Fast prediction method for approximating steady flow simulations over multiple domains

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(Simulation + Data + Learning); Towards Society 5.0
by h3-Open-BDEC

h3-Open-DDA in h3-Open-BDEC

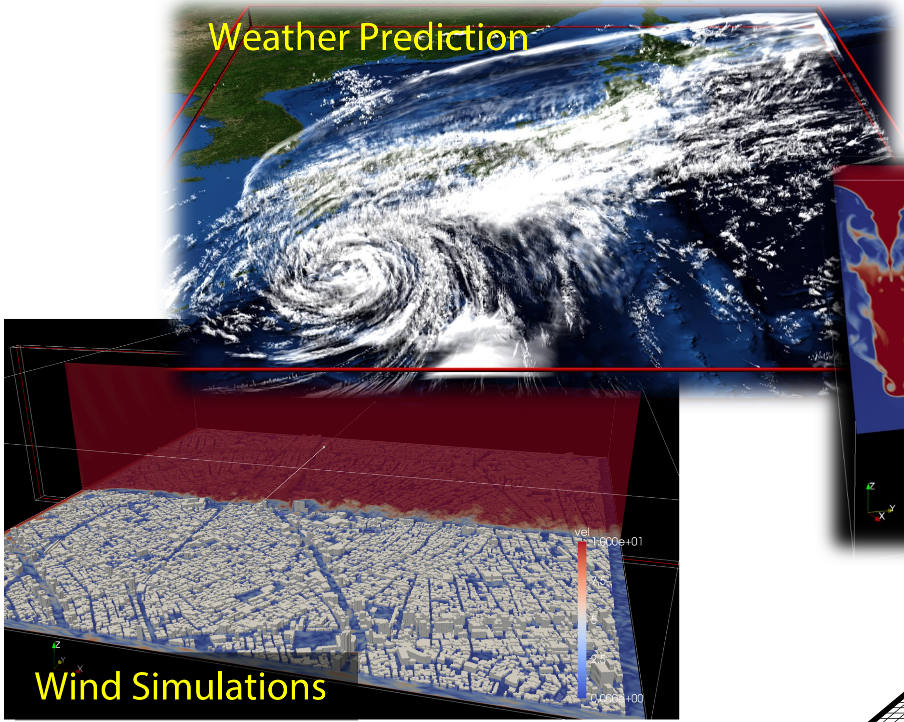
■h3-Open-DDA

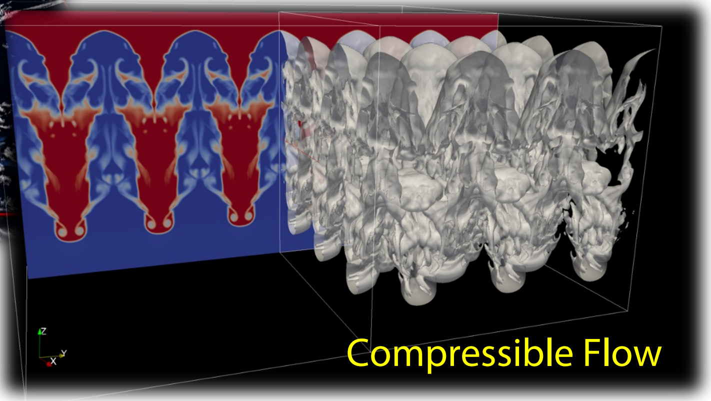
- Data Driven Approach (DDA)
  - Integration of simulation and machine learning
- Hierarchical DDA (hDDA)
  - Training data generation and learning in efficient and realistic time by simple model
  - Reducing computation time, computation volume, and power consumption (less than 1/10 of conventional methods)

■Research topics

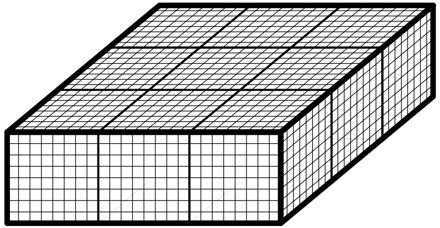
- Prediction of steady-state flow over multiple domains by combining deep learning and boundary conditions
- Development of a fast prediction method for time-dependent flows
- Enhancement of molecular dynamics simulation by machine learning

Target: Computational Fluid Dynamics

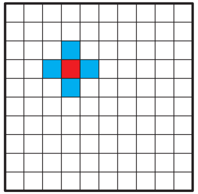




Computational cost of computational fluid dynamics is relatively high.



Computational domain



Stencil computations

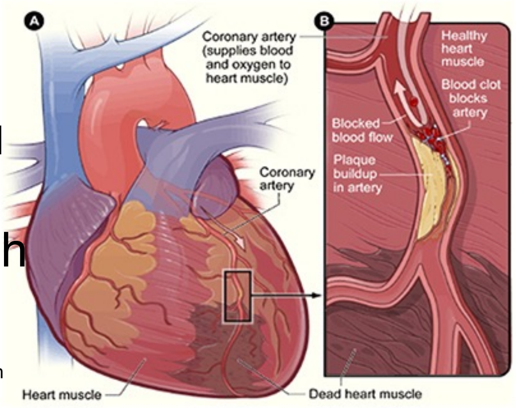
Goal: Fast Prediction of Blood Flow Simulation

■Background and Motivation

- Recently, computational fluid dynamics (CFD) has been used to compute the blood flow and to diagnose the severity of coronary stenosis.
- However, since CFD requires large computational resources, it is indispensable to accelerate the process of CFD analysis.
- In order to solve this problem, we will use deep learning to build a fast surrogate for approximating the large-scale 3D blood flow simulation.

■Challenge

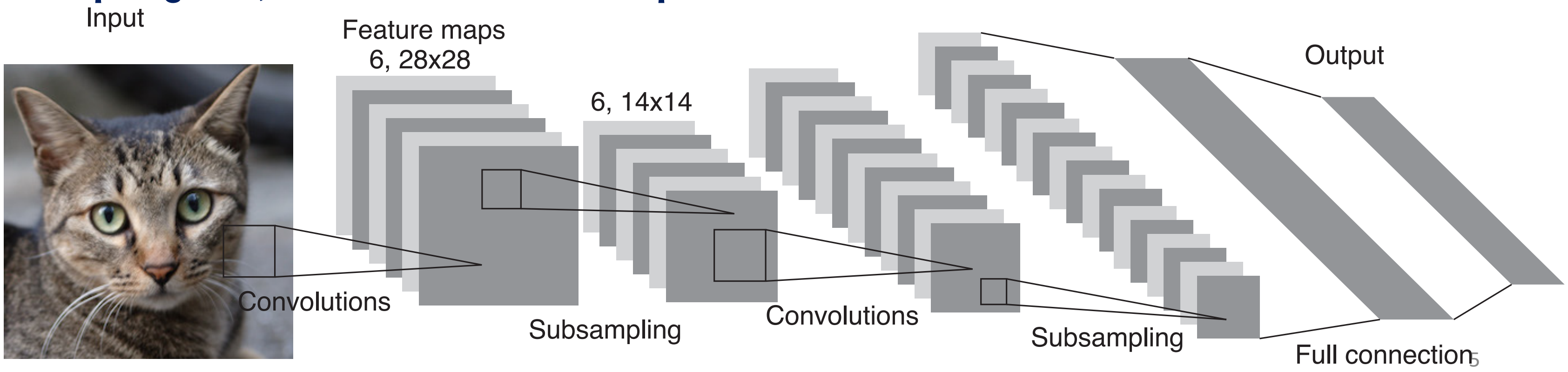
- Developing deep learning surrogate for 2D/3D steady flow
    - Training models on multiple GPUs using PyTorch and Horovod
    - Predicting flow around a complex shape.
- Developing a prediction method using deep learning with boundary exchange for 3D CFD simulation results



Adapted from https://www.drsureshbhagia.com/patient-guide/overview-of-coronary-artery-disease/

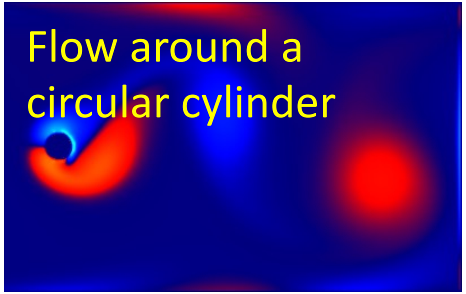
Deep learning / Convolutional Neural Network

- Deep learning is one of methods of machine learning based on neural networks.
- A deep neural network (DNN) is a neural network with multiple layers between the input and output layers.
- A convolutional neural network (CNN) is one of the representative of DNN.
- CNNs are utilized with great success in image recognition, analysis and classification.
- In our project, we use CNNs to predict the CFD simulations results.



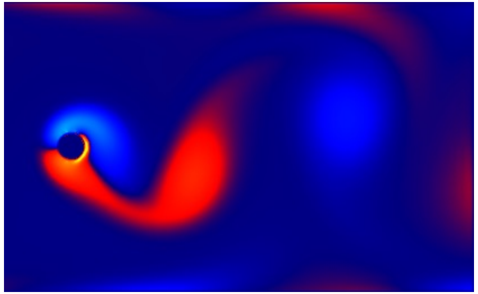
Fast prediction of CFD simulation results by DNN

Dataset



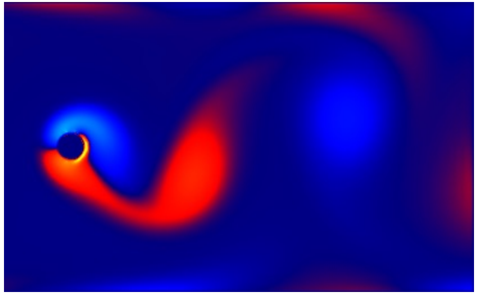
CFD simulation
(Lattice Boltzmann
methods)

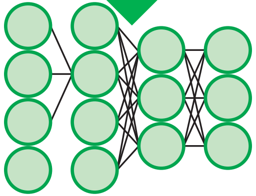
$$f_i(x + c_i \Delta t, t + \Delta t) = f_i(x,t) + \Omega_i(x,t)$$
$$\Omega_i(x,t) = -\frac{1}{\tau}(f_i(x,t) - f_i^{eq}(x,t))$$



Training

Prediction





Prediction of flow

Convolutional neural networks (CNNs) to predict simulation results

CNNs may become "faster simulator"

Datasets

■Steady flow

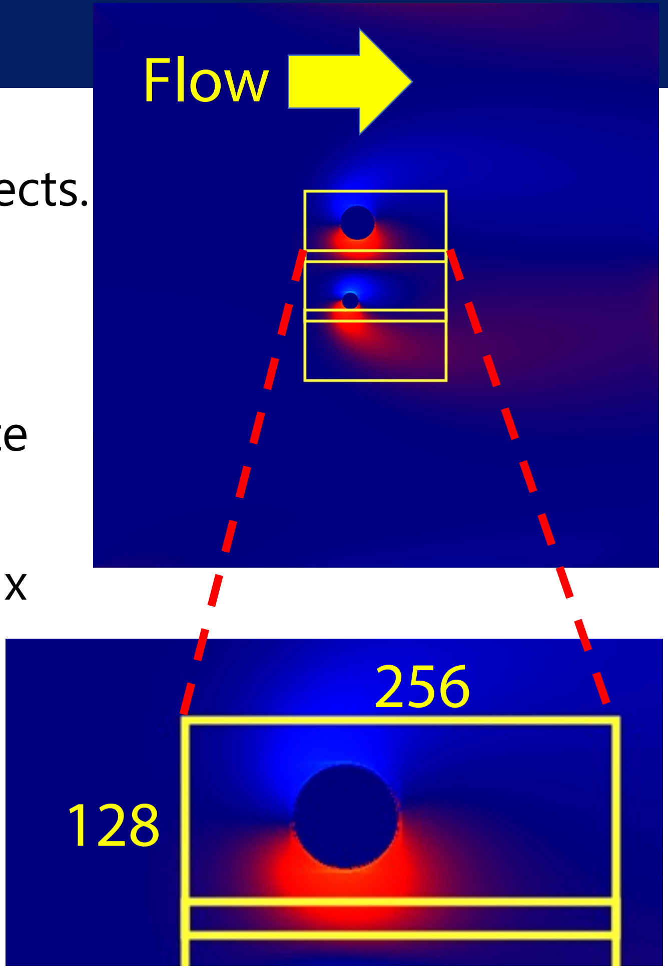
- The fluid flows along the x axis around objects.

■LBM (Lattice Boltzmann method) simulation results

- D2Q9 model (9 variables is used for discrete velocity)
- Re = 20,
- Region size: 256 x 128 (clipped from 1024 x 1024)
- 6 types of object shapes:
  - polygons (number of angles: 3-7)
  - cylinders.

■Input data: 256 x 128 (clipped)

- Training: 14515
- Validation: 1613

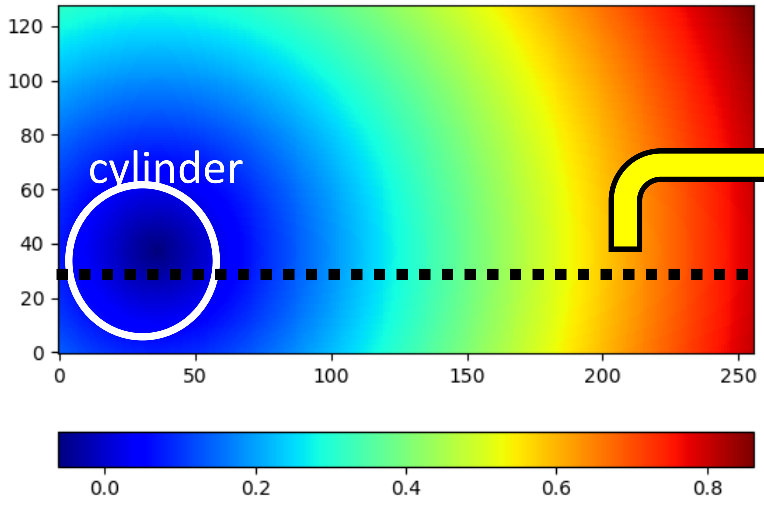


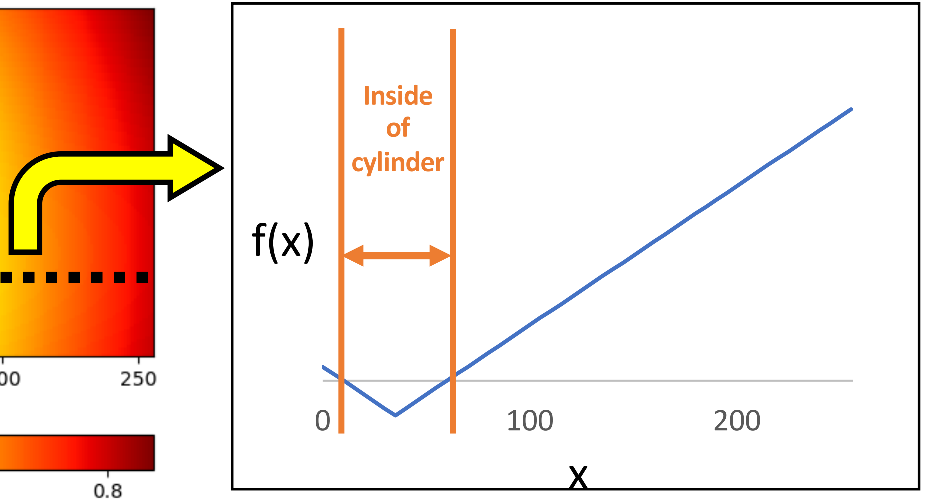
Singed distance function (SDF)

■SDF represents

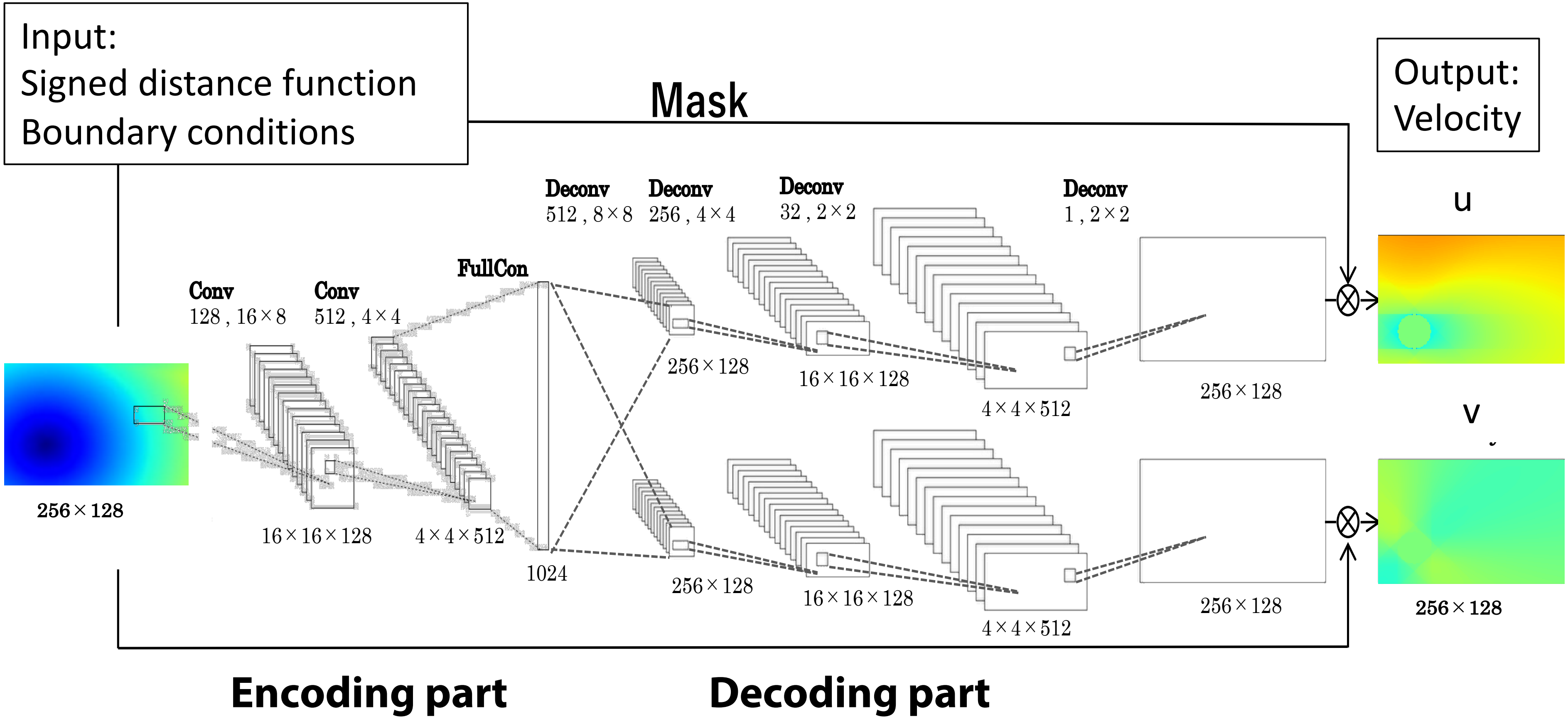
- the surface of the object as zero.
- the outside of the object as a positive distance.
- the inside of the object as a negative distance.

■A universal representation for different geometry shapes and works efficiently with neural networks





Network Architecture and Training

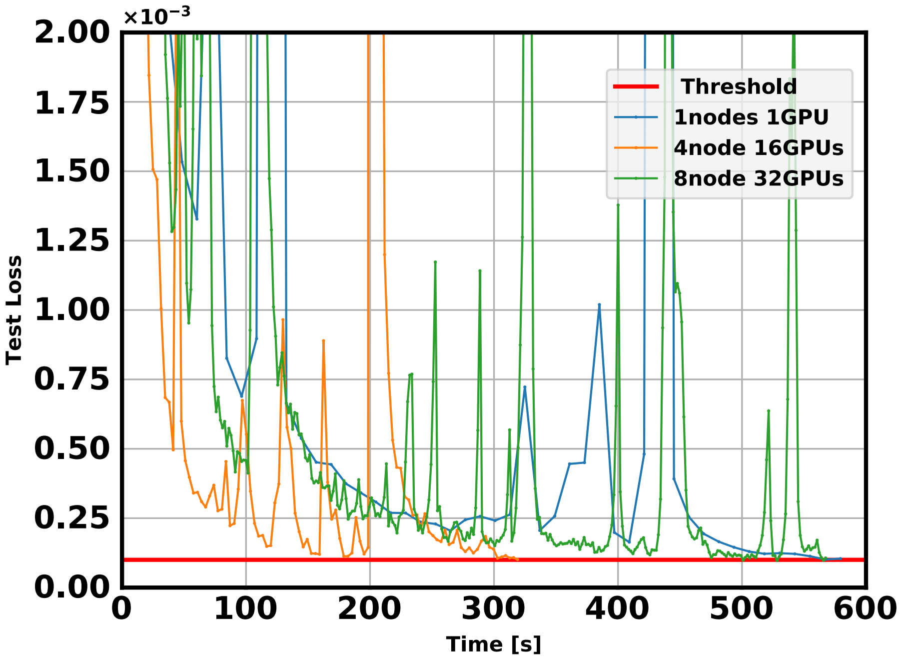


A modified version of the network architecture proposed in Guo et al. "Convolutional Neural Networks for Steady Flow Approximation", 2016

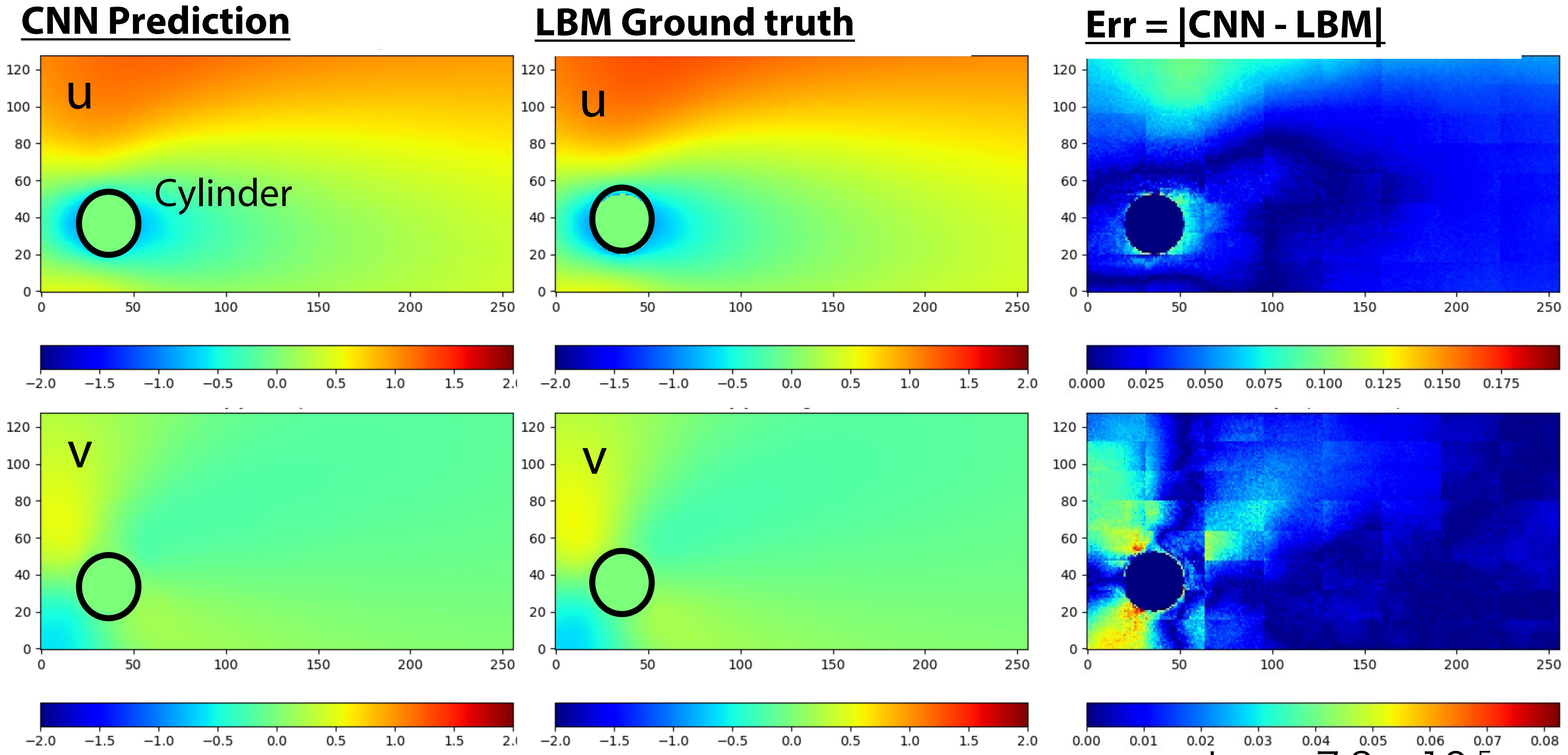
Accelerating training with multiple GPUs

■Implementing models with PyTorch and Horovod

Learning curves using multiple GPUs on Reedbush-L

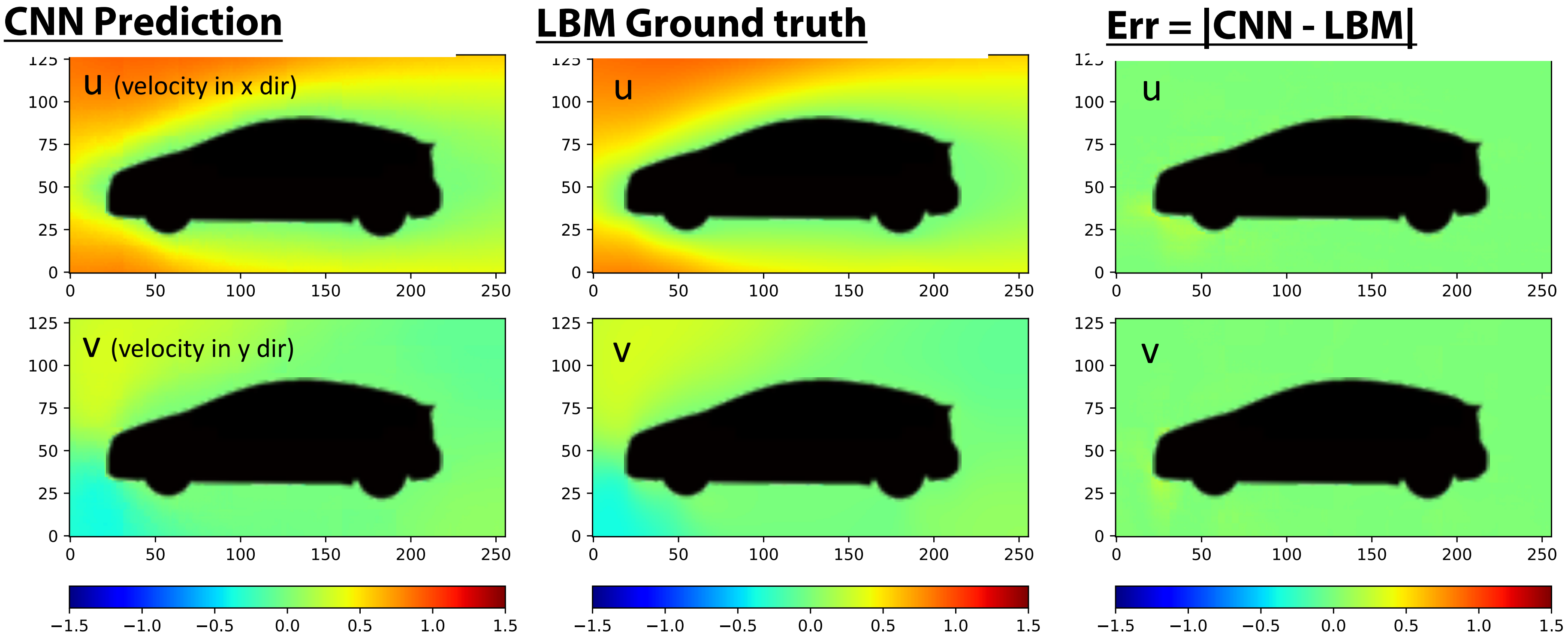


Prediction results for single domain



Loss: 7.3 x 10^{-5}

Prediction results for a complex shape

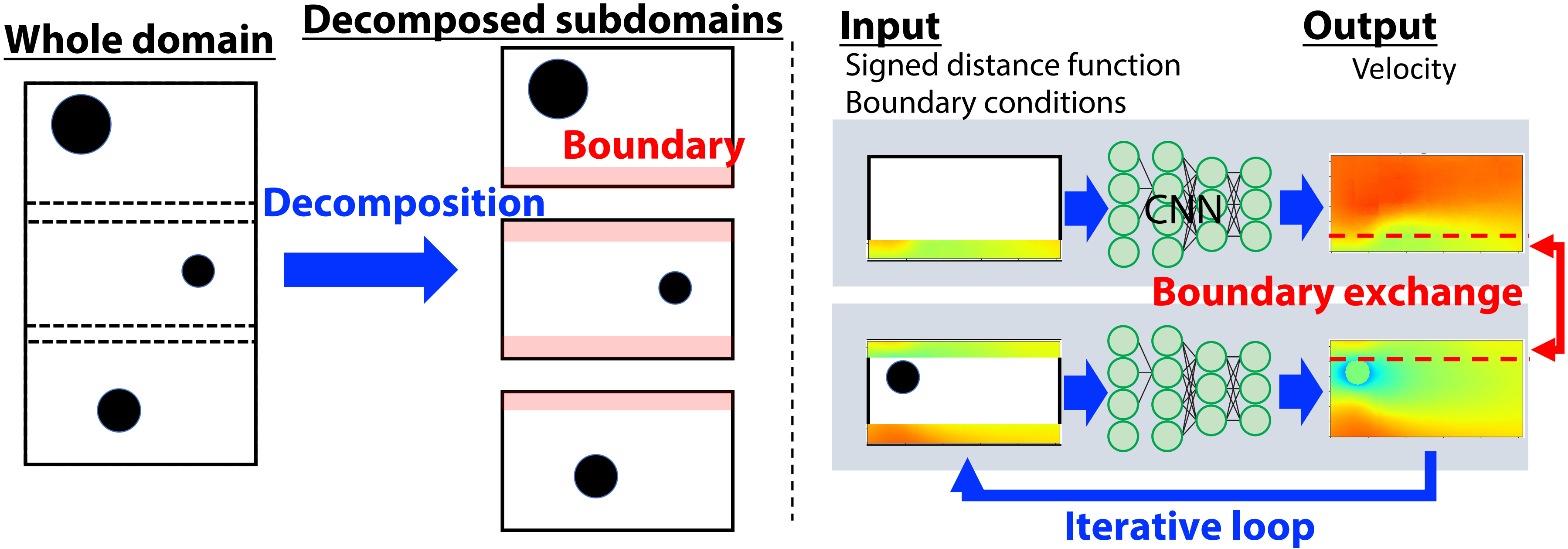


- **Computation time…** LBM (82,000steps) → 41.1 sec 、 CNN prediction → 0.6 sec

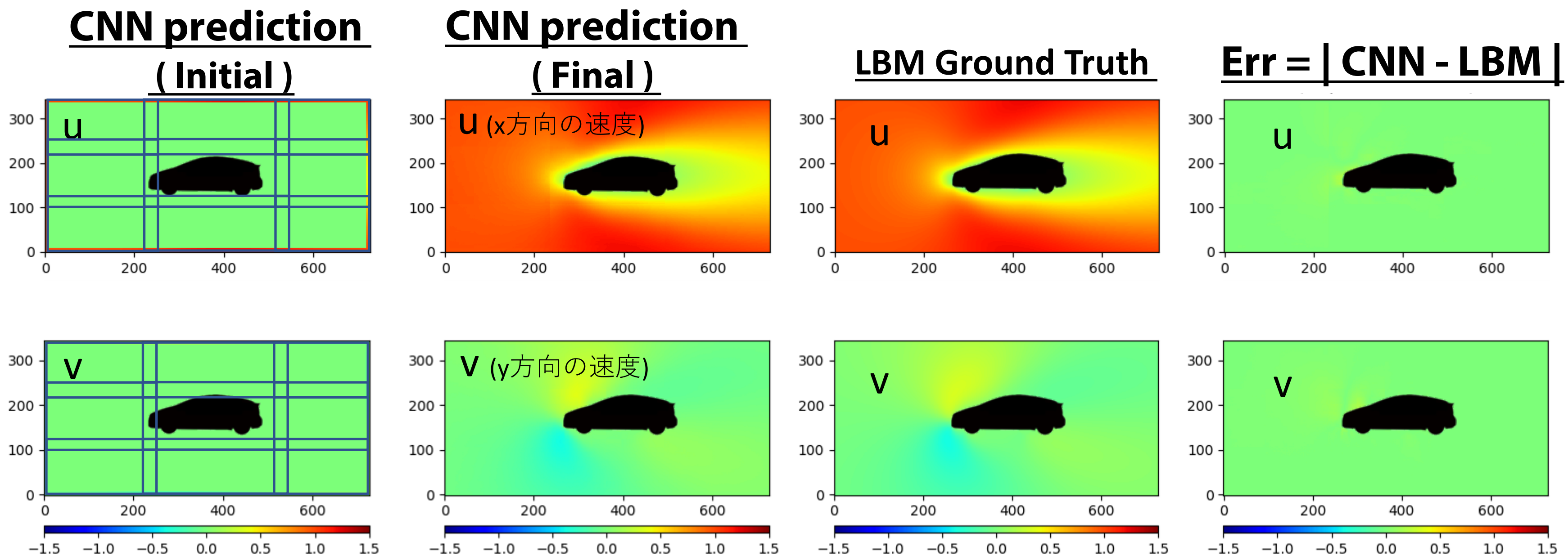
⇒ CNN prediction has achieved high accuracy with significant reduction in calculation time.

Prediction by CNN with boundary exchange

- The network model trained for a single domain is applied to the decomposed subdomains to predict the simulation results in each subdomain.
- In order to maintain consistency between values in the subdomains, boundary exchange between neighbor subdomains is performed.
- CNN and boundary exchange are performed iteratively until values converge.
- This method has no limitation for device (GPU) capacity.

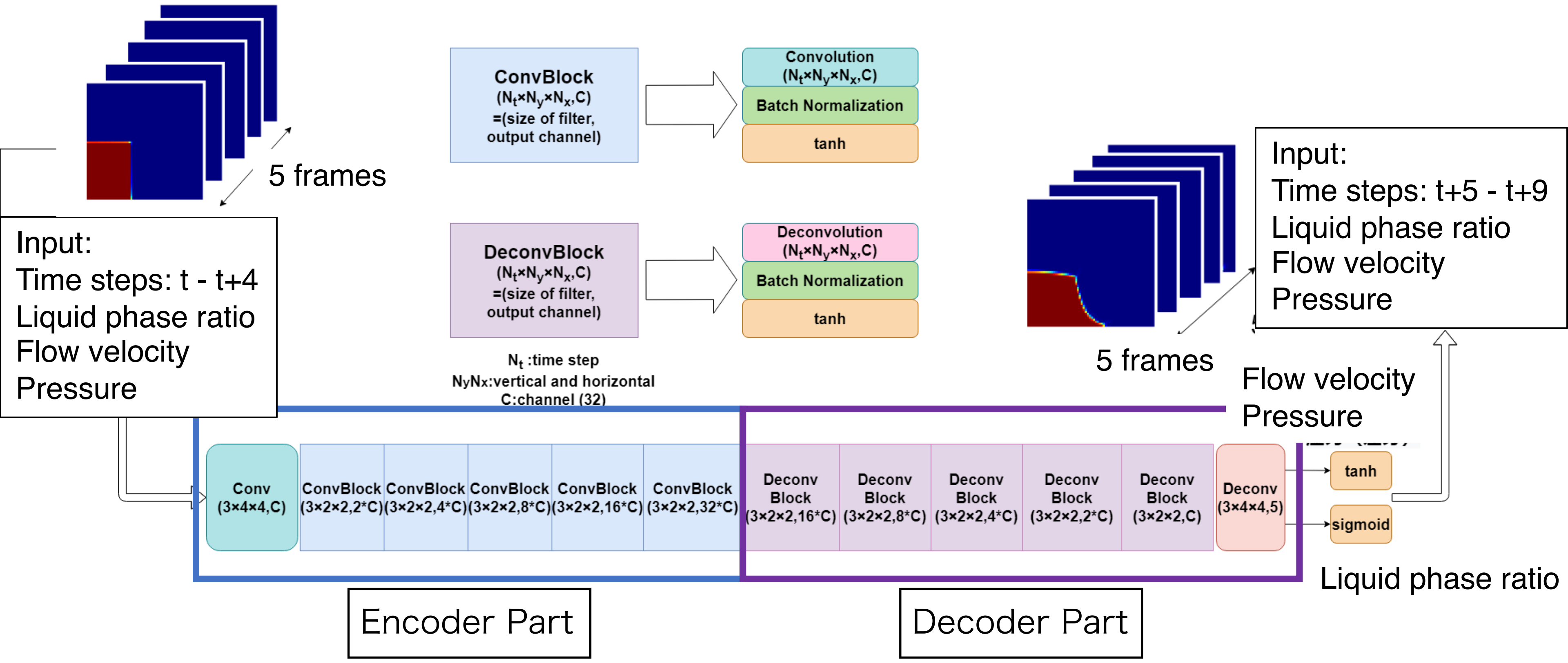


Predicted results using CNN with boundary exchange



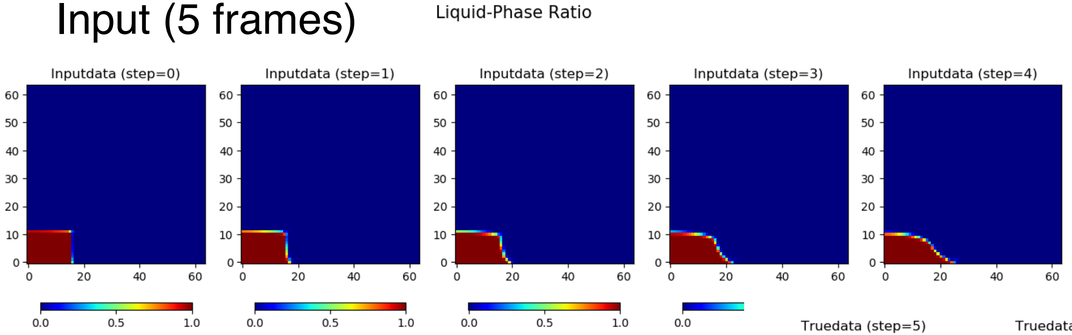
Domain size ：748 x 364 (9 decomposed subdomains)
Mean error ：3.89％
Comp. time ：3.82 s

Future plan: Extending to Time dependent flow



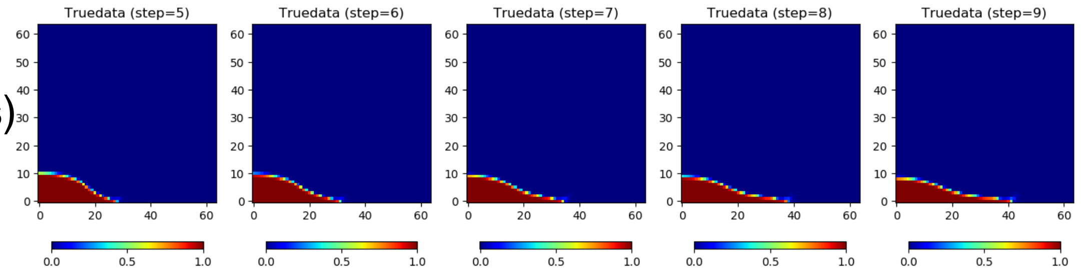
Prediction (Liquid phase ratio)

Input (5 frames)

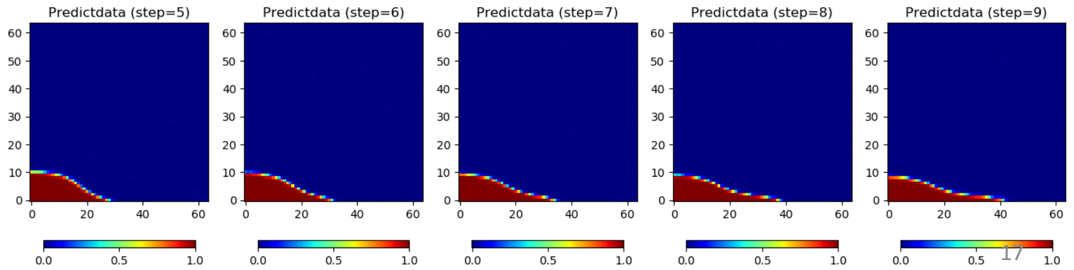


Datasets:
OpenFOAM simulation results (50 cases)

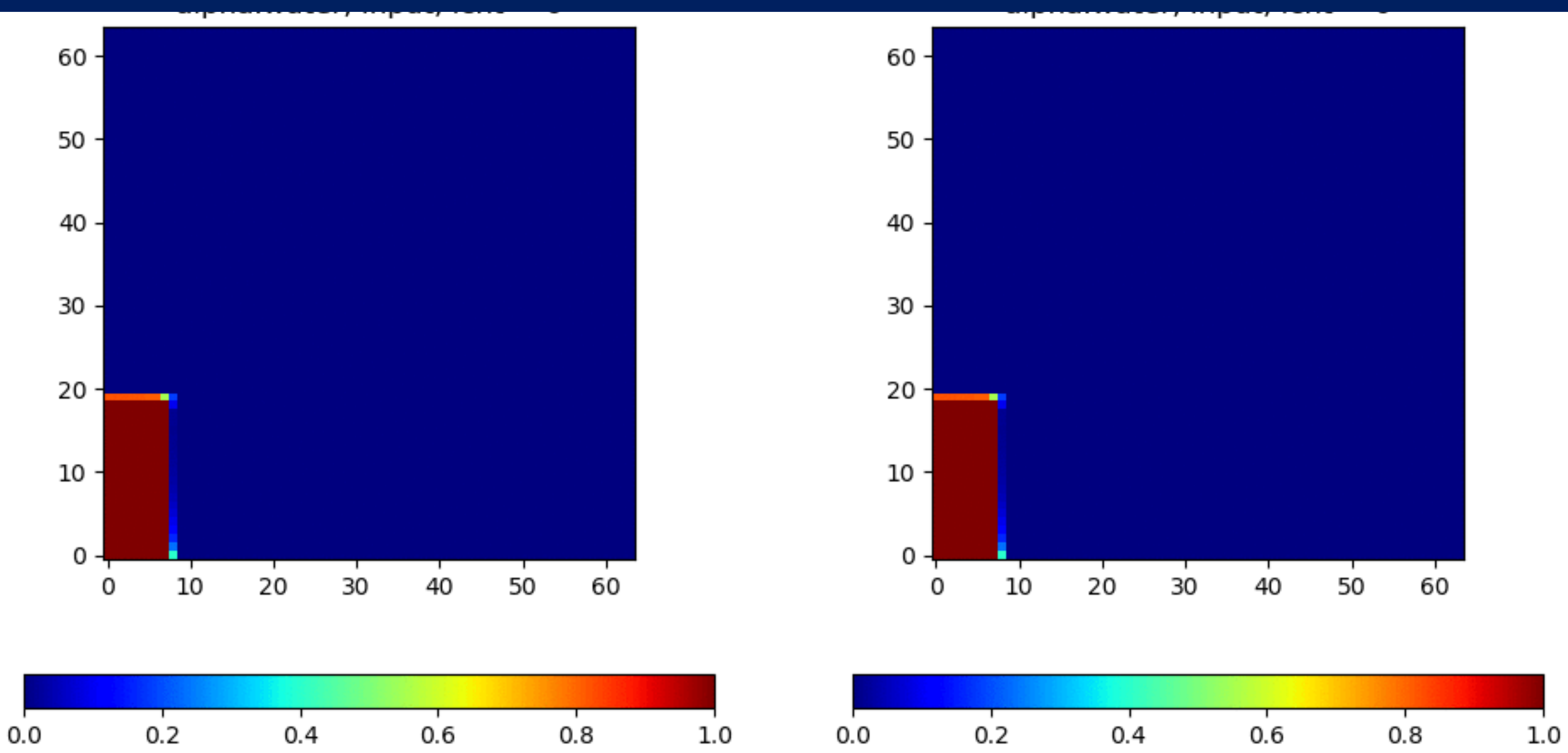
Ground truth (5 frames)



Prediction (5 frames)



Prediction result (Liquid phase ratio)



Ground truth (OpenFOAM) **CNN Prediction**

Conclusion

■Deep learning fast surrogate for steady flow

- Predicting the LBM results by using convolutional neural networks (CNNs).
  - Predicting flow around a complex shape.
- Predicting simulation results on large domain using CNNs with boundary exchange.
  - The proposed method has no limitation for device (GPU) capacity.

■Time dependent flow

- Predicting OpenFOAM simulation results using 3D CNN.

■Future works

- We will improve a prediction method for large-scale computational results.
- We will apply the fast surrogate for steady flow to blood simulations.
- We plan to extend our research to the development of fast prediction methods for time dependent flows.