Learning from Differentiable Physics to Simulate Liquids with Graph Networks

Bachelor’s Thesis in Informatics

29.04.2021

Jonathan Klimesch

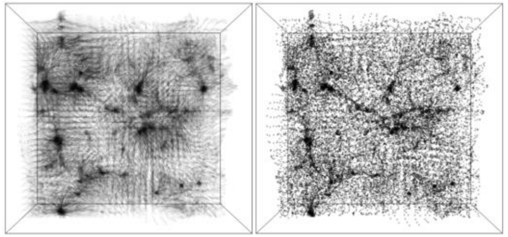
Prof. Dr. Nils Thuerey

M. Sc. Philipp Holl

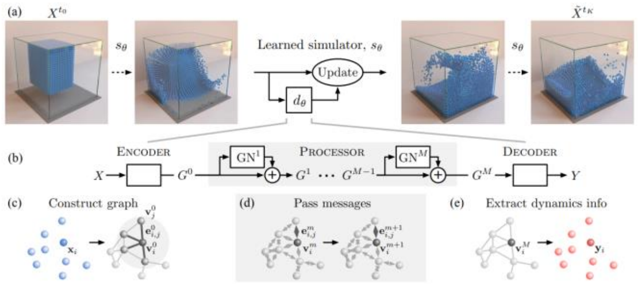
Motivation

U.S. National Oceanic and Atmospheric Administration (NOAA)
https://celebrating200years.noaa.gov/breakthroughs/climate_model/modeling_schematic.html

Motivation



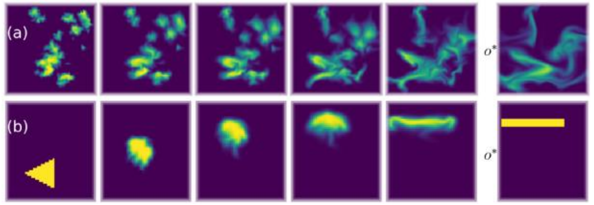
S. He, Y. Li, Y. Feng, S. Ho, S. Ravanbakhsh, W. Chen, and B. Póczos. Learning to predict the cosmological structure formation. 2019.



A. Sanchez-Gonzalez, J. Godwin, T. Pfaff, R. Ying, J. Leskovec, and Battaglia P.W. Learning to simulate complex physics with graph networks. 2020.

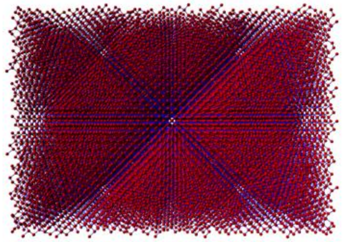
Graph Network-based Simulators (GNS)

ΦFlow



P. Holl, V. Koltun, and N. Thuerey. Learning to control pdes with differentiable physics. 2020.

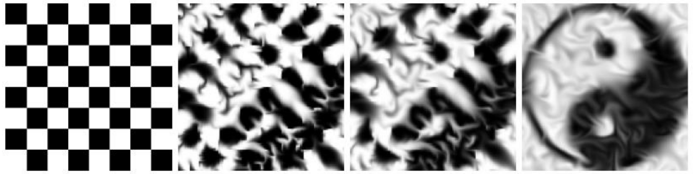
JAX, M.D.



S. Schoenholz and E. D. Cubuk. Jax, m.d.: End-to-end differentiable, hardware accelerated, molecular dynamics in pure python. 2019.

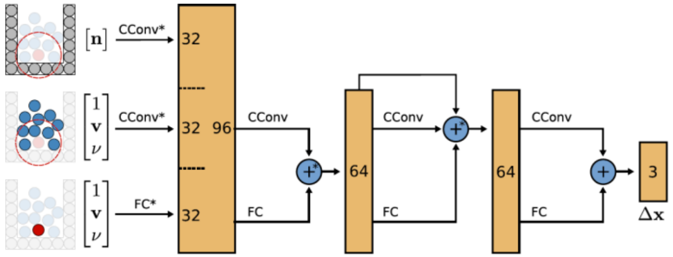
Differentiable Physics

DiffTaichi

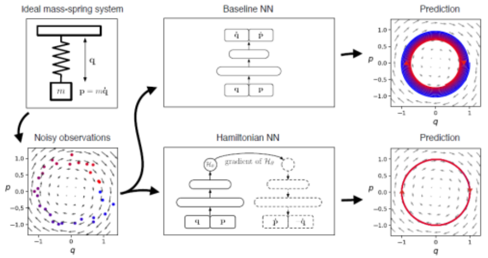


Y. Hu, L. Anderson, T. Li, Q. Sun, N. Carr, J. Ragan-Kelley, and F. Durand. Difftaichi: Differentiable programming for physical simulation. 2020.

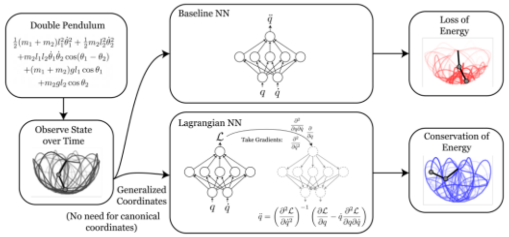
Learned Simulators / Physics-Informed Architectures



B. Ummenhofer, L. Prantl, N. Thuerey, and V. Koltun. Lagrangian fluid simulation with continuous convolutions. 2020.



S. Greydanus, M. Dzamba, and J. Yosinski. Hamiltonian neural networks. 2019.



M. Cranmer and S. Greydanus and Stephan Hoyer and P. Battaglia and D. Spergel and S. Ho. Lagrangian Neural Networks. 2020.

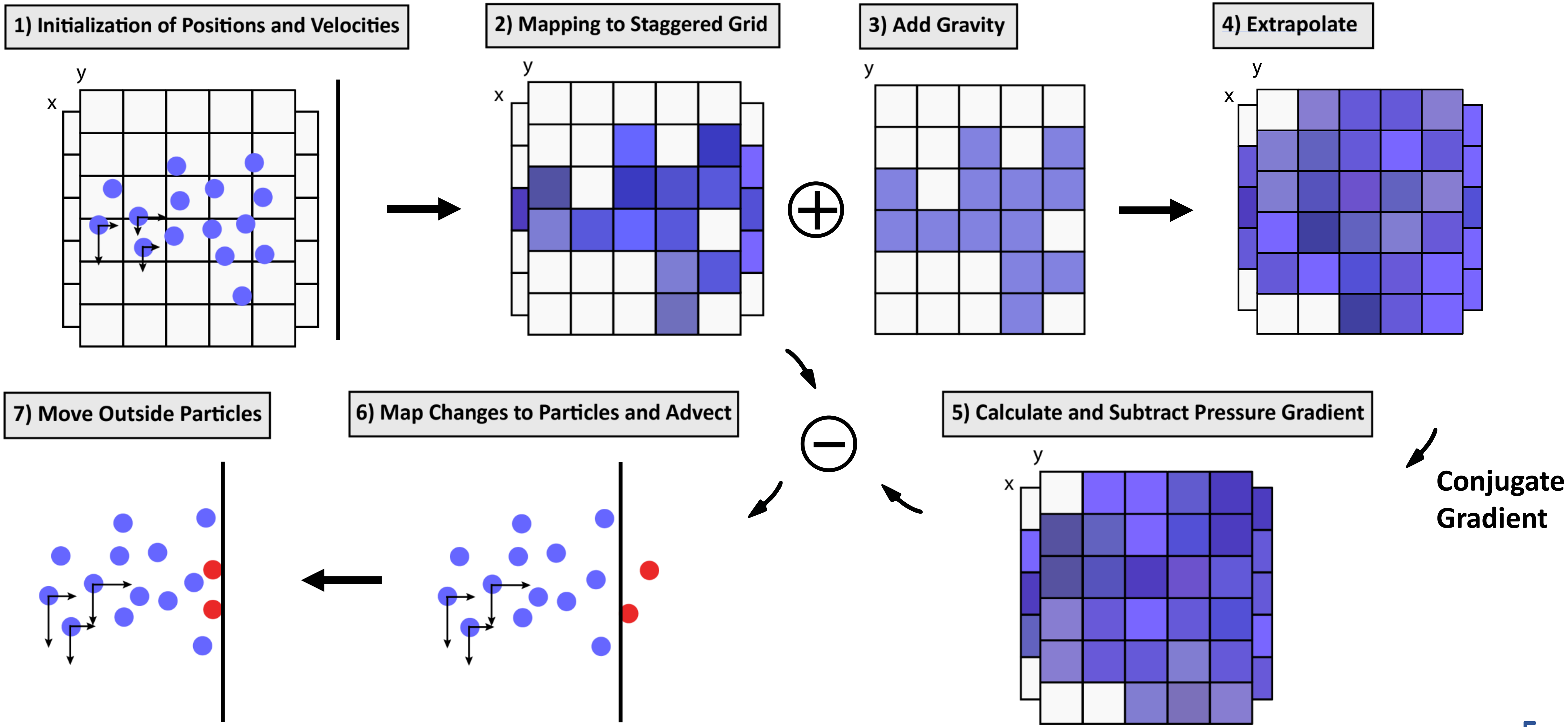
Goals

1. Differentiable FLIP simulator for $\Phi_{\mathbf{Flow}}$

2. Apply GNS to FLIP data

3. Extend GNS with new training variants

FLIP Algorithm



1) Initialization of Positions and Velocities

2) Mapping to Staggered Grid

3) Add Gravity

4) Extrapolate

5) Calculate and Subtract Pressure Gradient

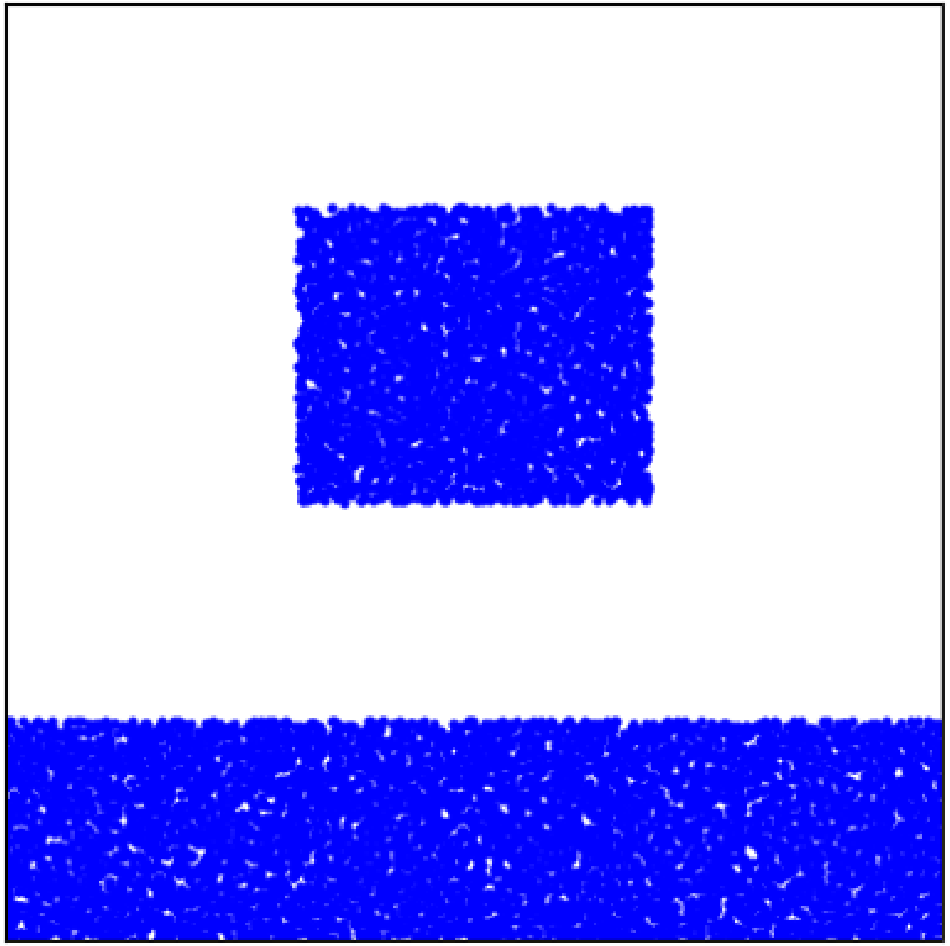
Conjugate Gradient

6) Map Changes to Particles and Advect

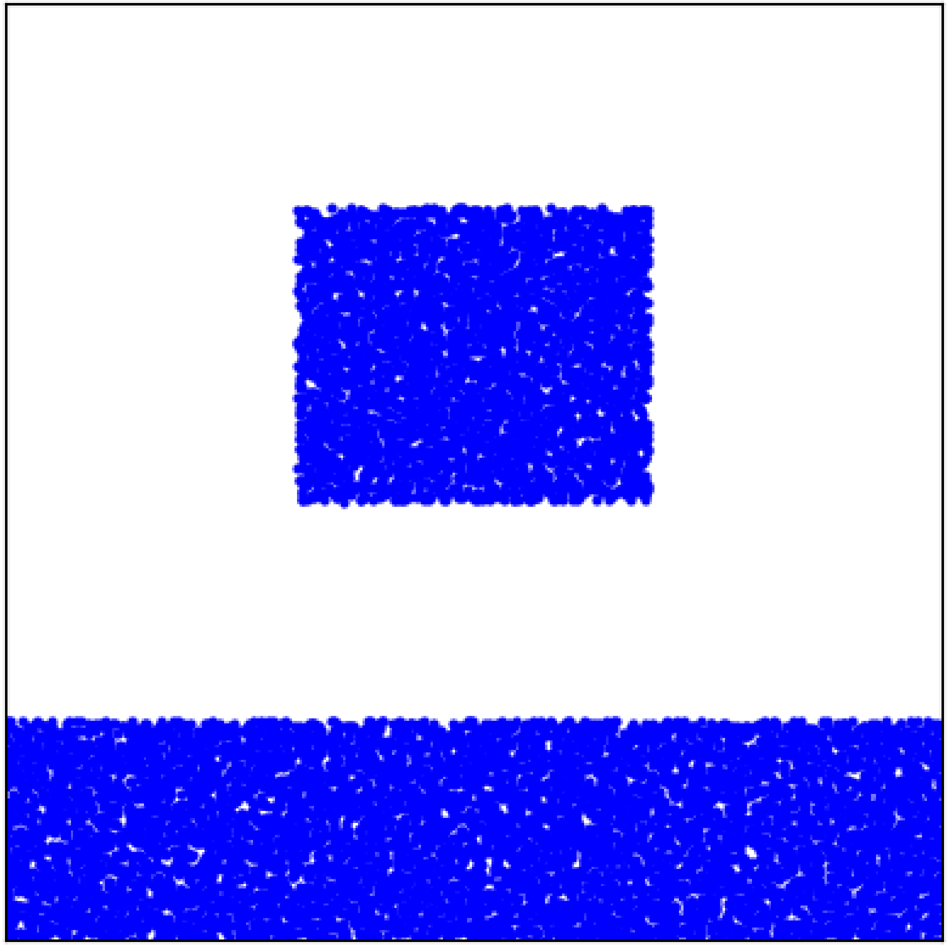
7) Move Outside Particles

Brackbill and Ruppel. 1986 / Zhu and Bridson. 2005

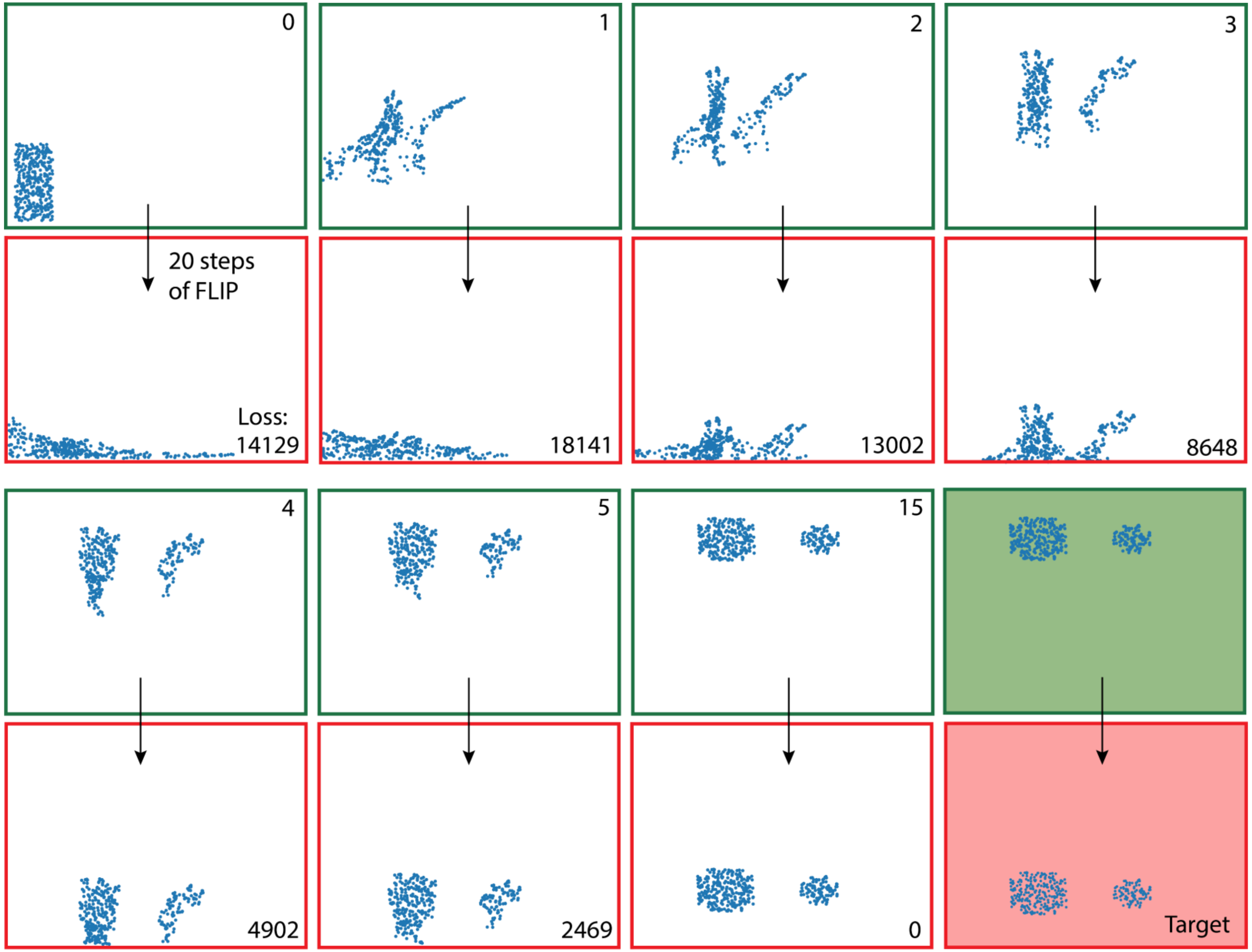
FLIP Verification - Simulation



FLIP Verification - Simulation

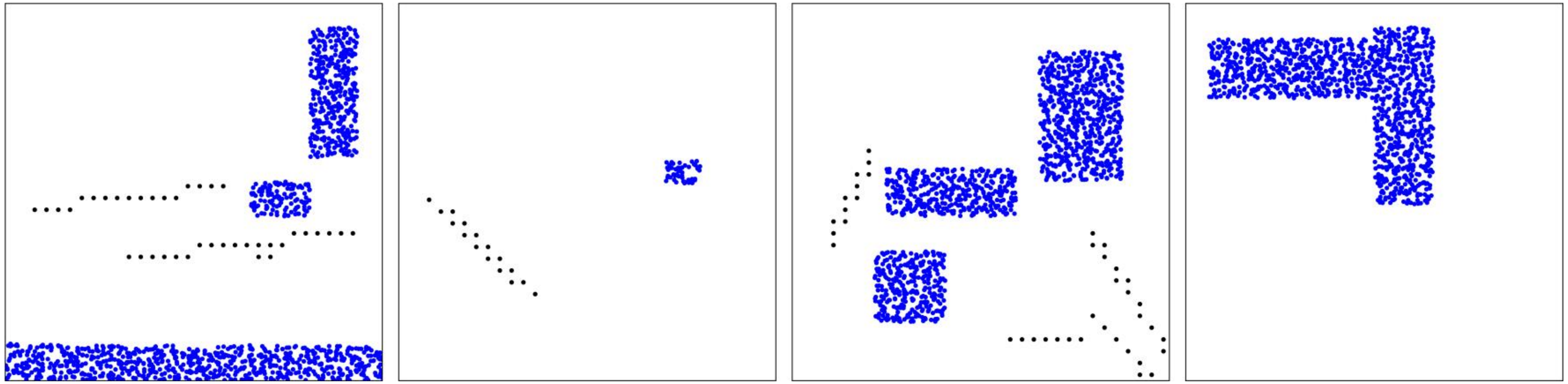


FLIP Simulation - Differentiability

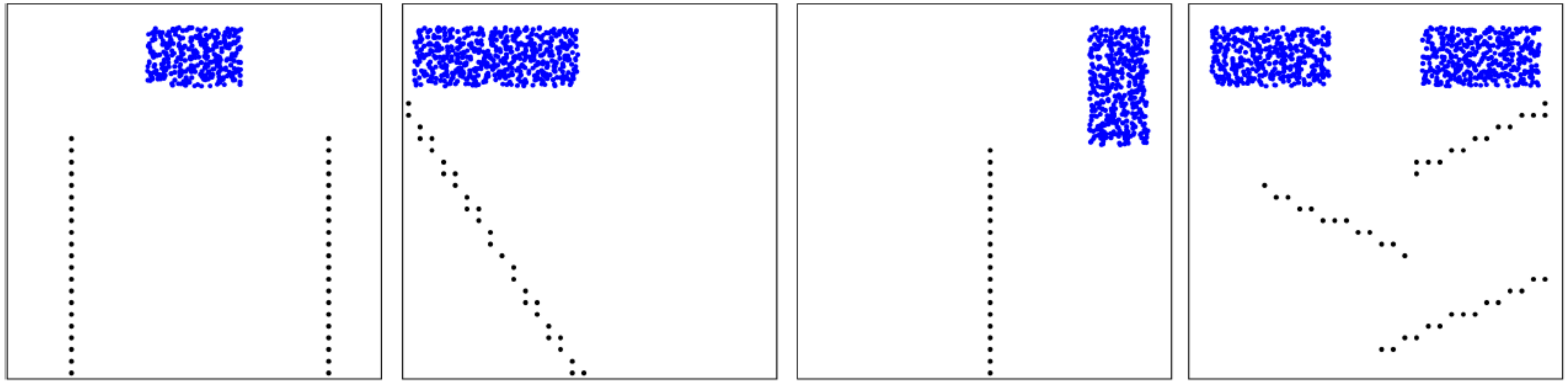


FLIP Dataset

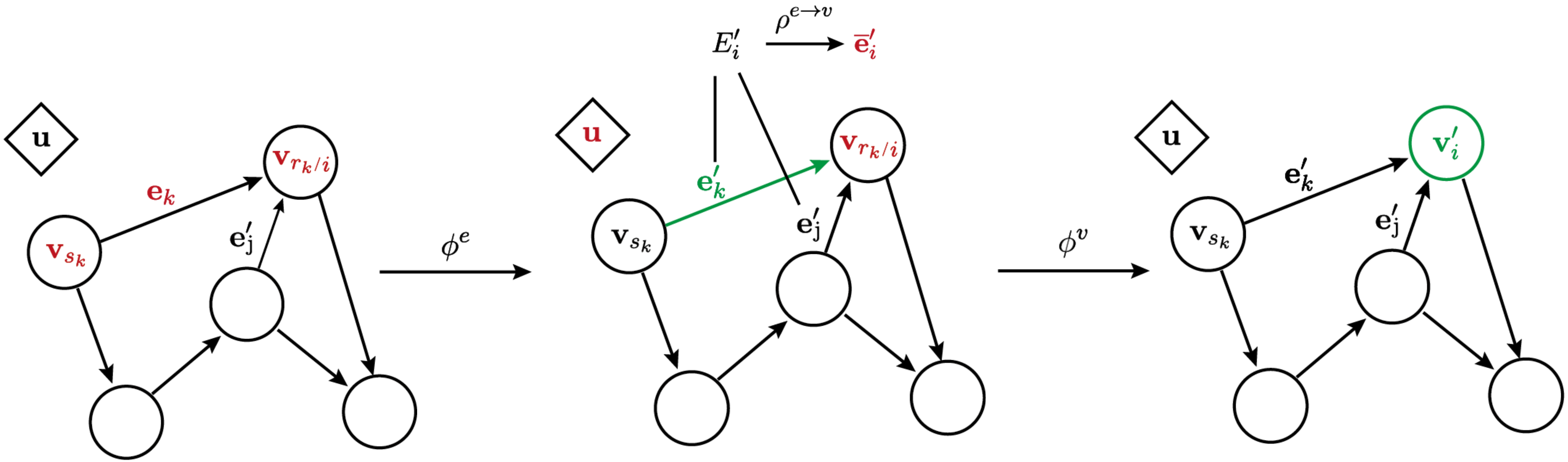
Training / Validation



Test



Graph Networks



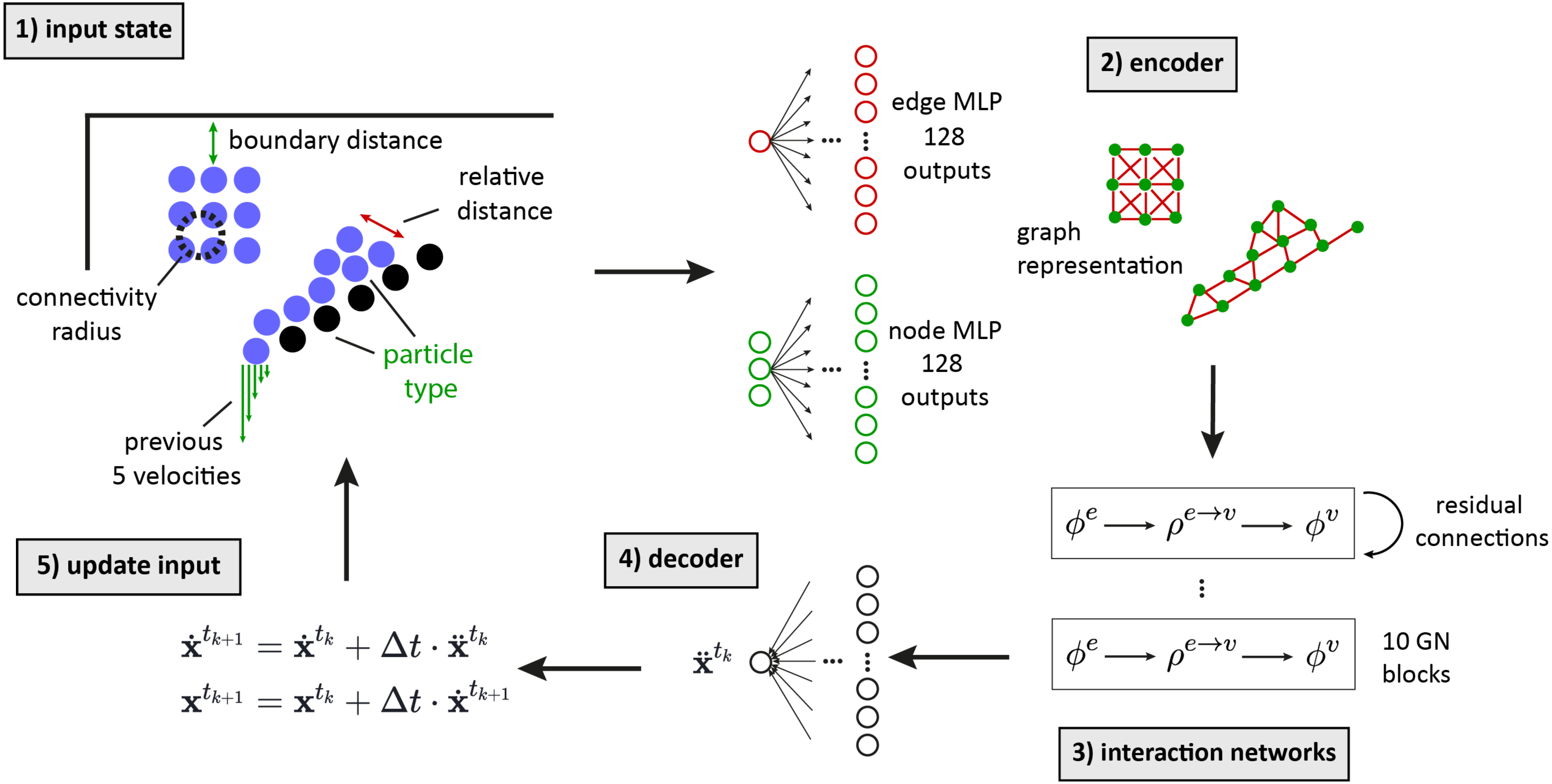
Edge update: $\mathbf{e}'_k = \phi^e\left(\mathbf{e}_k, \mathbf{v}_{r_k}, \mathbf{v}_{s_k}\right)$

Edge aggregation: $\overline{\mathbf{e}}'_i = \rho^{e\rightarrow v}\left(E'_i\right)$

Node update: $\mathbf{v}'_i = \phi^v\left(\overline{\mathbf{e}}'_i, \mathbf{v}_i, \mathbf{u}\right)$

Battaglia et al. 2018

Graph Network-based Simulators



1) input state

boundary distance

relative distance

connectivity radius

particle type

previous 5 velocities

edge MLP 128 outputs

node MLP 128 outputs

2) encoder

graph representation

$$\phi^e \longrightarrow \rho^{e\to v} \longrightarrow \phi^v$$

residual connections

$$\vdots$$

$$\phi^e \longrightarrow \rho^{e\to v} \longrightarrow \phi^v$$

10 GN blocks

3) interaction networks

4) decoder

$$\ddot{\mathbf{x}}^{t_k}$$

5) update input

$$\dot{\mathbf{x}}^{t_{k+1}} = \dot{\mathbf{x}}^{t_k} + \Delta t \cdot \ddot{\mathbf{x}}^{t_k}$$

$$\mathbf{x}^{t_{k+1}} = \mathbf{x}^{t_k} + \Delta t \cdot \dot{\mathbf{x}}^{t_{k+1}}$$

Sanchez-Gonzalez et al. 2020

Training Procedures and Quantitative Comparison

1-step-noise model (1sn)

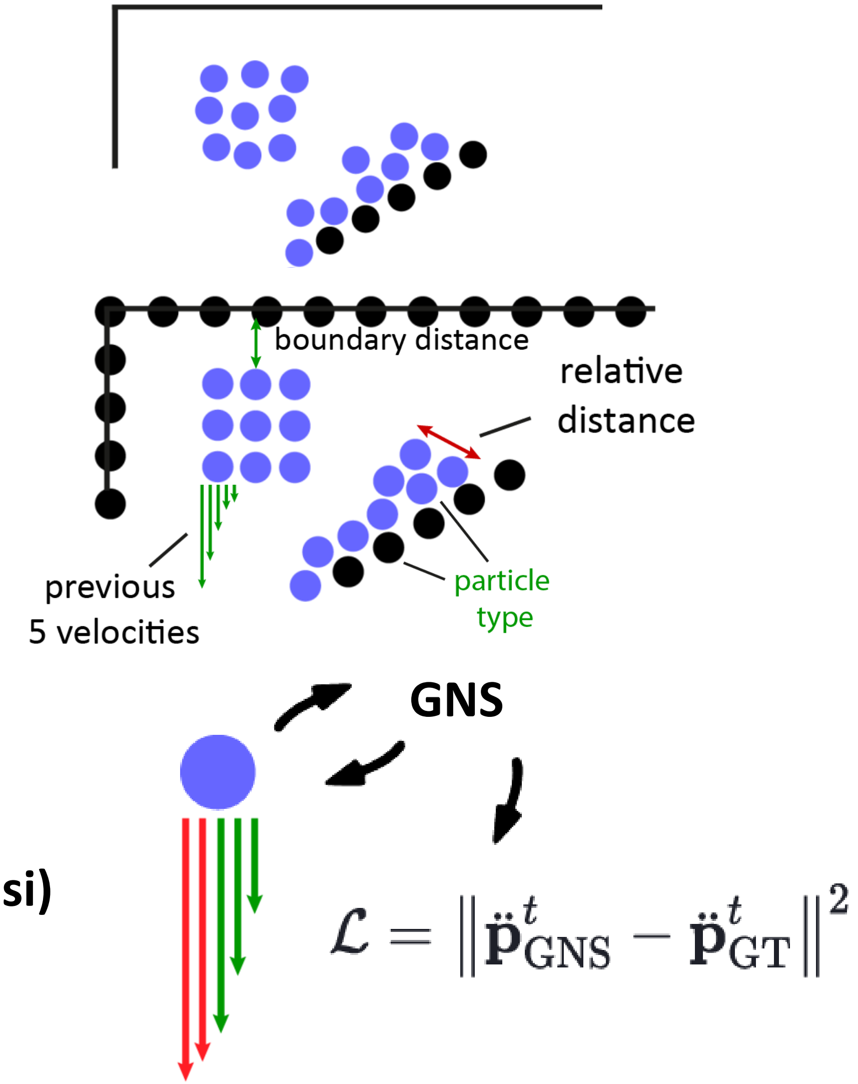
Sanchez-Gonzalez et al. 2020

$$\mathcal{L} = \left\| \ddot{\mathbf{p}}^{t}_{\mathrm{GNS}} - \ddot{\mathbf{p}}^{t}_{\mathrm{GT}} \right\|^{2}$$

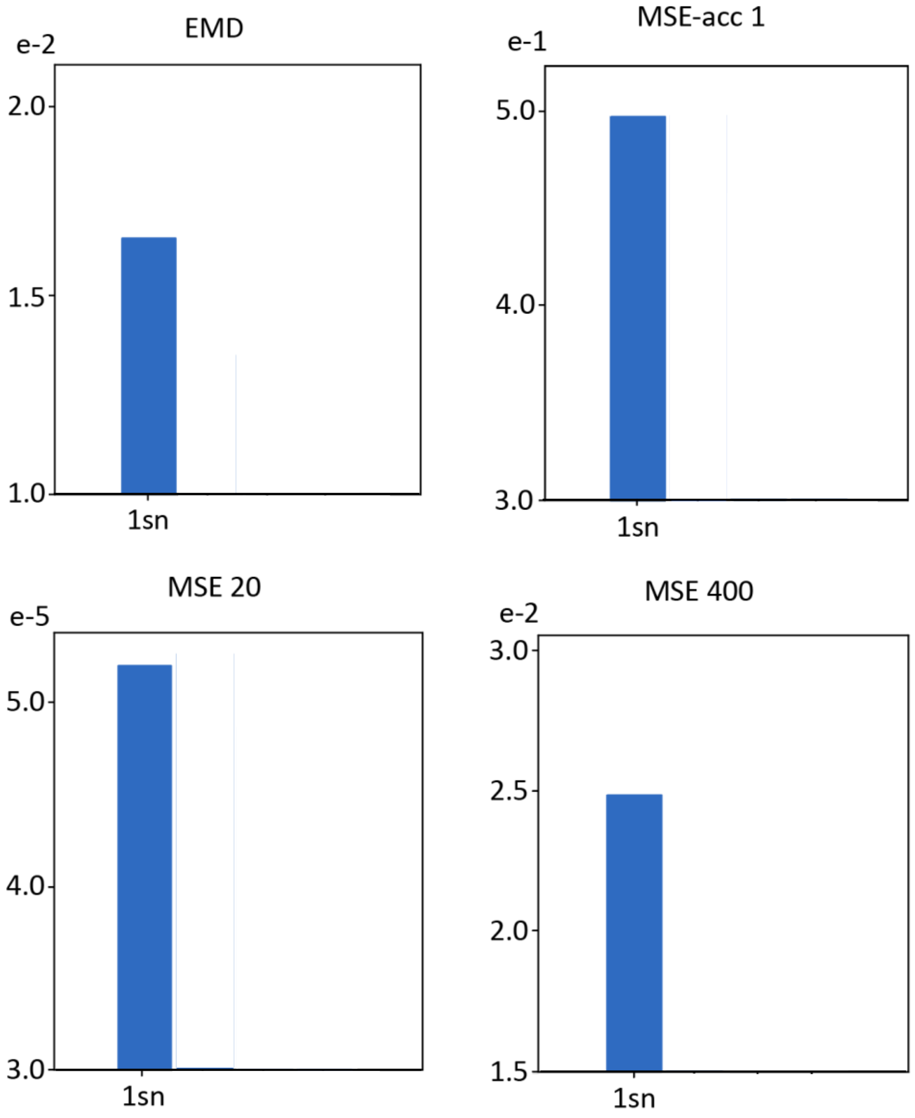
1-step-noise-bounded model (1snb)

2-step-scratch model (2ss)

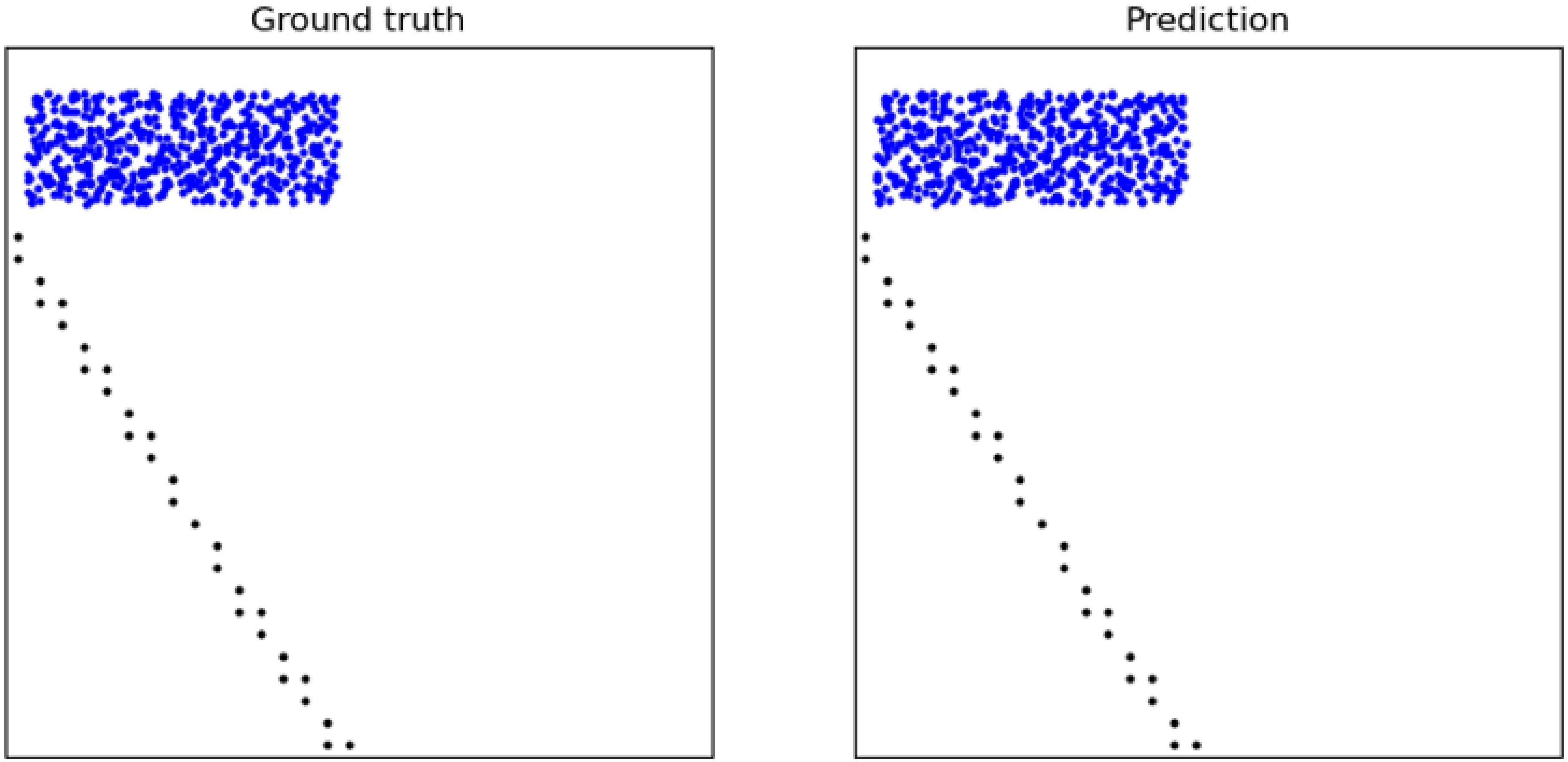
2-step-initialized model (2si)



$$\mathcal{L} = \left\| \ddot{\mathbf{p}}^{t}_{\mathrm{GNS}} - \ddot{\mathbf{p}}^{t}_{\mathrm{GT}} \right\|^{2}$$



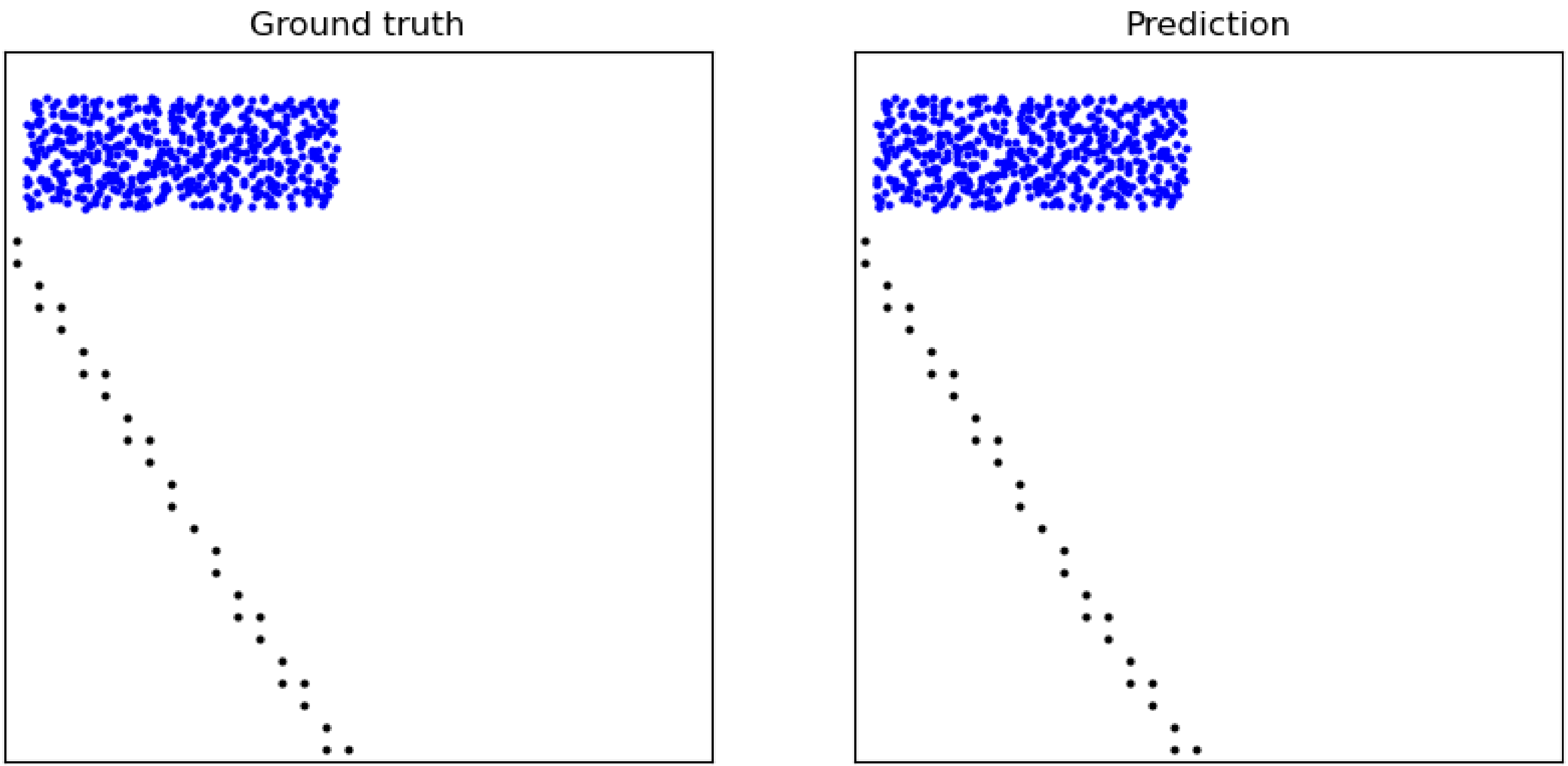
1-step-noise model



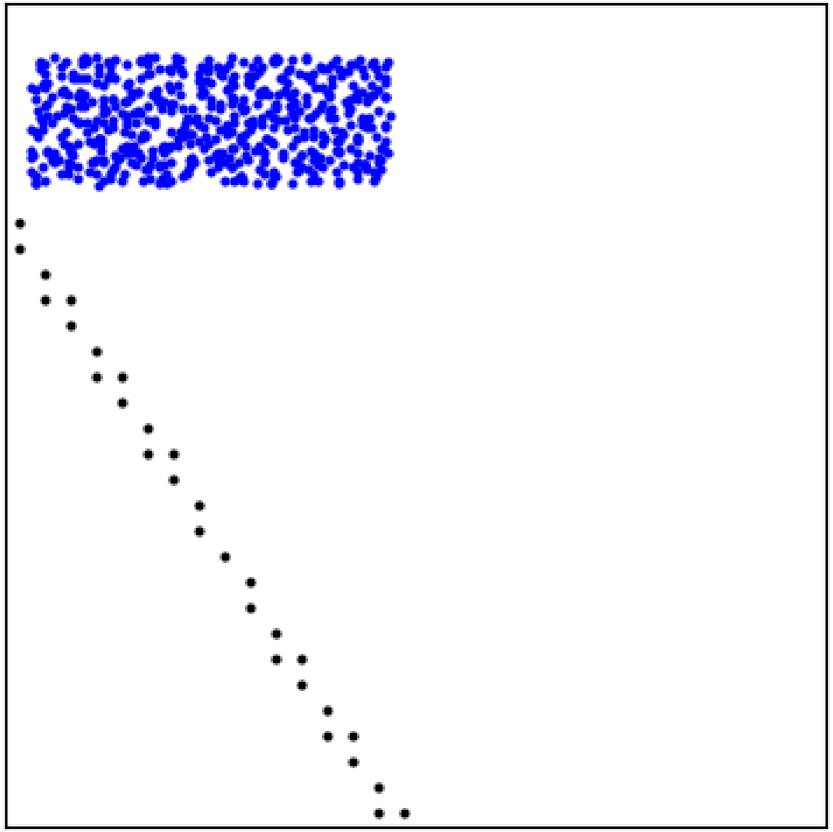
Ground truth

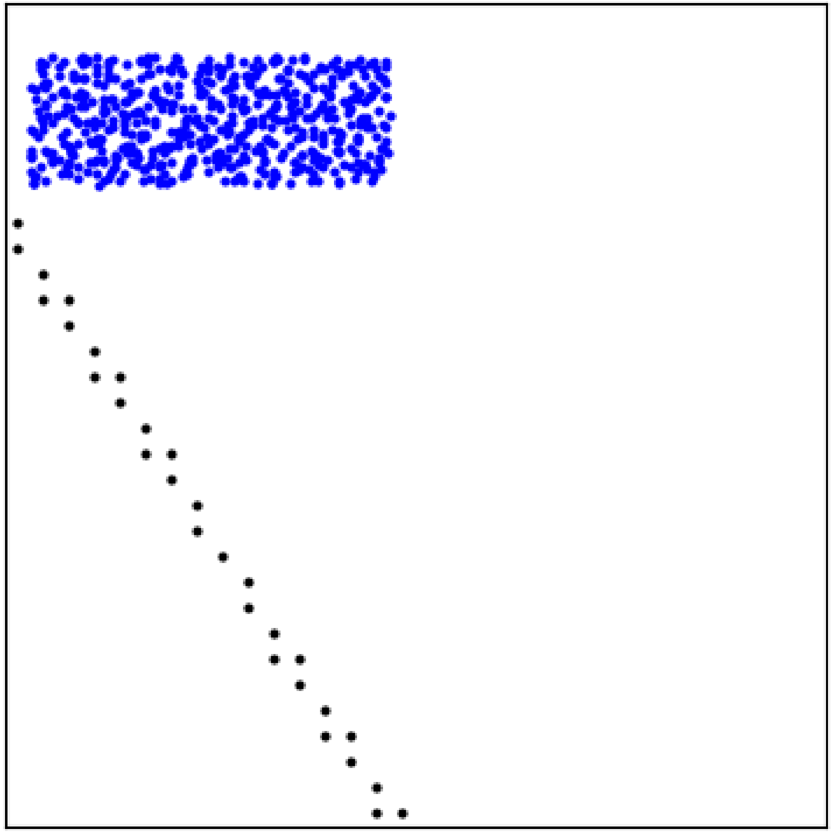
Prediction

1-step-noise model

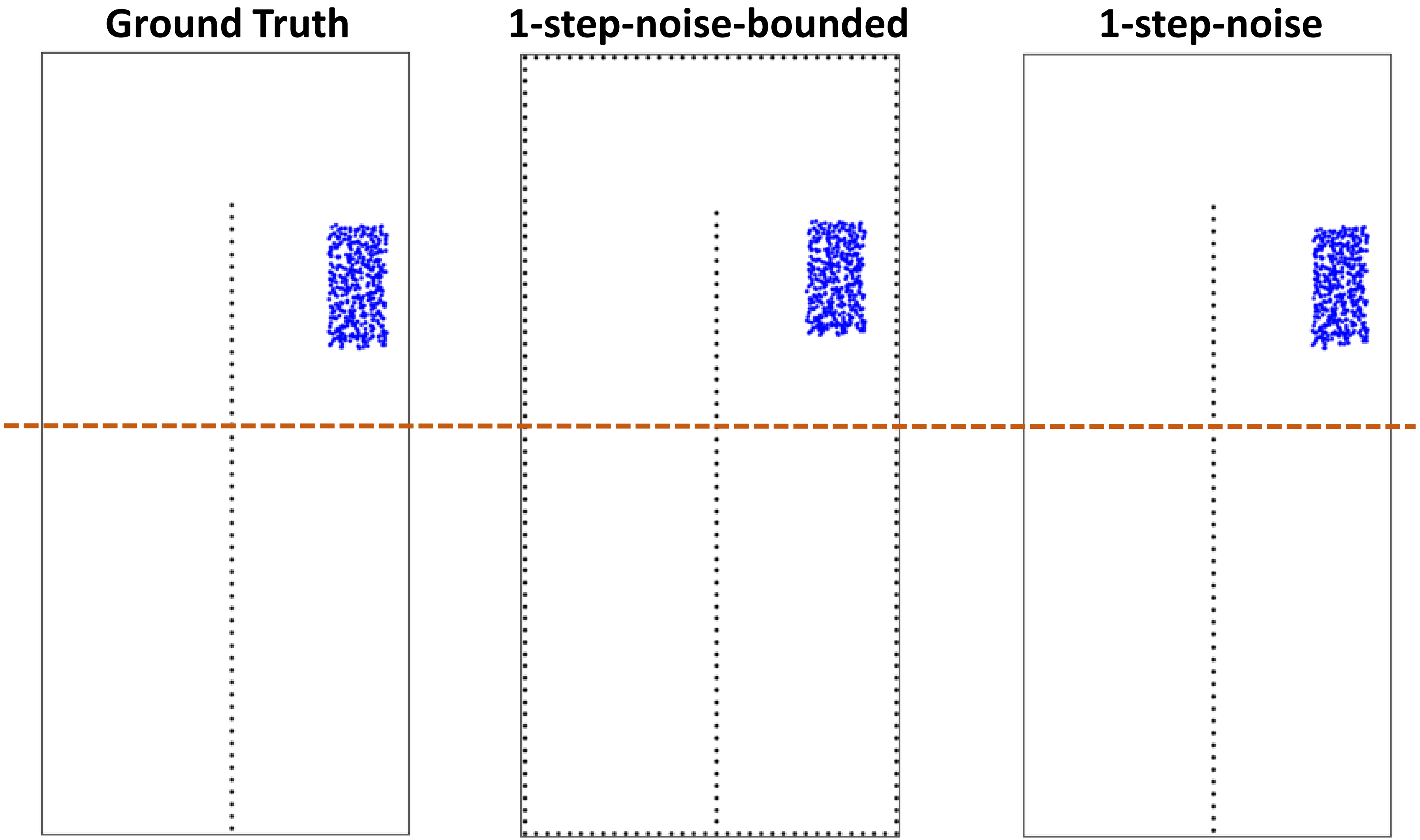


2-step-scratch model


Ground truth


Prediction

Generalization Test

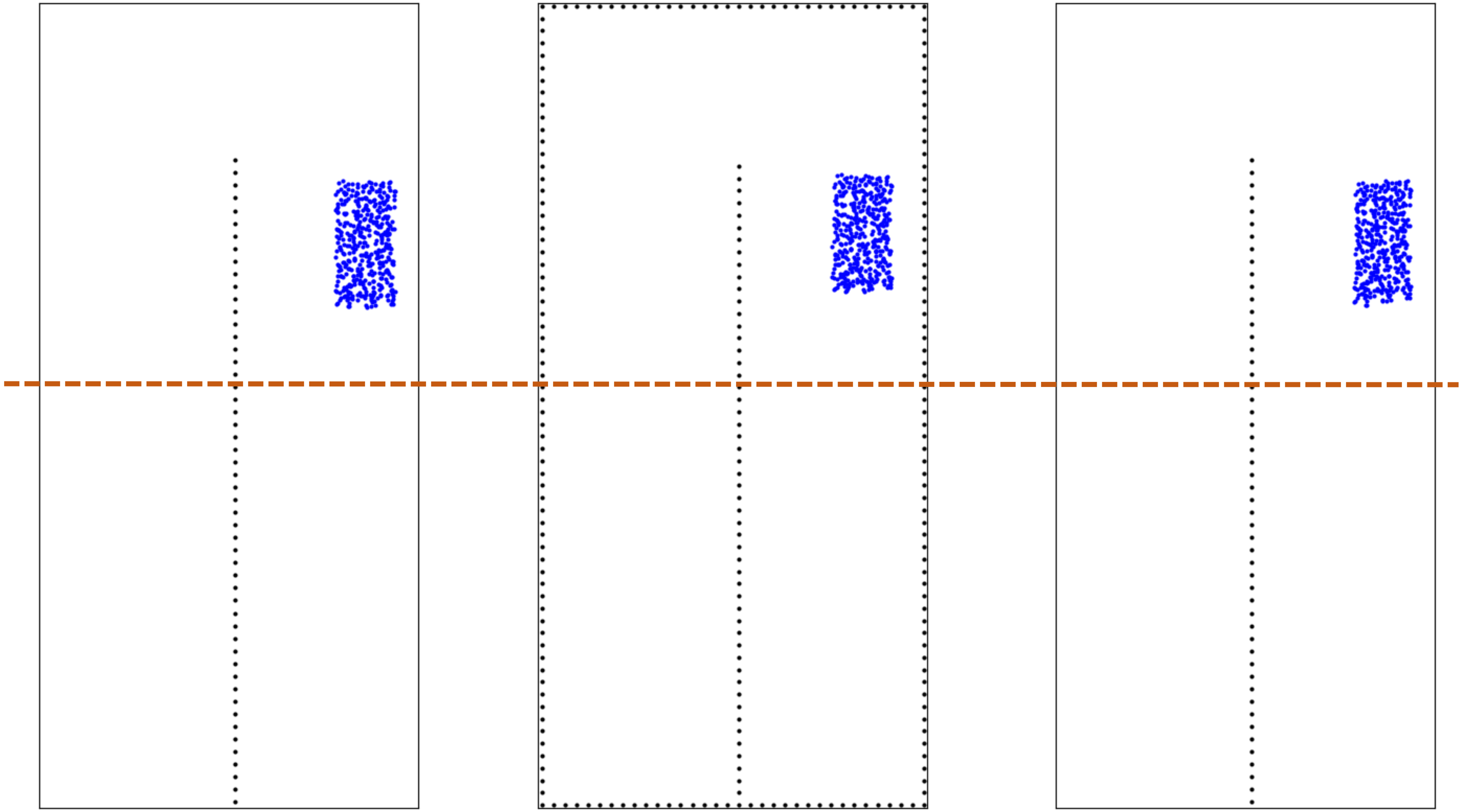


Ground Truth

1-step-noise-bounded

1-step-noise

Generalization Test



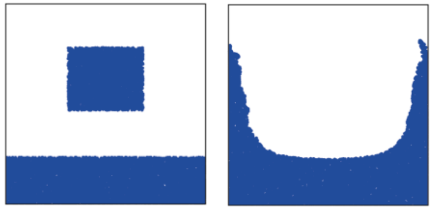
Ground Truth

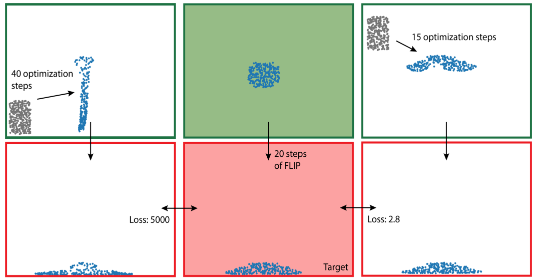
1-step-noise-bounded

1-step-noise

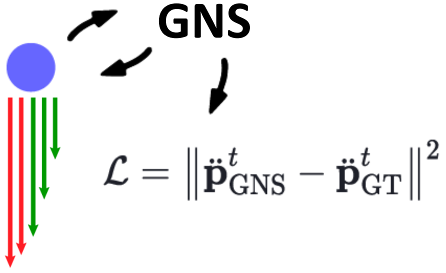
Conclusions and Outlook

- **Deep learning ↔ Differentiable physics**



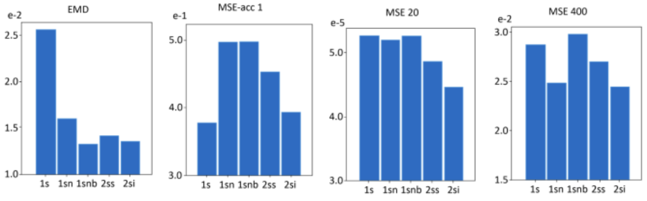


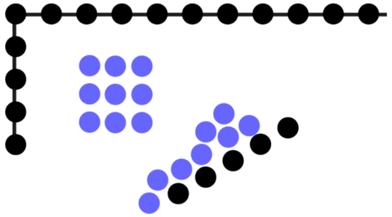
- **New error mitigation**



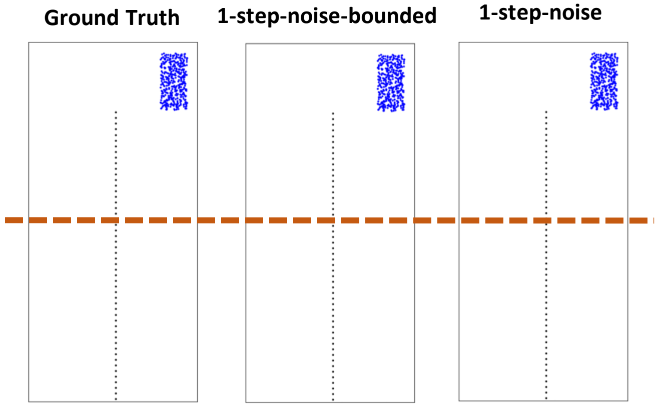
$$\mathcal{L} = \left\| \ddot{\mathbf{p}}^t_{\mathrm{GNS}} - \ddot{\mathbf{p}}^t_{\mathrm{GT}} \right\|^2$$

- **Improved generalization**





- **Weak physical understanding**



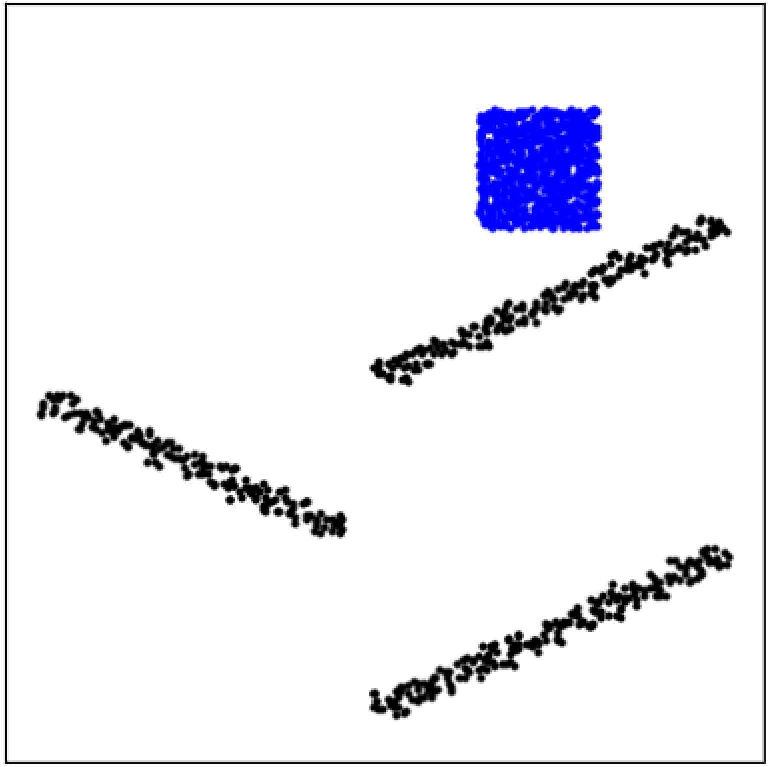
Physical biases **Inverse Problems**

Analyze reasoning **Improve FLIP**

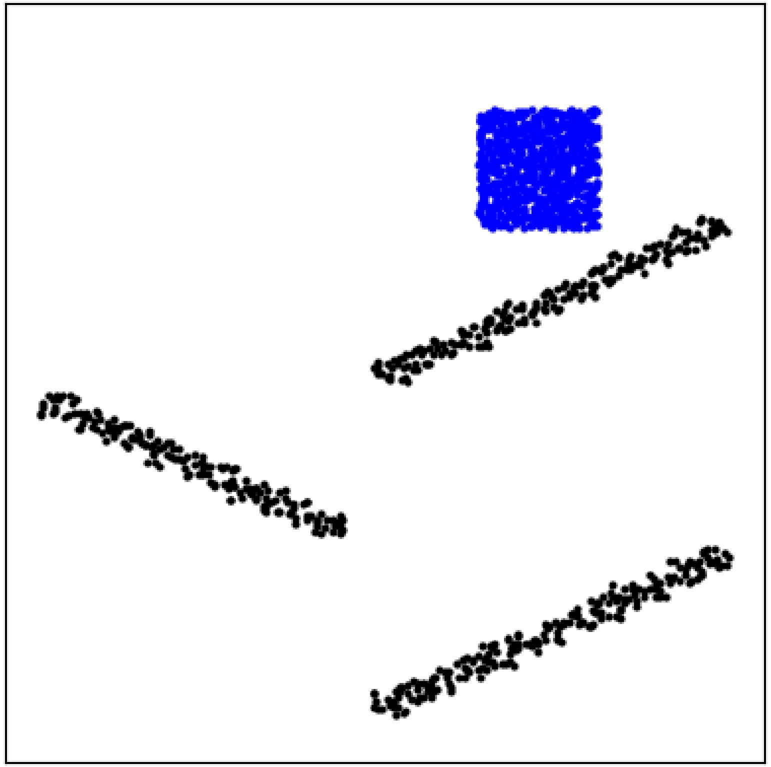
THANK YOU!

Appendix

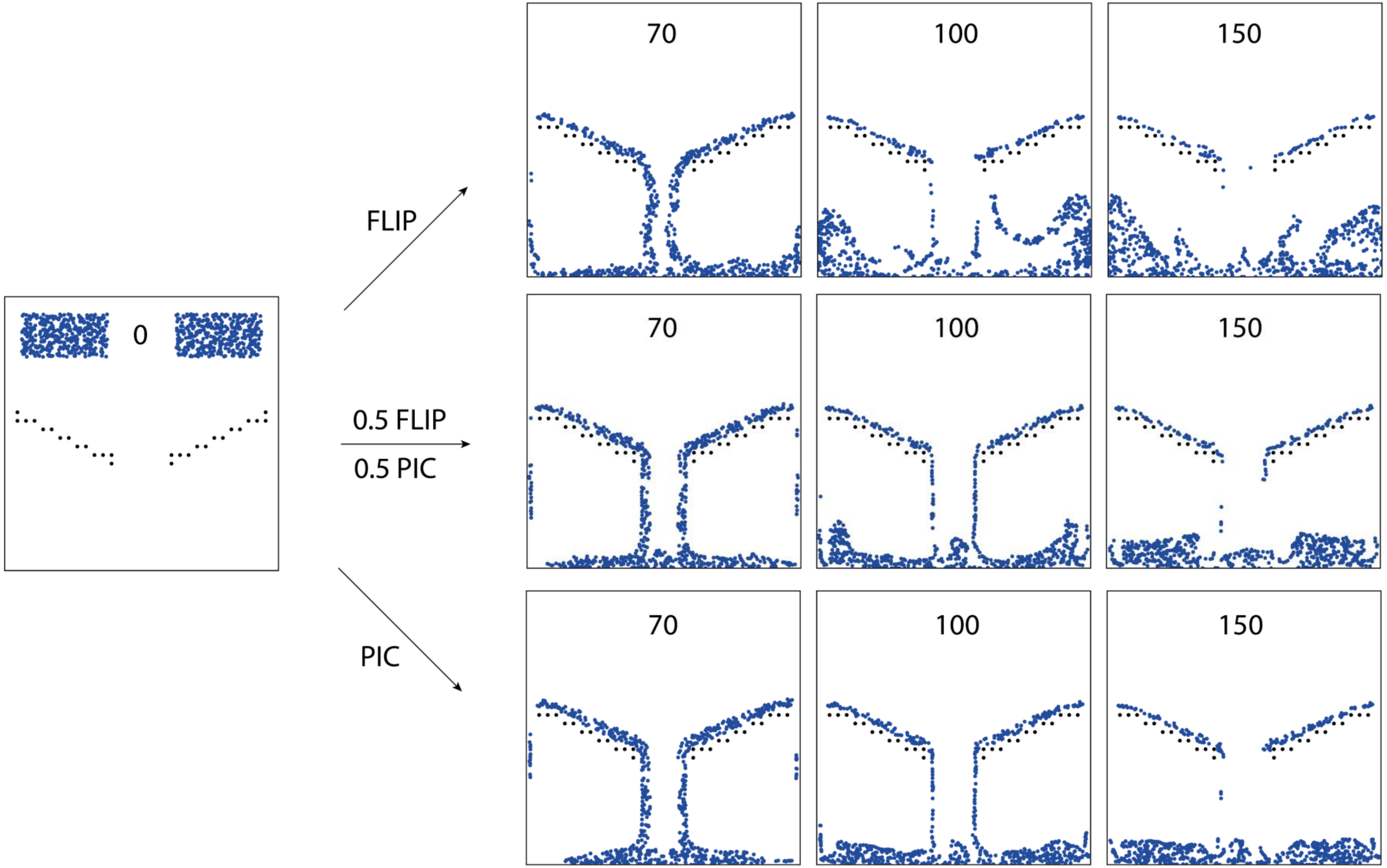
FLIP Verification - Simulation



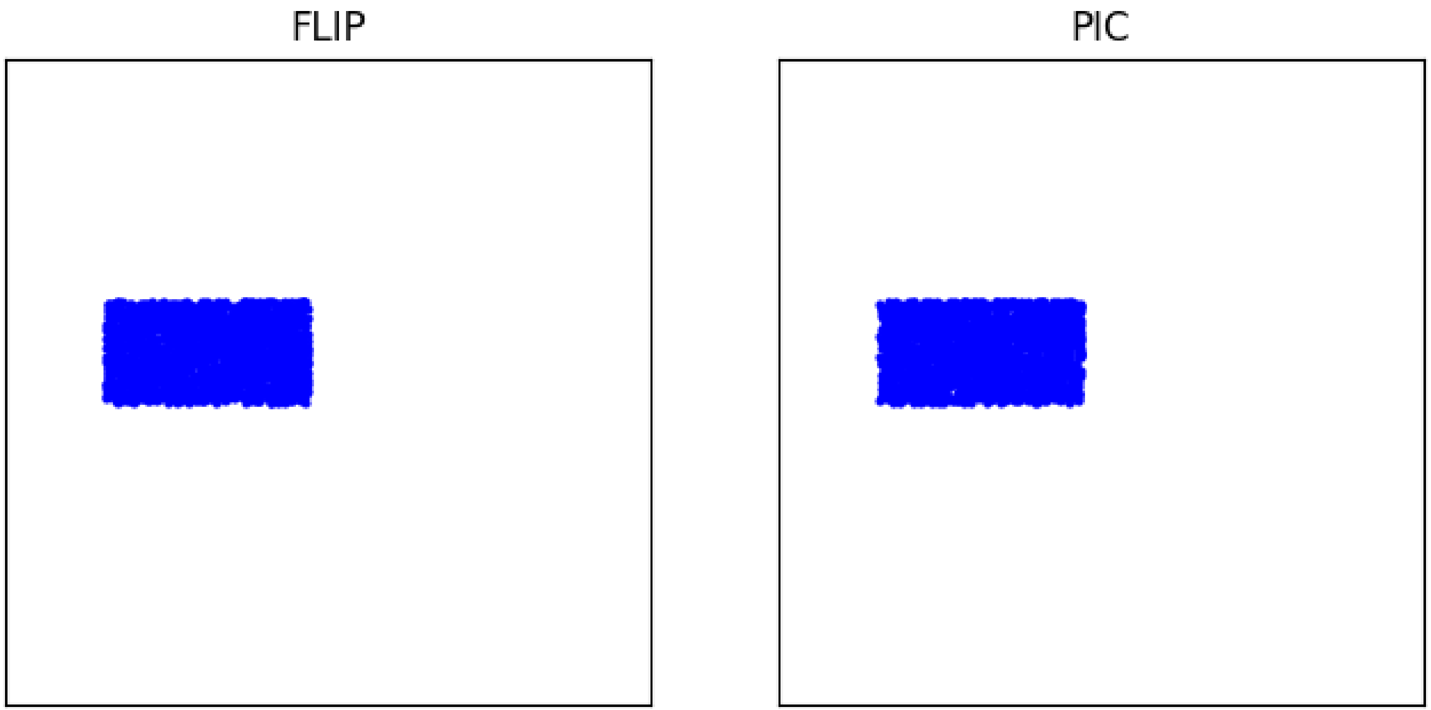
FLIP Verification - Simulation



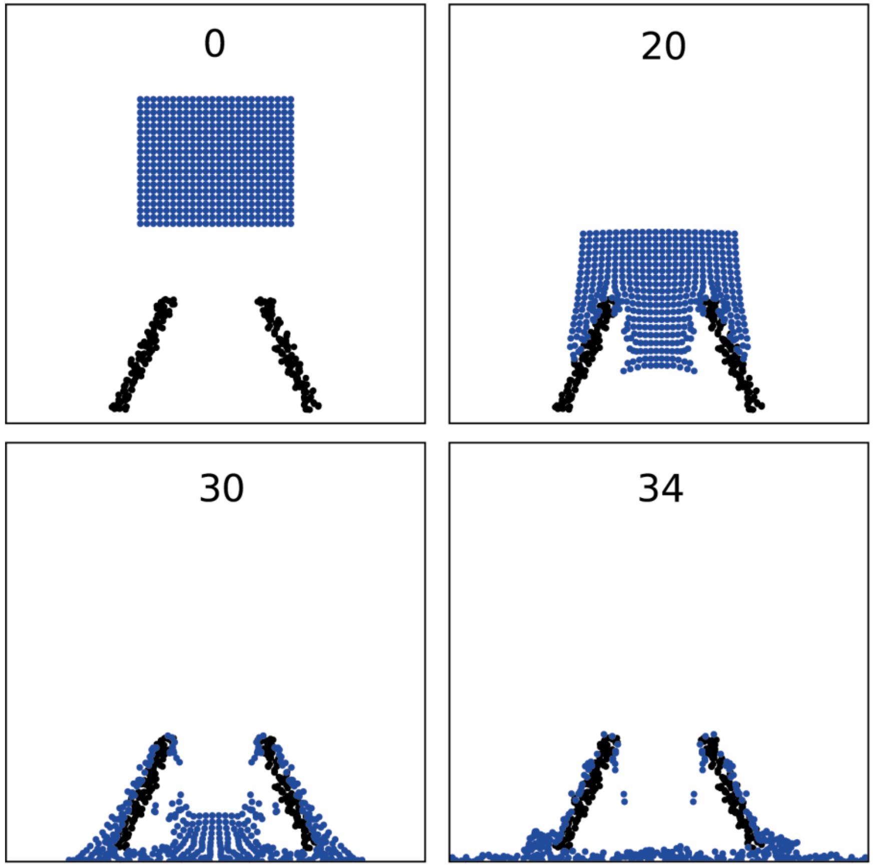
FLIP Verification - Artificial Viscosity

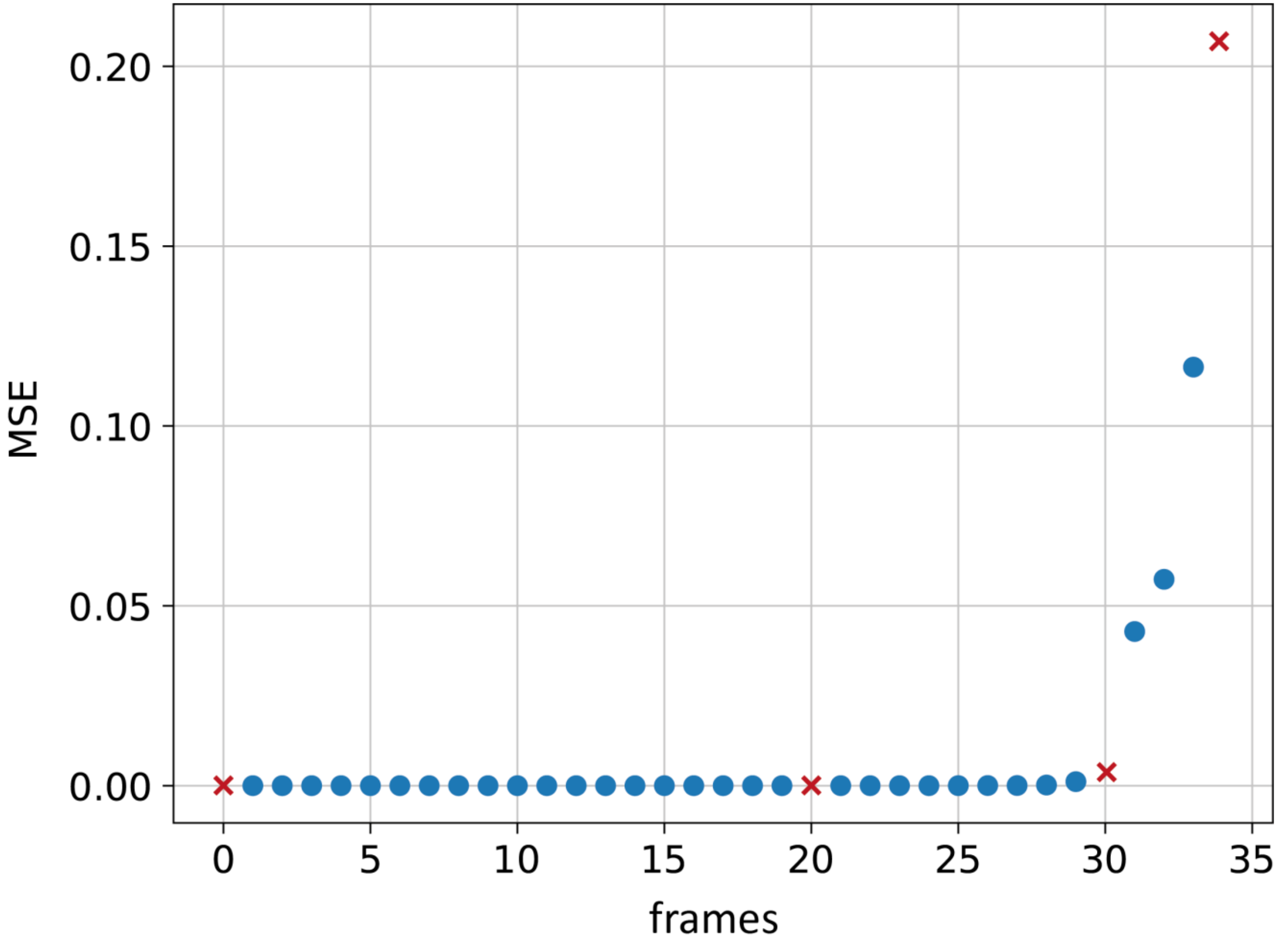


FLIP Verification - Artificial Viscosity

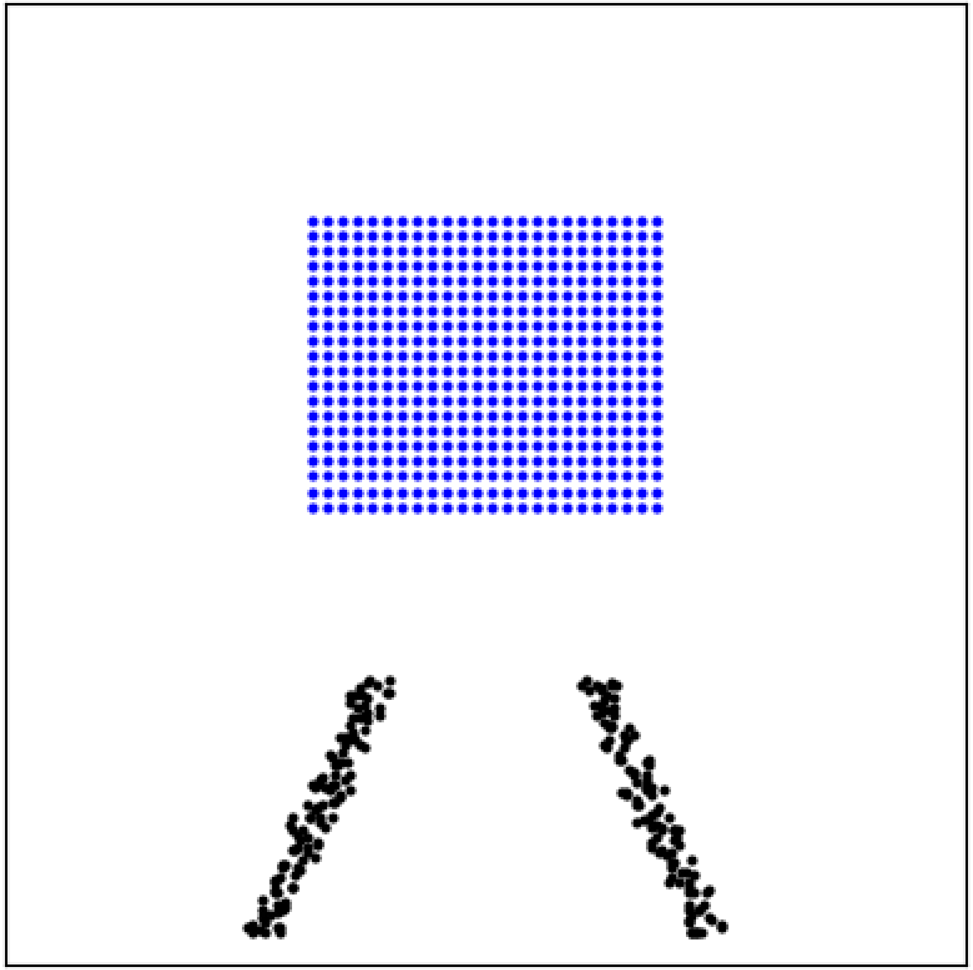


FLIP Verification - Symmetry Test

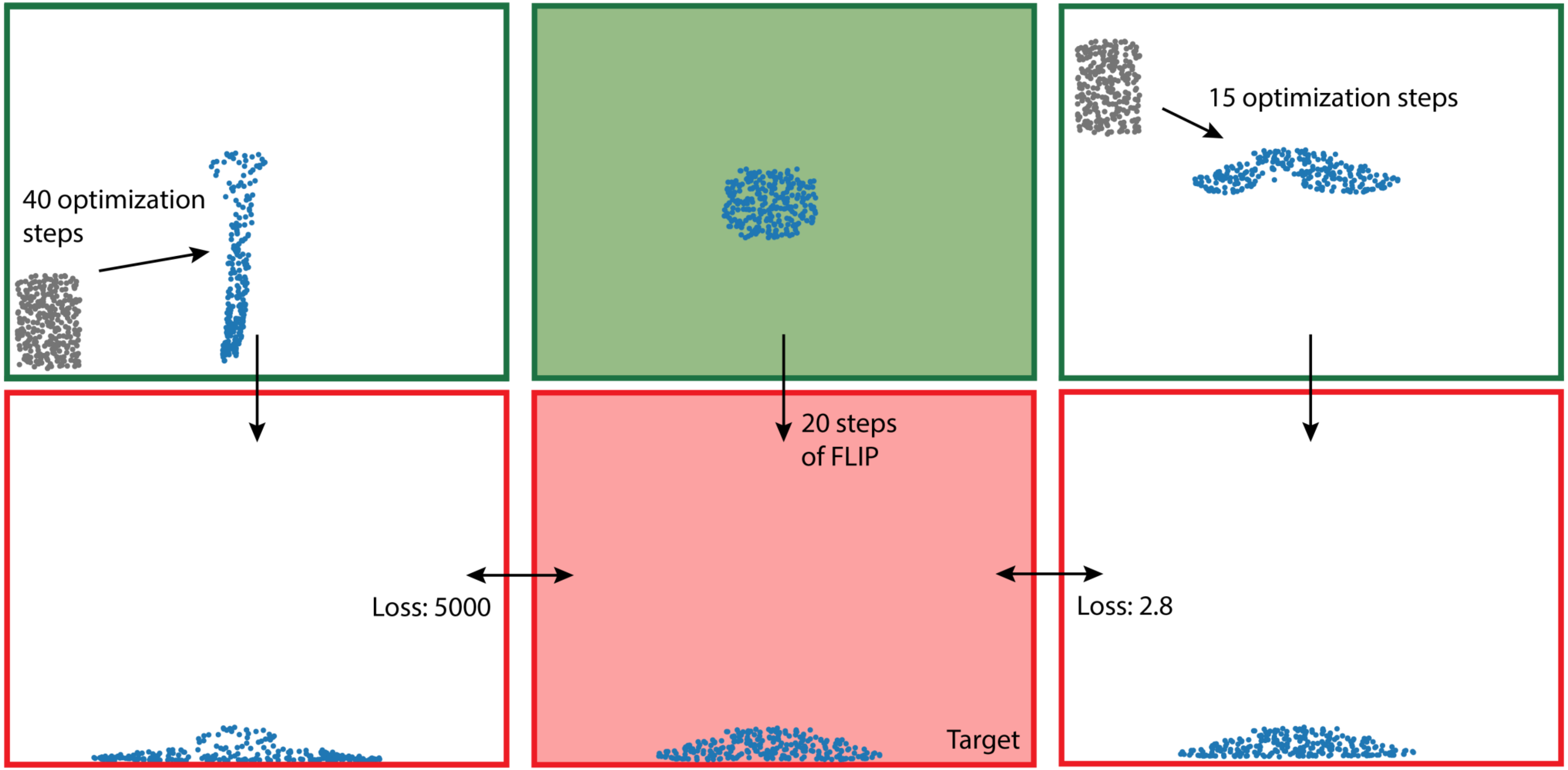




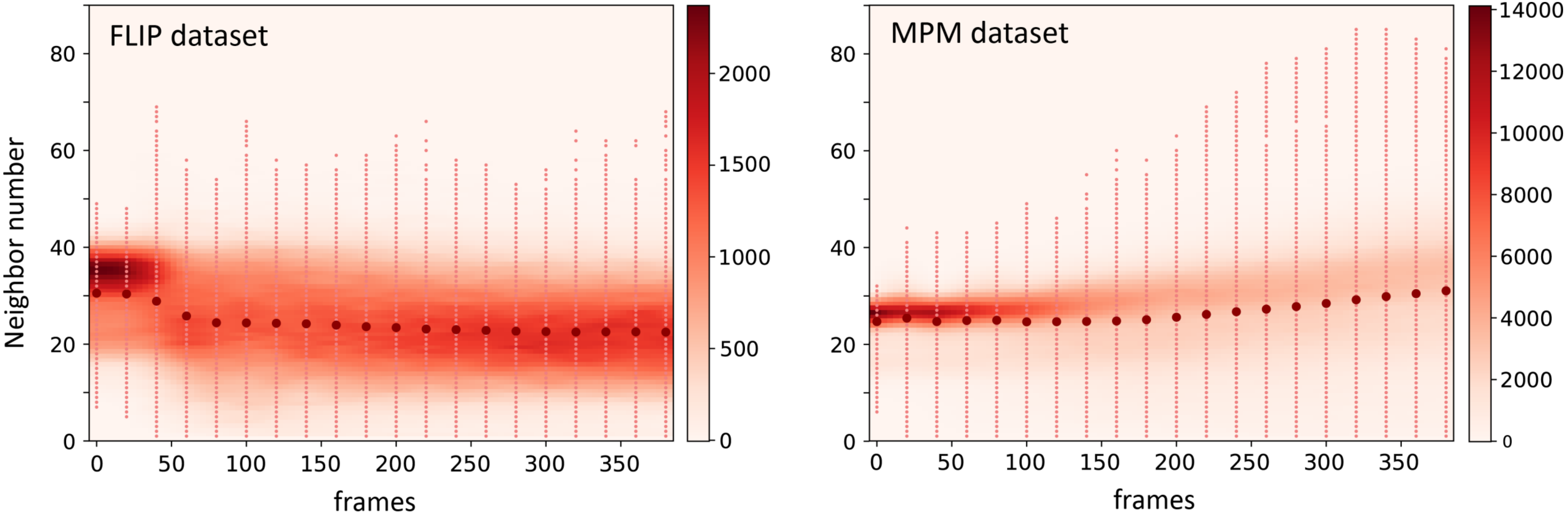
FLIP Verification - Symmetry



FLIP Simulation - Differentiability



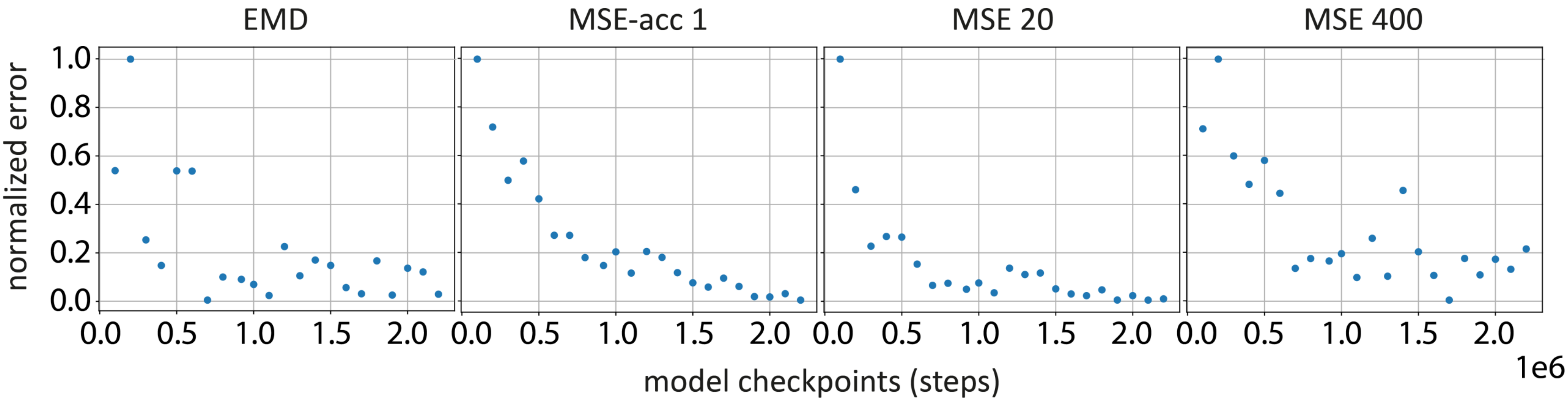
Radius Analysis



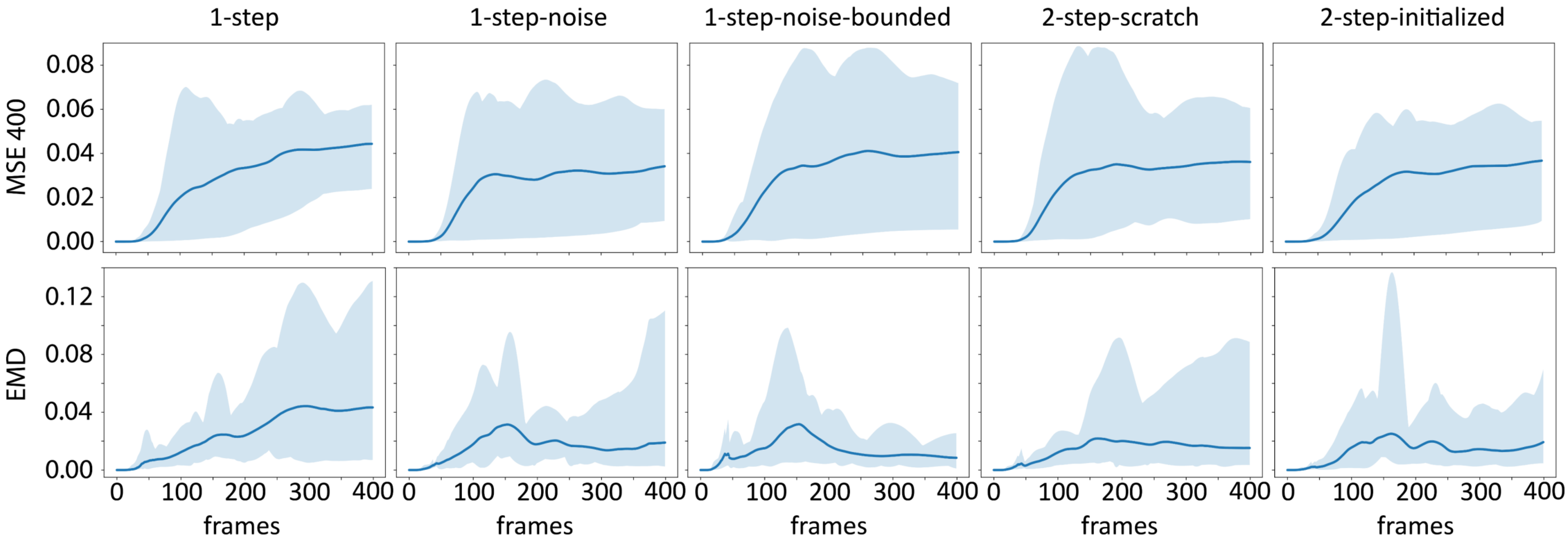
Training Details

- **Adam optimizer**
- **Exponential learning rate decay ($\mathbf{10^{-4}}$ to $\mathbf{10^{-6}}$)**
- **Domain size 0.8**
- **Connectivity radius 0.03**
- **Normalization to zero mean and unit variance**

Model Screening

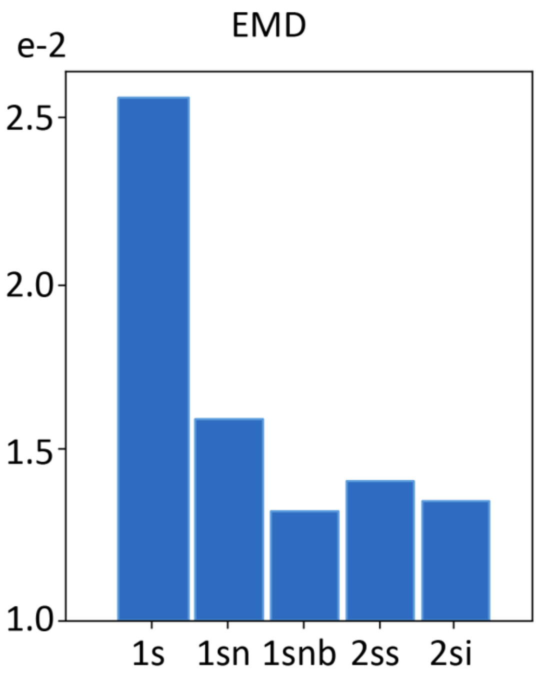


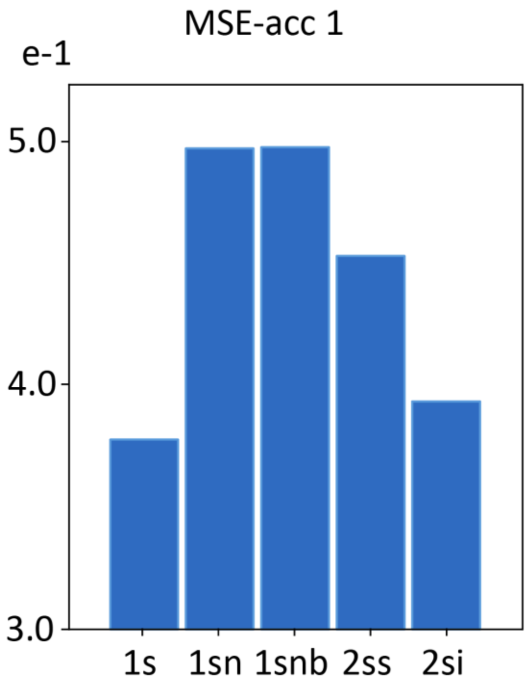
Error Trajectories

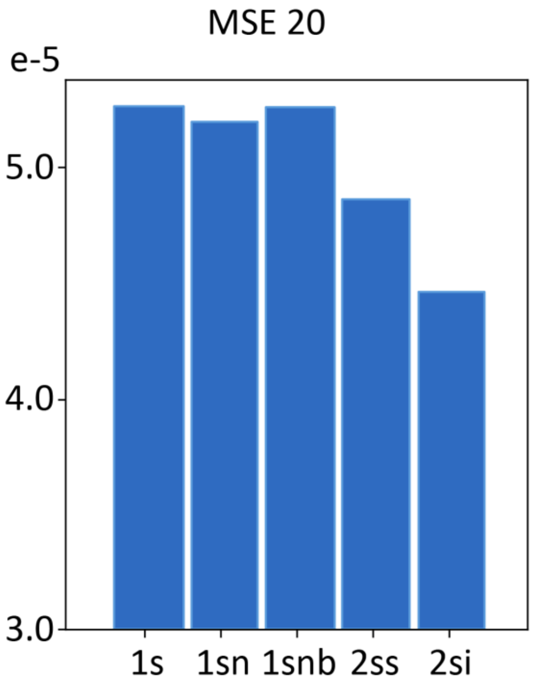


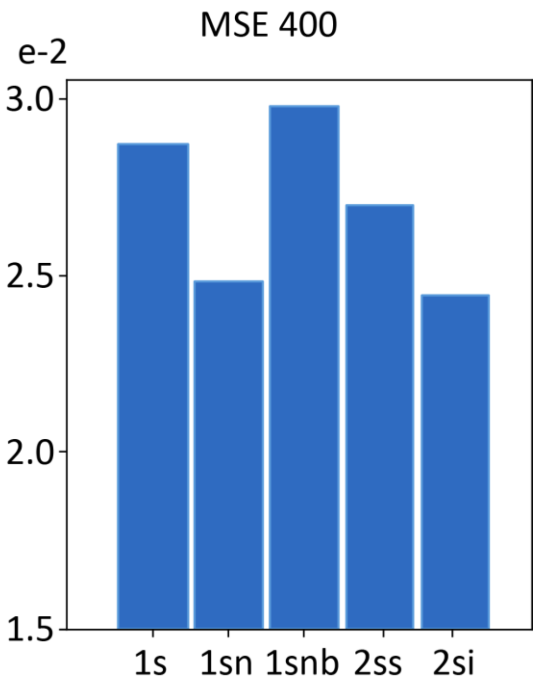
Quantitative Comparison

Model variant	EMD (10^{-2})	MSE-acc 1 (10^{-1})	MSE 20 (10^{-5})	MSE 400 (10^{-2})
1-step	2.598	**3.775**	5.653	2.853
1-step-noise	1.617	4.980	5.574	2.469
1-step-noise-bounded	**1.336**	4.985	5.648	2.959
2-step-scratch	1.428	4.535	5.181	2.682
2-step-initialized	1.367	3.933	**4.711**	**2.430**

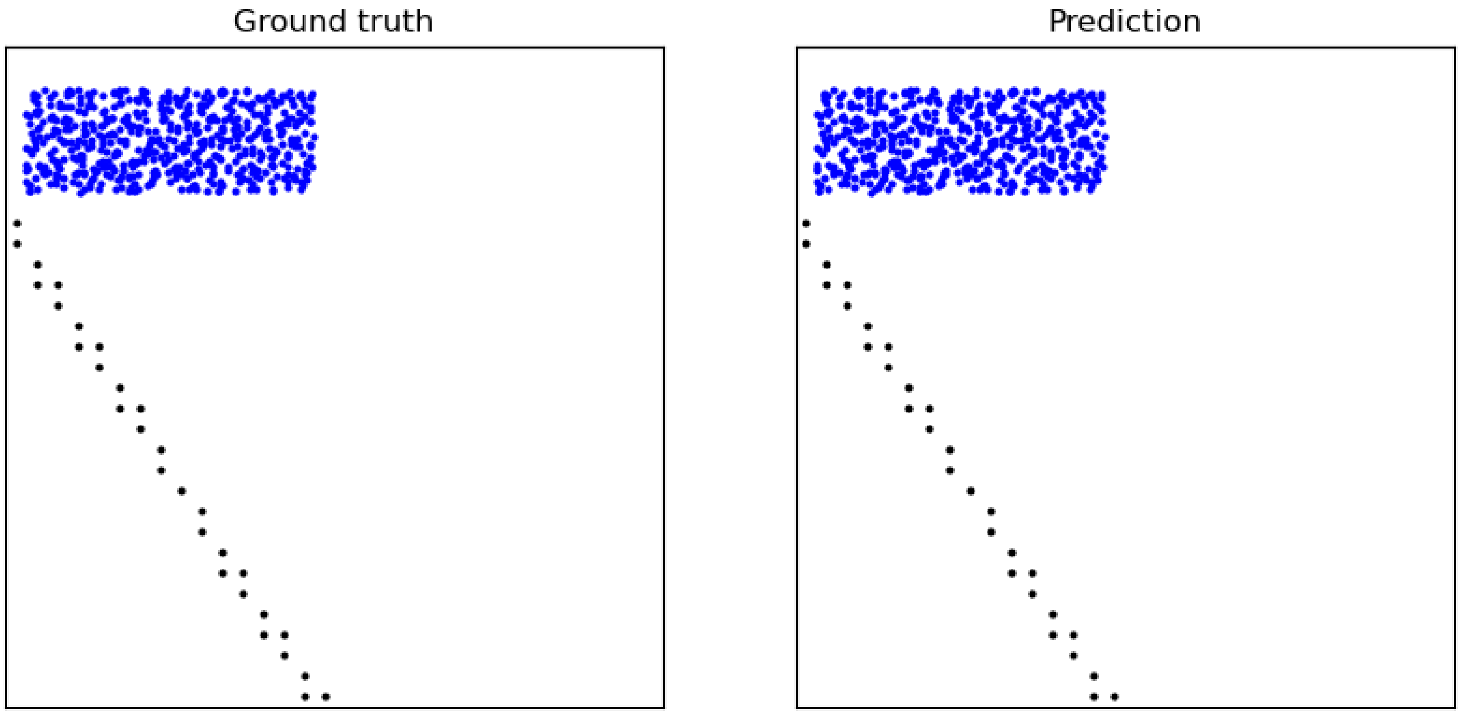




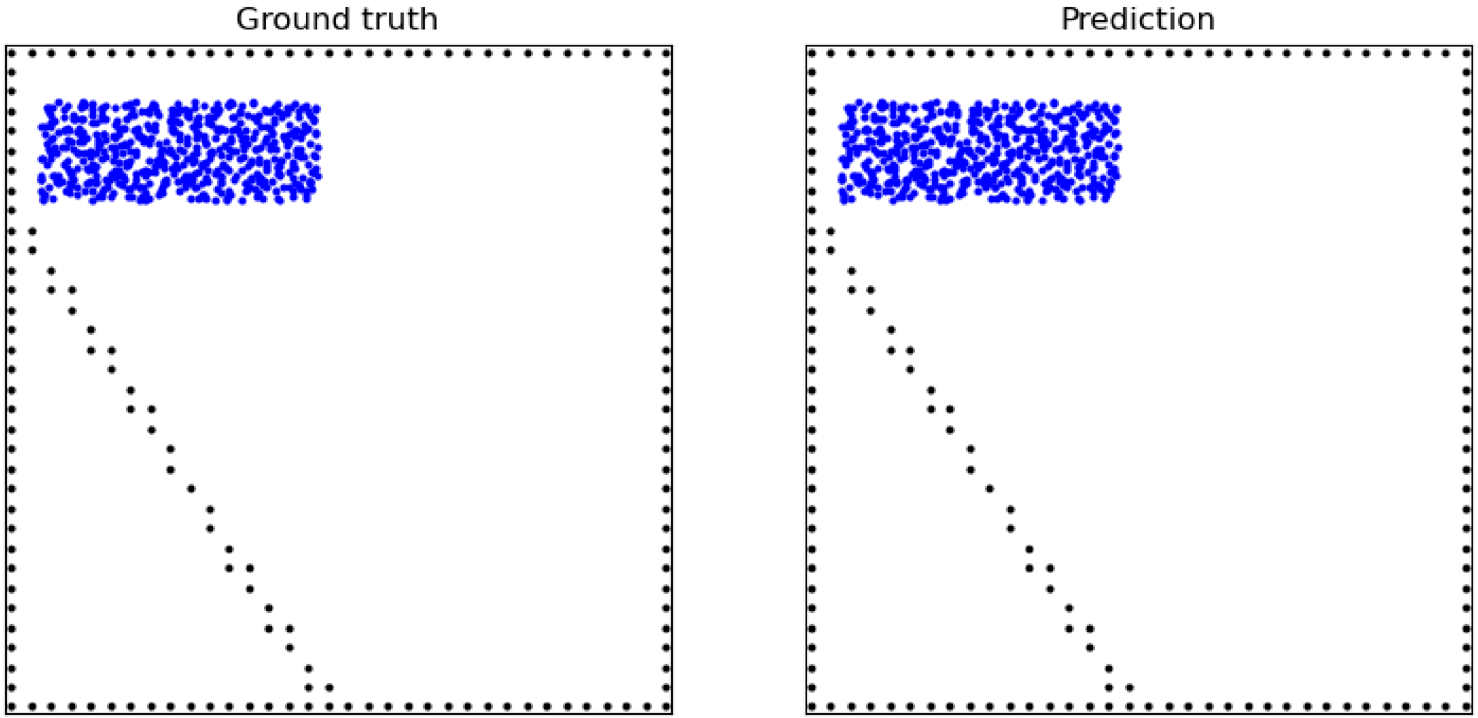




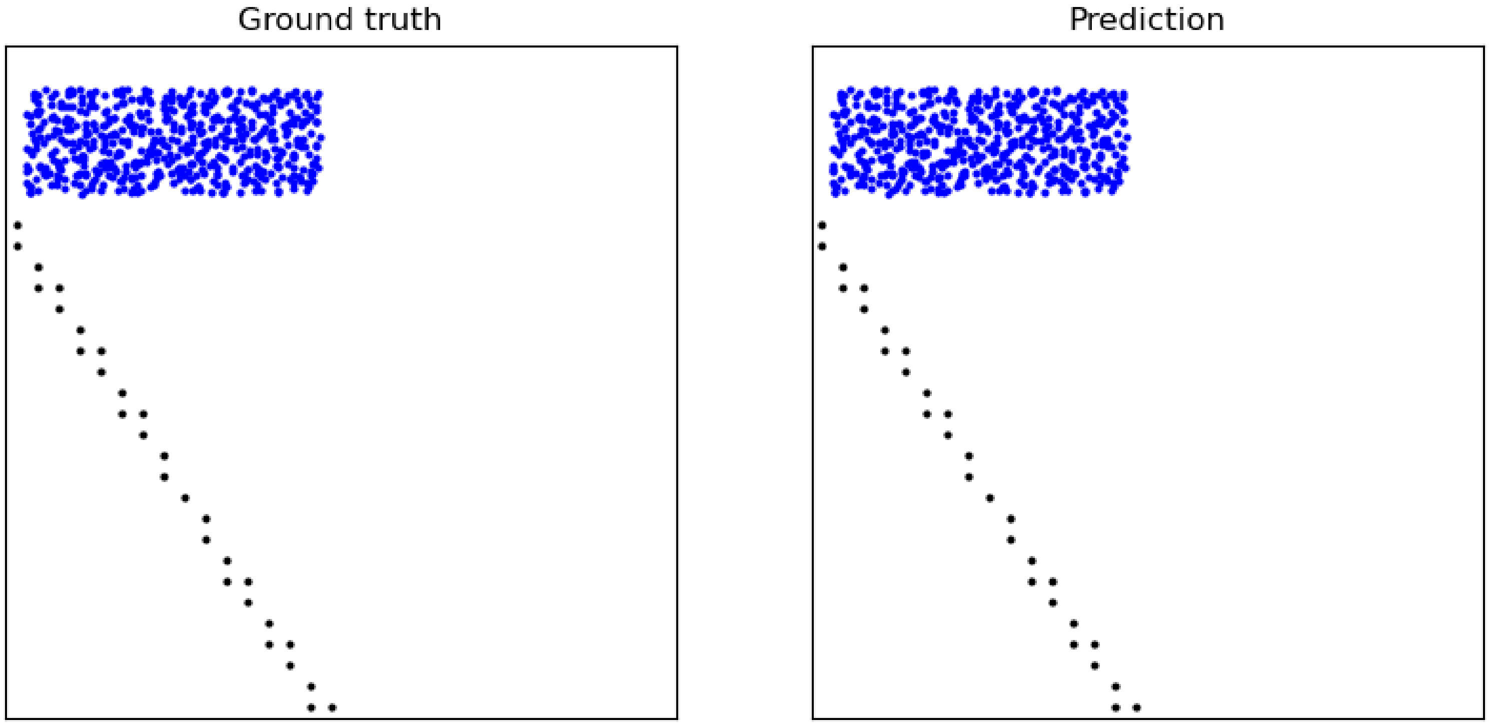
1-step model



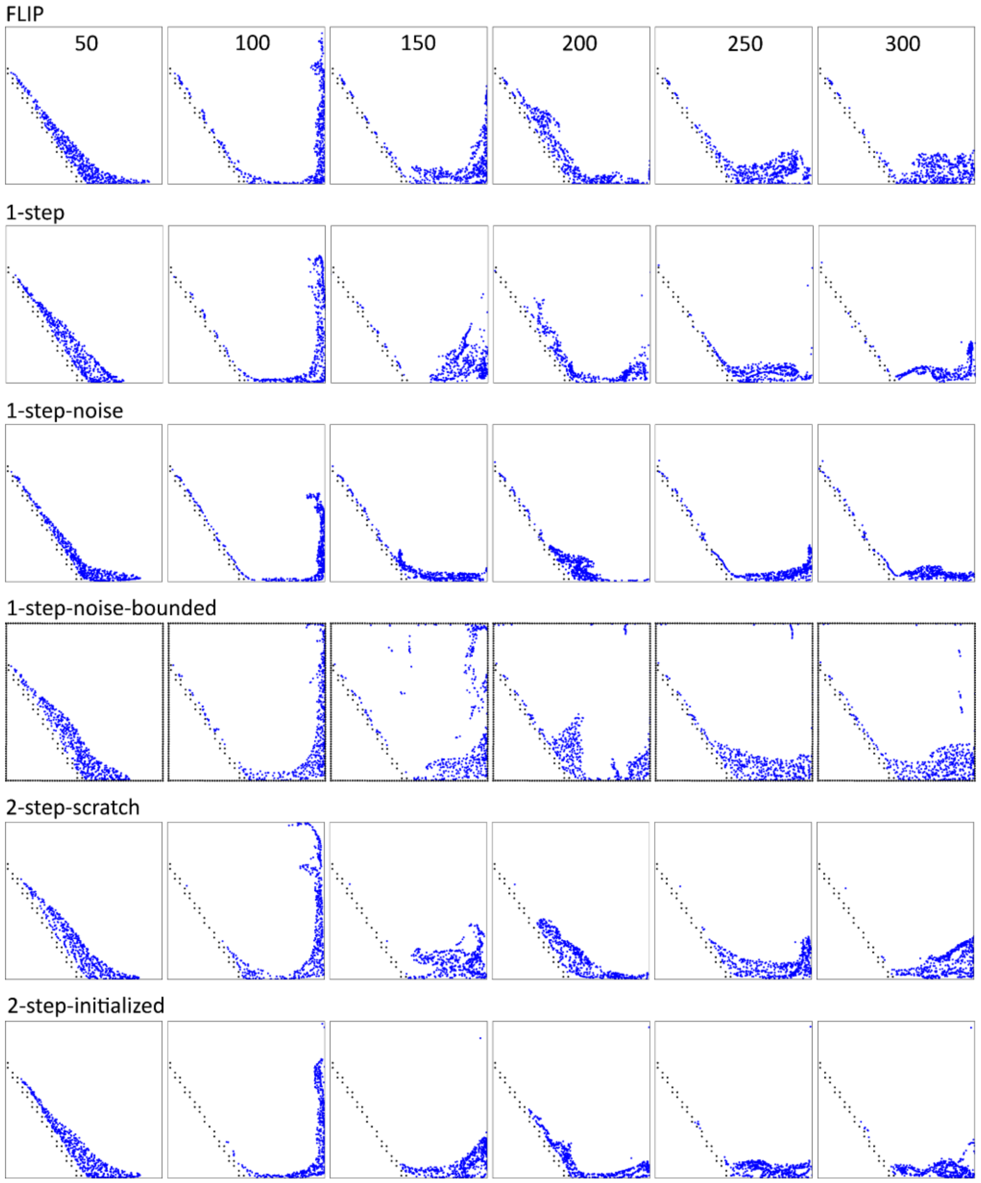
1-step-noise-bounded model



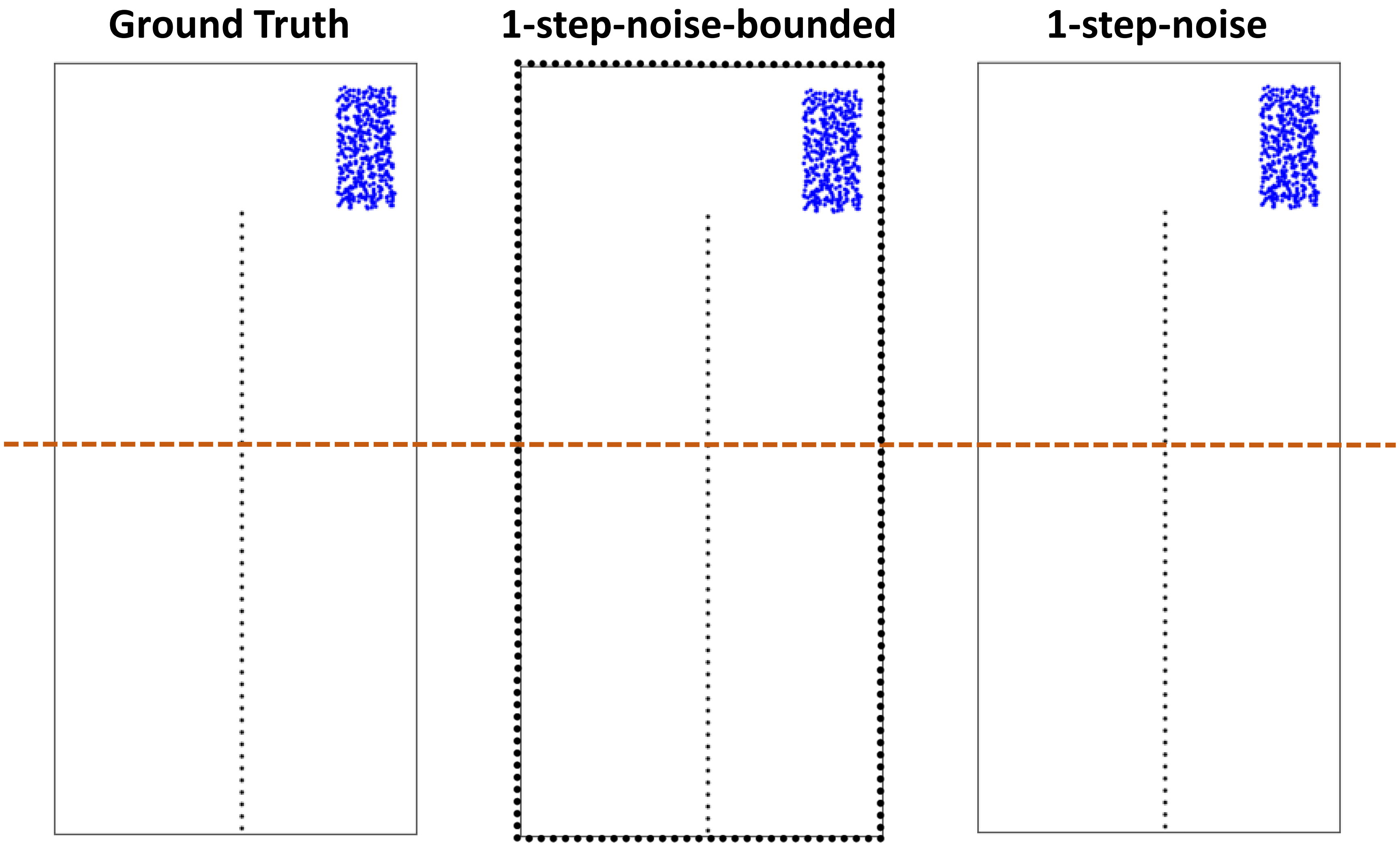
2-step-initialized model



Model Predictions



Generalization Test

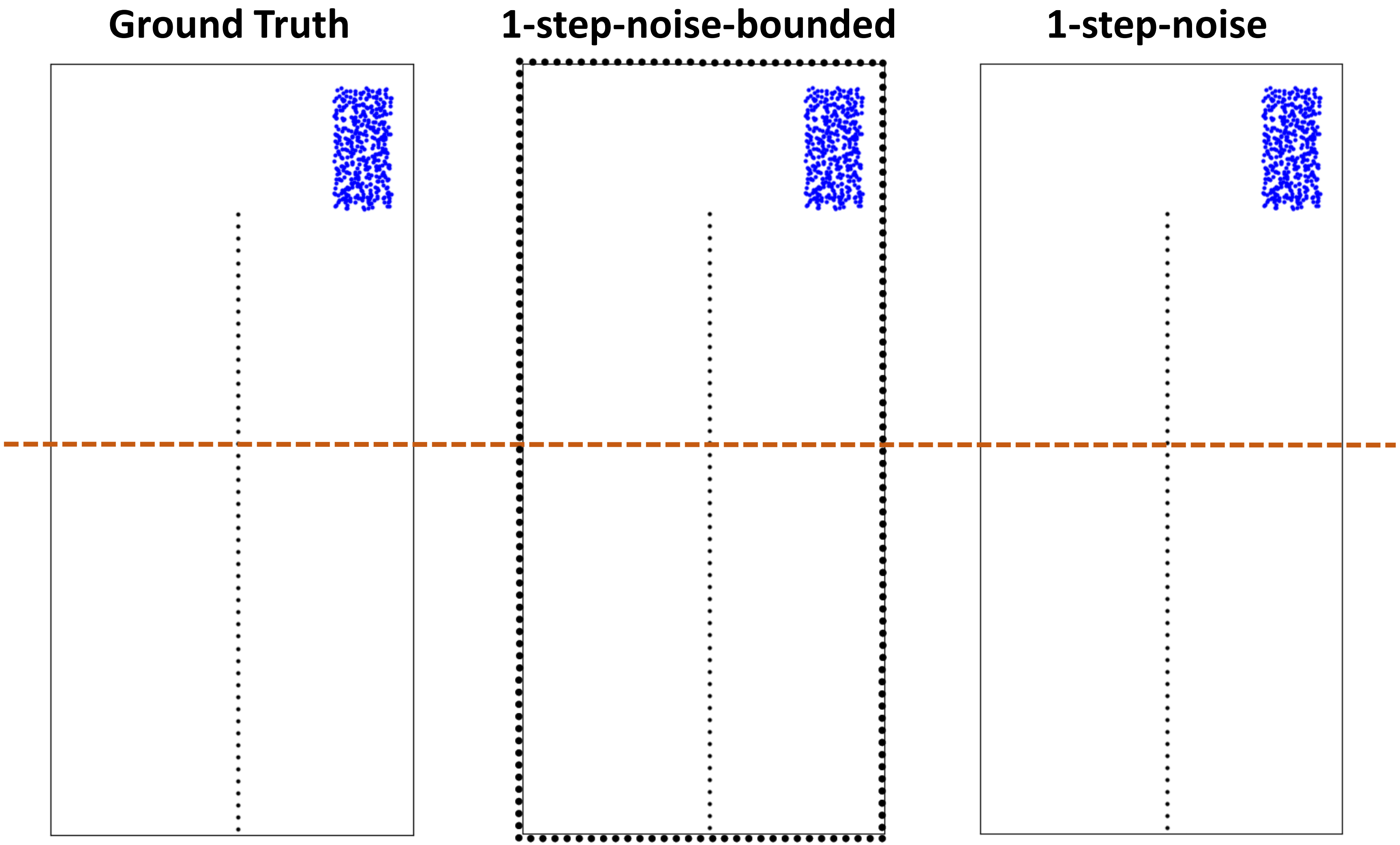


Ground Truth

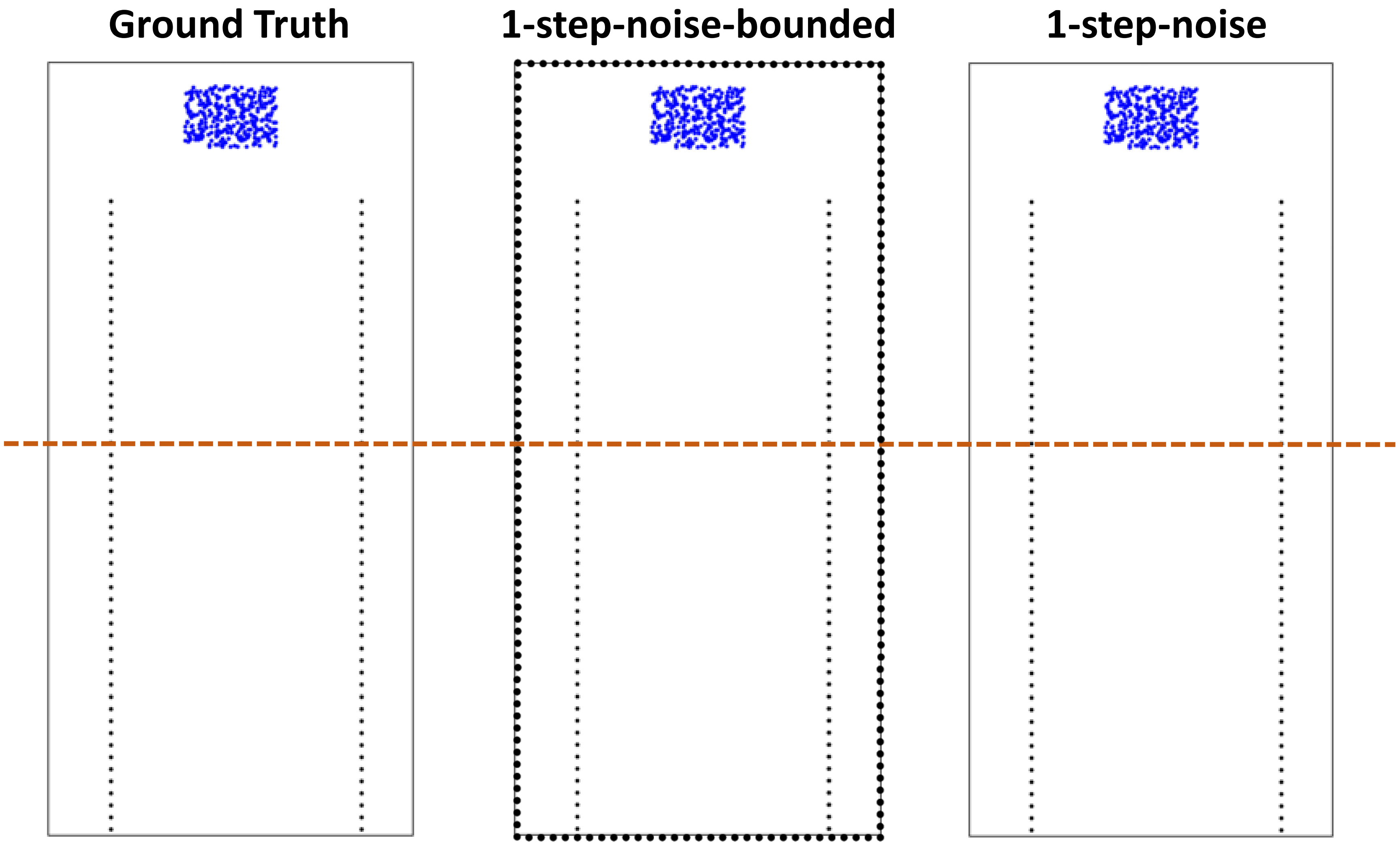
1-step-noise-bounded

1-step-noise

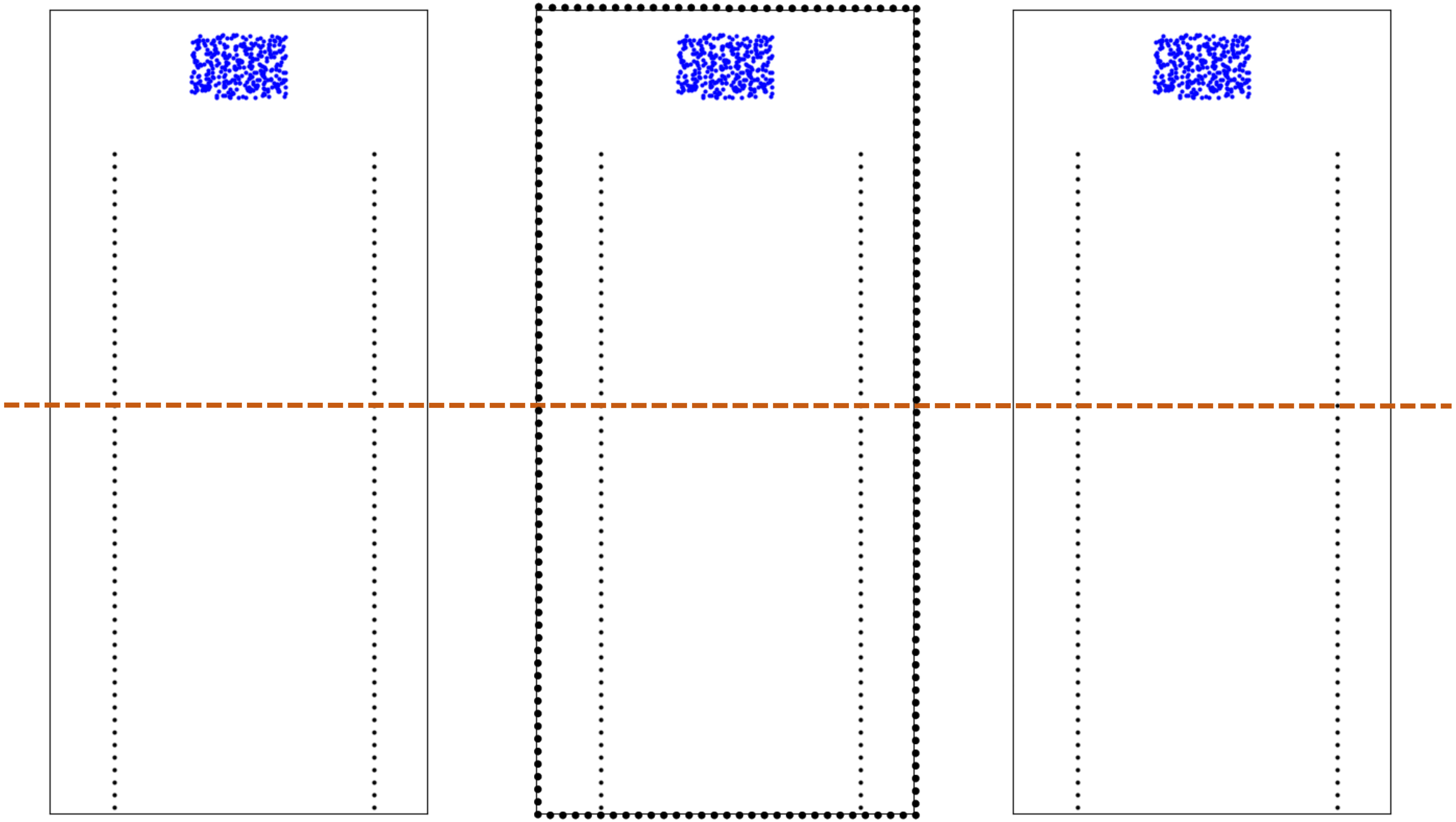
Generalization Test



Generalization Test



Generalization Test

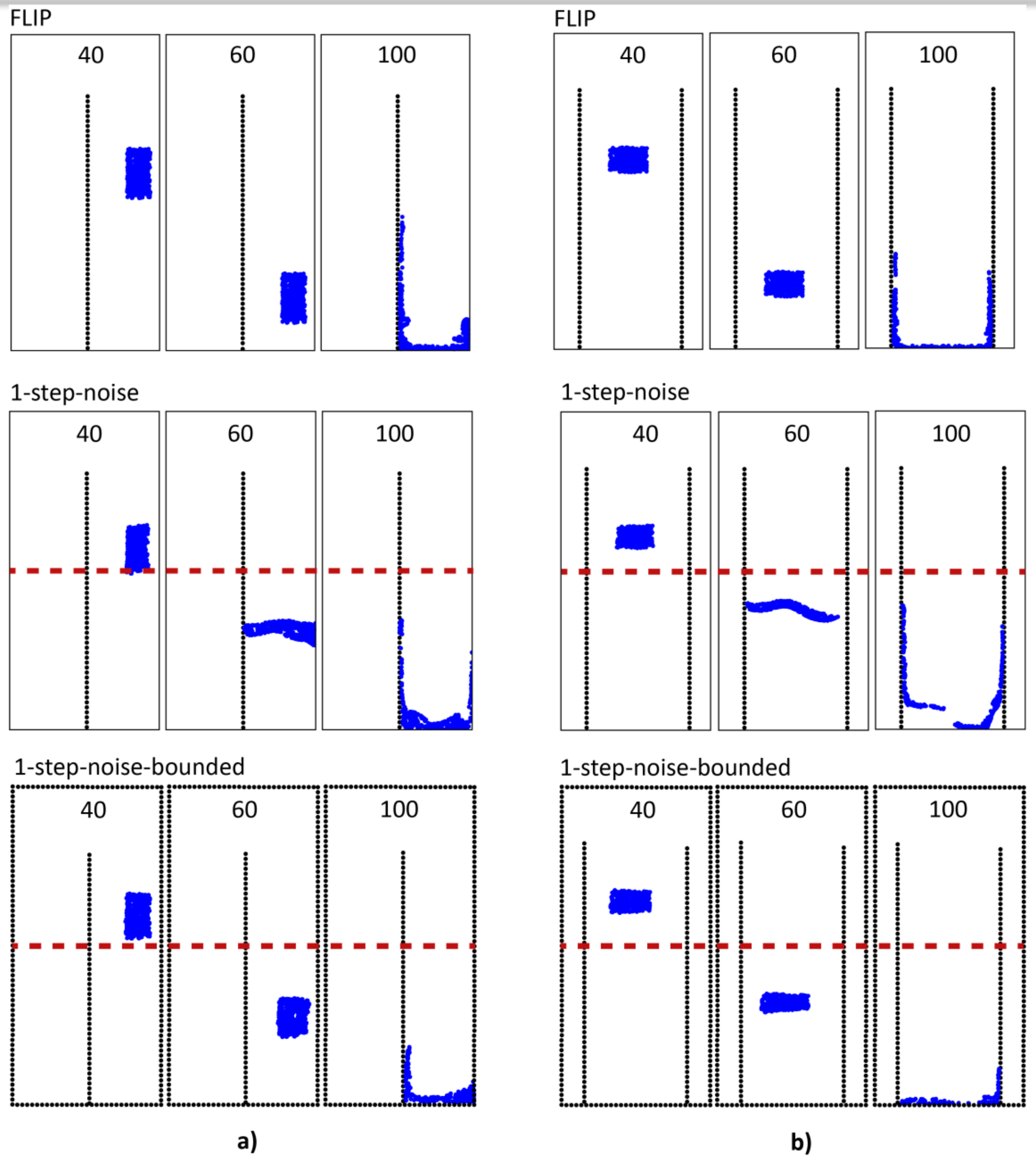


Ground Truth

1-step-noise-bounded

1-step-noise

Generalization Test


FLIP
40
60
100
FLIP
40
60
100
1-step-noise
40
60
100
1-step-noise
40
60
100
1-step-noise-bounded
40
60
100
1-step-noise-bounded
40
60
100
a)
b)