# MaST: Scale-Bridging Exploration of Transcritical Fluid Systems

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***Abstract* – Understanding the behavior of multi-component flow systems is a challenging task. This is especially true for mixtures in the transcritical regime, i.e. mixtures under very high pressure but at relatively low temperature, such as fuel injection processes in rocket chambers. The analysis of the underlying flow processes, e.g. droplet and bubble formation, requires detailed multiscale considerations, ranging from molecular properties to large-scale continuum flow field simulation and analysis. In our dtec.bw project "MaST: Macro/Micro-simulation of Phase Decomposition in the Transcritical Regime", we investigate such systems in a multi-disciplinary consortium. Various simulation techniques, including molecular dynamics simulation (MD), classical density functional theory (DFT), computational fluid dynamics (CFD) and scale-bridging molecular-continuum approaches, as well as experimental studies are developed, evaluated, and—where possible—compared for relevant flow scenarios. In this contribution, we report on first case studies, such as injection and multi-phase molecular simulation studies, and on the development of molecular-continuum simulation software for multi-phase and multi-component systems. We further discuss technological requirements for current and anticipated analyses in terms of both experimental set ups, which necessitate the establishment of a high-pressure chamber, and simulation studies, which, due to their high computational intensity, rely on high performance computing approaches.**

***Keyword – Computational fluid dynamics, molecular dynamics, density functional theory, injection, high performance computing***

NOMENCLATURE

| | |
|---|---|
| CFD | Computational fluid dynamics |
| DFT | Density functional theory |
| fps | Frames per second |
| MD | Molecular dynamics |

## I. INTRODUCTION

Injection processes play an essential role in a variety of application fields, such as process, automotive or aerospace engineering. One prominent example is given by the high-pressure injection of fuel into combustion chambers, as used in cars or rocket engines. The underlying process relies on one fluid streaming under extreme pressure conditions into the other, cf. FIGURE 1. Injection processes for such multi-component systems have already been explored for various operating conditions, i.e. various configurations of fluid densities, pressures and temperatures, for different kinds of components. However, the so-called transcritical regime, which is characterized by very high pressures but rather low temperatures, is still not well understood. The transcritical regime is common in the mentioned fuel injection processes. Its investigation is particularly challenging, since the derivation of macroscopic properties such as surface tension, which are required in thermodynamic analyses and CFD simulations, can only be evaluated through fine-scale computations, such as computationally intensive molecular dynamics simulations.

Therefore, the dtec.bw project "MaST: Macro/Micro-simulation of phase decomposition in the transcritical regime" strives to explore these complex flow systems by a highly interdisciplinary approach: experts from thermodynamics, process engineering, fluid dynamics, scientific and high performance computing have teamed up to explore the multi-component systems over a wide range of scales. For this purpose, numerical simulations and their high performance implementations, that are executable on supercomputers due to the simulations' inherently high computational demands, are developed and put into relation with each other to enable a length and time scale-bridging view on the matter, complemented by high-pressure experiments.

In the following, we outline the project developments achieved so far. We explain the injection processes, respective computational fluid dynamics (CFD)- and experiment-based

investigations and our collaborative approach in Section II. At the other end of the scale spectrum, molecular dynamics (MD) simulations are developed and used for investigation of vapor-liquid systems, which are detailed in Section III. Sections IV and V focus on classical density functional theory (DFT) and molecular-continuum simulation methods, which operate on scales between the fine-scale molecular regime and the coarse-scale CFD view. Section VI closes the discussion with a short summary and outlook to future project activities.

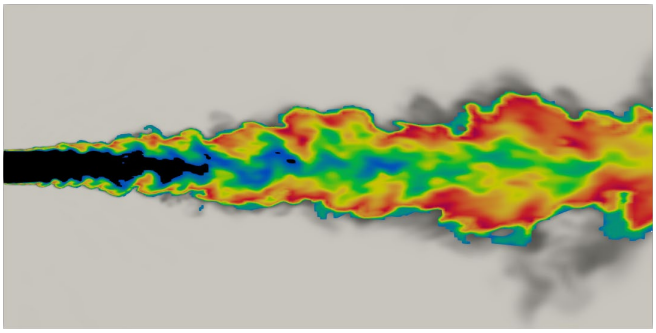

FIGURE 1: TRANSCRITICAL INJECTION OF CYCLO-PENTANE (TEMPERATURE 293 K) INTO NITROGEN (563 K) WITH PHASE SEPARATION DUE TO MULTICOMPONENT MIXING [1]. THE VOLUME FRACTION OF VAPOR IN THE MIXING ZONE IS VISUALIZED BY THE RAINBOW COLOR MAP. THE GRAY SCALE CORRESPONDS TO THE TEMPERATURE.

## II. A GLIMPSE INTO THE INVESTIGATION OF INJECTION PROCESSES: AN INTERIDISCIPLINARY EFFORT

### A. *Computational Fluid Dynamics for Injection Processes*

At the Institute of Applied Mathematics and Scientific Computing at the Universität der Bundeswehr München, numerical flow simulations are conducted in this project to investigate turbulent mixing and two-phase phenomena in liquid fuel injection and in shear layers. For this purpose, an extended version of the open-source flow solver *OpenFOAM* is used, containing a thermodynamic model that accounts for real gas thermodynamics and phase transition effects. The mixture of two fluids may have a higher critical point than the respective pure substance, resulting in a transition to a subcritical mixture and phase separation effects due to multicomponent mixing. Complex thermodynamic models are required to represent and capture these physical phenomena. FIGURE 1 shows a transcritical injection with phase separation due to multicomponent mixing. The two-phase region in the mixing zone is visualized by the rainbow color map.

### B. *Collaborations*

These considerations, that are made at the continuum scale (i.e., in the micro-sized, close-to-visible regime), require close interactions among the entire consortium, that is coordinated by Helmut-Schmidt-Universität Hamburg: reference MD data as well as detailed and accurate MD data for vapor-liquid equilibrium of selected fluid systems have been shared and discussed among the group at the Universität der Bundeswehr München and the group at TU Berlin to ensure consistency of the thermodynamic models at continuum scale [1] with actual molecular behavior. One essential building block consists in a precise formulation and use of equations of state for the underlying fluids. The latter has been subject to close collaboration of Universität der Bundeswehr München with the thermodynamics group at University of Stuttgart, who evaluate the classical DFT against MD simulations. To make respective MD simulations computationally feasible, the group at Technische Universität München collaborates with TU Berlin to improve the computational efficiency of the MD simulation software *ls1 mardyn* and to enable the respective large-scale simulations on supercomputers. This effort is complemented by interactions with the company MEGWARE Computer Vertrieb & Service GmbH to establish an optimal benchmarking platform for simulation software. This is to guarantee a robust performance optimization process, i.e. ensuring a continuous improvement in runtime, over and beyond the project period. To narrow the gap between continuum and molecular investigations, the group at Helmut-Schmidt-Universität Hamburg works on molecular-continuum simulation approaches which incorporate both CFD and MD simulations in a holistic approach. The group interacts with the CFD and MD experts at Universität der Bundeswehr München and TU Berlin and, for the sake of computational efficiency, with the group at Technische Universität München.

While most work in MaST focuses on the application and development of novel simulation techniques, experiments are necessary to validate the simulation results. For this purpose, a special high-pressure chamber is under procurement and installation at the Universität der Bundeswehr München, Institute of Thermodynamics. Selected configurations and operating points have been planned by the CFD and the experimentalist group, with FIGURE 1 illustrating one of these.

### C. *Preliminary Spray Experiments with Various Optical Techniques*

Spray experiments were conducted using three different optical diagnostic techniques; the focused shadowgraphy, Mie scattering measurement and high-speed infrared radiation (IR) imaging. The goal of the experiments is a preliminary test for the future work to provide validation data for the simulation groups for CFD and MD simulation, which can model the phase separation of the spray at the transcritical condition.

An optically accessible chamber [2] with quartz and sapphire windows was used to simulate high-pressure and temperature conditions relevant to IC engine and rocket injection as shown in FIGURE 2. Surrogate fuels such as ethanol and cyclo-pentane were injected into the heated nitrogen ambience. A high-pressure gasoline injector with a single injection hole was installed at the bottom of the chamber and the spray was injected in the opposite direction of the ambient nitrogen flow. A Photron Fastcam SA-Z camera with 40,000 fps was used for the shadowgraphy and the Mie scattering measurements. A Telops FAST M2k camera with 4,000 fps and a sapphire window at the imaging side were used for the IR imaging. A single green LED was utilized as the parallel light source for the shadowgraphy, and three perpendicularly arranged white LED flash lamps were applied for the Mie scattering technique. The experiments were conducted at the high-pressure (up to 55 bar for cyclo-pentane and 75 bar for ethanol) and high-temperature (up to 563 K for cyclo-pentane and 768 K for ethanol) chamber conditions.

Since the spray images were captured by the high-speed camera, the spray penetration and evaporation can be analyzed

[1] HTTPS://WWW.UNIBW.DE/NUMERIK-EN

frame by frame as shown in FIGURE 3. The penetration distance and the spray angle can be quantitatively measured from the images, and the instant jet speed can also be calculated. These databases will be used as the validation data for numerical simulations. Spray images from the three different optical techniques can be compared as shown in FIGURE 4; the shadow image shows the jet flow regardless of the phase (darker regions correspond to higher density, i.e. liquid fuel), the Mie image presents the existence of the liquid phase, and the IR image contains the information of

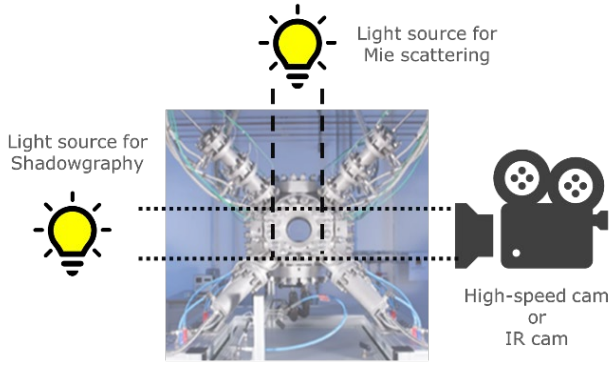


FIGURE 2: EXPERIMENTAL CHAMBER AND OPTICAL SETUP.

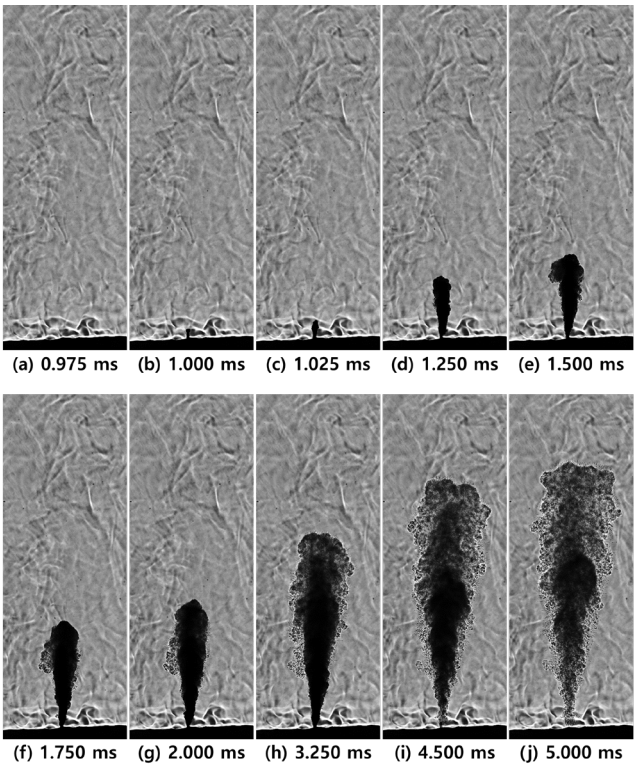


FIGURE 3: HIGH-SPEED SHADOW IMAGES OF THE FUEL JET.

concentration and temperature changes. Combining different methods can provide insight into how the phase change occurs at various ambient conditions. Based on this study, quantitative analysis methods will be developed and a database will be provided as validation data.

## III. MOLECULAR DYNAMICS SIMULATION FOR VAPOR-LIQUID SYSTEMS

To elucidate the behavior of vapor-liquid systems in the transcritical regime, atomistic MD simulations are carried out in this subproject. The goal is to directly sample structure and dynamics of the interacting phases during injection processes on the basis of molecular force field models. On the one hand, due to the extreme resolution in time and space, MD is limited to small, yet representative sections of these processes, see FIGURE 5. On the other hand, it is well-suited to yield the full suite of thermophysical properties that are required for models on coarser scales, such as CFD.

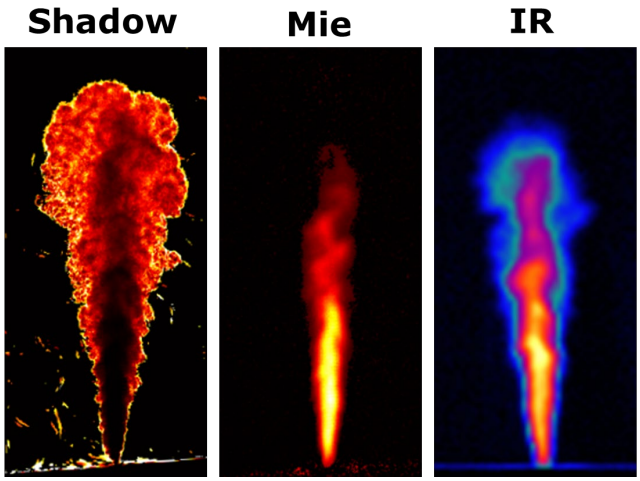


FIGURE 4: COMPARISON OF THREE DIAGNOSTIC METHODS.

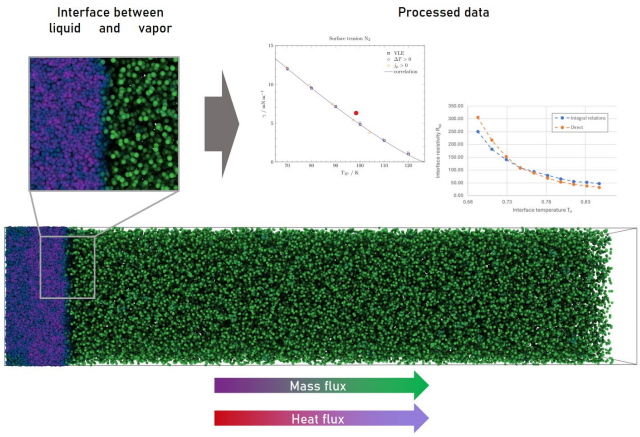


FIGURE 5: SNAPSHOT OF MD SIMULATION WITH MAGNIFIED VIEW ON INTERFACE. PARTICLES BELONGING TO THE LIQUID AND VAPOR ARE COLORED IN VIOLET AND GREEN, RESPECTIVELY.

One topic that was dealt with in the first phase of MaST was the question whether the surface tension under equilibrium conditions is the same as under strong non-equilibrium conditions. While prior work [3] focused on Lennard-Jones model fluids, the objective of the present work was the extension to more complex fluids, whose molecules need to be resolved by several interaction sites or which exhibit a significant polarity. Relying on a reverse non-equilibrium MD method [4], it was demonstrated that neither a large temperature gradient of up to $10^9$ K/m, nor a large mass flux density of up to 350 kg/m$^2$s have a significant impact, such that the surface tension depends solely on the local temperature at the interface.

Further work in MaST focused on a first-order phase transition phenomenon, i.e. the evaporation of a liquid. This process occurs in combustion chambers under the influence of strong non-equilibrium conditions, which are particularly

suitable for MD simulations. A series of MD simulations considering up to $10^6$ particles was utilized to investigate evaporation processes and derive the interface resistivities [5]. Applying a dedicated method [6] to keep the simulation scenario stationary allowed for better statistics and sampling of high-quality data. Varying the imposed parameters, like the bulk liquid temperature or the hydrodynamic velocity in the far field of the vapor, allows for the investigation of their influence on the most relevant quantities, i.e., heat and mass fluxes as well as interface resistivities. For evaporation into vacuum, the fluxes are found to be dependent only on the local temperature at the interface [7].

## IV. Density Functional Theory for Mixtures

Classical DFT in conjunction with, e.g., the PC-SAFT equation of state [8, 9, 10, 11], does not only provide physical properties of the vapor and liquid bulk phases of multi-component mixtures (vapor-liquid equilibria, densities, speed of sound, viscosities, thermal conductivities, diffusion coefficients, etc.), but also interfacial properties, i.e. surface tension. To support the development of physical-based interface models for CFD-based simulations, partners from University of Stuttgart work together with colleagues from TU Berlin to predict surface tension and tangential pressures over vapor-liquid interfaces. Classical DFT extends equations of state to inhomogeneous situations. In contrast to equations of state, DFT takes the surroundings (the density profile) into account and is therefore able to describe inhomogeneous fluids at the molecular level, for instance vapor-liquid interfaces or adsorbed molecules on solid surfaces.

Figure 6 exemplarily compares density and tangential pressure profiles for a binary oxygen/cyclohexane mixture from classical DFT with molecular dynamics results for a slab geometry. While the density profiles agree well (small deviations in the bulk phase are due to deviations in the liquid-vapor equilibrium), the tangential pressure profile is slightly offset, which requires further investigation in the future. Surface tensions are determined by integrating the tangential pressure profiles as in Figure 6, so that differences in surface tension can be attributed to differences in these profiles.

## V. High Performance Computing for Molecular Dynamics and Molecular-Continuum Simulations

Due to the very limited temporal and spatial scales, that MD simulations can resolve, boosting their computational performance on supercomputers is of utmost importance to the project MaST.

### A. *Boosting Performance of Molecular Dynamics: Auto-tuning for multi-site molecule representations*

Partners at Technische Universität München work on the optimization and parallelization of the software *ls1 mardyn*, which is used by the process engineering group from TU Berlin and which achieves high performance on state-of-the-art supercomputers [12]. This includes the particle simulation library *AutoPas*, which is used by *ls1 mardyn* and provides a black-box interface for the costly pairwise force calculation required at each time step in a MD simulation [13]. *AutoPas* selects from a large collection of algorithms the fastest way to calculate the forces acting on each molecule (auto-tuning). Such algorithms include particle containers, such as Linked Cells and Verlet lists, as well as symmetry optimizations (e.g., force balances according to Newton's third law (Newton3)), shared-memory parallel schemes, and vectorization to optimally leverage the entire CPU.

The MD simulation test bed *md-flexible*, used for the experimentation of *AutoPas*, is being extended from single-

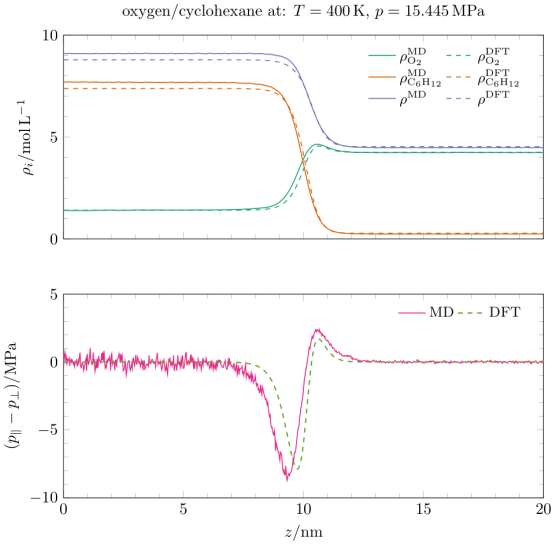


Figure 6: (Partial) density profiles (top) and difference between tangential and normal pressure, $p_\parallel$ and $p_\perp$ (bottom), for the vapor-liquid interface of the binary mixture of oxygen with cyclo-hexane from DFT and MD calculations.

site Lennard-Jones simulations to rigid-body multi-site simulations. In these, molecules are represented by a small number of fixed sites around a center-of-mass (CoM). The force acting between two molecules is thus the sum of the forces acting between the sites of the molecules, and so, large molecules require quadratically more computational time than small molecules. As *AutoPas* has only been used for particle simulations with uniform pairwise computational costs, MD simulations of molecules with different numbers of sites present a new, unique insight into the use of auto-tuning.

To demonstrate this, the runtime for the force calculation for a scenario with 27,000 molecules with varying numbers of sites was compared for all the algorithms available within *AutoPas*. In Figure 7, we see a comparison of the schemes

- lc_sliced_c02 (linked cells, slicing-based shared-memory parallelization), array-of-structures data structure, no Newton3 optimization, and
- the algorithm lc_c08 (linkd cells, 8-way cell-coloring scheme for shared-memory parallelization), array-of-structures data structure, no Newton3 optimization.

We see that in the 1-site case, lc_sliced_c02 is 21 % faster than lc_c08, but it is 17 % slower in the 5-site case. This demonstrates the advantages of tuning the algorithms used according to the number of sites. In future work, we strive to demonstrate this in full *ls1 mardyn*-based simulations. As part of this, input from partners of TU Berlin has resulted in realistic scenarios to experiment with, so that development of *AutoPas* in this direction can be guided by real world test cases.

The development of high performance software for supercomputers heavily relies on reproducibility of performance metrics such as floating point operations per second or, in the case of MD, molecule updates per second.

The research groups of Technische Universität München and Helmut-Schmidt-Universität Hamburg have teamed up with MEGWARE to leverage a prototype for continuous benchmarking for MaST-related MD simulation developments. One of the next steps in this regard is the

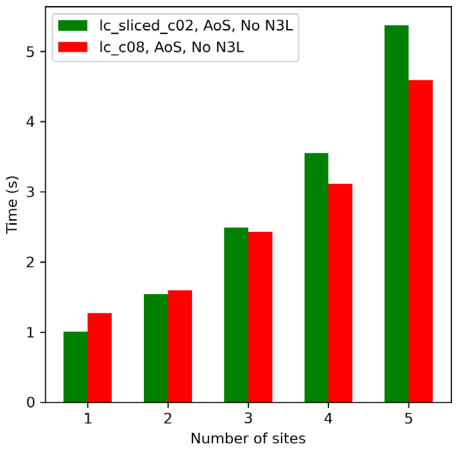


FIGURE 7: COMPARISON OF TWO ALGORITHMS FOR A RANGE OF NUMBERS OF SITES. FOR DETAILS ON THE SPECIFICS OF THESE ALGORITHMS, REFER TO GRATL ET AL. [13].

deployment of the benchmarking toolkit to the new supercomputer HSUper, which is hosted at Helmut-Schmidt-Universität and which has been extended by even more computational resources to enable the planned large-scale MD simulations.

### B. *Boosting Algorithmic Performance by a Multiscale Approach: Towards Molecular-continuum Simulations for Multiphase Systems*

When experimenting on supercomputers with highly optimized MD simulations, one inevitably runs into certain performance limits which are impossible to surpass. Considering very large domains with few rather small-sized regions requiring scrutiny, full sized MD simulations require big computational efforts and appear to be wasteful in terms of their use of HPC resources. Hence the team at Helmut-Schmidt-Universität Hamburg are developing and utilizing the macro-micro coupling tool *MaMiCo* [14], which couples concurrent CFD and MD simulations over large domains, allowing the use of specific solvers for specific regions. Having large CFD volumes in areas of uniform flow, with smaller MD regions only in areas of interest, the aim is to achieve high performance without compromising on the granularity or the quality of the results. Currently, the team at Helmut-Schmidt-Universität collaborate with partners from Technische Universität München and TU Berlin on coupling the solver stack of *ls1 mardyn/AutoPas*, and the independent coupling tool *preCICE* to *MaMiCo*.

To couple *ls1 mardyn* to *MaMiCo*, the necessary interfaces on the side of *MaMiCo* have been written and tested. *MaMiCo* can reliably couple with a single *ls1 mardyn/AutoPas* instance placed anywhere within a domain, regardless of whether the *ls1 mardyn* instance is running sequentially or parallel with MPI. Besides, *ls1 mardyn* was refactored to allow for single timestep simulation, and to allow external code to control the simulation steps. The remaining functionality was added via *ls1 mardyn's* plugin system, allowing us to inject coupling code at required moments in the simulation loop. The ensemble builds seamlessly with cmake, and is easy to set up and use. A successful simulation result of coupling *ls1 mardyn/AutoPas* and *OpenFOAM* is shown in FIGURE 9, for which the experimental setup can be seen in FIGURE 8.

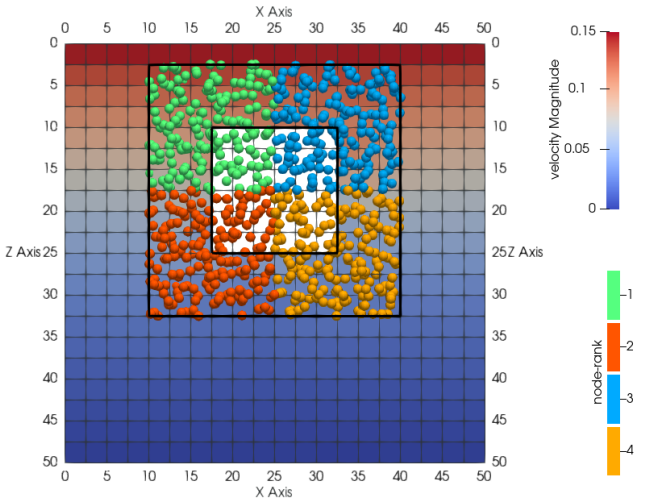


FIGURE 8: EXPERIMENTAL SETUP SHOWING THE CFD DOMAIN AND THE MD DOMAIN. THE AREA BETWEEN THE THICK-LINED BLACK BOXES DENOTES THE OVERLAP REGION IN WHICH CFD AND MD SOLVERS ARE COUPLED. THE GRID SHOWS THE MAMICO COUPLING CELLS.

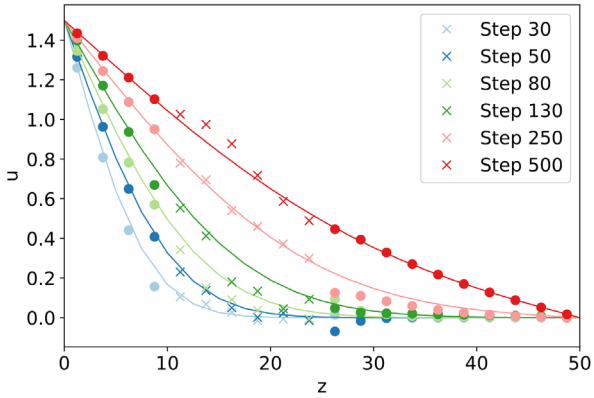


FIGURE 9: VELOCITY PROFILE IN A COUETTE FLOW SIMULATION, COUPLING LS1 MARDYN/AUTOPAS WITH OPENFOAM USING MAMICO. SOLID LINES DENOTE THE ANALYTICAL SOLUTION FOR THE FLUID FLOW VELOCITY IN X-DIRECTION, DOTS REPRESENT DATA EXTRACTED FROM OPENFOAM AND CROSSES REPRESENT DATA FROM LS1/AUTOPAS.

*MaMiCo* was designed to ease the coupling between MD and CFD solvers. In its core multiple coupling algorithms are present that can be used and reused between the multiple MD and CFD solvers. However, each CFD solver that is to be coupled requires the implementation of a specific *MaMiCo* interface. For more flexibility, we chose to couple the coupling library *preCICE* [15] with *MaMiCo*. Through this *MaMiCo-preCICE* coupling, multiple CFD solvers already adapted to *preCICE*, e.g. *OpenFOAM*, *FEniCS*, etc., shall become usable within *MaMiCo*. Furthermore, this allows us to use the steering methods and (in particular) the implicit coupling schemes of *preCICE*. This will be useful within the context of transcritical multiphase flow with potentially stiff transients which require such schemes. Finally, the interpolation functionalities coming with *preCICE* allow us to use unstructured grids within the CFD solver while using the usual Cartesian grid used for MD simulations.

In the very near future, a multiscale simulation with *ls1 mardyn/AutoPas* and *OpenFOAM* with *preCICE* is to be coupled through *MaMiCo* and executed on the new supercomputer HSUper at Helmut-Schmidt-Universität. This will enable us to compare results at appropriate granularities and verify the robustness of the coupling scheme. This test will then be extended to a variety of hardware, to check for compatibility and ease of use.

## VI. Summary and Outlook

We have outlined our current achievements in the dtec.bw project MaST to explore transcritical fluid systems across a wide range of temporal and spatial scales by a variety of simulation methods as well as by experiments. Fruitful collaborations have formed out from the very beginning of the project, which have enabled integral views on research findings, such as a first comparison of MD and DFT data, or information exchange on equations of state for thermodynamically consistent modeling in MD, CFD and molecular-continuum simulations. We look forward to deepening these collaborative investigations and to further following our joint research path in the future.

In order to enhance scientific exchange beyond the MaST research team, a workshop has been conducted mid of September 2022 with several renowned invited speakers. The participation from industrial partners such as MAN and Liebherr will help to stipulate the discussion also towards industrial applications and requirements in the future.

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References

[1] A. Doehring, N. Urban, T. Trummler, M. Pfitzner and M. Klein, "Assessment of a state-of-the-art thermodynamic modelling approach for CFD-simulations under trans- and supercritical conditions," in *4th International Seminar on Non-Ideal Compressible Fluid Dynamics for Propulsion & Power*, City University London, 2022.

[2] S. Riess, L. Weiss, A. Peter, J. Rezaei and M. Wensing, "Air entrainment and mixture distribution in diesel sprays investigated by optical measurement techniqes," *International Journal of Engine Research,* vol. 19, no. 1, pp. 120-133, 2018.

[3] M. Schweizer, H. Öttinger and T. Savin, "Nonequilibrium thermodynamics of an interface," *Physical Review E,* vol. 93, p. 052803, 2016.

[4] F. Müller-Plathe, "A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity," *The Journal of Chemical Physics,* vol. 106, no. 14, p. 6082, 1997.

[5] E. Johannessen and D. Bedeaux, "Integral relations for the heat and mass transfer resistivities of the liquid–vapor interface," *Physica A: Statistical Mechanics and its Applications,* vol. 370, no. 2, pp. 258-274, 2006.

[6] M. Heinen and J. Vrabec, "Evaporation sampled by stationary molecular dynamics simulation," *The Journal of Chemical Physics,* vol. 151, no. 4, p. 044704, 2019.

[7] S. Homes, M. Heinen, J. Vrabec and J. Fischer, "Evaporation driven by conductive heat transport," *Molecular Physics,* vol. 119, no. 15-16, p. e1836410, 2021.

[8] J. Gross and G. Sadowski, "Perturbed-Chain SAFT: An Equation of State Based on a Perturbation Theory for Chain Molecules," *Industrial & Engineering chemistry research,* vol. 40, no. 4, pp. 1244-1260, 2001.

[9] J. Gross, "A density functional theory for vapor-liquid interfaces using the PCP-SAFT equation of state," *The Journal of Chemical Physics,* vol. 131, no. 20, p. 204705, 2009.

[10] E. Sauer and J. Gross, "Classical Density Functional Theory for Liquid–Fluid Interfaces and Confined Systems: A Functional for the Perturbed-Chain Polar Statistical Associating Fluid Theory Equation of State," *Industrial & Engineering Chemistry Research,* vol. 56, no. 14, pp. 4119-4135, 2017.

[11] R. Stierle, E. Sauer, J. Eller, M. Theiss, P. Rehner, P. Ackermann and J. Gross, "Guide to efficient solution of PC-SAFT classical Density Functional Theory in various Coordinate Systems using fast Fourier and similar Transforms," *Fluid Phase Equilibria,* vol. 504, p. 112306, 2020.

[12] S. Seckler, F. Gratl, M. Heinen, J. Vrabec, H.-J. Bungartz and P. Neumann, "AutoPas in ls1 mardyn: Massively Parallel Particle Simulations with Node-Level Auto-Tuning," *Journal of Computational Science,* vol. 50, p. 101296, 2021.

[13] F. Gratl, S. Seckler, H.-J. Bungartz and P. Neumann, "N ways to simulate short-range particle systems: Automated algorithm selection with the node-level library AutoPas," *Computer Physics Communications,* vol. 273, p. 108262, 2022.

[14] P. Neumann, H. Flohr, R. Arora, P. Jarmatz, N. Tchipev and H.-J. Bungartz, "MaMiCo: Software design for parallel molecular-continuum flow simulations," *Computer Physics Communications,* vol. 200, pp. 324-335, 2016.

[15] G. Chourdakis, K. Davis, B. Rodenberg, M. Schulte, F. Simonis, B. Uekermann, G. Abrams, H.-J. Bungartz, L. Yau, I. Desai and K. Eder, "preCICE v2: A sustainable and user-friendly coupling library," *arXiv,* 2021.