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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 perform 3D blood flow simulations using OpenFOAM and lattice Boltzmann method (LBM) to generate data sets. We will build the prediction method for large-scale 3D results, which is based on a prototype of a prediction method developed in our previous research project.

predict the blood flow simulation by the proposed method using data sets generated by LBM and/or OpenFOAM. We will use Reedbush-L and Oakforst-PACS for the training and prediction. We will use Oakbridge-CX to perform OpenFOAM.

(4) Preliminary study of prediction methods for time evolution calculation

In order to obtain more accurate results, it is necessary to consider the time-dependent flow in the blood flow simulation. We will attempt to expand the proposed method to predict statistics of flow such as mean and variance of flow velocity. We will use Reedbush-H/L for this study.

3 Prediction for large-scale simulation



Coronary Artery Disease

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

Predicting simulation results in multiple domains

We have developed a method to predict the simulation results in large computational domains in 2D. This method combines neural network inference and 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. Convolutional neural network (CNN) and boundary exchange are performed iteratively until values converge.

Prediction method using CNN with boundary exchange



[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

<u>2 Research plan</u>

(1) Developing blood flow simulation based on lattice Boltzmann method (LBM)

As the study progressed, it was found that LBM may yield faster and more accurate results than OpenFOAM for blood flow simulations used as training data. In addition, since LBM uses structure grids, it is more suitable for deep learning. Then, in this current year, we attempt to extend our own LBM code to simulate blood flow. If LBM does not work for this purpose, we will use OpenFOAM as originally planned. We will use the following data sets for training: geometry models without patient-specific physi-ological information ("https://simtk.org/projects/cv-gmodels/", "http://simvascular.github.io/clinicalCase3.html"), and geometry models with patient-specific physiologi-cal information ("http://www.vascularmodel.com/sandbox/doku.php?id=repository" .) We will use Reed-bush-H/L to develop LBM-based simulation codes. (2) Improving the prediction method for results of large-scale simulation We have developed a prototype of prediction method for results of large-scale simulation by using deep learning inference and boundary exchange in the previous year. Since the proposed method currently only supports 2D computations with specific physical conditions, we will expand this method to 3D computations with various physical conditions. We will replace Chainer with PyTorch as the deep learning framework to use since development of Chainer has been discontinued. We will use Reedbush-H/L and Oakforst-PACS to train our neural network models.

(3) Applying the proposed method to 3D blood flow simulation generated by LBM/OpenFOAM

After the proposed method becomes able to predict various simulation results, we will verify that the proposed method can predict simulation results using simplified geometry for blood vessels. We will then attempt to

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