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A service-oriented approach for multiscale materials modelling and current challenges

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Macroscopic effects in complex materials arise from physical phenomena on multiple length (from nano-through micrometer) and time (from femto- through microsecond) scales and therefore properties of such materials can be predicted accurately basing on the properties of the contained building blocks. This makes not only the physical description easier to understand but also computer simulations of whole macroscopic devices feasible due to the effective linear scaling. However the application of multiscale methods in materials research is currently still a challenge. In particular, the diversity of the required fields of expertise limits the feasibility of multiscale techniques, especially for experimental and industrial researchers.

In the MMM@HPC project a significant effort has been done to enable non-expert users to use multiscale models. Using directed acyclic graphs, so-called workflows, and a service-oriented approach we implement sequential multiscale models in computer simulations by integration of existing methods operating on the individual scales. This approach is particularly practical and scales well for loosely hierarchically coupled sub-models. The main advantage is that the complexity of the individual methods is hidden and only parameters and data relevant for the overall workflow are exposed to the modeller and the end user. Also the technical details of the computing infrastructure are effectively hidden making the access to the resources and installed applications transparent.

In this contribution we will provide an overview of our progress in development and deployment of an e-infrastructure for multiscale modelling and discuss current and upcoming challenges such as the data complexity, licensing issues and sustainability, including the uptake of the methodology by the community and ensuring long-term support and operation of the infrastructure.

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