NN-EVP: A Physics-Informed Neural Network-Based Elasto-Viscoplastic Framework for Predictions of Grain Size-Aware Flow Response

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Abstract

We propose a physics-informed, neural network-based elasto-viscoplasticity (NN-EVP) constitutive modeling framework for predicting the flow response in metals as a function of underlying grain size. The developed NN-EVP algorithm is based on input convex neural networks (ICNNs) as a means to strictly enforce thermodynamic consistency, while allowing high expressivity towards model discovery from limited data. It utilizes state-of-the-art machine learning tools within PyTorch's high-performance library providing a flexible tool for data-driven, automated constitutive modeling. To test the performance of the framework, we generate synthetic stress–strain curves using a power law-based model with phenomenological hardening at small strains and test the trained model for strain amplitudes beyond the training data. Next, experimentally measured flow responses obtained from uniaxial deformations are used to train the framework under large plastic deformations. Additionally, the Hall–Petch relationship corresponding to grain size strengthening is discovered by training flow response as a function of grain size, also leading to efficient extrapolation. The present work demonstrates a successful integration of neural networks into elasto-viscoplastic constitutive laws, providing a robust automated framework for constitutive model discovery that can efficiently generalize, while also providing insights into predictions of flow response and grain size-property relationships in metals and metallic alloys under large plastic deformations.

1 Introduction

Owing to their polycrystalline nature, the anisotropic flow response of metals under large deformations heavily depends on the average grain size that forms the underlying microstructure. Traditional phenomenological approaches require manual parameter calibration, which can become mathematically constrained under complex loading histories. Purely data-driven architectures often risk producing predictions that violate fundamental thermodynamic bounds when operating outside the training distribution.

To address these limitations, this work develops a novel data-driven elasto-viscoplasticity framework based on neural networks (**NN-EVP**) that replaces historical power-law structures with generic, physics-informed networks capable of predicting macroscopic mechanical profiles in low-data regimes. By utilizing Input Convex Neural Networks (ICNNs), thermodynamic compliance is enforced by design, allowing microstructural features like grain boundaries and hardening curves to be learned directly from limited observation fields.

2 Methods and Thermodynamic Formulation

Under an additive strain split assumption appropriate for small-to-moderate configurations, the total strain tensor ϵ is decomposed into elastic (ϵ^e) and viscoplastic (ϵ^{vp}) parts:

$$\epsilon = \epsilon^e + \epsilon^{vp} \tag{1}$$

The specific free energy function Ψ is partitioned into elastic stiffness and internal viscoplastic hardening states governed by the internal scalar accumulation variable r:

$$\Psi = \Psi^e(\epsilon^e) + \Psi^{vp}(r) \tag{2}$$

Following the standard Coleman-Noll procedure, the true Cauchy stress tensor σ and its thermodynamic isotropic conjugate force R are derived via thermodynamic derivation:

$$\sigma = \frac{\partial \Psi}{\partial \epsilon^e} = \mathbb{C} : \epsilon^e, \quad R = \frac{\partial \Psi}{\partial r} \tag{3}$$

where $\mathbb{C}$ represents the fourth-order elastic stiffness tensor, uniquely defined for isotropic materials by the Young's modulus E and Poisson's ratio ν.

To preserve stability, the material evolution must comply with the second law of thermodynamics. We define a dual dissipation potential $\varphi^*(\sigma, R)$ satisfying the properties of non-negativity, including the origin ($\varphi^*(0) = 0$), and strict convexity across all operational coordinates. Invoking the normality rule, the viscoplastic strain rate $\dot{\epsilon}^{vp}$ yields:

$$\dot{\epsilon}^{vp} = \frac{\partial \varphi^*}{\partial \sigma}, \quad \dot{r} = -\frac{\partial \varphi^*}{\partial R} \tag{4}$$

This ensures that the internal dissipation expenditure remains unconditionally non-negative:

$$\sigma : \dot{\epsilon}^{vp} - R\dot{r} \geq \varphi^* \geq 0 \tag{5}$$

2.1 NN-EVP Architecture and Convex Bounds

The dual potential is represented directly using a feedforward network $\mathcal{NN}_{\phi^*}$ parameterized with non-negative layer-to-layer connection weights ($W_l \geq 0$) to enforce input convexity. To resolve scaling discrepancies without inducing gradient decay, a scalable Softplus activation function is established:

$$\mathcal{F}_l^{\mathcal{NN}_{\phi^*}}(x) = \frac{1}{\beta}\log(1 + e^{\beta x}) - \mathcal{F}_l^{\mathcal{NN}_{\phi^*}}(0) \tag{6}$$

where $\beta > 0$ represents an optimized scaling coefficient. To ensure a strict zero viscoplastic rate at a completely un-deformed configuration ($\sigma = 0$), a localized stress correction function $\varphi^c(\sigma) = \zeta\sigma_{eq}$ is added, mapping the final corrected flow output identically to:

$$\dot{\epsilon}^{vp} = \frac{\partial \mathcal{NN}_{\phi^*}}{\partial \sigma} - \frac{\partial \mathcal{NN}_{\phi^*}(0)}{\partial \sigma} \tag{7}$$

2.2 Isotropic Hardening Subnetwork

When hardening regimes are active, the active threshold stress level $R(r)$ evolves as a continuous function of r. Rather than imposing analytical parameterizations (e.g., Johnson-Cook or Voce), an unconstrained subnetwork $\mathcal{NN}_R(r)$ tracks strain-hardening development. To handle late-stage saturation during extensive mechanical configurations, a blended activation profile is implemented to relax early plateauing:

$$\mathcal{F}_l^{\mathcal{NN}_R}(x) = \alpha_1 \max(x, 0) + \alpha_2 \frac{e^{\beta x} - e^{-\beta x}}{e^{\beta x} + e^{-\beta x}} \tag{8}$$

where α_1 and α_2 denote tunable structural combination weights.

3 Grain Size-Aware Flow Response and Hall–Petch Discovery

In order to incorporate the Hall-Petch effect into the NN-EVP framework, we introduce a Hall-Petch neural network $\mathcal{NN}_{HP} = \mathcal{NN}_{HP}(d_{grain})$ in addition to the dual potential $\mathcal{NN}_{\phi^*}$ and the hardening neural network $\mathcal{NN}_R$. This allows us to learn and discover the Hall-Petch relationship. To remain consistent with thermodynamics laws, the following conditions are enforced on the Hall-Petch neural network $\mathcal{NN}_{HP}$:

- $\mathcal{NN}_{HP}$ is monotonically decreasing,
- $\mathcal{NN}_{HP}$ is always positive: $\mathcal{NN}_{HP} > 0$.

Notice that since the Hall-Petch term only affects the initial yield function and does not evolve during the deformation, an adaptive activation function here is not necessary.

As illustrated in Figure 1, the response of the Hall-Petch network $\mathcal{NN}_{HP}$ and the hardening network $\mathcal{NN}_R$ are combined to $\mathcal{NN}_R(r) + \mathcal{NN}_{HP}(d_{grain})$ and then used as an input to the dual potential network $\mathcal{NN}_{\phi^*}$. Material anisotropy is captured solely from variation in grain size. Capturing the material anisotropy due to crystallographic texture and slip-system-based deformation mechanisms requires incorporating the crystal plasticity framework which is planned for future research towards ML-enabled, physics-informed crystal plasticity.

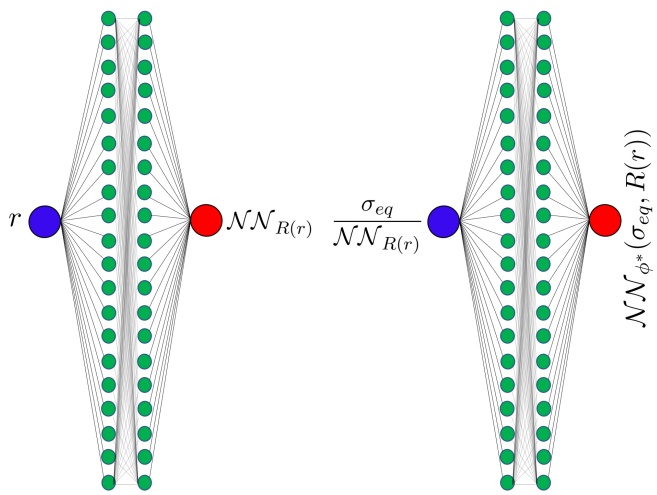

Figure 1: A schematic of neural network for elasto-viscoplasticity with isotropic hardening and Hall-Petch effects.

The multi-network architecture was optimized in PyTorch using the AdamW optimizer coupled with a cosine annealing scheduler decaying from $1e^{-2}$ to $1e^{-3}$. Total network parameters and operational field dimensions are summarized in Table 1.

Table 1: NN-EVP Network Optimization Field Metrics

Variable Coordinate Space	Input Layer Nodes	Optimized Trainable Parameters
Hardening Accumulation (r)	1	2648 Total Matrix Elements
Cauchy Stress State (σ)	6	(Across $\mathcal{NN}_{\phi^*}, \mathcal{NN}_R, \mathcal{NN}_{HP}$)

Initial verification was conducted against synthetically generated perfect viscoplastic benchmarks spanning rate sensitivity ranges of $n = 10, 20$, and 100. The training residual

converged rapidly to a normalized mean squared loss of $1e^{-5}$ within 100 epochs. Extrapolation accuracy was benchmarked by constraining training data strictly to 0.5% strain and parsing predictions up to 2.0% total strain (a 75% unseen test domain). A configuration balancing 80% adaptive tanh and 20% ReLU nodes successfully predicted the full continuous hardening curvature without premature numerical saturation.

To assess large plastic deformations, the framework was trained on experimental Nickel (Ni) flow response curves parsed via continuous nonlinear SciPy interpolation handlers up to 10% total mechanical strain. For multi-curve validation, tensile profiles of Copper (Cu) spanning four discrete grain size diameters ($2.1\,\mu$m, $3.4\,\mu$m, $7.1\,\mu$m, and $15\,\mu$m) were optimized in parallel. Upon recovering the isolated microstructural weights of $\mathcal{NN}_{HP}$ across extrapolated boundaries down to $0.5\,\mu$m and up to $500\,\mu$m, the network completely uncovered and recovered the expected linear Hall-Petch relationship in log-log scaling without any manual intervention. The parallel multi-curve capture of microstructural dependency is shown explicitly in Figure 2.

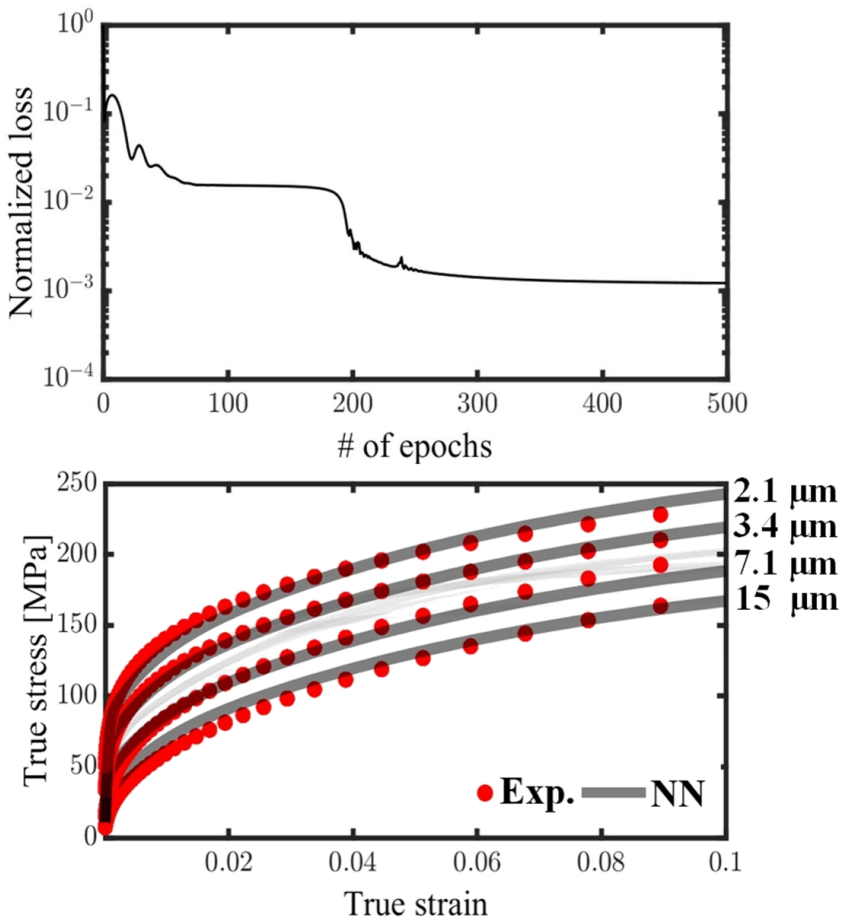

Figure 2: Multi-fit training of flow response in Cu for microstrucural grain sizes of 2.1-3.4-7.1-15 μm.

References

[1] A. Eghtesad, J. Tan, J. N. Fuhg, and N. Bouklas. NN-EVP: A physics informed neural network-based elasto-viscoplastic framework for predictions of grain size-aware flow response. *International Journal of Plasticity*, 181:104072, 2024.