

Selected topics in DL: Equivariance & Dynamics

Preliminary meeting

Unconstrained large-scale learning

User

What is the pH of a 0.10 M solution of NH_4F ? The K_a of NH_4^+ is 5.6×10^{-10} and the K_a of HF is 6.8×10^{-4} .

Thought for 4 seconds ▾

To determine the pH of a 0.10 M solution of ammonium fluoride (NH_4F), we'll need to consider the acid-base properties of its constituent ions when dissolved in water.

Step 1: Dissociation of NH_4F

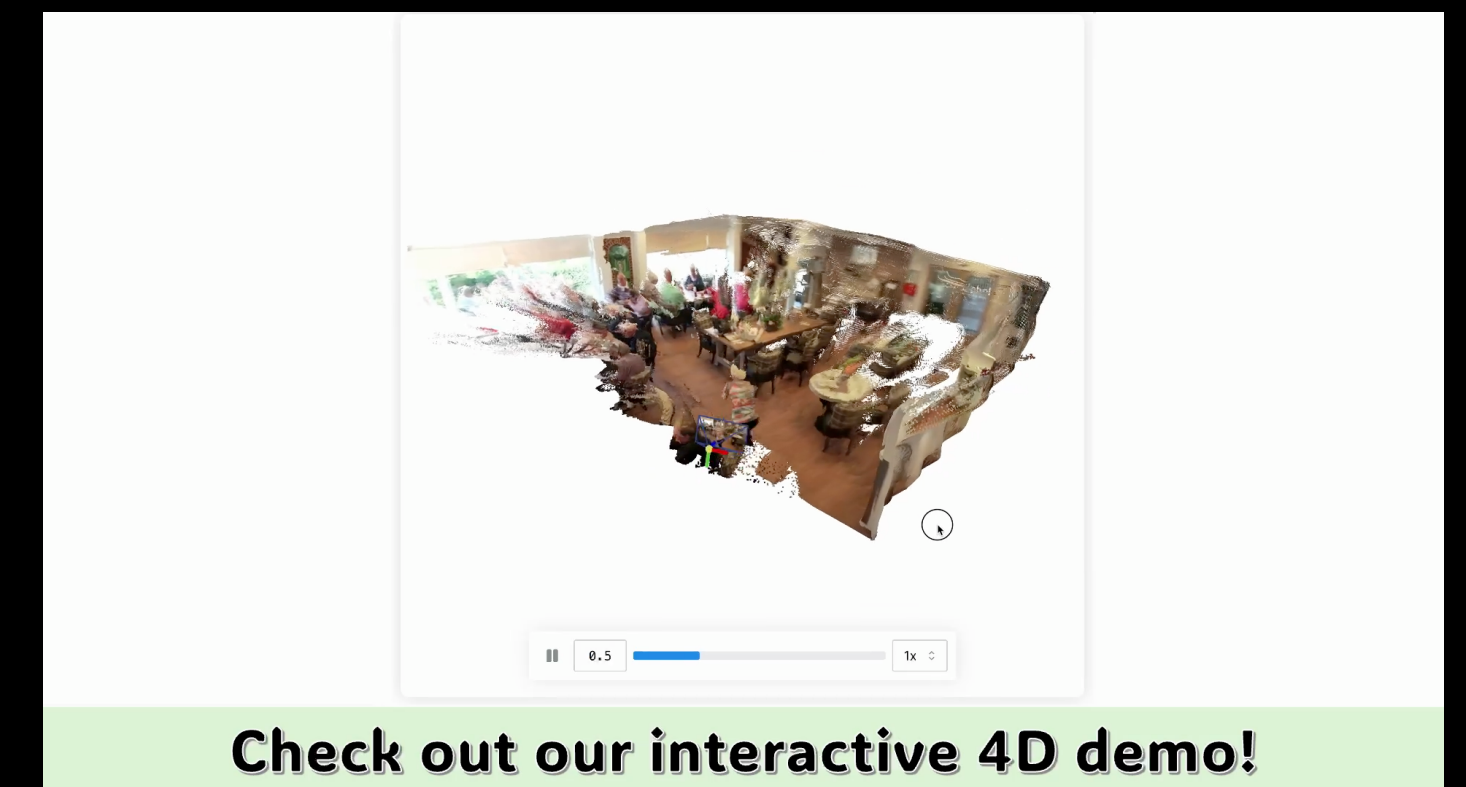
$$\text{NH}_4\text{F} \rightarrow \text{NH}_4^+ + \text{F}^-$$

Both NH_4^+ and F^- can react with water, affecting

Large language models



Segment Anything Model

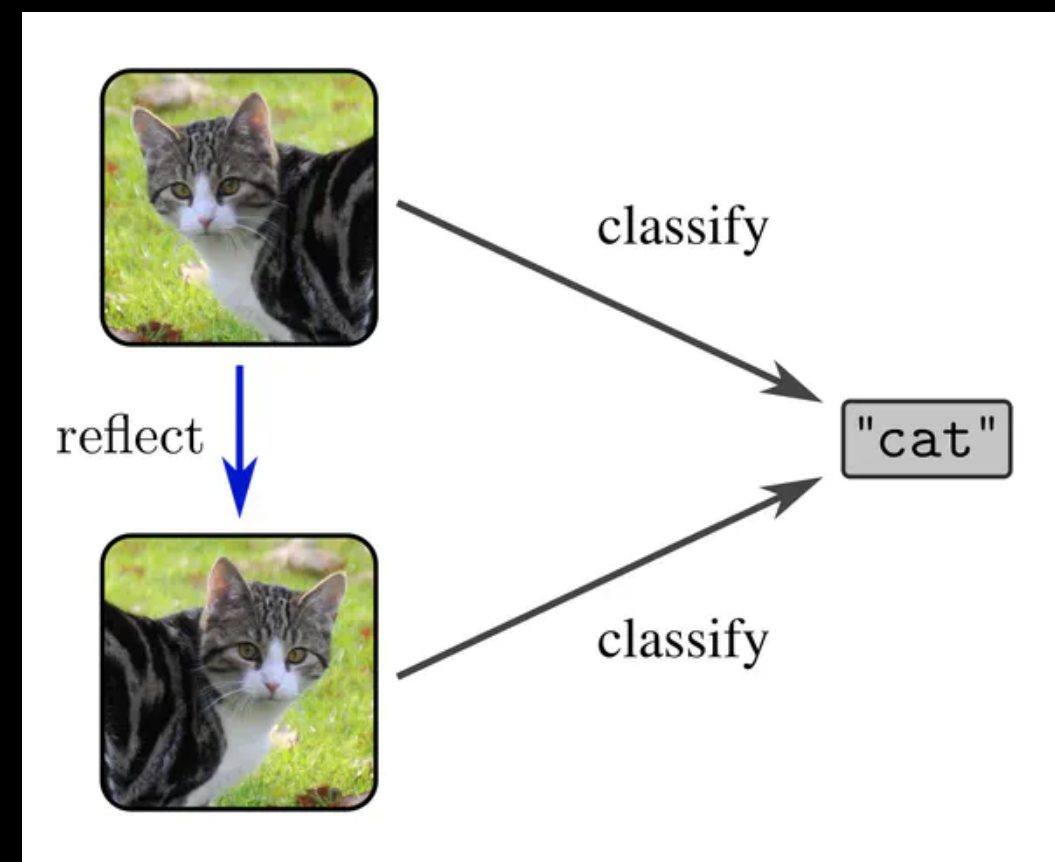


Check out our interactive 4D demo!

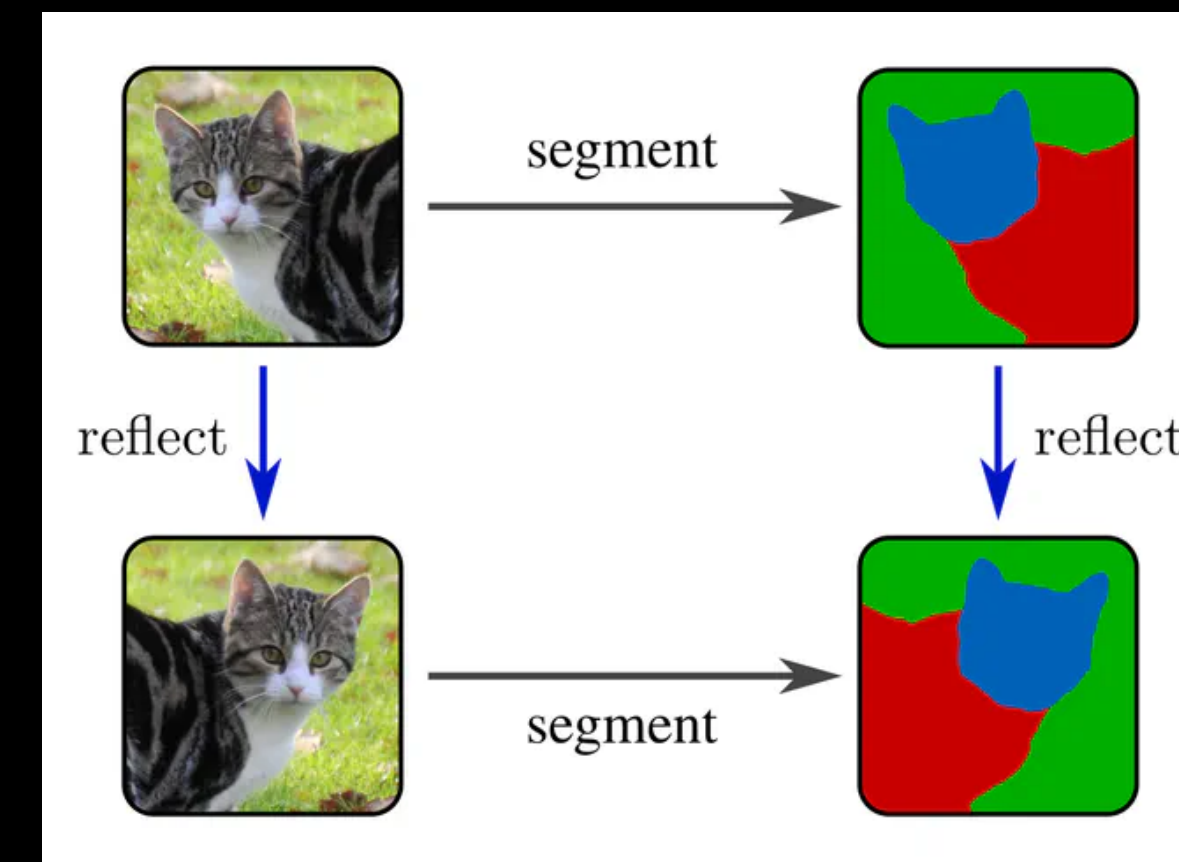
Dynamic Reconstruction
(MonST3R)

Structure-preserving learning

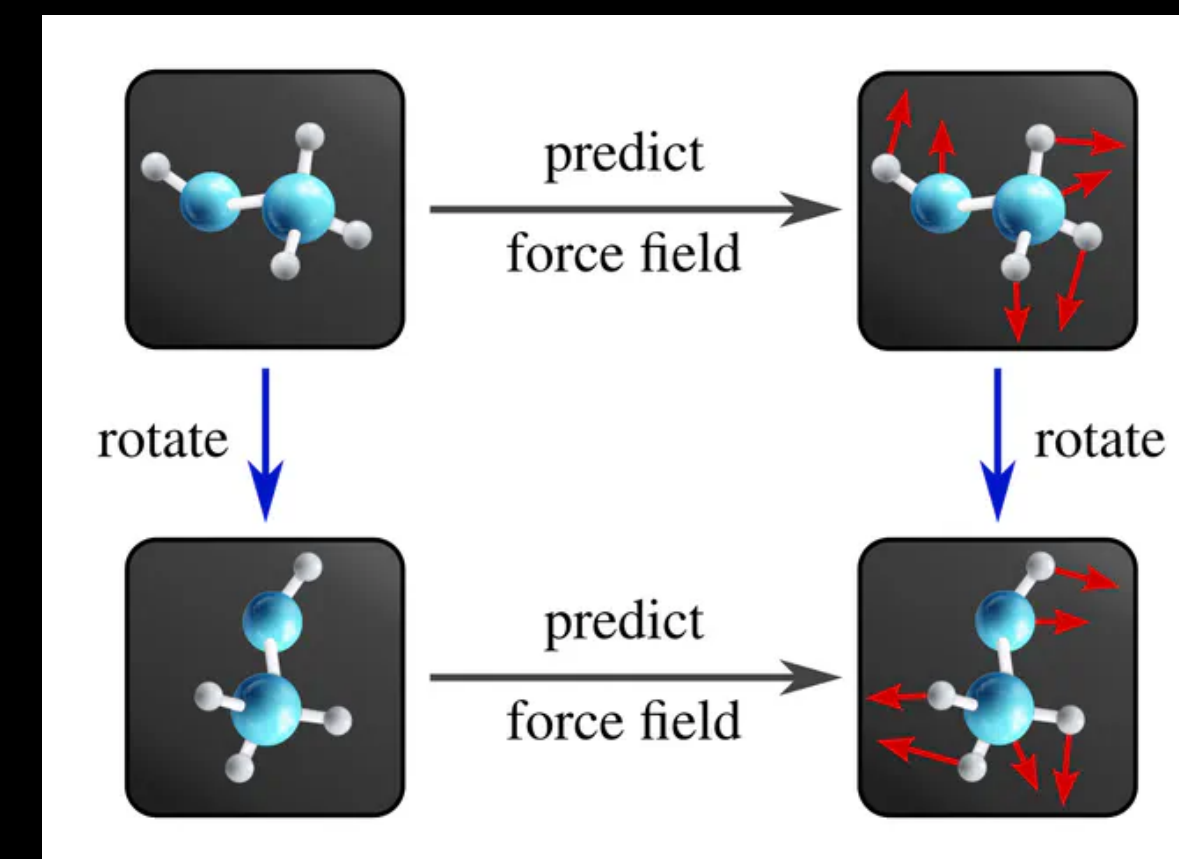
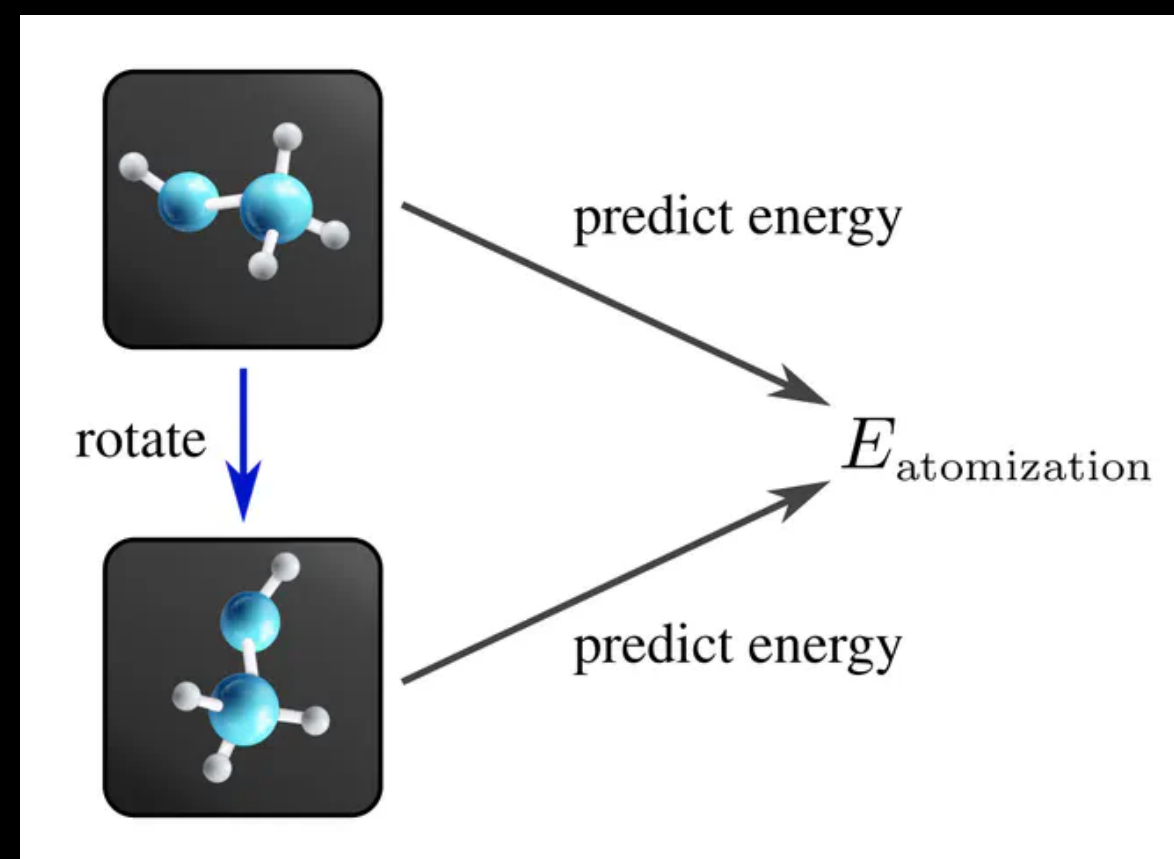
Symmetries



Invariance

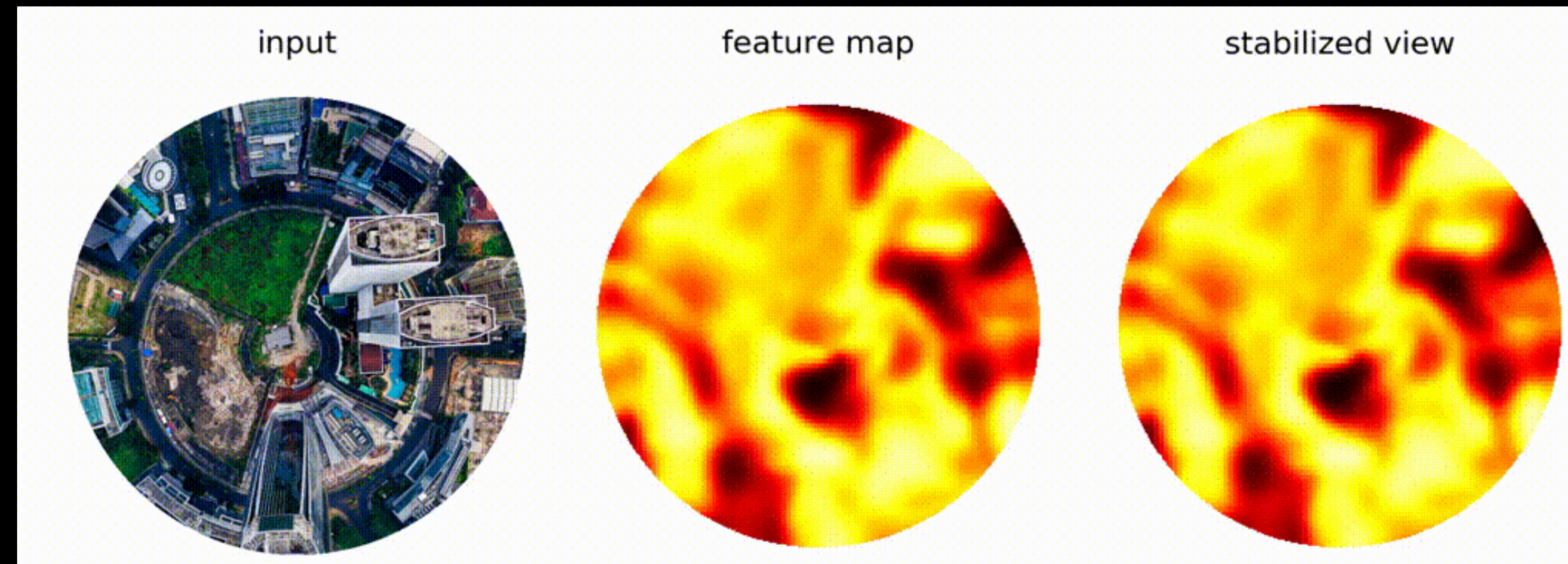


Equivariance

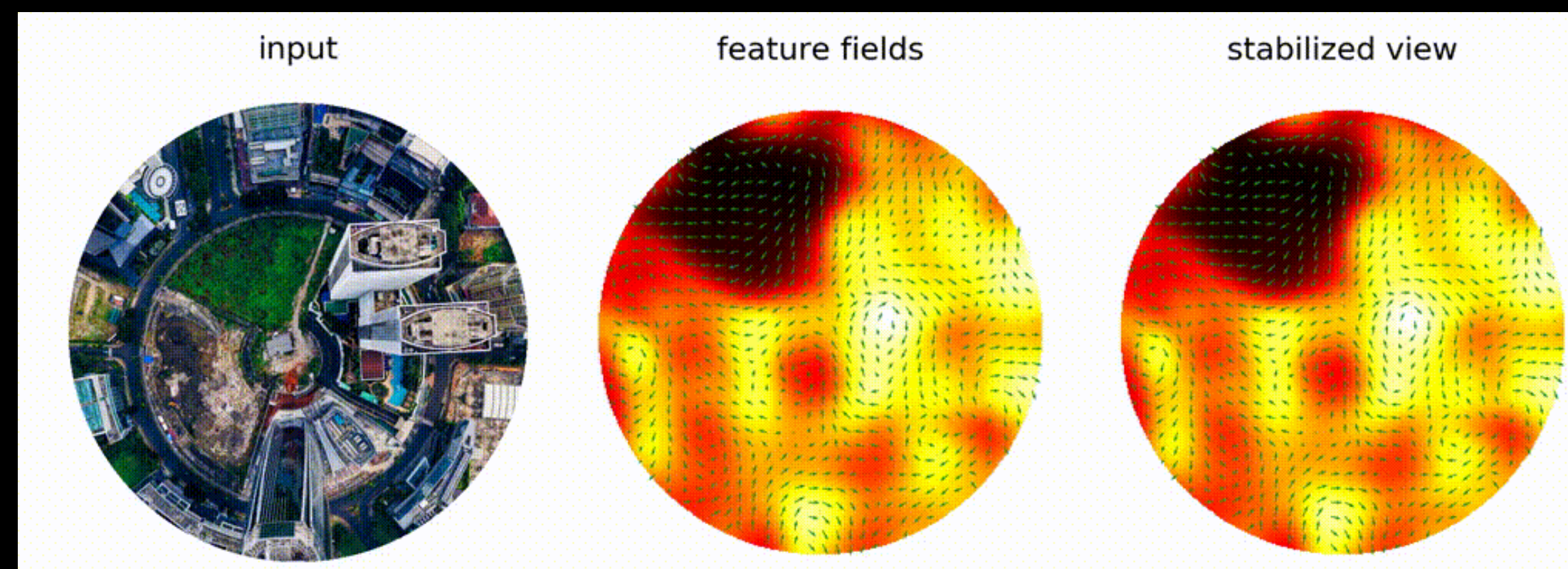


Structure-preserving learning

Symmetries



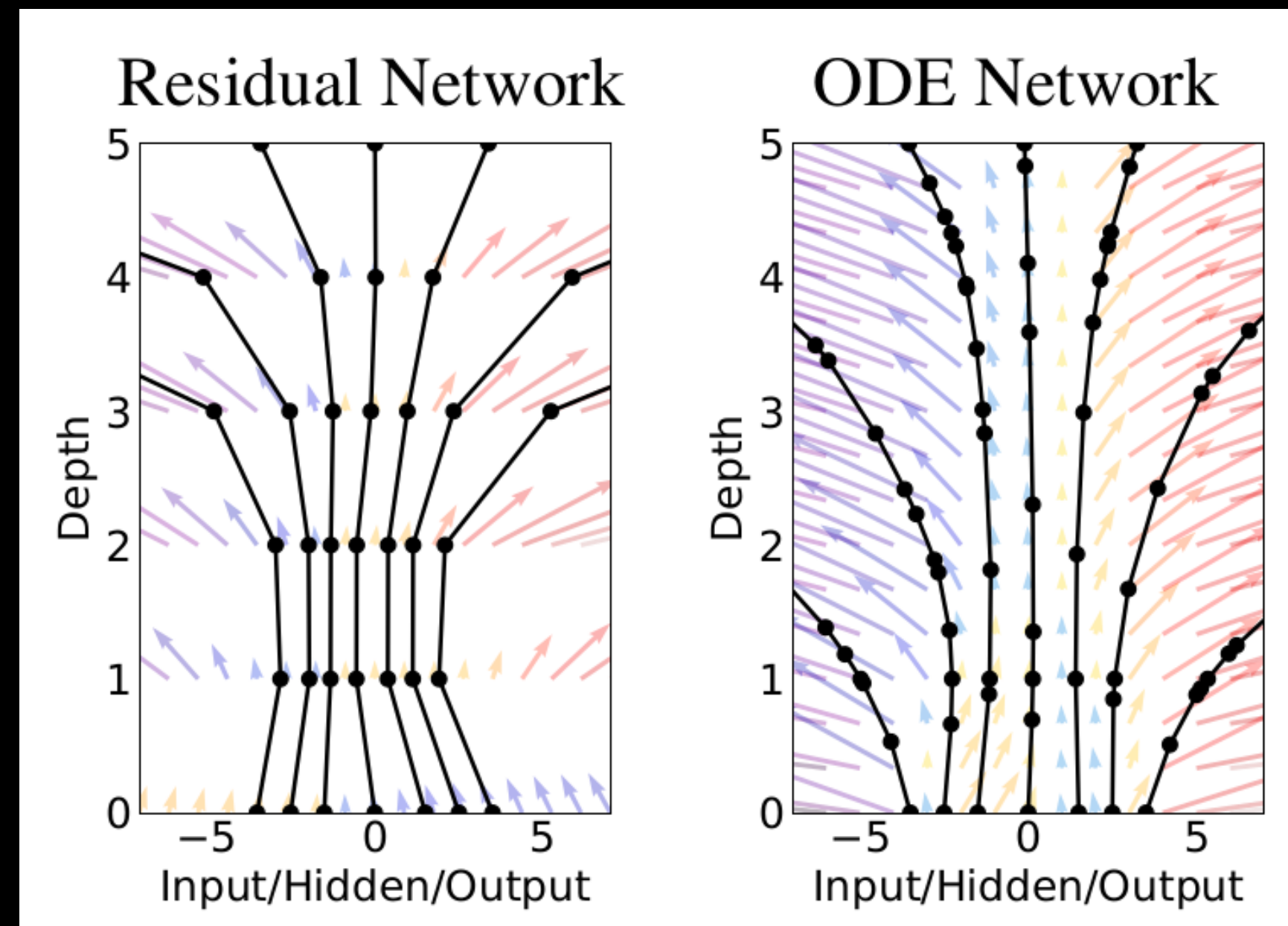
CNN



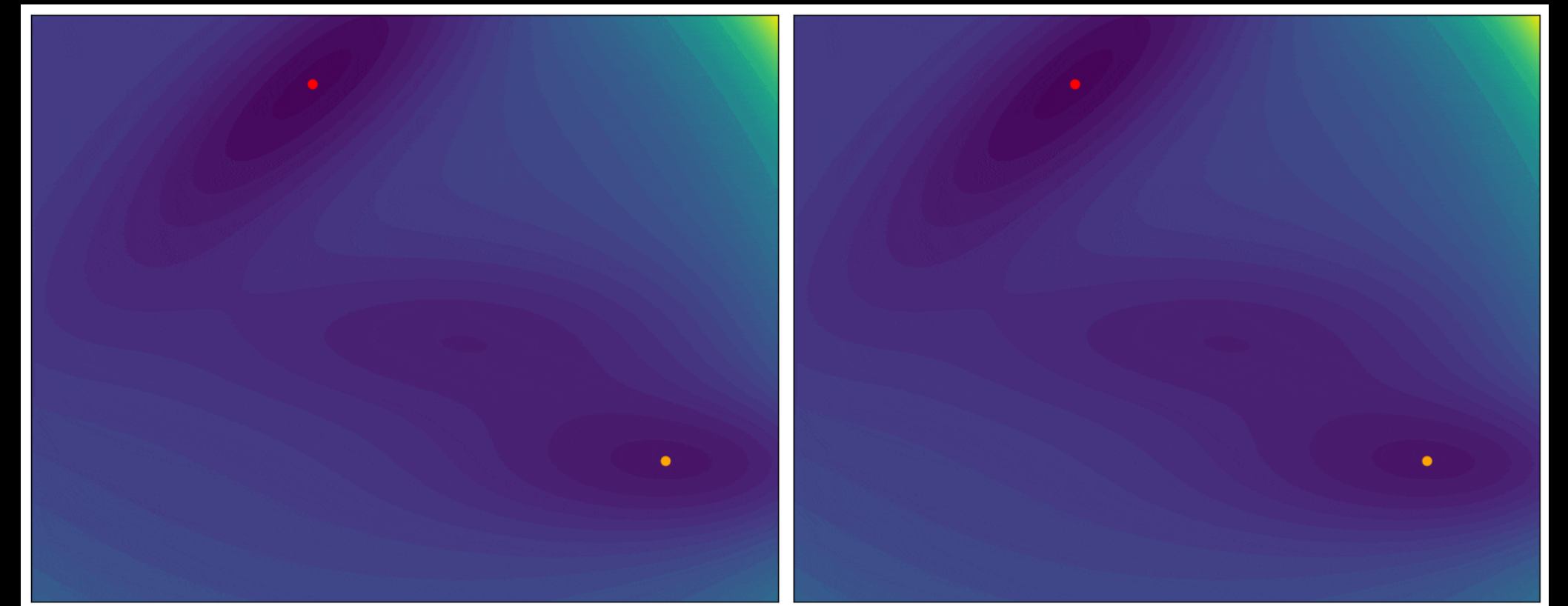
Group-CNN

Structure-preserving learning

Dynamics



Neural ODE
(Chen et al.)

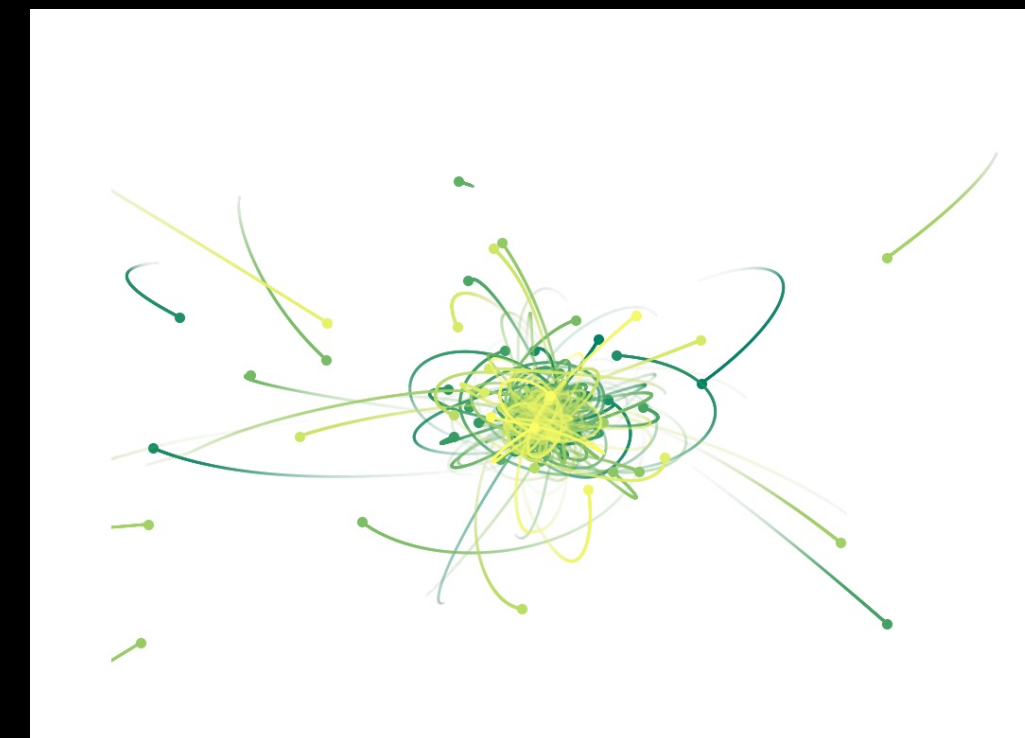


Path Sampling
(Du et al.)

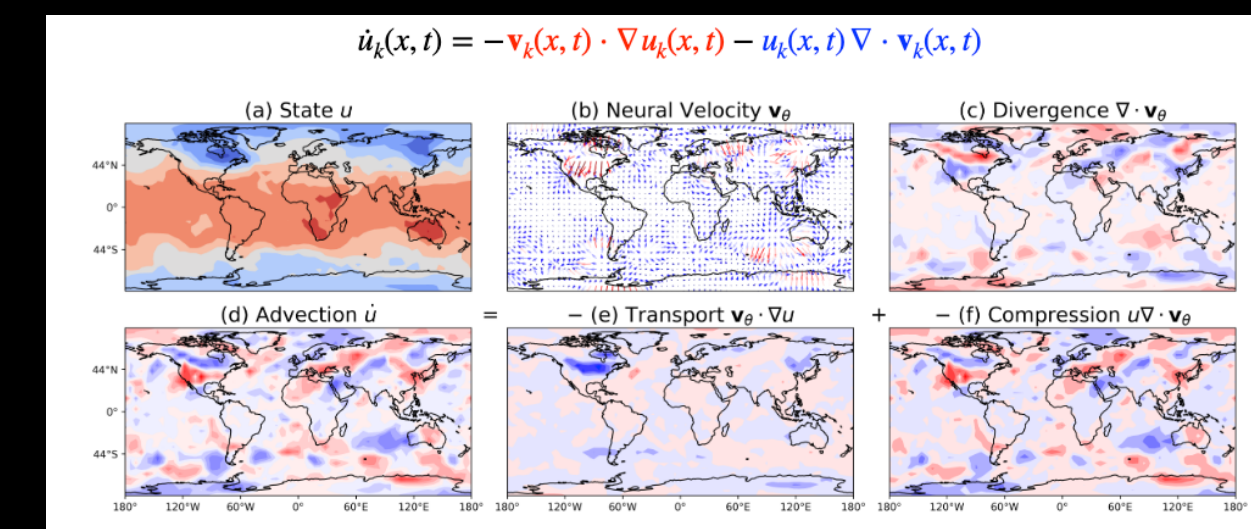
Structure-preserving learning

Applications

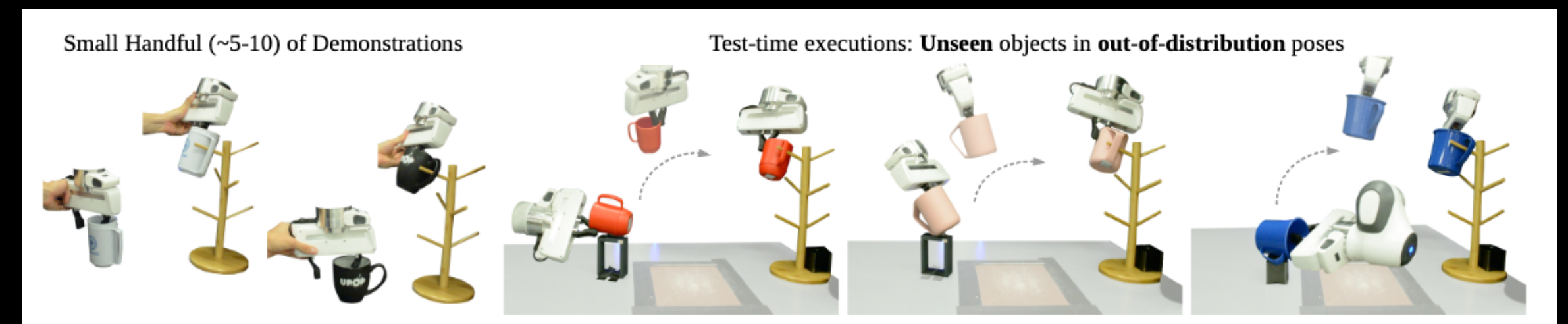
- Architectures with symmetry-preserving guarantees
- Efficient representation learning
 - Data efficiency
 - Compute efficiency*
- Architectures leveraging known dynamics



N-body dynamics



ClimODE



Neural Descriptor Fields

* Brehmer et al., Does Equivariance Matter at Scale?

Structure-preserving learning

Papers

No.	Paper
1	Group Equivariant Convolutional Networks
2	3D Steerable CNNs: Learning Rotationally Equivariant Features in Volumetric Data
3	SE(3)-Transformers: 3D Roto-Translation Equivariant Attention Networks
4	Equivariance with Learned Canonicalization Functions
5	Spherical Channels for Modeling Atomic Interactions
6	E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials
7	Geometric Algebra Transfromers
8	Neural Ordinary Differential Equations
9	Artificial Kuramoto Oscillatory Neurons
10	SE(3)-Stochastic Flow Matching for Protein Backbone Generation
11	Navigating Chemical Space with Latent Flows
12	Action Matching: Learning Stochastic Dynamics from Samples

Logistics*

- Plan to have 10 - 12 participants (through TUM Matching process)
 - Drop me an email so I don't miss your application!
- In-person session every other week
 - Tuesdays 14:30 - 16:30
- Two paper presentations in every session
 - 30 - 35 minutes presentation
 - 10 minutes discussion
- One early 'catch-up' session to review common DL models

Evaluation

- Major component (75%)
 - Paper presentation (40%)
 - Technical report (not a summary) (35%)
- Minor components (25%)
 - One paragraph paper summaries before every session (15%)
 - In-class participation (10%)

Warning

- First offering of the seminar
 - Expect some rough edges!
- Papers are dense in theory
 - ..which also makes it interesting
- I'm not an expert on these topics

Contact

- karnik.ram@tum.de
- CIT, 02.08.038
- <https://cvg.cit.tum.de/teaching/ss2025/dl-equi-dynam>