

# Understanding Emergent Dynamics through Modeling, Learning and Analysis

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November 25, 2025

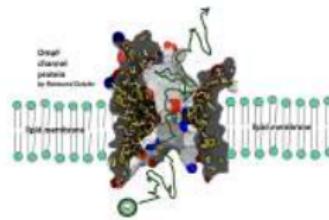
# Introduction

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# Motivation: Complex Dynamics



(a) Fish Milling



(b) Ion Transport

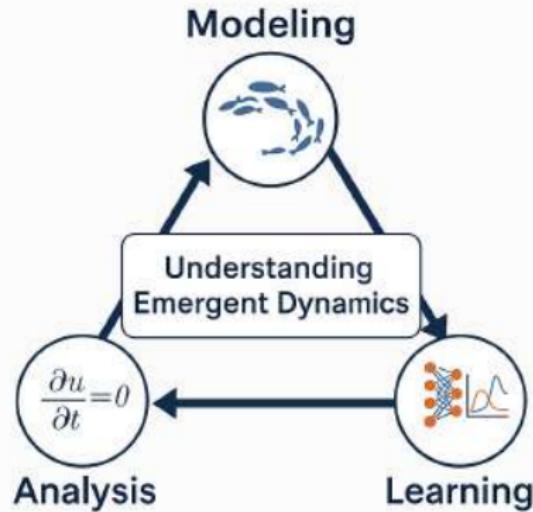


(c) Urban Crime

**Figure:** Complex dynamics arise from local interactions

# Motivation

- *What mechanisms generate complex behavior?*
- *How can we infer the underlying interaction laws from observations?*
- *How can we provide theoretical guarantees for the resulting models?*



# Outline

- 1 Introduction
- 2 Part I – Modeling
  - Synchronization and Swarming
  - Urban Crime Simulation
- 3 Part II – Learning
  - Learning Kernels
- 4 Part III – Analysis
  - Stability in Training PINNs
  - Ion transport: PNP
- 5 Synthesis and Outlook

# Part I – Modeling

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*Explain how local interactions create global patterns*

# Synchronization and Swarming

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*Patterns from phase-space coupling*

# Swarmalator Model <sup>1</sup>

*How simple “phase + spatial” interactions generate surprising states?*

$$\begin{aligned}\dot{x}_i &= \nu + \frac{J_i}{N} \sum_j^N \sin(x_j - x_i) \cos(\theta_j - \theta_i), \\ \dot{\theta}_i &= \omega + \frac{K_i}{N} \sum_j^N \sin(\theta_j - \theta_i) \cos(x_j - x_i), \quad (x_i, \theta_i) \in (\mathbb{S}^1, \mathbb{S}^1).\end{aligned}\tag{1}$$

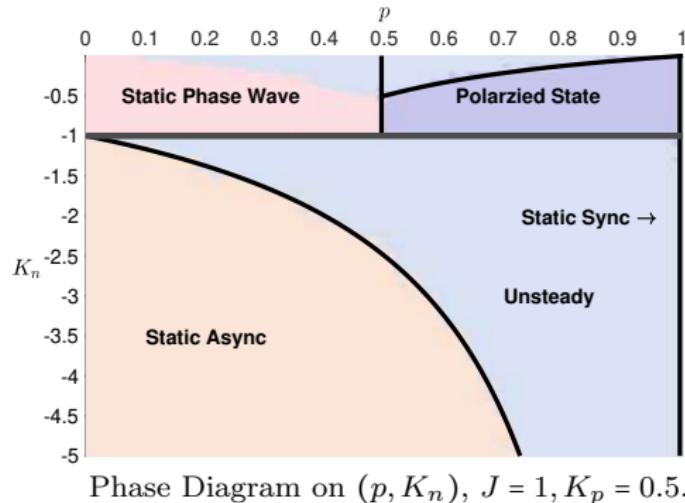
- Real systems couple **motion** and **phase dynamics** (cells, robots, etc.).
- $x_i$ -eq: attraction–repulsion forces (spatial swarming);  
 $\theta_i$ -eq: Kuramoto phase coupling (phase synchronization).
- $(\nu, \omega)$ : constant natural frequencies;  $(J_i, K_i)$ : couplings constants.
- Simple pairwise rules: interaction strength depends on **phase/spatial similarity**.
- **Minimal model** for exploring phase–spatial coupling and new emergent behaviors.
- **Energy:**  $E = -\frac{A}{2N} \sum_{i,j} \cos(x_j - x_i) \cos(\theta_j - \theta_i)$ , when  $\nu = \omega = 0$ ,  $J = K = A$ .
  - gradient flow:  $\dot{x}_i = -\frac{\partial E}{\partial x_i}$  ,  $\dot{\theta}_i = -\frac{\partial E}{\partial \theta_i}$ .

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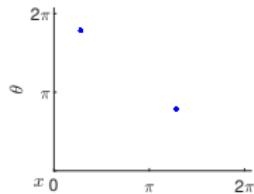
<sup>1</sup> O’Keeffe et al., 2017, *Nature communications*.

# Positive-attractive and Negative-repulsive Couplings

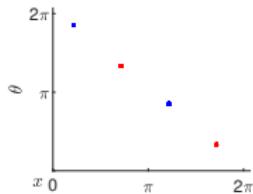
- Set  $J = 1$  and draw the phase coupling  $K$  from
  - 1  $h(K) = p\delta(K - K_p) + q\delta(K - K_n)$ , where  $p + q = 1$ ,  $K_p > 0$  and  $K_n < 0$
  - 2 Single Gaussian Distribution:  $h(K) \sim \mathcal{N}(\mu, \sigma|K)$
  - 3 Mixed Gaussian Distribution:  $h(K) \sim p\mathcal{N}(K_n, \sigma|K) + (1 - p)\mathcal{N}(K_p, \sigma|K)$
- **Linear Stability Analysis:** compute the Jacobian matrix to determine local stability via eigenvalue analysis.
- **Numerical Simulation:**  $W_{\pm} = S_{\pm} e^{-i\phi_{\pm}} := \frac{1}{N} \sum_{j=1}^N e^{i(x_j \pm \theta_j)}$  and  $V := \frac{1}{N} \sum_{j=1}^N \langle |\dot{x}_j| \rangle_t$ .



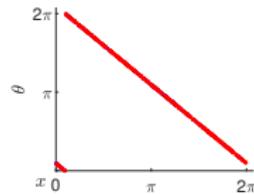
# Behavior and Pattern<sup>2</sup>



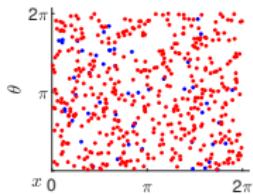
(a) Synchrony



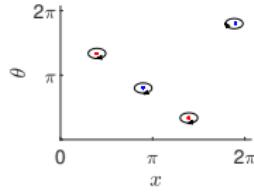
(b) Polarized State



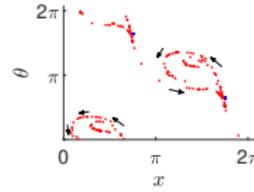
(c) Phase Wave



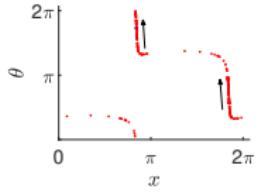
(d) Asynchrony



(e) Breathing



(f) Swirling



(g) Active Bands

**Figure:** Top row: Steady States. Bottom Row: Unsteady States. Swarmalators coupling with  $K_p$  and  $K_n$  are presented as blue dots and red dots, respectively.

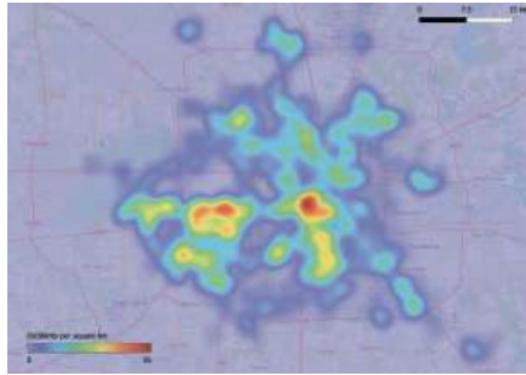
<sup>2</sup>Hao et al., 2023, *Physical Review E*.

# Urban Crime Simulation

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*From agent rules to city-scale hotspot patterns*

# Motivation & Contributions



*How local criminal decision-making and environmental factors generate city-scale crime patterns?*

## Goal

Build a **realistic, efficient, FEM framework** for burglary dynamics.

### Why agent-based model?

- Offender movement and burglary decisions are **probabilistic**
- ABM capture individual behavior

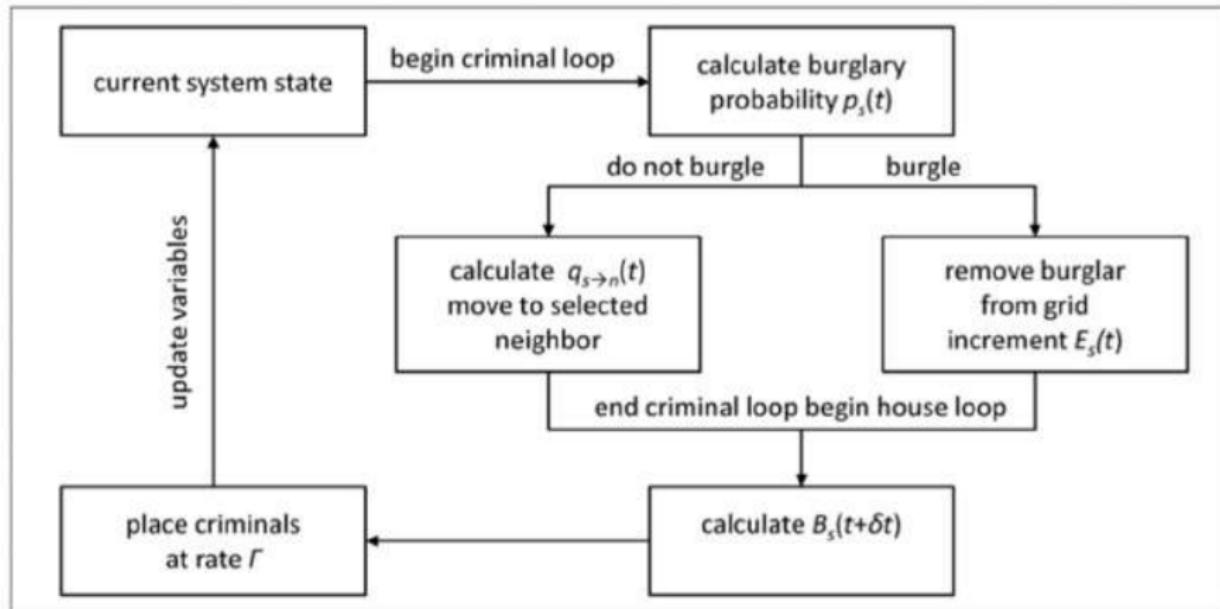
### Why PDE?

- Too many agents  $\Rightarrow$  expensive, noisy
- Hard to predict long-term patterns
- Large populations  $\Rightarrow$  **mean-field limit**: describing **aggregation**
- PDE reveals macroscopic mechanisms of hotspot formation

### Why Natural BCs & FEM?

- Offenders do not "wrap around" the domain
- Realistic city shapes, heterogeneous parameters
- Natural BCs enforced naturally

# Models<sup>3</sup>



<sup>3</sup>Short et al., 2008, *Mathematical Models and Methods in Applied Sciences*.

# Models

- Agent-based Model:

$$B_s(t + \Delta t) = \left[ (1 - \eta)B_s(t) + \frac{\eta}{4} \sum_{s' \sim s} B_{s'}(t) \right] (1 - \omega \Delta t) + \theta E_s(t)$$

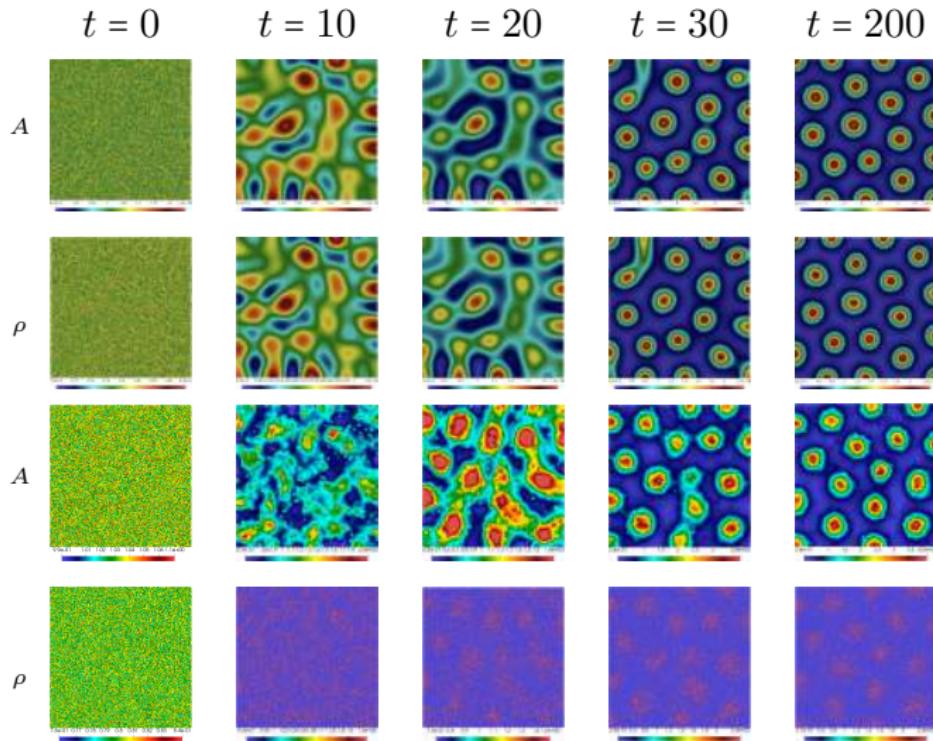
$$n_s(t + \Delta t) = A_s \sum_{s' \sim s} \frac{n_{s'}(t)[1 - p_{s'}(t)]}{T_{s'}(t)} + \Gamma \Delta t, \quad T_{s'}(t) = \sum_{s'' \sim s'} A_{s''}(t).$$

- $B_s$ : attractiveness at site  $s$ ;  $n_s$ : number of criminals at site  $s$ ;  $\Gamma$ : burglars generation rate;  $\theta$ : increase in attractiveness due to one burglary event;  $\omega$ : dynamic attractiveness decay rate;  $E_s(t)$  is the number of burglary events that occurred at site  $s$  during the time interval beginning at time  $t$ ;  $p_s(t) = 1 - e^{-A_s(t)\Delta t}$ : burglary probability.
- PDE Model (dimensionless mean-field limit):

$$\frac{\partial A}{\partial t} - \eta \Delta A + A - \rho A = -\eta \Delta A^{st} + A^{st}, \quad \frac{\partial \rho}{\partial t} - \nabla \cdot \left( \nabla \rho - \frac{2 \nabla A}{A} \rho \right) + \rho A = \frac{\Gamma \theta}{\omega^2}.$$

- $A = B + A^{st}$ ;  $\rho$ : density of criminals.
- $\eta$ : measures the significance of neighborhood effects;  $\frac{\Gamma \theta}{\omega^2}$ : influx of criminals.

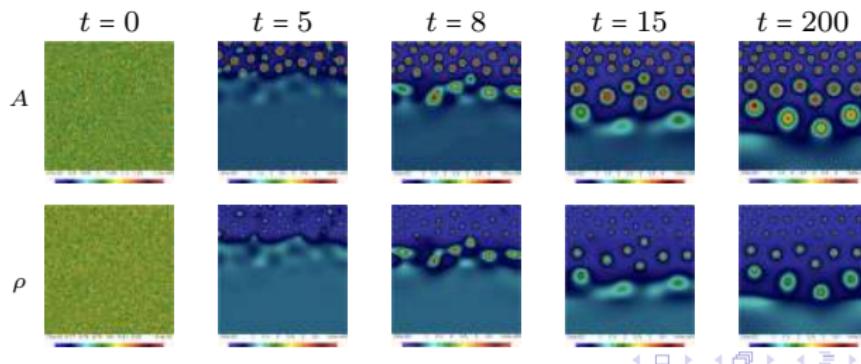
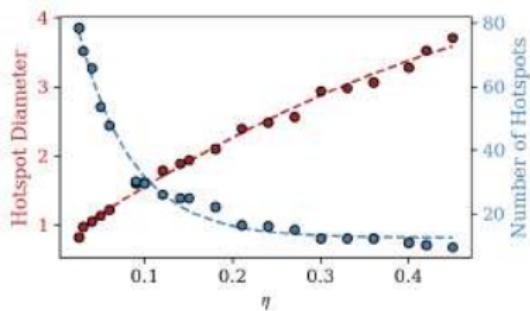
# FEM Framework and Patterns<sup>4</sup>



<sup>4</sup>Hao et al., 2025, *Mathematical Models and Methods in Applied Sciences*.

# How parameters affect the pattern?

- $\eta \in [0, 1]$  : measures the significance of neighborhood effects
- $\frac{\Gamma\theta}{\omega^2}$  : influx of criminals



# Robustness and Validation

$(h, \Delta t)$	Case 1			Case 2			Case 3		
	$10^{-3}$	$10^{-6}$	$10^{-9}$	$10^{-3}$	$10^{-6}$	$10^{-9}$	$10^{-3}$	$10^{-6}$	$10^{-9}$
$(\frac{16}{400}, \frac{1}{100})$	1.01	1.10	1.14	1.02	1.67	2.65	1.04	2.73	4.88
$(\frac{16}{200}, \frac{1}{50})$	1.01	1.11	1.26	1.04	1.89	2.96	1.08	3.06	5.93
$(\frac{16}{100}, \frac{1}{25})$	1.02	1.13	1.31	1.07	2.11	3.39	1.17	3.16	6.04
$(\frac{16}{100}, \frac{2}{25})$	1.03	1.15	1.38	1.11	2.34	4.17	-	-	-

**Table:** Average number of iterations over time required by the iterative splitting algorithm to meet the stopping crieterion with  $\text{tol}_1 = \text{tol}_2 = 10^{-3}, 10^{-6}, 10^{-9}$  for the three cases with different values of mesh size  $h$  and time step  $\Delta t$ .

# Spatial Heterogeneity & Complex Geometry

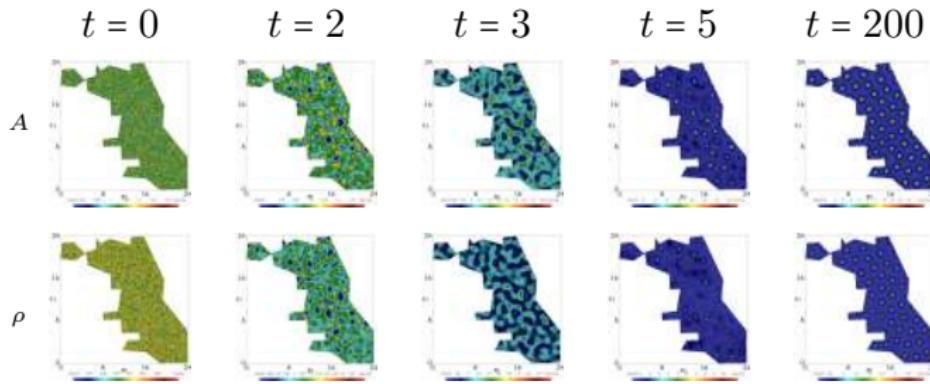


Figure: Chicago Simulation

Highway I-90 Animation:

$$A^{st}(\mathbf{x}) = \frac{1}{30} \cdot \exp\{-20 * (x_0 + x_1 - l)^2\} \cdot \left( x_0 > \frac{l}{2} \text{ } \& \text{ } x_1 < \frac{l}{2} \right) + \frac{1}{30} \cdot \chi_1(\mathbf{x}),$$

$$\frac{\Gamma(\mathbf{x})\theta}{\omega^2} = B_0(\mathbf{x}) = \exp\{-20 * (x_0 + x_1 - l)^2\} \cdot \left( x_0 > \frac{l}{2} \text{ } \& \text{ } x_1 < \frac{l}{2} \right) + 1 \cdot \chi_{0.1}(\mathbf{x}).$$

<https://github.com/baolihao/UrbanCrime-Sim>

# Part II – Learning

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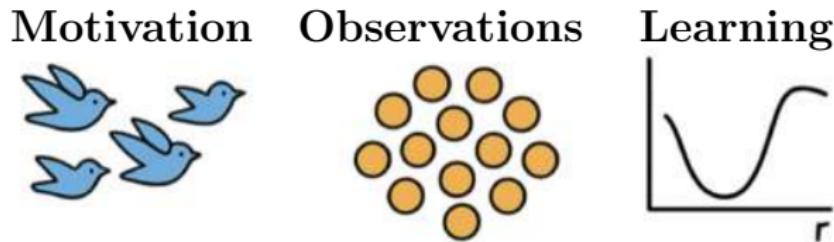
*Learn the hidden rules and dynamical laws from data*

# Learning Kernels

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*Recovering interaction laws from steady states*

# Motivation



- Many complex systems (flocking, swarming, opinion dynamics) evolve according to **unknown interaction laws**.
- Existing methods require **time-series data, large samples**, or assume simple parametric forms<sup>5</sup>.
- **Limited data:** We have only **steady-state snapshots** rather than full trajectories.
- **Highly underdetermined:** forces cancel out, time-scale disappears, and the system becomes **ill-conditioned**.
- Goal: develop a **robust, data-efficient framework** that can recover interaction laws **from a single steady-state snapshot**.

<sup>5</sup>Lu et al., 2019, *Proceedings of the National Academy of Sciences*.

# Problem Setup

- The first-order dynamics:

$$\dot{\mathbf{x}}_i = \sum_{j \neq i}^N \frac{1}{N} \phi^E(|\mathbf{x}_j - \mathbf{x}_i|) (\mathbf{x}_j - \mathbf{x}_i). \quad (2)$$

- The second-order dynamics:

$$\begin{cases} \dot{\mathbf{x}}_i &= \mathbf{v}_i, \\ \dot{\mathbf{v}}_i &= \sum_{j \neq i}^N \frac{1}{N} \left( \phi^E(|\mathbf{x}_j - \mathbf{x}_i|) (\mathbf{x}_j - \mathbf{x}_i) + \phi^A(|\mathbf{x}_j - \mathbf{x}_i|) (\mathbf{v}_j - \mathbf{v}_i) \right). \end{cases} \quad (3)$$

- Given: A set of single-time snapshots at steady state  $\{\mathbf{x}_{i,T_m}^m\}_{i,m=1}^{N,M}$  or  $\{\mathbf{x}_{i,T_m}^m, \mathbf{v}_{i,T_m}^m\}_{i,m=1}^{N,M}$ .
- Goal: Learn  $\phi^E$  or  $\phi^A$  to get approximated  $\hat{\phi}^E$  or  $(\hat{\phi}^E, \hat{\phi}^A)$ .

# Learning Framework

## Nonlinear Interaction Dynamics

$$0 = \sum_{j \neq i} \phi(r_{ij}) \mathbf{r}_{ij}$$



## Finite-Dimensional Representation of Kernel

$$\phi(r) \approx \sum_k \alpha_k \psi_k(r)$$



## Linear System at Steady State

$F(\alpha; \mathbf{x}) = A(\mathbf{x})\alpha = 0$ ,  $F$ : a **rank-deficient linear operator**



## Nullspace / Eigenstructure Extraction

**Ill-conditioning:**  $F(C\alpha; \mathbf{x}) = F(\alpha; \mathbf{x}) = 0, \forall C \in \mathbb{R}$



## Scaling Recovery (Time-Scaling or Energy)

Determine physical scale  $C$  of  $\hat{\phi}$ :  $\phi \sim C\hat{\phi}$

# Ill-conditioning & Regularization

At steady state:

$$\sum_{j \neq i} \phi(|\mathbf{x}_j - \mathbf{x}_i|) (\mathbf{x}_j - \mathbf{x}_i) = 0.$$

**Ill-conditioning:** Steady-state equations do not contain enough information to uniquely determine  $\phi$  without **additional constraints or scaling information**.

- **Empirical Distribution Regularization (and Learnability Check):**

$$\rho_T(r) = \mathbb{E}[\delta_{r_{i,j,T}}(r)], \quad r_{i,j,T} = |\mathbf{x}_{j,T} - \mathbf{x}_{i,T}|.$$

→  $\rho_T$  is not learnable when the geometry of the steady-state distribution does not produce enough linear constraints on  $\phi$  (Identifiability requires  $\dim \ker F \leq 1$ ).

- **Minimal Energy Direction (Crucial Missing Information):**

For gradient-flow dynamics, true steady states are **energy minimizers**:

$$E = \frac{1}{N} \sum_{i < j} U(|\mathbf{x}_j - \mathbf{x}_i|), \quad U'(r) = r \phi(r).$$

This provides the **missing information (but available)** to select the correct  $\phi$ .

→ Combined with  $\nabla E = 0$ , if the learned  $\phi$  increases  $E$ , flip its sign:  $\phi \leftarrow -\phi$ .

- **Time-scale Recovery:**

If one trajectory or a steady-state time  $T_m$  is known, estimate scaling  $C$  by minimizing

$$\|T_m - \hat{T}_m(C)\|.$$

# Results: Adaptive Learning

- The use of nonuniform knots allows to focus more on regions of the domain where data points are densely concentrated, while reducing resolution in regions with sparse data.

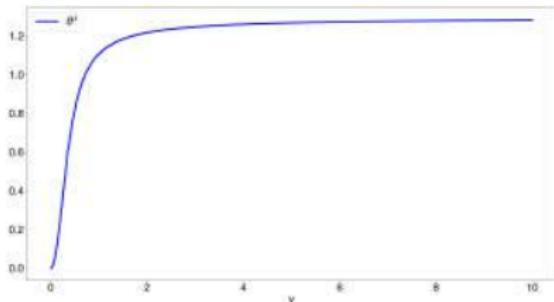
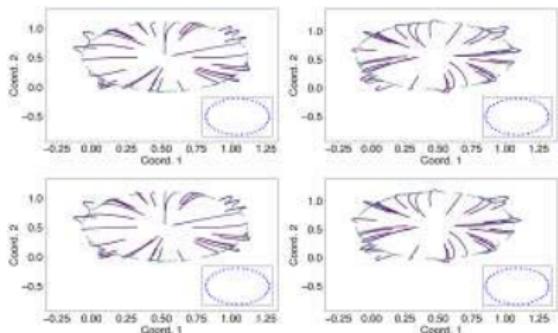
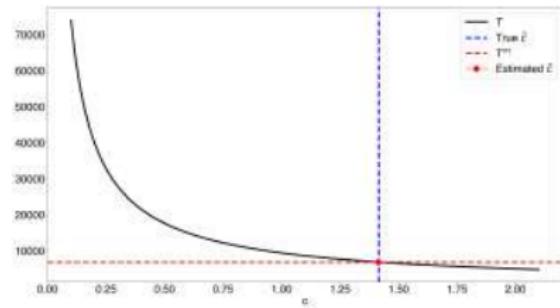
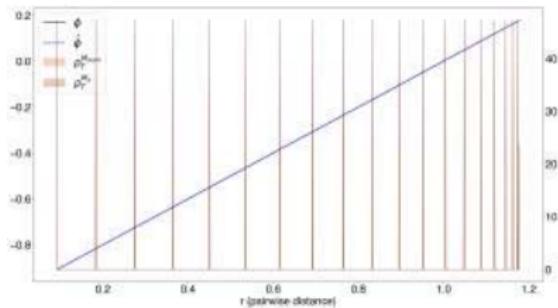


Figure: Kernel:  $r - 1$

# Results

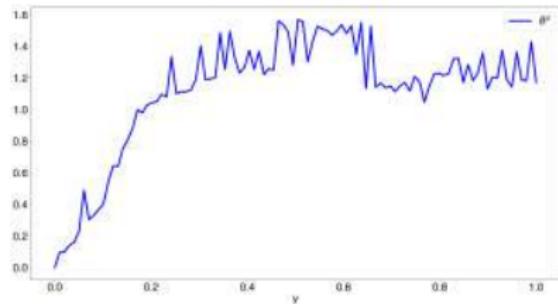
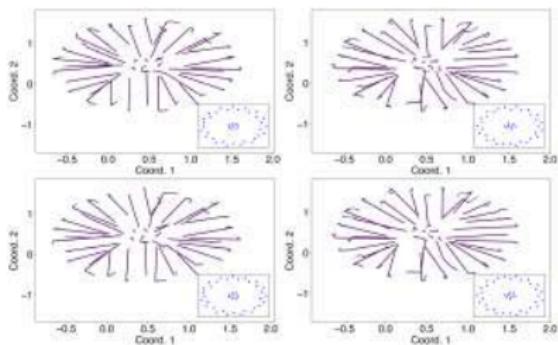
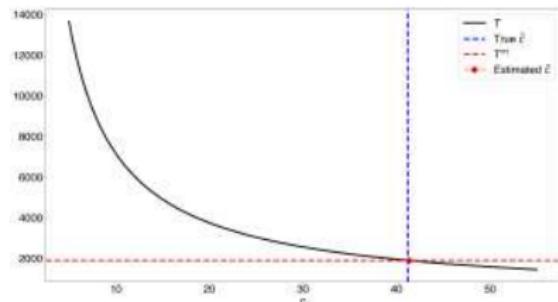
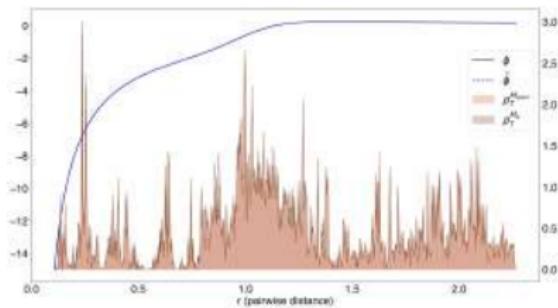


Figure: Kernel: tanh

# Results

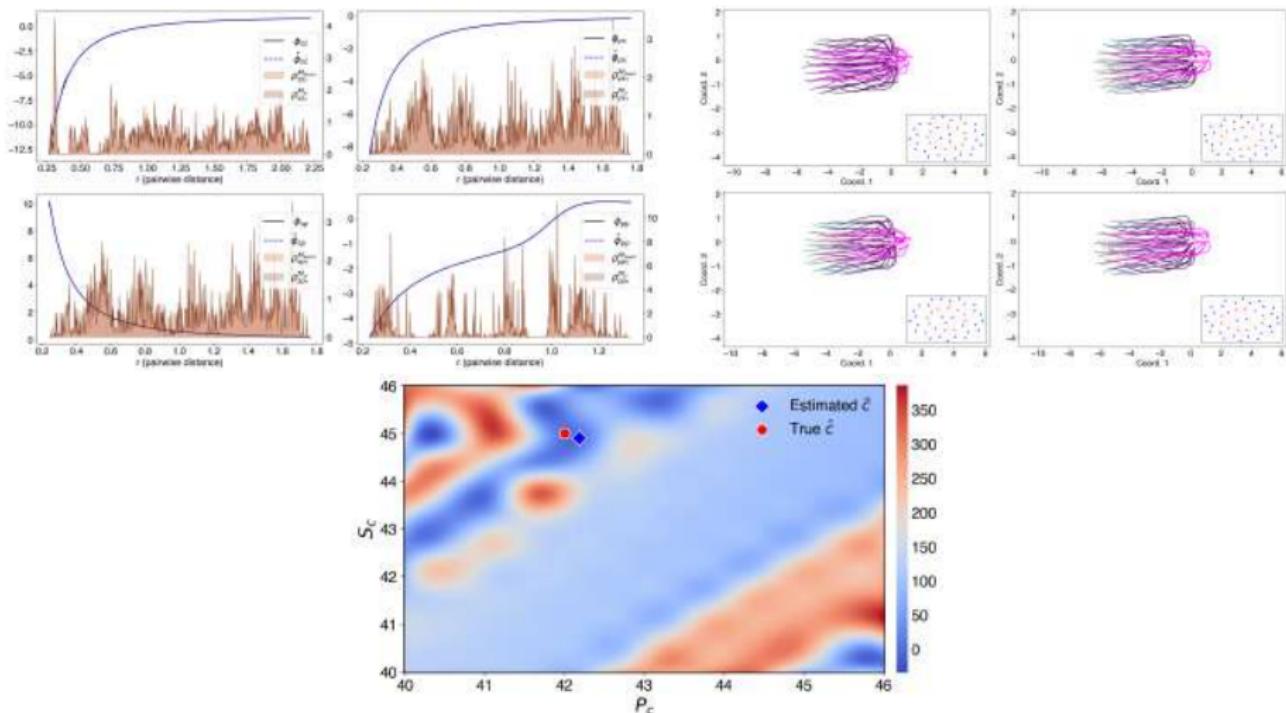


Figure: Kernel: Multi-species

# Results

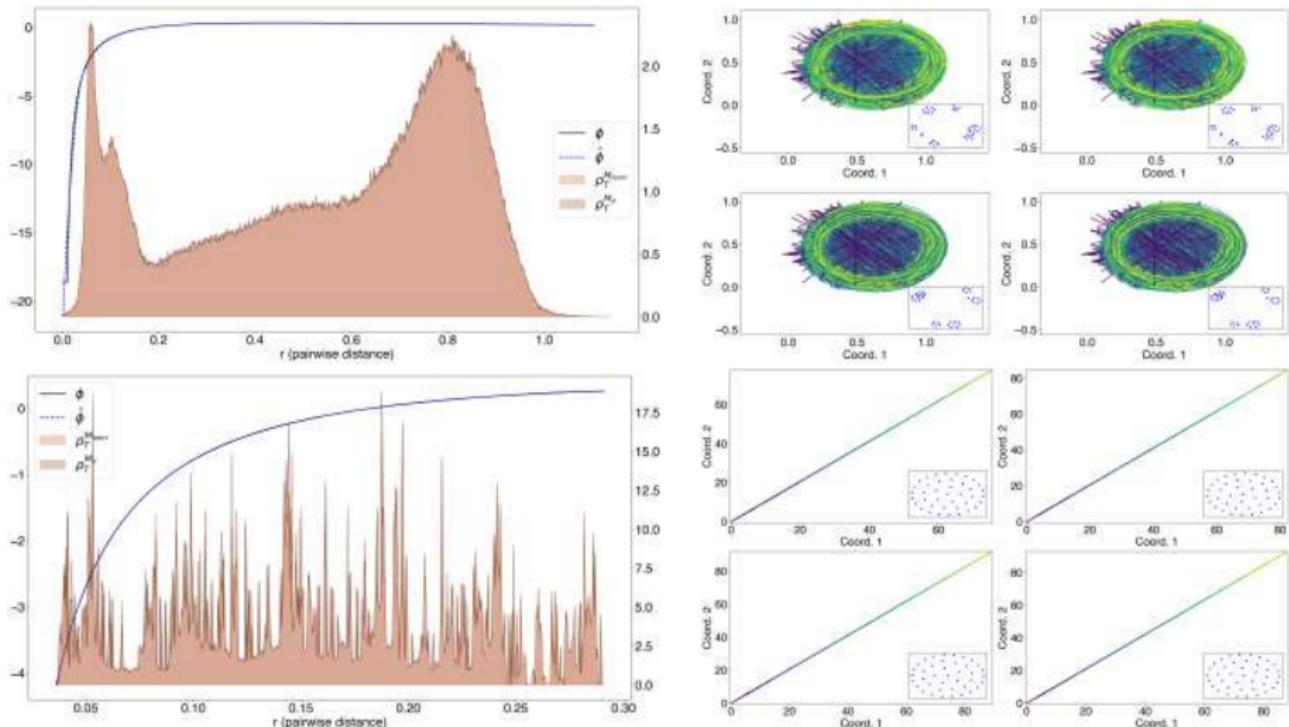


Figure: Kernel: Fish Milling & Flocking

# Part III – Analysis

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*Provide mathematical foundations for well-posedness*

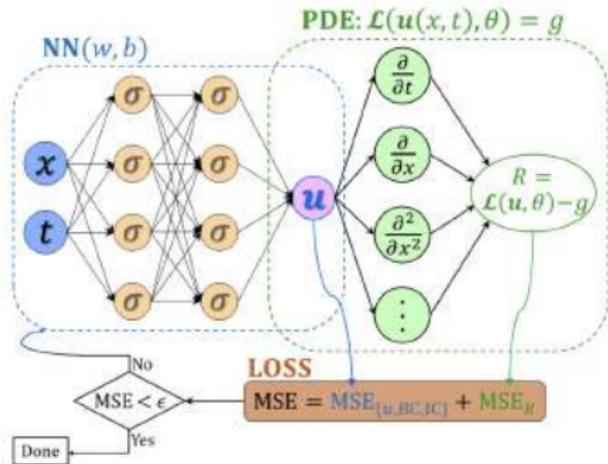
# Stability in Training PINNs

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*Stability in Training PINNs for Stiff PDEs: Why Initial Conditions Matter*

# Introduction to PINNs<sup>67</sup>

- PINNs integrate PDE constraints into deep learning



**Figure:** Schematic of PINN, where the loss function of PINN contains a mismatch in the given data on the state variables or boundary and initial conditions. The hyperparameters of PINN can be learned by minimizing the total loss  $\mathcal{L} = MSE_{IC} + MSE_{BC} + MSE_R$ .

<sup>6</sup>Lagaris et al., 1998, *IEEE transactions on neural networks*.

<sup>7</sup>Raissi et al., 2019, *Journal of Computational physics*.

# Motivation & Contributions

## Why enforcement of IC matters?

- Training PINNs on **stiff PDEs** is highly unstable.
- Stiff PDEs evolve on **widely varying time scales**.
- Explicit solvers struggle → stability hinges on **ICs**.
- Soft penalty causes severe **spectral bias**, and failure to propagate information away from  $t = 0$ .

## Main Contributions:

- Systematic **ablation study** of stabilization mechanisms for stiff PDEs.
- Show hard IC constraints are the dominance for stability and accuracy.
- Demonstrate effectiveness across **7 stiff PDE benchmarks** (AC, CH, GS, KS, LA, etc.).
- Provide an **NTK-based theoretical explanation** for why hard IC constraints reduce spectral bias and improve training decay rates.
- Show compatibility with advanced PINN techniques (causal PINNs, RBA PINNs, time-marching, etc.).

# Methodology

- PDE setup:  $u_t + \mathcal{P}(u) = f$  on  $(0, T] \times \Omega$ .
- **Hard constraint transformation:**

$$\tilde{u}(t, \mathbf{x}) = \psi(t, \mathbf{x}) + \phi(t, \mathbf{x})u_{\text{NN}}(t, \mathbf{x}),$$

with  $\psi(0, \mathbf{x}) = u_0(\mathbf{x})$ ,  $\phi(0, \mathbf{x}) = 0$  ensuring exact IC satisfaction.

- Standard PINN loss combines:

$$\mathcal{L} = \mathcal{L}_{\text{IC/BC}} + \mathcal{L}_{\text{R}}.$$

- HC-PINN loss:

$$\mathcal{L} = \mathcal{L}_{\text{R}}.$$

## Summary

- Hard ICs enforce the time direction in training, reducing spectral bias (**NTK**).
- Mimics traditional numerical solvers (exact ICs at  $t = 0$ ).
- Behaves like an implicit time integrator → more stable.

# Results

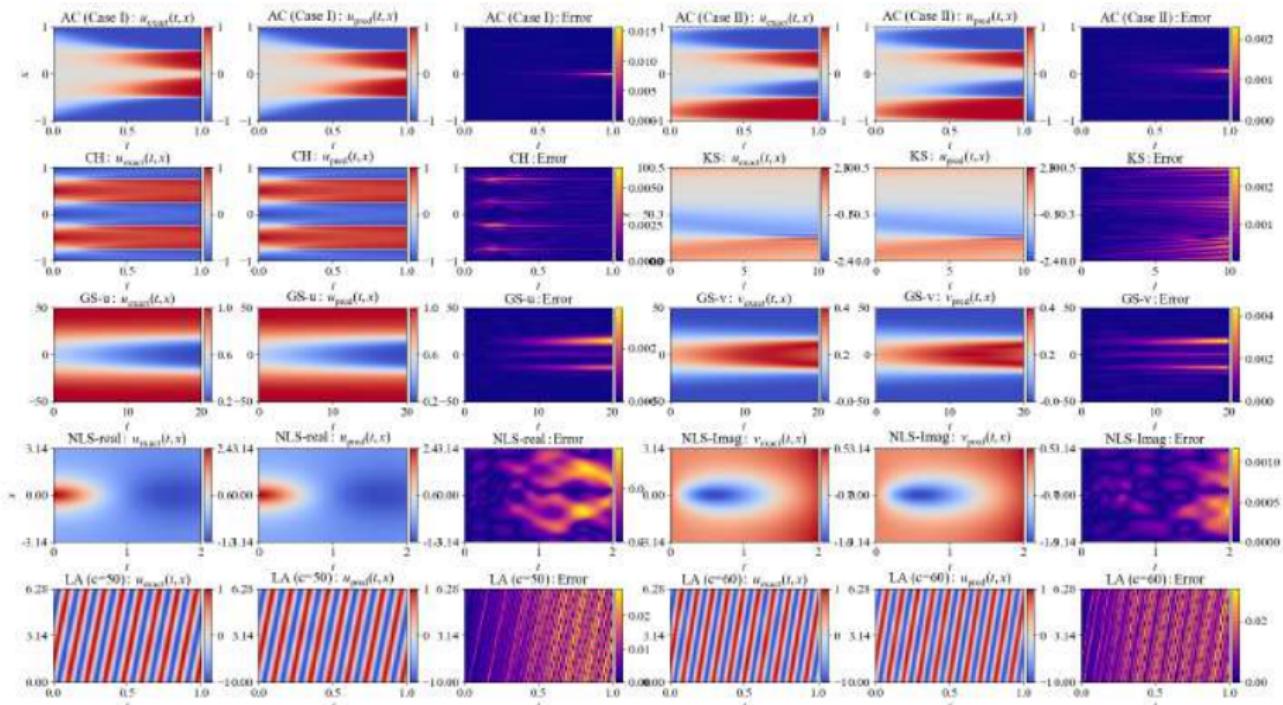


Figure: Benchmark Results: Truth vs HC-PINN vs Absolute Error.

# Results: Comparison

	Causal training (MLP) <sup>8</sup>	Enhanced RBA <sup>9</sup>	HC-PINNs
AC (Case I)	$6.95 \times 10^{-2}$	$2.62 \times 10^{-3}$	$8.29 \times 10^{-4}$
AC (Case II)	$1.78 \times 10^{-2}$	$1.08 \times 10^{-3}$	$2.14 \times 10^{-4}$
CH	$3.49 \times 10^{-1}$	$9.83 \times 10^{-2}$	$5.61 \times 10^{-4}$
KS	$2.72 \times 10^{-1}$	$3.64 \times 10^{-2}$	$5.37 \times 10^{-4}$

**Table:** Relative  $L^2$  errors after  $50k$  training iterations. All methods are implemented under the same  $50k$  iteration.

- HC-PINNs achieve much lower errors with fewer iterations!

<sup>8</sup>Wang et al., 2022, *arXiv preprint arXiv:2203.07404*.

<sup>9</sup>Anagnostopoulos et al., 2023, *arXiv preprint arXiv:2307.00379*.

# **Ion transport: PNP**

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*Rigorous analysis for complex ion transport PDEs*

# Variational Models<sup>10</sup>

- Variational models are useful in modeling problems in physics, biology, etc.
- Variational models leverages the laws of thermodynamics to model **chemo-mechanical effects across different scales** in a unified way:
  - 1st law of thermodynamics:  $\frac{d}{dt}(\mathcal{K} + \mathcal{U}) = \dot{\mathcal{W}} + \dot{\mathcal{Q}}$ .
  - 2nd law of thermodynamics:  $Td\mathcal{S} = \dot{\mathcal{Q}} + \Delta$  with  $\Delta \geq 0$ .

$\mathcal{K}$ : kinetic energy;  $\mathcal{F}$ : free energy;  $\dot{\mathcal{W}} = 0$ : rate of external work;  $\dot{\mathcal{Q}}$ : rate of heat absorbed;  $\Delta \geq 0$ : rate of entropy production.

## Energy-dissipation law (Isothermal Case)

$$\frac{d}{dt}E^{total} = \frac{d}{dt}(\mathcal{K} + \mathcal{F}) = \dot{\mathcal{W}} - \Delta,$$

where  $\mathcal{F} := \mathcal{U} - T\mathcal{S}$ .

- Capable to **incorporate multiscale chemo-mechanical coupling systematically** by choosing appropriate energy and the rate of energy-dissipation.
- Force (mechanical) and reaction rate (chemical) can be derived using **EnVarA**.

<sup>10</sup>Giga et al., 2018, *Handbook of mathematical analysis in mechanics of viscous fluids*.

# Introduction to PNP Equations 11

- **Ion transport is fundamental:** Appears in electrochemistry, physiology (ion channels), semiconductors, energy storage, porous media.
- **Microscopic description is too complex:** Direct particle-based models are computationally expensive.

Poisson-Nernst-Planck (PNP) Equations:

$$\begin{aligned}\partial_t c_i &= -\nabla \cdot \mathbf{J}_i, & \mathbf{J}_i &= -D_i \nabla c_i - \frac{D_i z_i e}{k_B T} c_i \nabla \phi, \\ -\nabla \cdot (\epsilon \nabla \phi) &= \sum_i z_i e c_i, & \text{where } i &= n, p.\end{aligned}$$

Energy and Dissipation:

$$\begin{aligned}E[c_n, c_p, \phi] &= \int_{\Omega} k_B T \left( c_n \ln \frac{c_n}{c_{n\infty}} + c_p \ln \frac{c_p}{c_{p\infty}} \right) + \frac{\epsilon}{2} |\nabla \phi|^2 dx. \\ \Delta &= \int_{\Omega} \frac{k_B T}{D_n} c_n |\mathbf{u}_n|^2 + \frac{k_B T}{D_p} c_p |\mathbf{u}_p|^2 dx.\end{aligned}$$

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<sup>11</sup>Xu et al., 2014, *Communications in Mathematical Physics*.

# PNP with Steric Effects<sup>12</sup> and Relative Drags

- Classical PNP is a dilute-solution mean-field model.
- High ionic concentration / crowding<sup>13</sup>: Finite size and excluded-volume effects lead to nonlinear correlations. Strong ion–ion and ion–solvent interactions require including steric repulsion, cross interactions.
- Coupled friction and relative drags<sup>14</sup>: In crowded electrolytes, ions do not move independently. When a cation moves, it drags nearby anions (cross diffusion).
- Modification:

$$\mathcal{A}^* = \int_{\Omega} k_B T \left( c_n \ln \frac{c_n}{c_{n\infty}} + c_p \ln \frac{c_p}{c_{p\infty}} + \frac{1}{2} g_{nn} c_n^2 + g_{np} c_n c_p + \frac{1}{2} g_{pp} c_p^2 \right) + \frac{\epsilon}{2} |\nabla \phi|^2 dx,$$

$$\Delta^* = \int_{\Omega} \frac{k_B T}{D_n} c_n |\mathbf{u}_n^*|^2 + \frac{k_B T}{D_p} c_p |\mathbf{u}_p^*|^2 + \frac{K_B T}{D_{n,p}} c_n c_p |\mathbf{u}_n^* - \mathbf{u}_p^*|^2 dx,$$

where  $g_{nn}, g_{pp} > 0$ : self-crowding repulsion and  $g_{np}$ : cross-crowding effect between cations and anions,  $D_{n,p}$  is a cross-diffusion or friction coefficient.

<sup>12</sup> Horng et al., 2012, *The Journal of Physical Chemistry B*.

<sup>13</sup> Hsieh, 2019, *Nonlinear Analysis: Real World Applications*.

<sup>14</sup> Hsieh et al., 2015, *Journal of Mathematical Analysis and Applications*.

# PNP with Steric Effects and Relative Drags

$$\partial_t c_n = \nabla \cdot \left[ \frac{D(1+c_n)}{1+c_n+c_p} \left( \nabla c_n + \frac{z_n e}{k_B T} c_n \nabla \phi + \frac{g_{nn}}{k_B T} c_n \nabla c_n + \frac{g_{np}}{k_B T} c_n \nabla c_p \right) \right.$$

$$\left. + \frac{D c_n}{1+c_n+c_p} \left( \nabla c_p + \frac{z_p e}{k_B T} c_p \nabla \phi + \frac{g_{pp}}{k_B T} c_p \nabla c_p + \frac{g_{np}}{k_B T} c_p \nabla c_n \right) \right],$$

$$\partial_t c_p = \nabla \cdot \left[ \frac{D(1+c_p)}{1+c_n+c_p} \left( \nabla c_p + \frac{z_p e}{k_B T} c_p \nabla \phi + \frac{g_{pp}}{k_B T} c_p \nabla c_p + \frac{g_{np}}{k_B T} c_p \nabla c_n \right) \right.$$

$$\left. + \frac{D c_p}{1+c_n+c_p} \left( \nabla c_n + \frac{z_n e}{k_B T} c_n \nabla \phi + \frac{g_{nn}}{k_B T} c_n \nabla c_n + \frac{g_{np}}{k_B T} c_n \nabla c_p \right) \right],$$

$$-\epsilon \Delta \phi = z_p c_p + z_e c_n.$$

- Produces diffusion matrices, can lose symmetry or positivity.
- Becomes degenerate, non-symmetric, and no longer variational.

# PNP with Steric Effects and Relative Drags

To simplify the equations, we let  $u = c_n + c_p$ ,  $v = c_n - c_p$ .

$$\begin{aligned}\partial_t u &= \nabla \cdot [\nabla u - v \nabla \phi + u \nabla u], \\ \partial_t v &= \nabla \cdot \left[ \frac{1}{1+u} (\nabla v - u \nabla \phi + v \nabla u) + \frac{v}{1+u} (\nabla u - v \nabla \phi + u \nabla u) \right], \\ \Delta \phi &= v,\end{aligned}\quad (4)$$

with boundary conditions:

$$\begin{aligned}(\nabla v - u \nabla \phi + v \nabla u) \cdot \nu &= 0, \\ (\nabla u - v \nabla \phi + u \nabla u) \cdot \nu &= 0, \\ \phi &= 0,\end{aligned}$$

and initial conditions:

$$\begin{aligned}u(x, 0) &= u^0(x) = c_n^0(x) + c_p^0(x) \in L^2(\Omega), \\ v(x, 0) &= v^0(x) = c_n^0(x) - c_p^0(x) \in L^2(\Omega).\end{aligned}$$

# Main Theorem and A Priori Estimate

## Lemma 1

Let  $(u, v)$  be the solution. Then there exist positive constants  $K_1, K_2$  and  $\gamma$  depending only on  $M_0, d$ , and  $\Omega$  such that

$$\begin{aligned} \frac{d}{dt} \left( \int_{\Omega} K_1 u^2 + v^2 \, dx \right) + \gamma \int_{\Omega} (|\nabla u|^2 + |\nabla v|^2) \, dx + K_1 \int_{\Omega} \bar{u}^* |\nabla u|^2 \, dx \\ \leq K_2 (1 + \|\bar{v}\|_{L^2(\Omega)}^4) \left( \int_{\Omega} K_1 u^2 + v^2 \, dx \right). \end{aligned}$$

## Main Theorem (Local Existence)

Suppose that the initial data  $c_{n,0}, c_{p,0} \in L^\infty(\Omega)$ . Then there exists  $t_0 > 0$  such that the PDE system 4 has a solution  $(c_n, c_p, \phi)$  with  $0 \leq c_n, c_p \in L^\infty((0, t_0); L^2(\Omega)) \cap L^2((0, t_0); H_1(\Omega))$  and  $\partial_t c_n, \partial_t c_p \in L^2((0, t_0); H^{-1}(\Omega))$ .

# Proof Outlines

## Fixed Point Framework:

- Define  $F((\bar{u}, \bar{v})) = (u, v)$  in  $X = \{(f, g) : f, g \in L^4((0, t_1); L^2(\Omega))\}$ .
- Truncation:  $f^* = \min\{\max(f, 0), 5M_0\}$
- The elliptic equation  $\Delta \bar{\phi} = \bar{v}$  couples the system.

## Galerkin Approximation and Compactness:

- Apply Galerkin's method to construct approximate  $(u^k, v^k)$ .
- Use the a priori estimate and Gronwall's inequality for uniform bounds:

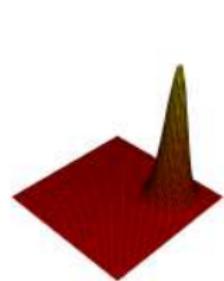
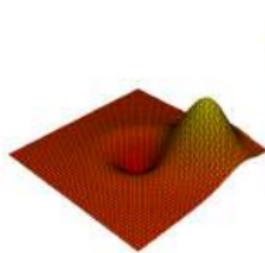
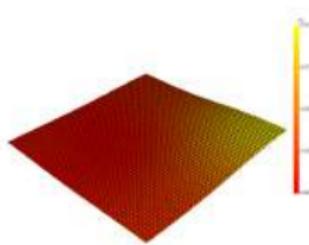
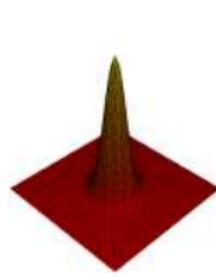
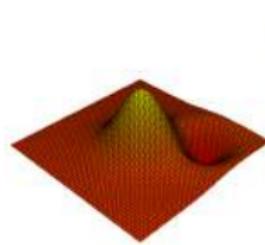
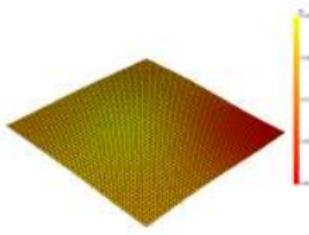
$$(u^k, v^k) \text{ bounded in } L_t^\infty L_x^2 \cap L_t^2 H_x^1.$$

- Compactness  $\Rightarrow$  continuity of  $F$  and  $F(B_R) \subset B_R$ .

## Passing to the Limit:

- Apply Schauder's fixed point theorem to obtain a fixed point  $(u, v)$ .
- Recover  $(c_n, c_p)$  and  $\phi$ , proving local existence and positivity.

# Results

(a)  $c_n$ : Time Step = 0(b)  $c_n$ : Time Step = 30(c)  $c_n$ : Time Step = 380(d)  $c_p$ : Time Step = 0(e)  $c_p$ : Time Step = 30(f)  $c_p$ : Time Step = 380

# Results

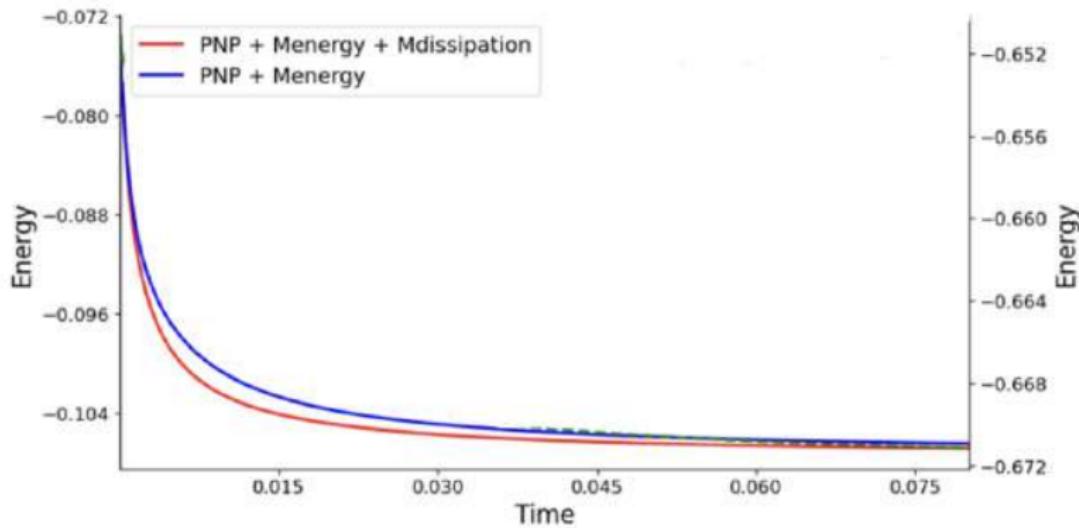


Figure: Comparison between different models

# Synthesis and Outlook

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# Conclusion

- Emergent behavior across physical, biological, and social systems can be explained by **interaction rules**.
  - Examples: Swarmalators; Crime models; Ion transport systems
- If emergent patterns reflect interaction rules, we can **recover** the rules from the patterns.
  - Examples: Learning kernels from steady states
- Predictive models require **mathematical foundations**: existence, stability, and structure.
  - Examples: Global existence for nonlinear PDEs; Stability in training PINNs

# Ongoing and Future Work

- ① **Synchronization and Swarming:** Extending this work to networked graph systems.
- ② **Crime Pattern Modeling:** Extending the model to include police response for data-driven predictive analytics and decision support in complex systems.
- ③ **Learning Kernels:** Developing a topological learning framework that leverages persistent homology to infer interaction laws from spatial patterns by integrating neighborhood density information with geometric and dynamical features of the data.
- ④ **PINNs:** Combining Physics-Informed Neural Networks with Graph Neural Networks to model biological interactions.
- ⑤ **Ion transport and PNP:** Ongoing work focuses on establishing the global existence of weak solutions near equilibrium.

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Thank you ! Happy Thanks Giving !

# Q&A

## QUESTIONS & ANSWERS