# A FRAMEWORK FOR PHYSICS-INFORMED REINFORCEMENT LEARNING WITH APPLICATIONS TO CELL MIGRATION

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## ABSTRACT

Many discrete systems in physical sciences can be modeled as an agent undergoing Markov Decision Process (MDP). In the abstract notion of MDP, every agent has a state that evolves over time, governed by the actions the agent chooses at each time step. These choices of the actions given the current state and the choices of the following state given the current state are stochastically determined by probability distributions referred to as the policy and transitions, respectively. The policy choice is intrinsically determined based on a reward maximization principle. These MDP-based models are well-suited for inference using Reinforcement Learning (RL) techniques [1].

The mean field behavior of the discrete agents is typically studied in the framework of Continuum physics. We have identified a particular class of MDP-based models that, at the continuum scale, are governed by the Fokker-Planck Equation. This gives us a physical notion of energy that these agents tend to minimize. The form of this energy can be inferred using data-driven approaches such as Variational System Identification (VSI) [2]. On the other hand, Inverse Reinforcement Learning (IRL) is an inverse problem of RL that uncovers the reward function of an MDP from the observed trajectories of an agent. We draw upon the connection between the energy minimization principle at the continuum level and expected reward maximization in MDP to inform transition probabilities in the IRL approach. This talk will present a physics-informed algorithm for estimating policies for these particular classes of agents. Our approach utilizes continuum-scale inference to facilitate a robust reinforcement learning procedure at the discrete level. Finally, we will show that our approach provides a computational advantage over the traditional fixed-point iteration techniques used in IRL.

As an application, we will study the migratory behavior of MDA-MB-231 breast cancer cells in a chemotaxis device [3]. The migratory behavior of biological cells is a complex and stochastic phenomenon that results from inter-cellular mechanisms and extra-cellular interactions. This highly stochastic behavior of cells is studied using discrete agent-based models. These cells exhibit a collective behavior modeled as a Fokker-Planck Equation at the continuum scale.

### REFERENCES

[1] Ziebart BD, et al. ”Modeling interaction via the principle of maximum causal entropy.” ICML 2010.

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[3] Ho K, et al. ”Cell-to-cell variability of dynamic CXCL12-CXCR4 signaling and morphological processes in chemotaxis.” *bioRxiv* 2022.05.19.492090.