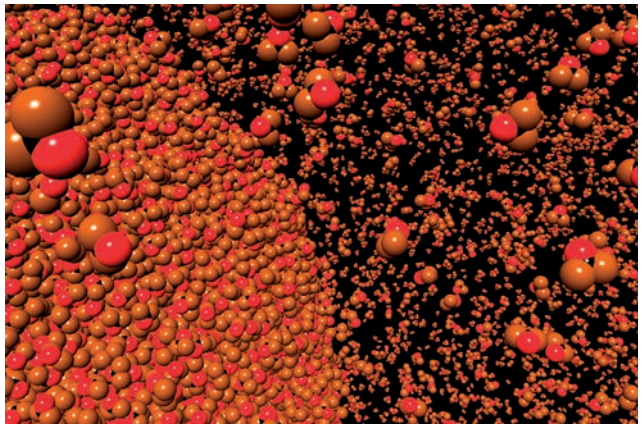
SkaSim

SkaSim - Scalable HPC-Codes for Molecular Simulation in the Chemical Industry

Molecular dynamics (MD) and Monte-Carlo (MC) simulations form the basis for investigating many relevant application scenarios in science and engineering. At the heart of these simulations lie physically meaningful and quantitative models of molecular interactions, requiring precise validation through state of the art ab initio calculations and experimental data. The extreme spatial and temporal resolution (individual molecules, femtoseconds) of such simulations allow for very reliable predictions of material properties, even where experiments are impossible or dangerous. However, this extreme resolution also implies substantial computational demands in order to investigate scenarios in a timely manner. The same holds true for nanofluidics: realistic insights, not obtainable experimentally, can be captured through simulation. Complex phenomena as for instance phase transitions (e.g. condensation) can be investigated on the molecular level, allowing new and more fundamental insights. However, as the dynamics of every molecule is evaluated explicitly, the number of simulated molecules needs to be considerable in order to capture the phenomena in question. Determining experimentally elusive properties of matter is attracting increasing attention from industry. Be it in process engineering, where the already highly optimized procedures can only be improved through better and more detailed data and understanding.



The computational power required to generate the quantity and quality of data required is significant. Thus, only through the efficient use of cutting-edge hardware can these demands be met. However, many relevant scenarios are far from trivial to simulate at scale, e.g. coinciding fluid and gaseous phases in a highly dynamic environment as in condensation or evaporation.
However, the industrial development of new products and processes will experience a fundamental change in the coming years. Expensive and oftentimes dangerous experiments can be replaced with safe and increasingly efficient and affordable simulations. For this transition to take place, simulations need to be performed with accuracies comparable to high-quality experiments. Besides the computational requirements, this calls for extremely accurate molecular models and, for complex scenarios, reliable new methodologies.

The challenges to simulate such scenarios efficiently are huge and will be addressed in SkaSim.

The interdisciplinary consortium is lead by the High Performance Computing Center Stuttgart (HLRS), and brings together a dozen partners from academia and industry. Molecular modelling and simulation is a key technology for the chemical industry of the future. Having started in July 2013, the BMBF project SkaSim will run for 36 months, carrying the molecular simulation technology forward, thus enabling new products, new processes and opening up new opportunities in science.

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