MSE 2024

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dgm.de

Topic M: Modelling and Simulation

M04: Hybrid data-driven modeling for scalable materials design

The Twin (Green and Digital) Transition asks for new advanced materials and requires fast adaption to varying process parameters. Classical approaches to materials discovery and process development are based on high-throughput experimental assessments. This quickly becomes infeasible as the number of possible chemical components and the number of process parameters increase.

Therefore, a data-driven modeling becomes an important tool in the process-structure-property-performance chain and complements the classical ICME approach to accelerate materials modeling and design. The development, modification and multi-scale application of these methods, including an efficient organization of research data management systems, is one of the key interests in academia and industry. Depending on the problem to be solved, such as modeling complex physical phenomena, predicting specific material properties, optimizing process parameters, or improving chemical compositions under constraints, different data-driven methods and models are employed. These include statistical and machine learning, active and deep learning, computer vision, natural language processing, multi-objective optimization, etc. They are applied to an increasing amount of experimental and simulation data to derive robust and efficient data-driven models.

To improve the understanding of complex phenomena in materials science applications, so-called hybrid models are used, combining physics-based material models for the underlying process-structure-property relationships (where available and applicable) with observations (where knowledge is limited). Well-constructed hybrid models generalize better and reduce the number of required experiments and simulations.

Topics of interest include but are not limited to the following research points:

- development of data-driven methods and their applications to simulations and experimental data,
- data-fusion of experimental and simulations data, i.e. hybrid approaches,
- consideration of uncertainties in related to experimental and simulation data
- hybrid models as physically-based data-driven modelling,
- sequential adaptive learning using Active Learning Loops for alloy design and optimization,
- acceleration of process simulation for predicting microstructures and their evolution,
- microstructure characterisation and reconstruction (e.g. 2D and 3D image-based methods),
- computer vision for analysis of microstructure evolution using traditional and deep learning methods,
- dimensionality reduction, features extraction and regression techniques for establishing process-structure-property-performance linkages or part of it.
- high-performance data processing techniques,
- research data management systems

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