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DATA-DRIVEN MODELING AND DESIGN OF MATERIALS

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MINISYMPOSIUM

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 modern composites and architected materials are key to a sustainable future. Driven by progress in digitization and high-throughput experiments that enhance data availability, the interest in data-driven techniques, which facilitate material design, is constantly increasing.

Research in the field of data-driven modeling and design of materials covers a wide range of topics. For instance, techniques for reconstructing microstructures may enable the generation of appropriate simulation domains, i.e., realistic representative or statistical volume elements. Computational homogenization of these microstructures facilitates prediction and understanding of the interplay between effective properties and microstructural features of complex materials. To describe the behavior of materials with high precision, model-free approaches that directly exploit data or techniques based on machine learning models that learn from data could be used. In this context, the trend to enrich machine learning approaches with knowledge from fundamental underlying physics enables 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 prediction of structure-property linkages for the computational design and optimization of materials and structures. Finally, the inverse design of suitable microstructures that ensure certain effective target properties is a task for which machine learning methods are predestined.

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

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