Selected topics in DL: Equivariance & Dynamics

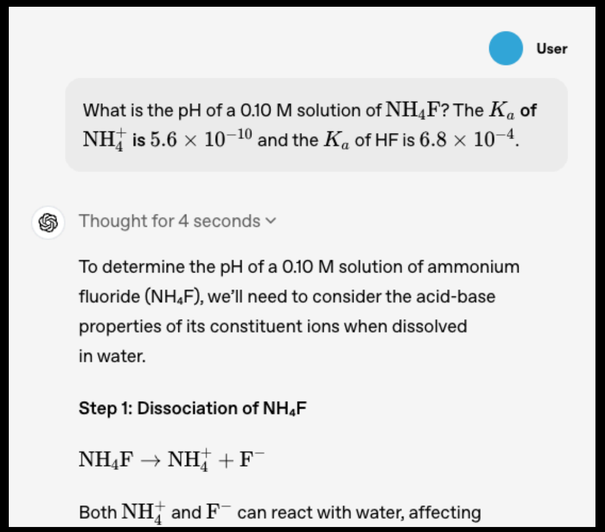
Preliminary meeting

CVG, 11.07.2025

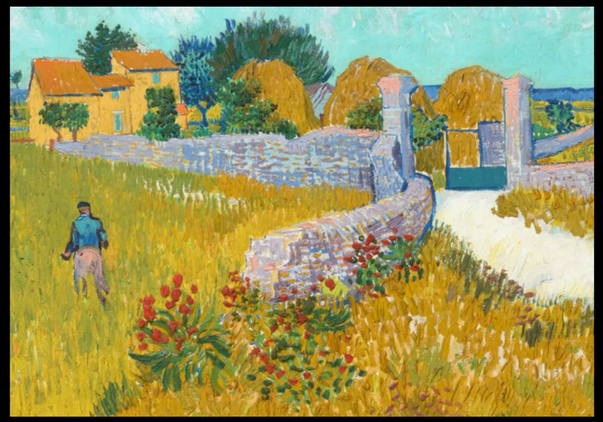
About me

- 2nd year PhD student in the Computer Vision Group
- Research focus: Machine learning for molecular science
  - Neural free energies for dynamical density functional theory
  - Interaction potentials for lattice-based simulations
- Application focus: Material discovery for carbon capture

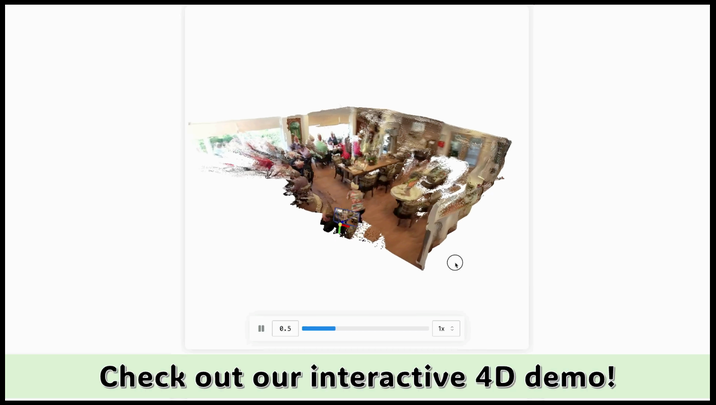
Unconstrained large-scale learning



Large language models



Segment Anything Model



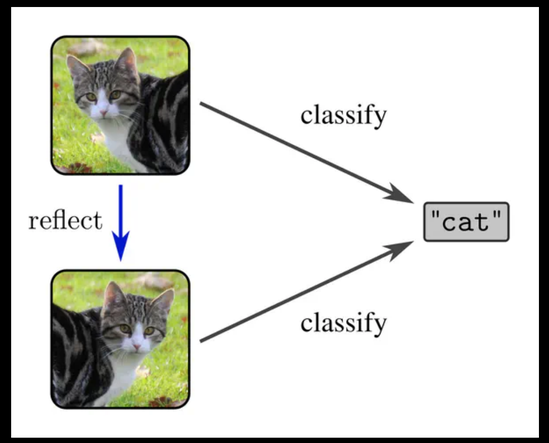
Dynamic Reconstruction (MonST3R)

Unconstrained large-scale learning

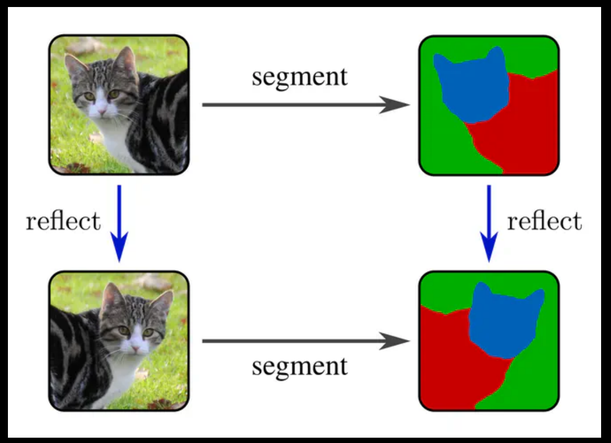
Is attention and scaling all you need?

Structure-preserving learning

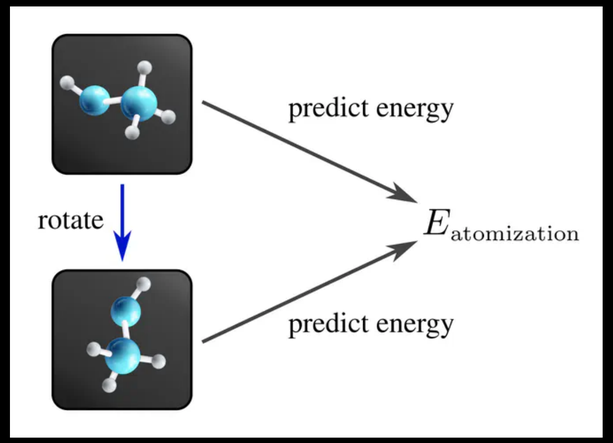
Symmetries

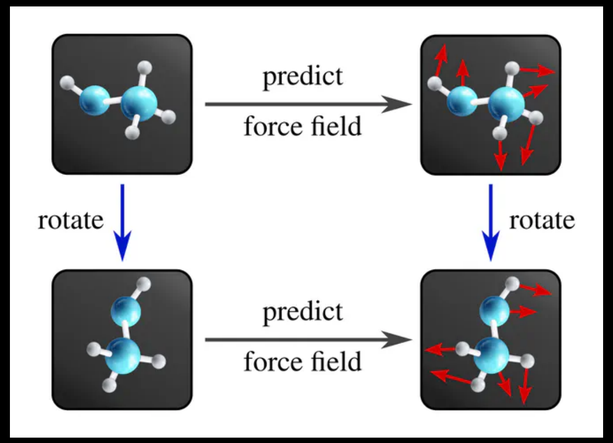


Invariance



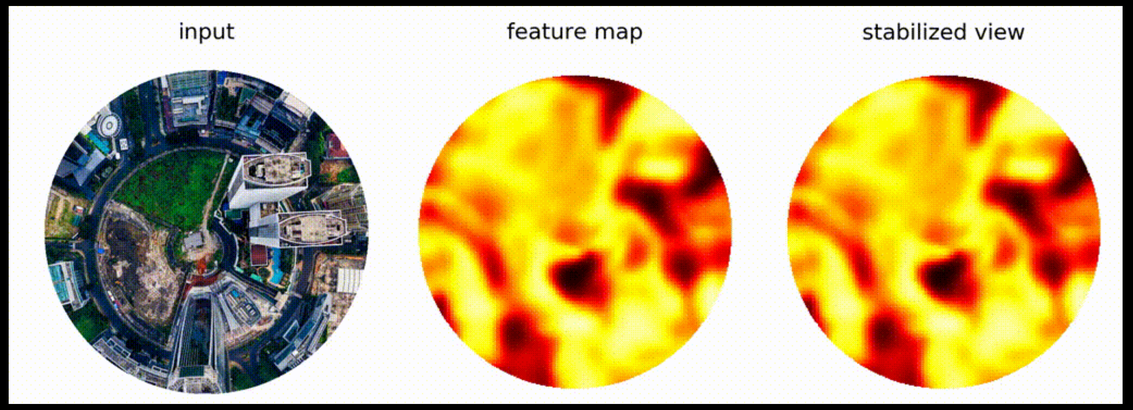
Equivariance



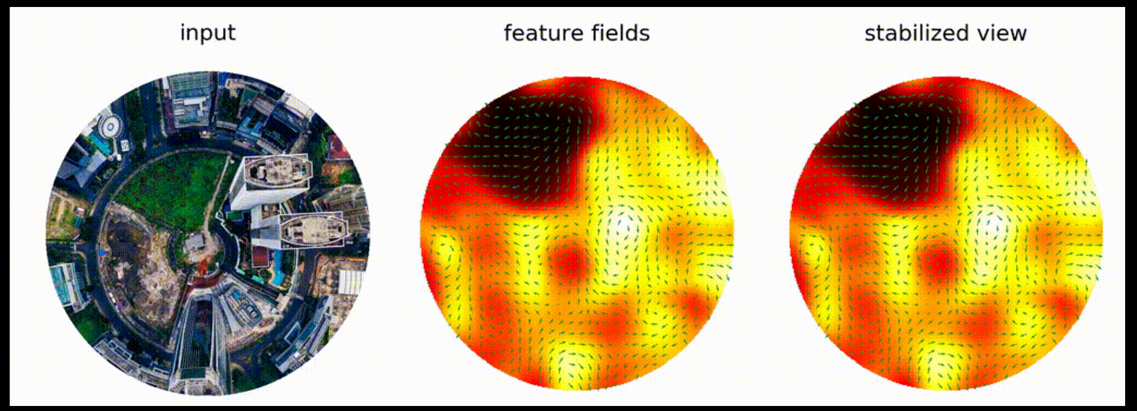


Structure-preserving learning

Symmetries



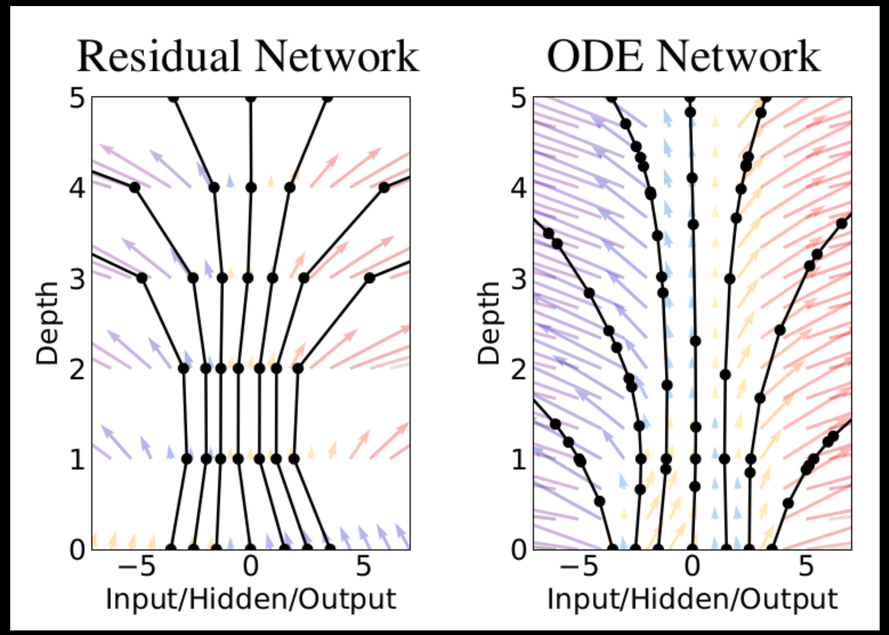
CNN



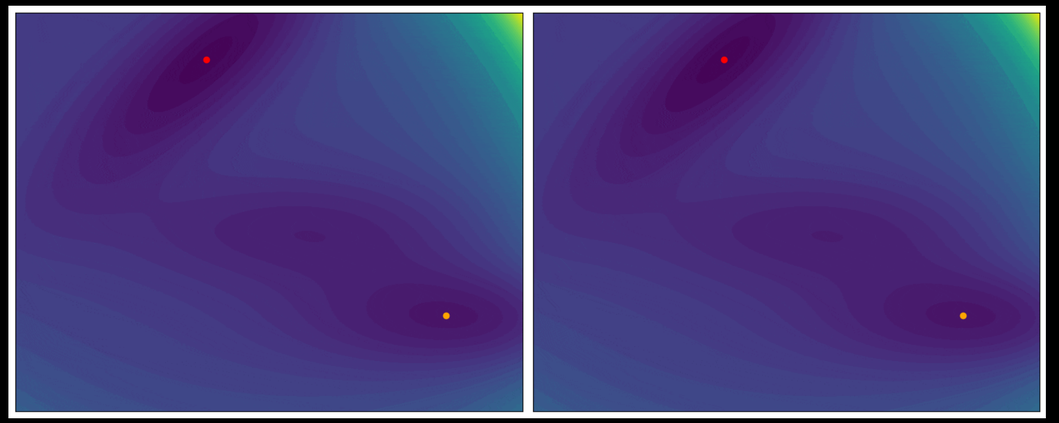
Group-CNN

Structure-preserving learning

Dynamics



Neural ODE
(Chen et al.)

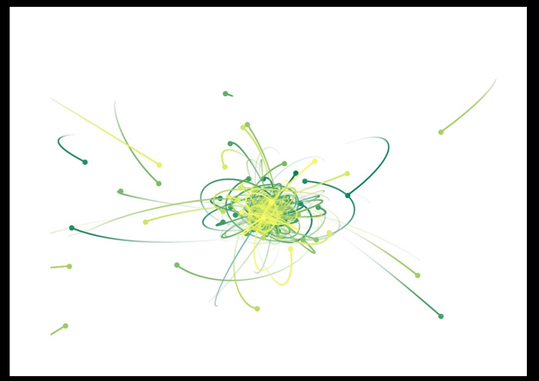


Path Sampling
(Du et al.)

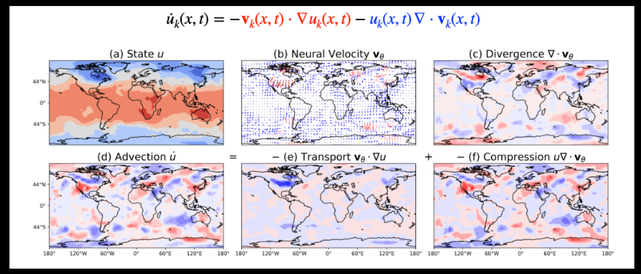
Structure-preserving learning

Applications

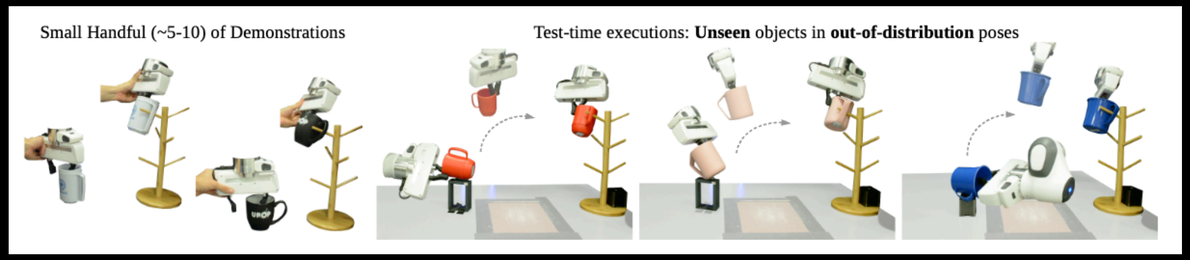
- Architectures with symmetry-preserving guarantees
- Efficient representation learning
  - Data efficiency
  - Compute efficiency*
- Architectures leveraging known dynamics



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

https://cvg.cit.tum.de/teaching/ss2025/dl-equi-dynam

Logistics*

- Plan to have 10 - 12 participants (from both TUM Math and TUM Informatik matching)
  - 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

* tentative

Evaluation

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

Why should you take this seminar

- Good overview of important papers and ideas in the sub-fields
- Get familiar with a useful toolkit for “AI4Science” problems and beyond
- Interesting theory inspired from mathematical physics and PDE communities
- Experience giving presentation, participating in discussions, and writing critical research review

Contact

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- CIT, 02.08.039

- https://cvg.cit.tum.de/teaching/ws2025/dl-equi-dynam