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Development of Fast Surrogate for Approximating Large-scale 3D Blood Flow Simulation

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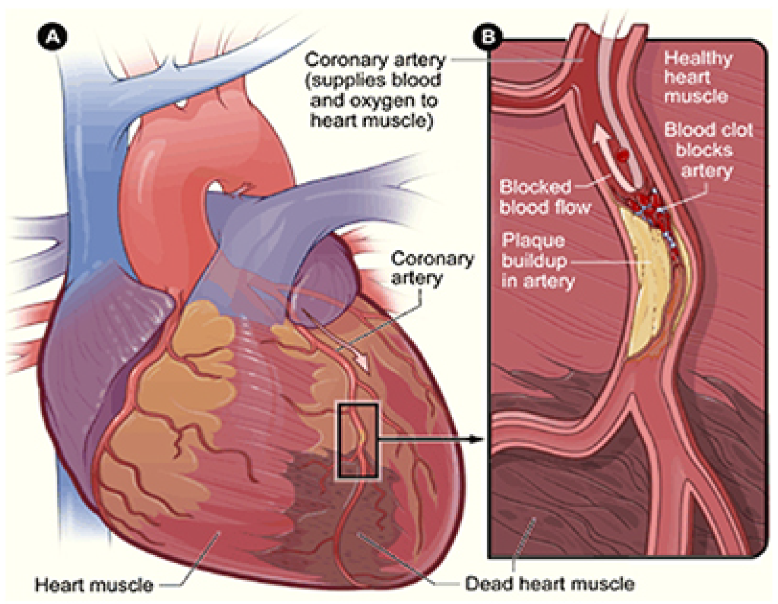
1 Background and Motivation

Coronary heart disease is a leading cause of death worldwide. The main cause of coronary heart disease is coronary stenosis, which is mainly due to atherosclerosis. In the normal situation, coronary arteries supply oxygenated blood to heart muscle. When atherosclerotic plaque appears on the artery wall, the corresponding artery wall becomes narrow. This stenosis reduces the amount of oxygenated blood delivered to heart muscles and thus cause myocardial ischemia. Fractional flow reserve (FFR) is defined as the ratio between distal pressure and proximal pressure and has been used as a standard tool to diagnose the severity of coronary stenosis [1].

Recently, computational fluid dynamics (CFD) has been used to compute the blood flow and FFR for patient-specific artery. In this method, patient specific artery geometries are extracted from medical images and used as wall boundaries in the subsequent simulation. Some clinical trials demonstrated that the method combining CFD and medical image is better than the method using medical image solely in diagnosing ischemic stenosis [1]. However, this method can be computationally demanding because it may take hours to perform CFD simulation [1, 2]. This drawback may limit the usage of this method in clinic practice. Therefore, it is indispensable to accelerate the process of CFD analysis.

In this study, we will use deep learning to build a fast surrogate for approximating the 3D blood flow simulation. We will also develop a parallelization method to make it possible to apply the deep learning to large scale geometry, which can contribute to realizing large-scale 3D blood flow simulation.

In this current year, we will develop a prediction method for large-scale computational results in 3D by combining a deep learning-based inference method for single-domain computational results with boundary exchange, which can contribute to realizing prediction of the large-scale 3D blood flow simulation. We will improve our in-house CFD solver, which is used to generate the training dataset, to be able to handle complex geometry. We will show that the proposed prediction method is effective for predicting the flow around complex geometry. Finally, we will apply the method to the prediction of flow in blood vessels.



Coronary Artery Disease

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

[1] Zhang J-M, Zhong L, Luo T, Lomarda AM, Huo Y, Yap J, et al. (2016) Simplified Models of Non-Invasive Fractional Flow Reserve Based on CT Images. PLoS ONE 11(5): e0153070.

[2] Itu, L., Rapaka, S., Passerini, T., Georgescu, B., Schwemmer, C., Schoebinger, M., . . . Comaniciu, D. (2016). A machine-learning ap-proach for computation of fractional flow reserve from coronary computed tomography. Journal of Applied Physiology,121(1), 42-52

2 Research plan

(1) Improving the prediction method for results of large-scale 3D simulation

In the previous year, we have developed a method for predicting the results of 2D computations over multiple domains, which is based on deep learning inference with boundary exchange. We have also developed a method for predicting the results of 3D computations for a single domain by deep learning. This year, we will integrate these two methods to develop a method for predicting 3D computational results over multiple domains. As our research progressed, unlike the 2D case, it was found that in 3D it is difficult to predict the flow velocity over the entire area of multiple domains from only the geometry and the velocity at the boundaries. To solve this problem, further development is needed. For example, we are considering a method that uses low-resolution predictions to guide inference. In addition, we plan to use fast storage to speed up data access and accelerate the DNN training for the 3D case. We will use RB-H/L, Wisteria to train DNN models.

(2) Development of lattice Boltzmann method (LBM) code for handling complex geometry

From the point of view of efficiently generating the expected training data, we have found it desirable to use our in-house GPU-based code for CFD simulations. For this reason, we plan to continue to improve and utilize our LBM code for this study. In the current year, we will improve this code to be able to handle complex geometry with multiple GPUs for efficient generation of training data. If necessary, we will introduce the adaptive mesh refinement (AMR) method, which is capable of localized high-resolution computation, in order to generate high-resolution training data. We will use GPUs on RB-H/L, Wisteria for developing the LBM code.

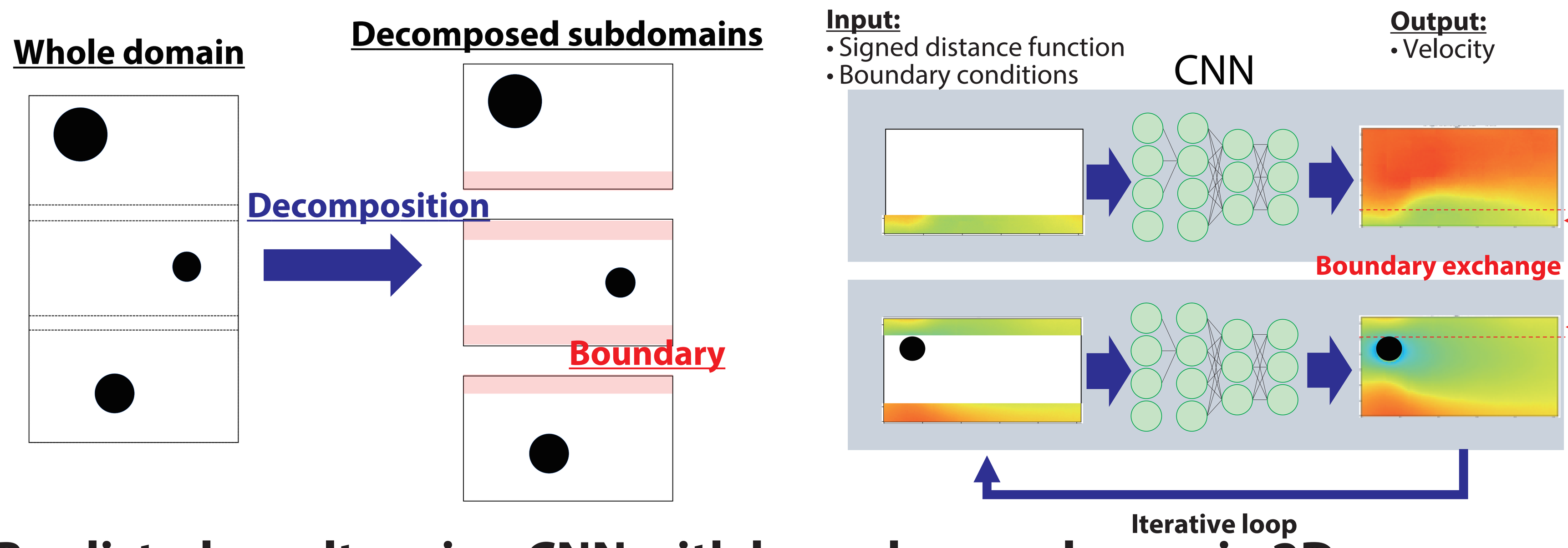
(3) Applying the proposed method to 3D flow around complex geometry and blood flow simulation

After the proposed method becomes able to predict various simulation results, we will train the DNN models using the LBM simulation results with the simplified geometry for blood vessels and verify that the proposed method can predict these results. We will then attempt to predict the blood flow simulation by the proposed method using the real geometry models with/without patient-specific physiological information. We will use Wisteria and OFP for the generation of the data sets and training the models.

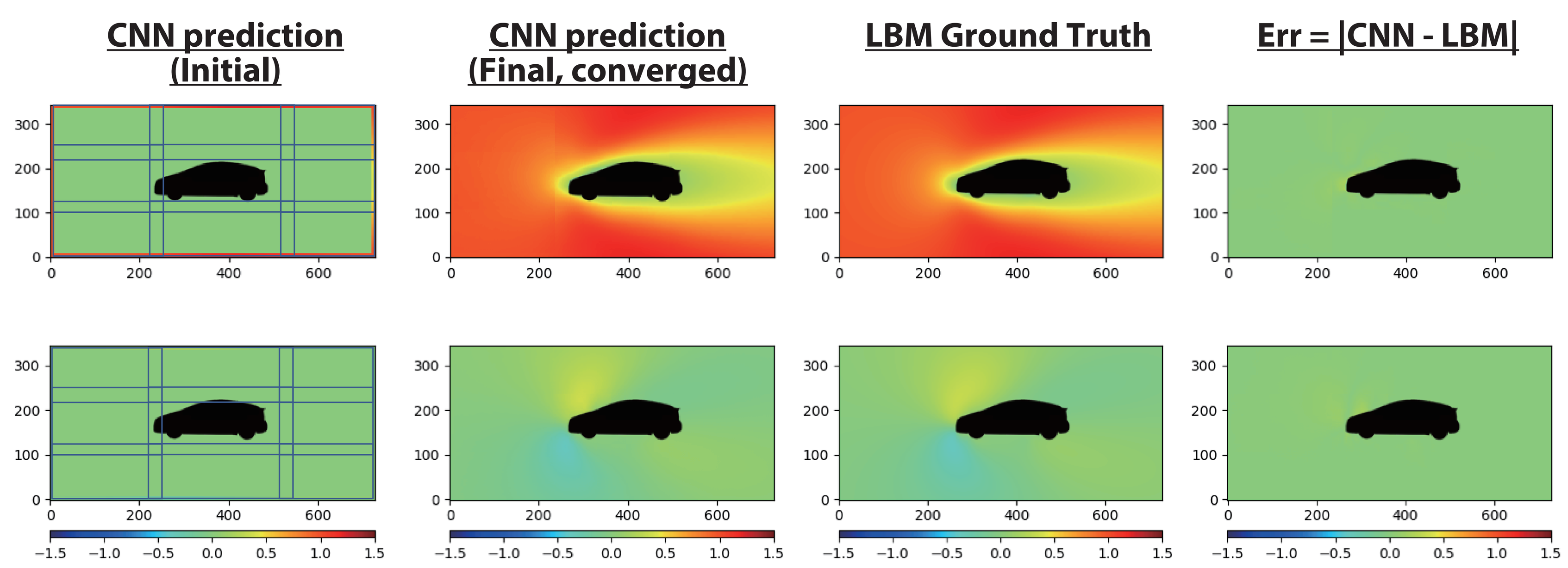
3 Prediction for large-scale simulation

Predicting simulation results 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, which is one of the DNN models, and boundary exchange are performed iteratively until values converge.
- This method has no limitation for device (GPU) capacity.

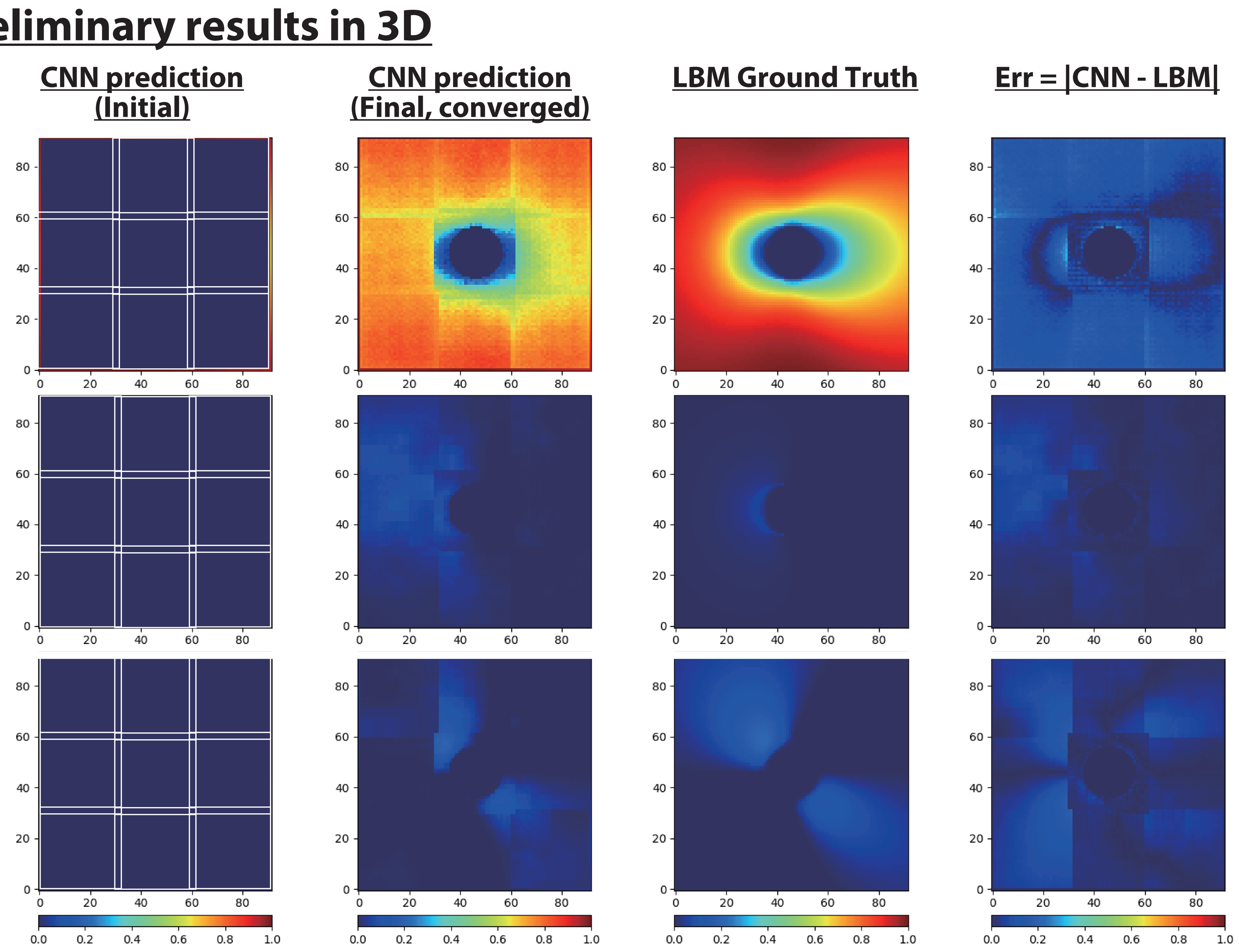


Predicted results using CNN with boundary exchange in 2D



- Domain size: 748 x 364 (9 decomposed subdomains)
- LBM simulations: D2Q9, Re =20, 6 types of object shapes.
- Training: 14515, Validation: 1613 (size: 256 x 128)

Preliminary results in 3D



- Cross section at y = 40
- Domain size: 87^3
- Training: 3110, Validation: 346 (size: 32^3)

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