GNN: Simulation

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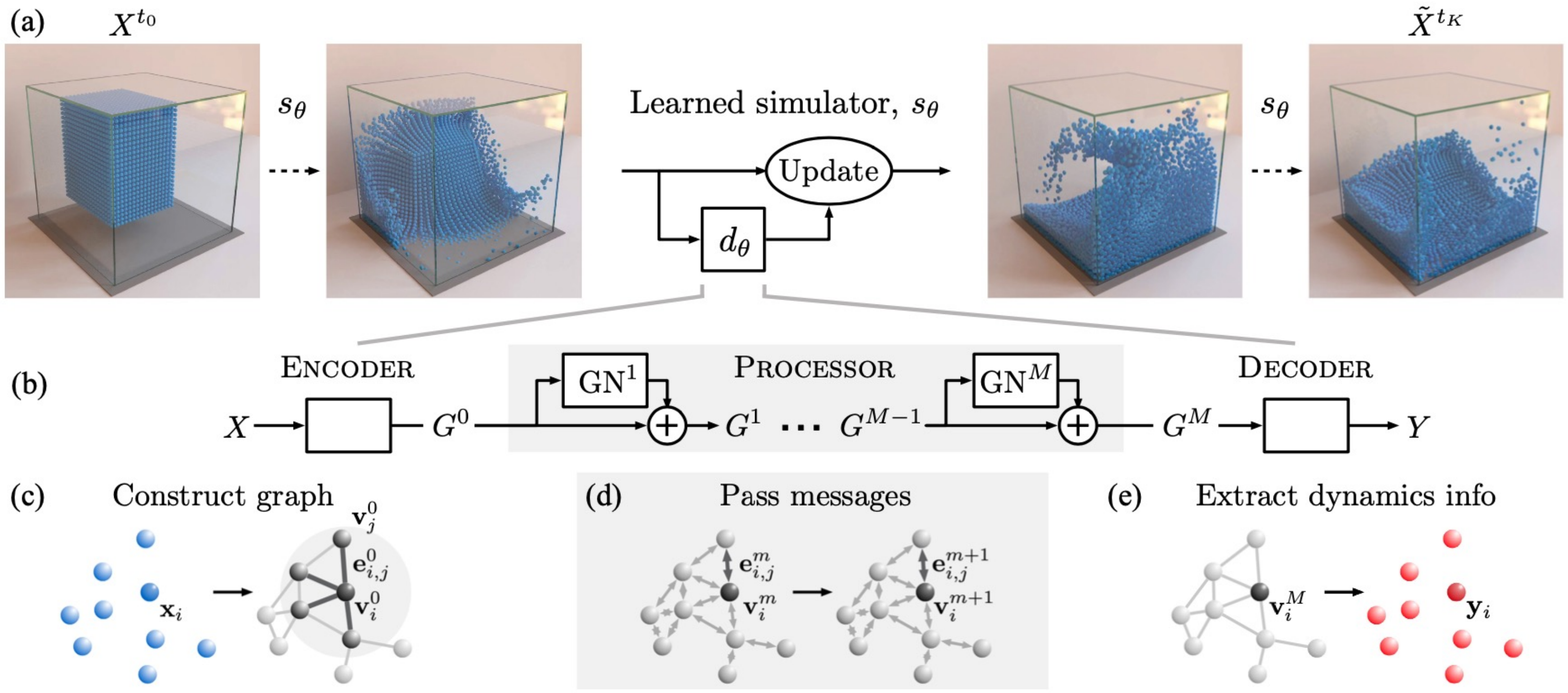
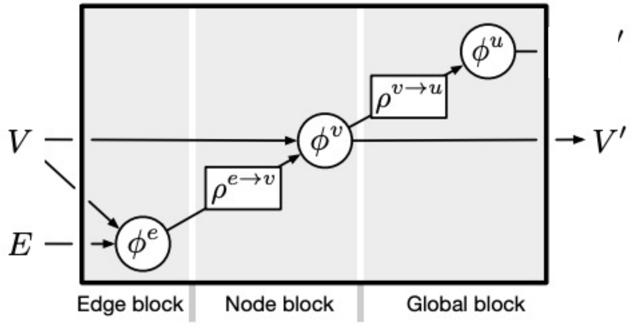
Background

- Realistic simulators of complex physics
    - Invaluable to many scientific and engineering disciplines.
    - Very expensive to create and use.
    - Trade off generality for accuracy.
    - Prohibitive for scaling up.
- Learning simulations from data
    - Use machine learning to train simulators directly from observed data.
    - Efficient and fast for predicting complex phenomena.
    - Difficult for standard end-to-end learning approaches to overcome.
- Graph Network-Based Simulator
    - Inductive biases.
    - Interpretability and generalization ability.

Graph Network-Based Simulator (GNS)

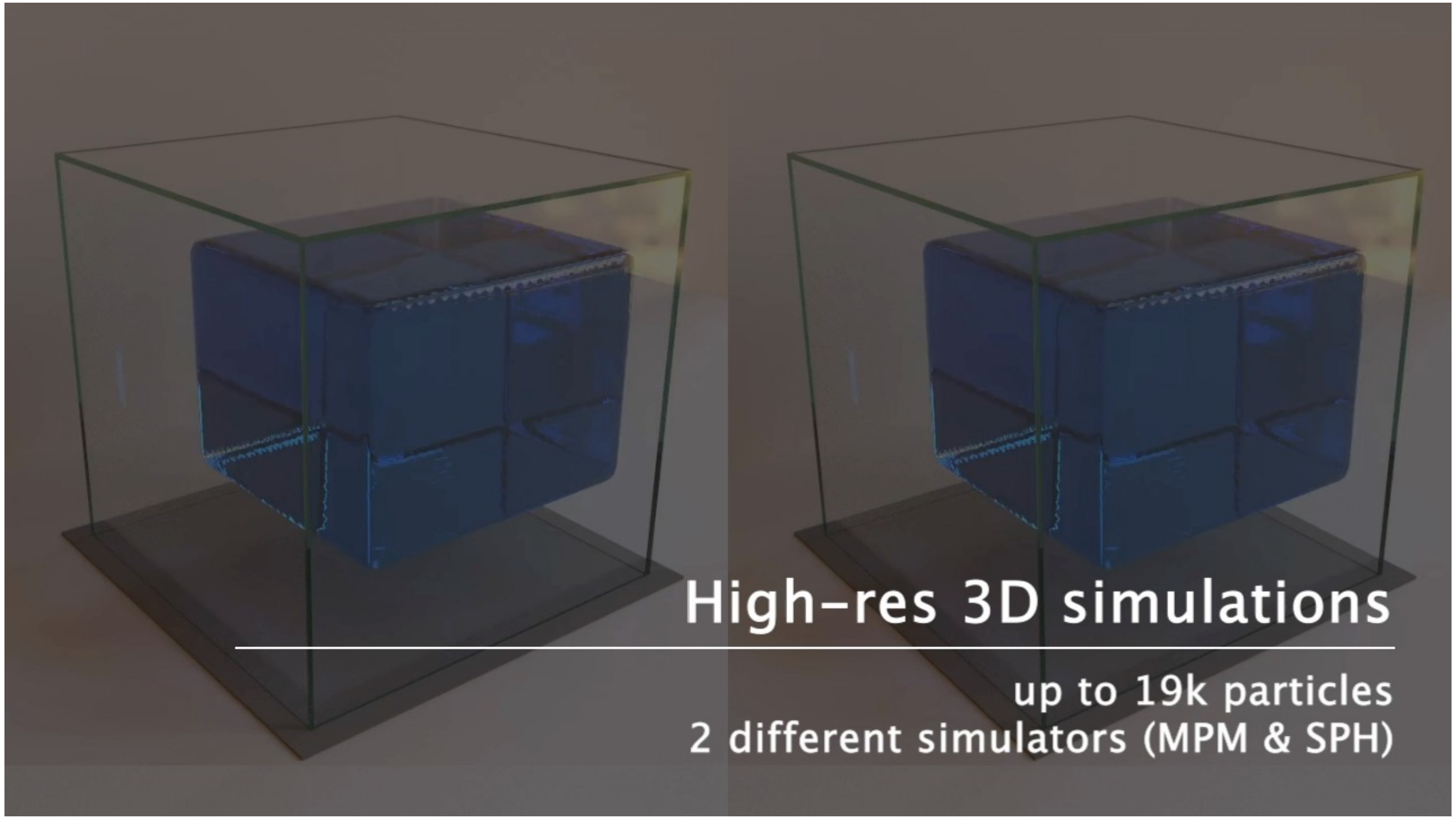




Message-passing neural network

A. Sanchez-Gonzalez, J. Godwin, T. Pfaff, R. Ying, J. Leskovec, and P. W. Battaglia, ‘Learning to Simulate Complex Physics with Graph Networks’, *arXiv:2002.09405 [physics, stat]*, Sep. 2020, Accessed: May 03, 2021.
P. W. Battaglia *et al.*, ‘Relational inductive biases, deep learning, and graph networks’, *arXiv:1806.01261 [cs, stat]*, Oct. 2018, Accessed: May 04, 2021.

Simulation Results



A. Sanchez-Gonzalez, J. Godwin, T. Pfaff, R. Ying, J. Leskovec, and P. W. Battaglia, 'Learning to Simulate Complex Physics with Graph Networks', *arXiv:2002.09405 [physics, stat]*, Sep. 2020, Accessed: May 03, 2021.

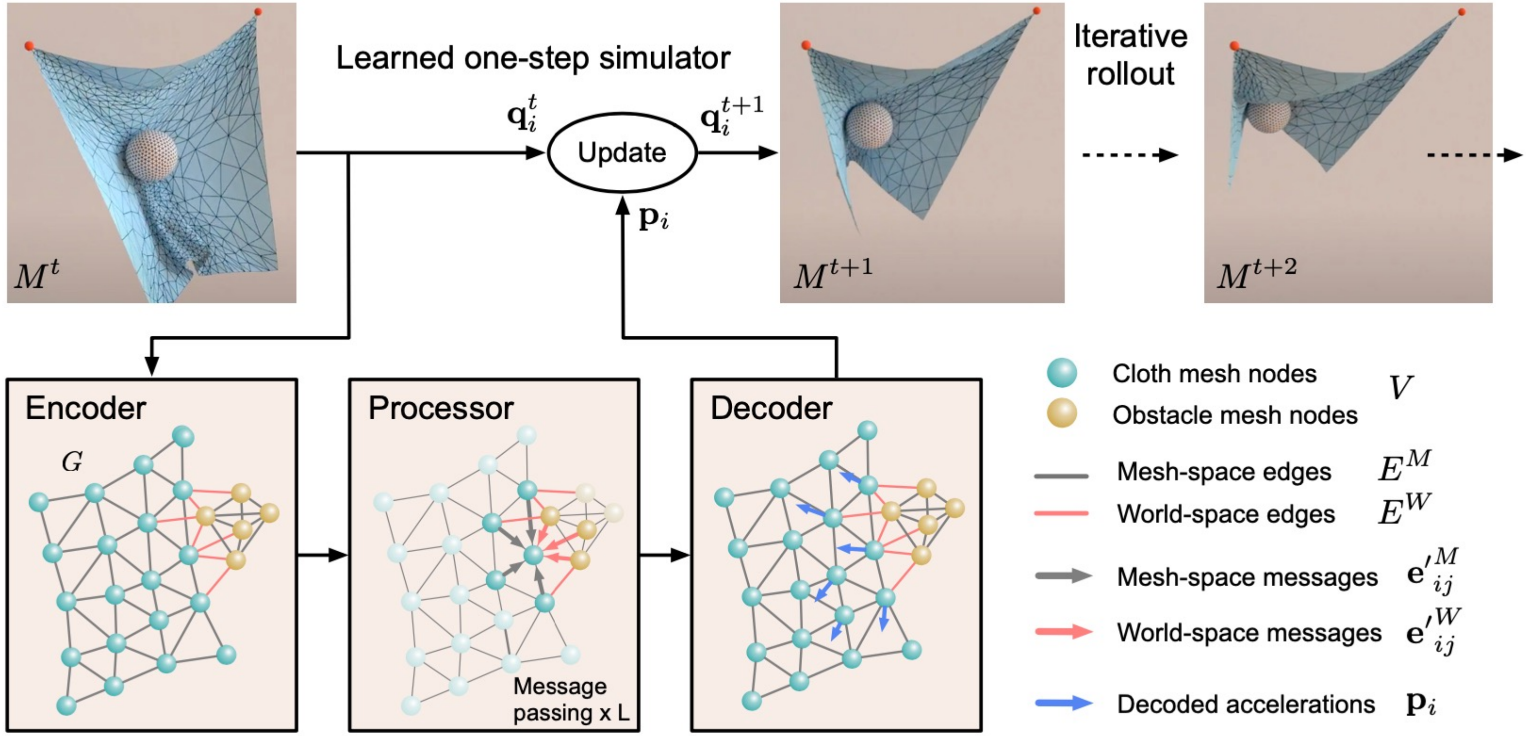
Performance

- A *general* approach to learning particle simulation.
- Simpler to implement.
- Accurate across fluid, rigid, and deformable material systems.
- High generalization ability.
- Robust to hyperparameter choices across various evaluation metrics.

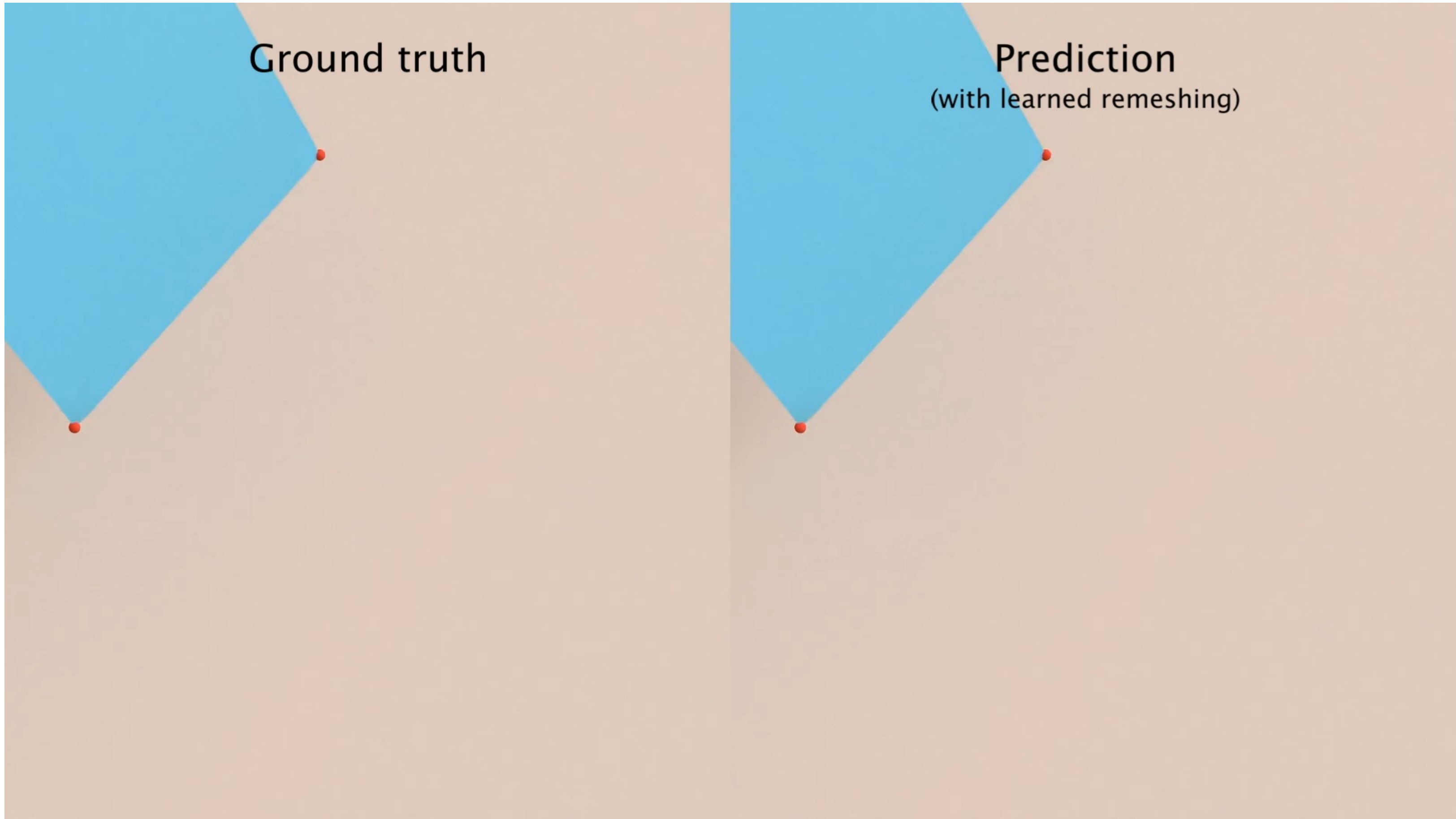
A. Sanchez-Gonzalez, J. Godwin, T. Pfaff, R. Ying, J. Leskovec, and P. W. Battaglia, 'Learning to Simulate Complex Physics with Graph Networks', *arXiv:2002.09405 [physics, stat]*, Sep. 2020, Accessed: May 03, 2021.

Variant: MESHGRAPHNETS
learning mesh-based simulations using graph neural networks

- Pass messages on a mesh graph.
- Adaptive remeshing.



T. Pfaff, M. Fortunato, A. Sanchez-Gonzalez, and P. W. Battaglia, 'Learning Mesh-Based Simulation with Graph Networks', *arXiv:2010.03409 [cs]*, Jan. 2021, Accessed: May 03, 2021.



T. Pfaff, M. Fortunato, A. Sanchez-Gonzalez, and P. W. Battaglia, ‘Learning Mesh-Based Simulation with Graph Networks’, *arXiv:2010.03409 [cs]*, Jan. 2021, Accessed: May 03, 2021.

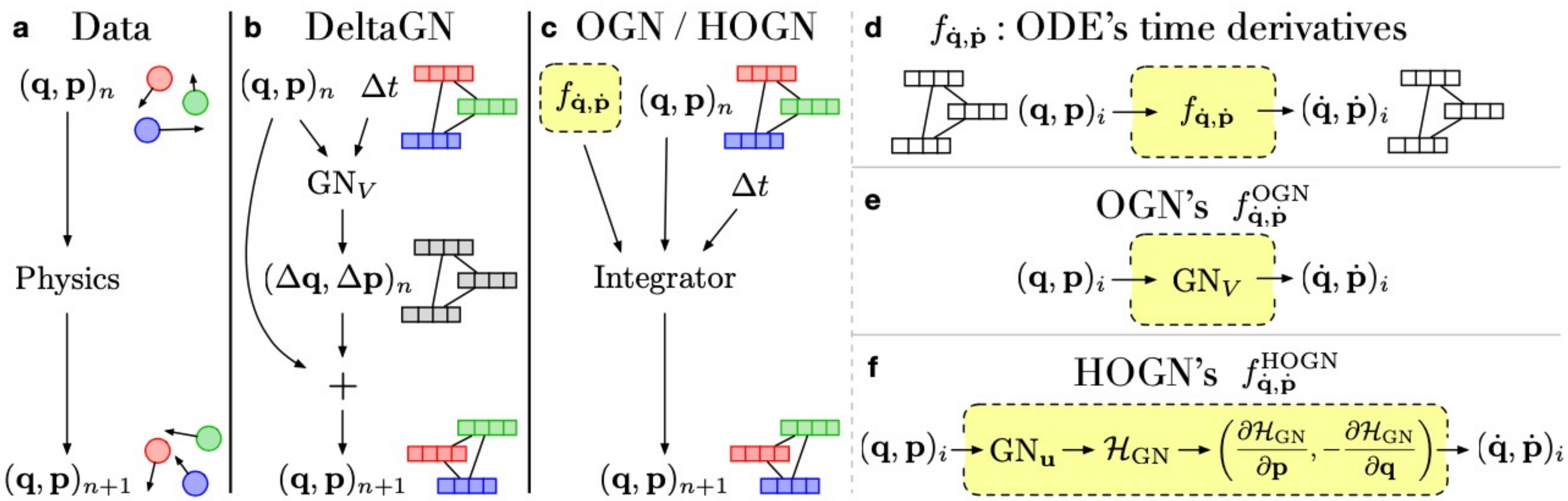
Inductive Biases of Graph Networks

- An inductive bias allows a learning algorithm to prioritize one solution (or interpretation) over another, independent of the observed data (Mitchell, 1980).

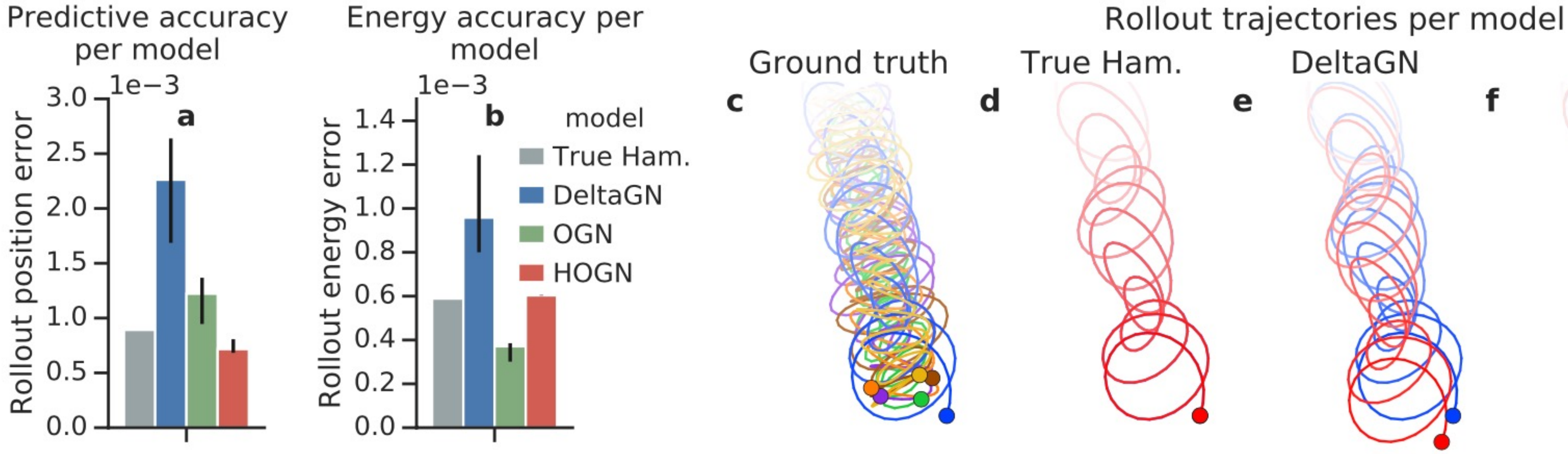
Component	**Entities**	**Relations**	**Rel. inductive bias**	**Invariance**
Fully connected	Units	All-to-all	Weak	-
Convolutional	Grid elements	Local	Locality	Spatial translation
Recurrent	Timesteps	Sequential	Sequentiality	Time translation
Graph network	Nodes	Edges	Arbitrary	Node, edge permutations

P. W. Battaglia *et al.*, 'Relational inductive biases, deep learning, and graph networks', *arXiv:1806.01261 [cs, stat]*, Oct. 2018, Accessed: May 04, 2021.

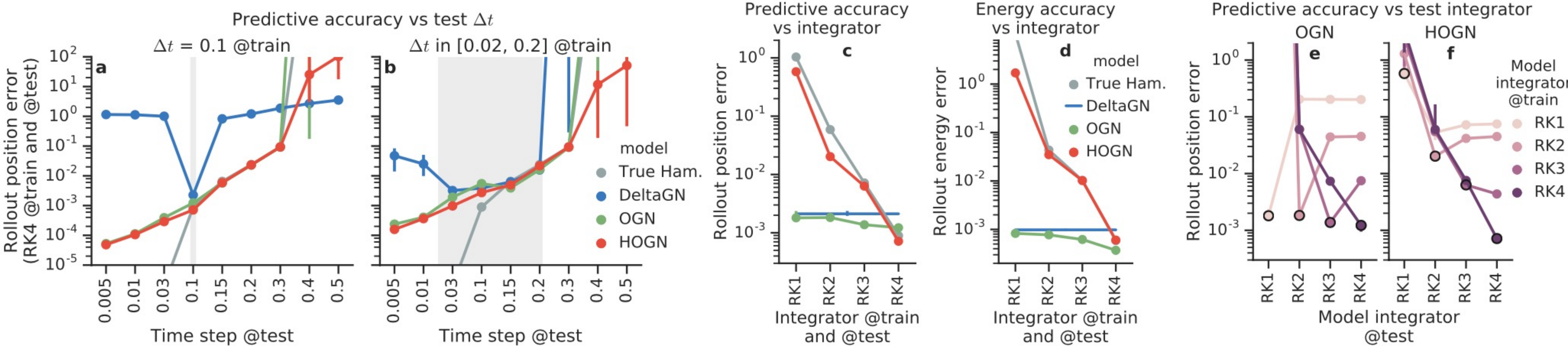
Hamiltonian Graph Networks with ODE Integrators



S. Greydanus, M. Dzamba, and J. Yosinski, 'Hamiltonian Neural Networks', *arXiv:1906.01563 [cs]*, Sep. 2019, Accessed: May 03, 2021.

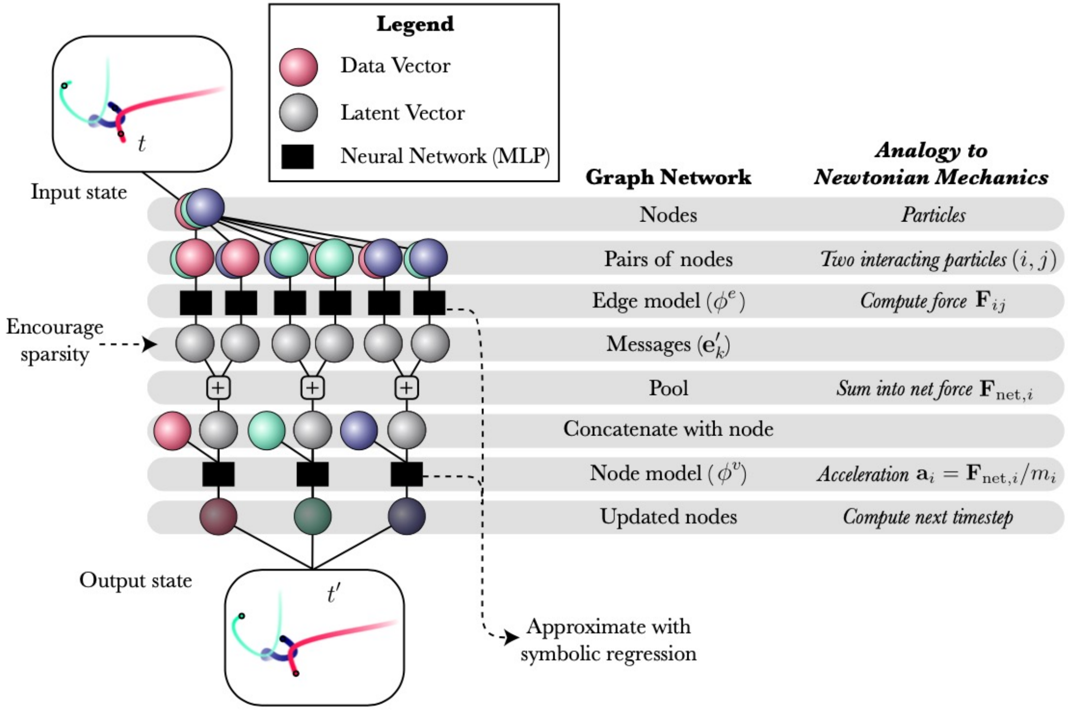


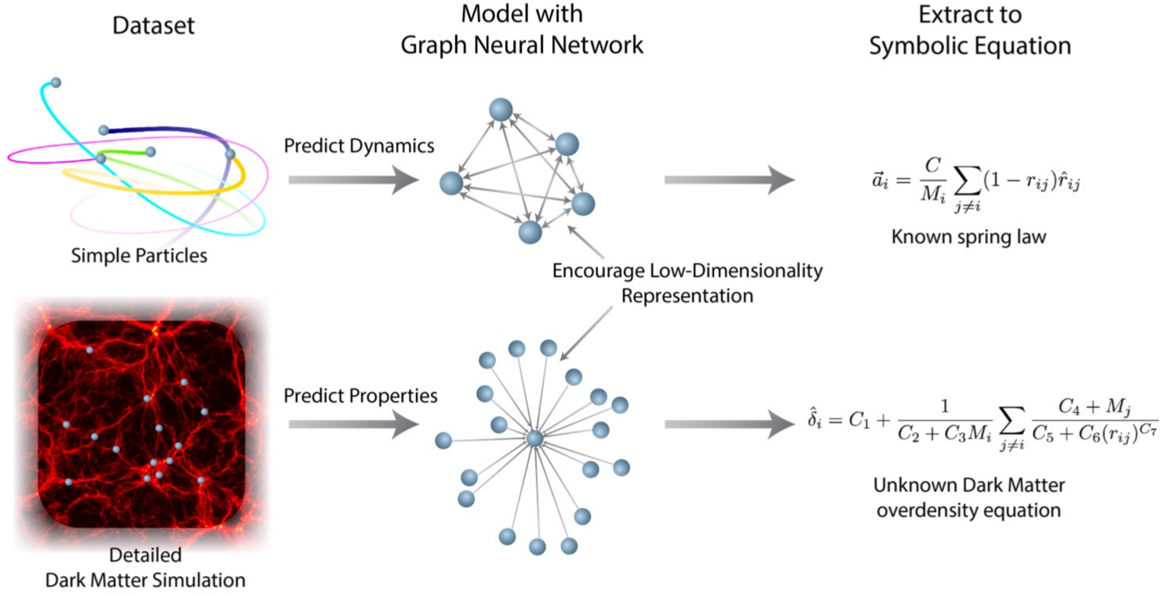
Predictive accuracy per model
Energy accuracy per model
Rollout trajectories per model
a
b
c
d
e
f
g
Ground truth
True Ham.
DeltaGN
OGN
HOGN
Rollout position error
Rollout energy error
1e−3
model
True Ham.
DeltaGN
OGN
HOGN



Predictive accuracy vs test Δt
Δt = 0.1 @train
Δt in [0.02, 0.2] @train
a
b
Rollout position error (RK4 @train and @test)
Time step @test
model
True Ham.
DeltaGN
OGN
HOGN
Predictive accuracy vs integrator
Energy accuracy vs integrator
c
d
Rollout position error
Rollout energy error
Integrator @train and @test
Predictive accuracy vs test integrator
OGN
HOGN
e
f
Model integrator @train
RK1
RK2
RK3
RK4
Model integrator @test

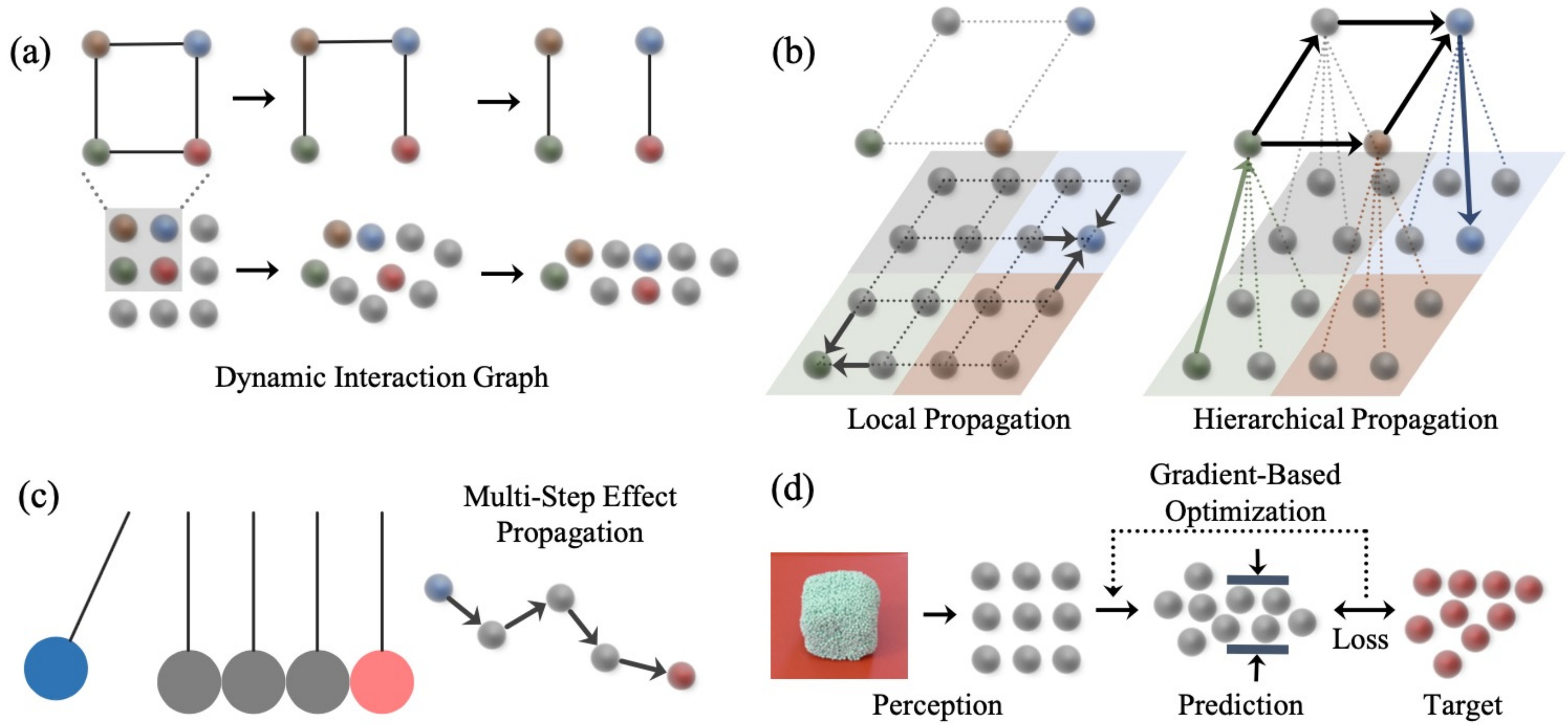
Discovering Symbolic Models from GNS





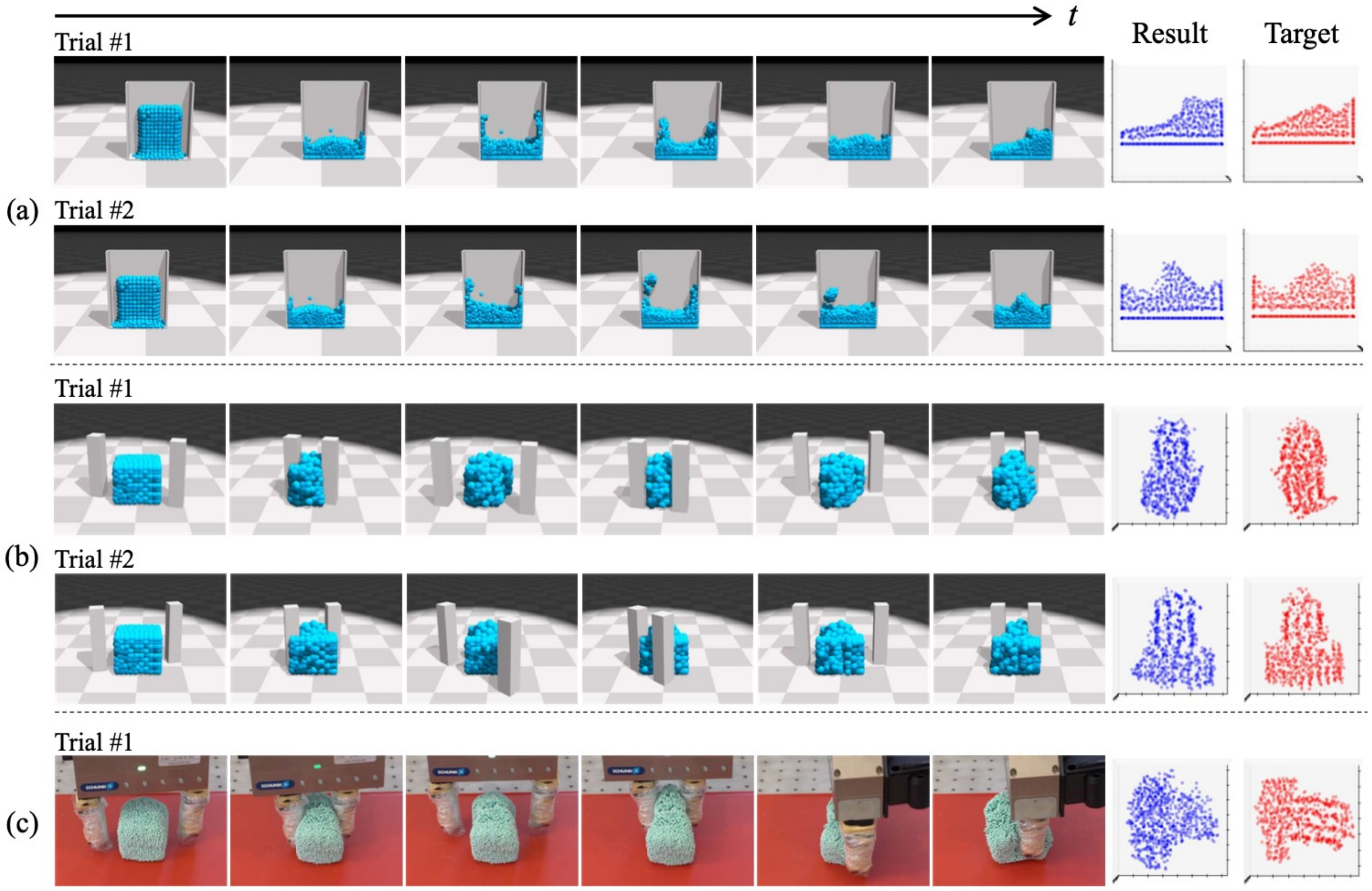
M. Cranmer *et al.*, 'Discovering Symbolic Models from Deep Learning with Inductive Biases', *arXiv:2006.11287 [astro-ph, physics:physics, stat]*, Nov. 2020, Accessed: May 03, 2021.

Learning Dynamics for Manipulation

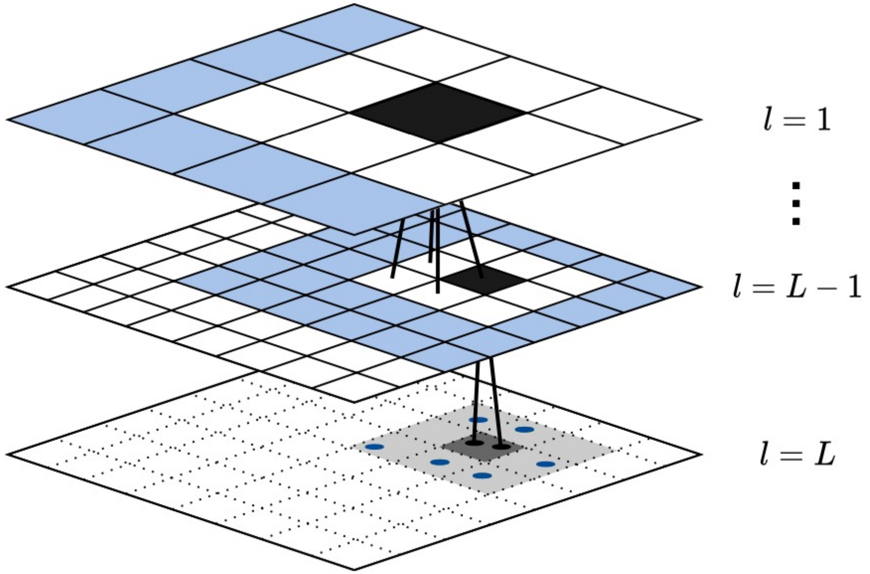


Y. Li, J. Wu, R. Tedrake, J. B. Tenenbaum, and A. Torralba, ‘Learning Particle Dynamics for Manipulating Rigid Bodies, Deformable Objects, and Fluids’, *arXiv:1810.01566 [physics, stat]*, Apr. 2019, Accessed: May 03, 2021.

Learning Dynamics for Manipulation



Scalable Graph Networks for Particle Simulations



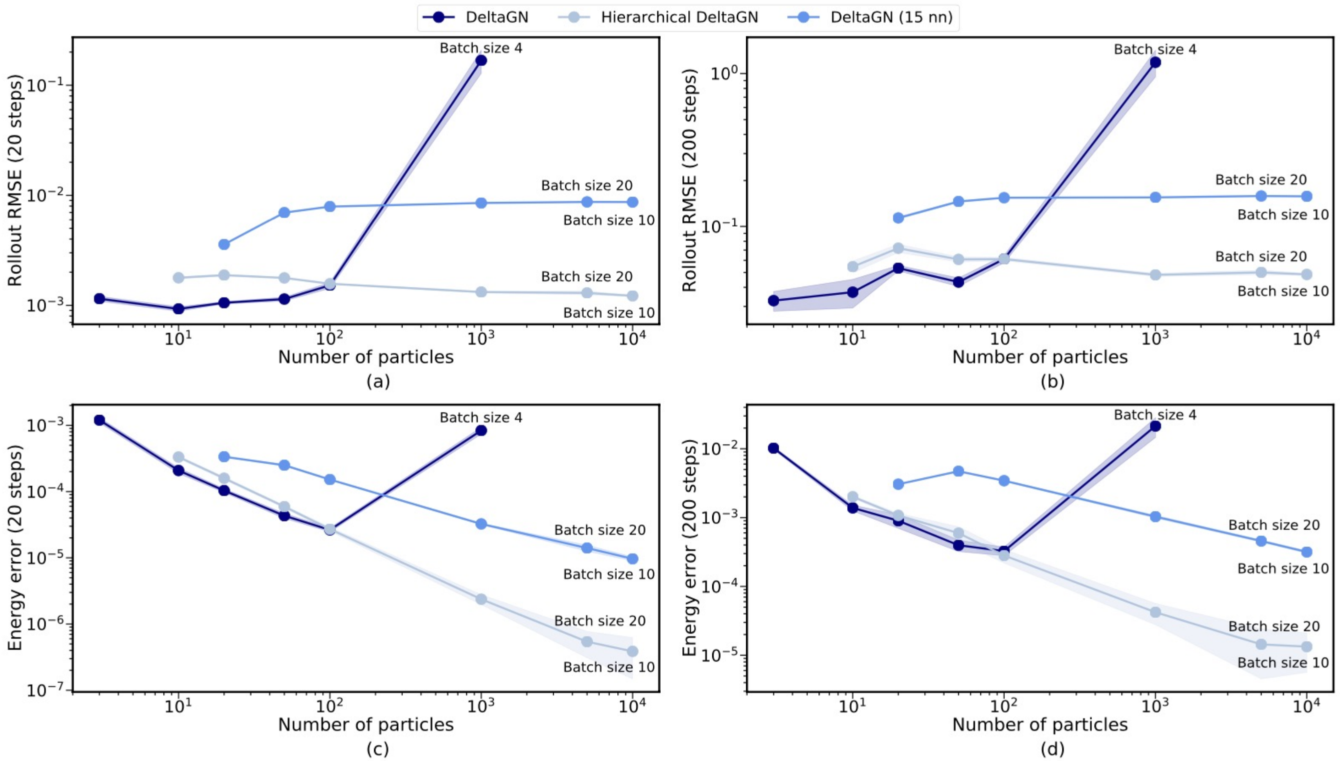
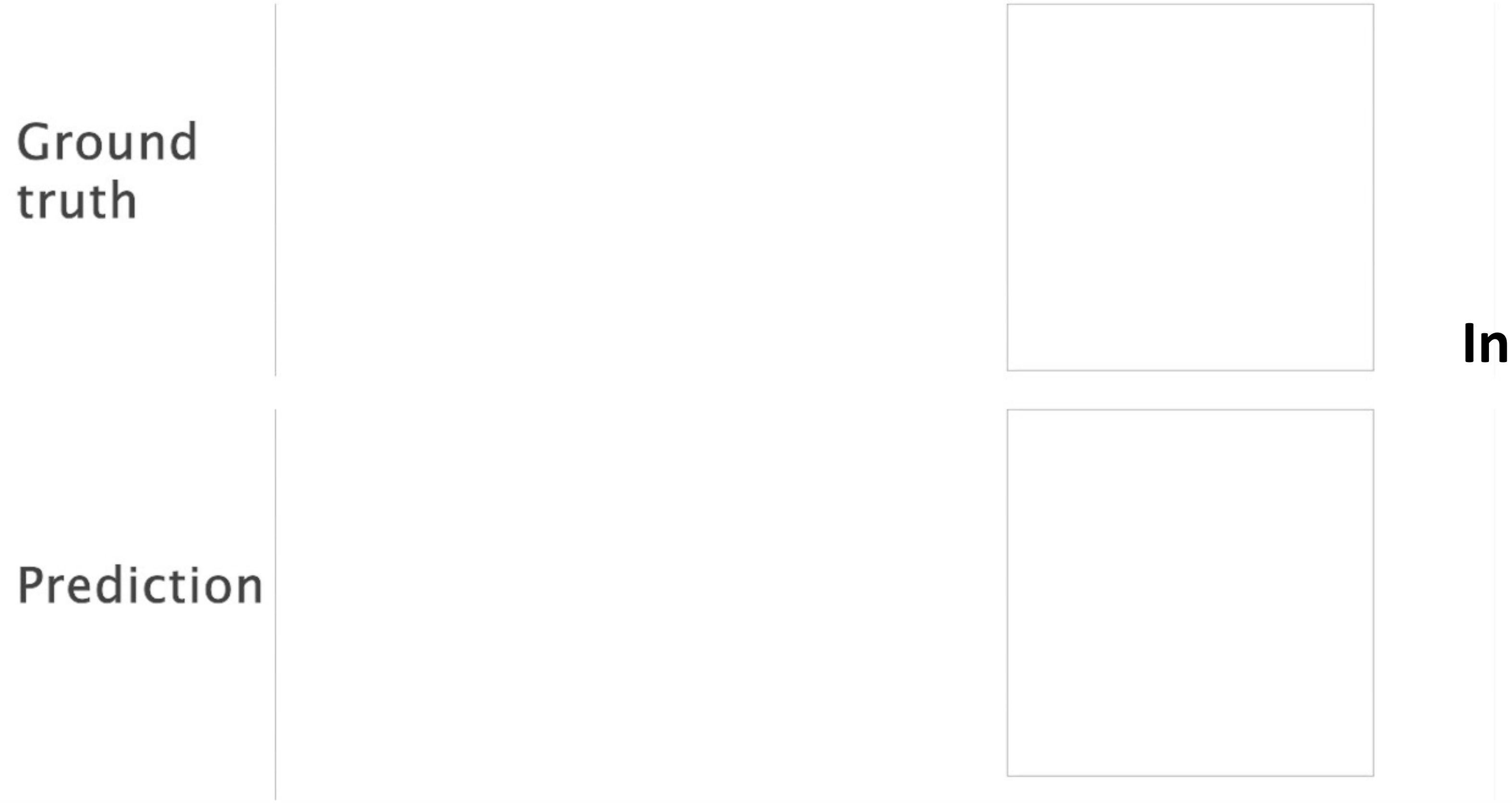


Figure 2: Models trained and evaluated on increasing particle counts. (a) 20 step rollout RMSE, (b) 200 step rollout RMSE, (c) energy error after 20 steps, (d) energy error after 200 steps. Batch sizes smaller than 100 were used if not enough memory was available (shown in the graph).

K. Martinkus, A. Lucchi, and N. Perraudin, 'Scalable Graph Networks for Particle Simulations', *arXiv:2010.06948 [astro-ph, physics:physics, stat]*, Mar. 2021, Accessed: May 03, 2021.

Limitations and Discussions



Incorporate physical laws?

A. Sanchez-Gonzalez, J. Godwin, T. Pfaff, R. Ying, J. Leskovec, and P. W. Battaglia, 'Learning to Simulate Complex Physics with Graph Networks', *arXiv:2002.09405 [physics, stat]*, Sep. 2020, Accessed: May 03, 2021.

Thank you!