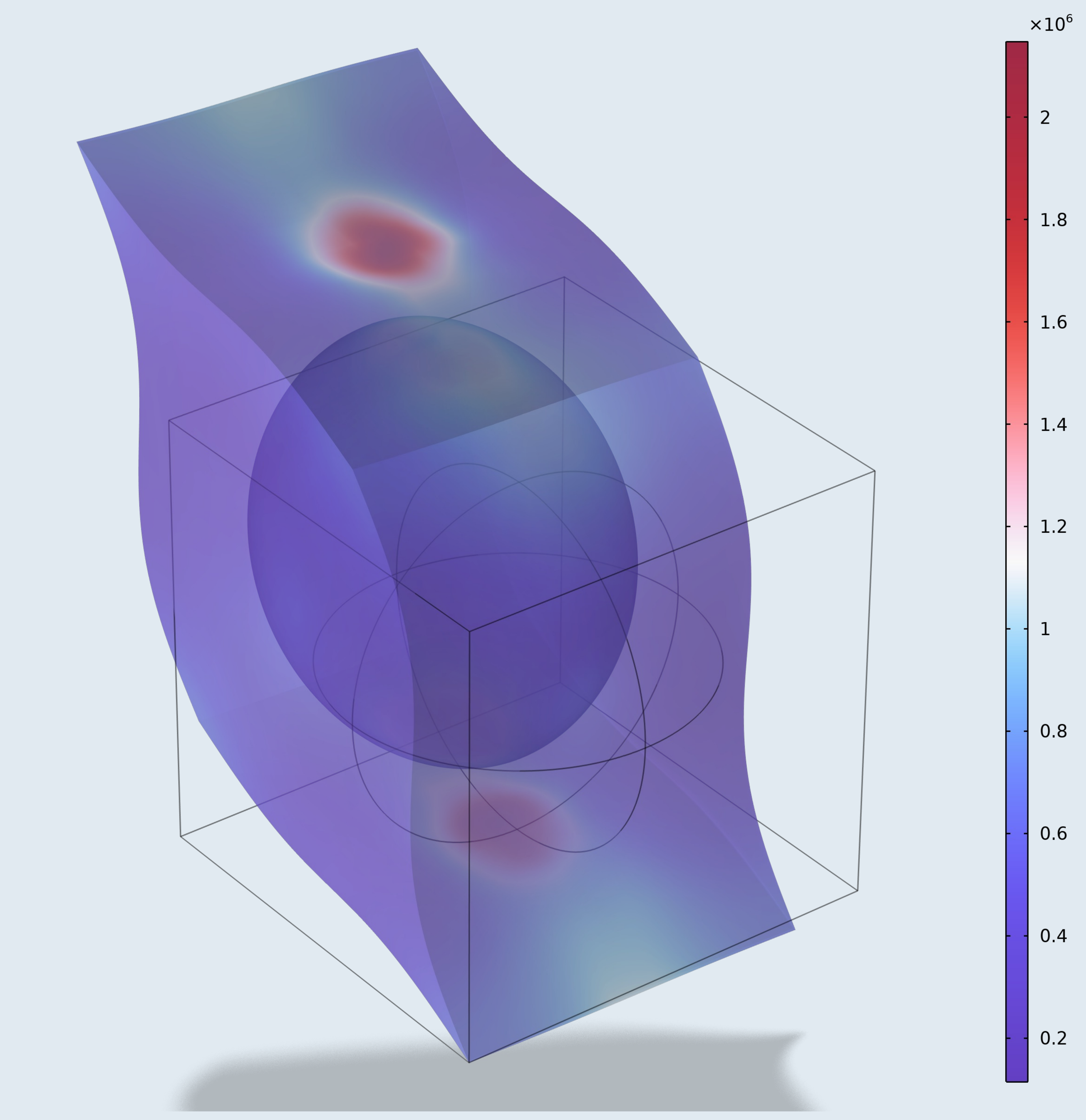

Nonlinear Homogenization of Metamaterials for Neural Network-Based Material Modeling

We built a pipeline to homogenize nonlinear metamaterials, train machine learning constitutive models and solve macroscopic FEA in COMSOL®.

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Project goals

In functional material design, achieving desired macroscopic properties through precise microstructural configurations remains a significant challenge. Numerical homogenization is a powerful computational approach to derive effective macroscopic properties of materials with complex microstructures.

Using COMSOL Multiphysics®, we generate detailed, high-fidelity homogenization data of microstructured materials. With these data, we calibrate physics-augmented neural network material models [1,2] that can accurately capture the complex behavior of heterogeneous materials within potential macroscopic digital twin applications [3,4].

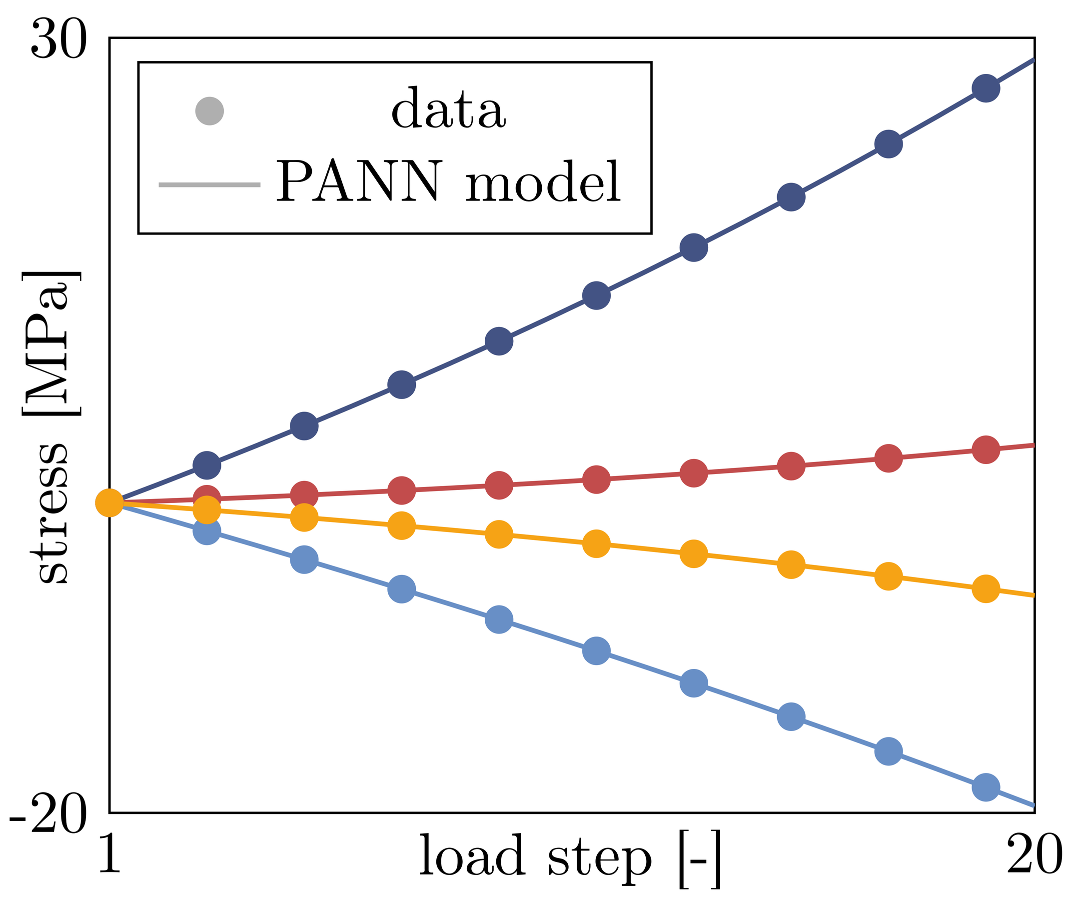

FIGURE 1. Homogenized First Piola-Kirchhoff stresses.

Nonlinear Homogenization

A spherical inclusion inside a material matrix is modeled with a user-defined, nearly incompressible hyperelastic Ogden material model, with a contrast of ten between the sphere and matrix material.

$$\psi = \sum_{p=1}^{N_O} \frac{\mu_p}{\alpha_p}\left[\sum_{\beta=1}^{N_\lambda} v_\beta \left(\lambda_\beta^{\mathrm{iso}}\right)^{\alpha_p} - 3\right] + \frac{\kappa}{4}\left(J^2 - 2\ln J - 1\right)$$

Our approach incorporates nonlinear material effects of finite strain elasticity. This encompasses modifying the Cell Periodicity boundary condition to accept variable deformation gradients. We homogenize the first Piola-Kirchhoff stress $\boldsymbol{P} = \partial_{\boldsymbol{F}}\, \psi$ and the tangent modulus $\mathbb{A} = \partial_{\boldsymbol{F}}\, \boldsymbol{P} = \partial^2_{\boldsymbol{F}\boldsymbol{F}} \psi$.

Neural Network-Based Material Model

The homogenized behavior of microstructures is often highly nonlinear. Thus, we envision using physics-augmented neural network constitutive models [1,2]. These models are formulated to fulfill important conditions such as thermodynamic consistency and convexity conditions by construction. They combine the extraordinary flexibility of neural networks with a sound mechanical basis. These material models are calibrated in a TensorFlow code using homogenization data generated with COMSOL Multiphysics®.

Currently, approaches are being investigated to include the calibrated neural network models back into macroscopic FEA simulations within COMSOL Multiphysics®.

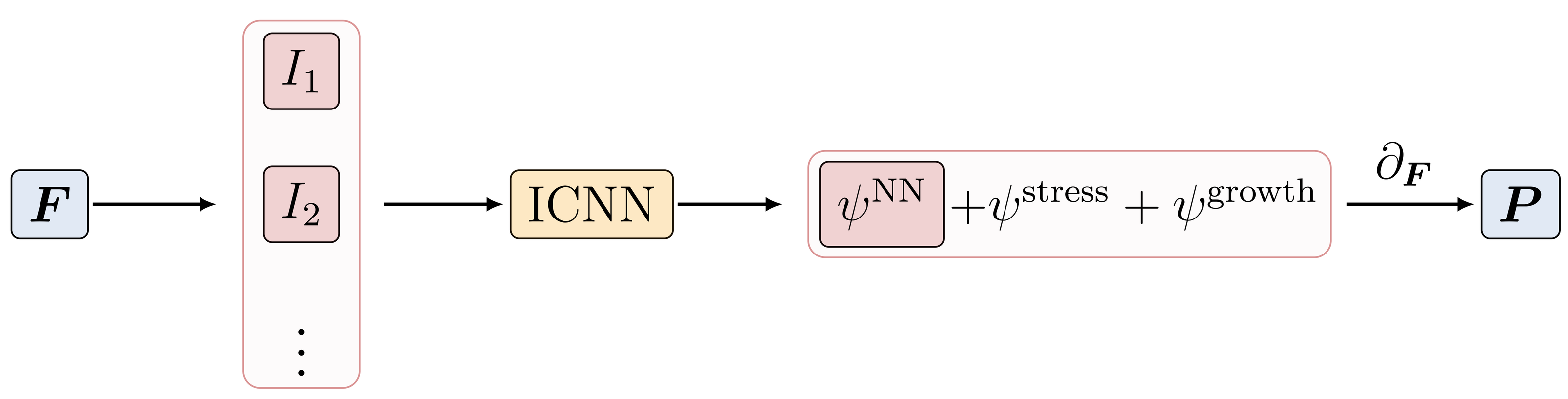

FIGURE 2. Hyperelastic physics-augmented neural network constitutive model.

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