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Data-based characterization, modeling and simulation of materials across scales

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Improving and accelerating materials development is an essential goal in science and industry, as innovative, tailored and optimized materials are key to saving resources. Thanks to the progressing digitalization, data-driven and machine learning approaches facilitating in-silico materials design and optimization have recently emerged. Research in this field covers a wide range of topics. Appropriate geometries that can be used, e.g., in computational homogenization approaches, are available through characterization and reconstruction of real microstructures. Also, data-driven approaches based on machine learning allow efficient computations across different temporal- and length-scales limiting or suppressing the assumptions on the material's constitutive behavior. In this context, data dependency is one of the key issues that can be reduced by adopting physics-constrained learning algorithms, which integrate mechanical knowledge directly in the training process. 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. Topics of interest covered within this mini-symposium include but are not limited to:

- Data-driven techniques in computational mechanics,
- Machine learning in the context of constitutive modeling,
- Microstructure characterization and reconstruction, e.g., 2D and 3D image-based methods,
- Data-based multiscale simulations,
- Machine learning applications for the acceleration of multiscale computations,
- Dimensionality reduction and regression techniques for establishing process-structure-property linkages or part of them.