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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 deep learning to build a fast surrogate for approximating the 3D blood flow simulation. In this year, we have developed the method that combines neural network inference and boundary exchange to predict the 3D simulation results in large computational domains. This method allows us to apply the same neural network architecture to any size of 3D 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 for large-scale deep learning
- Masashi Imano (The University of Tokyo): Advice and support for using OpenFOAM
- Hayato Shiba (The University of Tokyo): Advice and support of CFD and medical simulations
- Hiromichi Nagao (The University of Tokyo): Advice on machine learning methods
- Hiroya Matsuba (The University of Tokyo): Advice on machine learning execution environment
- 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
- Shota Suzuki (The University of Tokyo): Development of CFD simulations
- 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 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 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 FY2019

In our previous research, 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 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. We performed steady-state flow simulations with objects of simple shapes by using the lattice Boltzmann method (LBM). Using these results as training data sets, we trained the our neural networks. By using these networks with boundary exchange, our proposed method successfully predicted the results of a large-scale 2D steady flow.

5 Details of FY2020 Research Achievements

In this year, we improved the prediction method for 2D large-scale steady flow simulations. In the last year, we used Chainer as a deep learning framework to construct a convolutional neural network (CNN) model. However, since the development of Chainer was discontinued, we replaced it with PyTorch. We have trained this model on a single GPU and have also successfully trained it on multiple GPUs using Horovod. We have also developed a method for predicting 3D simulation results by extending the prediction method for 2D. We have also improved our LBM simulation code to enable the computation of flow around objects in order to exploit this code for the blood flow simulation.

5.1 Overview and update of the CNN prediction method for 2D simulations

In this section, we describe the overview and update of the proposed prediction method for 2D simulation results. In this year, all the network models developed last year using Chainer are implemented again using PyTorch.

The 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 the structure of the neural network used in this prediction method for 2D. 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 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

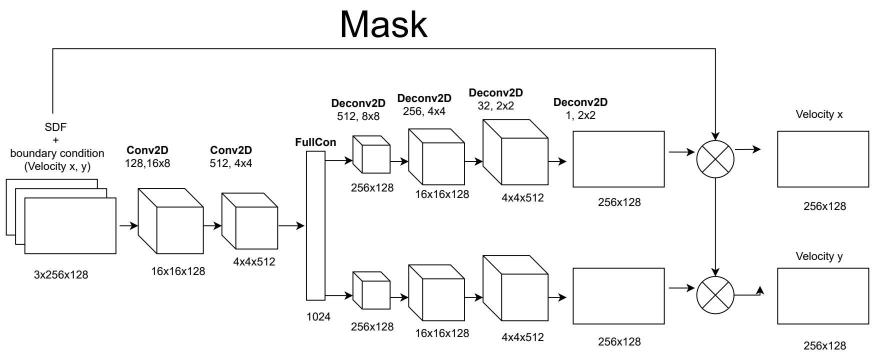

Figure1: Network architecture for 2D geometry.

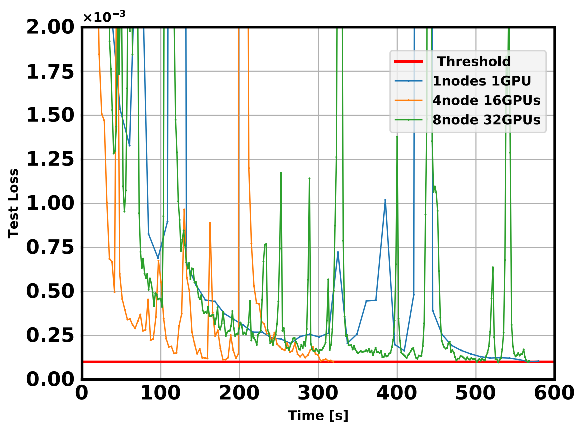

Figure2: Learning curves using multiple GPUs on Reedbush-L.

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 5 in order to improve the prediction accuracy, whereas it was set to 1 in the previous year.

In order to make training more efficient, we introduce Horovod to train neural networks with multiple GPUs. Figure 2 shows the learning curves when the number of GPUs used for training is varied. The Reedsbush-L supercomputer at the University of Tokyo was used for the training. We have succeeded in accelerating training with multiple GPUs.

5.2 CNN prediction method for the 3D simulation results

In this section, we describe the proposed prediction method for 3D simulation results.

Figure 3 shows the structure of the neural network used in this method for 3D. Similar to the 2D case, the object shape by SDF and the x, y and z flow velocity in the boundary region are given as inputs to the neural network, and the prediction of the velocity calculated by the LBM simulation over the entire computational domain is obtained as outputs. This model is also written using PyTorch.

We explain the data set of the neural network used in our method. First, we place one sphere in a 150 × 150 × 150 computational domain and simulate a fluid with a Reynolds number of 20 flowing from negative to positive in the x direction by LBM. The size and position of the spheres to be placed are changed to perform several steady flow simulations.

Next, 27 computational domains of 32 × 32 × 32 are cut out from the LBM simulation results in each 150 × 150 × 150 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 32 × 32 × 32 computational domain.

We thus prepare a total of 3,456 combinations of the LBM calculation results

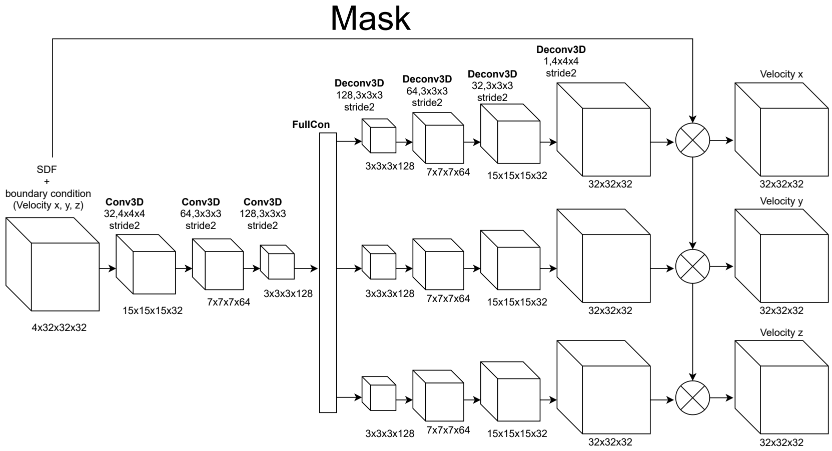

Figure3: Network architecture for 3D geometry.

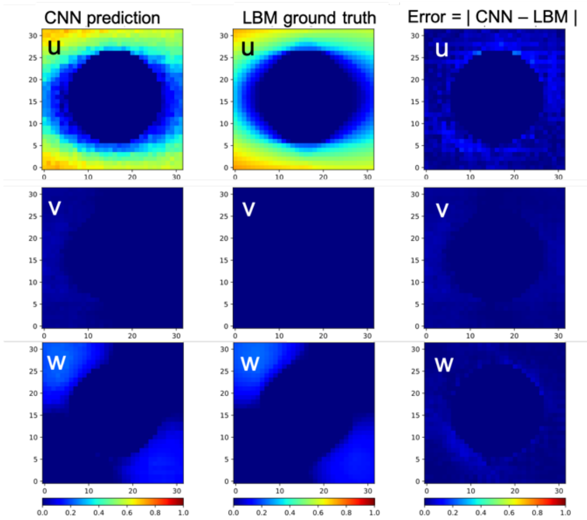

Figure4: Prediction results of a single domain in 3D. The CNN predictions, the LBM ground truth, and the error between the prediction and the ground truth at y = 16 are shown.

and SDF for the 32 × 32 × 32 domains, 3,110 for training and 346 for evaluation.

Figure 4 shows the results of the prediction using our trained model for 3D. 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 321 seconds (27,000 time steps) to reach the steady state using the LBM simulation code. On the other hand, the proposed method using CNN requires 0.6 seconds on one GPU. The proposed method can reduce the calculation time by 99%.

5.3 Prediction method using CNN with boundary exchange for the large-scale 3D simulation results

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 5 shows the prediction procedure of the LBM simulation results in this method. In this method, the entire prediction region is divided into 32 × 32 × 32 subregions and the simulation results in each subregion are predicted using the CNN model. The boundary regions of the neighboring subregions are overlapped. After the prediction is completed once, the prediction value of the boundary region is

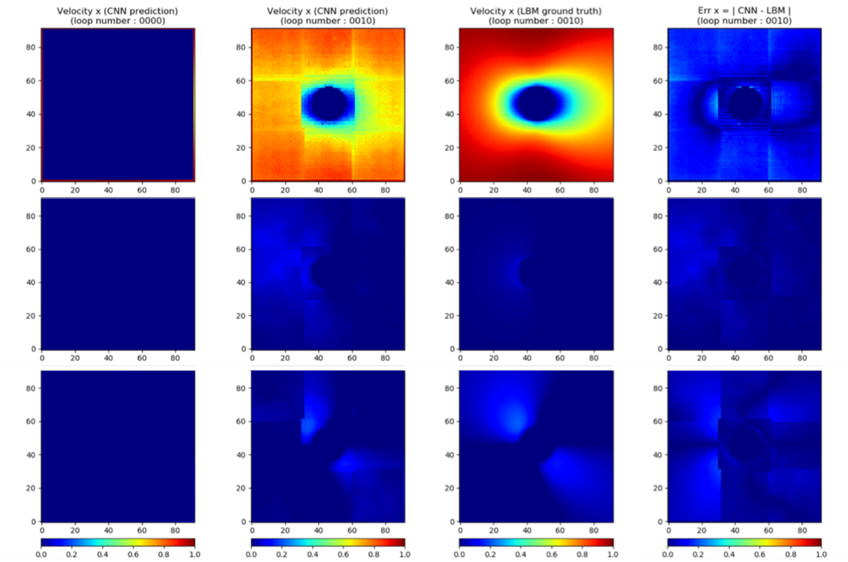

Figure 6: Prediction results over a large computational domain consisting of several subregions. The CNN predictions (initial and final values), the LBM ground truth, and the error between the prediction and the ground truth at y = 40 are shown.

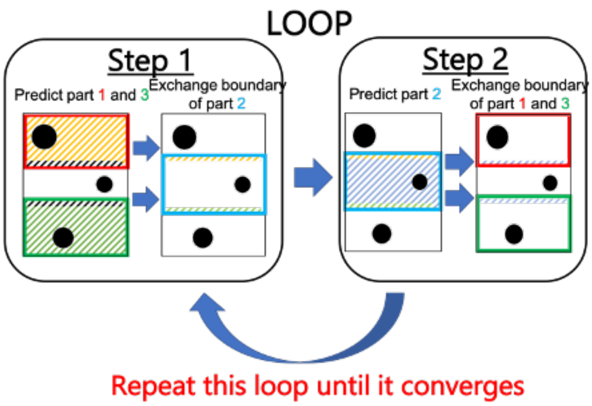

Figure 5: Prediction procedure using an iterative loop with boundary exchange.

obtained from the adjacent subregions, and the prediction is performed again by using this as the input. By repeating this process with an iterative loop, the values of the boundaries of subregions become continuous. The prediction result for the entire region is obtained. Note that although Figure 5 shows an example of three divisions in the y direction for simplicity, the number of divisions can be specified arbitrarily for the x, y and z directions.

Figure 6 shows the predicted results when a sphere is placed in a region of 87 × 87 × 87 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, y and z 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 10. In the prediction in this figure, the entire prediction region is divided into a total of 27 subregions, 3 in each 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 almost continuous at the final state for all directions. Although the errors are reduced by the iterative loops, the errors in the final state are still relatively large at the boundaries between subregions.

6 Progress during FY2020 and Future Prospects

In this research project, we have developed a prediction method for 2D large-scale steady-state flow simulations using deep learning inference and boundary exchange. We originally used Chainer as the framework for deep learning. However, since the development of Chainer was discontinued, we replaced it with PyTorch as we planned. We have introduced Horovod, which enables us to train the CNN models on multiple GPUs. We have extended the 2D method to predict large-scale 3D steady flow simulations. Unlike the results of 2D prediction, the results of 3D prediction by the proposed method still have a large error at the boundary regions of subdomains, which needs to be solved in the future.

The research plan for the next year is described below. We will improve a prediction method for large-scale computational results in 3D. 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. We will also 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.

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] Sora Hatayama, Takashi Shimokawabe and Naoyuki Onodera, “Steady Flow Prediction across Multiple Regions using Deep Learning and Boundary Exchange,” 3rd International Conference on. Computational Engineering and Science for Safety and Environmental Problems (COMPSAFE2020), Kobe, Japan, Dec. 2020.

[2] Hayato Shiba, Kengo Nakajima and Takashi Shimokawabe, “Data-driven approach for accelerated computing - a CFD example and beyond”, International Workshop on Machine Learning for Soft Matter 2021, Online, Feb. 2021.

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

[3] 畑山そら, 下川辺隆史, 小野寺直幸, “畳み込みニューラルネットワークと境界交換を用いた複数領域にまたがる定常流のシミュレーション結果の予測”, 第25回計算工学講演会, 小倉（オンライン開催）, 2020年6月.

[4] 畑山そら, 下川辺隆史, 小野寺直幸, “深層学習と境界交換を用いた複数領域にまたがる定常流のシミュレーション結果の予測”, 2020年並列／分散／協調処理に関する『福井』サマー・ワークショップ（SWoPP2020), 福井（オンライン開催）, 2020年7月.

[5] 長谷川敦, 下川辺隆史, “深層学習による混相流の時間発展シミュレーション結果の予測手法の検討”, 第177回

HPC 研究発表会，オンライン開催，2020 年 12 月.

(5) Published library and relating data

None

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

None