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

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Abstract 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. Recently, computational fluid dynamics (CFD) has been used to compute the blood flow for patient-specific artery with medical images in diagnosing ischemic stenosis. However, CFD simulation requires a lot of computational resources and time. Therefore, in order to use CFD in clinical practice, it is essential to accelerate CFD analysis. In this project, we will use geometric 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. In this year, we have developed the method that combines neural network inference and boundary exchange to predict the simulation results in large computational domains. It exploits neural network to predict the simulation results of each subdomain and exchanges boundary between neighbor subdomains to maintain consistency in them. This method allows us to apply the same neural network architecture to any size of input data.

1. Basic Information

(1) Collaborating JHPCN Centers

The University of Tokyo

(2) Research Areas

- ■ Very large-scale numerical computation
- ■ Very large-scale data processing
- □ Very large capacity network technology
- □ Very large-scale information systems

(3) Roles of Project Members

- Takashi Shimokawabe (The University of Tokyo): Development of a method for predicting large-scale simulation results
- Weichung Wang (National Taiwan University): Development of deep learning, surrogate modelling and algorithm designs
- Naoyuki Onodera (Japan Atomic Energy Agency): Advice and support to apply deep learning to CFD simulations
- Kengo Nakajima (The University of Tokyo): Advice and support for large-scale computations
- Toshihiro Hanawa (The University of Tokyo): Advice and support for large-scale deep learning
- Masashi Imano (The University of Tokyo): Advice and support for using OpenFOAM
- Shlok Mohta (The University of Tokyo): Development of a surrogate for predicting large-scale CFD simulation
- Sora Hatayama (The University of Tokyo): Development of a method for predicting large-scale simulation results
- Atsushi Hasegawa (The University of Tokyo): Development of a surrogate for predicting large-scale CFD simulation
- Cheng-Ying Chou (National Taiwan Normal University): Advice and support of CFD and medical imaging
- Che-Yu Hsu (National Taiwan University Hospital): Advice and support of medical backgrounds and knowledge
- Yikai Kan (National Taiwan University): Development of CFD simulations and deep learning
- Mei-Heng Yueh (National Taiwan Normal University): Development of

computational geometry

- Wanyun Yang (National Taiwan University): Development of CFD simulations and deep learning
- Yuehchou Lee (National Taiwan University): Development of CFD simulations and deep learning

2. Purpose and Significance of Research

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. 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. Recently, computational fluid dynamics (CFD) has been used to compute the blood flow and FFR for patient-specific artery. 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. However, this method can be computationally demanding because it may take hours to perform CFD simulation. 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 geometric 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. This method divides the large-scale geometry into multiple parts and applies deep learning in parallel to them. This makes it possible to approximate a large-scale 3D blood flow simulation.

3. Significance as JHPCN Joint Research Project

In this project, we are developing a fast surrogate that approximates 3D blood flow simulation using geometric deep learning and a parallelization method of the surrogate for applications with large-scale geometry. Since we perform a large number of CFD simulation to generate training data sets and train neural networks with these data sets to build the surrogate, a lot of computational resources are indispensable to realize this project. We uses a lattice Boltzmann method (LBM) code and OpenFOAM mainly as CFD solvers. Since LBM can achieve high performance on GPUs, we have exploited Reedbush-L at the University of Tokyo to generate the training data sets. We have also utilized Oakforst-PACS to generate the training data sets withy OpenFOAM. We have utilized both Oakforst-PACS and Reedbush-L for training deep neural networks, since the deep learning frameworks achieve high performance with Xeon Phi and GPUs, which are installed on Oakforst-PACS and Reedbush-L, respectively. This project is being carried out by collaborative research by blood flow experts, CFD experts, the experts of large-scale deep learning, and high-performance computing experts. Therefore, implemented as a JHPCN joint research project, this project has been able to effectively carry out collaborative research and achieve research results.

4. Outline of Research Achievements up to FY2018

Not applicable.

5. Details of FY2019 Research Achievements

The purpose of this study is to develop an a fast surrogate model that predicts steady flow simulation of blood flow using deep learning. In this fiscal year, we have developed (1) a prediction method for steady flow simulation using deep learning, and (2) a prediction method for large-scale simulation results by extending the (1) method. The original plan was to develop the prediction of the blood flow simulation using OpenFOAM. However, it was found that the lattice Boltzmann method (LBM) may be more effective in simulating blood flow simulations. In this fiscal year, the steady flow simulations for (1) and (2) were carried out with the LBM, and we focused on developing methods to predict these simulations.

5.1. Steady flow simulation using lattice Boltzmann method

The lattice Boltzmann method (LBM), which has attracted much attention in recent years, is used for efficient execution of large-scale simulations. In this study, we use the simulation results of steady flows with this method as training dataset to train a deep learning model and create a fast surrogate model. In the prediction of the steady-state flow around objects by deep learning, it is known that the signed distance function (SDF), which represents the distance to the geometry, is effective in improving the prediction accuracy. SDF is used for the LBM simulation and is utilized as inputs for prediction by deep learning models. Figure 1 shows an example of a signed distance function.

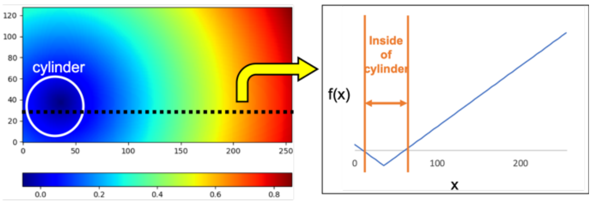

Figure1: SDF representation of a cylinder shape.

5.2. Prediction method for the simulation results of LBM using convolutional neural networks

In this section, we describe a method for predicting the LBM results by using convolutional neural networks (CNNs) for a certain region size. CNNs are neural networks containing convolutional layers and have been shown to be effective in the fields of geometric representation learning and image recognition. This method predicts the simulation results of the steady flow around a cylindrical or polygonal shape placed at an arbitrary location. The computational domain is 256×128, and the fluid flows from negative to positive in the x direction.

5.2.1. Network model

Figure 2 shows the structure of the neural network used in this method. In this method, the object shape by SDF and the flow velocity in the boundary region (boundary condition) are given as inputs to the neural network, and the prediction of the velocity obtained by the LBM simulation over the entire computational domain is obtained as outputs. The first part of the network is a common network in the x and y directions before a fully

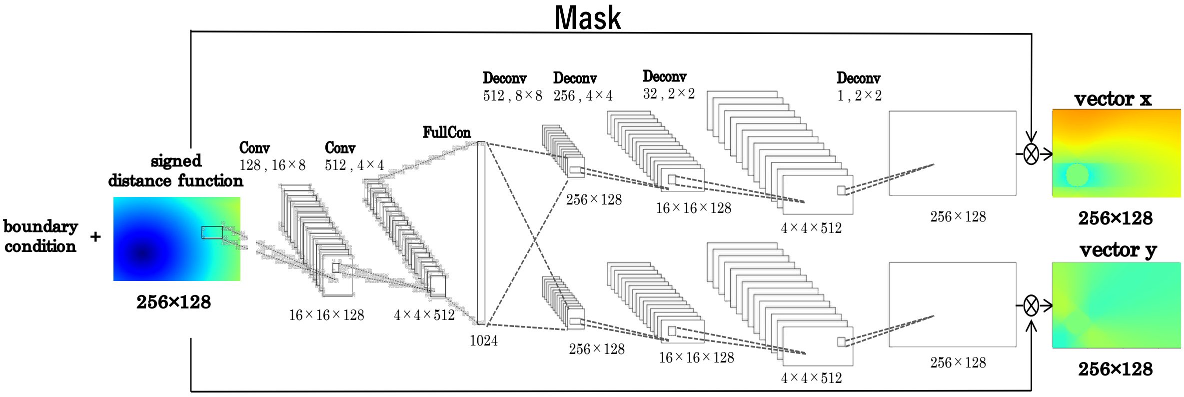

Figure2: Network architecture for 2D geometry.

connected layer, while the second part of the network is different in each direction. In addition, the existence of the geometrical shape at each grid point is obtained from the input SDF and applied to the CNN predictions as masks. As a result, only the predicted velocity in the fluid region where no object exists is considered as the final predicted velocity. The width of the boundary region used as a boundary condition is set to 1. The network used in this method is based on the one proposed by Guo, Li, and Iorio et al. In this study, the boundary conditions of the calculation region are used as input in addition to SDF in order to predict the steady flow over multiple regions using this network, while only SDF is used as input in the previous study.

In this study, Chainer is used as a deep learning framework. ReLU is used for the activation function, Xavier is used for initialization, and Adam is used for optimization. The learning rate is set to 1.0×10^{-4}.

5.2.2. Dataset

We explain the data set of the neural network used in our method.

First, we place one or two cylinders or polygons in a 1024 × 1024 computational domain and simulate a fluid with a Reynolds number of 20 flowing from negative to positive in the x direction by LBM. The number, type, size, and position of the cylinders or polygons to be placed are changed to perform several steady flow simulations. We use a total of six types of object shapes: polygons (number of angles: 3-7) and cylinders. 32 objects with different sizes are used for each type. For the placement of object shapes in the region, two patterns are prepared: one in which one type of object shape is placed and another in which two randomly selected object shapes are placed. We include the simulation results in which the two objects affect the flow together in the dataset.

Next, 21 computational domains of 256 × 128 are cut out from the LBM simulation results in each 1024 × 1024 domain. The areas to be cut out should not overlap each other. In order to use SDF as the input, we also prepare the SDF data corresponding to each 256 × 128 computational domain.

We thus prepare a total of 4,704 combinations of the LBM calculation results and SDF for the 256 × 128 domains, 3,528 for training and 1,176 for evaluation.

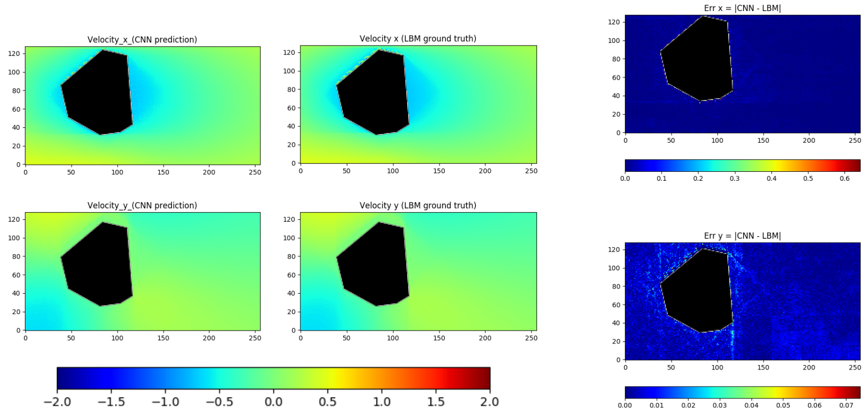

Figure 3: Prediction results of a single domain. The CNN predictions, the LBM ground truth, and the error between the prediction and the ground truth are shown.

5.2.3. Predicted result

Figure 3 shows the results of the prediction using our trained model. It can be seen that the proposed method is highly accurate. Using a single NVIDIA GPU (Tesla P100) on Reedbush supercomputer on the University of Tokyo, it takes 13.8 seconds (30,000 time steps) to reach the steady state using the LBM simulation code. On the other hand, the proposed method using CNN requires 0.006 seconds on one GPU. The proposed method can reduce the calculation time by 99%.

5.3. Expanding the prediction region by using boundary exchange

The method of predicting LBM simulation results using CNN described in Section 5.2 can only predict the results in the domain size of the data used in the training dataset. Therefore, in this study, we propose an extension of this method to be used for predicting computational results over a larger domain than the domain size of the data used in the training dataset. This proposed method allows us to apply the same neural network architecture to any size of input data.

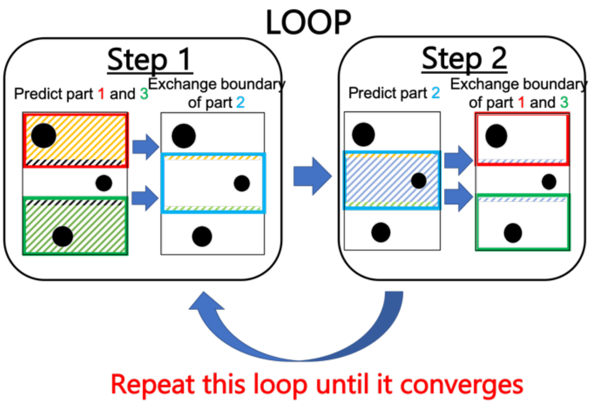

Figure 4: Prediction procedure using an iterative loop with boundary exchange.

5.3.1. Proposed prediction method

Figure 4 shows the prediction procedure of the LBM simulation results in this method. In this method, the entire prediction region is divided into 256 × 128 subregions and the simulation results in each subregion are predicted using the method described in Section 5.2. The boundary regions of the neighboring subregions are overlapped. After the prediction is completed once, the prediction value of the boundary region is obtained from the adjacent subregions, and the prediction is performed again by using this as the input. By repeating this process with

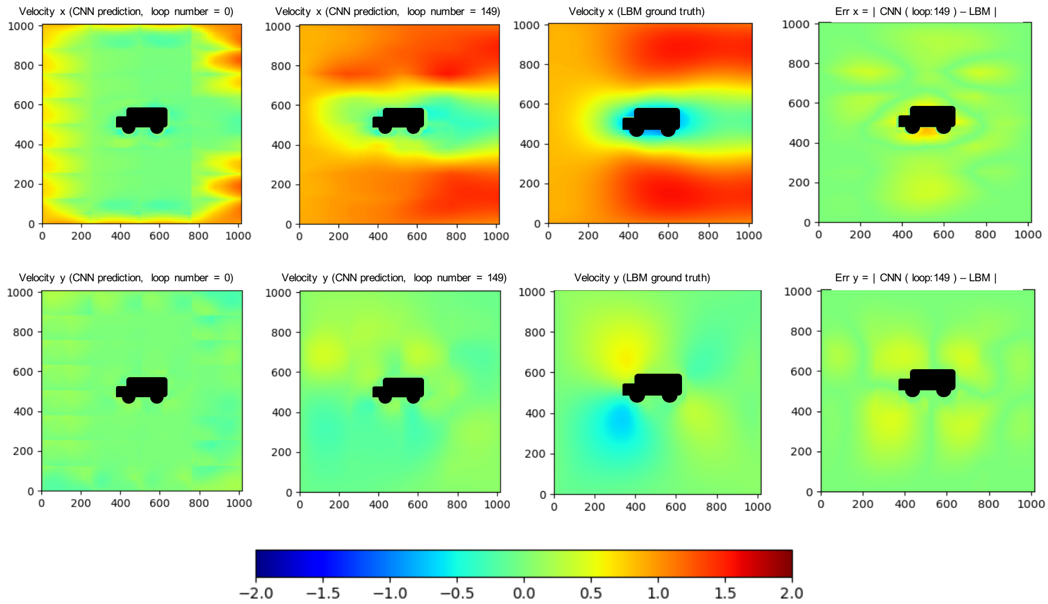

Figure 5: Prediction results over a large computational domain consisting of several subregions. The CNN predictions (initial and final values), the LBM ground truth, and the error between the prediction and the ground truth are shown.

an iterative loop, the values of the boundaries of subregions become continuous. The prediction result for the entire region is obtained. This method can be applied to any shapes of objects in the prediction region. The training data of the model for predicting subregions also includes a pattern in which an object is divided at the boundary of the subregion. Thus, the prediction can be made even for computational regions where there is an object in the boundary of the subregion. Note that although Figure 4 shows an example of three divisions in the y direction for simplicity, the number of divisions can be specified arbitrarily for both the x and y directions.

5.3.2. Predicted results

Figure 5 shows the predicted results when an object with a shape similar to a car is placed in a region of 1021 × 1017 and a fluid with a Reynolds number of 20 flows in the x positive direction. This figure shows the predictions of flow velocity in the x and y directions using this method, the ground truth of the velocity obtained by the LBM simulation, and the error between the predictions and the LBM ground truth. The prediction results show the initial and final value of the iterative loop. In this case, the final loop number is 149. The boundary width is set to 1. In the prediction in this figure, the entire prediction region is divided into a total of 32 subregions, 4 in the x direction and 8 in the y direction. It can be seen that the values of the predicted velocity are discontinuous between subregions at the initial state of the iterative loop but continuous at the final state for both the x and y directions. Although the errors are reduced by the iterative loops, the errors in the final state are still relatively large in the neighborhood of the object and at the boundaries between subregions.

6. Progress during FY2019 and Future Prospects

In this research project, 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. It exploits neural network to predict the simulation results of each subregion and exchanges boundary between neighbor subregions to maintain consistency in them. In order to apply this method to blood flow simulations, we are currently extending this method to 3D simulations.

The research plan for the next year is described below. 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 the next 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.

Since our 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. After the proposed method becomes able to predict various simulation results in 3D, we will verify that the proposed method can predict simulation results using simplified geometry for blood vessels. We will then attempt to predict the complex blood flow simulation by the proposed method using data sets generated by LBM and/or OpenFOAM.

7. List of Publications and Presentations

(1) Journal Papers (Refereed)

None.

(2) Proceedings of International Conferences (Refereed)

None.

(3) International conference Papers (Non-refereed)

[1] Takashi Shimokawabe, Naoyuki Onodera, Kengo Nakajima, Toshihiro Hanawa, Shlok Mohta and Weichung Wang, "Fast Surrogate for Approximating Large-scale CFD Simulations," the Asian Pacific Congress on Computational Mechanics (APCOM) 2019, Taipei, Dec. 2019.

[2] Sora Hatayama and Takashi Shimokawabe, "Steady Flow Prediction using Convolutional Neural Networks with Boundary Exchange," International Conference on High Performance Computing in Asia-Pacific Region (HPCAsia) 2020, Fukuoka, Japan, January, 2020. (poster)

(4) Presentations at domestic conference (Non-refereed)

[3] Shlok Mohta, Kengo Nakajima, and Takashi Shimokawabe, "Recurrent Neural Network based linear embeddings for non-linear dynamics evolution," 2019 年並列/分散/協調処理に関する『北見』 サマー・ワークショップ (SWoPP2019), 北見, 2019 年 7 月.

(5) Other (patents, press releases, books and so on)

None.