Machine Learning methods and, in particular, Artificial Neural Networks (ANNs) have demonstrated promising capabilities in material constitutive modeling. One of the main drawbacks of such approaches is the lack of a rigorous frame based on the laws of physics. This may render physically inconsistent the predictions of a trained network, which can be even dangerous for real applications.

Here we propose a new class of data-driven, physics-based, neural networks for constitutive modeling of strain rate independent processes at the material point level, which we define as Thermodynamics-based Artificial Neural Networks (TANNs). The two basic principles of thermodynamics are encoded in the network’s architecture by taking advantage of automatic differentiation to compute the numerical derivatives of a network with respect to its inputs. In this way, derivatives of the free-energy, the dissipation rate and their relation with the stress and internal state variables are hardwired in the network. Consequently, our network does not have to identify the underlying pattern of thermodynamic laws during training, reducing the need of large data-sets. Moreover the training is more efficient and robust, and the predictions more accurate. Finally and more important, the predictions remain thermodynamically consistent, even for unseen data. Based on these features, TANNs are a starting point for data-driven, physics-based constitutive modeling with neural networks.

We demonstrate the wide applicability of TANNs for modeling elasto-plastic materials, with strain hardening and strain softening. Detailed comparisons show that the predictions of TANNs outperform those of standard ANNs. TANNs ’ architecture is general, enabling applications to materials with different or more complex behavior, without any modification.