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DPK: Deep Neural Network Approximation of the First Piola-Kirchhoff Stress

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Abstract. This paper presents a specific network architecture for approximation of the first Piola-Kirchhoff stress. The neural network enables us to construct the constitutive relation based on both macroscopic observations and atomistic simulation data. In contrast to traditional deep learning models, this architecture is intrinsic symmetric, guarantees the frame-indifference and material-symmetry of stress. Specifically, we build the approximation network inspired by the Cauchy-Born rule and virial stress formula. Several numerical results and theory analyses are presented to illustrate the learnability and effectiveness of our network.

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Key words: Piola-Kirchhoff stress, deep neural networks, Cauchy-Born rule.

1 Introduction

Atomistic-based constitutive relation has played a critical role in multiscale modeling. With a proper description of macroscopic stress in the form of atomistic information, we can couple models based on continuum mechanics with models at microscopic scale [1], such as molecular dynamics (MD) and molecular statics (MS). In the last few decades, many research on the formulation [2–6], application [7–10] and simplification [11, 12] of various kinds of atomistic stress has been done. Among these, a well known and widely used atomistic-based stress for equilibrium and homogeneous system is the virial stress, which is firstly studied by Clausius in 1870 [13]. Formally, the virial stress is a sum of

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the multiplications of atoms positions and force, which can be easily computed in the molecular simulations. In practical multiscale modeling, however, we need to repeat this interatomic calculation in each coarse-grained patch [9, 10]. As a consequence, an easier-to-compute deformation-stress relation with atomic-level accuracy would make the multiscale modeling even more efficient.

On the other hand, with recent development of deep learning (DL) in traditional artificial intelligence (AI) domains, such as face recognition in computational visual (CV) and text classification in natural language processing (NLP), a lot of successes has also been achieved in the application of DL to scientific computation [14], e.g., using deep learning in speeding up the MD simulations [15, 16], solving differential equations [17–21], sampling equilibrium states in statistic mechanics [22], predicting multiphase flow [23], and identifying the constitutive law [24]. A significant difference in the utilization of DL in scientific computation from traditional AI problems is that, various constraints informed by different physical laws or boundary conditions must be considered. As a result, a physics-informed network is often wanted for the satisfaction of physical constraint. Furthermore, with a neural network enhanced by some physical knowledge, we can use less data in the training procedure.

In this article, we would build a special physics-informed network architecture for representation of the Piola-Kirchhoff stress (PK stress) in Lagrangian coordinates. Different from several existing works on the learning of constitutive relations with direct or indirect observed data by continuum model [25–28], we learn the PK stress directly from atomistic data driven by virial formulation, which supply the learning stress with an atomic-level accuracy. Furthermore, by constructing the network with symmetric operations in the crystallographic point symmetry group, this stress network is intrinsic symmetric, in the sense that the frame-indifference and material-symmetry of stress is exactly satisfied. In summary, our main contributions are as follows:

- We propose a novel deep neural network (DPK), for the representation of PK stress.
- The DPK stress is intrinsic symmetric and can be trained by virial stress.
- Several numerical results and theory analysis are given to illustrate the learnability, transferability and effectiveness of DPK.

The rest of this paper is organized as follows. In Section 2 we first review the PK stress and virial formulation, then propose the DPK stress and its simplification version. Several theorems on the symmetry, approximation and learnability will also be presented. After that, some numerical results will be shown in Section 3 to demonstrate the effectiveness and transferability of the simplified DPK stress. Finally in Section 4 we will give our main conclusions.