FLUID-STRUCTURE-CONTACT-INTERACTION BETWEEN LIQUID DROPLETS AND ROUGH SURFACES

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Summary
We present the continuum mechanical equations governing small liquid droplets in contact with rough substrate surfaces. Some remarks are given on the computational implementation of these equations within the finite element method, and a numerical example is shown for illustration. This work is motivated by the study of self-cleaning surface mechanisms.

INTRODUCTION

Some natural surfaces have remarkable self-cleaning capabilities. Particles polluting the surface adhere to passing water droplets and are thus removed. The mechanical principles behind this self-cleaning mechanism are very complex as they involve the coupling of several phenomena: These are the fluid flow inside the droplets, the surface tension of the droplet membrane, the contact with rough surfaces, the contact angle at the three-phase line, and the interaction between droplet and pollutants. In this work, we focus on the first four phenomena.

GOVERNING EQUATIONS

Flow field

We consider liquid droplets at small length scales, such that the effects of inertia are negligible. Further, the liquid is treated as incompressible. These conditions are known as the Stokes' flow model. According to this, the local momentum balance is given by

$$\operatorname{div}\boldsymbol{\sigma} + \rho\,\boldsymbol{b} = \boldsymbol{0}\,, \tag{1}$$

where $\boldsymbol{b}$ denotes the body forces and $\boldsymbol{\sigma}$ denotes the Cauchy stress tensor. Newtonian fluid behavior is considered such that

$$\boldsymbol{\sigma} = p\,\boldsymbol{I} + 2\mu\,\boldsymbol{d}\,, \tag{2}$$

where $\boldsymbol{d}$ is the symmetric part of the velocity gradient, i.e. $\boldsymbol{d} = \nabla^{\mathrm{s}}\boldsymbol{v}$. The fluid incompressibility is expressed by the equality constraint

$$g_{\mathrm{v}} = J - 1 = 0\,, \tag{3}$$

where $J := \det\boldsymbol{F}$ (the determinant of the deformation gradient) governs the local volume change. Since eq. (3) implies $\dot{J} = 0$, where $\dot{J} = J\operatorname{div}\boldsymbol{v}$, the incompressibility constraint is equivalent to $\operatorname{div}\boldsymbol{v} = 0$. In order to solve these equations, boundary conditions for the velocity and the stress field are required, i.e.

$$\begin{aligned} \boldsymbol{v} &= \bar{\boldsymbol{v}}\,, \qquad \text{for } \boldsymbol{x}_{\mathrm{s}} \in \partial_{\mathrm{v}}\mathcal{B}\,, \\ \boldsymbol{\sigma}\,\boldsymbol{n} &= \bar{\boldsymbol{t}}\,, \qquad \text{for } \boldsymbol{x}_{\mathrm{s}} \in \partial_{\mathrm{t}}\mathcal{B}\,. \end{aligned} \tag{4}$$

The velocity $\bar{\boldsymbol{v}}$ and the traction $\bar{\boldsymbol{t}}$ are imposed by the droplet membrane. In this regard, (4) correspond to the coupling conditions between the fluid domain $\mathcal{B}$ and the membrane domain $\partial\mathcal{B}$.

Droplet membrane

The droplet membrane is governed by the Young-Laplace equation

$$2H\gamma = \Delta p\,, \tag{5}$$

where H denotes the mean curvature of the membrane and γ denotes the surface tension of the fluid. Eq. (5) can be derived from a potential. Δp denotes the pressure difference across the membrane surface, which is given as

$$\Delta p = p - p_{\mathrm{c}}\,, \tag{6}$$

where p is the pressure of the fluid, which acts on the inside of the droplet membrane, and p_{c} is the contact pressure acting on the outside. In the special case of hydrostatic conditions (i.e. $\boldsymbol{v} = \boldsymbol{0}$) we have

$$p = p_0 - \rho g y\,, \tag{7}$$

where p_0 is the capillary pressure and $\rho g y$ is the hydrostatic pressure. In this case, p_0 is obtained from the incompressibility constraint (3), which can also be written as $\tilde{g}_{\mathrm{v}} = V - V_0 = 0$, where V and V_0 denote the current and the initial volume of the droplet, respectively. The membrane domain $\partial\mathcal{B}$ is considered closed and thus does not need boundary conditions.

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Surface contact

The contact pressure p_c is obtained from the impenetrability constraint

$$g_\mathrm{n}(\boldsymbol{x}_\mathrm{s}) \geq 0\,, \quad \forall\, \boldsymbol{x}_\mathrm{s} \in \partial\mathcal{B}\,. \tag{8}$$

Here g_n denotes the normal contact gap

$$g_\mathrm{n} = (\boldsymbol{x}_\mathrm{s} - \boldsymbol{x}_\mathrm{p}) \cdot \boldsymbol{n}_\mathrm{p} \tag{9}$$

between the membrane point $\boldsymbol{x}_\mathrm{s}$ and the substrate surface Γ_m. The unit vector $\boldsymbol{n}_\mathrm{p}$ denotes the surface normal of Γ_m at $\boldsymbol{x}_\mathrm{p}$, which is the solution of the minimum distance problem

$$\boldsymbol{x}_\mathrm{p}(\boldsymbol{x}_\mathrm{s}) = \min_{\forall\, \boldsymbol{x}_\mathrm{m} \in \Gamma_\mathrm{m}} (\boldsymbol{x}_\mathrm{s} - \boldsymbol{x}_\mathrm{m})\,, \quad \text{for } \boldsymbol{x}_\mathrm{s} \in \partial\mathcal{B}\,. \tag{10}$$

The contact pressure p_c is then governed by the contact conditions

$$\begin{cases} p_\mathrm{c} = 0\,, & \text{if } g_\mathrm{n} > 0\,, \\ p_\mathrm{c} > 0\,, & \text{if } g_\mathrm{n} = 0\,. \end{cases} \tag{11}$$

Line contact

The contact conditions at the triple line, where the liquid, solid and gas phases meet, are governed by the Young-Dupré equation

$$\gamma \cos\theta_\mathrm{c} = \gamma_\mathrm{SG} - \gamma_\mathrm{SL}\,, \tag{12}$$

where θ_c denotes the contact angle at the triple line, and γ_SG and γ_SL denote the surface tension at the solid-gas and solid-liquid interface. In consequence, an attractive line force, with magnitude $\gamma \sin\theta_\mathrm{c}$, acts at the triple line between the membrane and the substrate.

COMPUTATIONAL IMPLEMENTATION

All the equations above are implemented within the finite element method. We use quadrilateral Q2Q1 Taylor-Hood elements to solve Stokes' flow [1], and have developed a novel FE formulation for the droplet membrane in contact with the rough surface [2]. The penalty method [3] is used to enforce constraint (8) and equation (12). As an initial example, Fig. 1 shows the 2D solution of the membrane shape and the fluid velocity of a water droplet rolling over a rough surface, considering $\theta_\mathrm{c} = 155°$ and $V = 1.1\pi\mathrm{mm}^2$. For simplification, the flow field and the membrane deformation are

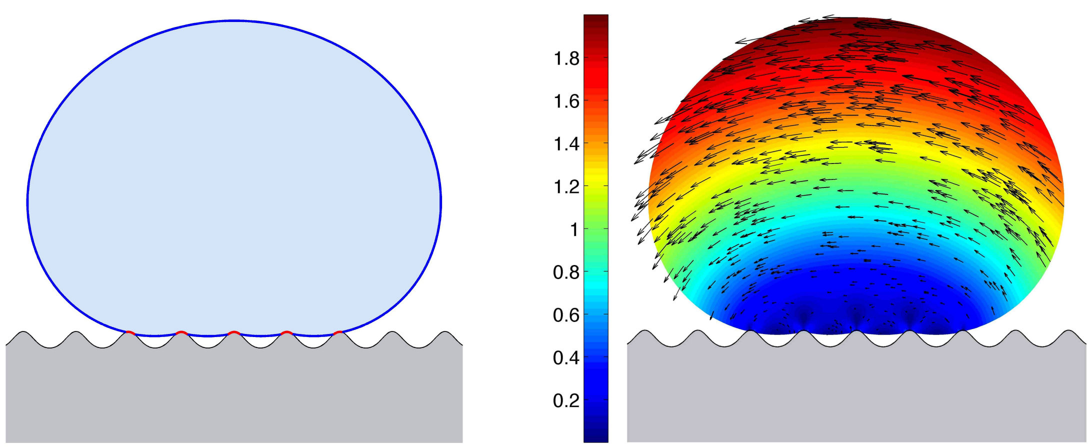

Figure 1. Liquid droplet rolling over a rough surface: membrane solution for rough surface contact (left); fluid velocity (right).

considered decoupled, computing first the membrane deformation, giving boundary $\partial\mathcal{B}$, and then the flow field, giving $\boldsymbol{v}$ and p within $\mathcal{B}$. We have therefore imposed a velocity field on $\partial\mathcal{B}$ that corresponds to a rolling motion of the droplet.

References

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