Towards a Microstructure Simulation Ecosystem

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The microstructure is the state variables determining the properties of any material and accordingly also of any component made from a material. The simulation of microstructure evolution even in complex metallic alloys has made enormous progress in the last decade. Respective simulation tools like MICRESS® [1] meanwhile are successfully used to tackle and to solve problems of industrial interest [2],[3],[4].
Microstructure evolution occurs at the boundary between processes occurring at the macroscopic scale of the component and the atomistic scale determining e.g. the properties of pure phases or the properties of interfaces. Microstructures further integrate all effects and phenomena occurring along the entire processing history of a component. Simulating the evolution of microstructures thus requires interoperability between a variety of simulation codes operating at different scales and also a seamless data exchange between experimental microstructure data and their simulated counterparts [5] as well as thermodynamic and kinetic data. This variety of tools and data eventually has to be orchestrated by suitable tools. Modular configurable workflows eventually must be executed on suitable grid-based platforms [6] or in a cloud-based infrastructure [7].
The information exchange within such an ecosystem must be based on format and data standards or even better on an ontology. The development of a microstructure ontology e.g. based on a first metadata description [8] is objective of a recent task group of the EMMC.

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