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Towards the Numerical Determination of the Splashing Threshold of Two-component Drop Film Interactions

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Introduction

The scenario of an impacting drop onto a film is highly relevant in many natural and technical systems. A fundamental and often required parameter of these interactions is the so called splashing threshold above which secondary droplets are generated (see figure 1).

For situations in which the liquids of drop and film differ, a general threshold correlation is unknown. Due to the limited amount of test liquids and their fixed properties, its experimental determination is, however, impossible and the threshold can, therefore, only be determined by means of a numerical parameter study. In this study we investigate the suitability of a numerical determination using the multiphase flow solver Free Surface 3D (FS3D).

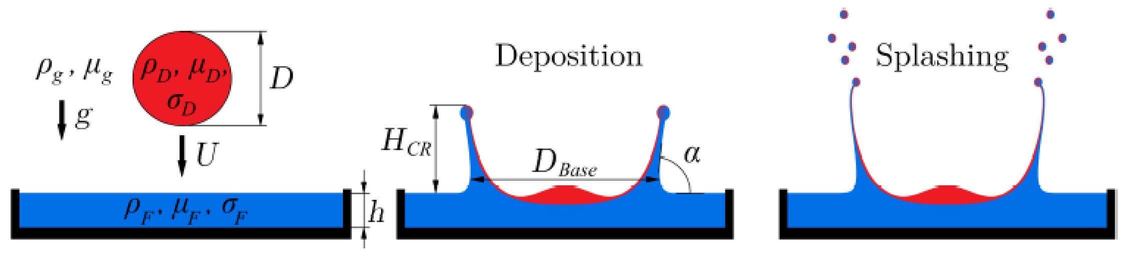

Fig. 1: Schematic setup of drop film interactions (left) and schematic sketch of the impact outcomes deposition (middle) and splashing (right). The regime in between deposition and splashing is called transition zone. Relevant non-dimensional parameters are $\delta = h/D$, $\overline{Re} = \bar{\rho}DU/\bar{\mu}$, $\overline{Oh} = \bar{\mu}/\sqrt{\bar{\rho}\bar{\sigma}D}$, where the overline means arithmetic mean of the liquid properties, and the property ratios $\chi = \rho_D/\rho_F$, $\lambda = \mu_D/\mu_F$, $\gamma = \sigma_D/\sigma_F$.

Numerical Method

FS3D is based on the Volume-of-Fluid (VOF) method and is capable of simulating multi-component liquids [1]. For the treatment of multiple liquids, additional VOF variables $\psi_i = V_i/V_f$ are introduced representing the species volume fractions in a control volume that is part of the liquid phase. Between these species a linear mixing behavior is assumed. The volume fraction of a species is advected analogously to the VOF variable f with the transport equation

$$\partial_t(f\psi_i) + \nabla\cdot(f\psi_i\boldsymbol{u}) = 0.$$

Since FS3D solves the conservation equations in a one-field formulation, local properties like the density are computed via $\rho(\boldsymbol{x},t) = \rho_l f(\boldsymbol{x},t) + \rho_g(1 - f(\boldsymbol{x},t))$ with $\rho_l = \sum_{i=1}^{n}\rho_{l,i}\psi_i$. The local viscosity is calculated by using the volume fraction based viscosity mixture model for binary liquid mixtures by Dey and Biswas [2]. The surface tension coefficient is set to a constant averaged value for the sake of simplicity.

Results

In order to identify the necessary grid resolution for an accurate reproduction of the impact morphology close to the splashing threshold, a detailed grid study was conducted. The numerical setup is similar to the one used by Kaufmann et al. [1]. As shown in figure 2, a very fine grid resolution is necessary in order to prevent unphysical disintegrations of the crown wall.

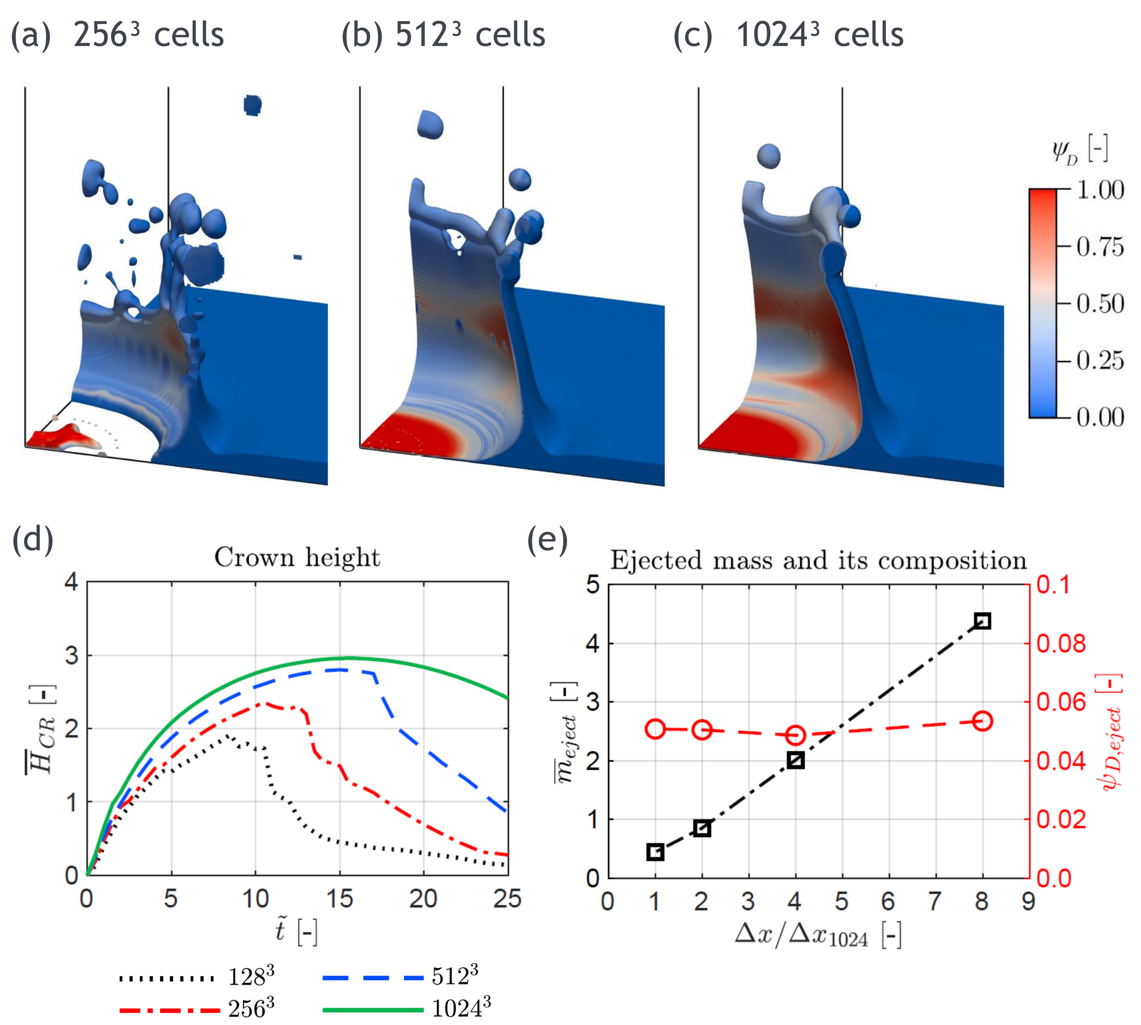

Fig. 2: (a-c) Impact morphology at $\tilde{t} = tU/D = 18$, (d) temporal evolution of the crown height $\overline{H}_{CR} = H_{CR}/D$, and (e) ejected mass normalized with the initial drop mass $\overline{m}_{eject} = m_{eject}/m_D$ and fraction of drop liquid of the ejected mass $\psi_{D,eject}$ over normalized grid cell size for the transition case for different grid resolutions.

Furthermore, three impact scenarios across existing empirical threshold correlations were simulated (see figure 3 and 4). The resulting impact morphologies and the corresponding shapes of the rim show that the regimes can be well reproduced.

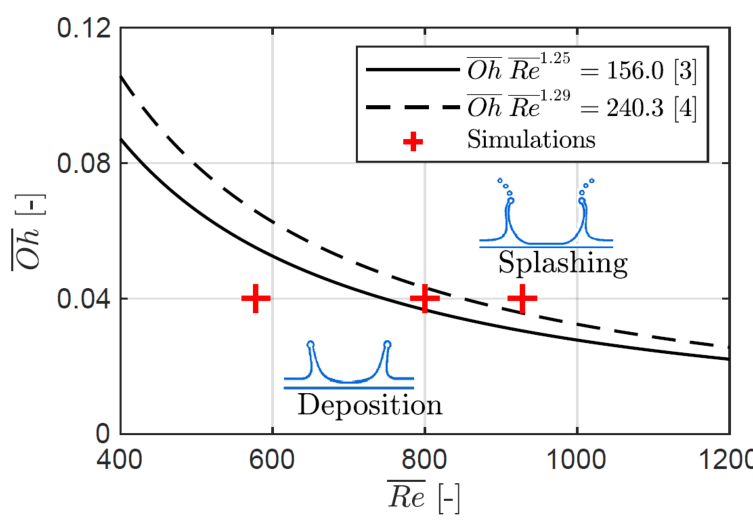

Fig. 3: $\overline{Oh}, \overline{Re}$-diagram for mapping of the simulated drop film interactions with corresponding impact regimes according to correlations by Geppert et al. [3] and Bernard et al. [4] for $\delta = 0.36$, $\overline{Oh} = 0.04$.

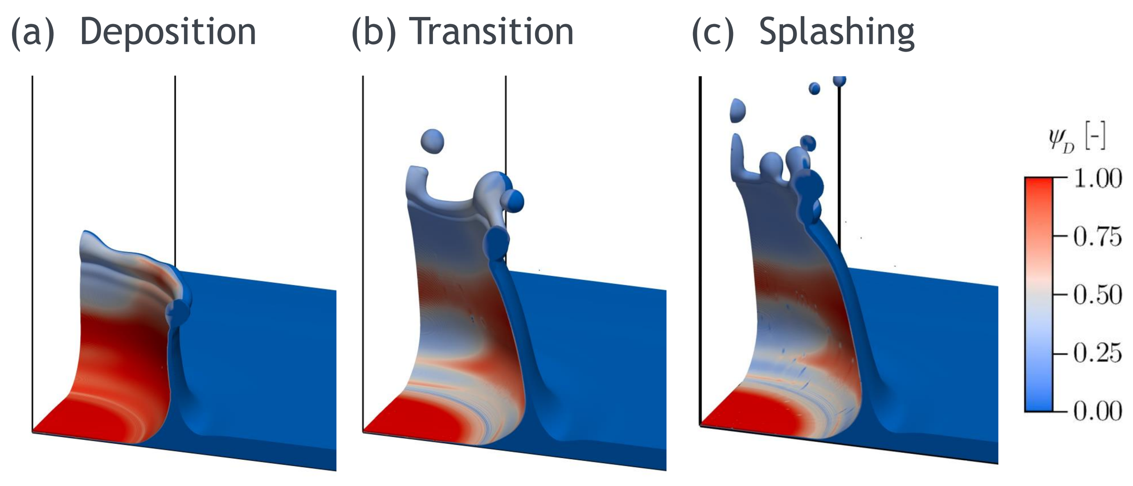

Fig. 4: Impact morphology for the simulated cases (a) deposition, (b) transition, and (c) splashing after the crown has reached its maximum height using a grid resolution of 1024³ cells.

A Further analysis of the ejected mass for all cases and several grid resolutions shows that a grid resolution below 1024³ cells results in a massive overestimation of the ejected mass, which will lead to a significant underestimation of the splashing threshold.

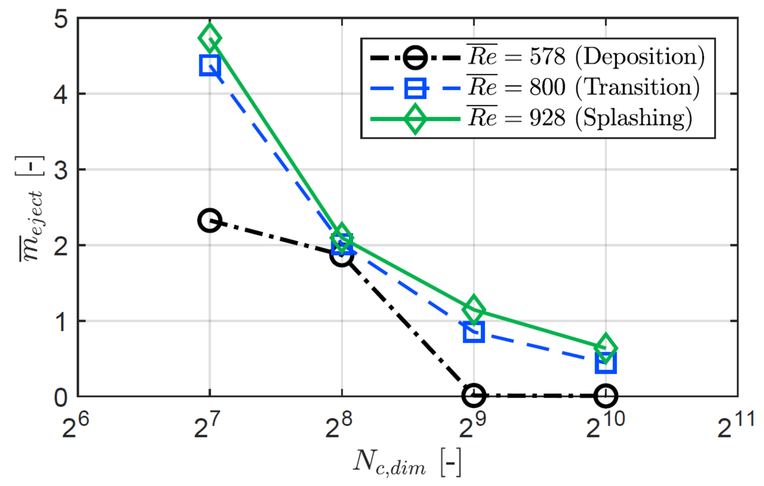

Fig. 5: Ejected mass $\overline{m}_{eject}$ of the simulated drop film interactions for different grid resolutions or number of grid cells per dimension $N_{c,dim}$, respectively.

Improvement of Computational Performance

A good parallel performance of FS3D is crucial for future investigations of drop film interactions. One of the main issues in the numerical framework is the efficient solution of the pressure Poisson equation resulting from the volume conservation in incompressible flows using the implemented Multigrid solver (MG). An unfavorable communication imbalance during the agglomeration and distribution of the computational domain onto one single processor leads to a high amount of idling processes. To overcome this issue, FS3D was adapted to use a tree structured communication during the coarsening and refining on the levels during the solution cycle.

A performance analysis for both FS3D code versions (optimized MG and original solver) was conducted measuring the scalability and parallel performance using both strong and weak scaling by estimating the number of solution cycles per hour (CPH). As shown in figure 6, the optimized solver outperforms the original one without tree structured communication in cases with more than 512 processors, achieving a performance speed-up of factor 20 for strong scaling and factor 10 for weak scaling at 4096 processors.

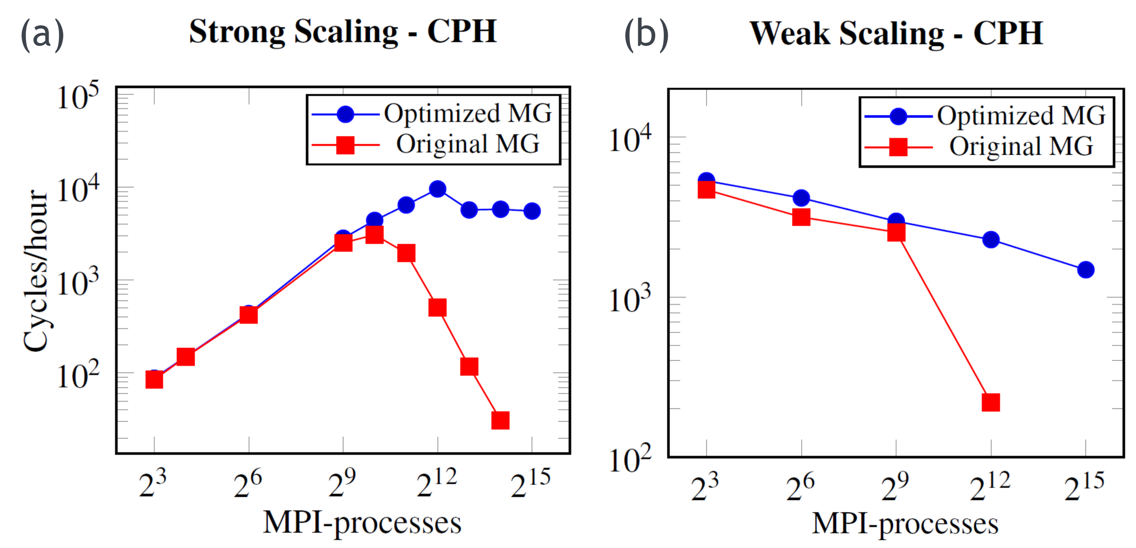

Fig. 6: Number of estimated cycles per hour (CPH) for the optimized and the originally implemented MG solver for (a) strong scaling with a fixed global domain size of 512³ grid cells and (b) weak scaling with a fixed domain size of 64³ grid cells per processor.

Conclusion

A detailed grid study revealed that by only very fine grid resolutions a premature breakup of the crown wall can be prevented. However, the composition of the secondary droplets can be predicted reliably for coarse grid resolutions. From the ejected masses and impact morphologies for the selected impact scenarios it can be concluded that FS3D is capable of reproducing the splashing threshold for two-component drop film interactions with sufficient accuracy. Since a good parallel performance is essential, the time-consuming MG solution cycle was optimized by implementing a tree structured communication architecture, leading to a speed-up of almost a factor of 20 compared to the original solver at peak performance.

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