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A new approach to 3D front-tracking simulation of grain growth

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Numerical modeling currently plays an important role in the scientific pursuit to predict, understand and interpret complex systems such as (sub-)structure in polycrystalline systems. Contrary to experimental methods, numerical modeling is unhindered by time- and length-scale constraints. Numerical models can thus be developed based on theory, be tested and validated with experiments and then applied to systems that are beyond the scope of experiments, such as the creeping of salt in diapirs or, in more general terms, the evolution of a microstructure. Already existing numerical models usually are designed to solve specific problems and can not easily be extended to other problems. Existing numerical simulation packages such as Elle that overcome these restrictions can be used to simulate different coupled processes, but are limited to two dimensions. We are currently developing new simulation software that will be capable of modeling coupled processes in three dimensions (xyz-space and time). The software is based on the principle of polyhedra enclosing a volume of material (such as one grain, one crustal block etc.). The polyhedra are bounded by facets and by changing the facets (e.g. their size, orientation etc.) the represented volume element changes its shape. This is a front-tracking approach. It is the change of energy across the front (facet) that can be calculated and changes the shape of the polyhedra. This setting is capable of simulating a large number of processes (such as grain growth, development of liquid networks along grain boundaries, diffusion etc.). We will present our first results using this new software and are especially looking for feedback on what should and should not be included in the software from potential future users.