From atoms to insights: How powerful data analysis tools help us understand and visualize atomic-level materials simulations

Alexander Stukowski

Atomistic simulation approaches such as molecular dynamics (MD) in conjunction with massively-parallel supercomputers and refined interatomic potentials can now reach material length scales directly comparable to experiment. They make it possible, for example, to study nanomechanical behavior of entire microstructures down to the atomic level in full detail and provide a wealth of information on the involved material defects and physical mechanisms.

However, the huge number of degrees of freedom in such large-scale simulations necessitates advanced data filtering and analysis techniques that help us deal with the inherent complexity of many materials processes and structures and allow us to compress the output data to be stored. The goal of ongoing research is therefore to develop smart computational methods that can reduce the simulation output to essential features and link atomistics with mesoscopic materials concepts such as grains, dislocation lines, surfaces and deformation fields – in other words, high-level descriptions that are more instrumental in gaining insights than the underlying all-atom model.

Furthermore, I will provide an overview of one of the leading data visualization tools in the field ("OVITO"), which is being developed in my group to work with outputs from particle simulation models.