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Physics-Enforced Neural Network Modeling of History-Dependent Materials

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Introduction

By now, it is well known that strictly enforcing physics in neural network-enhanced constitutive models offer several advantages over weakly (via penalty approaches) informing about physics. However, there has not been much comparison between different approaches of how physics are enforced. The most common approach in the literature is using Physics-Augmented Neural Networks (PANNs) describing scalar thermodynamic potentials using neural networks, and restrict these by certain positivity, monotonicity, and convexity requirements [1, 2]. An alternative approach is to describe the evolution laws directly by using neural networks, as the author did in [3]. This talk focus on the differences between these approaches, highlighted by a set of examples for viscoelastic and plastic material responses.

Theory

To illustrate the differences in the two approaches, we consider a standard viscoplastic model with isotropic hardening and a Norton overstress. We then have the following model equations,

$$\Psi = \frac{1}{2}:\left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\mathrm{p}}\right]:\mathbf{E}:\left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\mathrm{p}}\right] + \frac{1}{2}Hk^2 \tag{1a}$$

$$\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \boldsymbol{\epsilon}} = \mathbf{E}:\left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\mathrm{p}}\right], \qquad \kappa = -\frac{\partial \Psi}{\partial k} = -Hk \tag{1b}$$

$$\Phi = \sqrt{[3/2]\,\boldsymbol{\sigma}^{\mathrm{dev}}:\boldsymbol{\sigma}^{\mathrm{dev}}} - [Y_0 + \kappa], \qquad \Phi_{\mathrm{iso}} = \frac{\kappa^2}{2\kappa_\infty} \tag{1c}$$

$$\dot{\boldsymbol{\epsilon}}_{\boldsymbol{p}} = \dot{\lambda}\frac{\partial \Phi}{\partial \boldsymbol{\sigma}} = \dot{\lambda}\boldsymbol{\nu}, \qquad \dot{k} = \dot{\lambda}\left[\frac{\partial \Phi}{\partial k} + \frac{\partial \Phi_{\mathrm{iso}}}{\partial k}\right], \qquad g_\kappa \coloneqq \frac{\partial \Phi_{\mathrm{iso}}}{\partial k}, \dot{\lambda} = \frac{1}{t^*}\left[\frac{\langle \Phi \rangle}{Y_0}\right]^n \tag{1d}$$

For this setup, we have the physical requirement of the dissipation inequality,

$$\mathcal{D} = \dot{\lambda}[\Phi + Y_0 + \kappa g_\kappa] \geq 0 \tag{2}$$

PANN: Formulation based on potentials

If we want to enhance the model above by using PANNs, specifically focusing on the isotropic hardening, we replace the isotropic hardening potential, $\Phi_{\mathrm{iso}} = \mathcal{NN}_{PA}$, by an input-convex neural network (ICNN) [4]. For simplicity, let's consider that it only depends on the hardening, κ, such that the convexity gives,

$$\mathcal{NN}_{PA}(\kappa + \kappa^*) \geq \mathcal{NN}_{PA}(\kappa) + g_\kappa(\kappa)[\kappa^* - \kappa] \tag{3}$$

Reformulation and considering $\kappa^* = 0$, yields $g_\kappa(\kappa)\kappa \geq 0$, showing that convexity of is a sufficient requirement for a positive dissipation.

Evolution law augmentation

An alternative to using the PANN, $\mathcal{NN}_{PA}$, is to postulate a neural network enhanced variant of $g_\kappa(\kappa)$ directly. Following [3], this can be done by

$$g_\kappa = \kappa\,\mathcal{NN}_{PE}(\kappa) \tag{4}$$

The only requirement on $\mathcal{NN}_{PE}$ to ensure a positive dissipation is then that $\mathcal{NN}_{PE}$ is positive, which can be enforced by using a positive activation function in the last layer. In contrast to ICNNs, no constraints are put on the neural network weights during training.

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Results

An example of a non-convex Φ_{iso}, that still gives a positive dissipation, is

$$\Phi_{\text{iso}} = \frac{\kappa^2}{1+\kappa^2} \Rightarrow g_\kappa = \frac{2\kappa}{[1+\kappa^2]^2} \tag{5}$$

resulting in the hardening evolution illustrated in **Figure 1a.**

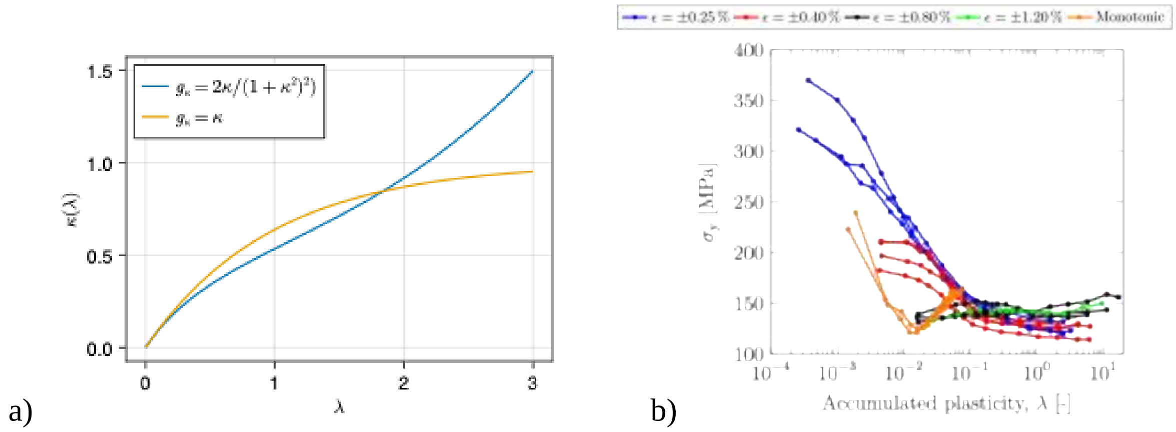

Figure 1: Evolution of isotropic hardening with plastic deformation using (a) a non-convex and convex potential, both ensuring a positive dissipation and (b) experimental results from [5].

The results in **Figure 1a** show that embedding the neural network in the evolution equations offer a greater modeling flexibility than using PANNs. However, the additional constraints enforced by the PANN-approach may be considered a knowledge-based constraint, here requiring a nonincreasing rate of hardening. On the other hand, the experimental results in **Figure 1b** show that non-monotonic responses can occur for real materials. While these results cannot be described by the single input hardening law given above ([3] used 6 invariants as inputs), they highlight that too much ansatz restrictions can prevent NN-enhanced models from reaching their full potential.

Concluding remarks

While many benefits of strictly enforcing physics in neural-network models for constitutive models are known in the literature, rather little is known about the differences between how these are constraints are enforced. This contribution aims to provide new insights in the consequences of different choices, particularly focusing on comparing PANNs and direct inclusion of neural networks in the evolution laws.

References

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