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Unified Finite Volume Physics Informed Deep Learning to Solve Heat Transfer Problems

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Abstract **–** As an alternative for the conventional numerical solver, the emerged physics informed neural network (PINN) has the capacity to solve partial differential equations (PDEs) with noisy data or partially missing physics. Thus, it has gained popularity in fluid dynamics, e.g., solving the heat transfer problems. Nevertheless, PINN struggles with low accuracy and high computational cost when the PDE solution contains multiple scales or steep gradients, which hinders its applications to high-Reynolds-number flows. To remedy the limitations, we propose a PINN approach that unifies the sub-domain decomposition, finite volume discretization and conventional numerical solver, termed as unified finite volume PINN (UFV-PINN). The output by neural network (NN) over the boundaries of agglomerated sub-domains functions as boundary conditions (BCs). Based on this, the conventional numerical solver further solves the PDEs. The gap between NN prediction and the solution by the conventional solver within the subdomain is taken as the new loss term to enforce the conservation law of PDE. As illustration, the steady-state Reynolds-averaged Navier-Stokes (RANS) equations and advection-diffusion equation (ADE) are solved. Numerical experiments are conducted to compare the performance of the proposed UFV-PINN and the standard-PINN, as well as the conventional finite volume (FV) solver. Results indicate that UFV-PINN obtains comparable accuracy to the numerical FV solver, while outperforms the standard-PINN to a large degree in terms of accuracy, computational time, and memory consumption. The proposed UFV-PINN is promising to serve as a powerful diagnostic tool in thermal fluids or surrogate model for thermal design.

Keywords**:** PINN, finite-volume discretization, PDE solver, RANS, heat transfer, design and optimization

1. Introduction

PDE solvers based on conventional numerical methods, e.g., finite-volume methods (FVMs), have been successfully applied to a wide variety of scientific and engineering problems [1]. They play the roles as indispensable diagnostic tools or design modules in fluid mechanics. However, with the enlarging computational domain or the wider spectra of scales encompassed in the simulated phenomenon, the number of grids is enlarged and the mesh size is refined. For example, the heat transfer problems with small diffusion coefficients in the large-scale fluid domain [2]. It not only intensifies the computation cost but also degrades the converge rates of iterative solutions because it is hard for the FVM solvers to eliminate the low-frequency errors on finely discretized grid cells [3]. This limitation becomes extremely severe on scenarios where repetitive simulations are required, for instance, optimization and reverse problems. Meanwhile, due to the strong nonlinearity of Navier-Stokes (NS) equations, a reasonable initial solution is vital to CFD simulation, otherwise the calculation will diverge [3]. Additionally, by reason of the complex code architecture to conduct forward solution efficiently [4], it is code-invasive and laborious to employ numerical solvers for reverse problems according to observational data.

As an alternative, PINN offers great flexibility toward the PDE solution process [5]. The PINN solves the PDE on a set of randomly generated or user-specified collocation points in the domain of definition. Such a feature endows PINN with the ability to break the curse of dimensionality for the cell number. The physical laws (namely PDE) and boundary conditions are adopted as penalty terms to train the NN. The partial derivative of the dependent variable with respect to the independent variable is calculated by the automatic differentiation, which is free of truncation error. Unlike the pure data-driven NN for the supervised learning, PINN can work in a data-free manner or merely with a few sampled data. Furthermore, both the forward and inverse problems are handled by PINN in the same way. It is natural for PINN to conduct the data assimilation, recovering the dense fields of quantities of interest from the sparse observation data. The obtained PDE solution by PINN is differentiable with respect to the independent variables. Thus, the trained PINN can seamlessly function as the surrogate model for the optimization problems.

Though flexible and elegant, PINN still suffers from low accuracy under many circumstances. By reason of the high-dimensional parameter space, PINN generally holds a non-convex total loss that tends to get stuck in local minimums or saddle points. PINN cannot tackle well with the problems exhibiting highly nonlinear, chaotic or multi-scale behavior [6]. Especially when the PDE parameters present heterogeneous across subdomains, the PINN fails to resolve the solution with discontinuity or sharp gradient. The physical problems like conjugate heat transfer are typically the scenarios that the PDE heterogeneity exists and pose formidable challenges to the PINN. The non-convex loss terms by BCs of PINN are hard to be minimized simultaneously. Weak consistency can also be noticed for the aforementioned stern problems, so that PINN may generate solutions varying enormously among different runs. In consequence, it is unreliable to directly apply the PINN in its native form (termed as standard-PINN) toward the realistic problems. The current applications of the PINN in heat transfer problem are limited to low-Reynolds-number flows [7].

2. Proposed Method

To improve the performance of PINN when faced with problems of higher Reynold number, we propose a PINN that unifies the sub-domain decomposition, finite volume discretization and the conventional numerical solver, termed as unified finite volume PINN. The whole framework is depicted in Figure 1. A NN parameterized by $\boldsymbol{\theta}$ takes the input by spatial coordinates (x_j, y_j, z_j) as well as the design parameters $\boldsymbol{\varphi}$. The output quantity (e.g., $\tilde{T}_{\partial\Omega_i}$) by NN over the boundaries of agglomerated subdomains $(\mathrm{e.g.}, \partial\Omega_i)$ functions as boundary conditions. Based on this, the embedded conventional numerical solver further solves the PDEs. The gap between neural network prediction (e.g., $\tilde{T}_{\Omega_i}$) and the solution by the conventional solver (e.g., $\hat{T}_{\Omega_j}$) within the subdomain is taken as the new loss term to enforce the conservation law of the PDE. To simulate the heat transfer, the RANS equations including conservation of momentum and continuity and the scalar transport equation are solved. Taking turbulence into account, the two governing equations for the *k*-epsilon turbulence model are also solved by the proposed technique [8]. Wall functions are adopted for the boundary condition treatment of the turbulence model [8]. When trained with a set of design parameters, the resultant UFV-PINN is exactly a surrogate model, which can be further utilized for optimization problems like the geometrical design for heat exchangers.

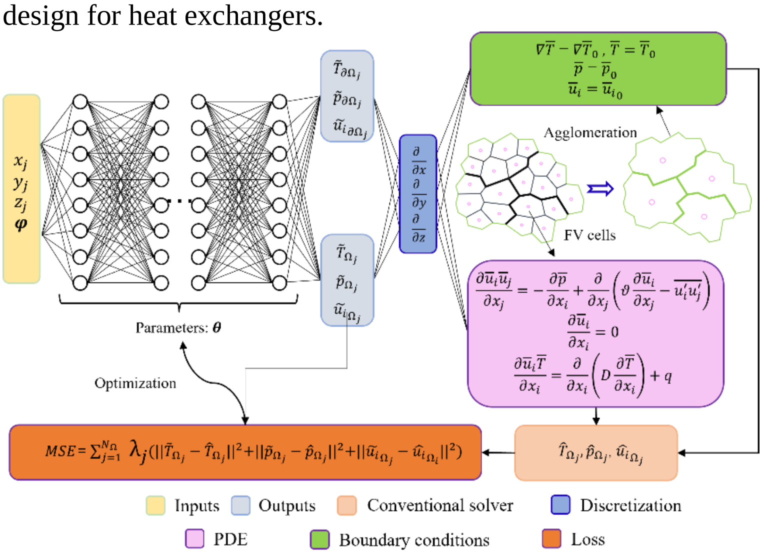

Fig. 1: The proposed unified finite-volume PINN.

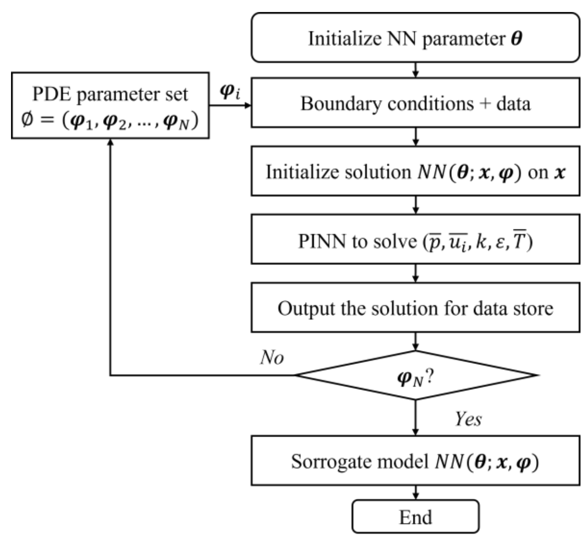

Fig. 2: Surrogate model by the UFV-PINN.

3. Numerical Experiments

We consider the heat transfer within a two-dimensional square cavity, where the flow is turbulent and relatively complex. The solution of the developed UFV-PINN is compared to the standard-PINN and conventional FV numerical solver. Figure 3 (a) exhibits the bi-unit square computational domain ranging within $\Omega = (0.0, 0.1)^2$. The domain is evenly evenly divided into 100 × 100 orthogonal FV cells, which are agglomerated into 10 × 10 subdomains. The Dirichlet and and Neumann BCs both exist for the heat transfer, as depicted by Figure 3 (a). As comparison, the FV solver OpenFOAM resolves the flow velocity field through solving the RANS equations with the BCs in Figure 3 (b). The incompressible flow is surrounded by walls, driven by the moving lid at the top boundary patch. It moves in the *x*-direction at the speed of 1 m/s while the other three walls are stationary. Due to the small kinematic viscosity ($\upsilon = 10^{-5}$), the flow is turbulent with Reynolds number around 10^4. With the standard *k*−epsilon model and the corresponding wall functions, the obtained turbulent heat diffusivity D is shown in Figure 3 (c), according to the calculated turbulent viscosity υ_t and turbulent Schmidt number S_t.=1.0.

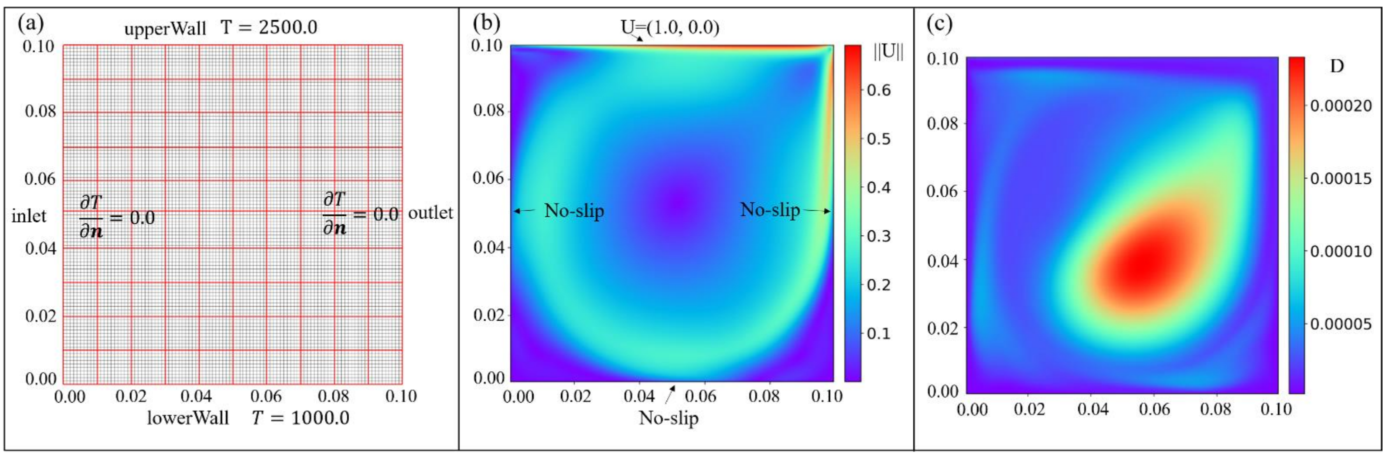

Fig. 3: Numerical settings for heat transfer within a square cavity a) the FV cells and subdomains; b) boundary conditions and velocity magnitude by OpenFOAM; c) the obtained turbulent heat diffusivity D

For both the standard- and UFV-PINNs, a fully connected NN with 5 hidden layers and 50 neurons in each hidden layer is used to approximate a single quantity to be solved. The layer-wise adaptive SiLU activation function is adopted to get non-linear output on each hidden neuron. The UFV-PINN and FV solver use upwind scheme for convection and central difference scheme for diffusion during the numerical discretization. All the FV cells in the agglomerated subdomains are collocated for the training of PINNs. We minimize the training loss constructed in Figure 1 through the Adam optimizer with a fixed learning rate 0.001. The training is iterated for 20,000 epochs to reach convergence.

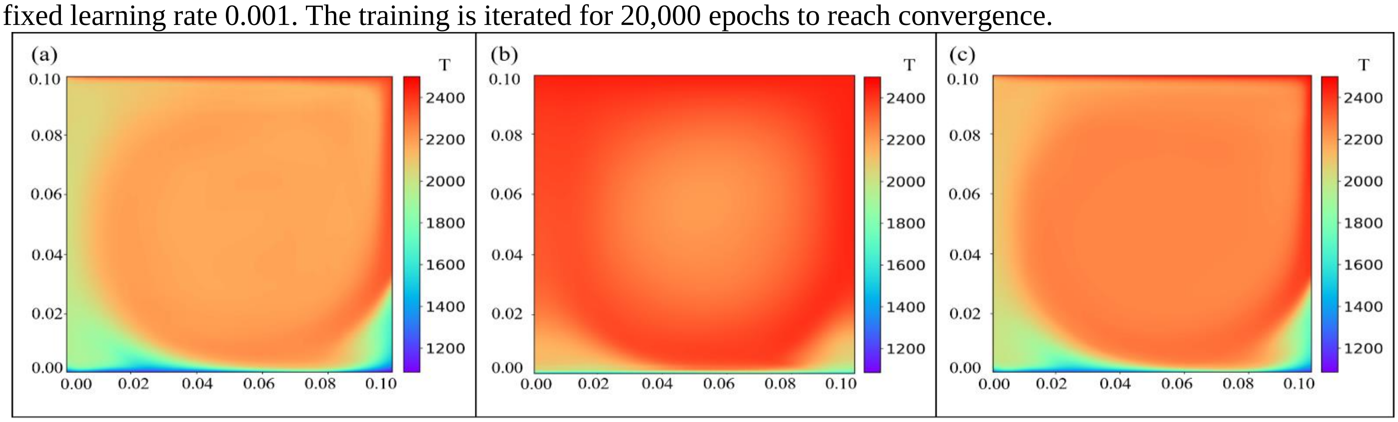

Fig. 4: Comparison of the solutions for the temperature field a) solved by OpenFOAM; b) solved by the standard-PINN; c) solved by the UFV-PINN.

The solutions are illustrated in Figure 4. It is evident that the solution by the UFV-PINN approximates to that of the conventional FV numerical solver. Opposite to this, the standard-PINN fails to capture the fine structures of the solution, indicating that the UFV-PINN is more accurate. Further analysis also shows that the UFV-PINN is more robust, time-efficient and less memory-consuming.

4. Conclusion

To extend the applicability of PINN in heat transfer problems of higher Reynolds number, we have proposed the UFV-PINN that unifies the sub-domain decomposition, finite volume discretization and conventional numerical solver. The preliminary results on the heat transfer within a square cavity validate that the UFV-PINN has attained largely enhanced abilities to solve the PDEs. Thus, it is promising to use the proposed solver as a powerful diagnostic tool in thermal fluids or surrogate model for the thermal optimization problems.

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