# Learning Evolution of Coupled Dynamical Systems with Integrated Data-driven and Model-based Approach

**Priyabrata Saha, Arslan Ali, Burhan A. Mudassar, Yun Long, Saibal Mukhopadhyay**
School of Electrical and Computer Engineering
Georgia Institute of Technology
{priyabratasaha, arslanali, burhan.mudassar, yunlong}@gatech.edu,
saibal.mukhopadhyay@ece.gatech.edu

## Abstract

We present a model-based and data-driven hybrid approach to learn the behavior of coupled PDE-ODE based dynamical systems. A coupled system is considered where an unknown multi-agent dynamics is masked by a known PDE-based dynamics. Data-driven deep neural networks are employed to unmask the hidden agents, learn their governing interaction dynamics and combined with a PDE-solver to predict the evolution of the coupled system.

## 1 Introduction

Understanding the behavior of dynamical systems is a fundamental problem in science and engineering. Classical approaches involve formulating ordinary or partial differential equations (ODEs or PDEs) based on physical reasoning, intuition, knowledge and verifying those with experiments and observations. Success of deep learning methods in complex sequence prediction tasks motivates to predict the evolution of dynamical system directly from observation data without rigorous formalization and experiments by human experts. However, a pure data-driven approach without any knowledge of the system is still not mature enough to capture complex dynamics. We consider to combine the data-driven approach with partial knowledge (known model) about the system to understand the behavior of such complex dynamical systems.

In this paper, we consider a coupled dynamical system where an unknown ODE-based multi-agent interaction dynamics perturbs a known PDE-based dynamics. Perturbing agents are not directly observable and masked under the known dynamics. Therefore, an unmasking network is used to unmask the perturbing agents from the observation of coupled system. Output of the unmasking network is the representational map of hidden agents in their state space. State codes of agents are fed to the **M**ulti-**ag**ent interaction **Net**work (MagNet) to predict the evolution of unknown multi-agent dynamics. Finally, a partial-differential-equation (PDE) solver use the predicted state codes and current observation map to forecast its evolution. Figure 1 shows the high-level diagram of our overall model.

We experiment with a diffusion system perturbed by some moving agents governed by unknown interaction dynamics and show long-term prediction capability of the proposed system.

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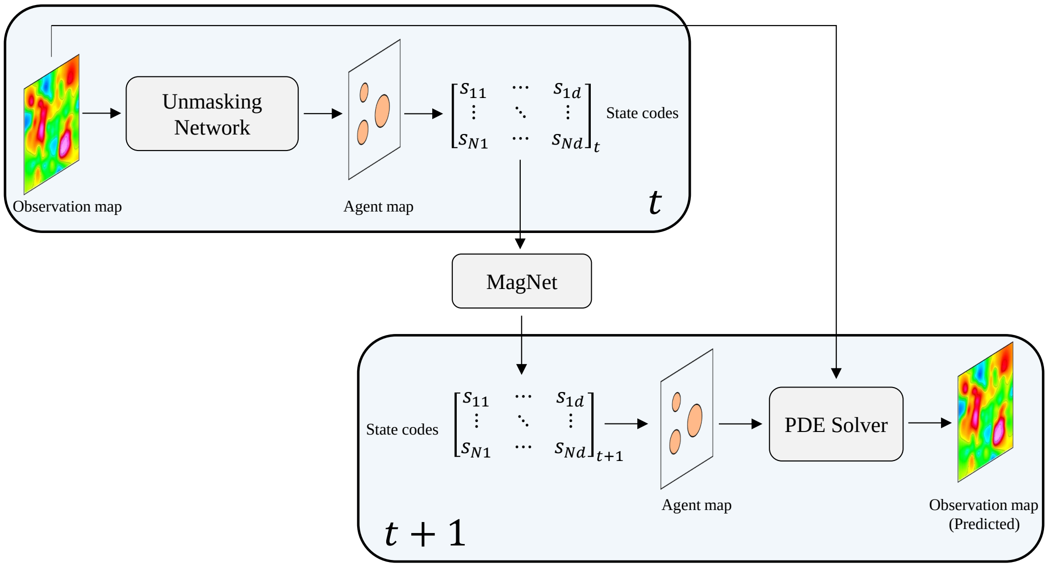


Figure 1: Hybrid network for evolution prediction of coupled dynamical system

# 2 Model

## 2.1 Mathematical formulation

The considered system couples an ODE-based source term to an inhomogeneous PDE. The following set of equations describes the considered coupled PDE-ODE system.

$$u_t(x,y,t) = \Psi\big(u, u_x, u_y, u_{xx}, u_{yy}, \cdots\big) + w(x,y,t) \tag{1}$$

$$u(x,y,0) = w(x,y,0) \tag{2}$$

$$w(x,y,t) = \Phi\left(x, y, \bigcup_{i=1}^{N} \mathbf{s}_i(t)\right) \tag{3}$$

$$\frac{d\mathbf{s}_i(t)}{dt} = F_i\left(\bigcup_{i=1}^{N} \mathbf{s}_i(t)\right) \quad \forall i \in \{1, 2, ..., N\} \tag{4}$$

We refer to $u$ as the observation map and $u(x,y,t)$ denotes the observed variable at position $(x,y)$ at time $t$. $w$ is the source term or external perturbation varying over space and time. Many dynamical systems involving the transport of some quantity (e.g. mass, heat etc.) follow equations similar to equation 1. The source term $w$ is a function of states of all agents contributing to the perturbation. $\mathbf{s}_i(t)$ denotes the state of $i^{th}$ agent at time $t$. $\bigcup_{i=1}^{N}$ denotes the union of all agents. We refer to $w$ as the agent map.

We assume that we know the masking dynamics (i.e. $\Psi$) as well as the conversion from state codes to agent map and its opposite (i.e. $\Phi$ and $\Phi^{-1}$). Therefore, given the agent map $w$ at some point in time, we can predict the evolution of observation map $u$ using a PDE solver. But, agent map is not directly observed and should be unmasked from the observation map. We use an unmasking network to find the inverse transform $\Theta$ such that $w = \Theta(u)$. The multi-agent ODE system (equation 4) is unknown and we propose a **M**ulti-**ag**ent interaction **Net**work (MagNet) to discover this dynamics.

### 2.2 Implementation

We implement the PDE solver (the forward network) using cellular neural network (CeNN) [1] as proposed in [2]. Dynamical structure of CeNN makes it suitable as a general purpose PDE solver [5]. Operations of CeNN can be implemented as convolution. The reason behind using CeNN-based PDE solver is that it can trained with backpropagation to learn the unknown physical parameters of the system.

The unmasking network is implemented by a fully convolutional pixel-to-pixel network. We use size-preserving convolution layers and maxpooling layers so that output size remains same as input size. However, if the size of the observation map is too large, then strided convolution followed by upsampling or deconvolution should be used. In this case, the unmasking network can be implemented by semantic segmentation network like [3].

Interaction networks(INs) by Battaglia et al. [4] can be used to learn the multi-agent interaction dynamics provided that object relation graph is available; but the relation graphs are often unknown in a real scenario. Moreover, input state vector to IN can include physical properties like agent's mass which may not be directly observable. We propose MagNet that learns the interaction dynamics solely from observational data (e.g. position, velocity). We use standard deep neural network components to implement the functions $F_i$'s. The proposed model is composed of two parts: a core network and a wrapper network. The core network shares parameters among all agents and learns the core interaction law present in the system, whereas the wrapper network is responsible for agent-specific attributes. If the attributes of the agents change, only the wrapper network needs to be fine-tuned online to adapt with the new set of agents.

## 3 Experiments and Results

### 3.1 Dataset

**Masking dynamics** We consider inhomogeneous heat diffusion system as the masking dynamics, which is delineated by the following PDE

$$\frac{\partial T}{\partial t} = D\,\Delta T + C\,T_{agent} \tag{5}$$

where $D$ is the diffusion coefficient and $C$ is the convection coefficient. $\Delta$ denotes the Laplace operator. $T$ is the temperature map defined over a two-dimensional space and $T_{agent}$ is the perturbation in temperature map due to agents (heat sources).

**Multi-agent interaction dynamics** Agents (heat sources) are physical objects with different mass moving in a two-dimensional space according to Newton's laws of motion. The forces acting on each agent are pairwise interaction forces. We consider two types of forces are acting simultaneously

- Interaction force due to invisible spring between each pair of agents. We consider different spring constants for different pairs.
- A repulsive inverse square law force between each pair. This force is proportional to the product of mass of the involved agent-pair (exactly same as gravitational attraction except the force is repulsive here). Inverse square law force makes the system highly nonlinear.

### 3.2 Results

All results are generated as solution to an initial value problem i.e. evolution of the system is predicted only from an initial observation, no intermediate observation is used.

**Performance of MagNet on multi-agent interaction dynamics** First, we consider four interacting objects (agents) with different mass and different pairwise spring constants. MagNet can predict the evolution of state codes for a long period of time with negligible error. Next, we increase the number of agents to eight and change spring constants between agent-pairs and masses of the agents. We only re-tune the wrapper network for the new set of agents while the core network parameters kept frozen. Visual evolution of ground truth and prediction are shown in Figure 2.

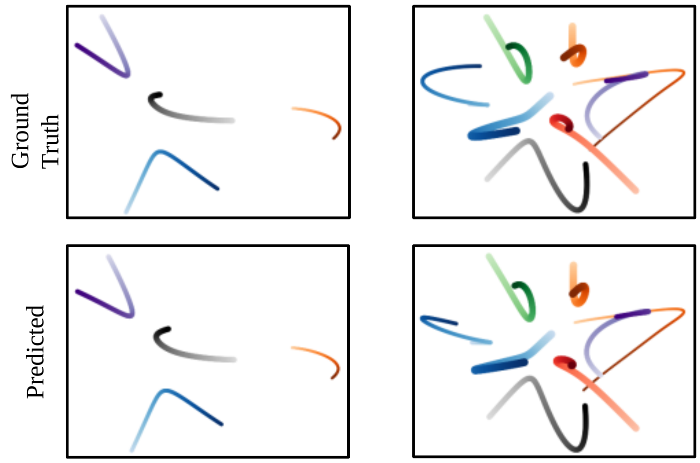


Figure 2: Visualization of evolution up to 200 timesteps. (a) Trajectory plot of four moving agents. Widths of the trajectories are proportional to the masses of corresponding agents. Predictions are from network trained from scratch. (b): Trajectory plot of eight moving agents. Predictions are from re-tuned wrapper network preceded by frozen core network trained with 4 agents.

**Performance of the combined model: Observation map to observation map prediction** Here we evaluate to the performance of the combined model (Figure 1). Agent maps are generated from the observation map using the unmasking network. Then, state code of agents are extracted from the agent map by computing weighted mean over pixel coordinates. Finally, an initial set of state codes is used by the MagNet to predict the evolution of state codes which are simultaneously converted to agent maps and fed to the PDE solver to predict the evolution of heat maps. Figure 3 shows the visual comparison. The peak-signal-to-noise-ratio (PSNR) between true heat maps and predicted heat maps shows high prediction accuracy.

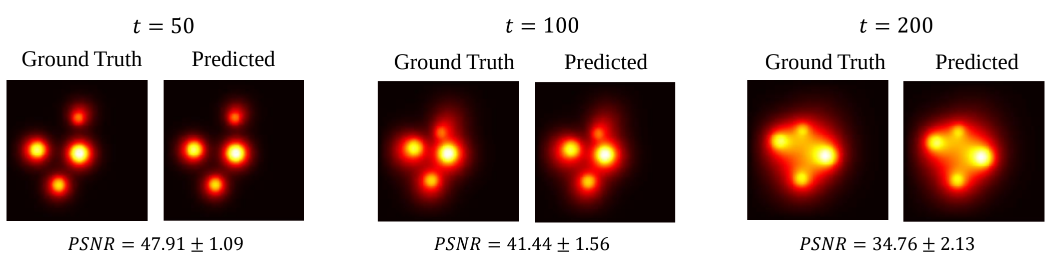


Figure 3: Visual comparison and PSNR between ground truth heatmaps and predicted heatmaps from the hybrid network. $t$ denotes the timestep. PSNR value (with 95% confidence interval) shown is the mean from 20 test sequences.

## 4 Conclusions

Combining the known models with data-driven learning is essential for accurate prediction of the evolution of complex dynamical systems. We demonstrated the application of such integration using an example involving a diffusion system with unknown dynamics of perturbing sources. Proposed approach can be generalized to a class of coupled dynamical systems where an unknown ODE-based dynamics couples with a known PDE-based dynamics.

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