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DATA-DRIVEN EXPLORATION AND DESIGN OF MATERIALS

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ABSTRACT

Improving and accelerating materials development is an important goal in science and industry, as innovative, tailored, and optimized materials ranging from metals and polymers to composites and architected materials are key to a sustainable future. With recent advances in machine learning and manufacturing technologies, tailoring the chemical composition and the microstructure of classical materials as well as the internal structure of architected materials for a targeted property, i.e., inverse design, has become feasible.

The inverse design process requires techniques to characterize and reconstruct numerical models of the local material structure. Computational homogenization of these microstructures facilitates prediction and understanding of the interplay between effective properties and microstructural features of complex materials. To describe the nonlinear, inelastic effective behavior of materials with high precision while explicitly considering design variables, neural networks enriched with knowledge from fundamental underlying physics enable an improved extrapolation capability and the use of sparse training data. Beyond constitutive modeling, data analysis and machine learning help to exploit knowledge from simulations in terms of surrogate models and are, therefore, key to the exploration and prediction of structure-property linkages for the computational design and optimization of materials and structures.

Topics of interest covered within this mini-symposium include but are not limited to:

- techniques for exploration and inversion of process-structure-property linkages,
- inverse design approaches for metals, polymers, composites, and architected materials,
- design approaches that account for crucial manufacturing constraints,
- machine learning in computational mechanics and constitutive modeling,
- data-driven multiscale simulations,
- microstructure characterization and reconstruction, e.g., 2D and 3D image-based methods, definition of descriptors
- numerical and experimental analysis of designer materials across scales.