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DATA-DRIVEN MODELING AND DESIGN OF ADDITIVELY MANUFACTURED MATERIALS AND STRUCTURES

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ABSTRACT

Speeding up the development of materials for additive manufacturing (AM) is a key objective in research and industry, as it is essential for realizing the technology's full potential and supporting sustainable production. This requires a deeper understanding of the interplay between material composition, processing parameters, the resulting microstructure, and the response under various loading conditions. As digitization advances and high-throughput simulations and experiments generate increasingly large datasets, interest in data-driven approaches to the design of materials and structures continues to grow. These approaches will make inverse design feasible, i.e., tailoring the chemical composition and microstructure of conventional materials, as well as the internal architecture of architected materials, to a targeted property.

Research on data-driven modeling and materials design for AM spans a broad range of topics. Thermodynamic modeling to predict phase formation, simulation of how microstructures form and evolve, and methods for reconstructing microstructures from image data all support the generation and parametrization of suitable representative or statistical volume elements. Computational homogenization of these microstructures enables the prediction of effective properties. To capture the behavior of AM materials and structures accurately, machine learning approaches can incorporate knowledge of the underlying physics, which improves extrapolation, allows training with sparse data, and permits design parameters to be integrated directly. Beyond constitutive modeling, data analysis and machine learning make it possible to extract knowledge from simulations in the form of surrogate models. They are therefore central to predicting process-structure-property relationships for the computational design and optimization of materials and structures.

This session welcomes contributions on data-driven methods for, but not limited to:

- Inverse, generative design and optimization of classical and architected materials,
- Design of materials for AM, e.g. metallic alloys, polymers, ceramics,
- AM process simulations to predict solidification and formation of phases and microstructures as well as resulting material properties,
- Techniques for exploring composition-process-structure-property linkages, in full or in part,
- Numerical and experimental analysis of designer materials,
- Deformation and fracture behavior of AM materials and structures.