Frame Invariance and Scalability of Neural Operators for Partial Differential Equations

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Abstract. Partial differential equations (PDEs) play a dominant role in the mathematical modeling of many complex dynamical processes. Solving these PDEs often requires prohibitively high computational costs, especially when multiple evaluations must be made for different parameters or conditions. After training, neural operators can provide PDEs solutions significantly faster than traditional PDE solvers. In this work, invariance properties and computational complexity of two neural operators are examined for transport PDE of a scalar quantity. Neural operator based on graph kernel network (GKN) operates on graph-structured data to incorporate nonlocal dependencies. Here we propose a modified formulation of GKN to achieve frame invariance. Vector cloud neural network (VCNN) is an alternate neural operator with embedded frame invariance which operates on point cloud data. GKN-based neural operator demonstrates slightly better predictive performance compared to VCNN. However, GKN requires an excessively high computational cost that increases quadratically with the increasing number of discretized objects as compared to a linear increase for VCNN.

1 Introduction

A wide class of important engineering and physical problems are governed by partial differential equations (PDEs) describing the conservation laws. Extensive research efforts have gone into formulating and solving these governing PDEs. Despite significant

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progress, major challenges remain related to the computational costs of solving complex PDEs for real life problems like turbulent flows, laminar-turbulence transition and climate modeling. To avoid these prohibitively high computational costs, developing accurate and efficient numerical approximations or surrogate models for PDEs has been a key area of research [1–4]. Machine learning based models [5–9] have the potential to provide significantly faster alternatives to the traditional methods [10,11] of surrogate modeling. For accuracy and physical realizability, it is desired that these machine learning based models closely mimic the properties of the governing PDEs.

One of the key features of these PDEs is *frame invariance*, which is an intrinsic property of all equations in classical mechanics from Newton's second law to Navier Stokes equations. It signifies that the behavior of the physical systems does not depend on the origin or orientation of the reference frame of the observer. An invariance principle reflects a basic symmetry and is a basic requirement of all physical equations and constitutive models [12–14]. It is related to the objectivity of modeling: different modelers choosing different reference frames should arrive at the *same* answer. A model is frame-invariant to a transformation if the transformation of the input data does not alter the output of the function or model. In the context of fluid mechanics, any scalar variable like pressure or velocity magnitude is independent of any translation or rotation of the reference frame. Specifically, for example, a vector-to-scalar constitutive mapping $f : q \mapsto \tau$ should remain unchanged in the frame rotated by matrix R, i.e., the same mapping should be valid for $f : Rq \mapsto \tau$. In other words, for any mapping $f : q \mapsto \tau$ to be frame-invariant, the mapping $f : q' \mapsto \tau$ should hold for any rotation matrix R, with $q' \equiv Rq$ being the input vector in the new, rotated coordinate system. Invariance with respect to other transformations (e.g., translation of origin or change of reference velocity) can be defined and interpreted similarly. For solid mechanics, the magnitude of the deformation tensor is invariant to the orientation of the reference frame or the origin of the frame – it is an objective quantity regardless of the observer. Clearly, any modeling equations or constitutive relations should faithfully reflect such invariance or symmetries. Furthermore, in the numerical solutions of these PDEs, frame invariance also requires permutational invariance, which ensures independence of the results from the order in which the discretized objects are indexed. Examples of such objects include elements, cells, grid points, or particles, depending on the specific numerical method used. In a hypothetical simple example, assume the scalar τ at a given location x_0 is a function of the vectors q_1, q_2, and q_3 at three cells in the neighborhood of x_0. The output τ must remain identical whether the input is (q_1, q_2, q_3), (q_3, q_2, q_1), or any other ordering of three vectors. In other words, permutation invariance demands that τ must only depend on the set as a whole and not on the ordering of its elements. Embedding these invariance properties in machine learning based models can significantly improve the generalizability of learned models [15–21].

In this paper, we have chosen an airfoil problem to investigate the impact of the frame-invariance property. However, this illustration on a simple geometry of airfoils should not, in any way, undermine the significance and impact of frame-invariance in practical applications. In many cases of aerodynamics simulations, it is straightforward to agree