Learning to Simulate Complex Physics with Graph Networks

Alvaro Sanchez-Gonzalez [*1] **Jonathan Godwin** [*1] **Tobias Pfaff** [*1] **Rex Ying** [*1 2] **Jure Leskovec** [2]
Peter W. Battaglia [1]

ICML 2020

From Deepmind & Stanford

Presentor: Yuanhao Xiong, Xiangning Chen, Li-Cheng Lan

Introduction

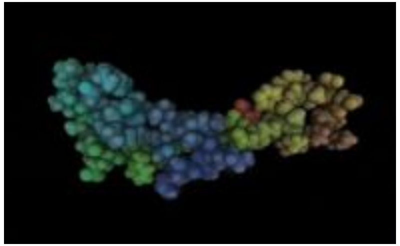
- Importance of simulation
  - Simulators of complex physics are invaluable to scientific and engineering disciplines
  - Largest supercomputers in the world

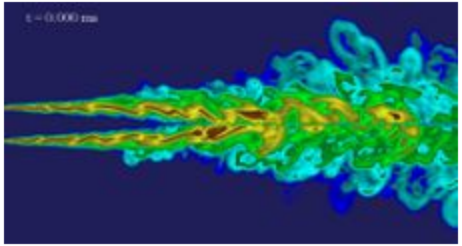
#1. "*Summit*" @ Oak Ridge: "A Sneak Peek at 19 Science **Simulations** for the Summit Supercomputer in 2019"

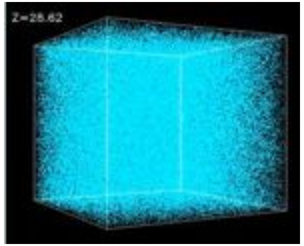
1. *Evolution of the universe*
2. *Whole-cell simulation*
3. *Inside a nuclear reactor*
4. *Post-Moore's Law graphene circuits*
5. *Formation of matter*
6. *Cell's molecular machine*
7. *Unpacking the nucleus*
8. *Mars landing*
9. *Deep learning for microscopy*
10. *Elements from star explosions*
11. *Cancer data*
12. *Earthquake resilience for cities*
13. *Nature of elusive neutrinos*
14. *Extreme weather with deep learning*
15. *Flexible, lightweight solar cells*
16. *Virtual fusion reactor*
17. *Unpredictable material properties*
18. *Genetic clues in the opioid crisis*
19. *Turbulent environments*

Introduction

- Difficulties in building a high-quality simulator
  - Can be very expensive to create and use
  - Entail years of engineering effort
  - Trade off generality for accuracy in a narrow range of settings
- Turn to learned simulators
  - Shared architectures
  - Accuracy-efficiency trade off
  - As accurate as the available data
  - ……







Introduction

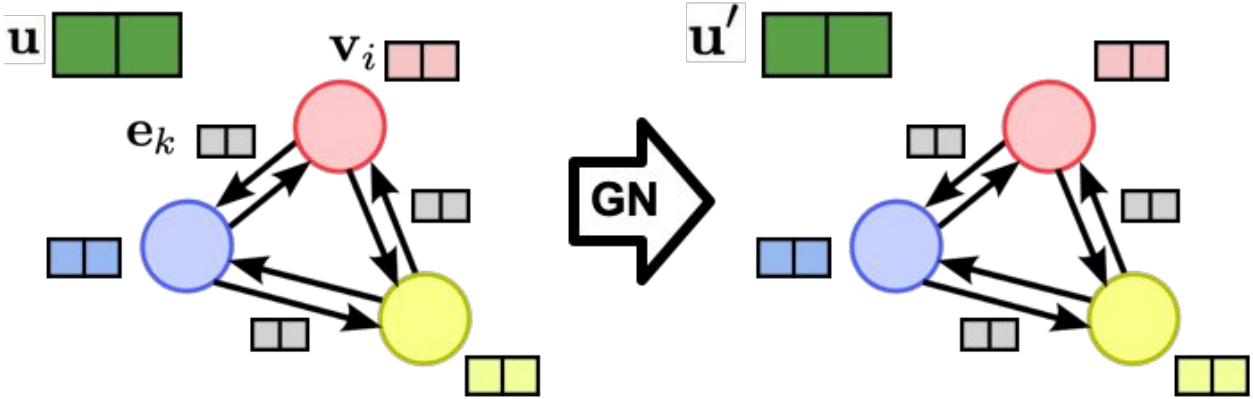
- Graph Network-based Simulators (GNS)
  - Rich physical states are represented by graphs of interacting particles
  - Complex dynamics are approximated by learned message-passing among nodes
  - Learn to accurately simulate a wide range of physical systems
  - Generalization to larger systems and longer steps

Related Work

- Particle-based simulation
  - States are represented as a set of particles, which encode mass, material,movement, etc. within local regions of space
  - Dynamics are computed on the basis of particles' interactions within their local neighborhoods
- Graph networks for learning forward dynamics
  - Interaction Networks
- Other baselines
  - DPI
  - CConv

Preliminaries

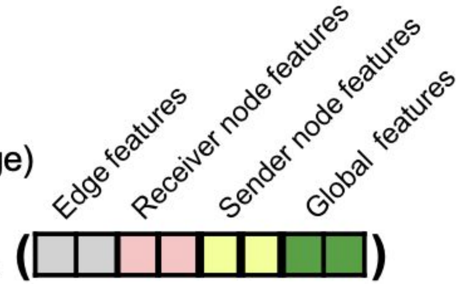
- Message passing network
  - Map an input graph to an output graph with the same structure but potentially different node, edge, and graph-level attributes

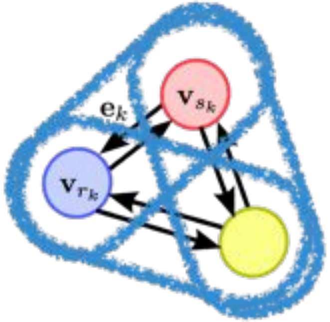


Preliminaries

Edge (message) function (for every edge)

$$\mathbf{e}'_k \leftarrow \phi^e\left(\mathbf{e}_k, \mathbf{v}_{r_k}, \mathbf{v}_{s_k}, \mathbf{u}\right) := \mathrm{NN}_e(\ \ )$$



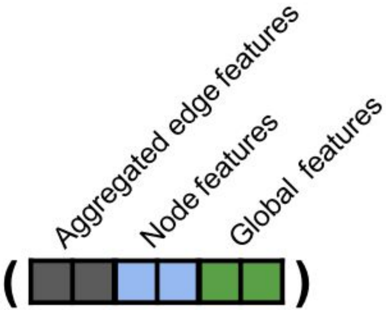


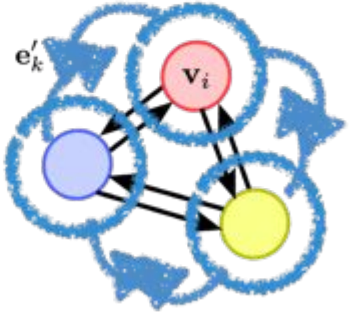
Receiver edge aggregation (Message pooling) (for every node)

$$\bar{\mathbf{e}}'_i \leftarrow \sum_{r_k = i} \mathbf{e}'_k$$

Node function (for every node)

$$\mathbf{v}'_i \leftarrow \phi^v\left(\bar{\mathbf{e}}'_i, \mathbf{v}_i, \mathbf{u}\right) := \mathrm{NN}_v(\ \ )$$





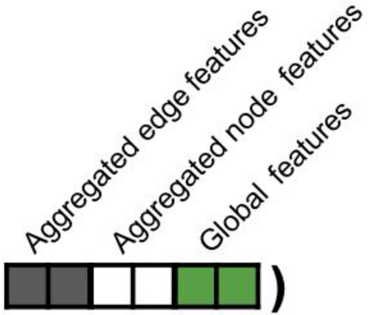
Preliminaries

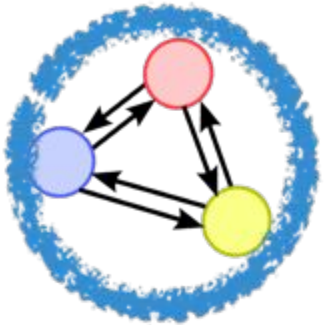
Global node and edge aggregation

$$\bar{\mathbf{v}}' \leftarrow \sum_i \mathbf{v}'_i \qquad \bar{\mathbf{e}}' \leftarrow \sum_k \mathbf{e}'_k$$

Global function

$$\mathbf{u}' \leftarrow \phi^u\left(\bar{\mathbf{e}}', \bar{\mathbf{v}}', \mathbf{u}\right) := \mathrm{NN}_u\big(\;\big)$$





Preliminaries

$$\dot{\boldsymbol{p}}^t = f(\boldsymbol{p}^t) = \boldsymbol{v}^t, \quad \boldsymbol{p}^{t_0} = \boldsymbol{p}^0$$

- Euler method
  - Explicit Euler

$$\boldsymbol{p}^{t_{k+1}} = \boldsymbol{p}^{t_k} + \Delta t \cdot f(\boldsymbol{p}^{t_k}) = \boldsymbol{p}^{t_k} + \Delta t \cdot \dot{\boldsymbol{p}}^{t_k}$$

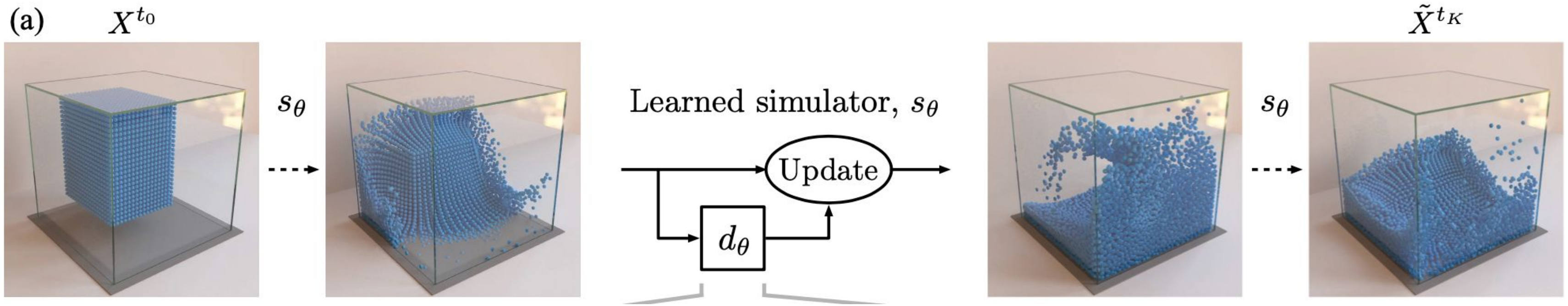
  - Implicit Euler

$$\boldsymbol{p}^{t_{k+1}} = \boldsymbol{p}^{t_k} + \Delta t \cdot f(\boldsymbol{p}^{t_{k+1}}) = \boldsymbol{p}^{t_k} + \Delta t \cdot \dot{\boldsymbol{p}}^{t_{k+1}}$$

  - Semi-implicit Euler

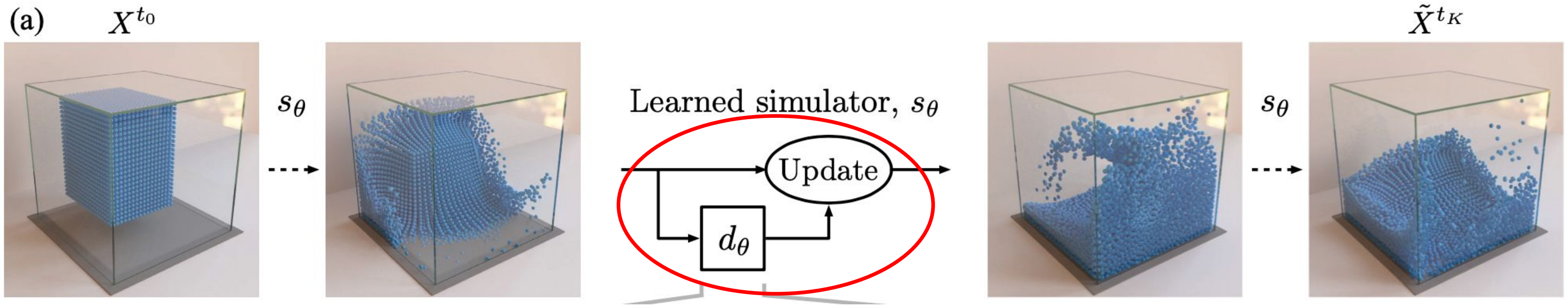
$$\begin{cases} \dot{\boldsymbol{p}}^t & = f(\boldsymbol{p}^t) = \boldsymbol{v}^t, \quad \boldsymbol{p}^{t_0} = \boldsymbol{p}^0 \\ \dot{\boldsymbol{v}}^t & = g(\boldsymbol{p}^t) = \ddot{\boldsymbol{p}}^t, \quad \boldsymbol{v}^{t_0} = \boldsymbol{v}^0 \end{cases} \Longrightarrow \begin{aligned} \dot{\mathbf{p}}^{t_{k+1}} &= \dot{\mathbf{p}}^{t_k} + \Delta t \cdot \ddot{\mathbf{p}}^{t_k} \\ \mathbf{p}^{t_{k+1}} &= \mathbf{p}^{t_k} + \Delta t \cdot \dot{\mathbf{p}}^{t_{k+1}} \end{aligned}$$

Formulation



- Obtain a simulator $s : \mathcal{X} \rightarrow \mathcal{X}$ to model the state dynamics ($X^t \in \mathcal{X}$ is the state of the world at time t)
- Given an initial state X^{t_0} and physical dynamics over K timesteps, we need to simulate a trajectory of states $\tilde{\mathbf{X}}^{t_{0:K}} = (X^{t_0}, \tilde{X}^{t_1}, \ldots, \tilde{X}^{t_K})$
- Rollout: Computed iteratively by $\tilde{X}^{t_{k+1}} = s(\tilde{X}^{t_k})$

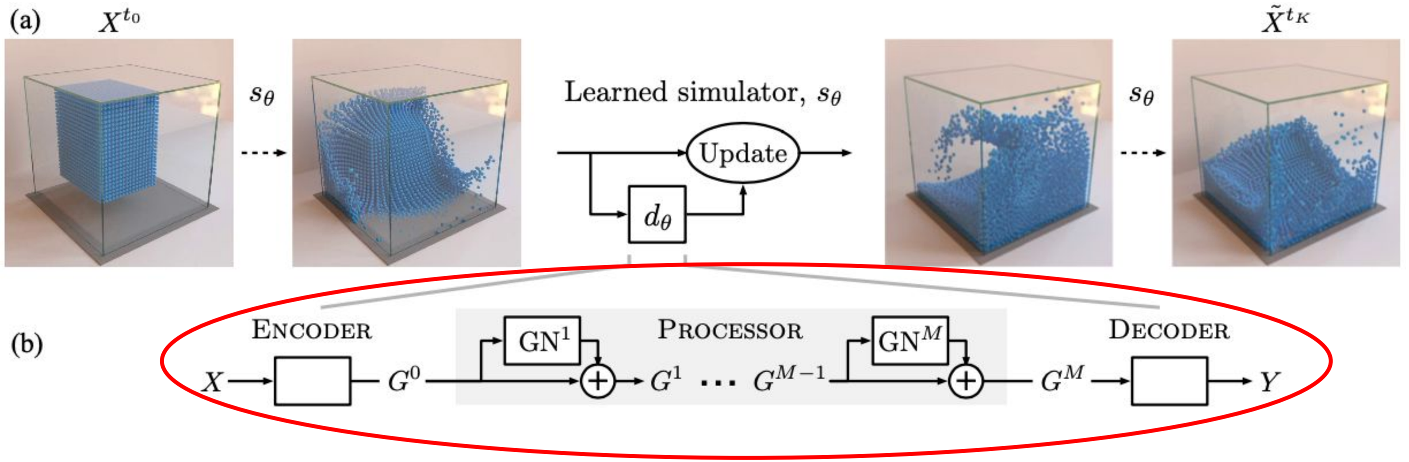
Pipeline



- First compute a function approximator $d_\theta : \mathcal{X} \rightarrow \mathcal{Y}$ mapping state to dynamics ($Y \in \mathcal{Y}$ represents the dynamics information, e.g., accelerations)

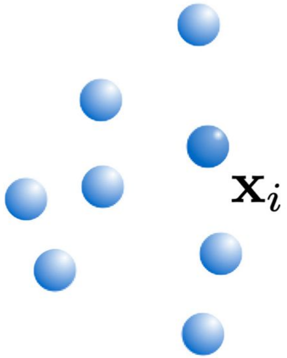
- Then the state is updated $\tilde{X}^{t_{k+1}} = \text{Update}(\tilde{X}^{t_k}, d_\theta)$ following some update mechanism (Euler integrator in this paper)

Structure of $d_\theta : \mathcal{X} \rightarrow \mathcal{Y}$



- Encoder: $\mathcal{X} \rightarrow \mathcal{G}$, embeds the raw state representations as a latent graph
- Processor: $\mathcal{G} \rightarrow \mathcal{G}$, message passing within the graph
- Decoder: $\mathcal{G} \rightarrow \mathcal{Y}$, extract the required dynamics information

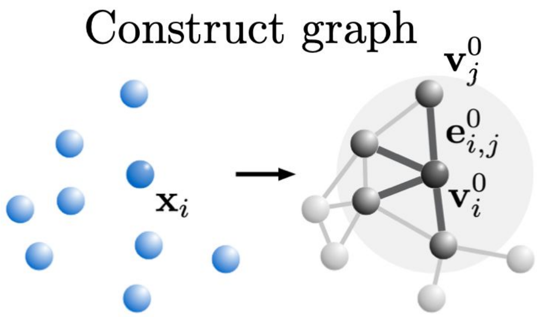
Input & Output Representation of $d_\theta : \mathcal{X} \rightarrow \mathcal{Y}$



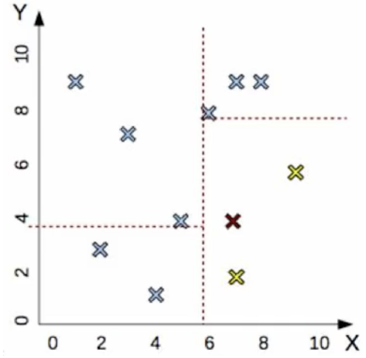
- **Input:**
  - Particle-based representation $X = (\mathbf{x}_0, \ldots, \mathbf{x}_N)$
  - Each of the N particles' $\mathbf{x}_i$ denotes its state
  - $\mathbf{x}_i^{t_k}$:position + C previous velocities + static material properties, e.g. water, sand
  - $\mathbf{x}_i^{t_k} = [\mathbf{p}_i^{t_k}, \dot{\mathbf{p}}_i^{t_{k-C+1}}, \ldots, \dot{\mathbf{p}}_i^{t_k}, \mathbf{f}_i]$
  - $\mathbf{r}_{i,j}$, pairwise properties, e.g., spring constant
  - Global properties of the system $\mathbf{g}$, e.g., external forces, global material properties

- **Outputs:**
  - Prediction targets: per-particle acceleration $\ddot{\mathbf{p}}_i$
  - $\dot{\mathbf{p}}_i$ and $\ddot{\mathbf{p}}_i$ are computed by finite differences

Encoder $\mathcal{X} \rightarrow \mathcal{G}$

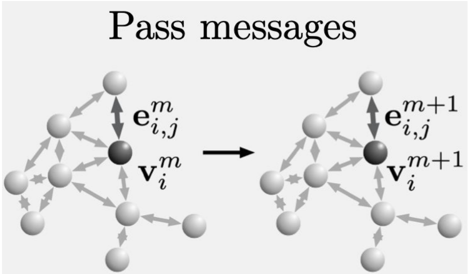


- Encodes the particle-based state representation as a latent graph $G^0 = \text{ENCODER}(X)$
- G^0 is constructed by assigning a ***node*** to each particle and adding ***edges*** between particles within certain distance R (using k-d tree algorithm)
  - Pick random dimension, find median, split data, repeat



- $G = (V, E, \mathbf{u})$, $\mathbf{v}_i \in V$, $\mathbf{e}_{i,j} \in E$, $\mathbf{u}$ represents the global properties
  - The node and vector embeddings are learned function
  - $\mathbf{v}_i = \varepsilon^v(\mathbf{x}_i)$, $\mathbf{x}_i$ is the node representations
  - $\mathbf{e}_{i,j} = \varepsilon^e(\mathbf{r}_{i,j})$, $\mathbf{r}_{i,j}$ is the pairwise properties, e.g., $\mathbf{r}_{i,j} = [(\mathbf{p}_i - \mathbf{p}_j), \|\mathbf{p}_i - \mathbf{p}_j\|]$

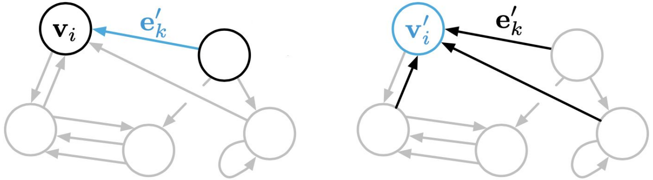
Processor $\mathcal{G} \rightarrow \mathcal{G}$



- Compute the final graph $G^M = \textsc{Processor}(G^0)$ via M steps of message-passing, where $G^{m+1} = \mathrm{GN}^{m+1}(G^m)$

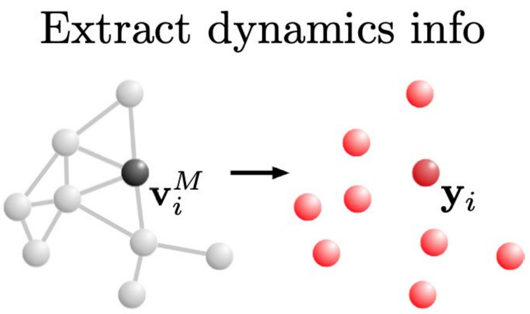
- Simply uses existed Graph Networks (GN)

$$\mathbf{e}'_k = \phi^e(\mathbf{e}_k, \mathbf{v}_{rk}, \mathbf{v}_{sk}) \tag{1}$$
$$\bar{\mathbf{e}}'_i = \rho^{e\rightarrow v}(E'_i),\ E'_i = \{(\mathbf{e}'_k,\ r_k, s_k)\}_{r_k=i,k=1:N^e} \tag{2}$$
$$\mathbf{v}'_i = \phi^v(\bar{\mathbf{e}}'_i, \mathbf{v}_i) \tag{3}$$



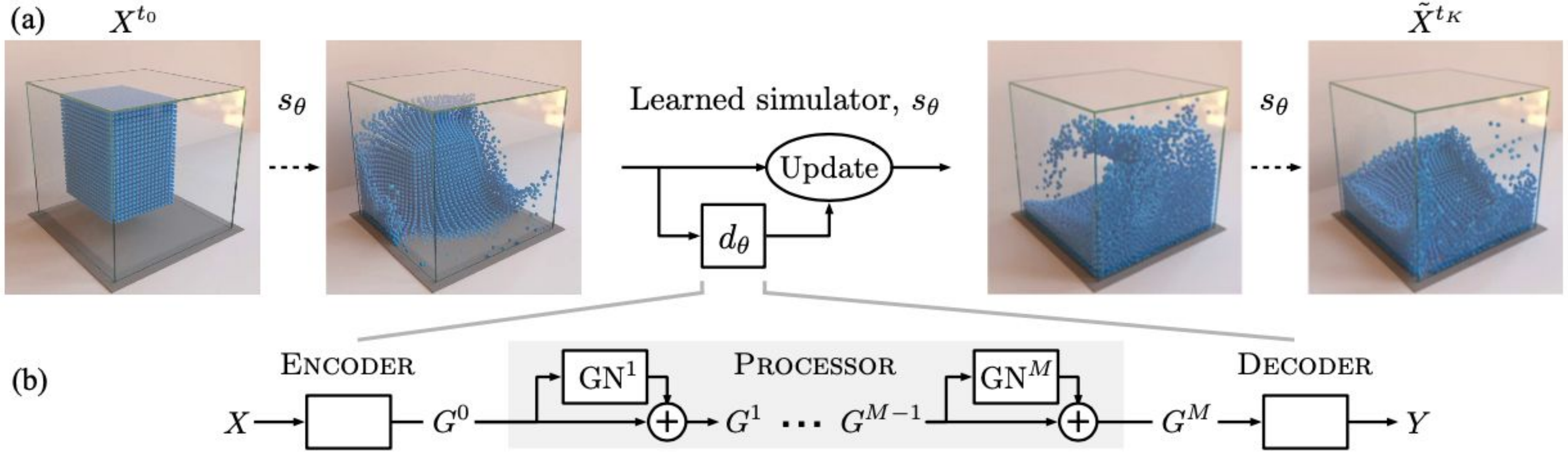
(a) Edge update (b) Node update

Decoder $\mathcal{G} \rightarrow \mathcal{Y}$



- Extracts dynamics information from the nodes of the final latent graph $\mathbf{y}_i = \delta^v(\mathbf{v}_i^M)$
- $\mathbf{y}_i$ is the per-node acceleration $\ddot{\mathbf{p}}_i$
- Then the future position and velocity are updated using an Euler integrator
- δ^v is also implemented as a MLP

As a whole

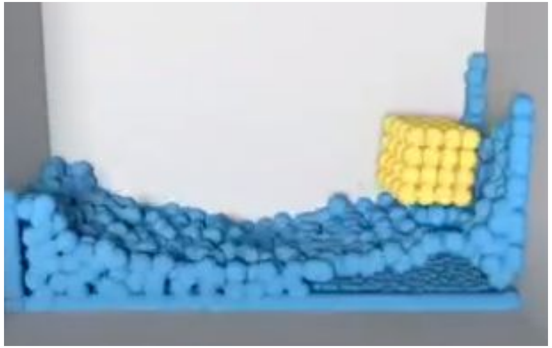

(a)
X^{t_0}
$\tilde{X}^{t_K}$
s_θ
Learned simulator, s_θ
Update
d_θ
s_θ
(b)
Encoder
Processor
Decoder
X
G^0
GN^1
G^1
G^{M-1}
GN^M
G^M
Y

Training

- Noise injection
  - Long rollouts can accumulate errors
  - Corrupt the input with Gaussian noise $\sim \mathcal{N}(0, \sigma_v = 0.0003)$
  - Autoencoder
- Normalize all input and target vectors to 0 mean and 1 variance
- Randomly sample particle pairs $(\mathbf{x}_i^{t_k}, \mathbf{x}_i^{t_{k+1}})$ from training trajectories
- Calculate $\ddot{\mathbf{p}}^{t_k} = \mathbf{p}^{t_{k+1}} - 2\mathbf{p}^{t_k} + \mathbf{p}^{t_{k-1}}$ (omitting constant Δt for simplicity)
- Loss function: $L(\mathbf{x}_i^{t_k}, \mathbf{x}_i^{t_{k+1}}; \theta) = \|d_\theta(\mathbf{x}_i^{t_k}) - \ddot{\mathbf{p}}_i^{t_k}\|^2$

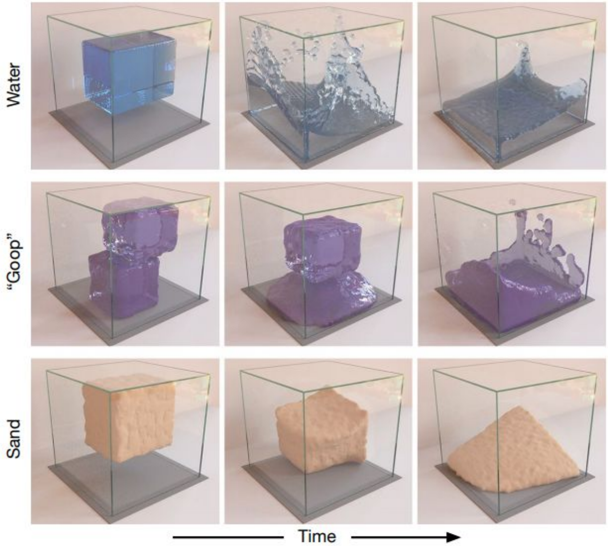
Physical Domains for Experiments

- BOXBATH
- WATER-3D
- WATER



Simulating Complex Materials

- Edge length of the container = 1.0
- Metric: particle-wise MSE
- Train one only 1-step

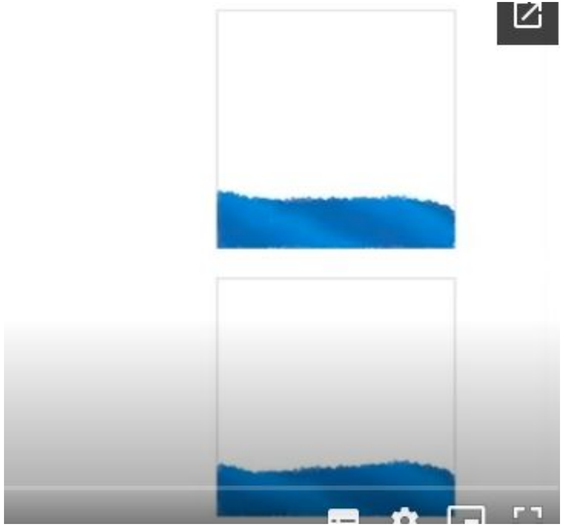


Experimental domain	N	K	1-step $(\times 10^{-9})$	Rollout $(\times 10^{-3})$
WATER-3D (SPH)	13k	800	8.66	10.1
SAND-3D	20k	350	1.42	0.554
GOOP-3D	14k	300	1.32	0.618
WATER-3D-S (SPH)	5.8k	800	9.66	9.52
BOXBATH (PBD)	1k	150	54.5	4.2
WATER	1.9k	1000	2.82	17.4
SAND	2k	320	6.23	2.37
GOOP	1.9k	400	2.91	1.89
MULTIMATERIAL	2k	1000	1.81	16.9
FLUIDSHAKE	1.3k	2000	2.1	20.1
WATERDROP	1k	1000	1.52	7.01
WATERDROP-XL	7.1k	1000	1.23	14.9
WATERRAMPS	2.3k	600	4.91	11.6
SANDRAMPS	3.3k	400	2.77	2.07
RANDOMFLOOR	3.4k	600	2.77	6.72
CONTINUOUS	4.3k	400	2.06	1.06

Table 1. List of maximum number of particles N, sequence length K, and quantitative model accuracy (MSE) on the held-out test set. All domain names are also hyperlinks to the video website.

Simulating Complex Materials

- FLUIDSHAKE
  - The container is being moved side-to-side
    - Causing splashes and irregular waves

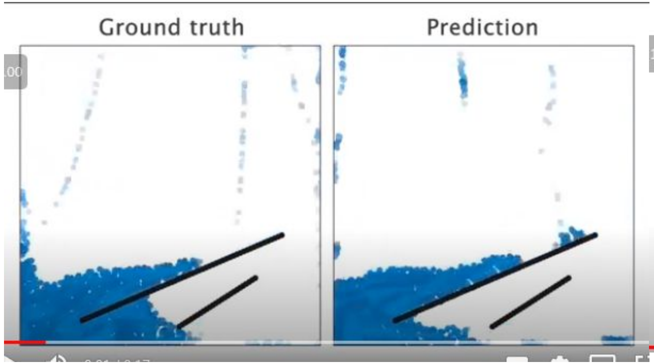


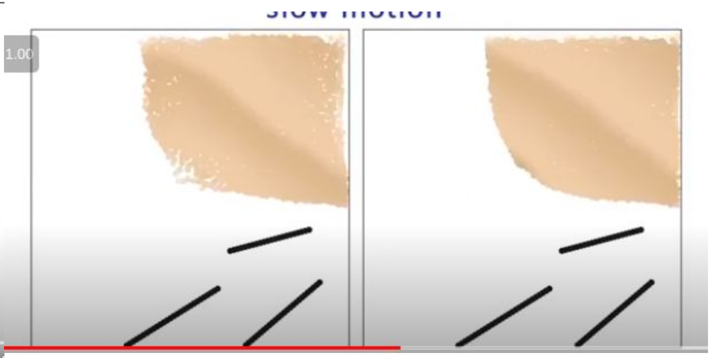
Experimental domain	N	K	1-step ($\times 10^{-9}$)	Rollout ($\times 10^{-3}$)
WATER-3D (SPH)	13k	800	8.66	10.1
SAND-3D	20k	350	1.42	0.554
GOOP-3D	14k	300	1.32	0.618
WATER-3D-S (SPH)	5.8k	800	9.66	9.52
BOXBATH (PBD)	1k	150	54.5	4.2
WATER	1.9k	1000	2.82	17.4
SAND	2k	320	6.23	2.37
GOOP	1.9k	400	2.91	1.89
MULTIMATERIAL	2k	1000	1.81	16.9
FLUIDSHAKE	1.3k	2000	2.1	20.1
WATERDROP	1k	1000	1.52	7.01
WATERDROP-XL	7.1k	1000	1.23	14.9
WATERRAMPS	2.3k	600	4.91	11.6
SANDRAMPS	3.3k	400	2.77	2.07
RANDOMFLOOR	3.4k	600	2.77	6.72
CONTINUOUS	4.3k	400	2.06	1.06

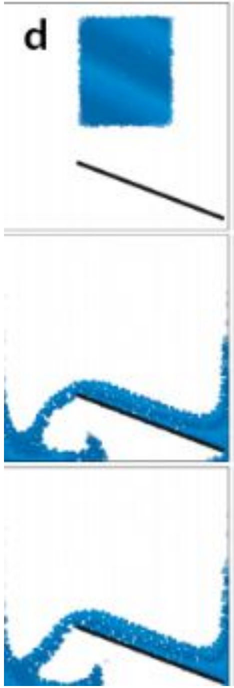
Table 1. List of maximum number of particles N, sequence length K, and quantitative model accuracy (MSE) on the held-out test set. All domain names are also hyperlinks to the video website.

Simulating Complex Materials

- Environment with complicated static obstacles (WATERRAMPS and SANDRAMPS)





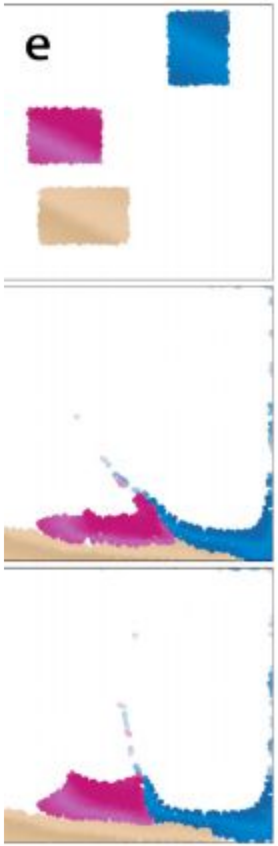


Simulating Complex Materials

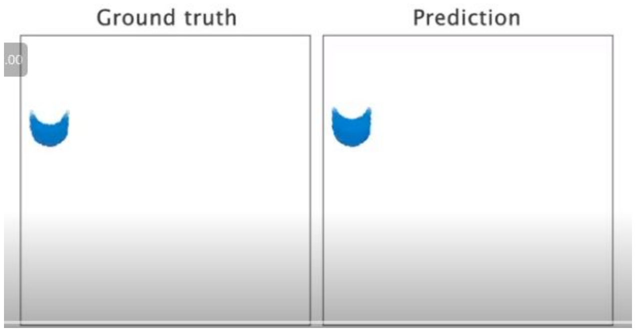
- Different friction angle (Continuous):
    - liquid (0°), sand (45°), or gravel (> 60°)
    - Train on [0, 30], [55, 80]
    - Test on [0, 90]
    - Can still be accurate on unseen angle

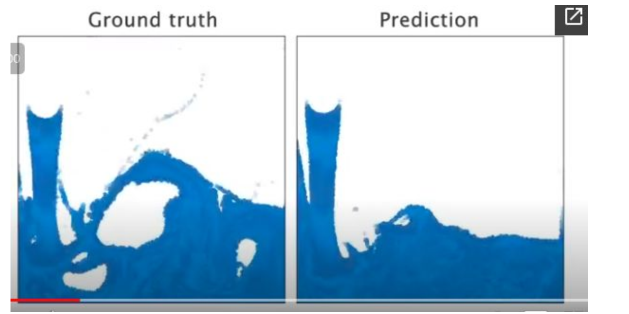
Multiple Interacting Materials

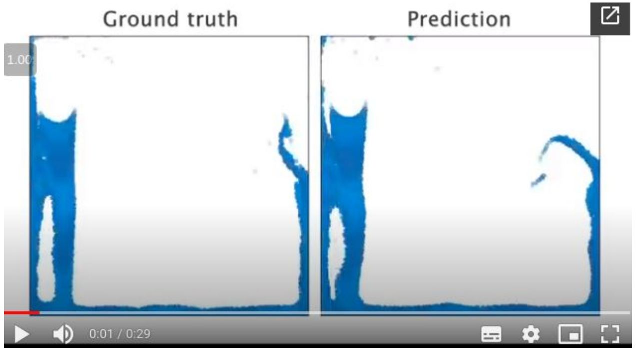
- Visually, thir model's performance in MULTIMATERIAL is comparable to its performance when trained on those materials individually

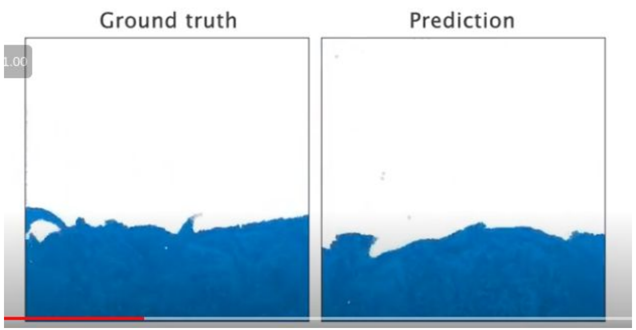


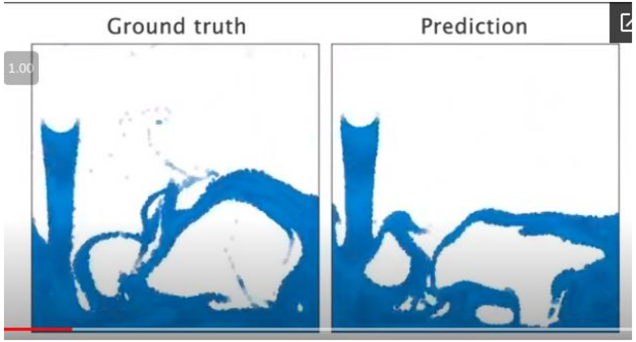
Generalization



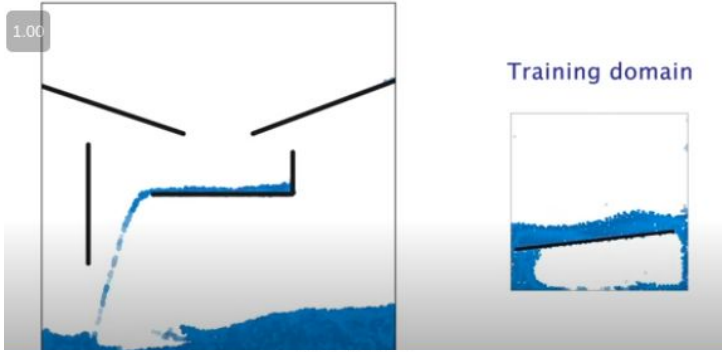


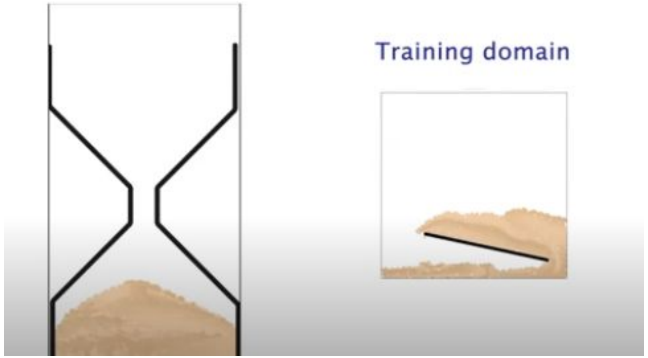


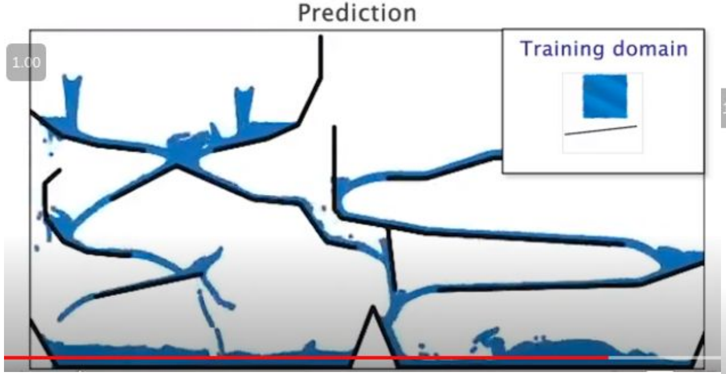


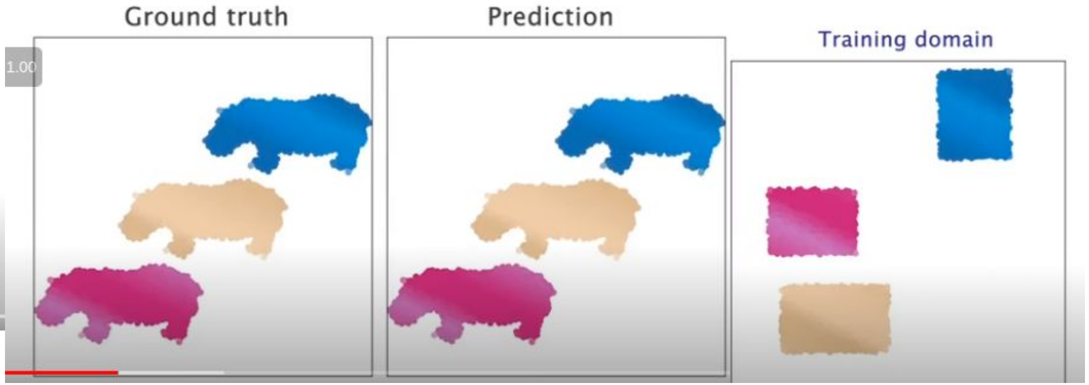


Generalization

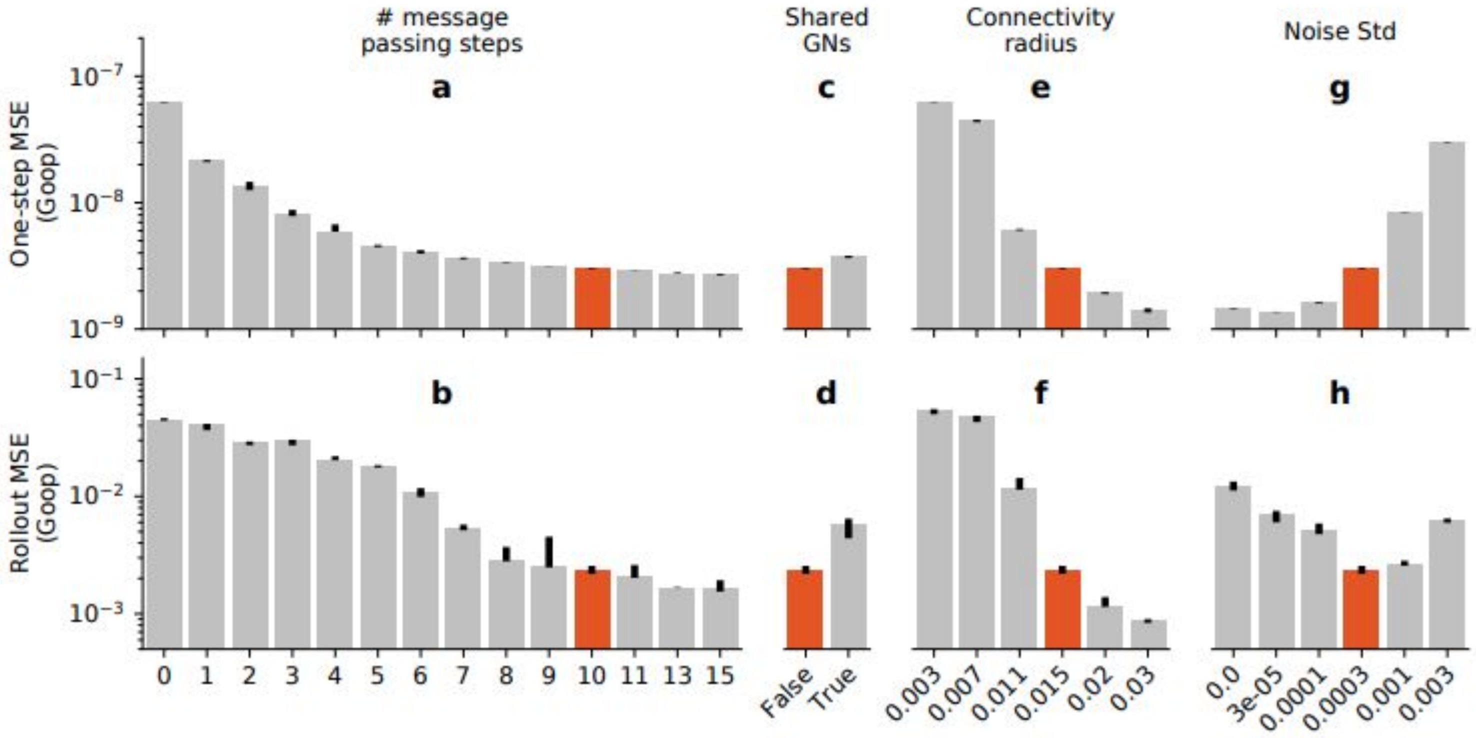






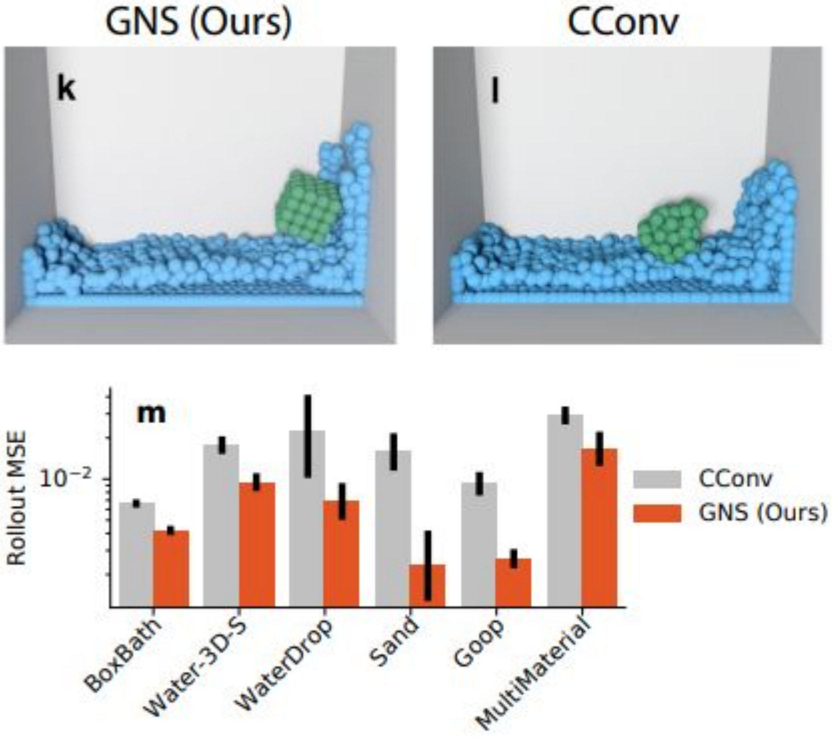


Analyzation



Comparisons to Previous Models

- They implement CConv with noise and multiple input states



Demo

Conclusion

- A powerful machine learning framework based on particle-based representations of physics and learned message-passing on graphs
- A simple architecture, but can learn to simulate dynamics of complex physics with tens of thousands of particles over thousands time steps
- More accurate, and has better generalization than previous approaches