INVERSE DESIGN OF MICROSTRUCTURES AND ARCHITECTED MATERIALS

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ABSTRACT

Inverse design of heterogeneous materials, microstructures, and architected solids is becoming an increasingly important topic in computational solid mechanics. The central challenge is to identify material architectures that achieve prescribed mechanical behavior while navigating high-dimensional design spaces, non-unique solutions, and expensive forward evaluations. Recent advances in artificial intelligence, data-driven modeling, and optimization methods offer new tools for addressing these challenges and for expanding the range of structures that can be explored and designed [1,2].

This Invited Minisymposium will focus on strategies for efficient exploration and optimization of complex material architectures. Of particular interest are approaches that reduce the dependence on large datasets generated through costly high-fidelity simulations or experiments. Surrogate models, reduced-order representations, and neural operators can accelerate repeated structure–property evaluations [2], while active learning and Bayesian optimization can guide the selection of informative or promising candidates under limited computational or experimental budgets [1]. Generative models offer a complementary route for addressing the non-uniqueness of inverse design by representing multiple candidate structures compatible with a desired response. Recent developments such as diffusion models and flow-matching approaches are particularly relevant for the generation of microstructures with prescribed effective properties or mechanical behavior. Learned latent and implicit representations, together with differentiable models and gradient-based optimization, further enable efficient search over complex geometric parameterizations. Contributions involving alternative learning-based, physics-guided, optimization-based, or hybrid strategies are equally encouraged.

Applications may encompass composites, porous and stochastic microstructures, and architected materials designed for prescribed stiffness, anisotropy, nonlinear response, stability, energy absorption, or other effective properties. The minisymposium aims to bring together researchers in computational solid mechanics, material modeling, optimization, and machine learning to exchange recent advances and foster reliable, data-efficient, and physically consistent approaches to inverse material design.

REFERENCES

[1] H. Danesh and H. Wessels, *Data-efficient Bayesian-guided design selection from large candidate sets: Application to hyperelastic stochastic metamaterials*, Materials & Design, 270, 116984, 2026.

[2] H. Eivazi and H. Wessels, *Physics-Informed Reduced-Order Operator Learning for Hyperelasticity in Continuum Micromechanics*, arXiv preprint, arXiv:2605.07738, 2026.