Introduction to fluid-solid interface problems and numerical methods

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Multi-phase fluid flow represents a class of common natural phenomena with a variety of practical implications.

**Microfluidics**

Fluid thread breakup under microfluidic confinement

**Lotus Effect**

Water drop on lotus plant

Water drops on surface with nano coatings

**Cell Membrane**
Two Phase Fluids on Flat and Rough Surface: Wetting Phenomena
Young’s Equation:

\[ \gamma_{SV} = \gamma_{SL} + \gamma \cos \theta_e, \]

Contact angle \( \theta_e < 90^\circ \), the surface is hydrophilic (亲水);
Contact angle \( \theta_e > 90^\circ \), the surface is hydrophobic (疏水)
Roughness enhanced wetting

Fig. 1 Water droplets on electrodeposited copper surfaces: (a) flat, (b) flat and hydrophobised, (c) textured and hydrophobised, (d) electron microscope image of an electrodeposited textured copper surface.
Contact angle hysteresis

The Hysteresis is due to impurity or roughness of the surface
Combined effects of roughness and hydrophobicity have been found to induce significant drag reduction for flow past these surfaces.

*Fastskin*
Moving Contact Line Problem

- No-slip boundary condition causes infinite energy dissipation in the Navier-Stokes model (Dussan and Davis, 1974)
- MD results show relative slip at contact line (Koplik, et al, 1988)
- Ad-hoc models are used to address the phenomena
Computer simulations of the dynamics of fluid molecules have circumvented the inability of hydrodynamics to explain how fluids spread.

Molecular dynamics (MD) simulations, in which materials are modelled on supercomputers at the level of their interacting molecules, have become an invaluable tool for studying complex systems on microscopic scales. Many problems in condensed matter physics and chemistry, which have otherwise eluded experimental and theoretical analysis, have been resolved with MD techniques. For three decades, most applications of MD have focused on equilibrium properties of solids, liquids, and other condensed systems. Recently, the availability of supercomputers has led to a proliferation of exciting studies involving inhomogeneous, non-equilibrium systems. New applications include studies of fluid dynamics, atomic force microscopy, micro-indentation and ‘stick-slip’ phenomena.

In treating a problem with MD techniques one always hopes to capture the physics at macroscopic scales. For many problems, attaining this goal requires system sizes that exceed computational limits. These barriers are rapidly being surmounted as new computers with more memory and faster processors become available. This is particularly evident in recent MD studies of convection, wetting and drying at solid surfaces, and the dynamics of tethered membranes and dense polymeric solutions. Here we show how MD studies have led to substantial insight into one of the more ubiquitous and poorly understood phenomena in our everyday lives: the spreading of fluids. This is an excellent example in which microscopic dynamics controls macroscopic behaviour.

Spreading phenomena are encountered whenever we sip coffee from a cup, drink Coke through a straw, butter our toast, or watch rain drops dance down window panes. Hardly a moment passes in a day when we are not confronted by them. Similarly, the spreading of many factors: surface roughness, chemical heterogeneity and non-Newtonian flow. For instance, surface defects can pin moving contact lines. This is clearly demonstrated when rain drops remain suspended on window panes rather than flowing down. Yet, even if we neglect these complications and consider only uniform smooth surfaces, understanding the basic mechanism of spreading remains exceedingly difficult. In fact, this problem has eluded both theoretical and experimental analysis for nearly a century.

The fundamental difficulty lies with the limitations of continuum hydrodynamics. In principle, a fluid spreading on a smooth surface can be described by the Navier–Stokes equations along with some appropriate boundary conditions (BCs). The usual BC assumed in fluid dynamics is the ‘no-slip’ condition: that is that the velocity of the fluid relative to the solid is zero at the interface. This condition works very well in describing macroscopic flow of single fluids e.g. water flowing in a pipe. However, when used to describe a spreading fluid, the no-slip condition leads to an unphysical
Sharp Interface model

![Diagram of a two phase domain](image)

Figure 1: Schematic diagram of a two phase domain.

The governing equations of unsteady, viscous, incompressible, and immiscible two fluid systems in three-dimensional space are the Navier-Stokes equations:

\[
\rho_i \left( \frac{\partial u_i}{\partial t} + u_i \cdotp \nabla u_i \right) = -\nabla p_i + \nabla \cdotp \left[ \eta_i \left( \nabla u_i + \nabla u_i^T \right) \right] + \rho_i g, \quad \text{in } \Omega_i,
\]

\[
\nabla \cdotp u_i = 0, \quad \text{in } \Omega_i,
\]

where \( \rho_i(x,t) \) is the density, \( u_i(x,t) = (u_1(x,t), u_2(x,t), u_3(x,t)) \) is the velocity, \( p_i(x,t) \) is the pressure, and \( \eta_i(x,t) \) is the viscosity of fluid \( i = 1, 2 \), the superscript \( T \) denotes transpose, and \( g \) is the gravitational force per unit mass. See Fig. 1 for the schematic diagram of a two phase domain. \( \Gamma \) is the interface of the two immiscible fluids and \( \mathbf{n} = (n_1, n_2, n_3) \) is the unit normal vector to the interface. On the interface \( \Gamma \), we have a normal jump condition

\[
p_2 - p_1 = \sigma \kappa + \left( 2 \eta n_k \frac{\partial u_k}{\partial n} \right)_2 - \left( 2 \eta n_k \frac{\partial u_k}{\partial n} \right)_1,
\]

where \( \sigma \) is the surface tension coefficient and \( \kappa \) is the mean curvature of the interface.
Phase Field Model

Consider two different fluids with densities $\rho_1$ and $\rho_2$. Define the composition field

$$\phi(x) = \frac{\rho_1 - \rho_2}{\rho_1 + \rho_2}$$

$$\phi(x) = \begin{cases} 
-1 & \text{for fluid 1} \\
0 & \text{at interface} \\
1 & \text{for fluid 2}
\end{cases}$$
Cahn-Hilliard Theory

The free energy functional

\[ F = \int \left[ \frac{1}{2} \varepsilon (\nabla \phi)^2 + \frac{1}{\varepsilon} f(\phi) \right] dx, \]

The Chemical Potential:

\[ \mu = \frac{\delta F}{\delta \phi} = -\varepsilon \nabla^2 \phi + \frac{1}{\varepsilon} f'(\phi) = -\varepsilon \nabla^2 \phi - \frac{1}{\varepsilon} (\phi - \phi^3) \]

\[ f(\phi) = -\frac{1}{2} \phi^2 + \frac{1}{4} \phi^4 \]
In equilibrium, we have
\[ \varepsilon \nabla^2 \varphi + \frac{1}{\varepsilon} (\varphi - \varphi^3) = 0 \]

Assuming it is 1-d in the direction \( z \) normal to the interface, we have
\[ \varepsilon \varphi_{zz} + \frac{1}{\varepsilon} (\varphi - \varphi^3) = 0 \]

\( \varphi(z) = \tanh\left( \frac{z}{\sqrt{2} \varepsilon} \right) \approx \begin{cases} -1 & z \to -\infty \\ 1 & z \to +\infty \end{cases} \)

\( \tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \)

Interface thickness \( \varepsilon \)

Interface energy \( \gamma = \varepsilon \int (\frac{\partial \varphi}{\partial z})^2 \, dz \)
\[ F = \int_{\Omega} \left[ \frac{1}{2} \varepsilon (\nabla \varphi)^2 + \frac{1}{\varepsilon} f(\varphi) \right] dx + \int_{\partial \Omega} \gamma_{wf}(\varphi) \]

\( \gamma_{wf}(\varphi) \) is the interface free energy density at the fluid solid boundary.

At the equilibrium,

\[
\begin{cases}
-\varepsilon \Delta \varphi + \frac{1}{\varepsilon} f'(\varphi) = 0 \quad \text{in } \Omega \\
\varepsilon \frac{\partial \varphi}{\partial n} + \frac{\partial \gamma}{\partial \varphi} = 0 \quad \text{in } \partial \Omega
\end{cases}
\]
Young’s Equation

\[ \int (\varepsilon \frac{\partial \phi}{\partial n} + \gamma \frac{\partial \gamma}{\partial x}) \frac{\partial \phi}{\partial x} \, dx = 0 \]

\[ \int \frac{\partial \gamma}{\partial \phi} \frac{\partial \phi}{\partial x} \, dx = \int \frac{\partial \gamma}{\partial \phi} \, d\phi = \gamma(-1) - \gamma(1) \]

\[ \int \varepsilon \frac{\partial \phi}{\partial n} \frac{\partial \phi}{\partial x} \, dx = \int \varepsilon \frac{\partial \phi}{\partial n} \, d\phi = \int \varepsilon \frac{\partial \phi}{\partial m} \, d\phi \cos(\theta_s) = \int \varepsilon \frac{\partial \phi}{\partial m} \frac{\partial \phi}{\partial m} \, dm \cos(\theta_s) \]

\[ = \int \varepsilon \left( \frac{\partial \phi}{\partial m} \right)^2 \, dm \cos(\theta_s) = \gamma \cos(\theta_s) \]

\[ \gamma \cos(\theta_s) = \gamma(-1) - \gamma(1) \]
Consider diffusion current: \( J = -M \nabla \mu, \quad \mu = \frac{\delta F}{\delta \varphi} \)

From conservation law,
\[
\frac{d}{dt} \int_{\Omega} \varphi dx = \int_{\partial\Omega} -\varphi v \cdot nds + \int_{\partial\Omega} -J \cdot nds
\]
\[
= -\int_{\Omega} \nabla \cdot (\varphi v) dx - \int_{\Omega} \nabla \cdot J
\]
\[
\Rightarrow \varphi_t + \nabla \cdot (\varphi v) = -\nabla \cdot J
\]

If there is no flow, i.e. \( v = 0 \), then we have the Cahn-Hilliard equation
\[
\varphi_t = -\nabla \cdot J = M \nabla \mu = M \Delta(-\varepsilon \Delta \varphi + \frac{1}{\varepsilon} f'(\varphi))
\]

Boundary conditions:
\[
J \cdot r = \frac{\partial \mu}{\partial n} = 0
\]
\[
\varepsilon \frac{\partial \varphi}{\partial n} + \frac{\partial \gamma}{\partial \varphi} = 0
\]
\[
\delta F = \int_\Omega \mu(\delta \phi) + \int_{\partial \Omega} L(\phi)(\delta \phi)
\]

\[
\mu = -\varepsilon \nabla^2 \phi - \frac{1}{\varepsilon} (\phi - \phi^3)
\]

chemical potential

\[
L(\phi) = \varepsilon \partial_n \phi + \frac{\partial \gamma_wf(\phi)}{\partial \phi}
\]

deviation from the equilibrium at the solid surface

\[
\mu \nabla \phi
\]

Capillary force density

\[
L(\phi) \partial_\tau \phi
\]

Uncompensated Young stress
Cahn-Hilliard-Navier-Stokes System for the Moving Contact Line Problem

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = M \nabla^2 \mu
\]

\[
\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = -\nabla p + \nabla \cdot \mathbf{\sigma} + \mu \nabla \phi + \mathbf{f}
\]

\[
\nabla \cdot \mathbf{v} = 0
\]

Qian, Wang, Sheng, *PRE, 03; PRL, 04, JFM, 06*
Wang, Qian, Sheng, *JFM, 08*
Boundary Conditions:
\[ \partial_n \mu = 0 \quad \text{and} \quad v_n = 0 \]

the boundary relaxation for surface
\[ \frac{\partial \varphi}{\partial t} + \mathbf{v} \cdot \nabla \varphi = -\Gamma L(\varphi) \]

and the generalized Navier Boundary Condition
\[ \beta \nu^{slip}_x = \eta [ \partial_z \nu_x ] + L(\varphi) \varphi_x \]

= tangential viscous stress + Young stress

The model can be derived from the Onsager’s principle: The Principle of Minimum Energy Dissipation
Quantitative agreement between molecular dynamic simulations and continuum simulations!
Comparison of experimental results and numerical simulations based on continuum model with GNBC


Measure the drag coefficient $\xi_i$ near MCL

\[ \frac{\xi_c}{\pi d} = \alpha \eta, \]
\[ \alpha = 0.8 \]

The black circles are the simulation results. Other symbols are experimental results from 6 different fibers.

This is the first time that an intrinsic property of MCL is ever measured experimentally.
Convex splitting scheme for the Cahn-Hilliard equation

(D.J. Eyre, 1998)

\[ \frac{\phi^{n+1} - \phi^n}{\Delta t} = \mathcal{L}_d \nabla^2 (\mu_1^{n+1} + \mu_2^n) \]

\[
\mu = -\epsilon^2 \nabla^2 \phi^{n+1} + s\phi^{n+1} - (1 + s)\phi^n + (\phi^n)^3 = \mu_1 + \mu_2
\]

(contractive)

(expansive)
Convex splitting for Cahn-Hilliard-Navier-Stokes

\[ \frac{\phi^{n+1} - \phi^n}{\Delta t} + v^{n+1} \cdot \nabla \phi^{n+1} = L_d \nabla^2 (\mu_1^{n+1} + \mu_2^{n}) \]

\[ R \left( \frac{v^{n+1} - v^n}{\Delta t} + v^{n+1} \cdot \nabla v^{n+1} \right) = -\nabla p^{n+1} + \Delta v^{n+1} + B\mu \nabla \phi^{n+1} \]

Here:

\[ \nabla \cdot v^{n+1} = 0 \]

\[ \mu = -\epsilon^2 \nabla^2 \phi^{n+1} + s\phi^{n+1} - (1 + s)\phi^n + (\phi^n)^3 = \mu_1 + \mu_2 \]

**contractive** \hspace{2cm} **expansive**

Boundary Conditions:

\[ \frac{\phi^{n+1} - \phi^n}{\delta t} + \tilde{v}_x^{n+1} \partial_x \phi^{n+1} = -\mathcal{V}_s [L(\phi^{n+1})] \]

\[ \tilde{v}_z^{n+1} = 0, \quad \partial_n \mu^{n+1} = 0 \]

\[ [\mathcal{L}_s (\phi^{n+1})]^{-1} (\tilde{v}_x^{slip})^{n+1} = B L(\phi^{n+1}) \partial_x \phi^{n+1} - \partial_n \tilde{v}_x^{n+1} \]

With linear splitting for boundary potential

\[ L(\phi^{n+1}) = \epsilon \partial_n \phi^{n+1} + \partial \gamma_{wf}(\phi^n) / \partial \phi + \tilde{\alpha}(\phi^{n+1} - \phi^n) \]
Energy Decaying Property

Theorem:
Assume \( \sup_{x \in \Omega} \{ |\phi^n(x)|, |\phi^{n+1}(x)| \} \leq M, M > 0 \).

If \( s \geq 3M^2 - 0.5, \alpha \geq \frac{C}{2}, C = |\frac{\sqrt{2}}{3} \cos \theta_{surf}^2 (\frac{\pi}{2})^2| \),

then

\[
\mathcal{B}[F(\phi^{n+1}) - F(\phi^n)] + \mathcal{R}[F_k(v^{n+1}) - F_k(v^n)] \\
\leq -\Delta t \mathcal{B} \mathcal{L}_d \| \nabla \mu \|_{2, \Omega}^2 - \Delta t \mathcal{B} \mathcal{V}_s \| L(\phi) \|_{2, \partial \Omega}^2 - \Delta t \| [\mathcal{L}_s(\phi)]^{-1/2} (v_{slip}^{n+1})^2 \|_{2, \partial \Omega}^2 \\
- \frac{1}{2} \Delta t \sum_{i,j=1}^2 \|(\partial_i v_{j}^{n+1} + \partial_j v_{i}^{n+1})^2 \|_{2, \Omega}^2 - \Delta t \| [\mathcal{L}_s(\phi)]^{-1} (v_{slip}^{n+1}, u_w) \|_{\partial \Omega}^2
\]

where

\[
F(\phi) = \int_{\Omega} \left[ \frac{1}{2} \epsilon^2 |\nabla \phi|^2 + \frac{(\phi^2 - 1)^2}{4} \right] dx + \int_{\partial \Omega} \epsilon \gamma_{wf}(\phi) ds
\]

is the total free energy,

\[
F_k(v) = \frac{1}{2} \int_{\Omega} |v|^2 dx
\]

is the bulk kinetic energy.
The incremental pressure-corrected scheme for NS

\[
\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} + 2v^n \cdot \nabla \phi^n - v^{n-1} \cdot \nabla \phi^{n-1} = \mathcal{L}_d \Delta \mu^{n+1}
\]

(4.26)

\[
\mathcal{R} \frac{3\tilde{v}^{n+1} - 4v^n + v^{n-1}}{2\delta t} + \mathcal{R}(2v^n \cdot \nabla v^n - v^{n-1} \cdot \nabla v^{n-1}) + \nabla p^n - \Delta \tilde{v}^{n+1} = B\mu^{n+1} \nabla \phi^{n+1}
\]

(4.27)

\[
\left\{ \begin{array}{l}
\mathcal{R}\left(\frac{3v^{n+1} - 3\tilde{v}^{n+1}}{2\delta t}\right) + \nabla(p^{n+1} - p^n + \nabla \cdot \tilde{v}^{n+1}) = 0 \\
\nabla \cdot v^{n+1} = 0, \quad v^{n+1} \cdot n|_{T,B} = 0
\end{array} \right.
\]

(4.28)

Here \(\mu^{n+1} = -\epsilon \Delta \phi^{n+1} + s\phi^{n+1}/\epsilon - 2(1+s)\phi^n + (1+s)\phi^{n-1}/\epsilon + 2(\phi^n)^3/\epsilon - (\phi^{n-1})^3/\epsilon\).

At top and bottom boundaries,

\[
\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\delta t} + 2v_x^n \partial_x \phi^n - v_x^{n-1} \partial_x \phi^{n-1} = -V_s[L(\phi^{n+1})]
\]

\[
\tilde{v}_z^{n+1} = 0, \quad \partial_n \mu^{n+1} = 0
\]

\[
[\mathcal{L}_s(\phi^{n+1})]^{-1}(\tilde{v}_x^{slip})^{n+1} = BL(\phi^{n+1}) \partial_x \phi^{n+1} - \partial_n \tilde{v}_x^{n+1}
\]
The consistent splitting scheme for NS

H. Johnston, J.G. Liu, 2004

\[
\frac{\mathcal{R}(3v^{n+1} - 4v^n + v^{n-1})}{2\delta t} + \mathcal{R}(2v^n \cdot \nabla v^n - v^{n-1} \cdot \nabla v^{n-1}) + \nabla p^n - \Delta v^{n+1} = \mathcal{B}\mu^{n+1}\nabla \phi^{n+1}
\]

(4.29)

\[
\begin{cases}
\Delta p^{n+1} = -\mathcal{R}\nabla \cdot (v^{n+1} \cdot \nabla v^{n+1}) + \mathcal{B}\nabla \cdot (\mu^{n+1}\nabla \phi^{n+1}) \\
\frac{\partial p^{n+1}}{\partial n}|_{T,B} = -n \cdot (\nabla \times \nabla \times v^{n+1}) + n \cdot (\mathcal{B}\mu^{n+1}\nabla \phi^{n+1}) \\
\frac{\partial p^{n+1}}{\partial n}|_{L,R} = 0
\end{cases}
\]

(4.30)
The incremental pressure-correction scheme has the second order accuracy for all quantities but not for pressure when the interface intersects with the boundary.

\[
\begin{array}{ccccccc}
\text{(nr.nz)} & \phi & \text{rate} & u & \text{rate} & v & \text{rate} \\
(128,64)-(256,128) & 4.01e-03 & 2.57e-04 & 2.08e-04 & 6.58e-02 \\
(256,128)-(512,256) & 8.27e-04 & 2.28 & 5.88e-05 & 2.13 & 4.87e-05 & 2.10 & 1.18e-02 & 2.48 \\
(512,256)-(1024,512) & 1.97e-04 & 2.07 & 1.47e-05 & 2.00 & 1.23e-05 & 1.99 & 4.48e-03 & 1.40 \\
(1024,512)-(2048,1024) & 4.87e-05 & 2.02 & 3.67e-06 & 2.00 & 3.09e-06 & 1.99 & 1.82e-03 & 1.30 \\
\end{array}
\]

Table 1: $L_2$ norm of the error and convergence rate for phase function $\phi$, velocity $v$, pressure $p$ at $T = 0.375$ with different grids. The results are obtained with the incremental pressure-correction scheme for Couette flow with static contact angle $\theta_{\text{surf}}^* = 77.6^\circ$. The results show second order accuracy for all quantities $\phi$, $v$ but not for $p$.

\[
\begin{array}{ccccccc}
\text{(nr.nz)} & \phi & \text{rate} & u & \text{rate} & v & \text{rate} & p & \text{rate} \\
(128,64)-(256,128) & 1.99e-03 & 5.47e-05 & 4.97e-05 & 1.27e-01 \\
(256,128)-(512,256) & 4.40e-04 & 2.18 & 1.15e-05 & 2.25 & 1.11e-05 & 2.16 & 2.98e-02 & 2.09 \\
(512,256)-(1024,512) & 1.08e-04 & 2.03 & 2.84e-06 & 2.02 & 2.73e-06 & 2.03 & 7.43e-03 & 2.01 \\
(1024,512)-(2048,1024) & 2.68e-05 & 2.01 & 7.07e-07 & 2.01 & 6.78e-07 & 2.01 & 1.88e-03 & 1.98 \\
\end{array}
\]

The incremental pressure-correction scheme has the second order accuracy for all quantities when the interface doesn’t intersects with the boundary.
The consistent splitting scheme has the second order accuracy for all quantities even when the interface intersects with the boundary.

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<th>$\phi$</th>
<th>rate</th>
<th>u</th>
<th>rate</th>
<th>v</th>
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Table 3: $L_2$ norm of the error and convergence rate for phase function $\phi$, velocity $v$, pressure $p$ at $T = 0.375$ with different grids. The results are obtained with the consistent splitting scheme for Couette flow with static contact angle $\theta_{surf} = 77.6^\circ$. The results show second order accuracy for all quantities $\phi$, $v$ and $p$. 
Adaptive Finite Element Method

- Adaptive strategy: *posteriori error estimates*

Use the jump of gradient across interface of adjacent elements for both $\phi$ and $u$.

\[
\eta_T(\phi_h) = \left( \sum_{e \in \Omega_T} \int_e h^3 \left( \frac{\partial \phi_h}{\partial n_e} \right)^2 \, de \right)^{\frac{1}{2}},
\]

\[
\eta_T(u_h) = \left( \sum_{e \in \Omega_T} \int_e h^3 \left( \frac{\partial u_h}{\partial n_e} \cdot \frac{\partial u_h}{\partial n_e} \right) \, de \right)^{\frac{1}{2}}.
\]

Due to the fact that the phase variable decays much faster away from the interface than the velocity variable, we use the indicator $\eta_T(\phi_h)$ to refine and coarsen the mesh, then use $\eta_T(u_h)$ only to refine the mesh.
Wenzel to Cassie-Baxter transition

Figure 1: Schematic diagram of a droplet suspended on an array of pillars.
\[ \theta_s = 30^0 \]
\[ \theta_s = 100^0 \]
In the total free energy functional $f$ the bulk free energy density $f_k \downarrow l$ is generally chosen to be a double well function

$$f_k \downarrow l = t_w k t^2 l^2.$$ 

In this case the state $\downarrow l = t$ represents the liquid phase and $\downarrow l = t$ represents the vapor phase. The surface free energy density $f_k \downarrow l$ is an interpolation between $SV = k t l$ and $SL = k t l$ in the form of

$$f_k \downarrow l = SV + SL t^2 SV^2 SL^2 \sin^2 \downarrow l.$$ 

Then from the Young's equation

$$\uparrow w = LV \cos \uparrow u \downarrow l.$$ 

We use a convex temporal splitting scheme and finite element spatial discretization to solve the system numerically. The scheme is linear and unconditionally stable, and it's convenient for complex geometries. Details of the finite element scheme is given in [8].

Figure 3: Normalized surface free energy against the penetration depth when (a) $\theta_e < \theta_{e,c}$, and (b) $\theta_e > \theta_{e,c}$.  $a=0.125, b=d=0.05$, $\theta_{e,c} = 101.31^\circ$, $R_c = 0.1796$

There is a critical $\theta_{e,c}$,

1. $\theta_e > \theta_{e,c} \Rightarrow$ Cassie-Baxter state (no penetration)
2. $\theta_e < \theta_{e,c}$, if $R < R_c \Rightarrow$ Cassie-Baxter state
3. $R > R_c \Rightarrow$ Wenzel state
Roughness enhanced wetting: Wenzel State

\[ \theta_s = 30^\circ \]

\[ \theta_s = 60^\circ \]

\[ \cos \theta_e = r \cos \theta_s \]

\[ r = \frac{\text{real substrate area}}{\text{area projection onto the horizontal plane}} > 1 \]
Roughness enhanced wetting: Cassie-Baxter State

\[ \theta_s = 110^\circ \]

\[ \theta_s = 150^\circ \]

Droplet sits suspended on top of posts with air beneath it

\[ \cos \theta_e = \lambda \cos \theta_e + (1 - \lambda) \]

\( \lambda \): fraction of the solid-liquid interface below the drop
Modelling of droplet impacting

- Droplet Diameter $D_0$
- Velocity $V_0$
- Solid Substrate
- Spreading
- Splashing
- Rebound

- Surface Properties
  - Surface energy
  - Roughness
  - Chemical homogeneity
  - Temperature

- Droplet Properties
  - Droplet Size
  - Impact Velocity
  - Surface Tension
  - Temperature

- Two-phase Properties
  - Density Ratio
  - Viscosity Ratio
Droplet Impacting (Qian Zhang)

Adherence

Partial bouncing

Bouncing

Splashing
The buoyancy driven droplet through a fluid-fluid interface, $Re=0.01$  
(Yi Shi)

Figure 1. Visual and audio recordings of impact. (a,b) Photographs of the impact of two spheres striking only in watertight cavitation by a water/air interface on their surface. Impact of a perfectly wetting sphere, with static contact angle $\theta_s \approx 15^\circ$ (a); impact of a hydrophobic sphere with static contact angle $\theta_s \approx 100^\circ$ (b). The impact velocity was 5.0 m s$^{-1}$ in both cases, corresponding to a 1.25 m height drop. The photographs were taken 15.5 ms (c) and 15.9 ms (d) after initial impact. (e-f) Time-dependent audio recordings of the impacts, as measured by a microphone $\approx 10$ cm from the impact point, for a hydrophobic (c) and a hydrophobic (d) sphere. The signal is proportional to the acoustic pressure emitted during the impact. The axes on the vertical scale are arbitrary (but identical). A big 'splash' is evident for the hydrophobic sphere, whereas a tiny 'plop' is heard for the hydrophobic sphere. The sound is associated with the rapid closure of the cavity (not shown).
For hydrophilic sphere, the film is seen to follow the sphere and closes up at the pole of the sphere.
For hydrophobic sphere, the film is seen to detach from the sphere before reaching the pole leading to cavity formation and air entrainment.
Drop Formation and Dripping-Jetting Transition
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• At low flow rates, surface tension causes the water to form drops.

• At higher flow rates, jetting occurs when the inertial forces of the water exceed surface tension force.
• Two phase drop formation and manipulations are important to the applications in microfluidics

Utata et al, PRL (2007)
Figure 2.1: (a) Dripping regime. (b) The first class jetting generated by increasing the flow rate of outer fluid above a threshold while keeping the flow rate of inner fluid constant. (c) The second class jetting generated by increasing the flow rate of inner fluid above a threshold while keeping the flow rate of outer fluid constant.
Figure 9. Comparison of the time sequence of drop shapes. Left half part is taken from Zhang’s experiment [Z99b], right half part is our numerical results.
\[ C_{out} = \frac{\eta_o u_o}{\gamma} \]
\[ W_{in} = \frac{\rho_i d_{tip} u_i^2}{\gamma} \]

**Figure 10.** Comparison of the state diagrams of the dripping to jetting transition in a co-flowing stream as a function of \( C_{out} \) and \( W_{in} \). The upper graph is numerical results, and the lower one is taken from the experiment carried by Utada *et al.* [UFNSW07]
Bifurcation Diagram

Time interval between $i$th and $(i-1)$th drop as function of inner fluid velocity