From Diffusion to Membrane Potential: A Progressive Simulation Framework for Teaching Electrochemical Signalling and Dynamical Systems in Computational Neuroscience

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Abstract

Students are commonly introduced to membrane potential through equilibrium equations before developing an intuitive understanding of the underlying mechanisms that give rise to electrochemical signalling. This often leads to procedural understanding without conceptual insight. This paper presents a pedagogical framework that introduces membrane potential through a sequence of progressively constrained particle-based simulations. The framework is designed for undergraduate computational neuroscience teaching and simultaneously introduces diffusion, selective permeability, electrochemical forces, dynamical systems, and numerical integration via Euler updates. The simulations are intentionally simplified and serve as conceptual models rather than biophysically accurate representations. The approach allows students to observe how membrane potential emerges from interacting dynamical processes before formal exposure to equilibrium equations or conductance-based neuron models. All accompanying code is provided in an openly available repository to support reuse and adaptation in teaching contexts.

Introduction and Pedagogical Framework

Membrane potential is a foundational concept in neuroscience and physiology, underpinning neuronal signalling, synaptic transmission, and action potential generation. Despite its importance, students are frequently introduced to membrane potential through equilibrium equations such as the Nernst equation or the Goldman–Hodgkin–Katz (GHK) equation before developing an intuitive understanding of the underlying mechanisms. While mathematically precise, this approach often leads to procedural competence without conceptual insight, as students learn to apply equations without understanding how voltage differences emerge from ion movement.

A central instructional difficulty arises from the gap between microscopic processes and macroscopic descriptions. Diffusion, selective permeability, and electrical forces operate simultaneously and interactively, yet traditional instruction often presents them in isolation or only at equilibrium.

Students therefore encounter membrane potential as a static property rather than as the result of interacting dynamical processes. This difficulty is compounded in computational neuroscience education, where students are also required to understand dynamical systems and numerical integration methods before developing intuition about how simple update rules produce behaviour over time.

The framework presented here addresses these challenges through a sequence of progressively constrained particle-based simulations designed to introduce electrochemical signalling as an emergent dynamical phenomenon. Rather than beginning with analytical expressions, the approach allows students to observe how diffusion, spatial constraints, selective permeability, and electrical forces combine to produce stable charge imbalances across a membrane-like boundary. Formal equations can then be introduced as compact descriptions of behaviour that students have already observed.

The instructional design is guided by three principles. First, new mechanisms are introduced incrementally. Each stage of the progression adds a single additional constraint or force while preserving previously introduced dynamics, allowing students to attribute changes in system behaviour to identifiable causes. Second, visual intuition precedes formalism. Animated particle motion provides a concrete representation of otherwise abstract processes, reducing cognitive load and supporting causal reasoning. Third, numerical methods are introduced implicitly through physical interpretation. All simulations evolve according to simple Euler-style updates,

$$x_{t+1} = x_t + f(x_t)\Delta t, \tag{1}$$

allowing students to encounter time-stepped dynamical systems in an intuitive setting prior to formal exposure to differential equations.

The simulations are intentionally simplified and do not aim to reproduce the biophysical accuracy of real membranes. Instead, they function as conceptual models that highlight causal relationships between diffusion, permeability, and electrical forces. Within this framework, membrane potential is presented not as an imposed property but as a stable outcome emerging from interacting dynamical processes.

Simulation Progression

The instructional sequence consists of several stages, each introducing one additional physical principle.

Diffusion as a Dynamical Process

The initial simulation introduces diffusion as a stochastic dynamical system in which particles undergo Brownian motion in two spatial dimensions. Each particle is described by a state vector containing its position,

$$\mathbf{x}_i(t) = \begin{bmatrix} x_i(t) \\ y_i(t) \end{bmatrix}, \tag{2}$$

and the system evolves through time according to random increments drawn from a zero-mean Gaussian distribution. The resulting motion corresponds to a discrete approximation of a diffusion process in which spatial distributions spread over time without directional bias.

The update rule for each particle can be written as

$$x_i(t + \Delta t) = x_i(t) + \sigma\, \eta_x \sqrt{\Delta t}, \tag{3}$$

$$y_i(t + \Delta t) = y_i(t) + \sigma\, \eta_y \sqrt{\Delta t}, \tag{4}$$

where η_x and η_y are independent samples from a standard normal distribution and σ controls the diffusion strength. In continuous time, this corresponds to a stochastic differential equation of the form

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{\xi}(t), \tag{5}$$

where $\boldsymbol{\xi}(t)$ represents temporally uncorrelated noise.

From a dynamical systems perspective, the simulation introduces three core ideas. First, the system possesses a state that evolves over time. Second, the future state depends only on the current state and an update rule. Third, complex macroscopic behaviour (spatial spreading) emerges from repeated application of simple local updates.

The numerical implementation follows a simple Euler-style update in which the state at the next timestep is computed directly from the current state and a change term. In pseudocode, the update rule can be expressed as:

```
for each timestep t:
    for each particle i:
        dx <- random_normal(0, sigma)
        dy <- random_normal(0, sigma)

        x[i] <- x[i] + dx * dt
        y[i] <- y[i] + dy * dt
```

At this stage no biological interpretation is introduced. The goal is to establish an intuitive understanding of diffusion as a dynamical process and to familiarize students with state variables, time evolution, and numerical integration before additional forces or constraints are introduced in later stages of the progression.

It should be noted that the diffusion process implemented here is a simplified phenomenological model rather than a physically complete description of molecular motion. The random increments

represent the net effect of many microscopic collisions and are chosen for conceptual clarity rather than biophysical accuracy. Spatial and temporal scales are therefore arbitrary, and no attempt is made to match physical diffusion constants. These simplifications are intentional, allowing students to focus on the dynamical principles of state evolution and stochastic change before additional biological constraints are introduced in later stages.

Diffusion Through Spatial Constraints

The second stage introduces spatial constraints by separating the environment into two compartments divided by a wall containing a narrow opening (channel). Particle motion remains purely diffusive, but movement between compartments is restricted by geometry. This allows students to observe how structural constraints alone can regulate transport without introducing new forces or changes to the underlying diffusion process.

The dynamical update rule from the previous section remains unchanged,

$$x_i(t + \Delta t) = x_i(t) + \sigma\, \eta_x \sqrt{\Delta t}, \tag{6}$$

$$y_i(t + \Delta t) = y_i(t) + \sigma\, \eta_y \sqrt{\Delta t}, \tag{7}$$

but an additional boundary condition is introduced. If a particle attempts to cross the separating wall outside the channel region, the attempted movement is rejected and the particle remains on its previous side. Formally, this can be written as

$$x_i(t + \Delta t) = \begin{cases} x_i(t), & \text{if crossing outside channel} \\ x_i(t + \Delta t), & \text{otherwise.} \end{cases} \tag{8}$$

From a dynamical systems perspective, this stage introduces the idea that system behaviour can change not only through forces but also through constraints on state transitions. The underlying stochastic dynamics remain identical, yet the macroscopic behaviour differs because certain transitions between states are no longer permitted.

In pseudocode, the update rule becomes:

```
for each timestep t:
    for each particle i:
        dx <- random_normal(0, sigma)
        dy <- random_normal(0, sigma)

        new_x <- x[i] + dx * dt
        new_y <- y[i] + dy * dt

        if crossing_wall(new_x) and not in_channel(y[i]):
            new_x <- x[i]

        x[i] <- new_x
        y[i] <- new_y
```

This stage introduces the important pedagogical idea that permeability can arise from geometry alone. Particles do not change how they move locally; instead, the environment constrains which movements are allowed globally. This provides an intuitive foundation for later introduction of selective ion channels.

As in the previous section, the environment is intentionally simplified. Boundaries are treated as perfectly reflecting outside the channel, and no interactions between particles are included. The goal is not to model physical membrane structure accurately, but to isolate the effect of spatial constraints on diffusive transport before additional mechanisms are introduced.

Channel width is used as a proxy for permeability, representing the probability that a particle undergoing diffusion both encounters and successfully traverses a pathway across the membrane. From a physical perspective, permeability here combines geometric accessibility with an implicit transmission probability, analogous to coarse-graining the effects of diffusive encounter rate, pore accessibility, and passage energetics into a single effective parameter. The model therefore does not attempt to represent the microscopic structure or electrostatic selectivity of biological ion channels, but instead captures the macroscopic consequence that increased permeability corresponds to an increased flux for a given concentration difference.

Selective Permeability

The next stage extends the constrained diffusion model by introducing multiple particle types that experience different permeability through the separating membrane. Particles continue to undergo identical diffusive motion, but each type is restricted to a distinct channel region. This introduces selective permeability without introducing additional forces, allowing students to observe how differential transport can arise purely from constraints on allowed state transitions.

The dynamical update rule for particle motion remains unchanged,

$$x_i(t + \Delta t) = x_i(t) + \sigma\, \eta_x \sqrt{\Delta t}, \tag{9}$$

$$y_i(t + \Delta t) = y_i(t) + \sigma\, \eta_y \sqrt{\Delta t}, \tag{10}$$

but the boundary condition now depends on particle type. Let s_i denote the species identity of particle i, and let the allowed channel region for that species be defined by the interval $[y_{\min}^{(s_i)}, y_{\max}^{(s_i)}]$. A crossing attempt is permitted only if

$$y_i(t) \in [y_{\min}^{(s_i)}, y_{\max}^{(s_i)}]. \tag{11}$$

Otherwise, the attempted transition is rejected and the particle remains in its previous position along the constrained axis.

From a dynamical systems perspective, this stage demonstrates that system behaviour may differ between state variables that evolve under identical local rules. The stochastic motion governing individual particles is unchanged, yet macroscopic transport differs because accessibility of state transitions is now species-dependent. This provides an intuitive analogue of ion-selective membrane channels, in which permeability differs between ion species despite similar underlying thermal motion.

In pseudocode, the update rule becomes:

```
for each timestep t:
    for each particle i:
        dx <- random_normal(0, sigma)
        dy <- random_normal(0, sigma)

        new_x <- x[i] + dx * dt
        new_y <- y[i] + dy * dt

        if crossing_wall(new_x) and
           not in_channel(y[i], species[i]):
            new_x <- x[i]

        x[i] <- new_x
        y[i] <- new_y
```

Pedagogically, this stage introduces the central biological idea that membrane transport can differ between species even when underlying motion is governed by the same physical processes. Differences in permeability therefore arise from constraints on allowed transitions rather than differences in diffusive behaviour itself.

As in previous sections, the representation is intentionally simplified. Selectivity is implemented geometrically rather than through energetic or electrostatic mechanisms, and channel width serves

as a coarse-grained proxy for permeability. The goal is to isolate the functional consequence of selective transport before introducing electrochemical forces in the following stage.

Electrochemical Drift

The next stage introduces electrical forces as a directional bias on otherwise diffusive motion. Particles continue to undergo stochastic Brownian motion, but their movement is now additionally influenced by an attractive or repulsive interaction with a charged region. This allows students to observe how deterministic forces interact with stochastic dynamics to produce directed transport.

The dynamical update rule is extended by adding a drift term to the diffusive update. Let $\mathbf{x}_i(t)$ denote the position of particle i, and let $\mathbf{x}_q$ denote the position of a fixed charge source. The update rule becomes

$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \sigma\boldsymbol{\eta}\sqrt{\Delta t} + \mathbf{F}(\mathbf{x}_i)\Delta t, \tag{12}$$

where $\boldsymbol{\eta}$ is a vector of independent Gaussian random variables and $\mathbf{F}(\mathbf{x}_i)$ represents a position-dependent drift term. In the present model, the drift is implemented as a distance-normalized attraction or repulsion,

$$\mathbf{F}(\mathbf{x}_i) = k\frac{\mathbf{x}_q - \mathbf{x}_i}{\|\mathbf{x}_q - \mathbf{x}_i\|}, \tag{13}$$

where k controls the strength of the electrical influence.

From a dynamical systems perspective, this stage introduces the important idea that system evolution may arise from the combination of stochastic and deterministic components. Diffusion alone produces unbiased spreading, whereas the addition of a drift term produces net flux even in the presence of random motion. Students therefore observe how directional behaviour can emerge without removing stochastic variability.

In pseudocode, the update rule becomes:

```
for each timestep t:
    for each particle i:
        dx_noise <- random_normal(0, sigma)
        dy_noise <- random_normal(0, sigma)

        force <- electric_force(position[i])

        new_x <- x[i] + (dx_noise + force.x) * dt
        new_y <- y[i] + (dy_noise + force.y) * dt

        apply_boundary_conditions()

        x[i] <- new_x
        y[i] <- new_y
```

Pedagogically, this stage introduces the concept of electrochemical gradients as the interaction between random thermal motion and directional forces. Rather than presenting electrical influence as an abstract potential, students observe how local update rules produce macroscopic transport behaviour over time.

The electrical interaction implemented here is intentionally simplified. The force term is not derived from a self-consistent electrostatic field and does not model charge redistribution within the medium. Instead, it provides a conceptual representation of how electrical forces bias diffusion, allowing the role of drift in electrochemical transport to be introduced before more complex multi-ion interactions are considered.

Multiple Ion Species and Emergent Membrane Potential

The final stage of the progression combines selective permeability and electrochemical drift by introducing multiple particle species with different charge signs and unequal permeability. Particles continue to evolve according to the same underlying dynamical rule, but now experience competing influences arising from diffusion, electrical drift, and species-dependent access to the membrane channel. This interaction produces a stable imbalance between compartments that serves as a qualitative analogue of membrane potential.

The dynamical update rule extends the previous formulation by allowing the drift term to depend on particle charge. Let $q_i \in \{-1, +1\}$ denote the charge associated with particle i. The update rule becomes

$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \sigma\boldsymbol{\eta}\sqrt{\Delta t} + q_i\mathbf{F}(\mathbf{x}_i)\Delta t, \tag{14}$$

where particles of opposite charge experience drift in opposite directions. Channel accessibility continues to depend on particle species as described in the previous section.

When multiple species are present simultaneously, particles that preferentially move in opposite

directions compete for access to the membrane channel. Over time, this competition produces a steady state in which diffusive motion and electrical drift balance one another. The system no longer evolves toward uniform spatial mixing, but instead approaches a stable configuration in which net flux across the membrane is approximately zero despite ongoing particle motion.

From a dynamical systems perspective, this stage introduces the concept of an emergent equilibrium or attractor. The steady state is not imposed externally but arises from the interaction of previously introduced mechanisms. Students therefore observe how stable macroscopic behaviour can emerge from continuous microscopic dynamics.

In pseudocode, the update rule becomes:

```
for each timestep t:
    for each particle i:
        dx_noise <- random_normal(0, sigma)
        dy_noise <- random_normal(0, sigma)

        force <- electric_force(position[i])

        new_x <- x[i] + (dx_noise + charge[i]*force.x) * dt
        new_y <- y[i] + (dy_noise + charge[i]*force.y) * dt

        apply_species_specific_channel_rules()

        x[i] <- new_x
        y[i] <- new_y
```

To provide a measurable quantity analogous to membrane potential, a simple proxy is introduced based on the net charge imbalance between compartments. Although this measure does not represent physical voltage, it allows students to observe how unequal permeability and opposing drift directions produce a stable charge difference across the membrane.

The model remains intentionally simplified. Real biological membranes maintain near electroneutrality in bulk solution, with voltage arising from charge separation confined to a thin region near the membrane surface. In contrast, the present simulations allow compartment-wide charge imbalance for pedagogical clarity. The goal is to illustrate how permeability-weighted ion movement gives rise to stable electrochemical states before introducing formal equilibrium descriptions such as the Nernst or Goldman–Hodgkin–Katz equations.

Instructional Context

The simulation framework is used within an undergraduate computational neuroscience unit as a mechanism for revisiting electrochemical signalling that students were previously introduced to in an earlier introductory neuroscience course. In the introductory setting, membrane potential is

presented through conceptual diagrams and textbook explanations typical of first-year neuroscience instruction. In the later computational neuroscience unit, the same biological concepts are revisited through a progression of simulations that reframe membrane potential as the outcome of interacting dynamical processes.

This progression serves two instructional purposes. First, it reinforces prior biological knowledge by providing a mechanistic interpretation of electrical signalling in nerve cells. Second, it introduces students to dynamical systems thinking through a familiar biological example. Rather than encountering dynamical systems as abstract mathematical objects, students observe how system state evolves through iterative update rules and how stable behaviour emerges from competing processes over time.

In this way, the simulations function as a bridge between qualitative biological explanations and computational modelling of physical systems more broadly. Students encounter state variables, time evolution, and steady-state behaviour in a visually interpretable context, which supports later formal introduction of differential equations and Euler integration as mathematical descriptions of system dynamics.

All simulation code is provided in an openly available companion repository located here:
https://github.com/crossley/crossleylab/tree/main/code/electrochemical_signals_progression

This allows instructors to adapt the materials for lecture demonstrations, laboratory exercises, or computational assignments.

Limitations

The simulations presented in this work are intentionally simplified and are not intended as biophysically accurate models of membrane electrophysiology. Their purpose is pedagogical: to isolate and visually demonstrate the causal relationships between diffusion, selective permeability, and electrical influences in a form that supports conceptual understanding of dynamical processes.

Several simplifying assumptions are particularly important. First, the simulations permit net charge imbalance across entire compartments, whereas real biological systems maintain near electroneutrality in bulk solution. In biological membranes, voltage arises from charge separation confined to a thin region near the membrane surface rather than from large-scale redistribution of charge throughout intracellular or extracellular space. Allowing compartment- wide imbalance in the present model makes the emergence of stable states more visually apparent but exaggerates the spatial scale at which charge separation occurs.

Second, electrical forces are implemented as externally specified drift terms rather than being derived from self-consistent electrostatic fields. The model does not include field generation from charge redistribution, ionic screening, or spatial variation in electric potential. The electrical interaction should therefore be interpreted as a conceptual bias on diffusive motion rather than a solution to Poisson-type field equations.

Third, channel selectivity is represented geometrically through channel width, which serves as a coarse-grained proxy for permeability. In biological ion channels, permeability arises from a combination of structural constraints, electrostatic interactions, and energetic selectivity. The present representation intentionally compresses these mechanisms into a single effective parameter in order to isolate their macroscopic consequences for transport.

These simplifications are deliberate and reflect the instructional goal of introducing dynamical intuition before physical realism. More detailed biophysical models, including conductance-based descriptions and self-consistent electrical dynamics, can be introduced subsequently once students have developed an understanding of how membrane potential emerges from interacting dynamical processes.

Conclusion

This paper presents a progressive simulation framework for teaching electrochemical signalling and membrane potential through dynamical intuition. By introducing diffusion, spatial constraints, selective permeability, and electrical drift incrementally, the framework allows students to observe how stable electrochemical behaviour emerges from simple update rules. Membrane potential is therefore encountered as the outcome of interacting dynamical processes rather than as a quantity defined solely by equilibrium equations.

The approach addresses a common instructional challenge in neuroscience education, namely the introduction of analytical descriptions prior to mechanistic understanding. By reversing this order and emphasizing visual and computational intuition, students develop a causal understanding of how permeability and electrochemical forces give rise to stable states. This provides a foundation upon which formal treatments, including Nernst and Goldman–Hodgkin–Katz descriptions and conductance-based neuron models, can be introduced more effectively.

Beyond its biological application, the framework provides a natural entry point to dynamical systems thinking and computational modelling of physical systems. Students encounter state evolution, steady states, and iterative numerical updates in a concrete setting before engaging with formal mathematical representations. In this way, the progression supports both neuroscience and computational learning objectives.

The simulations are intended as complementary teaching tools rather than replacements for analytical approaches. When integrated with traditional instruction, they provide an intuitive bridge between qualitative explanation and quantitative modelling, supporting deeper conceptual understanding of electrochemical signalling in nerve cells.