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Reliable Machine Learning for Data-Driven Nonlinear Elasticity and Viscoelasticity

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Summary — We present a mechanics-informed machine learning framework for the data-driven constitutive modeling of nonlinearly elastic and viscoelastic materials. By design, it forces the architecture of a neural network to satisfy a list of hard constraints, including: dynamic stability, material stability, and internal variable stability; objectivity; consistency; fading memory; recovery of elasticity; and the 2nd law of thermodynamics. We show that embedding these notions in a learning approach reduces sensitivity to noise and promotes robustness to inputs outside the training domain.
Keywords — Constitutive modeling; Data-driven; Neural network; Physics-informed; Thermodynamics; Viscoelasticity

1. Introduction

Constitutive modeling of materials exhibiting a highly nonlinear behavior is among the most intensely researched fields within solid mechanics, because of its complexity and importance for engineering problems. The complexity is exacerbated when the instantaneous stress depends not only on the instantaneous strain, but on the entire deformation history. Historically, constitutive modeling has been performed using one of two main approaches: (1) phenomenological modeling based on empirical observations; and (2) mechanistic modeling derived from first principles based on the material's underlying structure.

Phenomenological models are appealing – and often unavoidable – in the context of highly heterogeneous materials with complex or even ambiguous micro-structures. However, they are subject to the usual shortcomings of empirical relationships. Namely, they can violate some fundamental principles that govern the material they describe; and they typically require heuristic choices of parameterized functions whose parameters are fitted. Furthermore, they can be sensitive to data sparsity or noise and can suffer from overfitting. While mechanistic models avoid these problems, they are typically formulated on a material-by-material basis and their derivations can be infeasible for moderately complex materials. Hence, they cannot necessarily be constructed using a single, comprehensive, modeling framework.

2. Data-driven constitutive modeling using machine learning

With the advent of machine learning (ML), the use of deep artificial neural networks (ANNs) for constitutive modeling has gained prominence. This is partly due to the universal approximation property of an ANN; and to its fast online execution speed. For these reasons, regression-based ANNs have been explored for constitutive modeling as early as in [1] and demonstrated a strong potential. They have been applied to model kinematic hardening [2] and to generate implicit models for material viscoplasticity [3]. In the absence of paired stress-strain training data, ANN frameworks have also been proposed for learning constitutive relations from indirect observations [4]. With the emergence of automatic differentiation in ML, they have become even more attractive, particularly in the context of constitutive modeling for finite element (FE) analysis and/or optimization, when the computation of tangent modulus matrices and/or parameter sensitivities is required. ANN frameworks have also gained popularity for accelerating the homogenization of nonlinear multi-scale FE computations [5, 6].

Nonetheless, ANNs are not without shortcomings for data-driven constitutive modeling. In their standard form, they are built to simply map input data to output data – typically without fundamental restrictions. Thus, when such ANNs are exploited in a physics-based numerical simulation, they can violate some laws of physics, in which case confidence in the simulation-based predictions is reduced. Indeed, in the context of FE analysis, it was observed that purely regression-based constitutive models may lead to various instabilities and nonphysical phenomena [7]. At least for this reason, the literature has witnessed most recently a surge of papers proposing ML-based frameworks that attempt to inform or constrain ANNs with knowledge of mechanics and thermodynamics, in view of making their application to constitutive modeling more robust.

3. Mechanics-informed machine learning for nonlinear elasticity

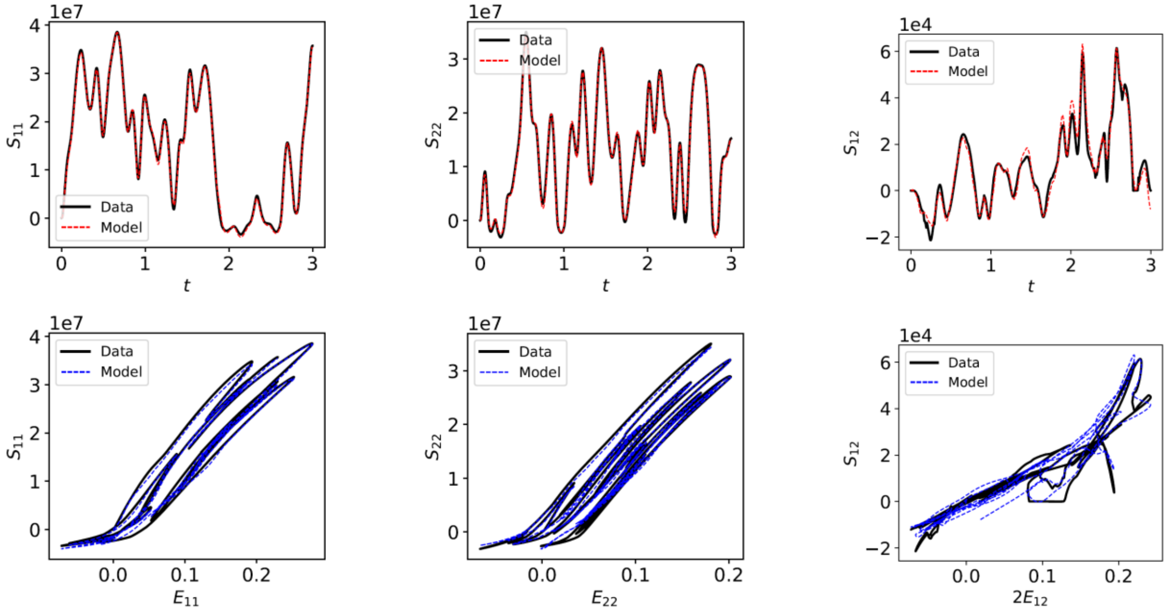
In particular, we have recently proposed in [8], in collaboration with Dr. Philip Avery at Stanford University, a computational framework for data-driven constitutive modeling that is broadly mechanics-informed, but is limited to nonlinear elasticity. This framework enforces on the ANN's network architecture a long list of desirable mathematical properties that guarantees the satisfaction of an even longer list of physical constraints, including: objectivity; consistency (preservation of rigid body modes); dynamic stability; and material stability. Furthermore, we have shown that embedding such notions in a learning approach reduces a model's sensitivity to noise and promotes its robustness to inputs outside the training domain. We have highlighted the merits of such a learning approach using several FE analysis examples; and demonstrated its potential for ensuring the computational tractability of multi-scale applications such as those associated with the fluid-structure simulation of the supersonic inflation dynamics of a parachute system with a canopy made of a woven fabric.

4. Mechanics-informed machine learning for nonlinear elasticity

In this lecture, which is based to a large degree on [9], we specifically set the context to viscoelasticity. In this setting, the instantaneous stress depends in general on the entire strain history, but does not experience permanent deformations. We extend the aforementioned framework for data-driven constitutive modeling [8] to the viscoelastic setting to capture the time-dependent behavior of the material. To this end, we first derive general mathematical restrictions on the functions arising in the development of a viscoelastic constitutive law. Next, we describe the adaptation of these restrictions to the construction of an ANN and its training using stress-strain data. Finally, we demonstrate the ability of the resulting ANN to learn highly nonlinear viscoelastic material responses generated by a synthetic model and a FE-based multi-scale homogenization of a woven fabric; and illustrate the merits of this framework using two different representative FE analyses.

5. Sample result

We include below a self-explanatory example of the performance of our reliable, mechanics-informed computational framework for machine learning data-driven constitutive modeling. We will discuss many more examples during the lecture that demonstrate the merits of this framework.



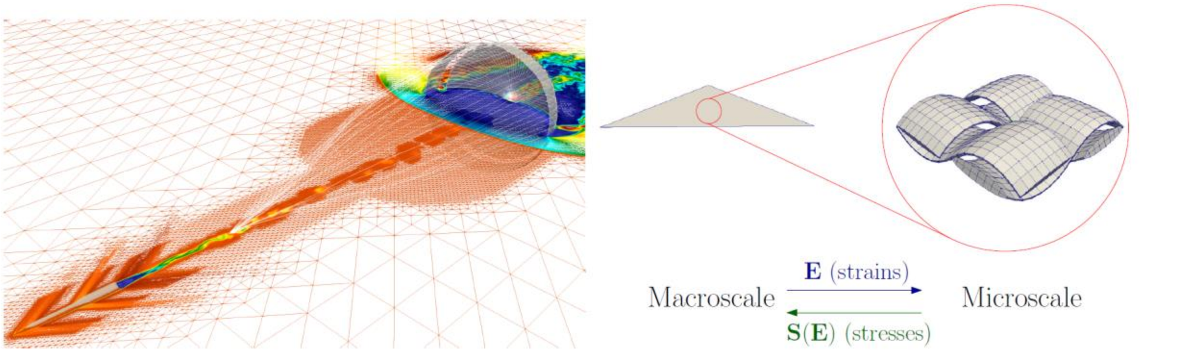


Figure 1 – Machine-learned nonlinear multiscale viscoelastic constitutive model and exploitation in a multiscale fluid-structure simulation of the supersonic inflation dynamics of a parachute system with a canopy made of a woven fabric and with soft braided suspension lines

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