LEARNING LAGRANGIAN FLUID DYNAMICS WITH GRAPH NEURAL NETWORKS

Anonymous authors
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ABSTRACT

We present a data-driven model for fluid simulation under Lagrangian representation. Our model uses graph to describe fluid field, where physical quantities are encoded as node and edge features. Instead of directly predicting the acceleration or position correction given current state, we decompose the simulation scheme into separate parts - advection, collision and pressure projection. For these different reasoning tasks, we propose two kinds of graph neural network structures, node-focused networks and edge-focused networks. Our tests show that the learned model can produce accurate results and remain stable in scenarios with large amount of particles and different geometries. Unlike many previous works, further tests demonstrate that our model is able to retain many important physical properties of incompressible fluids, such as minor divergence and reasonable pressure distribution. Additionally, our model can adopt a range of time step sizes different from ones using in the training set, which indicates its robust generalization capability.

1 INTRODUCTION

For many science and engineering problems, fluids is an essential integral part. How to simulate fluid dynamics accurately has long been studied by researchers and a large class of numerical models have been developed. However, computing high-quality fluid simulation is still computationally expensive despite the advances in computing power. Also, the time a high-quality numerical model uses usually increase drastically when resolution of scene scales up. A common way to alleviate computing cost in many situations is using data-driven model. Recent progress in machine learning domain opens up the possibility for employing learning algorithms to understand and model fluid dynamics.

In this paper, we propose a graph based data-driven fluid dynamics model (Fluid Graph Network, FGN), which consists of simple multi-layer perceptron and graph inductive architecture inspired from GraphSAGE (Hamilton et al., 2017) and (Kipf and Welling, 2016). Our model predicts and integrates forward the movement of incompressible fluid based on observations. Compared to previous works in this domain (Ummenhofer et al., 2020; Sanchez-Gonzalez et al., 2020), our model enjoys traceability of physical properties of the system, like pressure distribution and minor velocity divergence. Experiments reveal that our model can remain stable in long-term simulation, and it also preserves the divergence-free property of fluid field. Our model is entailed and customized for fluid simulation, however as it uses standard deep learning building blocks and takes universal feature (positions, velocities, particle density) under Lagrangian framework as input, it can be extended to simulation of other dynamics under Lagrangian framework.

2 RELATED WORKS

Our model is build upon Lagrangian representation of fluid, where continuous fluid are discretized and approximated by a set of particles. The most prominent advantage of Lagrangian methods is that, particle boundary is the material interface, which makes boundary condition easy to impose, especially when material interface is large and changing violently. A well-known Lagrangian method is Smooth Particle Hydrodynamics (SPH) (Monaghan, 1988). SPH and its variants are widely used in numerical physic simulation, especially fluid dynamics under various environments. Particle-based fluid simulation (Müller et al., 2003) introduces SPH model to generate realistic fluid visual effects.

Moving particle semi-implicit method (MPS) (Koshizuka and Oka, 1996) markedly improves accuracy and stability of incompressible fluid simulation by introducing a pressure projection procedure that emulates Eulerian grid methods. Weakly compressible SPH (Becker and Teschner, 2007) introduces equation of state to model the pressure during simulation. Predictive-corrective incompressible SPH (Solenthaler and Pajarola, 2009) and divergence-free SPH (Bender and Koschier, 2015) uses iterative method to improve the accuracy of pressure calculation in incompressible flow simulation.

Modelling fluid dynamics in a data-driven way have been explored and studied by many researchers. With advances in machine learning algorithms, especially deep learning ones, many high-fidelity data-driven models employing machine learning algorithms have been built. Ladický et al. (2015) reformulate the Navier-Stokes equation as an regression problem and build a regressor using random forest, which significantly boosts the calculation efficiency. Tompson et al. (2016), Xiao et al. (2020) learns the pressure projection under Eulerian framework with convolutional neural network, which accelerates the fluid simulation. Wiewel et al. (2018) brings significant speed-up by learning a reduced order presentation and predicting pressure field with a LSTM-based model. Morton et al. (2018) learns the dynamics of airflow around a cylinder based on Koopman theory. de Avila Belbute-Peres et al. (2020) predicts fluid flow by combining grid-based method with graph neural networks.

Learning and reasoning particle dynamics under a graph representation has the following benefits and conveniences. First, particle-based methods model physic phenomenon as interactions between particles within an area. This locality impose an inductive bias for learning under Lagrangian framework: dynamics have strong locality. The locality of unstructured data under Lagrangian representation can be captured by convolutional operators on the graph (Kipf and Welling, 2016). Second, unlike Eulerian grid-based methods, Lagrangian particle-based methods do not have explicit and structured grid, which makes standard Convolutional Neural Network (CNN) cannot be directly applied to particles without feature processing (Wang et al., 2018; Ummenhofer et al., 2020). Third, many dynamics are based on pairwise relation between particles, like collision, which can be easily interpreted as edge attributes of graph. Given these factors, recently there have been a rich class of works that uses graph neural network (Scarselli et al., 2009) to learn and reason about physics under Lagrangian framework. (Battaglia et al., 2016; Chang et al., 2016; Sanchez-Gonzalez et al., 2018; Li et al., 2018; Mrowca et al., 2018)

3 MODEL

3.1 FLUID DYNAMICS

The governing equation for incompressible fluids are the Navier-Stokes equation and continuity equation as follow (Batchelor, 2000):

$$\frac{D\mathbf{u}}{Dt} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} + \mathbf{g}, \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0. \tag{2}$$

To describe the fluid field, there are two kinds of systems, Eulerian and Lagrangian ones and in this work, we adopt a Lagrangian system. A common method to solve Navier-Stokes equation and discretize fluid under Lagrangian framework is Smooth Particle Hydrodynamics (SPH) method (Monaghan, 1988), where physical quantities at an arbitrary point in the space is approximated by the states of nearby particles.

In SPH, an arbitrary scalar (or vector) field $A(\mathbf{r})$ at location $\mathbf{r}$ can be represented by a convolution:

$$A(\mathbf{r}) = \int A(\mathbf{r}') W(|\mathbf{r} - \mathbf{r}'|, h) \, dV(\mathbf{r}'), \tag{3}$$

where W is weighting function or smooth kernel as defined in SPH, h is the smoothing length, which defines the range of particles to be considered and $V(\mathbf{r}')$ is the volume at $\mathbf{r}$. Numerically, the interpolation can be approximated by replacing the integration with summation.

Based on this model, equation equation 1 and equation 2 can be discretized. The discrete equation system is usually solved under a predictor-corrector scheme, prediction based on advection and correction based on physical properties (such as divergence free constraints).

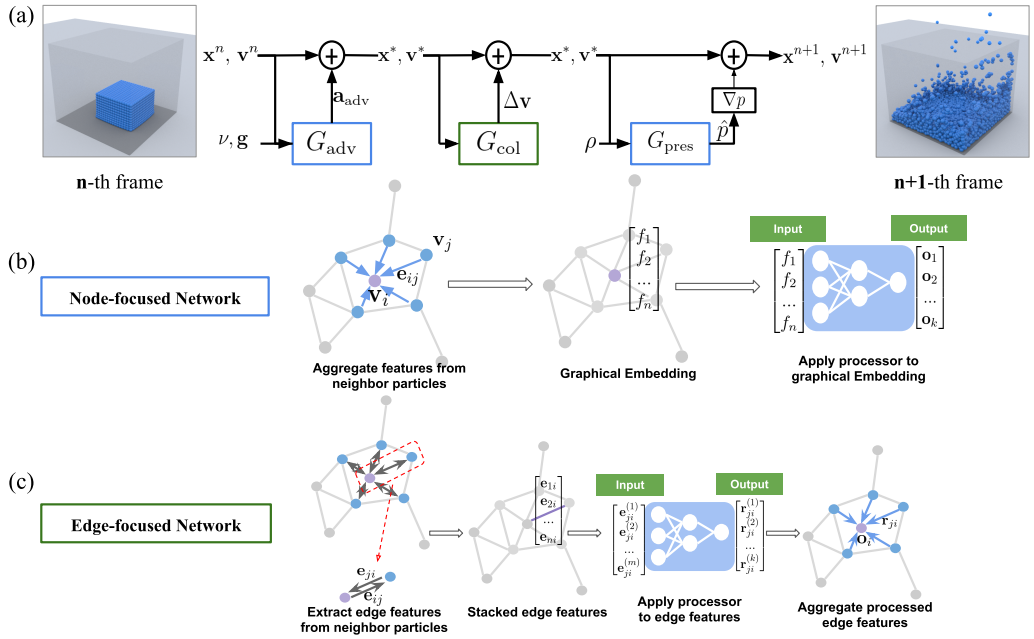

Figure 1: **(a)** Schematic of our FGN model. G_{adv} applies the effect of body force and viscosity to the fluids. G_{pres} predicts the pressure. G_{col} handles collision between particles. **(b)** In node-focused network, input are encoded as nodal features, and then passed to shared processor. Advection and pressure projection are particle-wise effect, where body force field and pressure field pose influences on each particle separately. **(c)** In edge-focused network, input are encoded as edge features of a directed graph, then features lying on edges are passed to shared processor. Collision net aims to predict a pairwise effect, which can be easily represented as edge attributes between each pair of particles.

3.2 MODEL

Fluids is a time-dependent dynamical system, where location of particles, $\mathbf{r}$, is described by equation of form: $d\mathbf{r}/dt = f(\mathbf{r})$. When building a data-driven model to learn and solve this system, we assume the system is Markovian, that is, the state of the system at time step $n+1$ depends only on the state of previous time step n. The update mechanism in our model can be represented as:

$$\{\mathbf{x}^{n+1}, \mathbf{v}^{n+1}\} = G_\theta\left(\{\mathbf{x}^n, \mathbf{v}^n\}\right). \tag{4}$$

Here $\{\mathbf{x}^n, \mathbf{v}^n\}$ denotes the positional information and velocity of fluid field at time step n. Data-driven model G_θ, parameterized by θ , maps the state of time step n to time step $n+1$.

In order to build a robust and generalized data-driven model, the structure of our model is physic-informed, which enables the model to give interpretable output without losing physical properties of the system. In general, our model mimics the predictor-corrector scheme and includes three parts, advection net, collision net and pressure net. They can be divided into two types of graph network (GN) according to the network structure (Battaglia et al., 2018). Specifically, advection net and pressure net are node-focused graph network, while collision net is edge-focused network. As each of these networks has specific task and different output, they are trained on different data separately.

Node-focused Graph Network Advection net is responsible for the prediction of advection effect and pressure net is responsible for pressure projection. Considering a particle i, the node-focused graph network first aggregates nodal features from neighbor particles $\{v_j | \forall j \in \mathcal{N}(i)\}$ and output an graphical embedding $\mathbf{f}_i$. Then the embedding $\mathbf{f}_i$ will be passed to a processor g_R, which takes embedding as input and output the desirable physical quantities o_i (i.e. acceleration $\mathbf{a}$ in advection net and pressure p in pressure net).

$$o_i = g_R\left(g_A\left(V_i\right)\right), V_i = \{v_j\}_{\forall j \in \mathcal{N}(i)} \tag{5}$$

Edge-focused Graph Network To handle the interaction between fluid particles and solid wall or obstacles, we propose a graph network which is responsible for predicting this effect of collision. As relative position and relative velocity will have different signs based on different observation perspective (e.g. relative velocity $v_{ij} = -v_{ji}$), thus the graph in collision net is directed. In collision net, relative features, e_{ij} (relative positions, relative velocities between particle i and j), are passed to processor f_R as edge features. The processor then predicts the relationship r_{ij} between nodes based on input edge features. Finally we aggregates the output relationship via aggregator f_A, in order to gather the influence from all nearby particles and predict an overall effect o_i on center particle i. The whole process is defined as:

$$o_i = f_A\left(f_R\left(E_i\right)\right), E_i = \{e_{ij}\}_{\forall j \in \mathcal{N}(i)} \tag{6}$$

The advantage of using relative position and velocity instead of global ones as input feature, is that it explicitly imposes an spatial invariance to the network, since collision between two particles is invariant to the global positions they are at.

4 IMPLEMENTATION

We adopt the numerical model in SPH to evaluate the physical quantities like particle density and differential operators like gradient. To construct a graph representation for particles, we establish edges between particles within control radius.

4.1 UPDATE SCHEME

In general, given the state (position $\mathbf{x}^n$ and velocity $\mathbf{v}^n$) of current time step n, we derive the state of next time step $n+1$ by passing the state information through advection net, collision net and pressure net sequentially. The input features to advection net are positions and velocities of particles, $[\mathbf{x}^n, \mathbf{v}^n]$, along with $\mathbf{g}$, which indicates the external body force per mass of fluid, and viscosity parameter ν, which denotes the magnitude of fluid viscosity. The advection net predicts acceleration of particles:

$$\mathbf{a}^{\text{adv}} = G_{\text{adv}}\left(\mathbf{x}^n, \mathbf{v}^n, \mathbf{g}, \nu\right), \tag{7}$$

and updates the state of fluid particles to an intermediate state $[\mathbf{x}^*, \mathbf{v}^*]$.

$$\mathbf{v}^* = \mathbf{v}^n + \mathbf{a}^{\text{adv}}\Delta t, \qquad \mathbf{x}^* = \mathbf{x}^n + \mathbf{v}^*\Delta t. \tag{8}$$

Where $\mathbf{a}^{\text{adv}} = [\mathbf{a}_1^{\text{adv}}, ..., \mathbf{a}_N^{\text{adv}}]$, $\mathbf{x}^n = [\mathbf{x}_1^n, ..., \mathbf{v}_N^n]$, $\mathbf{v}^n = [\mathbf{v}_1^n, ..., \mathbf{v}_N^n]$ for particles $i \in \{1, .., N\}$. We will use the same notation in following illustration.

The collision net takes relative positions and velocities between particles, $[\mathbf{x}_i^* - \mathbf{x}_j^*, \mathbf{v}_i^* - \mathbf{v}_j^*]$ as input, and predicts correction to the velocity,

$$\Delta\mathbf{v} = G_{\text{col}}(\mathbf{x}_r^*, \mathbf{v}_r^*), \tag{9}$$

where $[\mathbf{x}_r^*, \mathbf{v}_r^*]$ denotes the relative position and velocity in intermediate state. The velocity is then updated with predicted correction:

$$\mathbf{v}^* \leftarrow \mathbf{v}^* + \Delta\mathbf{v}. \tag{10}$$

The updated intermediate position and velocity are taken as input by the pressure net, along with particle number density $\boldsymbol{\rho}$.

$$\hat{\mathbf{p}} = G_{\text{pres}}(\mathbf{x}^*, \mathbf{v}^*, \boldsymbol{\rho}). \tag{11}$$

The state of fluid field is then updated to next time step $n+1$,

$$\mathbf{v}^{n+1} = \mathbf{v}^* - \frac{\nabla\hat{\mathbf{p}}}{\rho_c}\Delta t, \qquad \mathbf{x}^{n+1} = \mathbf{x}^* + \mathbf{v}^{n+1}\Delta t. \tag{12}$$

Where $\hat{\mathbf{p}} = [\hat{p}_1, ..., \hat{p}_N]$, $\boldsymbol{\rho} = [\rho_1, ..., \rho_N]$, ρ_c is the density parameter of fluid. Predicting pressure of fluid field using particle density and velocity is based on the observation that advection will incur a temporary compression on fluid body, which means fluid density has changed. Therefore the goal of pressure net is to impose a pressure projection to mitigate these deviations.

During the above calculation, the global positional information is only used to construct graph on fluid particles and will not be passed into aggregator and processor as features. Relative position and particle density are normalized before input.

4.2 NETWORK ARCHITECTURES

For node-focused graph network,to capture a smooth response of the field with respect to spatial location, the aggregation from layer $l-1$ to l is defined as:

$$\mathbf{a}_i^{(l)} = \frac{\sum \mathbf{f}_j^{(l-1)} W\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|, h\right)}{\sum W\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|, h\right)} + \mathbf{f}_i^{(l-1)}, \forall j \in \mathcal{N}(i), \tag{13}$$

$$\mathbf{f}_i^{(l)} = \sigma\left(\mathbf{W} \cdot \mathbf{a}_i^{(l)}\right), \tag{14}$$

where the aggregator sums up the features $\mathbf{f}_j^{(l-1)}$ from neighbor vertices $\{v_j | j \in \mathcal{N}(i)\}$ using smooth kernel as weight function, and here self-connection is added to every vertex. Linear transformation $\mathbf{W}$ and non-linear transformation σ are then applied to the aggregated features. In practice we found that two layer of aggregations is enough for the model to produce reasonably accurate output.(Adding more aggregation layers does not bring in significant improvements).

As for the edge-focused network, the aggregation is simply defined as:

$$\mathbf{a}_i = \sum_{j \in \mathcal{N}(i)} \mathbf{W} \cdot \mathbf{r}_{ji}, \tag{15}$$

where $\mathbf{r}_{ji}$ is edge feature processed by processor, $\mathbf{W}$ is a linear transformation matrix. The aggregation in the edge-focused network is at the last layer, so no non-linearity is included here.

The processors in both networks are implemented as shared MLP, where they are shared among nodes or edges depending on network types (e.g. in node-focused network, processor is MLP shared among each node). In node-focused network, the processor has three hidden layers, with the input node embedding $\mathbf{f}$ of size 128. In edge-focused network, the processor has four hidden layers, with input edge attributes $[\mathbf{x}_r, \mathbf{v}_r]$ of size 6.

5 EXPERIMENTS

5.1 TRAINING

Dataset We use moving particle semi-implicit method (MPS) (Koshizuka and Oka, 1996) with an improved pressure solver (Lee et al., 2011) to generate high-fidelity simulation data of incompressible flow. MPS is a numerical method based on SPH which prioritizes accuracy over calculation speed. It enforces the incompressibility of fluid field by solving the pressure Poisson equation. We created 20 scenes by randomly placing fluid blocks, solid obstacles, initializing fluid particles with random velocity (See A.2 for full detail of dataset generation and training strategy).

Loss Function and Optimization We train three networks, advection net, collision net and pressure net separately. Each network is trained in a supervised way by optimizing the mean squared error between prediction $\hat{y}$ and ground truth y.

$$L = \frac{1}{N} \sum_{i=1}^{N} ||y_i - \hat{y}_i||_2^2 \tag{16}$$

We normalize particle density before inputting into pressure net, which accelerates and stabilizes training. In the processor, we add LayerNorm (Ba et al., 2016) after activation to each layer (except for the output layer). The parameters of the model are optimized with Adam (Kingma and Ba, 2014) optimizer. We implement the model in PyTorch. All the training and experiments are mainly carried out on NVIDIA GTX 1080Ti GPU.

5.2 EVALUATION

Baselines Besides the comparison against ground truth data, we also compare our model to two recent works which use data-driven approaches to simulate fluids under Lagrangian framework. Ummenhofer et al. (2020) use continuous convolutional kernel to learn fluid dynamics and they reported that their model has outperformed other works in this domain. Sanchez-Gonzalez et al.

Case	Model	Density error		Velocity divergence		Average Chamfer distance (mm)	
		Mean	Max	Mean	Max	Mean	Max
Dam Collapse	FGN (this work)	**0.0561**	**0.1390**	**0.0196**	**0.0280**	**24.2**	**30.1**
	GNS	0.0898	0.3387	0.0210	0.0311	26.1	33.1
	CConv	0.1811	0.2947	0.0338	0.1700	31.4	44.0
	Ground Truth	0.0380	0.0711	0.0190	0.0268	-	-
Water Fall	FGN (this work)	**0.0541**	**0.1350**	**0.0207**	0.0431	**24.8**	**29.6**
	GNS	0.1035	0.3512	0.0223	**0.0399**	25.6	31.8
	CConv	0.2783	0.4121	0.0668	0.2882	40.4	61.5
	Ground Truth	0.0429	0.0966	0.0196	0.0398	-	-

Table 1: Quantitative accuracy analysis. For resolution, the dam collapse case contains about 10k particles and water fall case contains about 80k particles. We report the mean and maximum value of density error and velocity divergence over the whole simulation sequence. We also report the modified average Chamfer distance between the results of each model and ground truth data.

Case	Model	Density error		Velocity divergence		Average Chamfer distance (mm)	
		Mean	Max	Mean	Max	Mean	Max
Dam Collapse	FGN (this work)	**0.0461**	**0.0900**	**0.0195**	**0.0280**	**24.2**	**30.1**
	GCN	0.0939	0.3832	0.0196	0.0293	27.7	31.6
	SAGE	0.0935	0.3597	0.0196	0.0289	26.4	31.3
	MLP	0.0963	0.3624	0.0196	0.0289	28.5	32.8
	Ground Truth	0.0380	0.0710	0.0190	0.0268	-	-
Water Fall	FGN (this work)	**0.0541**	**0.1350**	**0.0207**	**0.0431**	**24.8**	**29.6**
	GCN	0.0794	0.3373	0.0210	0.0433	25.5	31.7
	SAGE	0.0769	0.3254	0.0209	0.0432	25.3	31.4
	MLP	0.0830	0.2967	0.0209	0.0433	26.3	32.4
	Ground Truth	0.0429	0.0966	0.0196	0.0398	-	-

Table 2: Quantitative ablation study. All aggregators have two layers. In general, they give similar performance on overall position prediction (similar Chamfer distance error), yet our model significantly improves the the quality of predictions in terms of maintaining a constant density.

(2020) propose a graph network-based simulator (GNS) as a general-purpose physic simulator under Lagrangian representation. Our model and GNS both transform and pass message of fluid field via a graph structure, but GNS consists of a far larger and deeper network with multiple sub-blocks and thus contains much more parameters than ours. For all baseline models, we adopt the same training strategy from original papers but train them on our dataset (See A.4 for full detail).

Metrics To conduct quantitative analysis, we evaluate models based on several metrics. We first report a modified version of Chamfer Distance between the simulated results of different models and ground truth sequence. We drop the symmetric part in the Chamfer Distance, and defined modified Chamfer distance for two collections of particles X, Y as:

$$L\left(X, Y\right) = \frac{1}{N} \sum_{\mathbf{x} \in X} \min_{\mathbf{y} \in Y} d\left(\mathbf{x}, \mathbf{y}\right), \tag{17}$$

where N is the total particle number of point cloud collection X, and distance function $d(\mathbf{x}, \mathbf{y})$ is evaluated using L2-norm $\|\mathbf{x} - \mathbf{y}\|_2$. We also investigate two essential physical quantities for incompressible fluid simulation - velocity divergence and particle density deviation of fluid field.

6 RESULTS

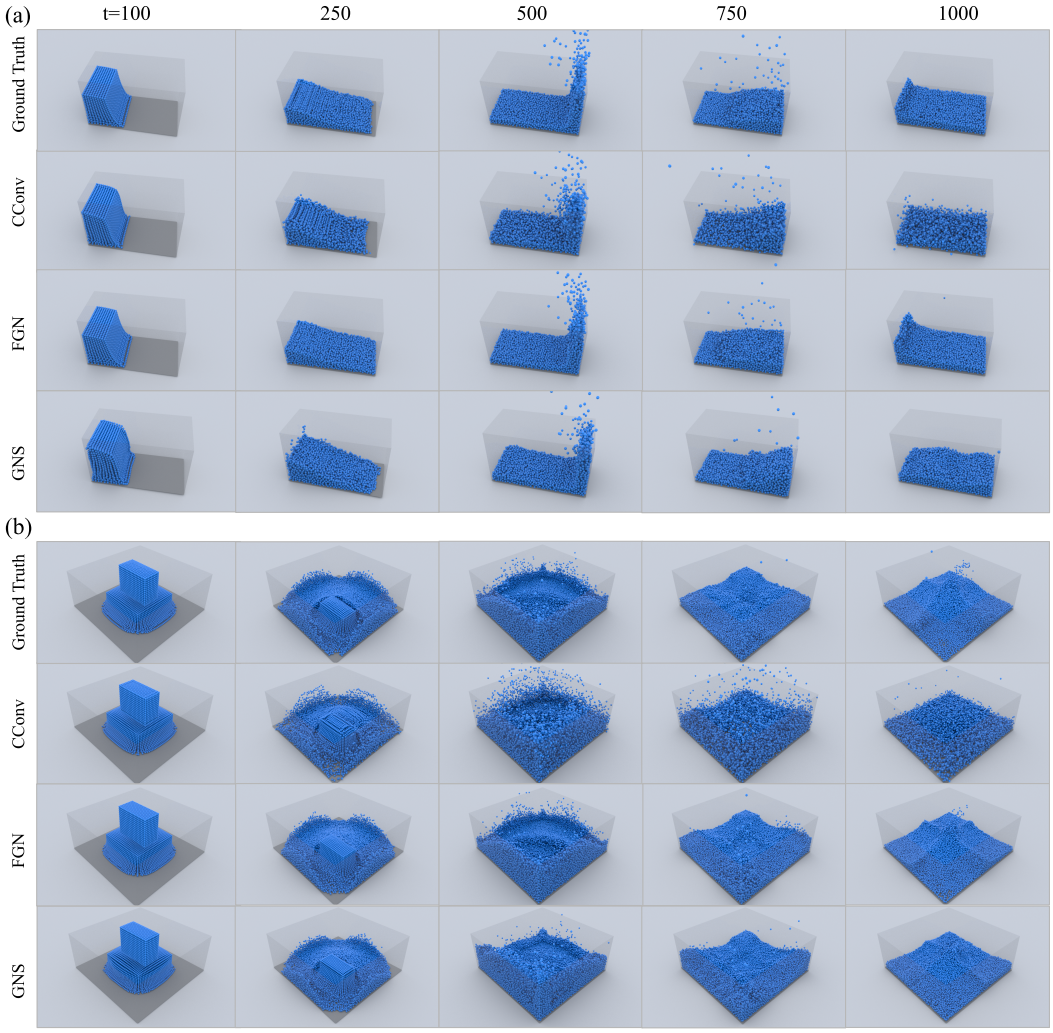

Figure 2: **(a)** Qualitative comparison of dam collapse. **(b)** Qualitative comparison of water fall. In CConv and GNS, we can observe oscillation on the free surface of fluids, while the results generated from our model maintains a much more compact and smoother shape. After a long time steps, CConv's result fail to maintain smooth and compact fluid distributions and GNS' prediction is significantly slower than ground truth, while our model's prediction has minor difference from ground truth.

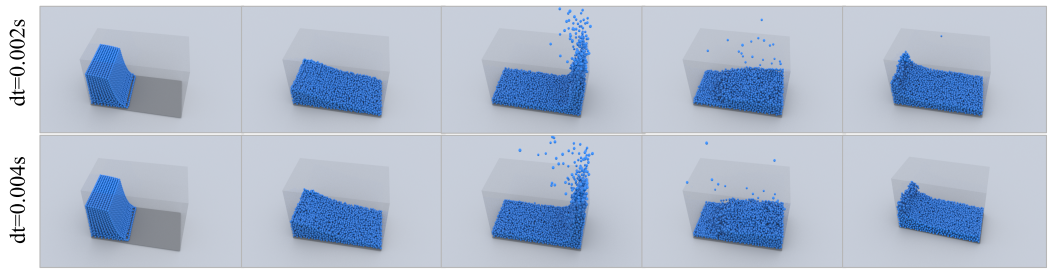

Figure 3: Qualitative comparison of different time step sizes. We use different time step size to simulate with our model. Despite the training set is generated with a time step size of 0.002s, our model can be generalized to a larger time step size with a neglectable increase in error. Other models diverge immediately when extrapolate to time step size different from training data.

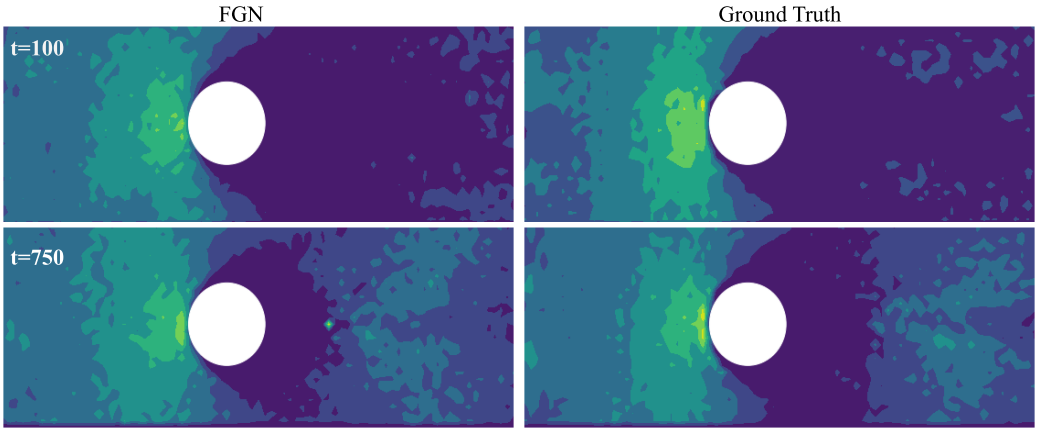

Figure 4: Pressure distribution contour. Our model can learn to generate reasonable pressure distribution agreed with ground truth, which captures the shape of shifting high pressure and low pressure region.

Performance In order to measure the performance of our FGN model as simulator, we performed simulation on different cases. In the two cases, dam collapse and water fall, we study the physical property of simulation results and its earth mover distance to ground truth data. Quantitative results over the whole simulation sequence are listed in Table 1 (See A.3 for detailed figures).

Generalization To test out model's capability of generalization. We apply our model to test cases with conditions beyond training distributions. In the first case, we study how our model will predict pressure distribution of circular flow around a cylinder. This scene contains an inflow on the left side which keeps emitting particles during simulation and an outflow on the right side. Additionally, we challenge our model's robustness by applying different time step sizes to it.

Ablation Study We test and compare the performance of different types of aggregators used in pressure net, as pressure net has the largest influence on prediction accuracy [1]. We compare our aggregator against graph convolution networks (GCN) from Kipf and Welling (2016), Hamilton et al. (2017)'s graph SAGE using mean aggregator and MLP *w/o* any graph aggregation operation. The evaluation metrics are same as those used in performance comparison against baselines. Results are listed in Table 2.

7 Conclusion

In this paper, we presented a data-driven Lagrangian fluid model for incompressible flow simulation by decomposing simulation scheme as separate reasoning tasks based on Navier-Stokes equation. It can preserve many essential physical properties of the fluid field such as low volume compression, and predict reasonable pressure distribution. Our model also has generalization capability, where it can remain stable when extrapolating to a wide range of different geometries and adopting different time step sizes. In general, our work is an advance in learning on unstructured data with graph neural networks, and enriches the paradigm of combining learning-based methods with physical models.

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[1] During preliminary experiment, we find that aggregators in advection net do not have significant impact on overall model performance when viscosity parameter of fluids is small, therefore ablation results on it are not listed here.

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APPENDIX A

A.1 IMPLEMENTATION DETAILS

Graph construction We build the graph by establishing edges between particles within limit radius. We perform the neighborhood searching on GPU by using cell sort algorithm. All the edge attributes are stored in sparse matrices. Although the limit radius does not have significant impact on training loss and larger limit radius will increase the computing cost drastically, we found that small limit radius can influence the long-term stability of the model. For advection net and pressure projection net, we select the limit radius to be three times the particle diameter D (D = 0.050m), and 0.9D for collision net.

Numerical model In general, we calculate all the gradient operators and smooth kernel based on numerical model of SPH.

In SPH model, particle density is defined as:

$$n_i = \sum_{i \neq j} W\left(|\mathbf{r}_i - \mathbf{r}_j|, h\right), \forall j \in \mathcal{N}(i). \tag{18}$$

For scalar quantity ϕ_i at location $\mathbf{r}_i$, we approximate its gradient by:

$$\nabla \phi_i = \frac{d}{n^*} \sum_j (\phi_j - \phi_i) \nabla W_{ij}, \tag{19}$$

where n^* is the constant particle number density derived by calculating the maximum particle number density at the initial frame, d is the dimension of the problem, W_{ij} denotes the smooth kernel function value between particle i and j. Similarly velocity divergence is defined as:

$$\nabla \cdot \mathbf{v}_i = \frac{d}{n^*} \sum_j (\mathbf{v}_j - \mathbf{v}_i) \cdot \nabla W_{ij}, \tag{20}$$

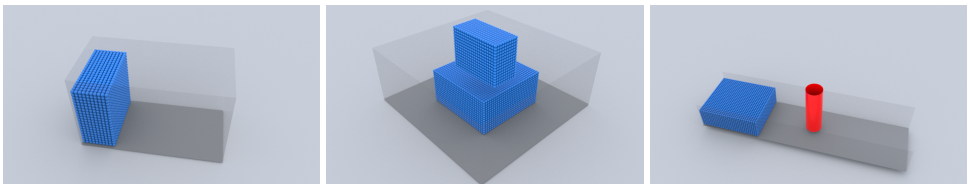
We adopt the same smooth kernel function from Koshizuka and Oka (1996), which is very simple to evaluate.

$$W_{ij} = \begin{cases} \frac{h}{||\mathbf{r}_i - \mathbf{r}_j||_2} - 1 & \text{if } ||\mathbf{r}_i - \mathbf{r}_j||_2 < h \\ 0 & \text{if } ||\mathbf{r}_i - \mathbf{r}_j||_2 \geq h \end{cases} \tag{21}$$

A.2 TRAINING

Dataset Generation We place scene objects in boxes with different shapes and initialize velocity uniformly sampled from $\mathcal{U}(0, 0.1)$. We simulate each scene to 1000 time steps with step size $dt = 0.002$.

Strategy We train each network for 100,000 iterations of gradient updates and decay learning rate from 0.001 to 0.0000625. For the training of three sub-networks (advection net, collision net, pressure net), the batch size of each network is 16, 4 and 32 respectively. To allow the mini-batching of different graph, we mini-batch the adjacency matrix from different scenes by creating a large sparse matrix and stack adjacency matrix on the diagonals.



(a) Dam Collapse (b) Water Fall (c) Flow around Cylinder

Figure 5: Visualizations of initial condition settings in evaluation scenarios

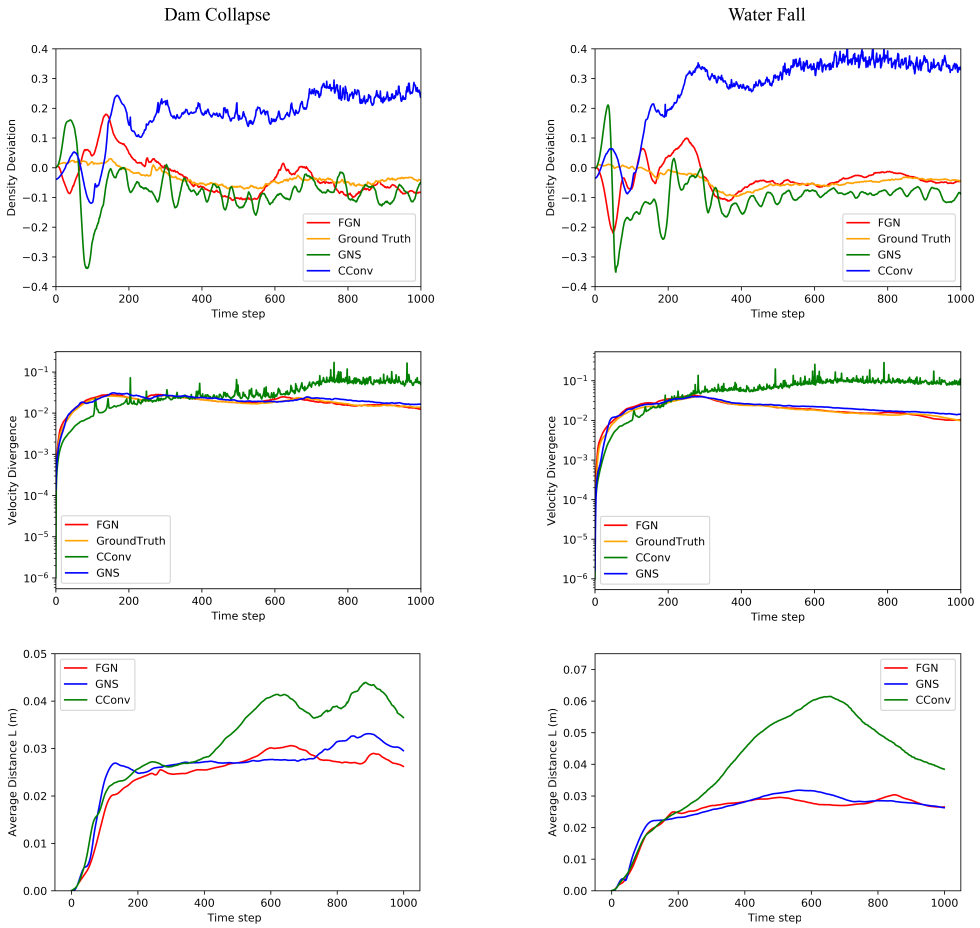


Figure 6: Error trend with respect to time. The density deviation of our model remain close to zero despite some oscillation at first. Although GNS also maintain a low density deviation, its average density oscillate much more severely. This is consistent with the qualitative comparison, in which the fluid surface from GNS is oscillating and less compact. CConv fails to maintain constant density and its density increases significantly after collision to the wall boundary. Both our model and GNS can predict a low divergence velocity field while CConv fails to capture this property. This somehow explains why CConv struggles to maintain constant density.The average earth mover distance to the ground truth data accumulates at first and stabilizes after system is in equilibrium. CConv has larger earth mover distance while graph-based model's distances are generally smaller.

A.3 Metrics Evaluation Details

We show how error under different evaluation metrics change as a function of time in Figure 6.

A.4 Baselines Implementation

Continuous Convolution We use the open-source implementation from Ummenhofer et al. (2020) [2]. To give a fair benchmark result we train their network with our dataset. As in our work, we model solid obstacles and wall as virtual particles, so we transform these virtual particles into surface and corresponding normals before inputting them into CConv network. The original CConv uses a time step size of 0.02s, but given such a large time step size, the qualitative results can be distinct from ground truth and other model with smaller time step size. Hence during training and comparison we adopt a time step size of 0.002s for CConv model.

[2]https://github.com/intel-isl/DeepLagrangianFluids

Graph Network-based Simulator We implemented GNS following the description in Sanchez-Gonzalez et al. (2020). We build GNS with 10 unshared GN blocks, conditioned on 5 previous velocities and input relative positions as edge features. We chose the connectivity radius to be 2.1D, so that the number of neighbors is around 20. Sanchez-Gonzalez et al. (2020) use finite difference to calculate acceleration and velocity, but in our implementation we explicitly maintain an array to store the velocities of all particles. Additionally, we do not use learned embedding but simple zero and one to indicate particle material type, as in our testing domain there are only two kinds of particles - solid and fluid. The loss function and training procedure are implemented as described in Sanchez-Gonzalez et al. (2020), including noise injection and similar normalization techniques.

For the implementation of GN block, as Sanchez-Gonzalez et al. (2020) states "We use GNs without global features or global updates (similar to an interaction network)", so we implement the GN block update mechanism following the description in Battaglia et al. (2018).

$$\mathbf{e}'_k = \phi^e(\mathbf{e}_k, \mathbf{v}_{r_k}, \mathbf{v}_{s_k}, \mathbf{u}) \tag{22}$$

$$\mathbf{v}'_i = \phi^v(\hat{\mathbf{e}}'_k, \mathbf{v}_i, \mathbf{u}) \tag{23}$$

$$\hat{\mathbf{e}}'_i = \rho^{e \to v}\left(E'_i\right) \tag{24}$$

where ϕ is the update function and implemented as MLP here, ρ is aggregation function which aggregates all the edge attributes to its center vertex, $\mathbf{u}$ is the global feature and here we append them to the nodal features as input feature, r_k denotes receiver vertices and s_k denotes sender vertices.

In the testing stage, as authors did not state how to set initial velocities, so we just warm start the simulation by calculating the first 5 frames using MPS method and apply GNS to the rest frames.