Data Driven Engineering II: Advaced Topics

Graph Neural Networks II

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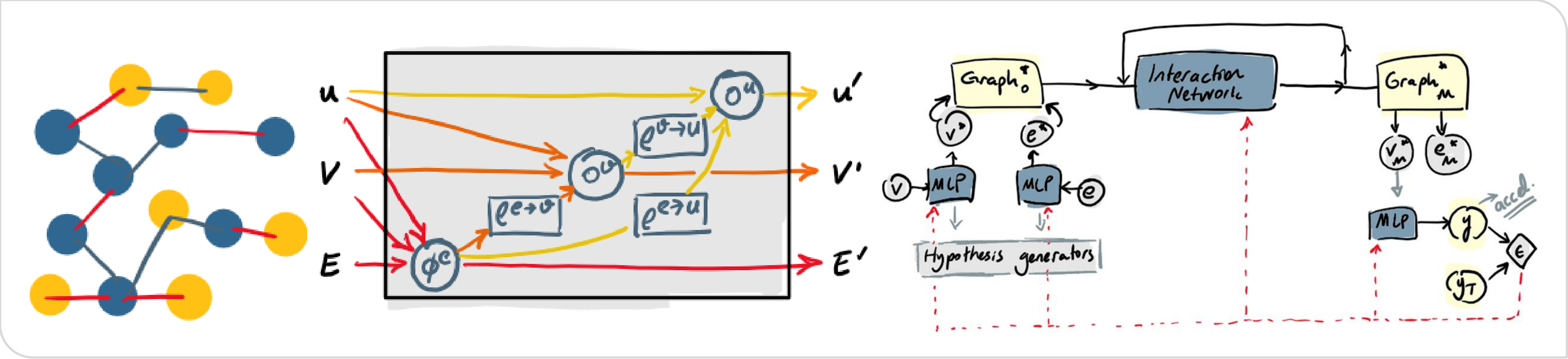


Graph Neural Networks :

1) GNN Basics

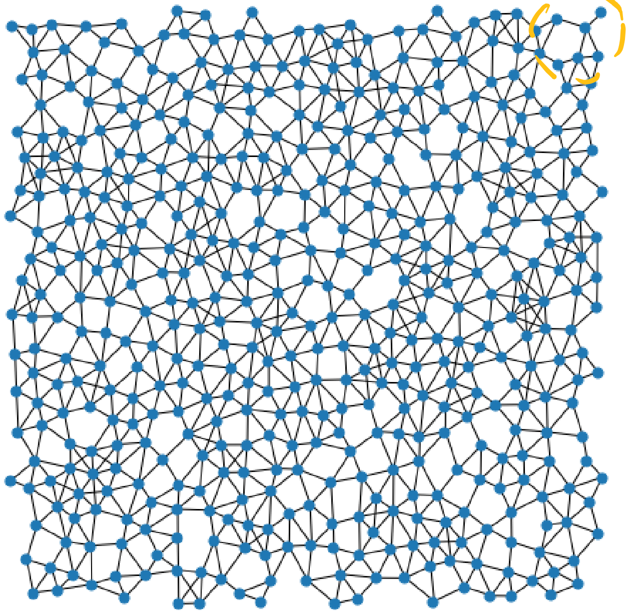
2) How GNN works

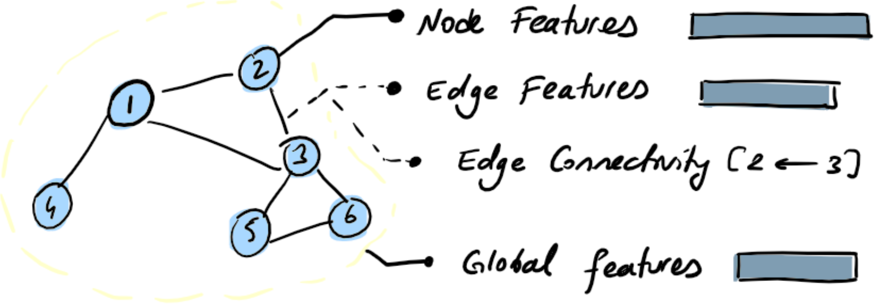
3) Basic architectures

4) Coding : ~~Graph Nets library~~
"PyTorch Geometric"

5) Graph Autoencoders; modelling transport phenomena

Understanding Graph Network :





Node Features

Edge Features

Edge Connectivity [2 ← 3]

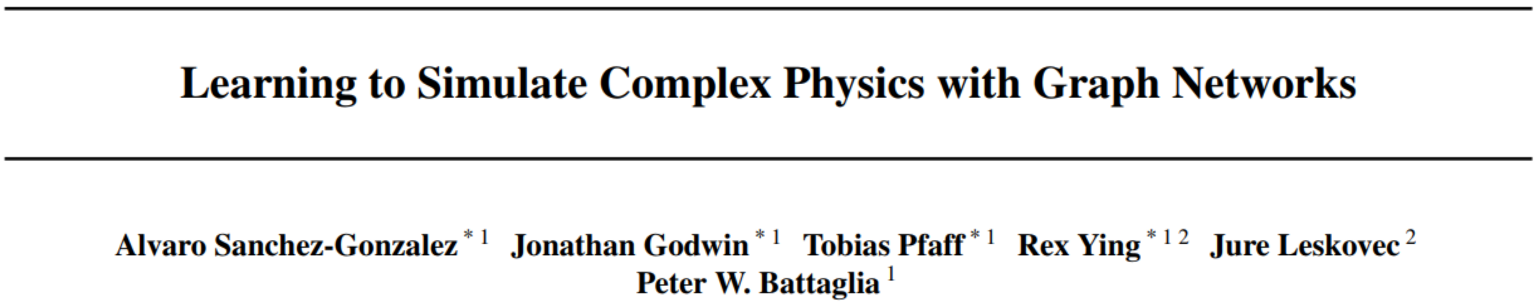
Global features

Obj

(i) Node Level Tasks ↗ Classification
↘ Regression

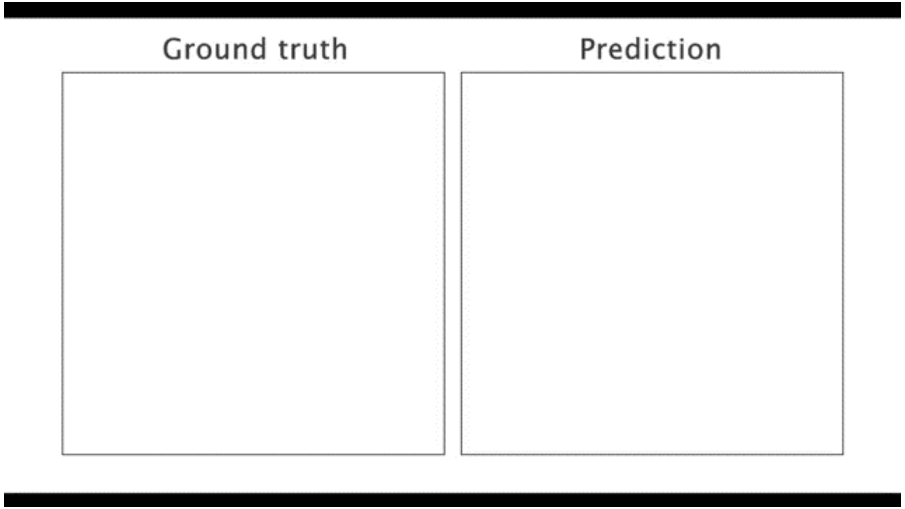
(ii) Edges ⇒ Connectivity
--> Recommendation Systems
--> Link Predictions

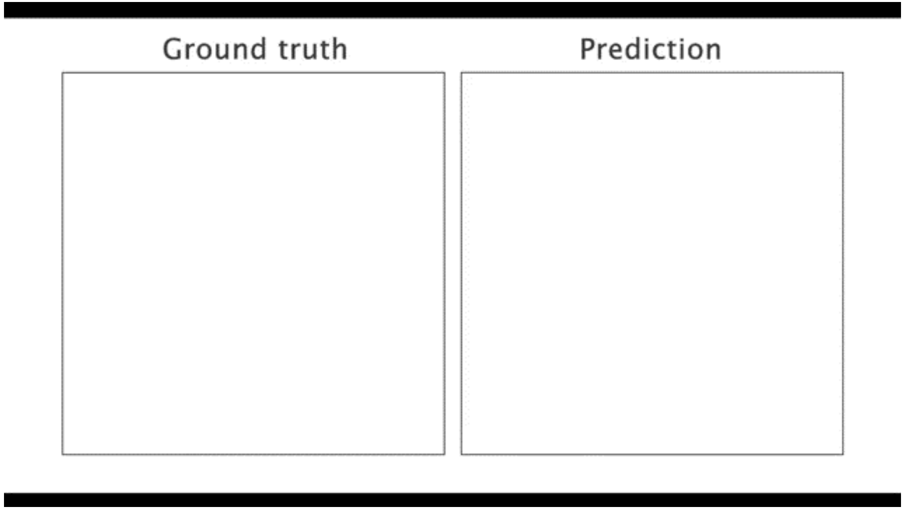
(iii) Graph Level Tasks → Class.
→ Regression



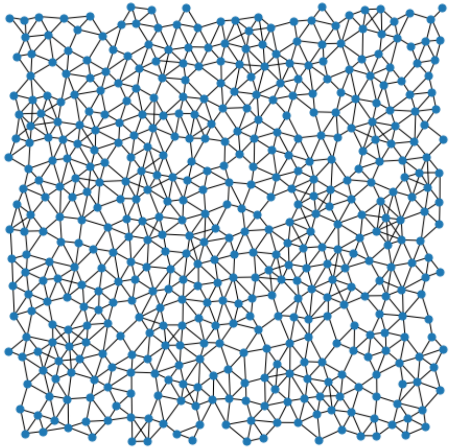
Learning to Simulate Complex Physics with Graph Networks

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





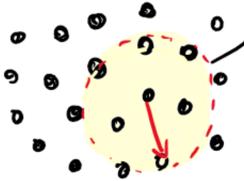
Case Study :



Data ○→ Seq. length of events [1000]

- 2D // 3D
- box bounds

- Radius of influence



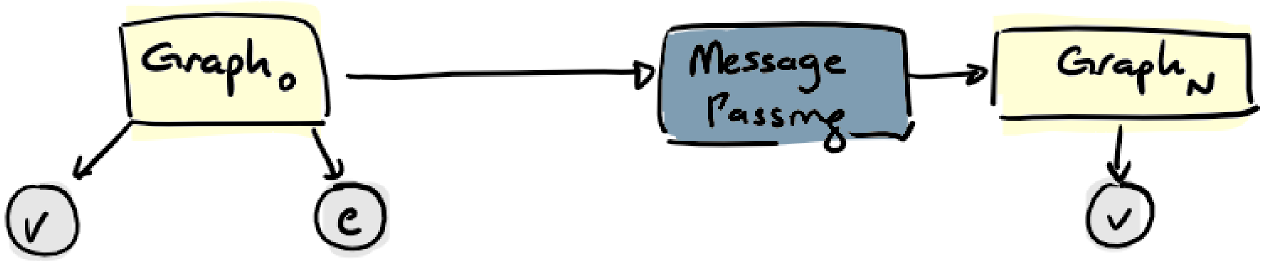
- Statistics for normalization
- Fluid type & position of each element.

* Closed system : No inlet/outlet

⇓ Fixed size Data for a given case

Case Study:

Basic Idea:



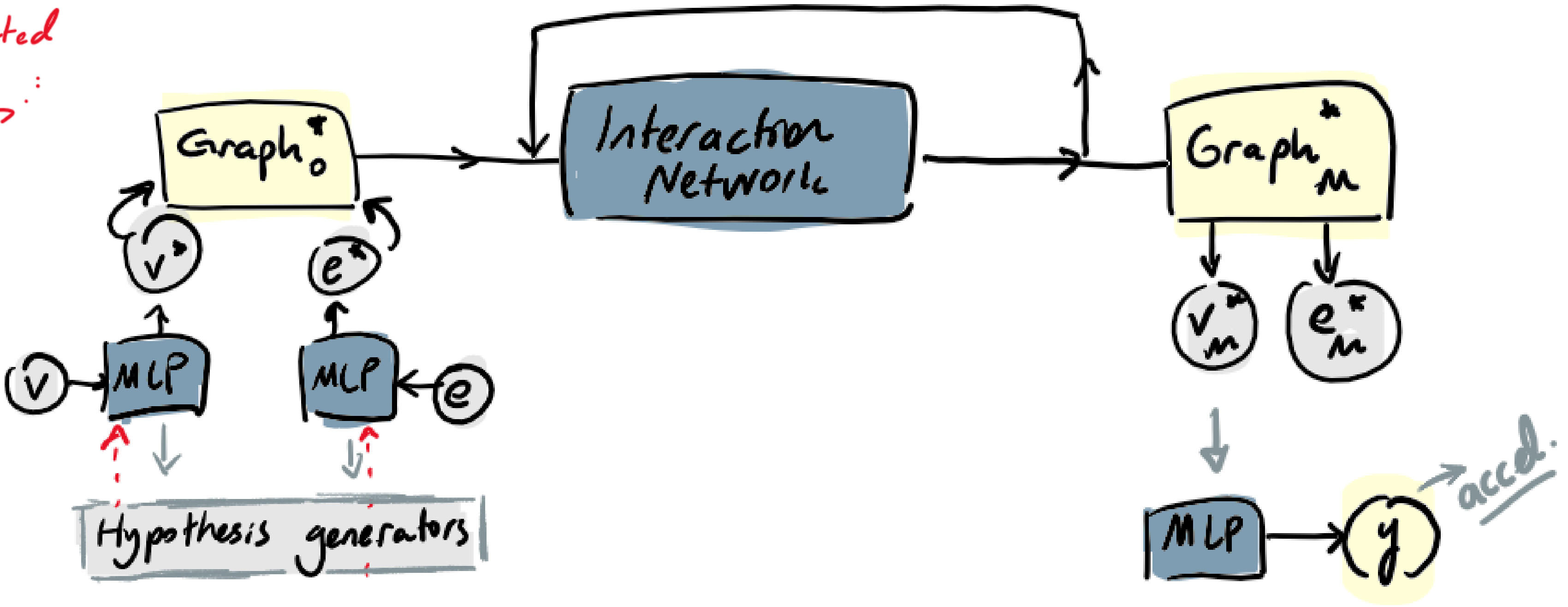
- velocities (5)
- Distance to boundaries
- Particle type

- Distance ij
- Displacements

- Acceleration

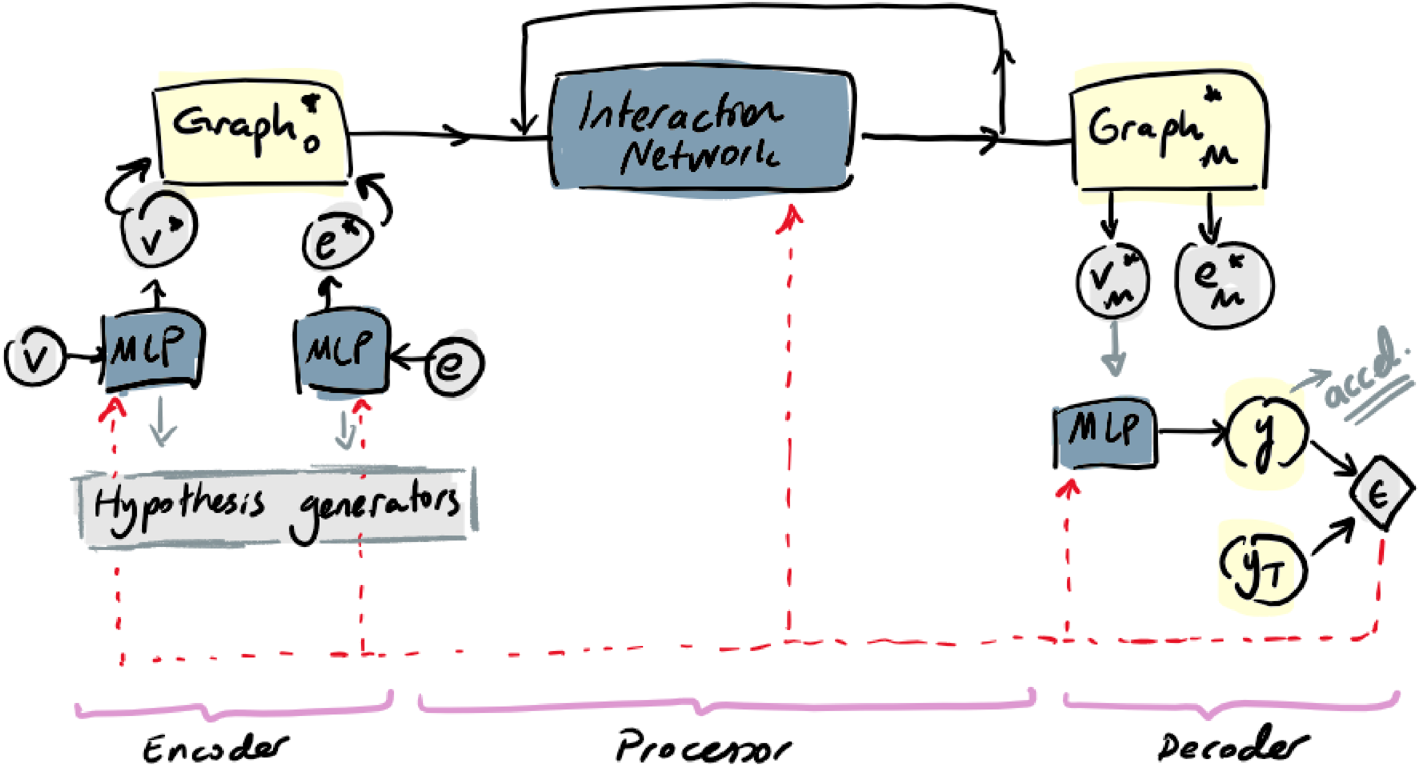
Case Study:

Implemented idea:



Case Study :

Implemented idea :



Interaction Network :

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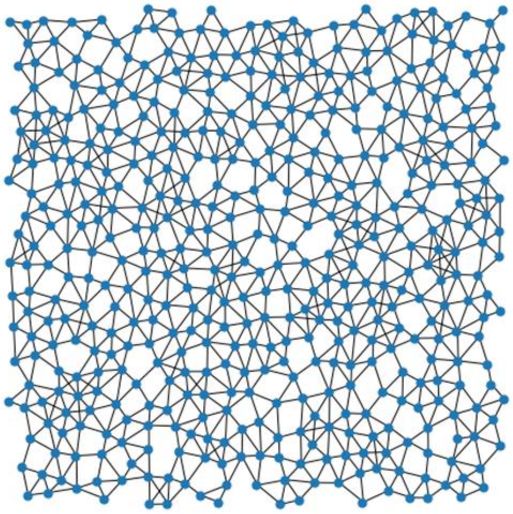
idea ⇒ hidden states of nodes v_i updated (I) according to the info. passed (II) from neighbours (III)



$$\underbrace{h_i^{(k+1)} = \phi_{update}}\left(\underbrace{h_i^{(k)}, \phi_{aggregate}^{(k)}}\left(\underbrace{\{h_j^{(k)}, \forall j \in \mathcal{N}(i)\}}\right)\right)$$

③ Update

- $v_i' \leftarrow v_i + f(v_i, Agg_i)$
- $e_{ij}' \leftarrow e_{ij} + f(Msg_{ij})$
- $g' \leftarrow g + f(\dots)$

② Message Aggregation

$$Agg_i = f(Msg_{i*})$$

↓

$$Agg_i = \sum_j Msg_{ij}$$

① Message Generation:

- Node i features
- Node j features
- Edge features
- Global features

$$Msg_{i,j} \leftarrow [v_i, v_j, e_{ij}, g]$$

Data for training

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WaterDrop
Water
Sand
Goop
MultiMaterial
RandomFloor
WaterRamps
SandRamps
FluidShake
FluidShakeBox
Continuous
WaterDrop-XL
Water-3D
Sand-3D
Goop-3D

Check

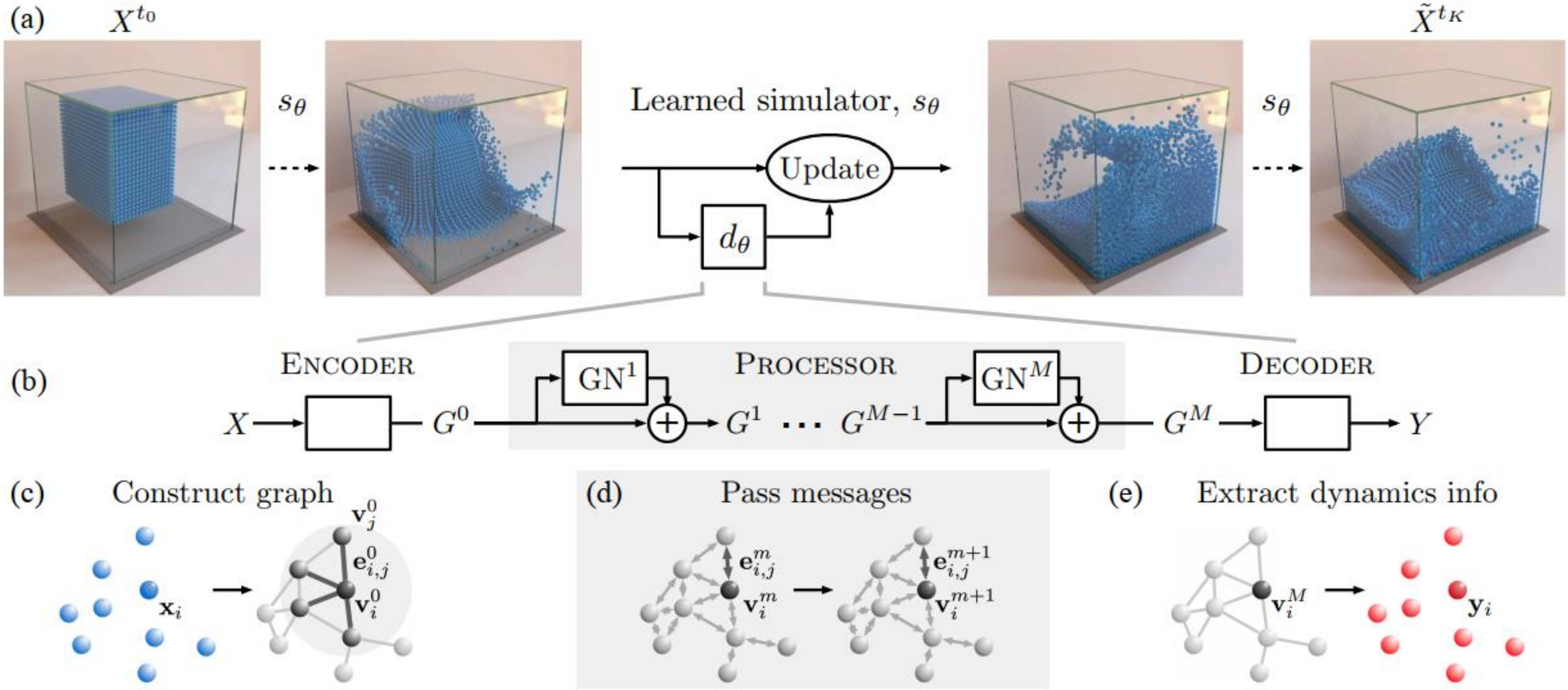
"download_dataset.sh"

* "WaterDrop"

Ateliers & Saveurs in Montreal

colab

Graph Neural Networks


(a)
X^{t_0}
s_θ
Learned simulator, s_θ
Update
d_θ
s_θ
$\tilde{X}^{t_K}$
(b)
ENCODER
PROCESSOR
DECODER
X
G^0
GN^1
G^1
G^{M-1}
GN^M
G^M
Y
(c)
Construct graph
$\mathbf{x}_i$
$\mathbf{v}_j^0$
$\mathbf{e}_{i,j}^0$
$\mathbf{v}_i^0$
(d)
Pass messages
$\mathbf{e}_{i,j}^m$
$\mathbf{v}_i^m$
$\mathbf{e}_{i,j}^{m+1}$
$\mathbf{v}_i^{m+1}$
(e)
Extract dynamics info
$\mathbf{v}_i^M$
$\mathbf{y}_i$