Latent Field Discovery in Interacting Dynamical Systems with Neural Fields

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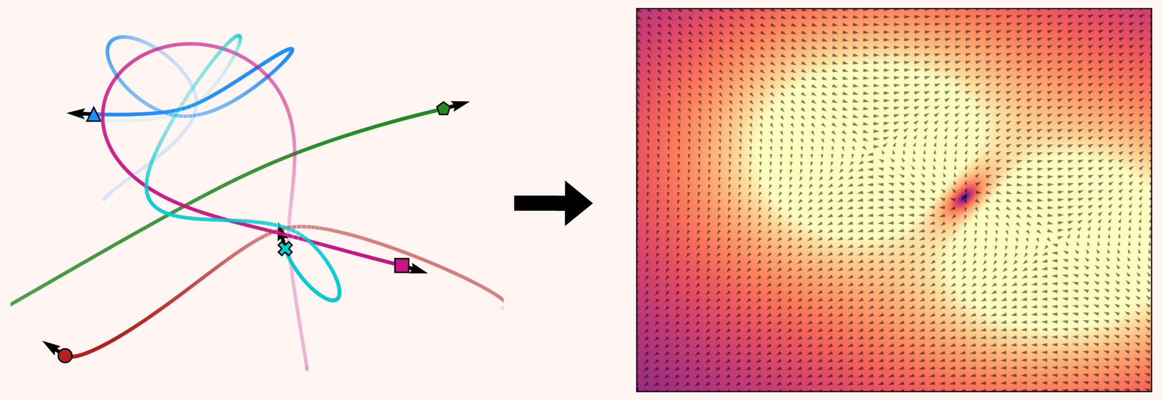
TL;DR: Field discovery in interacting systems

TL;DR We discover global fields in interacting systems, inferring them from the dynamics alone, using neural fields.

Abstract Systems of interacting objects often evolve under the influence of underlying field effects that govern their dynamics, yet previous works have abstracted away from such effects, and assume that systems evolve in a vacuum. In this work, we focus on discovering these fields, and infer them from the observed dynamics alone, without directly observing them. We theorize the presence of latent force fields, and propose neural fields to learn them. Since the observed dynamics constitute the net effect of local object interactions and global field effects, recently popularized equivariant networks are inapplicable, as they fail to capture global information. To address this, we propose to disentangle local object interactions –which are SE(3) equivariant and depend on relative states– from external global field effects –which depend on absolute states. We model the interactions with equivariant graph networks, and combine them with neural fields in a novel graph network that integrates field forces. Our experiments show that we can accurately discover the underlying fields in charged particles settings, traffic scenes, and gravitational n-body problems, and effectively use them to learn the system and forecast future trajectories.



We term our method *Aether*, inspired by the postulated medium that permeates all throughout space and allows for propagation of light.

Keywords Graph Neural Networks, Neural Fields, Field Discovery, Equivariance, Interacting Dynamical Systems, Geometric Graphs

Introduction – Interacting systems are everywhere...

- Colliding particles
- N-body systems
- Molecules
- Traffic scenes

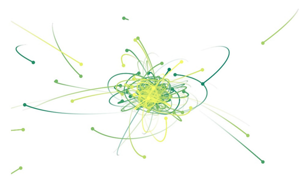


Figure credit: [2]

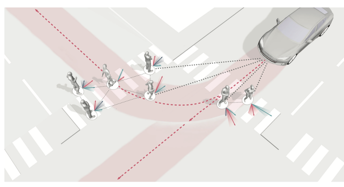


Figure credit: [8]

...but they do not evolve in a vacuum

- Electromagnetic fields
- Gravitational fields
- "Social" fields
  - Road network
  - Traffic rules

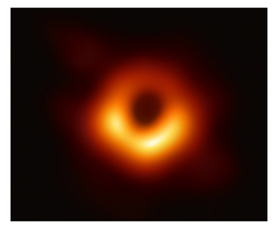


Figure credit: [10]

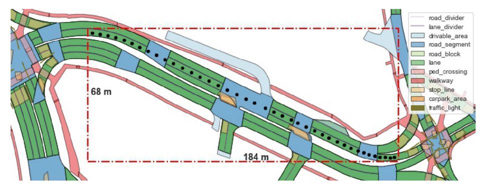
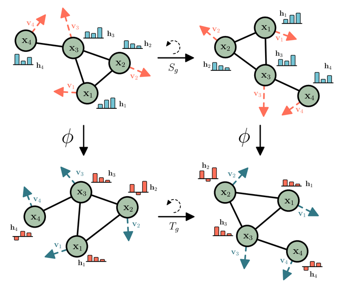


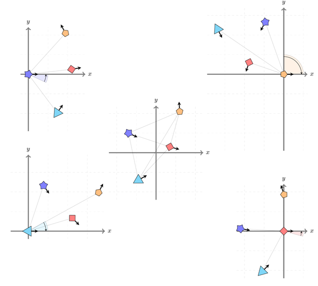
Figure credit: [3]

Related work – Equivariant graph networks

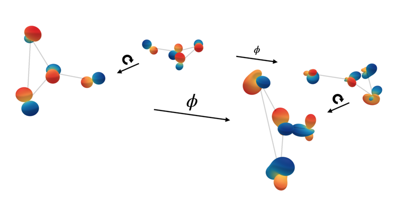
Strictly equivariant graph networks exhibit increased robustness and performance, while maintaining parameter efficiency due to weight sharing.



(a) EGNN [9]



(b) LoCS [7]

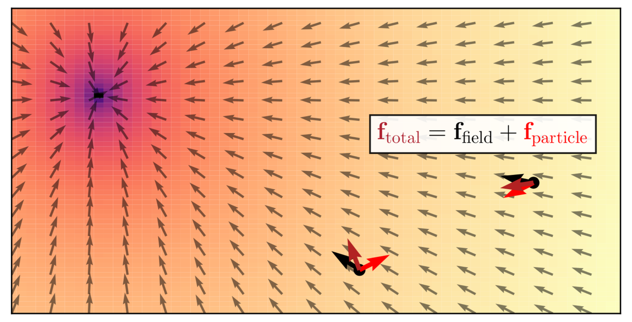


(c) SEGNN [2]

However, they are **incompatible** with global field effects.

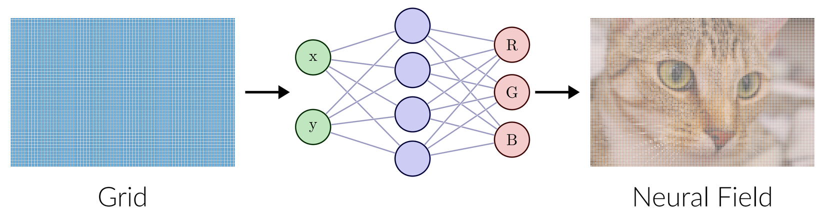
Motivation – Entangled equivariance

Object interactions depend on local information, while underlying field effects depend on global states. Interactions are equivariant to a group of transformations; field effects are not.

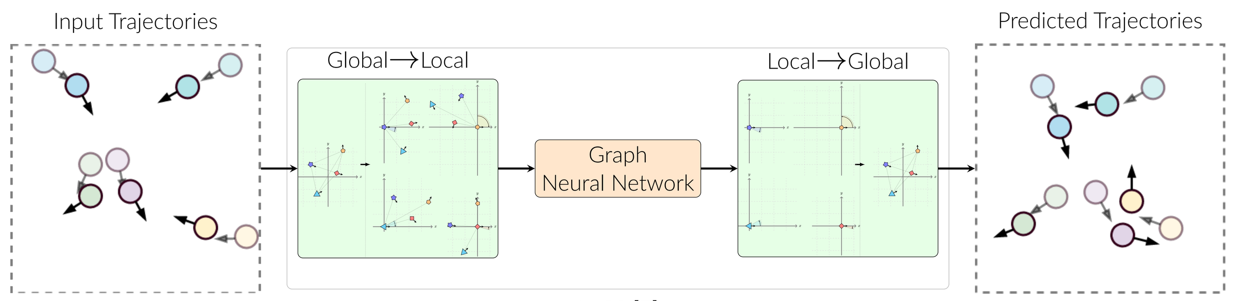


We only observe the net effect of the two constituents. We refer to this as *entangled equivariance*.

Background – Neural fields primer



Background – Equivariant graph network backbone



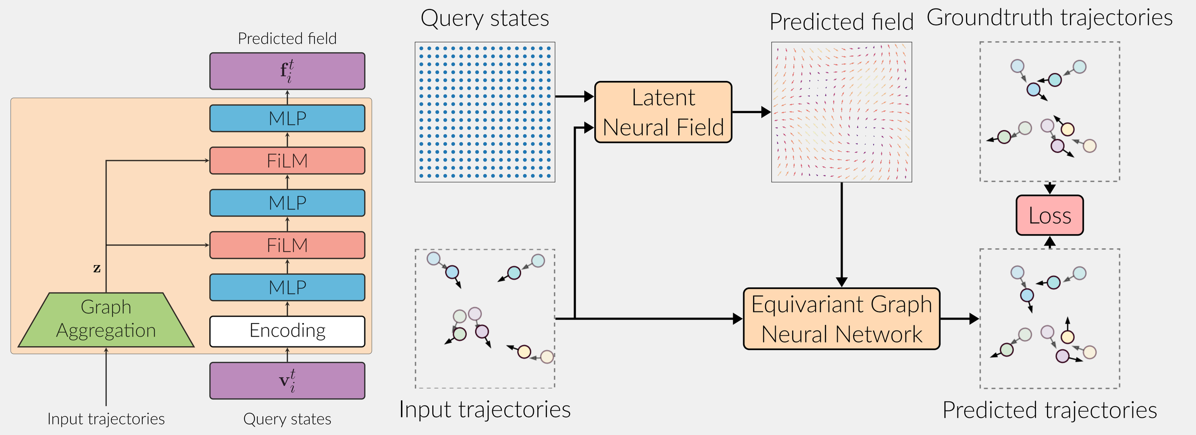
LoCS [7]

$$\mathbf{x}_i = \begin{Bmatrix} \mathbf{p}_i, & \text{positions} \\ \mathbf{u}_i, & \text{velocities} \end{Bmatrix} \rightarrow \mathbf{v}_i = \begin{Bmatrix} \mathbf{p}_i & \text{positions} \\ \mathbf{u}_i, & \text{velocities} \\ \boldsymbol{\omega}_i, & \text{orientations} \end{Bmatrix}$$

$$\begin{aligned} \mathbf{v}_{j|i} &= \text{Global2Local}(\mathbf{v}_j, \mathbf{v}_i) \\ \boldsymbol{\Delta}\mathbf{x}_{i|i} &= \text{GNN}\Big(\mathbf{v}_{i|i}, \{\mathbf{v}_{j|i}\}_{j\in\mathcal{N}(i)}\Big) \\ \boldsymbol{\Delta}\mathbf{x}_i &= \text{Local2Global}\big(\boldsymbol{\Delta}\mathbf{x}_{i|i}\big) \\ \hat{\mathbf{x}}_i &= \mathbf{x}_i + \boldsymbol{\Delta}\mathbf{x}_i \end{aligned}$$

Method – Aether Architecture

We model object interactions with equivariant graph networks [7], and field effects with neural fields. We hypothesize that field effects can be attributed to force fields, and therefore, our neural fields learn to discover latent force fields.



(a) Latent Neural Field (b) *Aether* pipeline

The pipeline of our method, *Aether*. In the latent neural field (a), a graph aggregation module summarizes the input trajectories in a latent variable $\mathbf{z}$. Query states from input trajectories, alongside $\mathbf{z}$, are fed to a neural field that predicts a latent force field. In (b), a graph network integrates predicted forces with input trajectories to predict future trajectories. The graph aggregation module and the FiLM layers exist only in a dynamic field setting.

$$\begin{aligned} \mathbf{h}_{j,i}^{(1)} &= f_e^{(1)}\Big(\Big[\mathbf{v}_{j|i}, \boxed{\mathbf{f}_{j|i}}, \mathbf{v}_{i|i}, \boxed{\mathbf{f}_{i|i}}\Big]\Big) \\ \mathbf{h}_i^{(1)} &= f_v^{(1)}\left(g_v\Big(\Big[\mathbf{v}_{i|i}, \boxed{\mathbf{f}_{i|i}}\Big]\Big) + \frac{1}{|\mathcal{N}(i)|}\sum_{j\in\mathcal{N}(i)} \mathbf{h}_{j,i}^{(1)}\right) \end{aligned}$$

$$\begin{aligned} \mathbf{h}_{j,i}^{(l)} &= f_e^{(l)}\Big(\Big[\mathbf{h}_i^{(l-1)}, \mathbf{h}_{j,i}^{(l-1)}, \mathbf{h}_j^{(l-1)}\Big]\Big) \\ \mathbf{h}_i^{(l)} &= f_v^{(l)}\left(\mathbf{h}_i^{(l-1)} + \frac{1}{|\mathcal{N}(i)|}\sum_{j\in\mathcal{N}(i)} \mathbf{h}_{j,i}^{(l)}\right) \\ \hat{\mathbf{x}}_i &= \mathbf{x}_i + \mathbf{R}_i \cdot f_o\big(\mathbf{h}_i^L\big) \end{aligned}$$

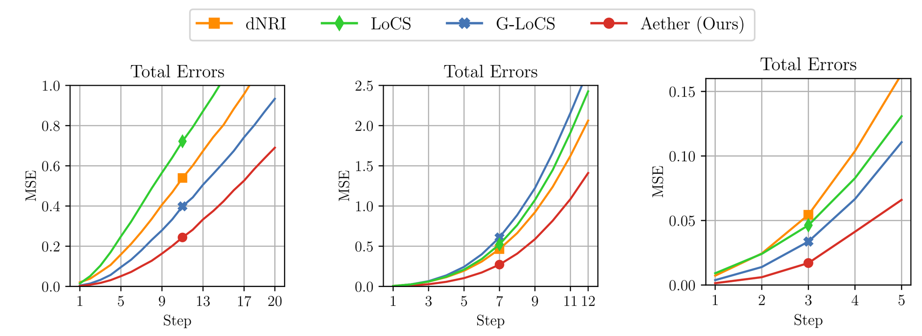
Method – Approximate equivariance

We also propose *G-LoCS*, an *approximately equivariant* graph network that integrates global information and still operates in local coordinate frames. We augment the graph with an auxiliary node-object corresponding to the global coordinate frame, *i.e.* an object positioned at the origin, and oriented to match the x-axis, $\mathbf{x}_{\mathcal{O}} = [\mathbf{p}_{\mathcal{O}}, \mathbf{u}_{\mathcal{O}}] \simeq [\mathbf{0}, \hat{\mathbf{x}}]$.

Experiments

Static field settings
- 2D electrostatic field
- 3D Lorentz force field [4]
- Traffic scenes, inD [1]

Dynamic field settings
- 3D gravitational fields



(a) Electrostatic field (b) inD (c) Gravity

Table 1. MSE on Lorentz force field. †: Results taken from ClofNet [4].

Method	MSE (↓)	No. parameters
GNN †	0.0908	104,387
SE(3) Transformer † [5]	0.1438	1,763,134
EGNN † [9]	0.0368	134,020
ClofNet † [4]	0.0251	160,964
LoCS [7]	0.0238	130,307
Aether (ours)	**0.0129**	132,822

Experiments – Ablation studies

Table 2. (a) Ablation study on the importance of the learned field. Our discovered field is almost as helpful as the groundtruth for at least 10 timesteps. (b) Ablation study on the importance of a sequential architecture. A parallel architecture is not as effective as the sequential approach. (c) Ablation study on the choice of equivariant GNN backbone. Our method is agnostic to the choice of equivariant GNN backbone; it is beneficial for a number of strictly equivariant networks. (d) Ablation study on using conditional neural fields for static fields. Conditional neural fields can be used in static settings, at the expense of more parameters and higher inference time.

(a) Electrostatic field

Method	MSE@10 (↓)
Particle Oracle	0.1847
Force Oracle	0.1883
Aether	0.2015

(b) Lorentz force field

Method	MSE (↓)
LoCS [7]	0.0238
Aether	**0.0129**
Parallel Aether	0.0211

(c) Lorentz force field

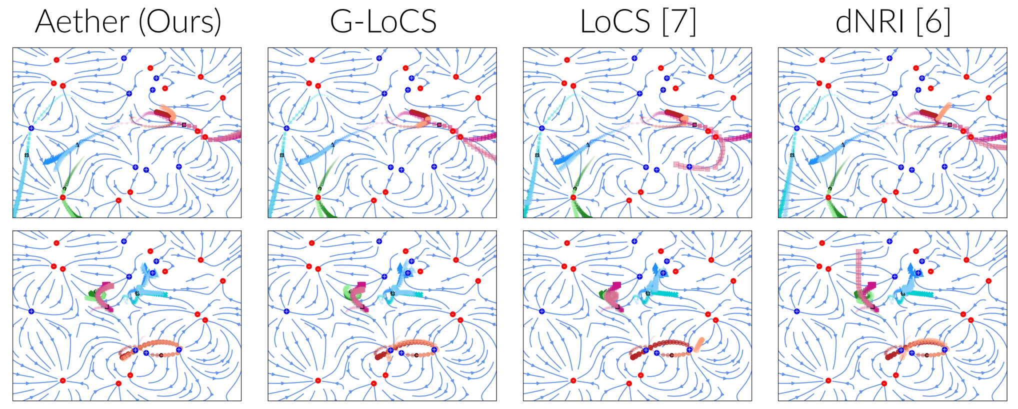
Method	MSE (↓)
EGNN [9]	0.0368
EGNN+Aether	**0.0254**

(d) Lorentz force field

Method	MSE (↓)	No. parameters	Inference Time
LoCS [7]	0.0238	130,307	0.0033
Aether	0.0129	132,822	0.0037
Conditional Aether	0.0131	142,807	0.0047

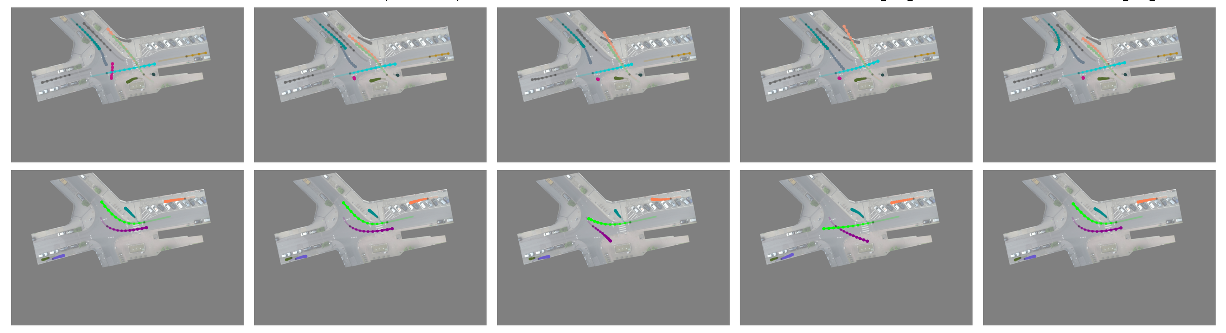
Qualitative results – Electrostatic field

Aether (Ours) G-LoCS LoCS [7] dNRI [6]



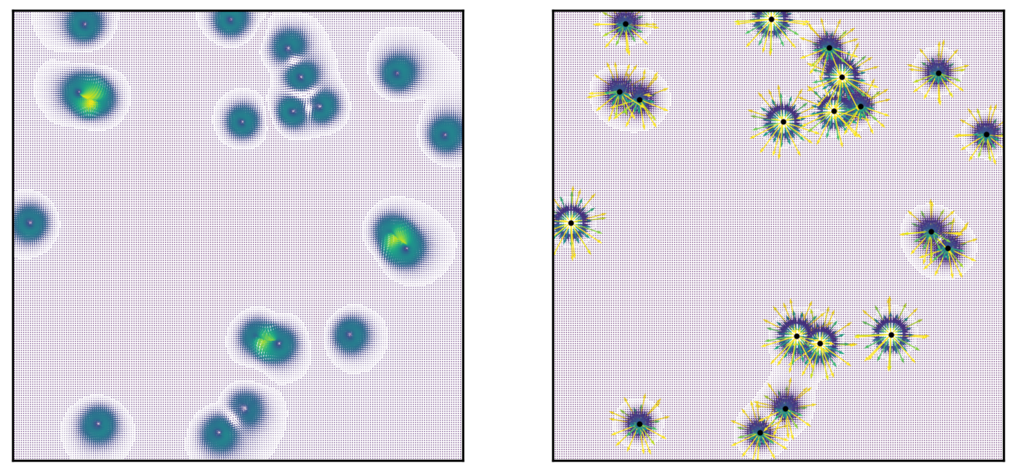
Qualitative results – Traffic scenes

Groundtruth Aether (Ours) G-LoCS LoCS [7] dNRI [6]

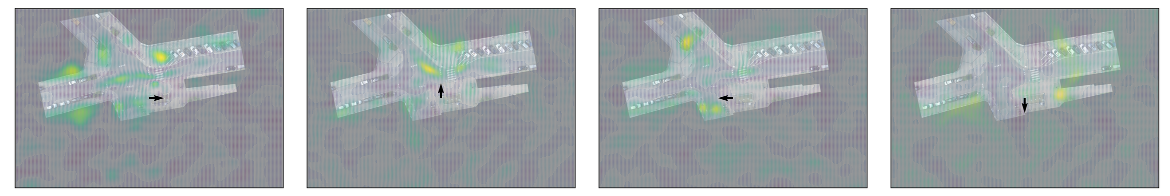


Qualitative results – Discovered fields

Predicted Field Groundtruth Field



Aether can effectively discover the underlying electrostatic field.



Discovered field on inD [1]. For clarity, we only visualize the field for discrete input orientations in $C_4 = \left\{0, \frac{\pi}{2}, \pi, \frac{3\pi}{2}\right\}$.

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