SIMULATING POLYURETHANE FOAMS USING THE MODENA MULTI-SCALE SIMULATION FRAMEWORK

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The MoDeNa project [1] aims at developing, demonstrating and assessing an easy-to-use multi-scale software framework application under an open-source licensing scheme that delivers models with feasible computational loads for process and product design of complex materials. The concept of MoDeNa is an interconnected multi-scale software framework. As application cases we consider polyurethane foams (PU), which are excellent examples of a large turnover product produced in a variety of qualities and of which the properties are the result of designing and controlling the material structure on all levels of scale, from the molecule to the final product. Hence, four scales will be linked together by this framework namely the nano-, micro-, meso-, and macroscale where OpenFOAM is deployed on the macroscale scale.

Multi-scale coupling requires the exchange of information between software instances developed for specific scales in a consistent way. In order to achieve this, generating consistent representations for models and data is necessary. The information exchange is governed by protocols and may occur in two ways, namely:

- "forward mapping" (passing information from the microscopic to the macroscopic scale in upward direction)
- "backward mapping" (passing information from the macroscopic to the microscopic scale in downward direction)

"Forward mapping" is relatively straightforward, while "backward mapping" inevitably requires iteration since changing the operating conditions at the fine level changes the feedback to the coarse level. "Backward mapping" can be realised by "two-way coupling" or by "fitting surrogate models". The first approach usually requires exchange of large amounts of data during runtime that may be expensive either due to the complexity of the data exchange or the computational cost associated with executing the microscopic-scale simulation. In such cases, replacing the microscopic-scale simulation with a surrogate model presents the only viable alternative. This operation inherently constitutes a transfer of data across scales and MoDeNa is unique in that it focuses on this approach.

The MoDeNa framework handles the communication across scales through recipes and adapters. Recipes perform simulations by executing applications (in-house codes or external software packages such as FOAM, Materials Studio, PC-Saft) for a given set of inputs. Adapters handle the communication with the MoDeNa software framework. Both, recipes and adapters are application specific.

The software framework consists of an orchestrator, a database and a interface library. The orchestrator is based on FireWorks [2] and constitutes the backbone of the software framework in that it schedules simulations and operations required by the framework. The NoSQL database MongoDB [3] is used to store the state of the work-flow as well as the surrogate models together with associated data. The interface library consists of two parts: A high-level python module providing access to the database as well as design of experiments and regression analysis capabilities by building on MongoEngine [4] and R [5], respectively. The second part is a low-level library providing unified access to the surrogate models. This component is written in C to ensure interoperability across platforms and target applications while providing the computationally efficient model execution required by the applications.

The macroscale model for the expanding PU foam is formulated in OpenFOAM and interconnectivity of the scales is realised through the MoDeNa software framework. The macroscale model is based on Computational Fluid Dynamics (CFD) combined with a Population Balance Equation (PBE). The CFD-PBE is targeted at 3D simulations of industrial-scale foaming processes. A new solver (`PUFoam`) is formulated, implemented and validated within the OpenFOAM software structure. The solver accounts for three major physical phenomena taking place within the PU foam: variation of material properties, evolution of bubbles size distribution and kinetics of the reactions.

The general procedure to perform a communication between different scales starts with instantiation of the surrogate model which is the read from the database. After allocating the required memory for the input and output arguments of the surrogate model, the model is called, the results are retrieved and used in the macroscale tool. For example, the bubble growth rate is needed to simulate the growth of bubbles via PBE. However, the growth rate itself depends on the dynamic characteristics of the foam during the foaming process and is too expensive to calculate on a cell-by-cell basis. By using the MoDeNa framework the growth rate is wrapped into a surrogate model with parameters dynamically fitted

to detailed simulations. The information is then applied in the `PUFoam` solver to realistically represent the state of gas bubbles within the foam at a much lower computational cost.

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References

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