Material modeling via Thermodynamics-based Artificial Neural Networks

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From data-driven to physics-based neural networks material modeling

- 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**.
- 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).

Thermodynamics principles

Under isothermal transformations and small strain regime, the **first law of thermodynamics** reads

$$\dot{\mathsf{F}} = \sigma \cdot \dot{\varepsilon} - \mathsf{D},$$

with F and $\dot{\mathsf{F}}$ the specific Helmholtz free energy (per unit volume) and its rate of change; σ the Cauchy stress tensor; ε and $\dot{\varepsilon}$ the small strain tensor and its rate of change; D the rate of mechanical dissipation. '$\cdot$' denotes contraction of adjacent indices.
From the **second law of thermodynamics** the rate of dissipation must be non-negative,

$$\mathsf{D} \geq 0.$$

For strain-rate independent materials

$$\mathsf{F} := \widetilde{\mathsf{F}}\left(\varepsilon, \mathcal{Z}\right) \quad \text{and} \quad \mathsf{D} := \widetilde{\mathsf{D}}\left(\varepsilon, \mathcal{Z}, \dot{\mathcal{Z}}\right),$$

where D is homogeneous of first-order (rate independency) in $\dot{\mathcal{Z}}$ and $\mathcal{Z} = (\zeta_i, \dots, \zeta_N)$ denotes a set of N (additional) internal state variables. It can be proven that

$$\sigma = \frac{\partial \mathsf{F}}{\partial \varepsilon}, \quad \mathsf{D} = -\sum_i \frac{\partial \mathsf{F}}{\partial \zeta_i} \cdot \dot{\zeta}_i = \sum_i \chi_i \cdot \dot{\zeta}_i.$$

Artificial Neural Networks

ANNs can be regarded as non-linear operators, composed of an assembly of mutually connected processing units−nodes−, which take an input signal $\mathcal{I}$ and return the output $\mathcal{O}$, namely

$$\mathcal{O} = \mathsf{ANN}@\mathcal{I}.$$

The signal flows from layer $(l-1)$ to layer (l) according to

$$p_k^{(l)} = \mathcal{A}^{(l)}(z_k^{(l)}),$$

with

$$z_k^{(l)} = \sum_s (w_{ks}^{(l)} p_s^{(l-1)}) + b_k^{(l)},$$

where $p_k^{(l)}$ is the output of node k, at layer (l); $\mathcal{A}^{(l)}$ is the activation function of layer (l); $w_{ks}^{(l)}$ is the *weight* between the s-th node in layer $(l-1)$ and the k-th node in layer (l); and $b_k^{(l)}$ are the *biases* of layer (l).

References

(+) Houlsby and Puzrin, 2007. Principles of Hyperplasticity. Springer Science Business Media.

(†) Masi et al., 2020. Thermodynamics-based Artificial Neural Networks for constitutive modeling. arXiv preprint arXiv:2005.12183.

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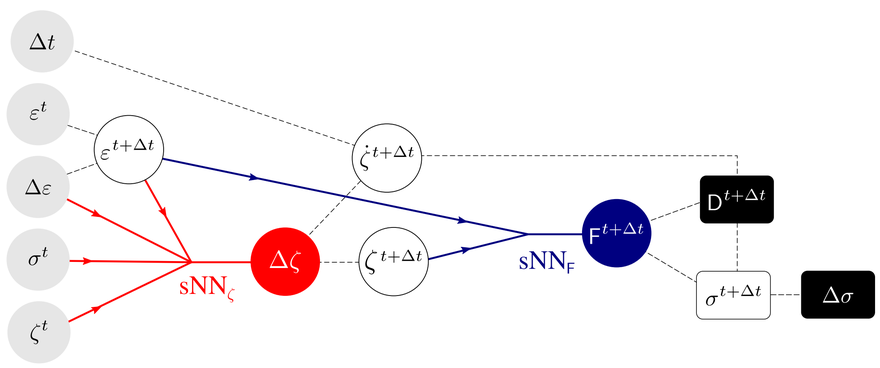
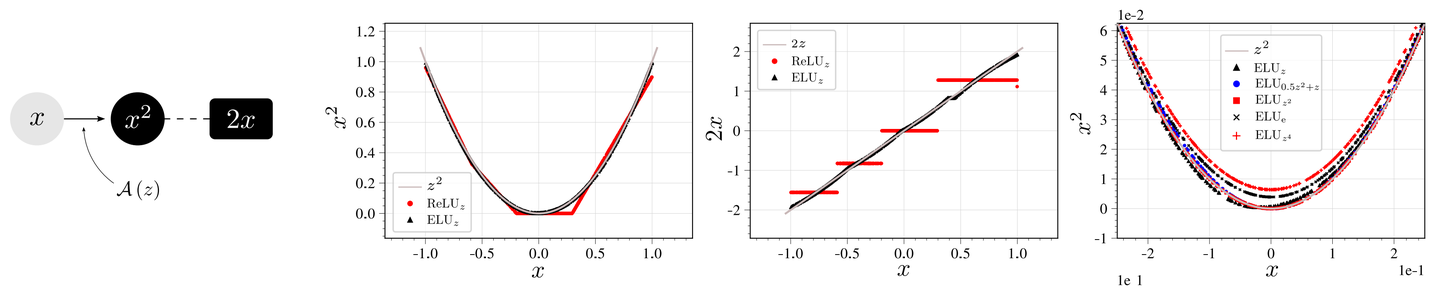
Architecture



1. $\varepsilon^{t+\Delta t} := \varepsilon^t + \Delta\varepsilon$
2. $\Delta\zeta = \mathsf{sNN}_\zeta@\left(\varepsilon^{t+\Delta t}, \Delta\varepsilon^t, \sigma^t, \zeta^t\right)$
3. $\dot{\zeta}^{t+1} \approx \frac{\Delta\zeta}{\Delta t}$, $\zeta^{t+1} := \zeta^t + \Delta\zeta^t$
4. $\mathsf{F}^{t+\Delta t} = \mathsf{sNN}_\mathsf{F}@(\varepsilon^{t+\Delta t}, \zeta^{t+\Delta t})$
5. $\mathsf{D}^{t+\Delta t} := -\dfrac{\partial \mathsf{F}^{t+\Delta t}}{\partial \zeta^{t+\Delta t}} \cdot \dot{\zeta}^{t+\Delta t}$
6. $\Delta\sigma := \dfrac{\partial \mathsf{F}^{t+\Delta t}}{\partial \varepsilon^{t+\Delta t}} - \sigma^t$

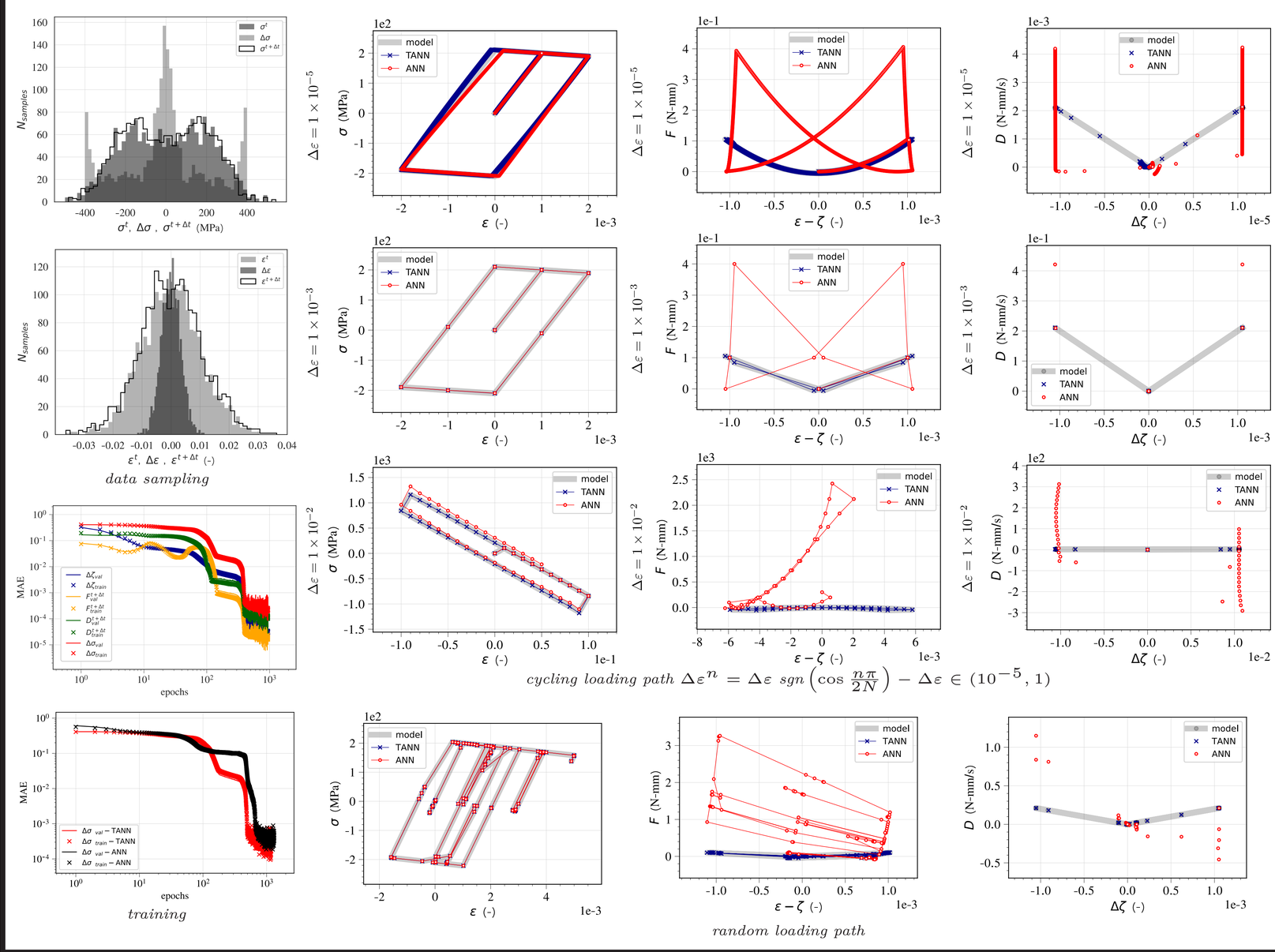
Second-order vanishing gradient

When dealing with TANNs, the issue of **second-order vanishing gradients** may arise. Similar to the first-order variant, it involves the **second derivatives of the activation functions**. Classical activation functions are not suitable choices.



Performance of TANNs vs standard ANNs

TANNs display **efficient and robust training**, and more **accurate predictions**. More important, TANNs predictions are always **thermodynamically consistent**, even for unseen data.



Concluding remarks

Thermodynamics-based Artificial Neural Networks (TANNs) do not have to identify the underlying pattern of thermodynamic laws during training, reducing the need of large data-sets and improving the **robustness** and the **performance** of **predictions**. The **predictions** remain **thermodynamically consistent**, even for unseen data. TANNs are excellent candidates for replacing constitutive calculations at Finite Element incremental formulations in solid mechanics.

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