

Soft geometric inductive bias

for object centric dynamics

Soft Geometric Inductive Bias for Object Centric Dynamics

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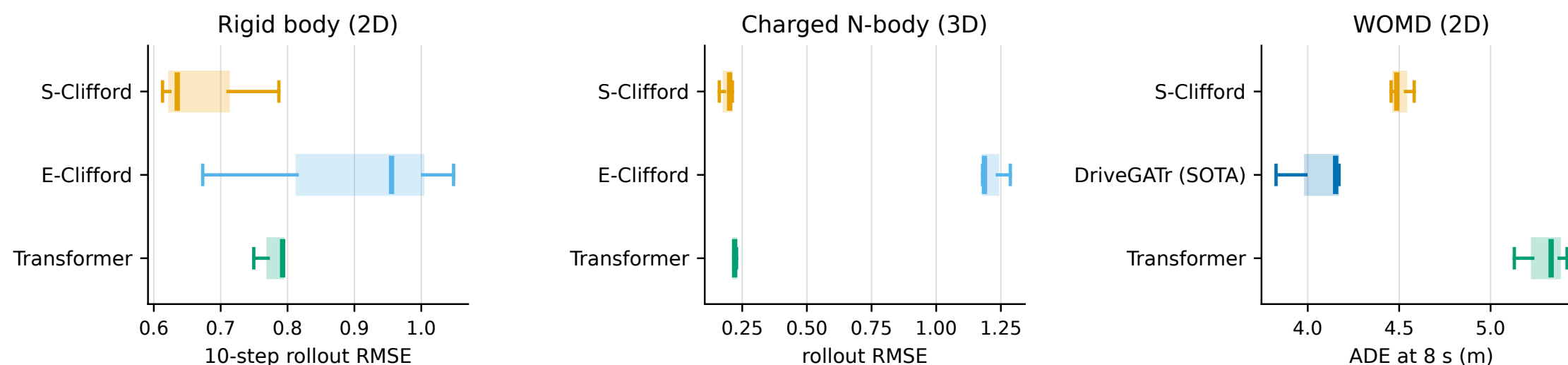
Christopher L Buckley³

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Max Planck Institute of Animal Behavior

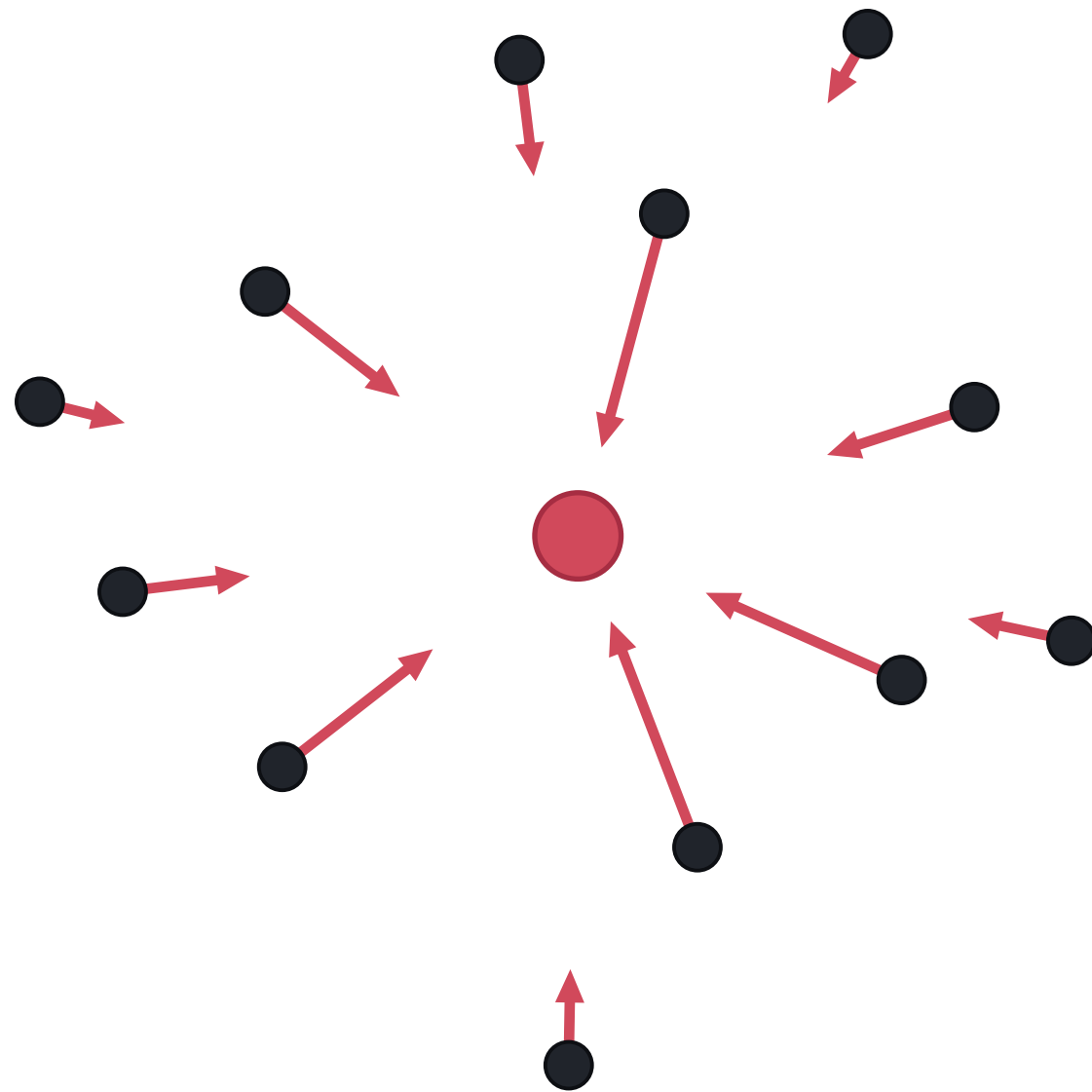
⁴Kodamai

³Department of Informatics
University of Sussex



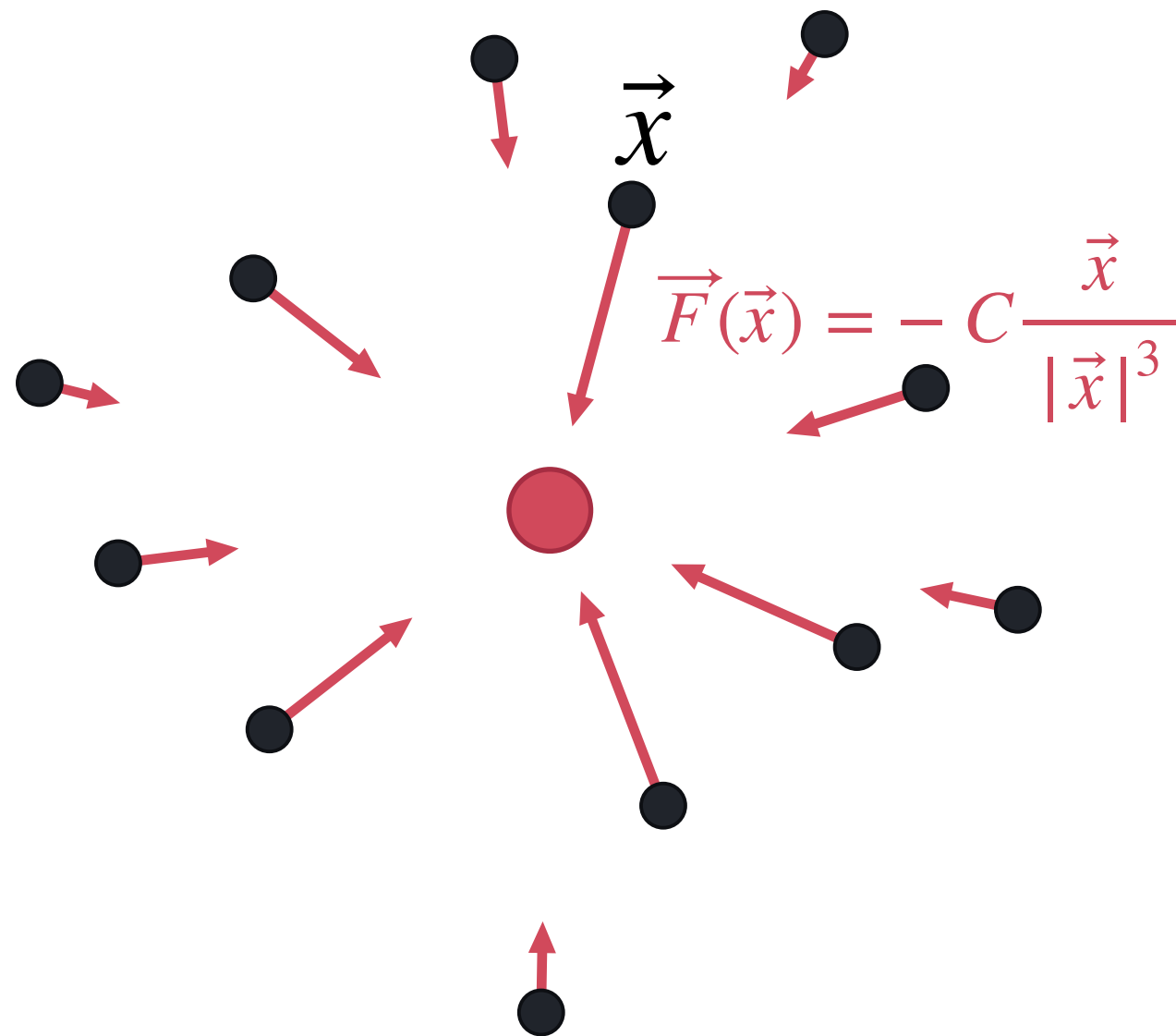
Inductive bias

Example: learn force field between two charged particles



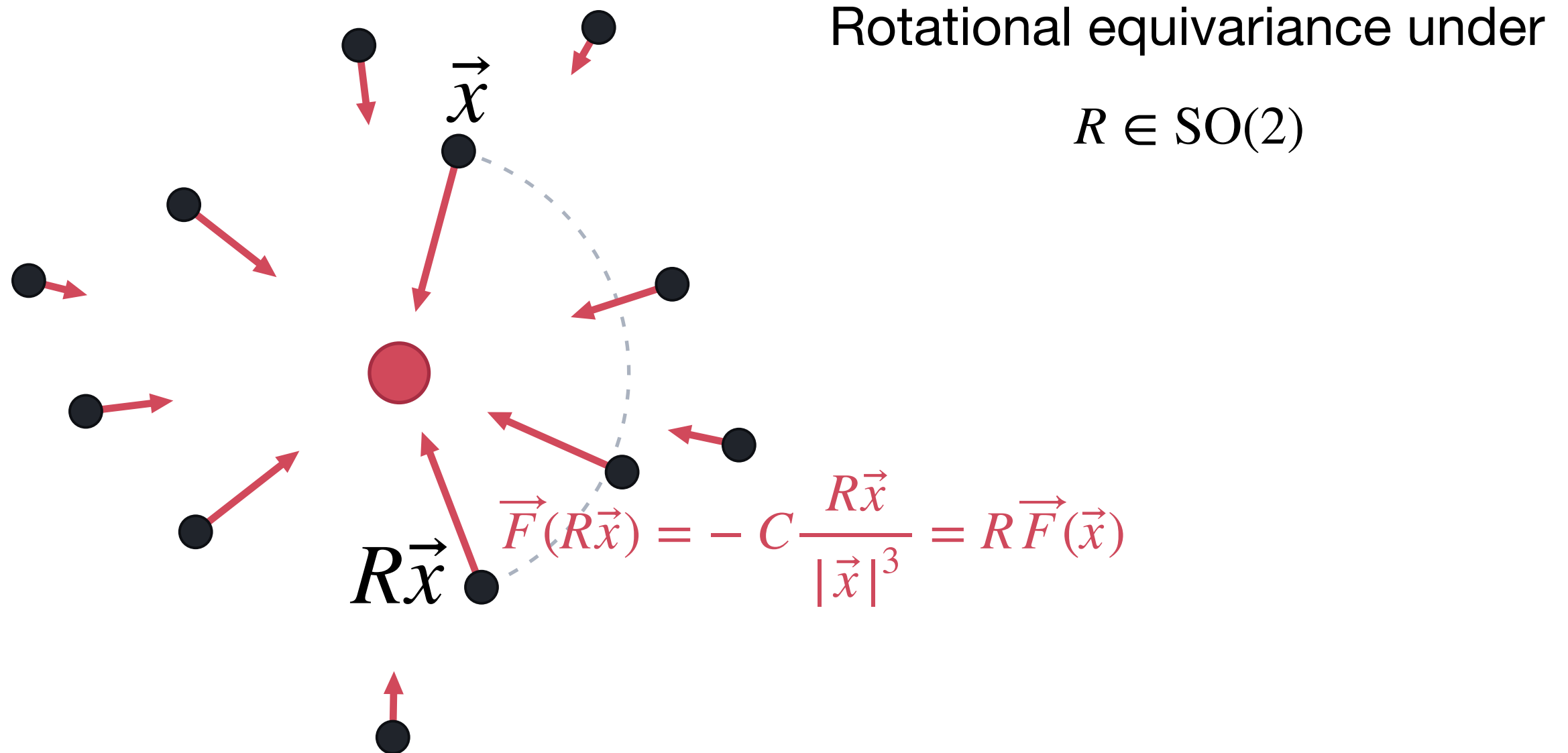
Inductive bias

Example: learn force field between two charged particles



Inductive bias

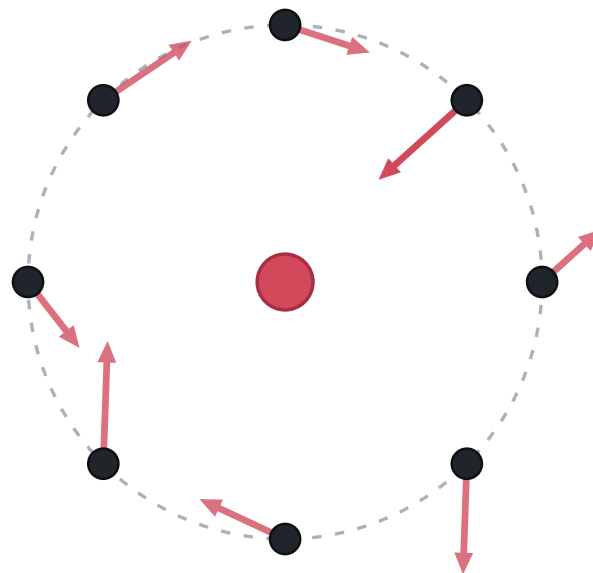
Example: learn force field between two charged particles



Inductive bias

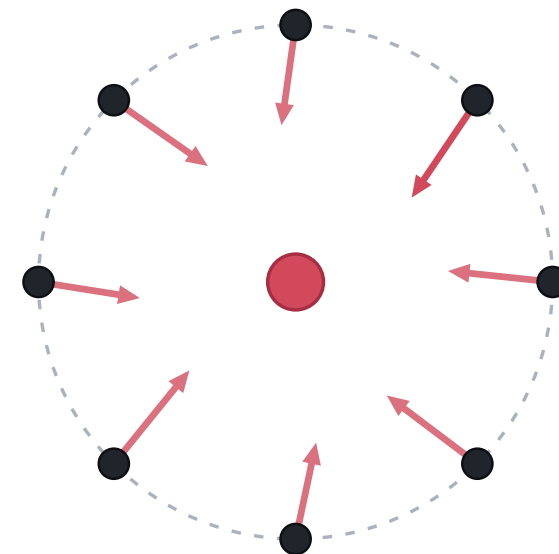
Equivariance

Untrained

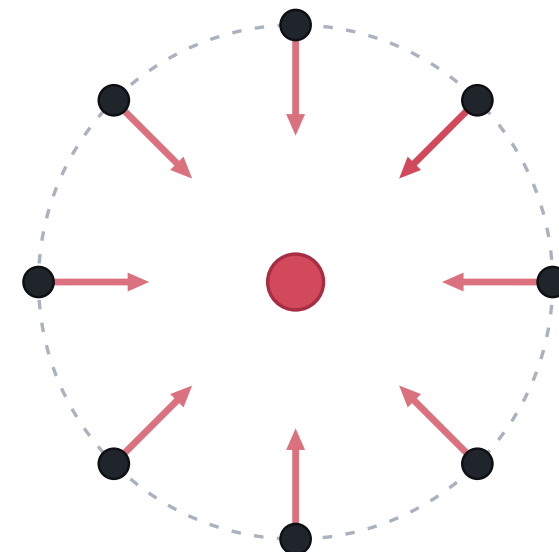
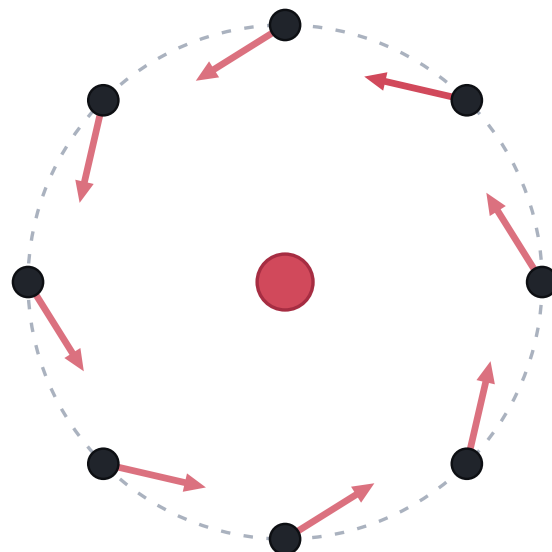


Unconstrained
model

Trained

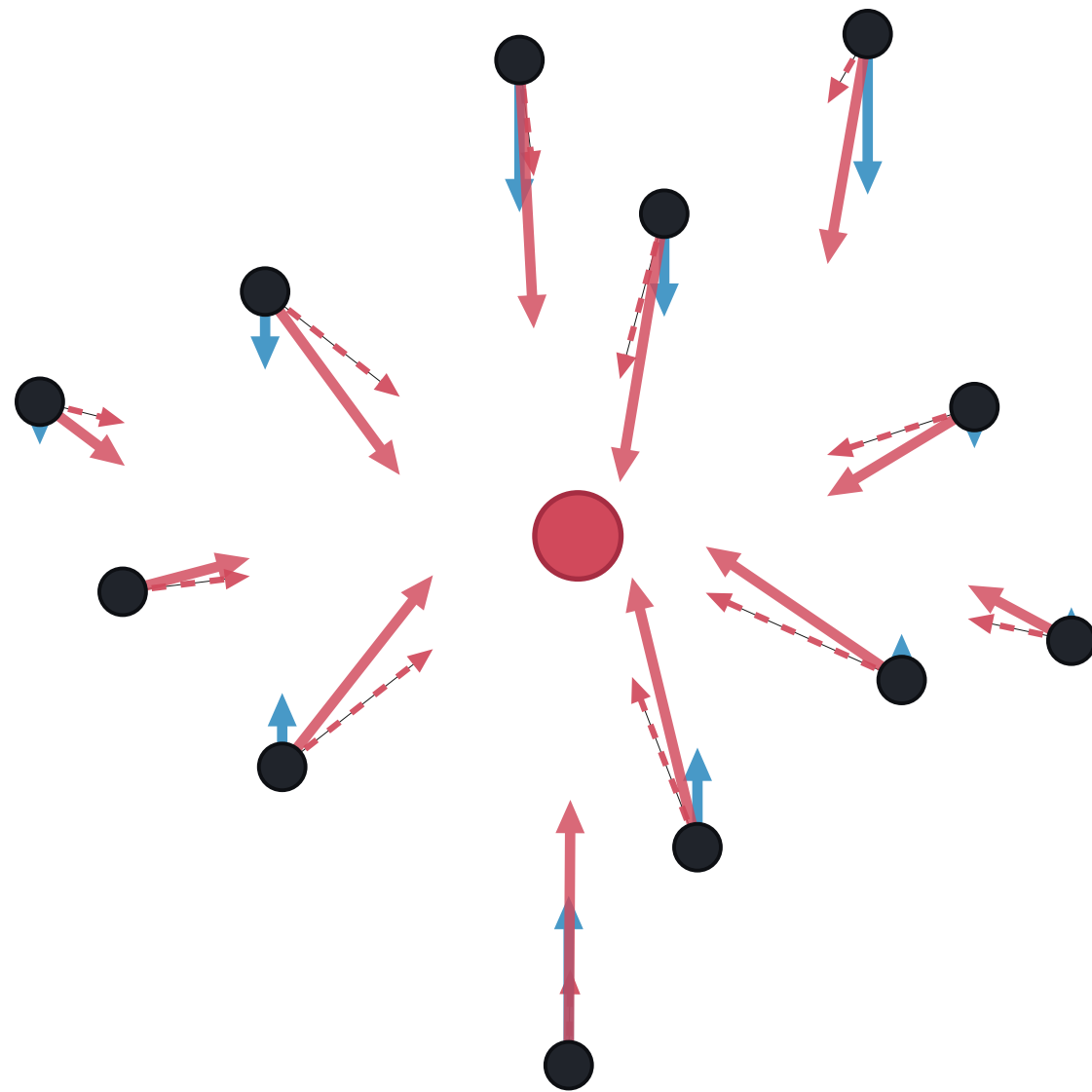


Equivariant
model



Broken equivariance

Example: anisotropic potential



Approximate symmetry

Prior work

Boundary conditions

Omitted context

External forces

$$f(gx) \neq gf(x)$$

Noise

$$f(gx, gc) = gf(x, c)$$

Finzi et al., “Residual Pathway Priors for Soft Equivariance Constraints,” **NeurIPS**, 2021.

Wang et al., “Approximately Equivariant Networks for Imperfectly Symmetric Dynamics,” **ICML**, 2022.

Romero et al., “Learning Partial Equivariances From Data,” **NeurIPS**, 2022.

van der Ouderaa et al., “Relaxing Equivariance Constraints with Non-stationary Continuous Filters,” **NeurIPS**, 2022.

Kim et al., “Regularizing Towards Soft Equivariance Under Mixed Symmetries,” **ICML**, 2023.

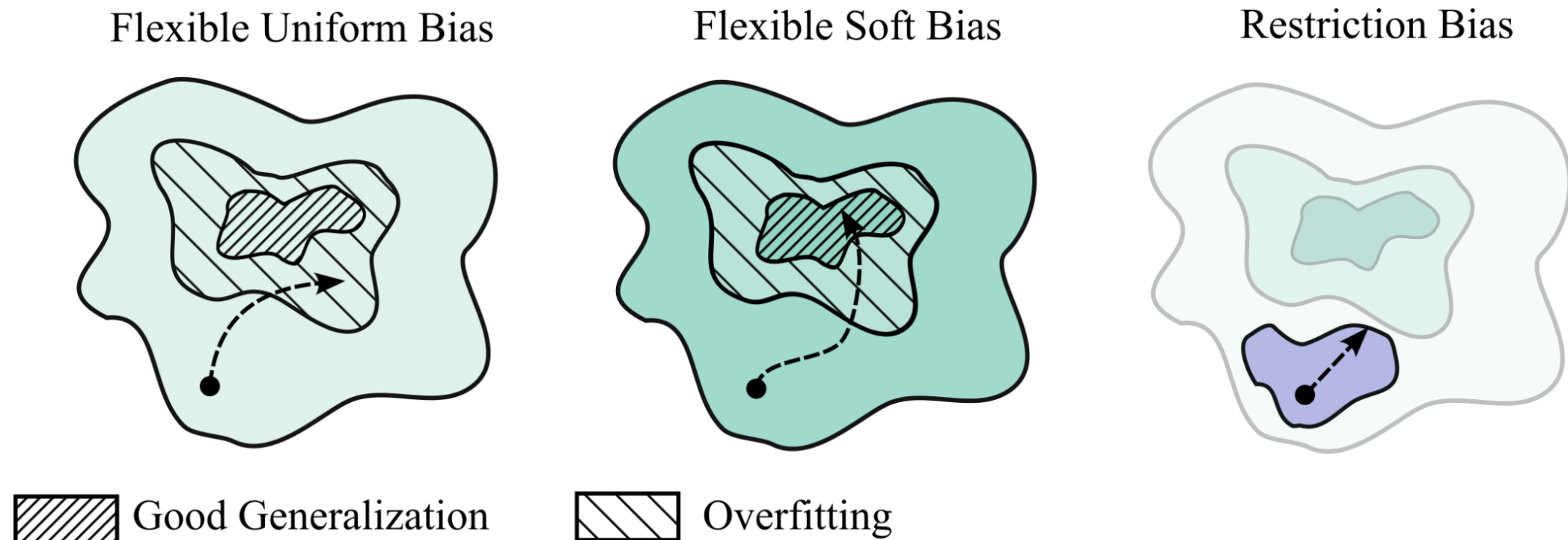
Petrache et al., “Approximation-Generalization Trade-offs under (Approximate) Group Equivariance,” **NeurIPS**, 2023.

Huang et al., “Approximately Equivariant Graph Networks,” **NeurIPS**, 2023.

Ashman et al., “Approximately Equivariant Neural Processes,” **NeurIPS**, 2024

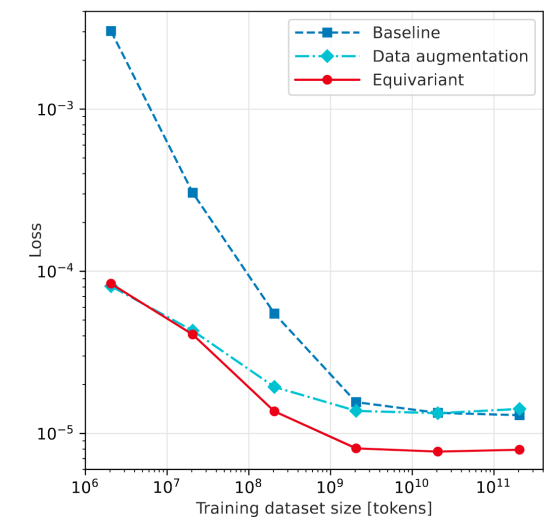
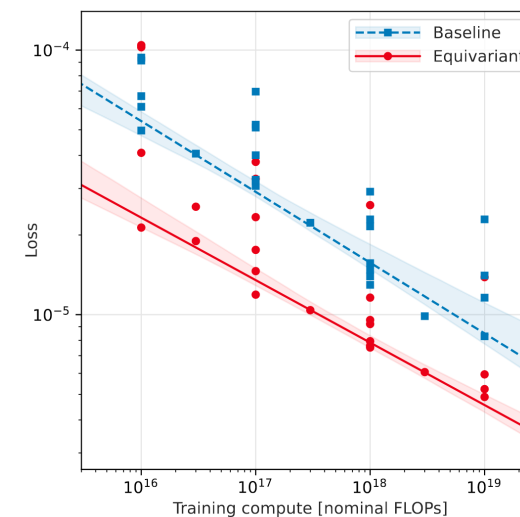
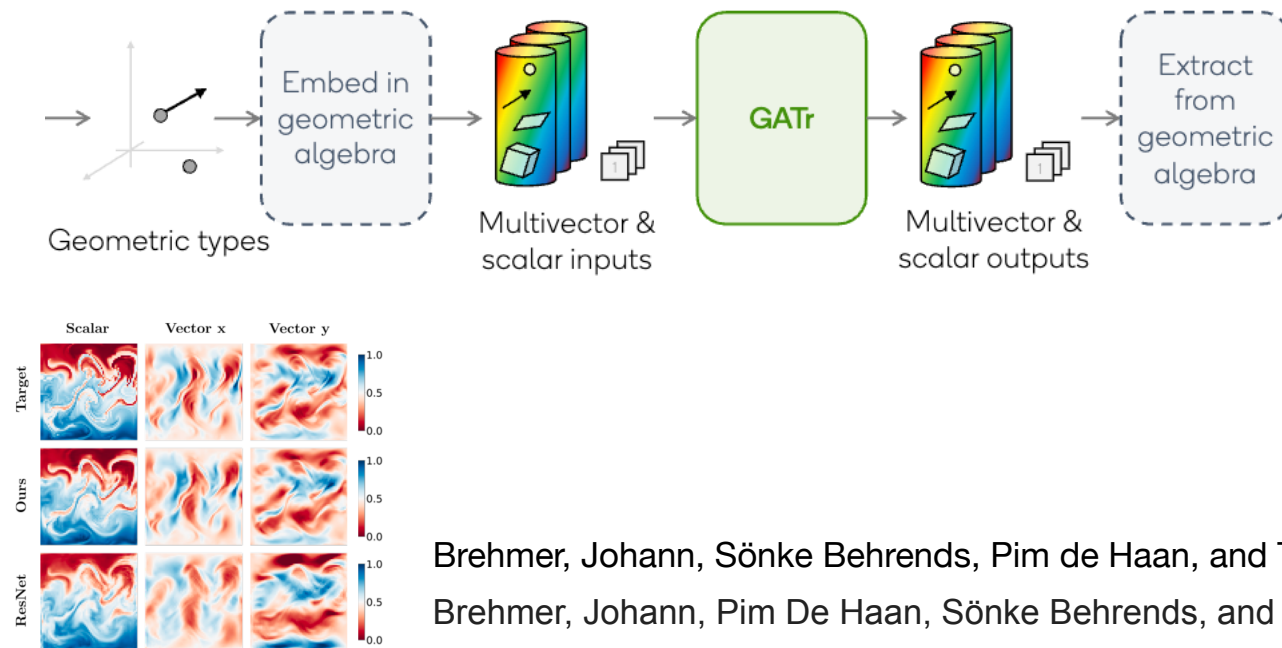
Inductive bias

What is the right amount?



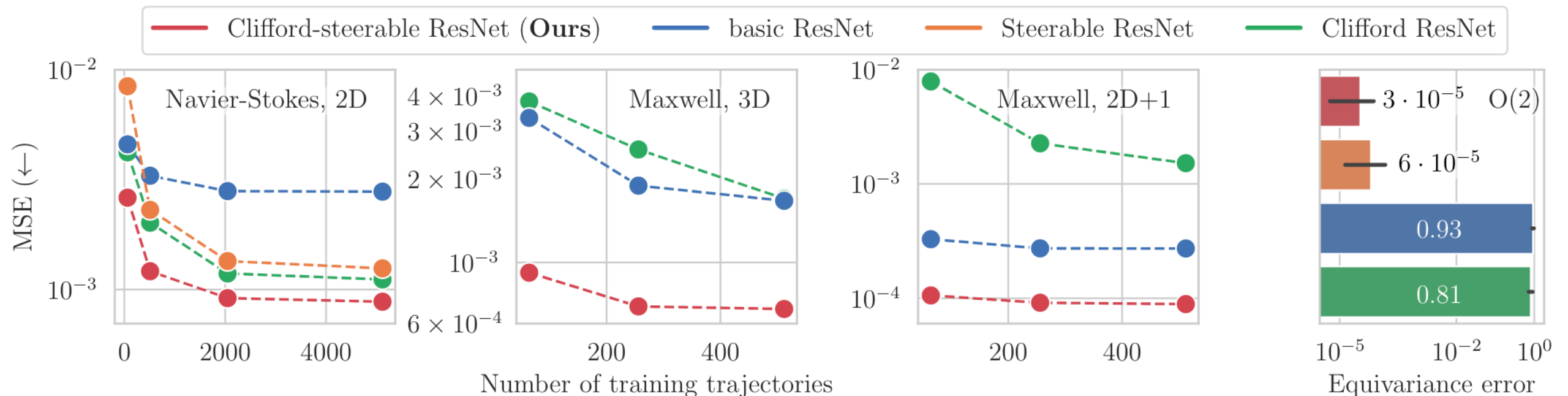
Geometric inductive bias

Clifford algebra neural networks



Brehmer, Johann, Sönke Behrends, Pim de Haan, and Taco Cohen. "Does Equivariance Matter at Scale?" **TMLR**, arXiv:2410.23179

Brehmer, Johann, Pim De Haan, Sönke Behrends, and Taco S. Cohen. "Geometric algebra transformer." **NeurIPS 2023**



Zhdanov, Maksim, David Ruhe, Maurice Weiler, Ana Lucic, Johannes Brandstetter, and Patrick Forré. "Clifford-steerable convolutional neural networks." **ICML 2024**

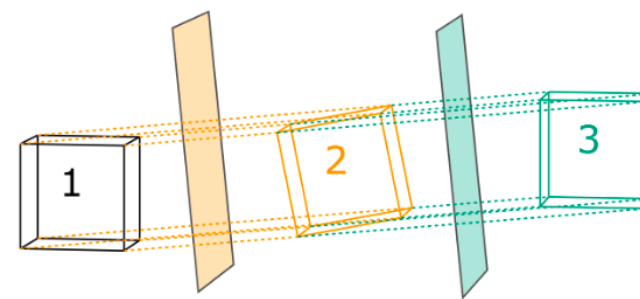
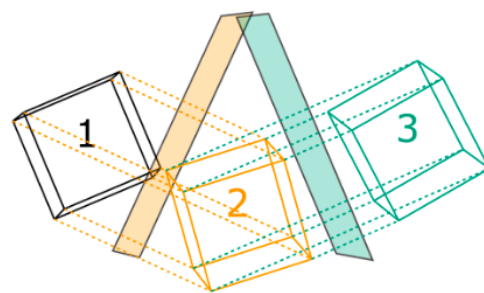
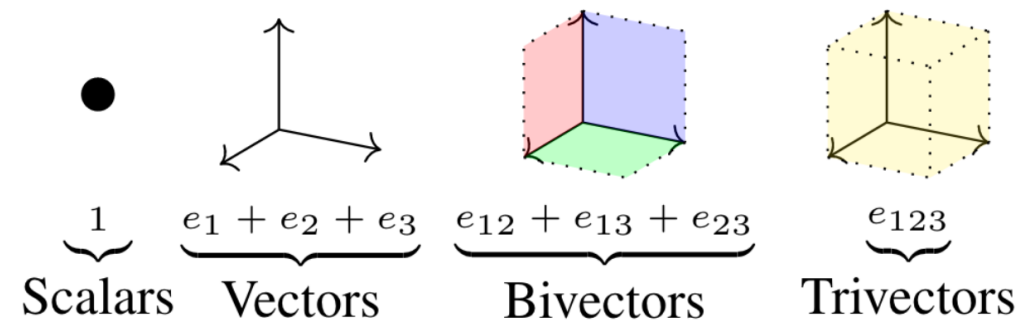
Geometric inductive bias

Clifford algebra / Geometric algebra

$$\mathbf{e}_i \mathbf{e}_i \in \{+1, -1, 0\}$$

$$\mathbf{e}_i \mathbf{e}_j = -\mathbf{e}_j \mathbf{e}_i \quad (i \neq j)$$

$$x = x_s + x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + x_3 \mathbf{e}_3 + x_{12} \mathbf{e}_1 \mathbf{e}_2 + x_{13} \mathbf{e}_1 \mathbf{e}_3 + x_{23} \mathbf{e}_2 \mathbf{e}_3 + x_{123} \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3$$



Ruhe, David, Jayesh K. Gupta, Steven De Keninck, Max Welling, and Johannes Brandstetter. "Geometric clifford algebra networks." ICML, 2023.

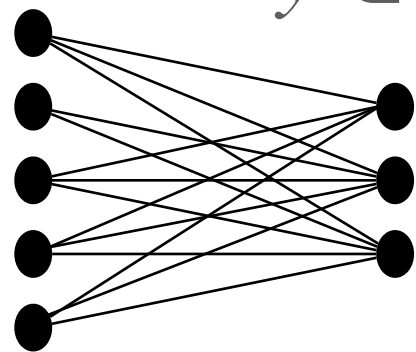
Brehmer, Johann, Pim de Haan, Sönke Behrends, and Taco Cohen. "Geometric Algebra Transformer," NeurIPS 2023

Geometric inductive bias

Clifford algebra neural networks

MLP

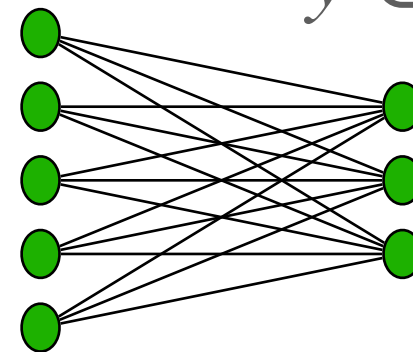
$x \in \mathbb{R}^m$
 $y \in \mathbb{R}^n$



$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

Clifford MLP

$x \in \mathbb{R}^m \times \mathbb{R}^8$
 $y \in \mathbb{R}^n \times \mathbb{R}^8$



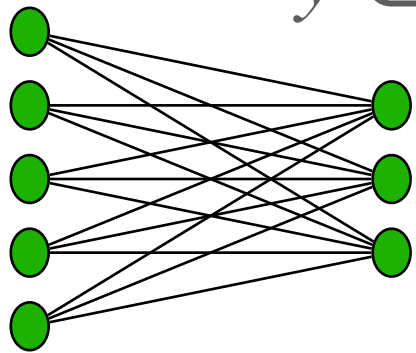
$$\begin{bmatrix} \mathbf{a}_{11} & \mathbf{a}_{12} & \cdots & \mathbf{a}_{1m} \\ \mathbf{a}_{21} & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_{n1} & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nm} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_m \end{bmatrix}$$

Geometric inductive bias

Clifford algebra: implementation

$$x \in \mathbb{R}^m \times \mathbb{R}^8$$

$$y \in \mathbb{R}^n \times \mathbb{R}^8$$



$$\begin{bmatrix} \mathbf{a}_{11} & \mathbf{a}_{12} & \cdots & \mathbf{a}_{1m} \\ \mathbf{a}_{21} & \mathbf{a}_{22} & \cdots & \mathbf{a}_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_{n1} & \mathbf{a}_{n2} & \cdots & \mathbf{a}_{nm} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_m \end{bmatrix}$$

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

$$\mathbf{y}^i(x) = \mathbf{a}^{ij} \mathbf{x}_j = (a^{ij\alpha} \mathbf{e}_\alpha)(x_j^\beta \mathbf{e}_\beta)$$

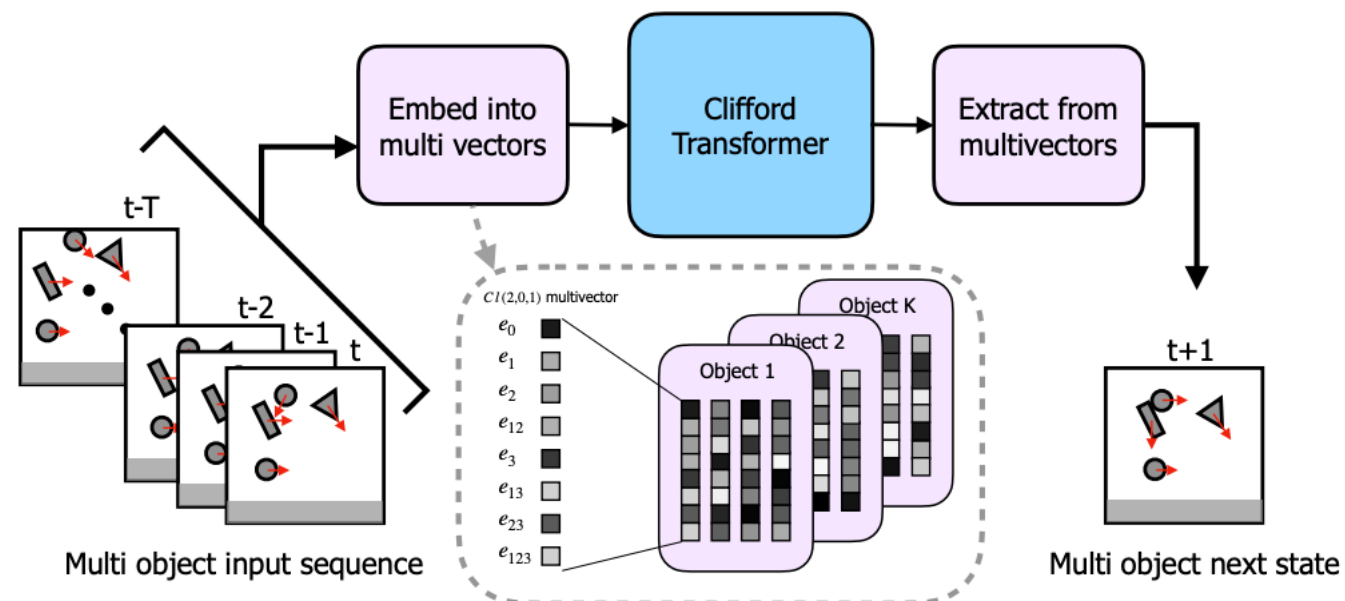
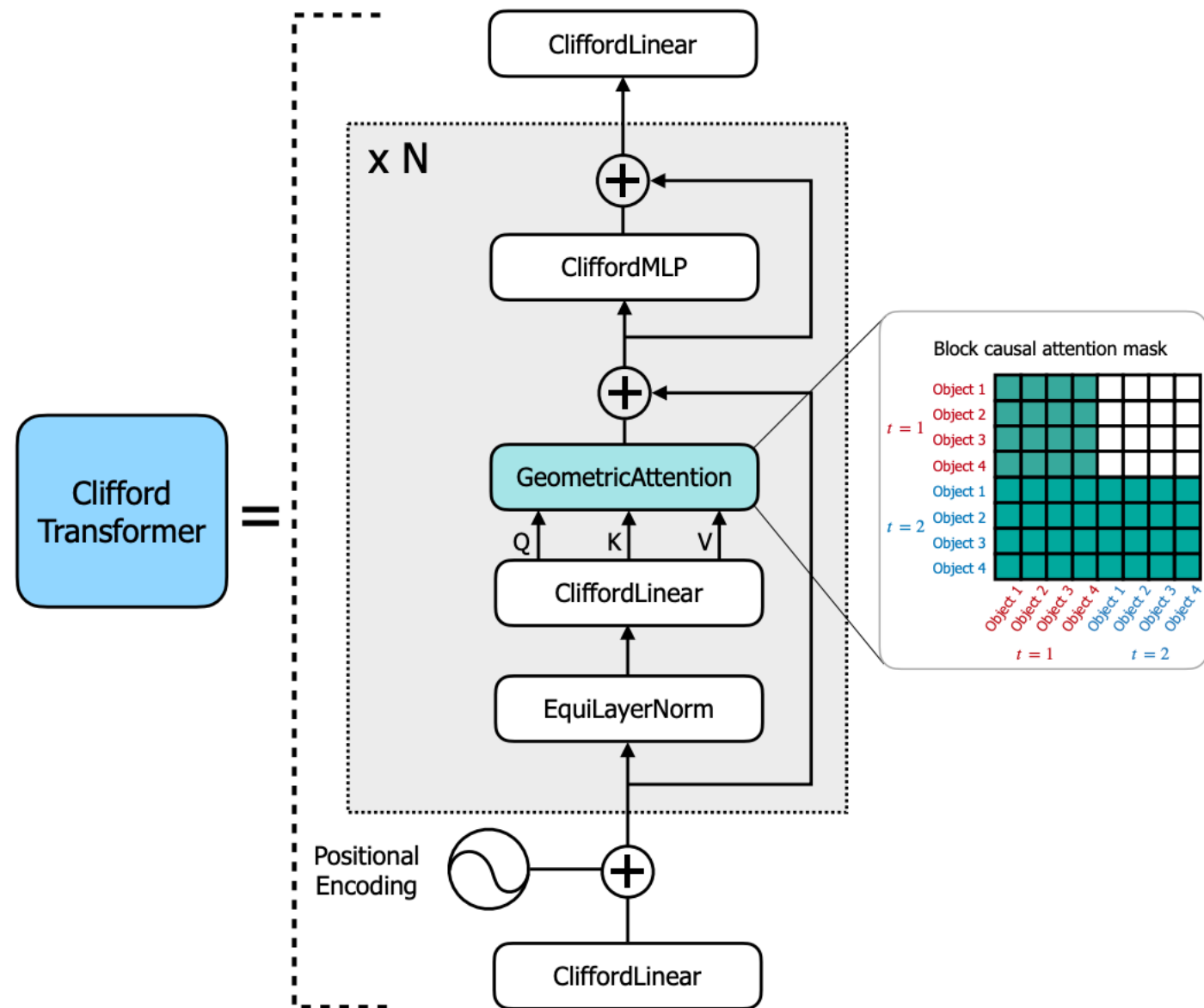
$$= a^{ij\alpha} x_j^\beta \mathbf{e}_\alpha \mathbf{e}_\beta$$

$$= a^{ij\alpha} x_j^\beta f_{\alpha\beta\gamma} \mathbf{e}^\gamma$$

[m, n, 8] [8, 8, 8]

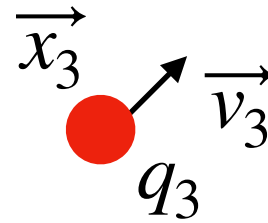
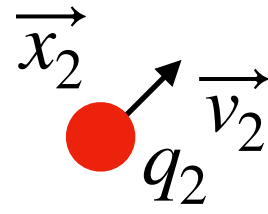
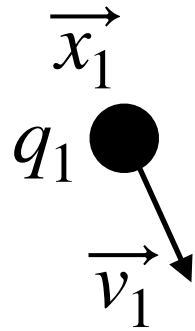
`einsum("ijk,kj,klm", W, x, f)`

[m, 8]



Object centric dynamics

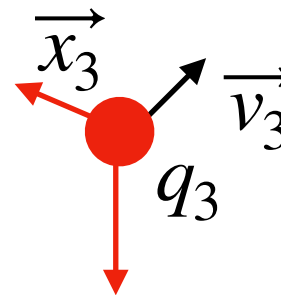
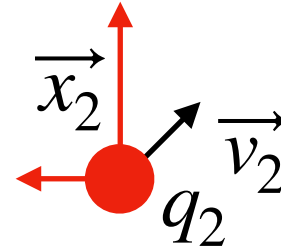
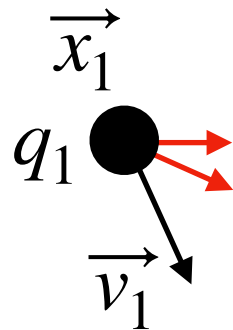
charged particles



Object centric dynamics

charged particles

State



Dynamics

$$\vec{F}_i = \sum_{j \neq i} q_i q_j \frac{\vec{x}_j - \vec{x}_i}{|\vec{x}_j - \vec{x}_i|^2}$$

$$\frac{d\vec{v}_i}{dt} = \vec{F}_i$$

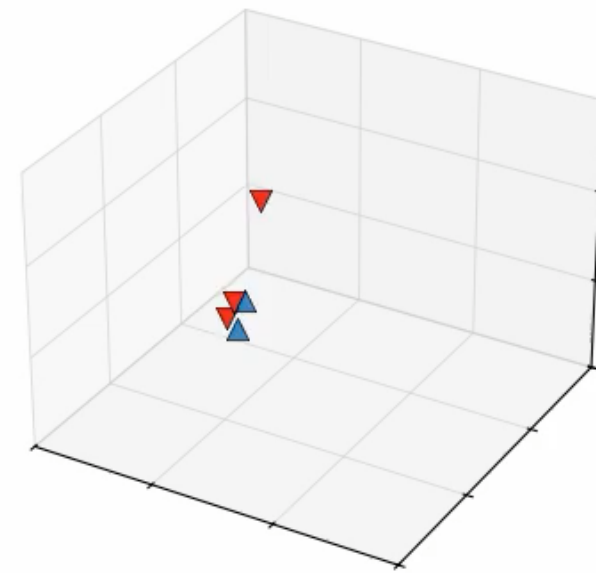
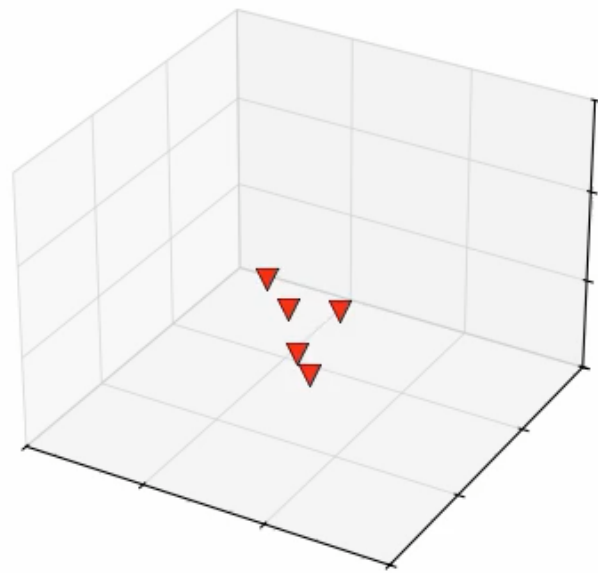
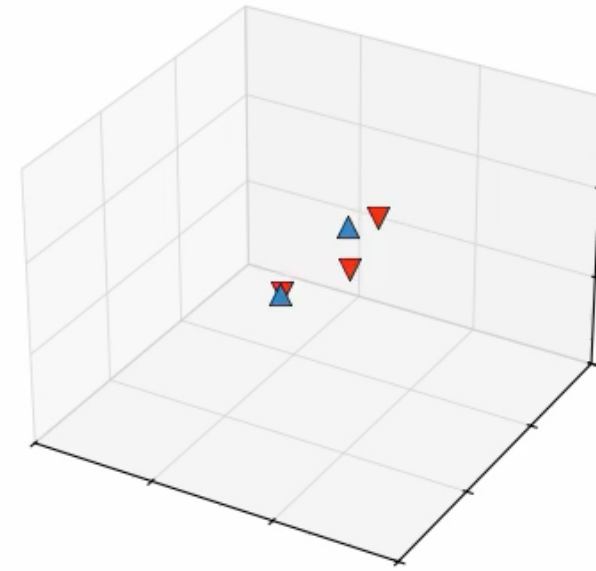
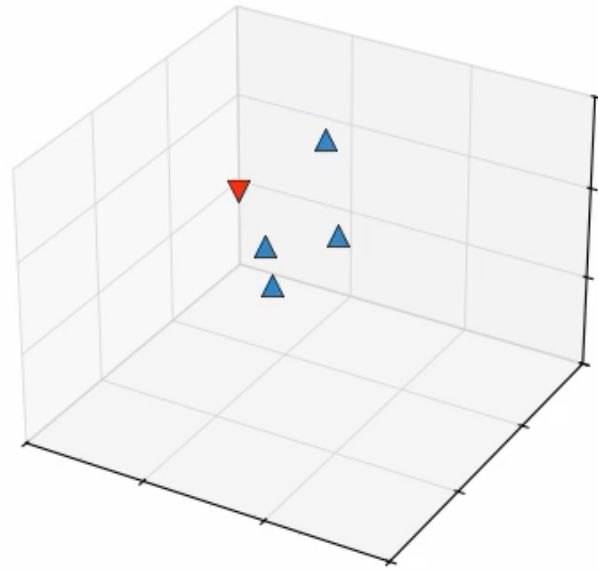
Task

predict $\vec{x}_i(t + \Delta t)$
 $\vec{v}_i(t + \Delta t)$

given $\vec{x}_i(t)$
 $\vec{v}_i(t)$
 q_i

Object centric dynamics

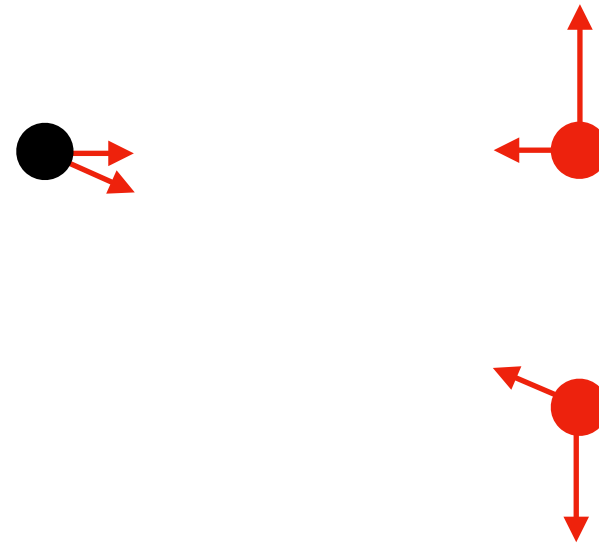
charged particles



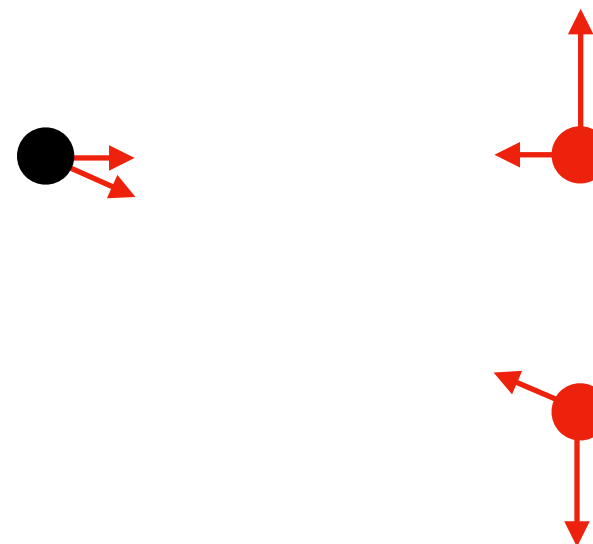
— Ground truth ▲ + charge ▼ - charge

Equivariance

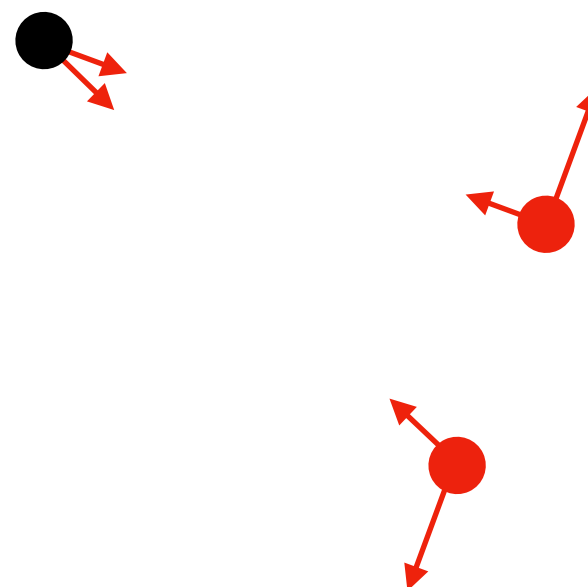
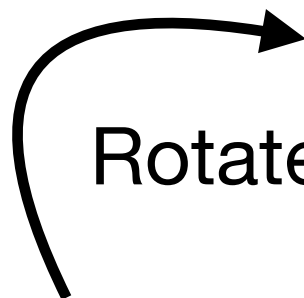
Euclidean group



Translate

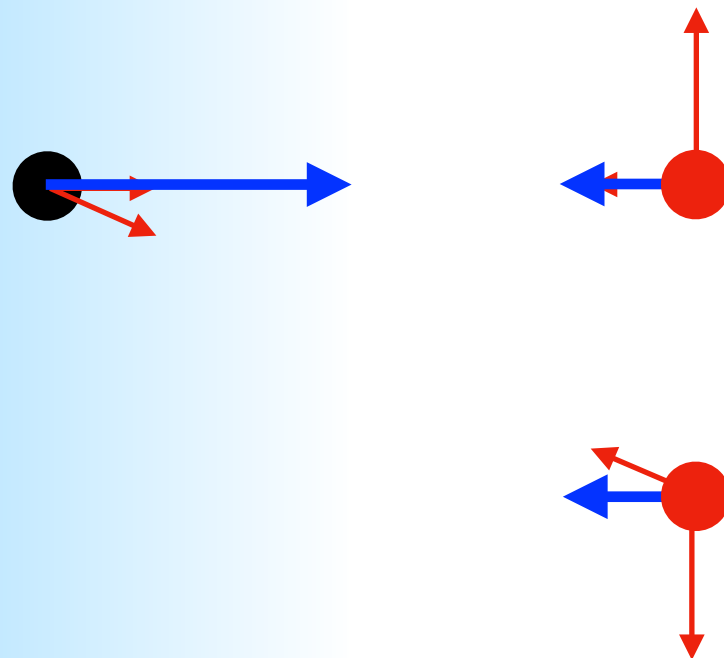


Rotate



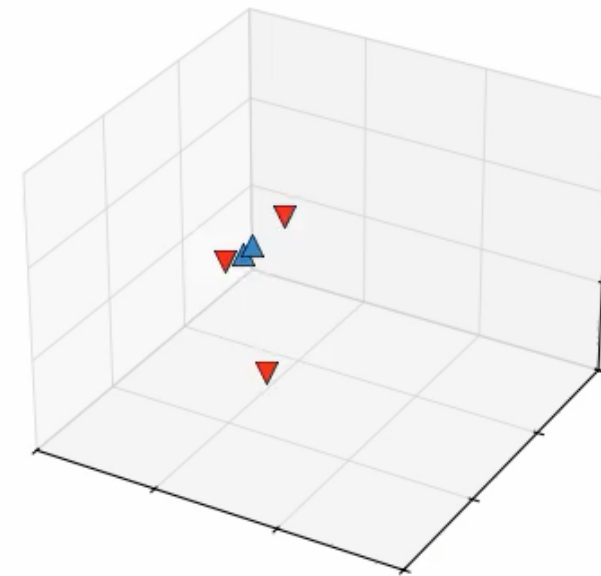
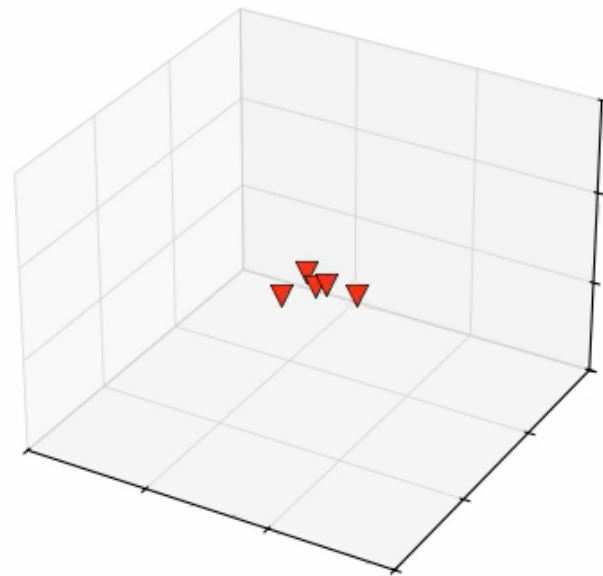
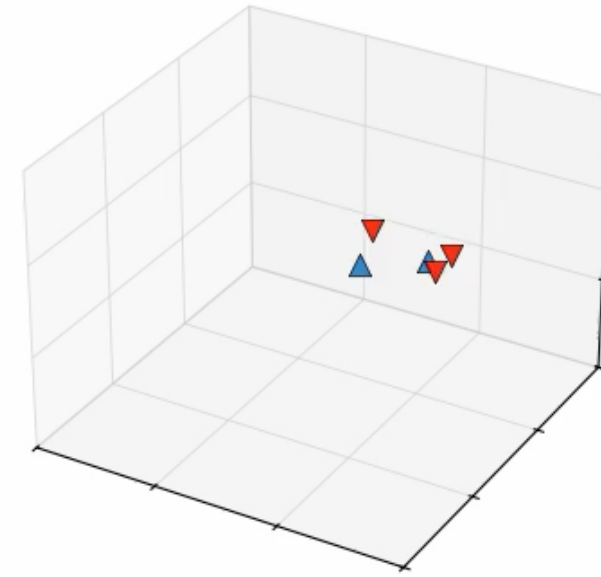
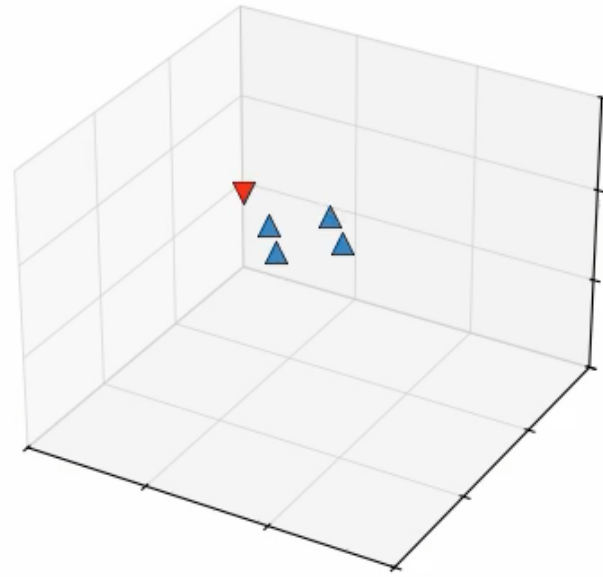
Broken equivariance

charged particles



Broken equivariance

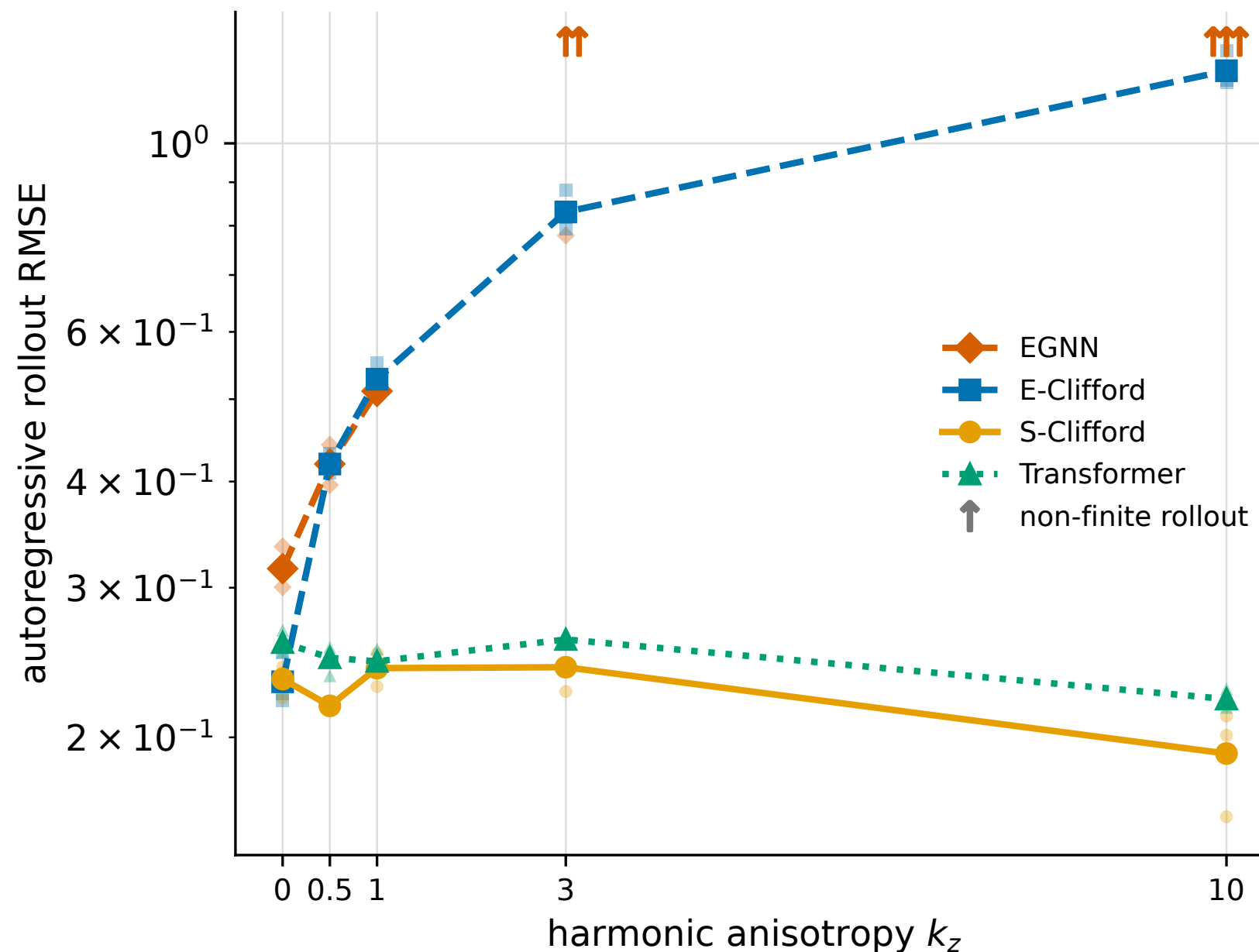
charged particles



— Ground truth ▲ + charge ▼ - charge

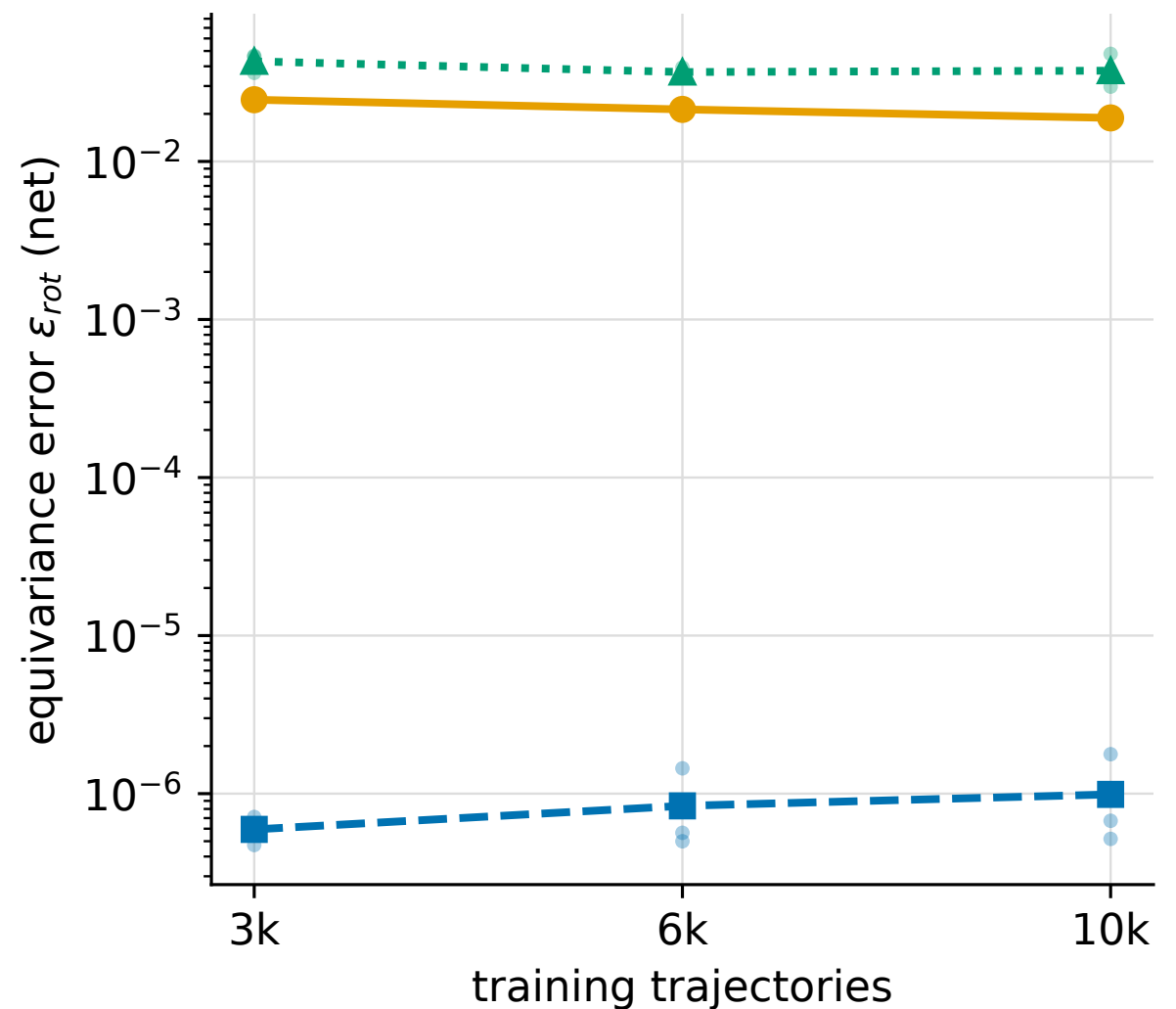
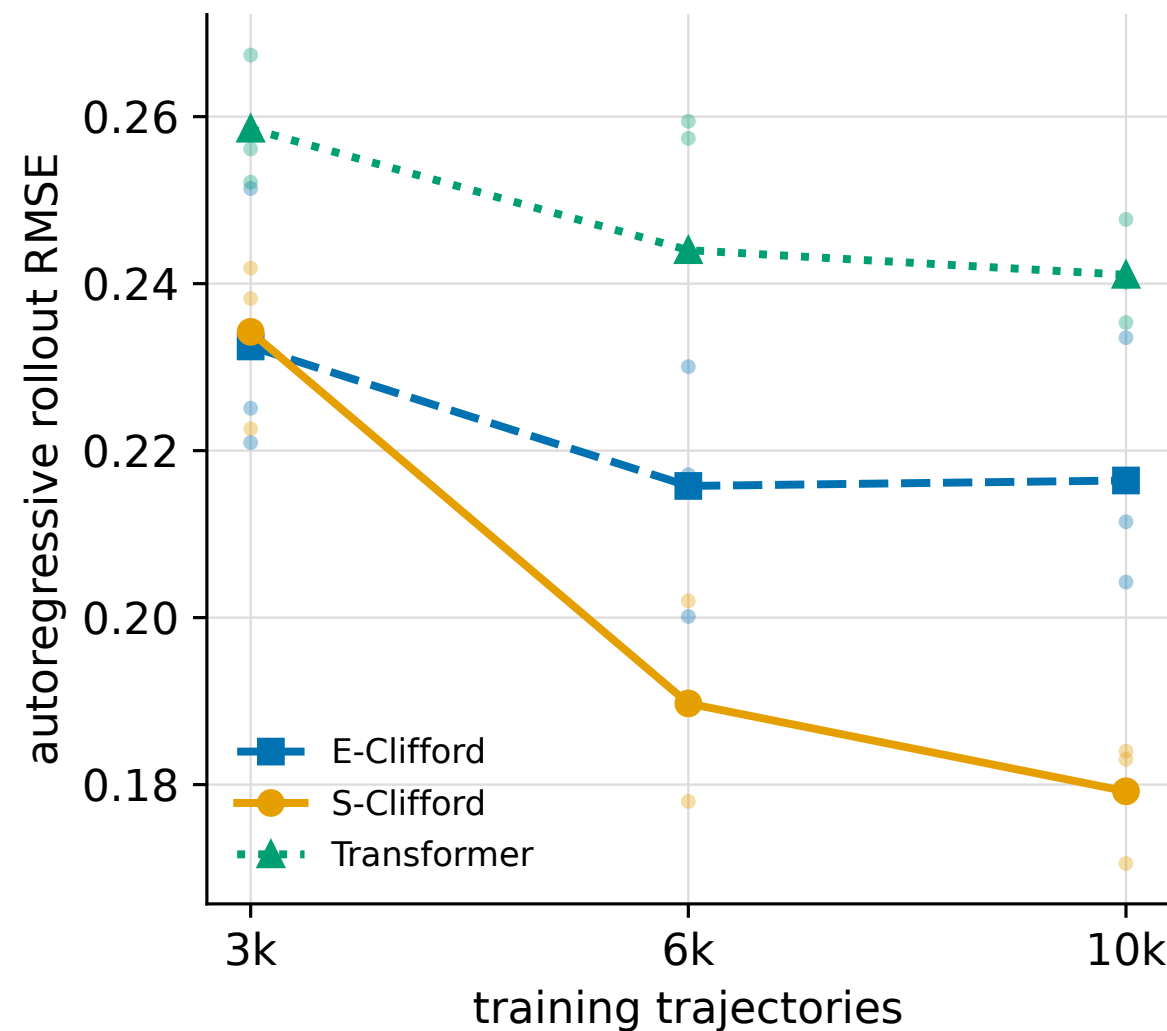
Results

charged particles with broken equivariance



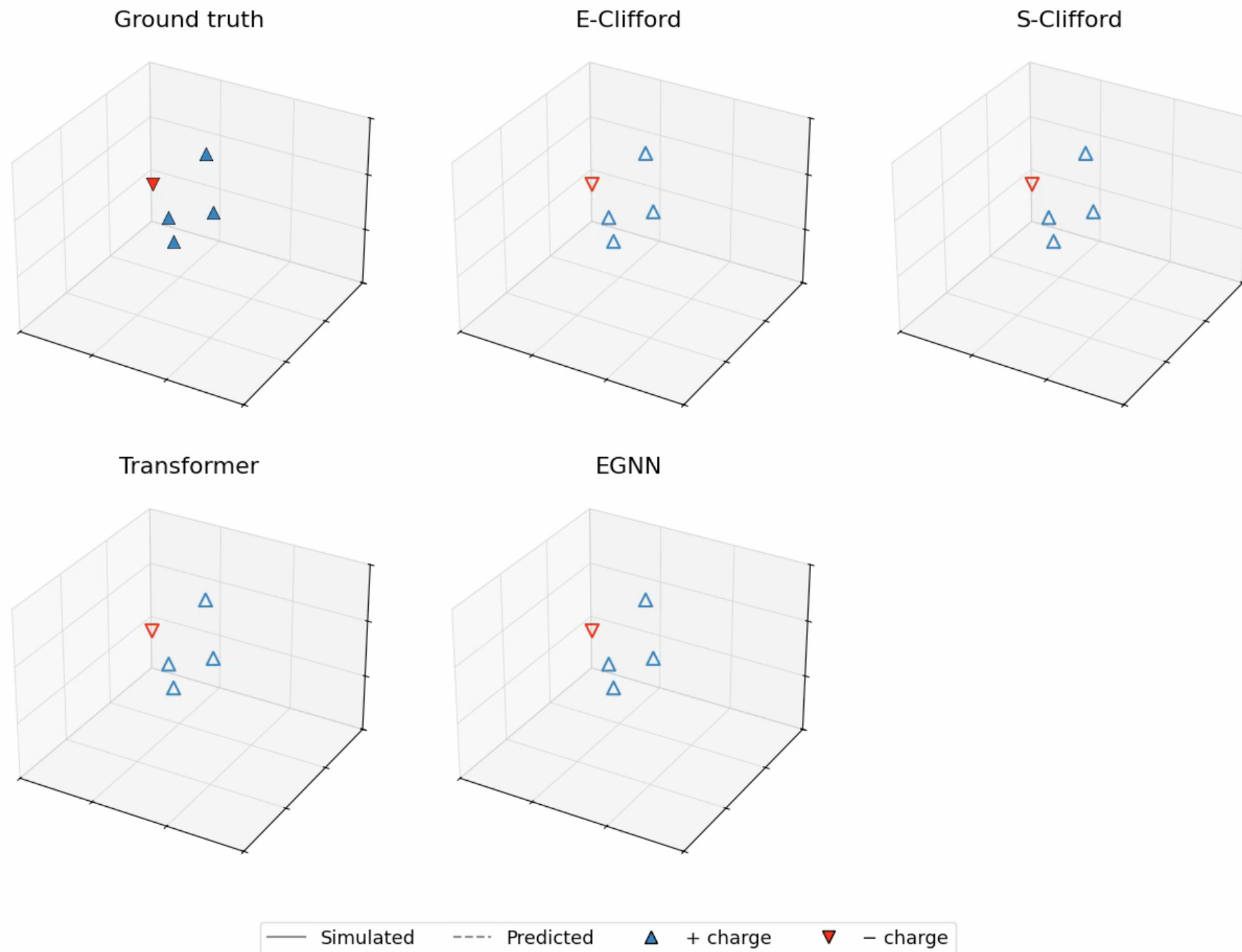
Results

charged particles: data scale with unbroken symmetry



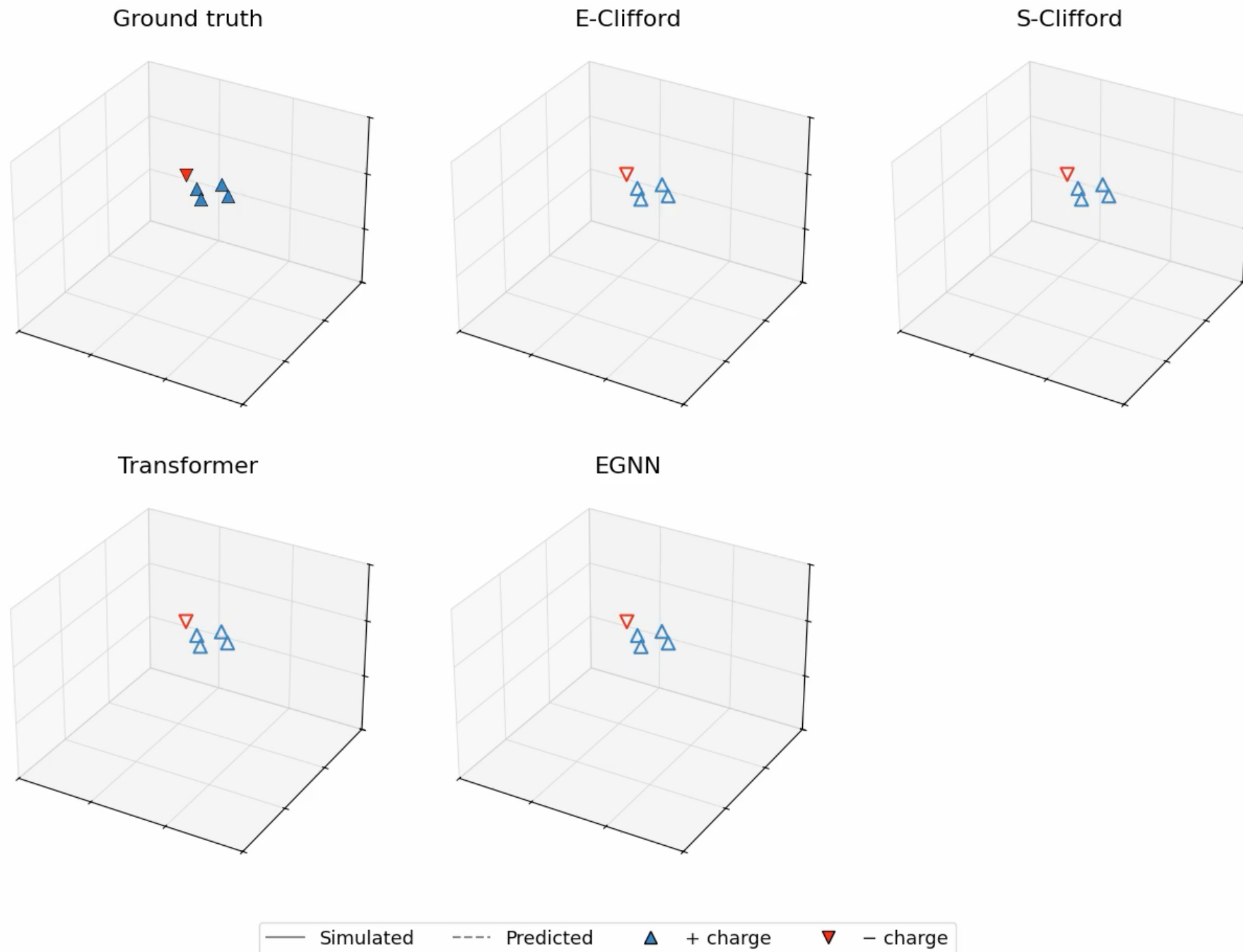
Results

charged particles: rollouts with **unbroken** symmetry



Results

charged particles: rollouts with **broken** symmetry



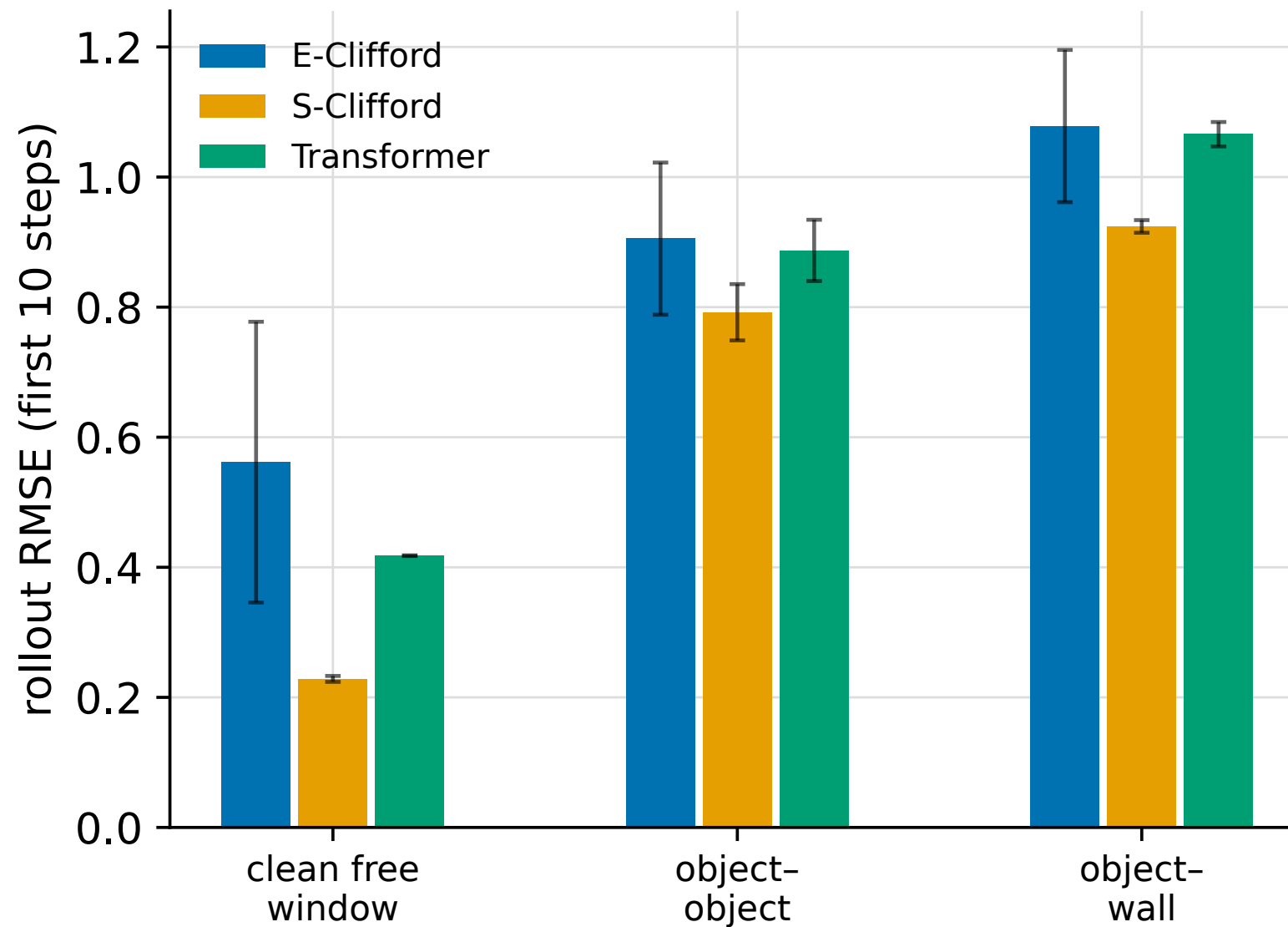
Results

2d rigid body dynamics (Kinetix)



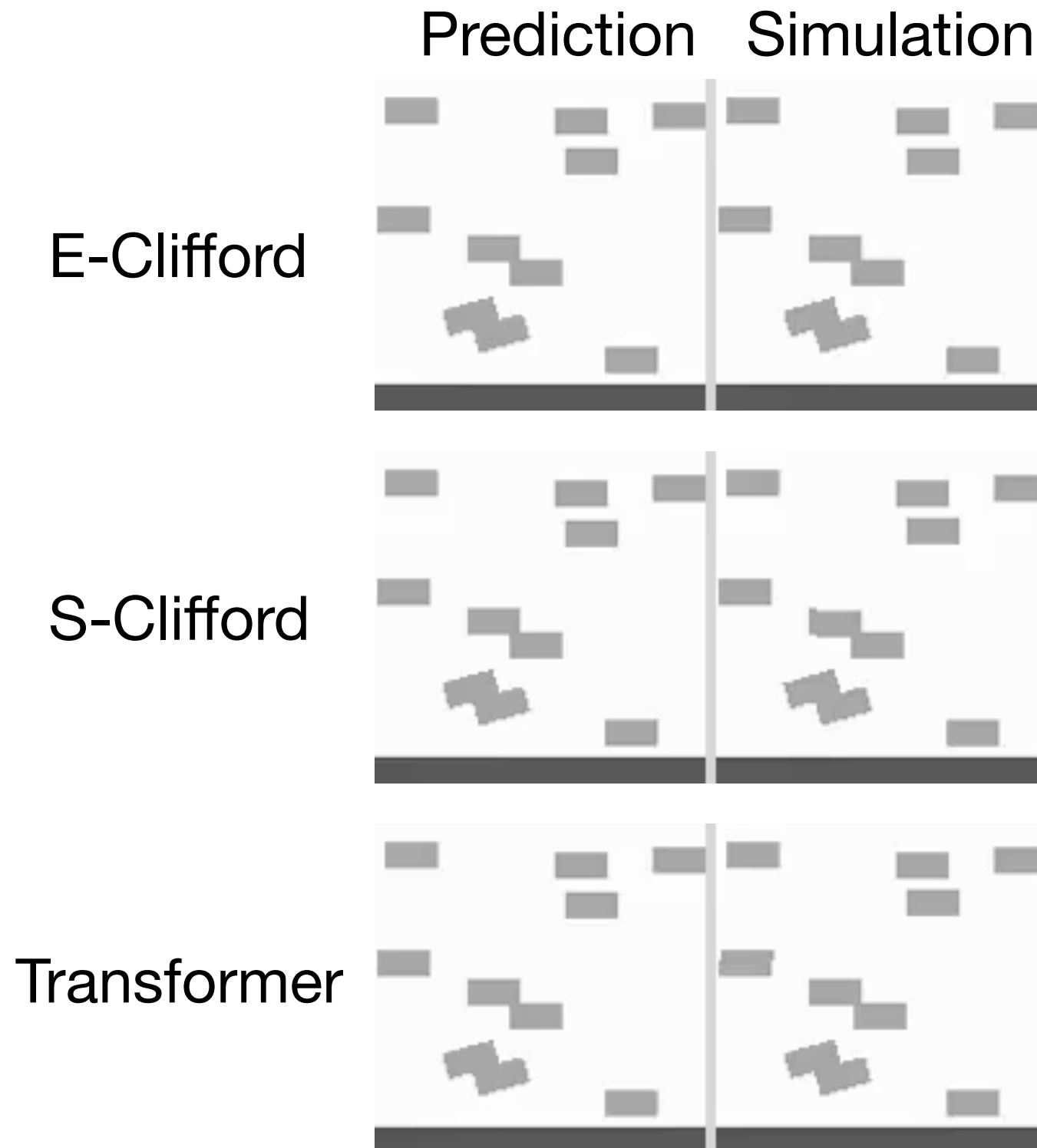
Results

2d rigid body dynamics (Kinetix)



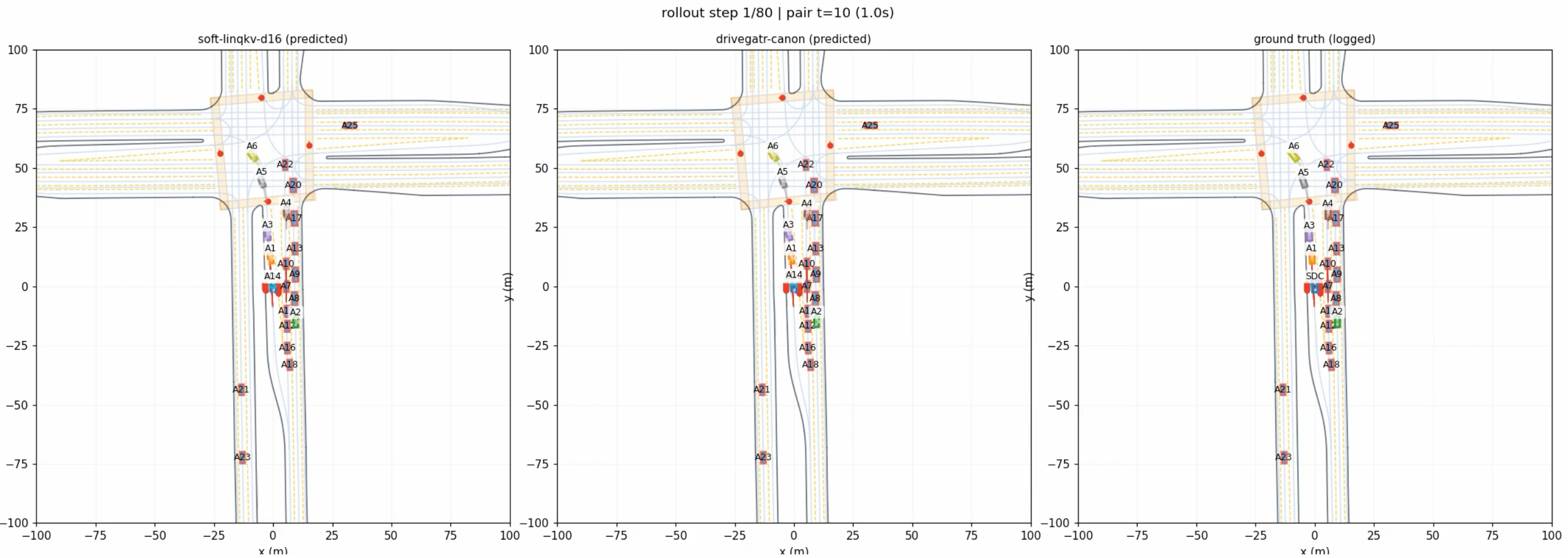
Results

2d rigid body dynamics (Kinetix)



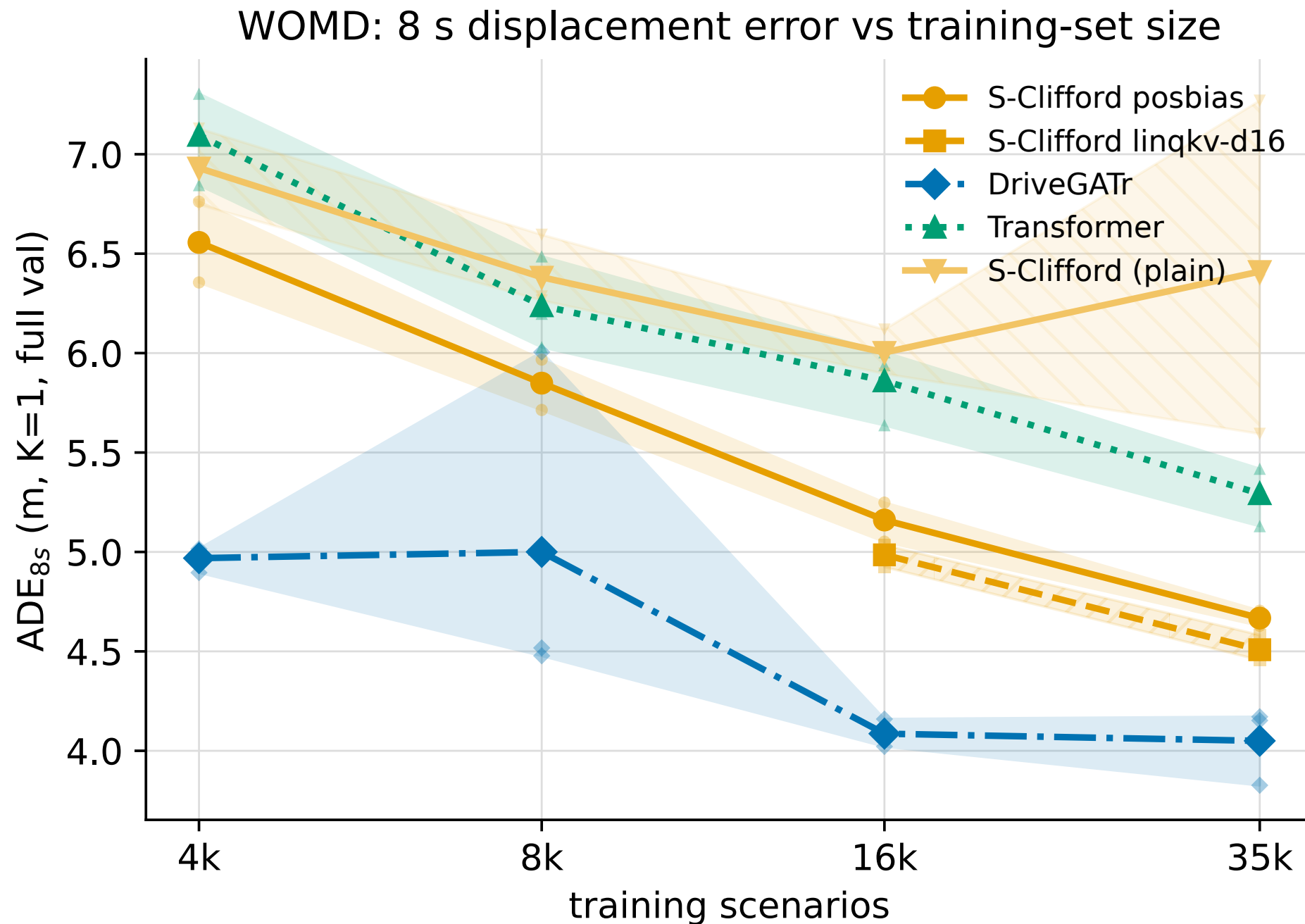
Results

2d multi-agent trajectory prediction (WOMD)



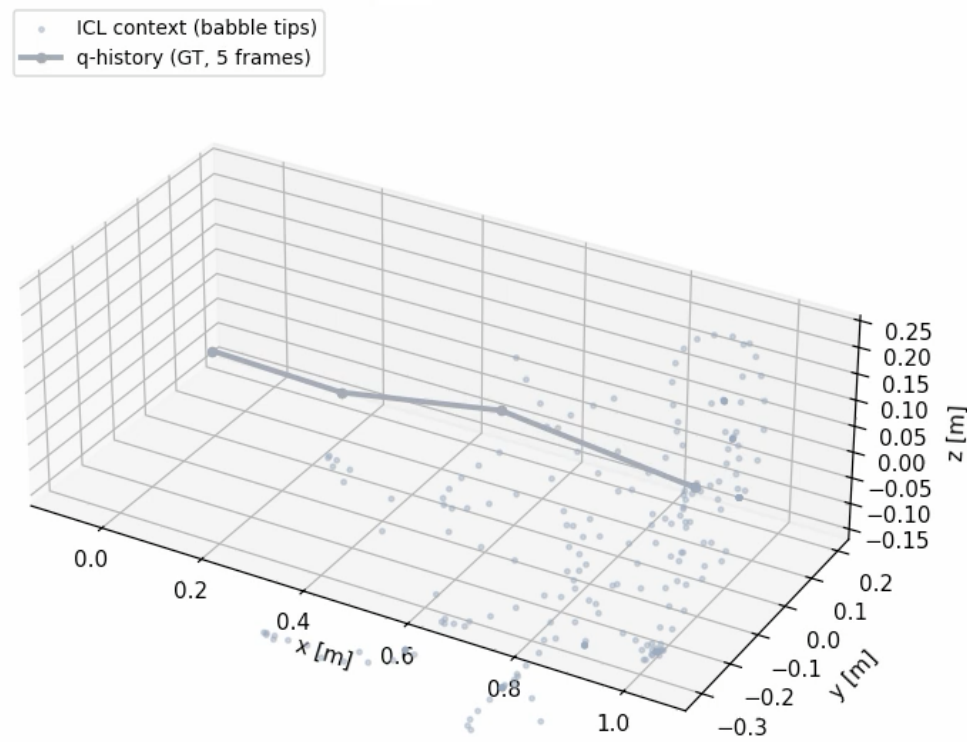
Results

2d multi-agent trajectory prediction (WOMD)

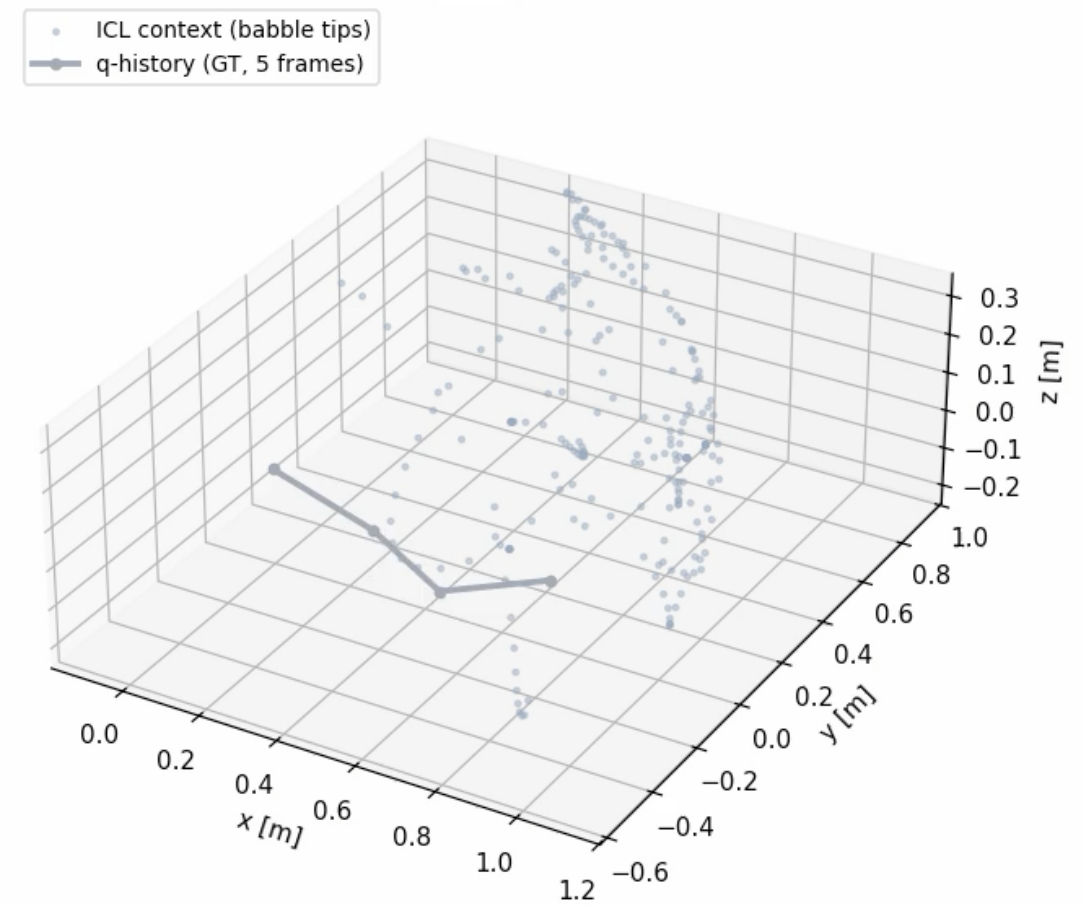


Outlook

best 1 (mean tip ADE 0.021 m) | ICL ctx=240 babble frames
soft-clifford-d8: fde 0.029m ade 0.017m | vanilla-d8: fde 0.039m ade 0.026m
q-history 1/5



median arm 1 (mean tip ADE 0.055 m) | ICL ctx=240 babble frames
soft-clifford-d8: fde 0.052m ade 0.040m | vanilla-d8: fde 0.055m ade 0.069m
q-history 1/5



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