_x p] \delta(x - x_b) + [p] \delta'(x - x_b),$$

where $[p] = p_r(x_b^+, t) - p_l(x_b^-, t)$. Returning to the diffusion portion of the generator in Eq. (2), we expand as

$\partial_x (D \partial_x p) = (\partial_x D)(\partial_x p) + D \partial_x^2 p$. The first term does not give rise to any δ' terms, since $\partial_x D \sim \delta(x - x_b)$.

Deriving BCs IV

As for the second, we see that it amounts to $D(x_b)[p]\delta'(x - x_b)$. But then it must be that this term equals the two terms proportional to δ' in Eq. (2), amounting to the self-consistency relation

$$D(x_b) (p_r(x_b^+, t) - p_l(x_b^-, t)) = (4\lambda - 1)\varsigma p(x_b, t) - D_r^2 \nu_r \frac{\partial p(x_b, t)}{\partial x}.$$

The left-hand side is defined in terms of the constructed, piecewise functions Eq. (10) whereas the right is the density derived from the master. The precise interpretation of this condition depends upon how one is to understand the behaviour at the membrane $x = x_b$; typically each of D , p and $\partial_x p$ are understood as some linear combination of the left and right limits of their respective functions. Note that, independent of interpretation, we correctly observe reduction to the “leather boundary condition”² when $D_r = D_l$.

Deriving the distribution identity

We show here the distribution identity

$$\delta'(x - a)f(a) = \delta'(x - a)f(x) + \delta(x - a)\partial_x f(x),$$

for a test function f used in the derivation of the FPE formulation of the problem. Consider another test function φ ,

$$\langle \delta'_a f(a), \varphi \rangle = f(a) \langle \delta'_a, \varphi \rangle = -f(a) \varphi'(a).$$

As for the right-hand side,

$$\langle \delta'_a f + \delta_a f', \varphi \rangle = \langle (\delta_a f)', \varphi \rangle = -\langle \delta_a, f \varphi' \rangle = -f(a) \varphi'(a),$$

as required.