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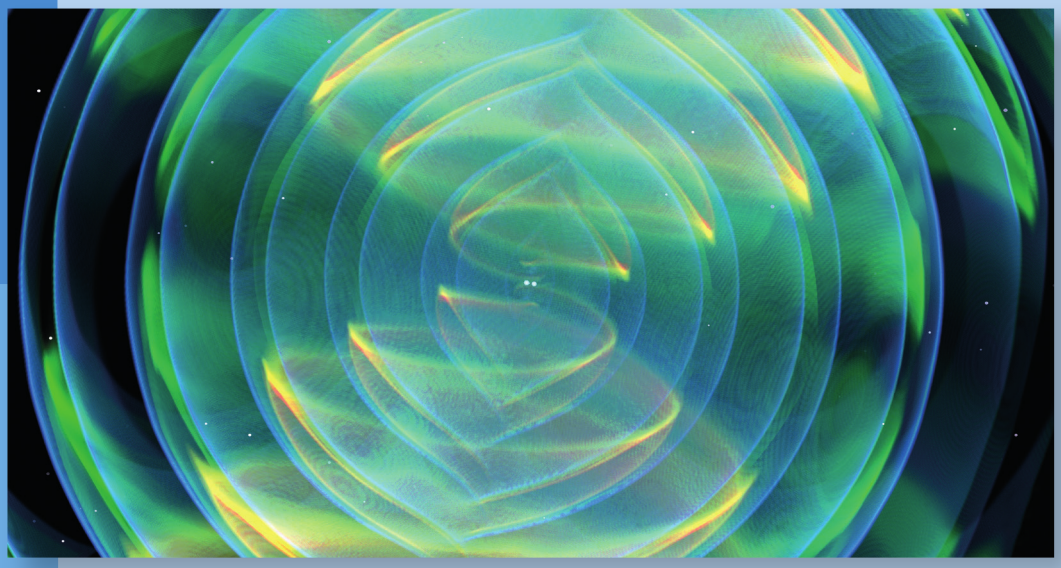

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Massively-parallel molecular dynamics simulation of fluids at interfaces

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Thermodynamics and Energy Technology, Universität Paderborn

SuperMUC Project ID: pr48te

Introduction

Molecular modelling and simulation is an established method for describing and predicting thermodynamic properties of fluids. It is well suitable for investigating phenomena on small length and time scales; often, however, scale-bridging series of simulations are needed to facilitate a reliable extrapolation from the nanoscale to the respective technically relevant length and time scales. The supercomputing project SPARLAMPE ("Scalable, Performant And Resilient Large-scale Applications of Molecular Process Engineering") examines interfacial properties of fluids, their contact with solid materials, interfacial fluctuations and finite-size effects, linear transport coefficients in the bulk and at interfaces and surfaces as well as transport processes near and far from equilibrium. These phenomena are investigated by massively-parallel molecular dynamics (MD) simulation, based on quantitatively reliable classical-mechanical force fields. The simulation results are combined to obtain an understanding of the complex processes undergone by cutting liquids during machining, in particular in the region of contact between the tool and the work piece.

With efficiently parallelized MD codes, scale-bridging simulation approaches for systems containing up to a trillion molecules have become feasible in recent years. Here, the program *ls1 mardyn* is used, i.e., an in-house code which is developed in collaboration with multiple academic partners [1], beside LAMMPS, which is externally developed free software.

Results and Methods

Nine publications have so far appeared on the basis of the computational resources allocated by LRZ within the SPARLAMPE supercomputing project. The representative results which are briefly illustrated here concern quantitatively accurate modelling of the vapour-liquid surface tension of real fluids [2], cf. Figure 1, wetting of structured surfaces [3], cf. Figure 2, and molecular simulation of the processes experienced by cutting liquids during nano-machining operations [4], cf. Figure 3.

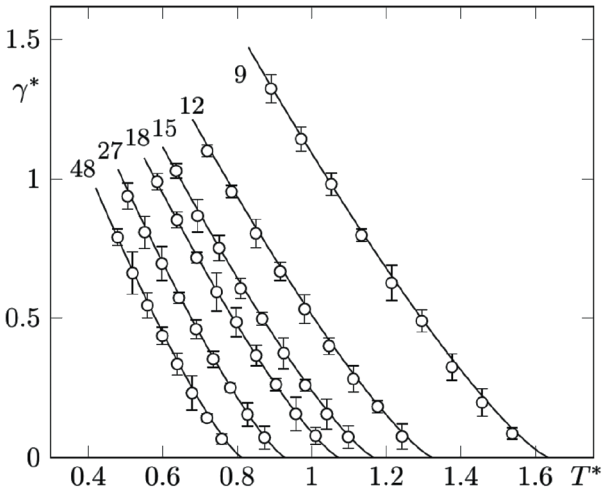

Figure 1: Surface tension over temperature (as dimensionless reduced quantities) for the Mie-6 class of fluid models, which has three parameters. By systematic exploration of the parameter space, the behaviour of the whole model class can be captured and correlated [2]. On this basis, molecular models can be adjusted to bulk and interfacial properties of real fluids, e.g., by multicriteria optimization.

The present MD simulations were carried out with *ls1 mardyn* [1-3] as well as LAMMPS [4]; the boundary conditions mainly correspond to the canonical ensemble, i.e., to constant N, V, and T. Concerning computational requirements, four major types of simulation runs exist:

(1) Test runs with small systems, or production runs for small single-phase systems; supercomputing resources were not needed for this purpose, except for very few test runs concerning the SuperMUC environment itself. Such simulations are always required to a limited extent.

(2) Scenarios where of the order of 30 to 300 simulations need to be carried out with different model pa-

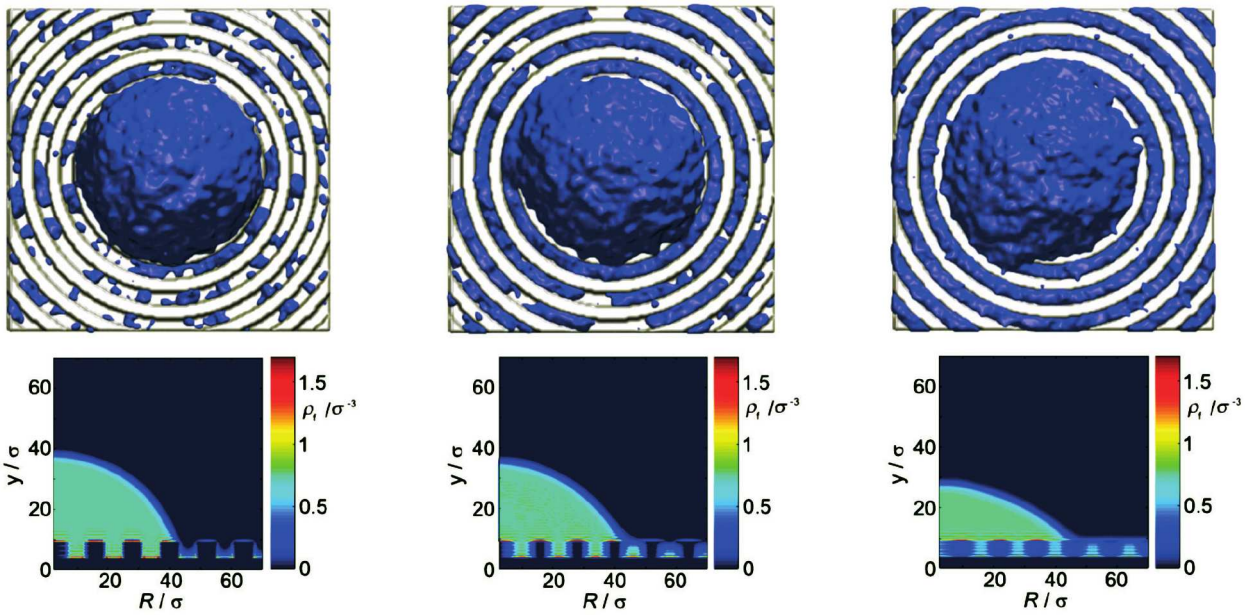

Figure 2: Three snapshots from a single simulation of a sessile droplet on a solid substrate which is structured by concentric cylindrical grooves; spreading of the droplet, i.e., a special case of wetting dynamics, is observed here [3]. The present regime follows a spreading mechanism conjectured by de Gennes: Thereby, first a metastable state is established (left), which breaks down by nucleation of a bridge (middle). The bridge continuously grows in azimuthal direction; depending on the boundary conditions, the final state may exhibit symmetry breaking (right).

rameters or boundary conditions, where the simulated systems are heterogeneous (which makes them computationally less trivial and requires a greater number of simulation time steps) and typically contain of the order of 30000 to 300000 molecules. The vapour-liquid surface tension simulations [2] and the three-phase simulations of sessile droplets on structured solid substrates [3] are of this type.

(3) Scenarios where a small series of computationally intensive production runs need to be carried out; large systems, particularly if they involve fluid-solid contact and even more so if the simulated scenarios are inherently dynamic in nature, also require a large number of simulation time steps. Here, this is the case for the MD simulations of nano-machining processes [4], cf. Figure 3, where five million interaction sites were included, and

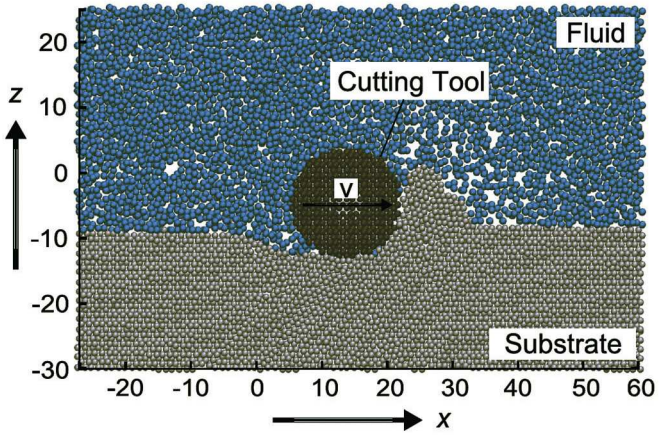

Figure 3: Scenario considered in MD simulations of nano-machining. The influence of the unlike interaction between the fluid and the solid components (substrate and cutting tool) on the friction coefficient was discussed for the truncated-shifted Lennard-Jones potential [4].

even though the simulation parameters were varied to a lesser extent than for the other scenarios, simulations needed to be repeated a few times to facilitate an assessment of the validity and the uncertainty of the simulation outcome.

(4) Scaling tests in the narrow sense, where simulations are conducted with the main purpose of analysing the strong and/or weak scaling of a code for a particular application scenario on a particular platform. These simulations by design typically cover all the range of available scales, up to the whole cluster. Nonetheless, the resource requirements are limited, given that only few time steps are needed. No such results are shown here; however, from such a test on SuperMUC, the present MD code *ls1 mardyn* holds the standing MD world record in terms of system size. Ongoing work, which is still in progress, will extend these results by performance tests that compare *ls1 mardyn* to LAMMPS, GROMACS, and further MD codes, on SuperMUC and on other platforms.

References and Links

[1] http://www.ls1-mardyn.de/

[2] S. Werth, K. Stöbener, M. Horsch, and H. Hasse. 2017. Simultaneous description of bulk and interfacial properties of fluids by the Mie potential. Mol. Phys. 115, 9-12, 1017-1030.

[3] S. Becker, M. Kohns, H. M. Urbassek, M. Horsch, and H. Hasse. 2017. Static and dynamic wetting behavior of drops on impregnated structured walls by molecular dynamics simulation. J. Phys. Chem. C 121, 23, 12669-12683.

[4] M. P. Lautenschlaeger, S. Stephan, M. T. Horsch, B. Kirsch, J. C. Aurich, and H. Hasse. 2018. Effects of lubrication on friction and heat transfer in machining processes on the nanoscale: A molecular dynamics approach. Procedia CIRP 67, 296-301.

In this book, the Leibniz Supercomputing Centre (LRZ), a member of the Gauss Centre for Supercomputing (GCS), reports on the results of numerical simulations, performed in 2016 and 2017 on the SuperMUC petascale system. More than 110 project reports give an impressive overview of the utilization of SuperMUC, the Tier-0 system of the Bavarian Academy of Sciences and Humanities.

SuperMUC Phase 1 began user operation in July, 2012, and **SuperMUC Phase 2** (picture above) became operational in May 2015. Each system segment has a peak performance of more than 3 PFLOP/s. Both phases are based on Intel x86 architecture and are coupled via a common parallel file system (GPFS). They are independently operated, but offer an identical programming environment. A detailed system description can be found in the appendix.

The articles provide an overview of the broad range of applications that use high performance computing to solve the most challenging scientific problems. For each project, the scientific background is described, along with the results achieved and the methodology used. References for further reading are included with each report.

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