Speedy and highly accurate prediction of flow phenomena

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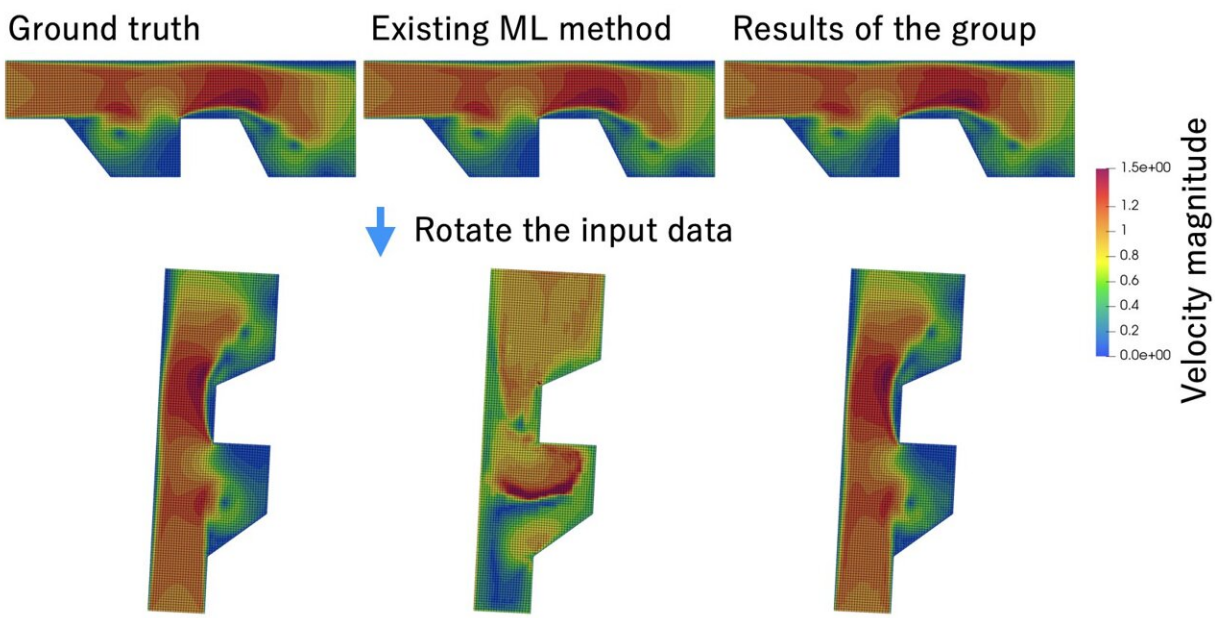


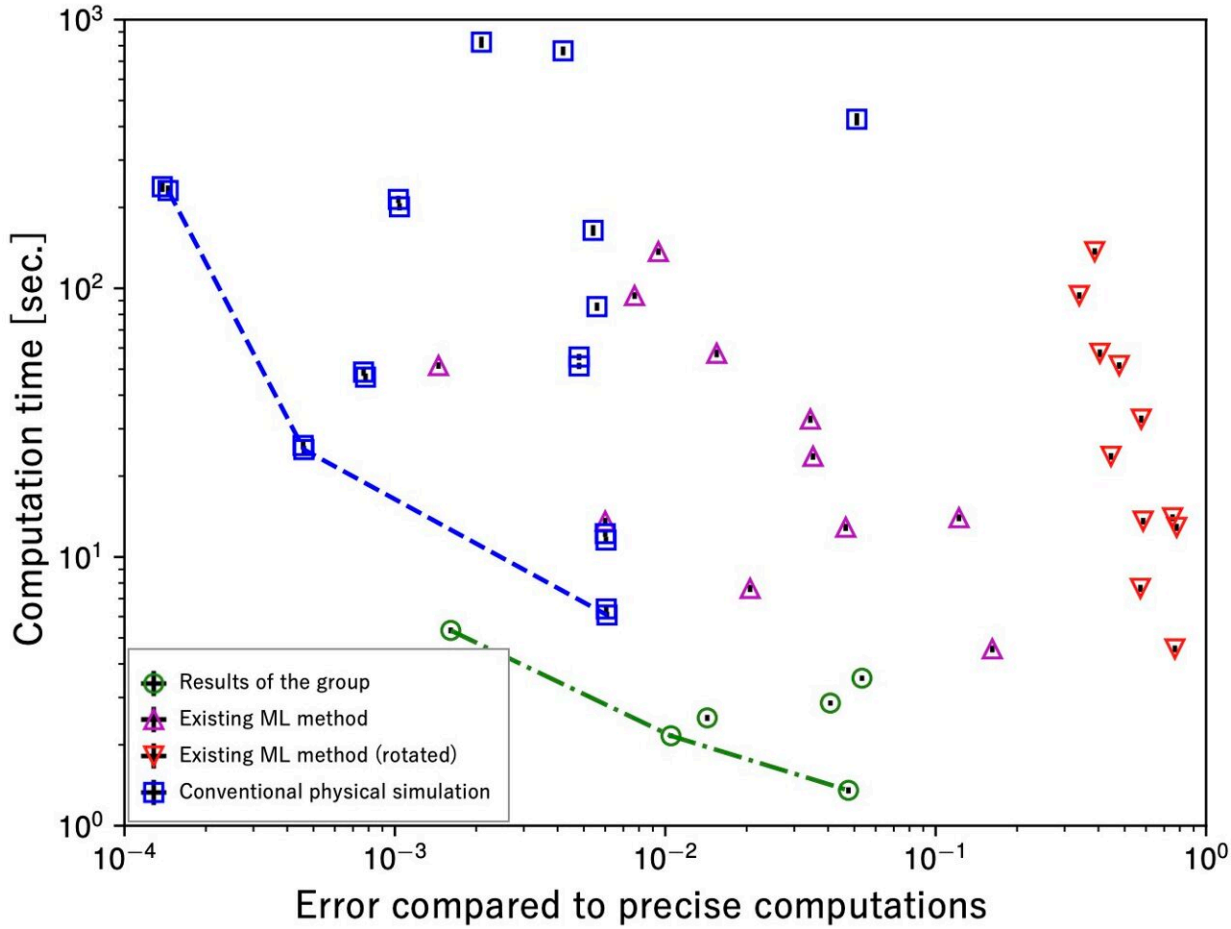
Visual comparison between ground truth (left), an existing ML method [Brandstetter et al. ICLR. 2022] (center), and results produced by the group (right). Physical phenomena can be observed from different viewpoints, resulting in varying appearances. Nevertheless, the fundamental essence of the phenomena should remain the same, which is commonly known as 'symmetry.' Unlike the existing approach, the proposed method maintains accuracy under rotation by taking into account the physical symmetry. Credit: Masanobu Horie

A research group led by Masanobu Horie at RICOS Co. Ltd. in collaboration with Assistant Professor Naoto Mitsume of Tsukuba

University, have successfully used AI to realize highly accurate and high-speed predictions of the flow of water and air and other phenomena. This technology achieves a sophisticated balance between accuracy and computation time (measured on the same computer) that was not achievable with existing physical simulations and other AI methods. The paper is published on the *arXiv* pre-print server.

Physical simulations are the mainstream methods for predicting flow phenomena. However, there is a trade-off between accuracy and computation time; high-accuracy analysis of the phenomena requires a long computation time, and simplifying the process to shorten the computation time reduces prediction accuracy. In recent years, extensive research has been conducted on constructing models that predict physical phenomena using a fundamental AI technology known as machine learning. However, this approach was often not applicable to simulations under complex conditions as handled in conventional physical simulations, and there were issues in terms of reliability and versatility.

By combining physical simulations and machine learning, this research group realized a high-speed prediction model that guarantees reliability and versatility, while leveraging the strengths of machine learning to make predictions based on existing data. The group achieved high-speed predictions without significantly compromising the accuracy compared to conventional physical simulations by having the model learn from highly accurate simulation data prepared in advance. In addition, this newly-developed technology theoretically proves that prediction accuracy does not deteriorate, whereas prediction accuracy dropped with existing machine learning technology when observing the same phenomenon from a different perspective.



Comparison of computation time and errors from the ground truth. The fast and accurate prediction is represented by the bottom left part of the figure. The proposed method (green) achieves a favorable speed-accuracy tradeoff that cannot be obtained with conventional physical simulation (blue) or existing machine learning models proposed by Brandstetter et al. [ICLR 2022] (magenta and red). Credit: Masanobu Horie

In the physical simulations of flow phenomena, boundary conditions are given for phenomena, such as considering the parts of "openings where air enters" and "walls that do not allow air to pass through." However, existing machine learning technology could not strictly take such specific conditions into account. The new technology successfully combines

machine learning algorithms with a rigorous treatment of the boundary conditions by formulating correspondence between input physical conditions and those in the abstract, high-dimensional data space handled by machine learning algorithms.

This was realized by embedding the computational methods of physical simulations in a machine learning algorithm, which is a unique feature of this technology. This time, the research group succeeded in showing the possibility that machine learning can have the same versatility as conventional physical simulation without losing the advantages of machine learning.

This technology is expected to accelerate the evaluation process by simulating flow phenomena, which can be a bottleneck in design and manufacturing, and improve the efficiency of the entire design and manufacturing processes. It may also be an important step to increasing the accuracy of weather forecasts and to improving the efficiency of ventilation systems to prevent the spread of infectious diseases caused by droplets.

More information: Masanobu Horie et al, Physics-Embedded Neural Networks: Graph Neural PDE Solvers with Mixed Boundary Conditions, *arXiv* (2022). DOI: 10.48550/arxiv.2205.11912

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