Design of Physics-Aware Neural Networks: Symmetry constraints

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Hyperelastic material models are widely used to represent nonlinear behavior of engineering materials, such as rubber and foam. These models are equipped with a hyperelastic potential W, which needs to obey certain constraints to be physically meaningful. Recently, the consideration of such constraints, e.g. material symmetry, in machine-learned hyperelastic potentials has become an active field of research and the different methodologies available in the literature shall be investigated within the framework of this project.

Motivation

Established principles from materials modeling can be translated into basic **invariant** and **equivariant** operations, commonly found in machine learning. For example, objectivity and material symmetry transformations may be perceived as:

- **Invariant** operations on $W(\boldsymbol{F})$

$$\text{Objectivity} \rightarrow W(\boldsymbol{F}) = W(\boldsymbol{QF}) \quad \forall \boldsymbol{Q} \in SO(3) \tag{1}$$

$$\text{Symmetry} \rightarrow W(\boldsymbol{F}) = W(\boldsymbol{FG}) \quad \forall \boldsymbol{G} \in \mathcal{G} \subseteq SO(3) \tag{2}$$

- **Equivariant** operations on $\boldsymbol{P}(\boldsymbol{F}) = D_{\boldsymbol{F}} W(\boldsymbol{F}))$

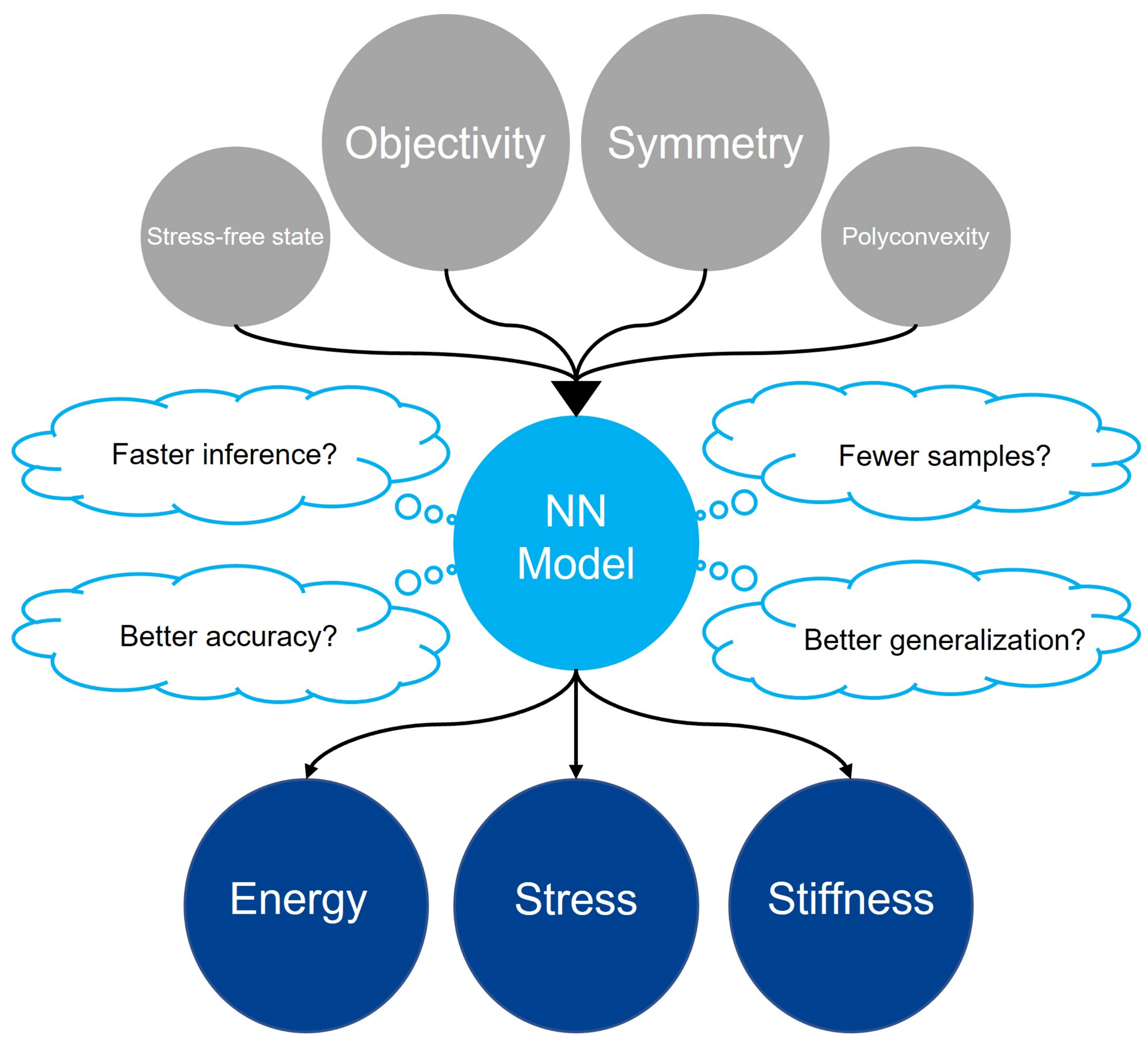
$$\text{Obejctivity} \rightarrow \boldsymbol{P}(\boldsymbol{QF}) = \boldsymbol{QP}(\boldsymbol{F}) \quad \forall \boldsymbol{Q} \in SO(3) \tag{3}$$

$$\text{Symmetry} \rightarrow \boldsymbol{P}(\boldsymbol{FG}) = \boldsymbol{P}(\boldsymbol{F})\boldsymbol{G} \quad \forall \boldsymbol{G} \in \mathcal{G} \subseteq SO(3) \tag{4}$$

The fulfillment of such transformations, either in an exact or approximated fashion, by a machine-learned hyperelastic potential $W^{ML}(\boldsymbol{F})$ is of upmost interest in this project.

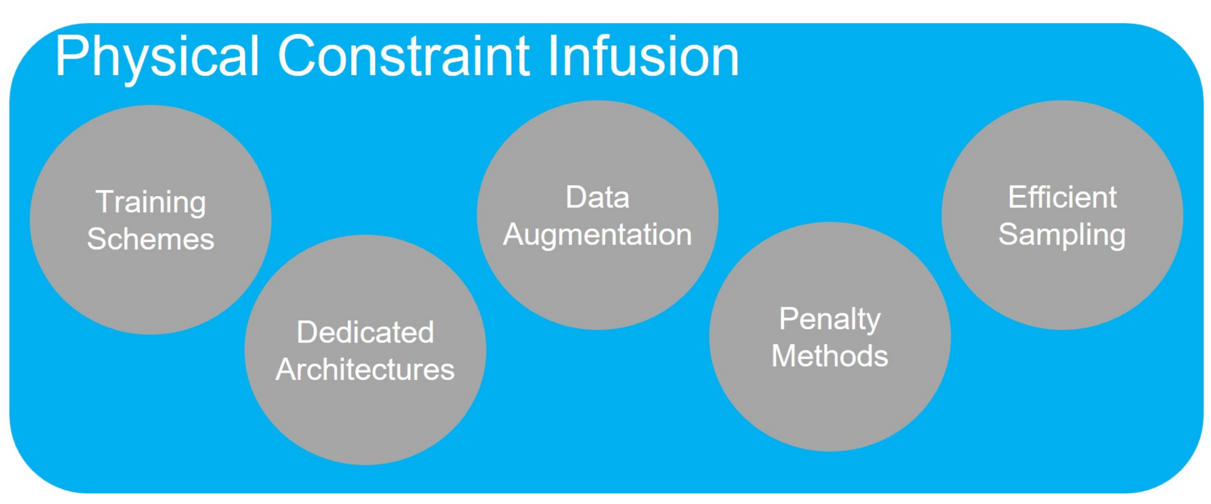
Research Questions

- How to efficiently incorporate physical constraints in the machine-learning model?
- How does the fulfillment of such constraints influence model accuracy?
- Does such fulfillment enable improvement of model features?
- How do the input and output features correlate?



Methods

- Data augmentation, penalty methods and dedicated machine-learning architectures are options to apply physical constraints in a machine-learning model



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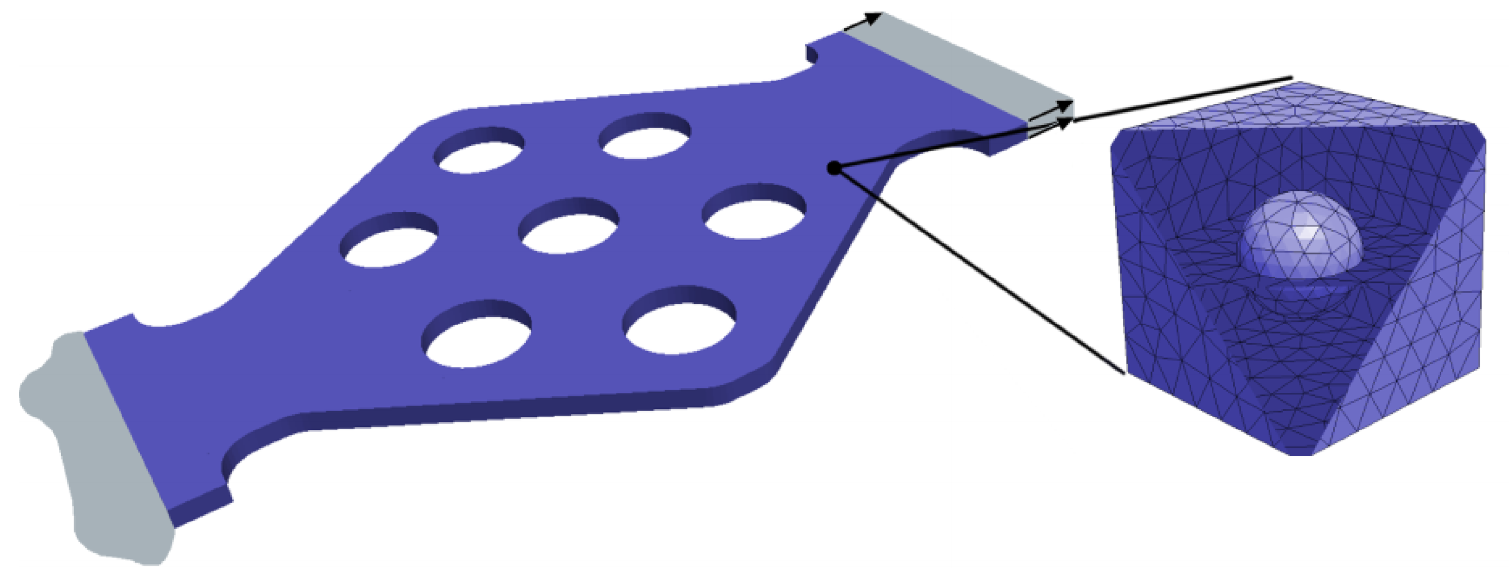
Applications

- Multiscale simulations can benefit from machine-learning models due to fast inference and evaluation, but are they still physically meaningful?



- Multi-parametric dependencies, e.g., additional geometry and material parameters

State-of-the-art

Group Symmetrization [1]

$$W^{ML}(\boldsymbol{F}) = \frac{1}{\#(\mathcal{G})} \sum_{\boldsymbol{G} \in \mathcal{G}} W_0(\boldsymbol{FG}),$$

where $\#(\mathcal{G})$ is the number of symmetry transformations in the corresponding symmetry group $\mathcal{G}$.

Constitutive Artificial Neural Networks (CANNs) [2]

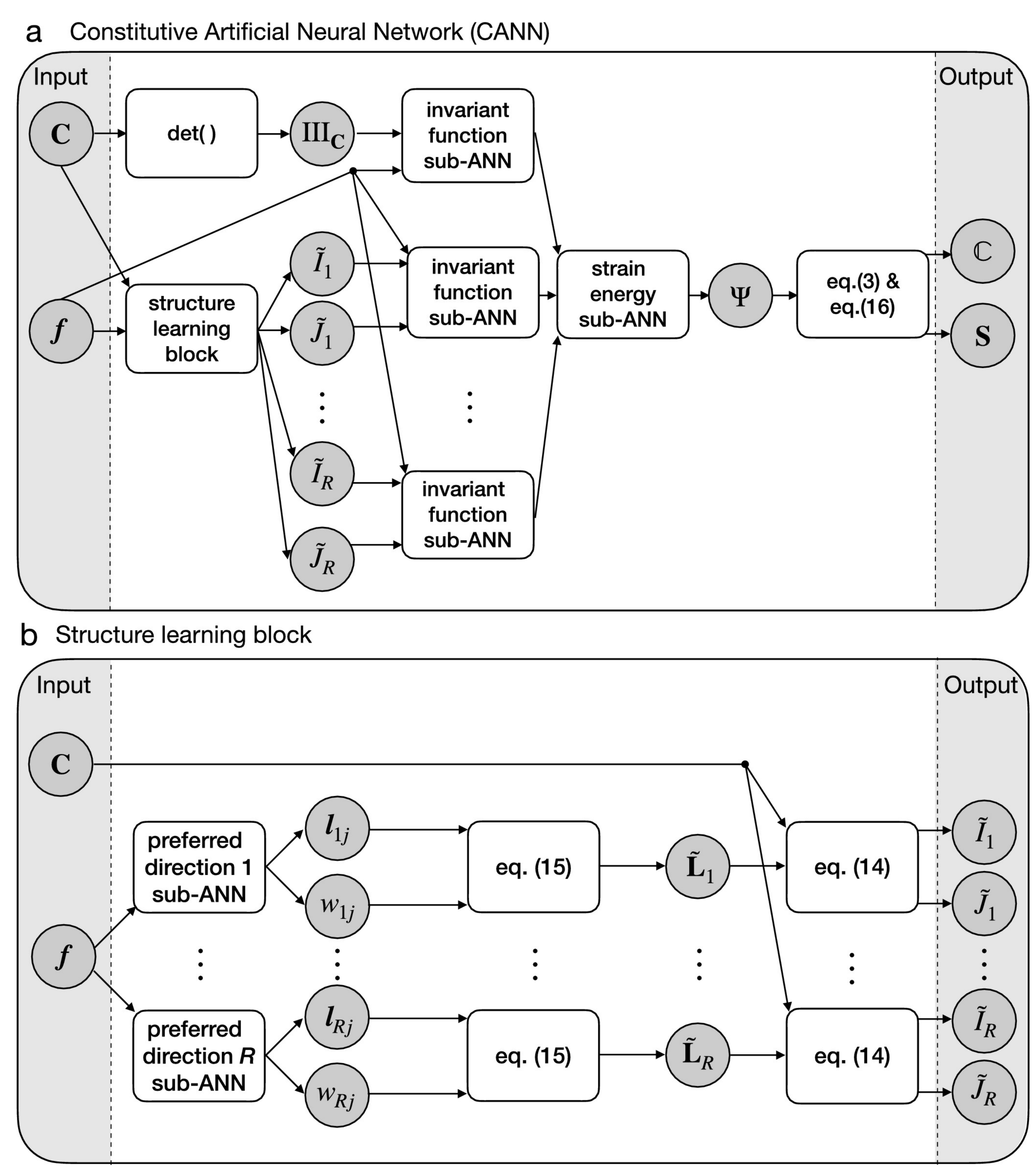


Figure from [2]

References

[1] Mauricio Fernández, Mostafa Jamshidian, Thomas Böhlke, Kristian Kersting, and Oliver Weeger.
Anisotropic hyperelastic constitutive models for finite deformations combining material theory and data-driven approaches with application to cubic lattice metamaterials.
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[2] Kevin Linka, Markus Hillgärtner, Kian P Abdolazizi, Roland C Aydin, Mikhail Itskov, and Christian J Cyron.
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