Numerical Upscaling for Droplet Impact on rough Walls

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Introduction

The reliable simulation of liquid droplet impact on surfaces is still a challenge. One issue in this context is the importance of compressible effects for even relatively small impact speeds. This problem has been studied for flat perfect walls, but very little has been done for textured walls, when micro-level structures affect the macroscopic flow field.

![Image](image.png)

Figure 1: The physical problem: Droplet impact on rough wall

- Droplet impact on perfect flat wall analyzed in [1] using compressible inviscid (Euler) model.
- Comparable numerical study for textured walls has not been started up to now.
- Direct Numerical Simulation using compressible Navier–Stokes equations is too complicated for realistically textured geometries.
- For incompressible flows effective boundary conditions for viscous flow on rough boundaries have been suggested, e.g. [2].
- Extension to compressible flows carried out in [3], but the derivation of effective boundary conditions for complex flows is far from being complete, hence numerical upscaling techniques are needed.

Modelling

The upscaling approach requires smooth solutions, therefore a diffuse interface model instead of sharp interface one is used. For the same reason we cannot use a Euler model and rely on an extension of the Navier–Stokes equations for two phase flows.

![Image](image.png)

Figure 2: Diffuse Interface

Navier–Stokes–Allen–Cahn system (NSAC)

We consider the isothermal compressible system [4] in \((0, T) \times \Omega\)

\[
\begin{align*}
\partial_t \rho + \text{div}(\rho \mathbf{v}) &= 0, \\
\partial_t (\rho \mathbf{v}) + \text{div}(\rho \mathbf{v} \otimes \mathbf{v} + P \mathbf{I}) &= \text{div}(\mathbf{S}), \\
\partial_t \rho \mathbf{v} + \text{div}(\rho \mathbf{v} \otimes \mathbf{v}) &= -\partial_p F(\rho, \phi, \nabla \phi)
\end{align*}
\]

with boundary conditions \(\mathbf{v} = 0, \nabla \phi = 0\) on \((0, T) \times \partial \Omega\).

- Phase field parameter \(\phi \in [0, 1]\)
- Viscous part \(\mathbf{S}\) of the stress tensor
- Free energy density \(F(\rho, \phi, \nabla \phi) = \frac{1}{2} \rho \|\nabla \phi\|^2 + \frac{1}{2} \rho F(\phi) + \nabla \phi \otimes \nabla \phi \frac{\partial^2 F}{\partial \phi^2}\)
- Nonlinear interpolation \(\psi(\phi)\) of free energies of pure phases
- Pressure \(P(\rho, \phi, \nabla \phi) = \left( -\frac{\partial F(\phi)}{\partial \phi} + I + \nabla \phi \otimes \nabla \phi \frac{\partial F}{\partial \phi^2} \right)\)

![Image](image.png)

Figure 3: Double well potential

![Image](image.png)

Figure 4: Phase field

Upscaling strategy

Resolving the micro-scale structure is infeasible due to high computational cost. The idea to overcome this issue is to perform simulations on a virtually smooth domain \(\Omega_0\), and include micro-scale effects through effective boundary conditions. To obtain these conditions cell problems corresponding to each roughness element have to be solved. The zeroth-order solution \((\rho_0, \mathbf{v}_0, \phi_0)\) on the (smooth) domain \(\Omega_0\) enters the cell problem.

This leads to the following procedure:

1. Solve the zeroth order problem
   \[
   \begin{align*}
   \mathcal{L}_{\text{NSAC}}(\rho_0, \mathbf{v}_0, \phi_0) &= 0 \quad \text{in } (0, T) \times \Omega_0, \\
   B(\rho_0, \mathbf{v}_0, \phi_0) &= 0 \quad \text{on } (0, T) \times \partial \Omega_0
   \end{align*}
   \]

2. In each time step solve for each roughness element the corresponding cell problem
3. Compute the effective boundary conditions
4. Solve the effective problem
   \[
   \begin{align*}
   \mathcal{L}_{\text{NSAC}}(\rho, \mathbf{v}, \phi) &= 0 \quad \text{in } (0, T) \times \Omega, \\
   B(\rho, \mathbf{v}, \phi) &= 0 \quad \text{on } (0, T) \times \partial \Omega
   \end{align*}
   \]

5. In this way, the effective boundary conditions are obtained, and the upscaling approach yields approximations to the zeroth-order solution.

Future Work

- Investigate wellposedness of the derived cell problem.
- Implementation in 2D, test numerically if cell problems can be further simplified.
- Use reduced basis methods since cell problems are parameter dependent.
- Consider non-isothermal extension of the underlying model.
- Extension to 3D.

References


