Small scale fluid dynamics, interfaces and numerics

Paul Vigneaux[•]

[•] Unité de Mathématiques Pures et Appliquées
Ecole Normale Supérieure de Lyon – France

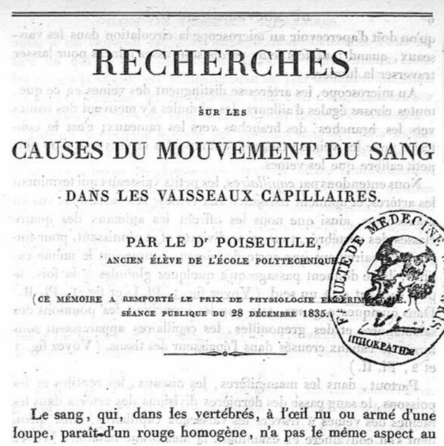
CEMRACS 2015 :
Coupling Multi-Physics Models involving Fluids.
CIRM. July 20 – 24, 2015

Outline

Outline

A bit of history

∼ **1840** : Jean L. M. Poiseuille. Pioneering experiments of liquid flows in capillaries, 30-150μm diameters



RECHERCHES

SUR LES

CAUSES DU MOUVEMENT DU SANG

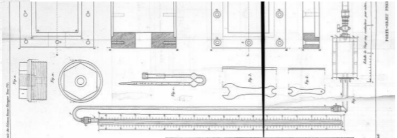
DANS LES VAISSEAUX CAPILLAIRES.

PAR LE Dr POISEUILLE,

ANCIEN ÉLÈVE DE L'ÉCOLE POLYTECHNIQUE.

(CE MÉMOIRE A REMPORTÉ LE PRIX DE PHYSIOLOGIE EXPÉRIMENTALE.
SÉANCE PUBLIQUE DU 28 DÉCEMBRE 1835.)

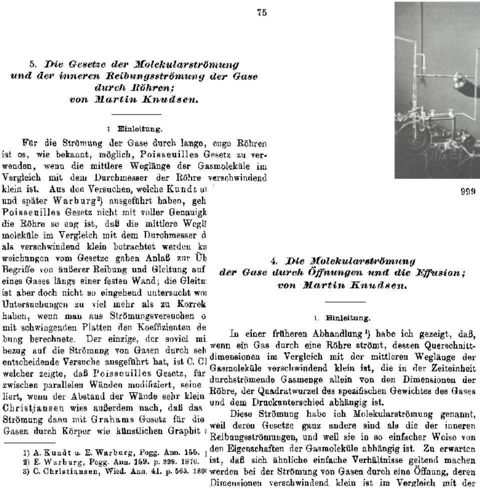
Le sang, qui, dans les vertébrés, à l'œil nu ou armé d'une loupe, paraît d'un rouge homogène, n'a pas le même aspect au



Recherches sur les causes du mouvement du sang dans les vaisseaux capillaires. Paris, Imprimerie royale, 1839.

A bit of history

$\sim$ **1909** : Martin H. C. Knudsen. Gas flows in the *transition* and *free molecular* regimes



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5. *Die Gesetze der Molekularströmung und der inneren Reibungsströmung der Gase durch Röhren;*

von Martin Knudsen.

1 **Einleitung.**

Für die Strömung der Gase durch lange, enge Röhren
ist es, wie bekannt, möglich, Poisseuilles Gesetz zu verwenden, wenn die mittlere Weglänge der Gasmoleküle im
Vergleich mit dem Durchmesser der Röhre verschwindend
klein ist. Aus den Versuchen, welche Kundt u
und später Warburg[2]) ausgeführt haben, geh
Poisseuilles Gesetz nicht mit voller Genauigk
die Röhre so eng ist, daß die mittlere Wegl
moleküle im Vergleich mit dem Durchmesser d
als verschwindend klein betrachtet werden ka
weichungen vom Gesetze gaben Anlaß zur Üb
Begriffe von äußerer Reibung und Gleitung auf
eines Gases längs einer festen Wand; die Gleitu
ist aber doch nicht so eingehend untersucht wo
Untersuchungen zu viel mehr als zu Korrek
haben, wenn man aus Strömungsversuchen o
mit schwingenden Platten den Koeffizienten de
bung berechnete. Der einzige, der soviel mi
bezug auf die Strömung von Gasen durch seh
entscheidende Versuche ausgeführt hat, ist C. Cl
welcher zeigte, daß Poisseuilles Gesetz, für
zwischen parallelen Wänden modifiziert, seine
liert, wenn der Abstand der Wände sehr klein
Christiansen wies außerdem nach, daß das
Strömung dann mit Grahams Gesetz für die
Gasen durch Körper wie künstlichen Graphit

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1) A. Kundt u. E. Warburg, Pogg. Ann. 155.
2) E. Warburg, Pogg. Ann. 159. p. 399. 1876.
3) C. Christiansen, Wied. Ann. 41. p. 565. 189

999

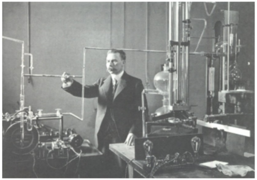
4. *Die Molekularströmung der Gase durch Öffnungen und die Effusion;*

von Martin Knudsen.

1. **Einleitung.**

In einer früheren Abhandlung[1]) habe ich gezeigt, daß, wenn ein Gas durch eine Röhre strömt, dessen Querschnittdimensionen im Vergleich mit der mittleren Weglänge der Gasmoleküle verschwindend klein ist, die in der Zeiteinheit durchströmende Gasmenge allein von den Dimensionen der Röhre, der Quadratwurzel des spezifischen Gewichtes des Gases und dem Druckunterschied abhängig ist.

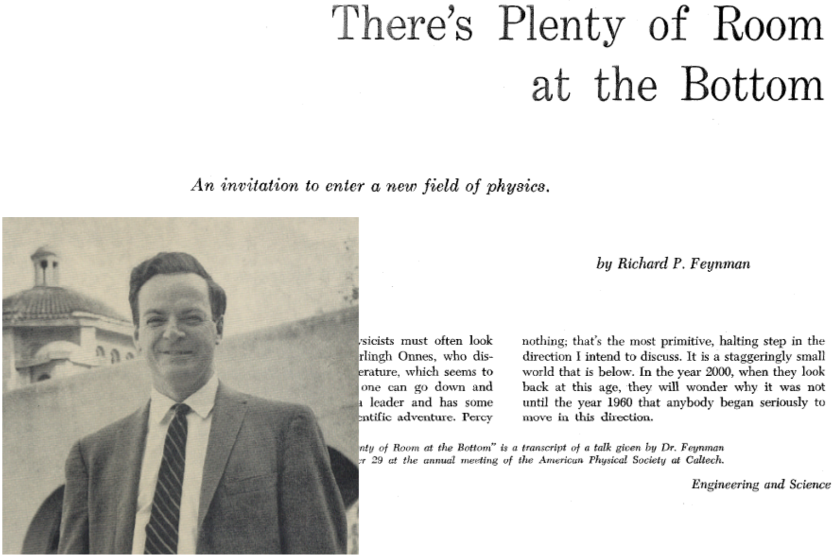
Diese Strömung habe ich Molekularströmung genannt, weil deren Gesetze ganz andere sind als die der inneren Reibungsströmungen, und weil sie in so einfacher Weise von den Eigenschaften der Gasmoleküle abhängig ist. Zu erwarten ist, daß sich ähnliche einfache Verhältnisse geltend machen werden bei der Strömung von Gasen durch eine Öffnung, deren Dimensionen verschwindend klein ist im Vergleich mit der



Annalen der Physik : 33(1), pp 75–130 ; 33(5), pp 999–1016

A bit of history

1959 : December 29th, Richard Feynman's talk at Caltech



There's Plenty of Room at the Bottom

An invitation to enter a new field of physics.

by Richard P. Feynman

sicists must often look
rlingh Onnes, who dis-
erature, which seems to
one can go down and
leader and has some
ntific adventure. Percy

nothing; that's the most primitive, halting step in the direction I intend to discuss. It is a staggeringly small world that is below. In the year 2000, when they look back at this age, they will wonder why it was not until the year 1960 that anybody began seriously to move in this direction.

nty of Room at the Bottom" is a transcript of a talk given by Dr. Feynman
r 29 at the annual meeting of the American Physical Society at Caltech.

Engineering and Science

A bit of history – Modern times

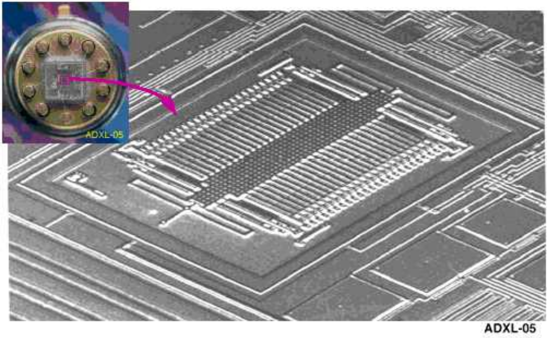
Until the 90's, academic literature rather sparse. Indeed :

- "**Fluidics**" : in the 60's – 70's
    - initiated in the USSR
    - ... then developed in the USA and Europe
    - Goal : design "fluidic computers" – spatial applications
    - ... design "pneumatic" devices $\Leftrightarrow$ electronic devices
    - Typical sizes : $\sim n.100\ \mu m$ – millimetres
- "Explosion" of μ**electronics** knockouted pneumatic computers
- **MEMS** : massively developed in the 80's
    - based on the "silicon"'s expertise
    - broad spectrum of applications at μ-scale
    - $\Rightarrow$, in particular, revival of fluids flow experiments
    - $\Rightarrow$ rose new questions on μ-scale Fluid Dynamics

Two big commercial success in the '80 – '90, among others

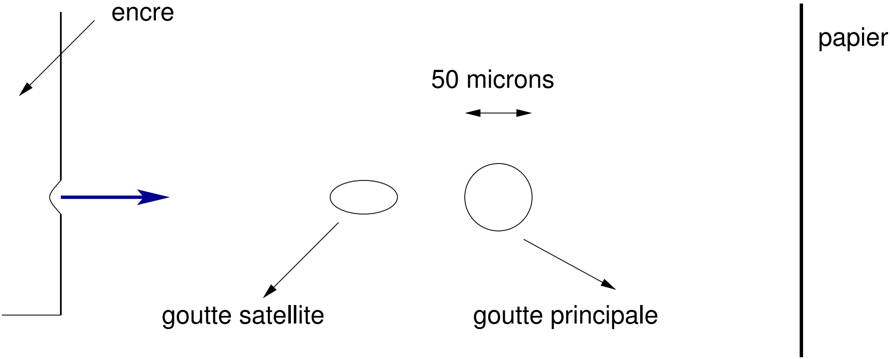
- Airbags
- Ink-Jet printers

MEMS for Airbags



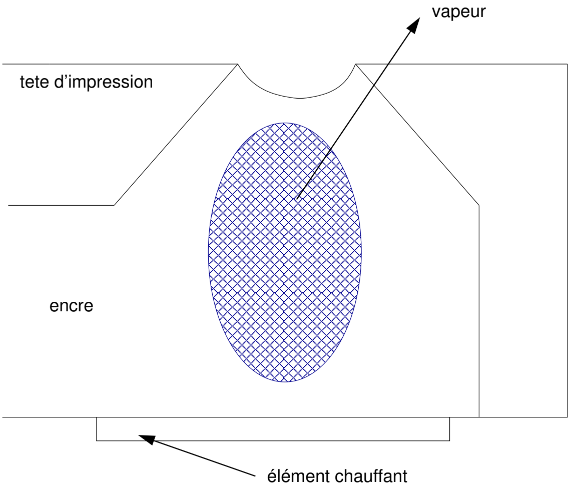
- Integrated system on a silicon wafer
- Not only the detector (accelerometer) ...
- but also : information analysis, signal processing...
- all in a few millimetres.
- Easily reproduced (tens of millions) and Cheap !

Ink-Jet Printers



Need to control the satellite drop for printing quality

Ink-Jet Printers – Prevent the printhead to be stuck



"Wind... effect" : Off/On

Ink-Jet Printers

Impressive review by H. Wijshoff (Physics Reports, 2010)
→ collab. with the leading group of D. Lohse (U. of Twente)

More generally about “Printers” : Droplet dispenser

Change ink by a chemical/biological product

⇒ massive parallelism of tests ⇒ Omics Big Data

More generally about MEMS :

Success thanks to :

knowledge acquired of the exotic physics at the microscale

Microfilms, Medicine and “Lab-on-chip”

Micropumps and Drug injection :

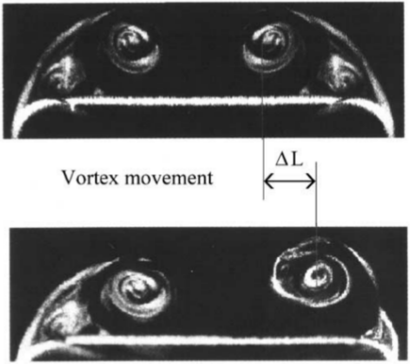
- insulin in liver
- Bactofen in spinal cord
- → improvement of patient comfort

Increased integration on micro-chips :

- various functions :
  - transport
  - mixing
  - characterisation
  - commercialised ex. : myocardial proteins (in 15 minutes)
- → bio / chemical microreactors
- → search new types of drugs and medical treatments

Microfluidics and Flow control

- Aeronautics : MEMS acting on vortices on the leading edge of a wing ⇒ control of the lift

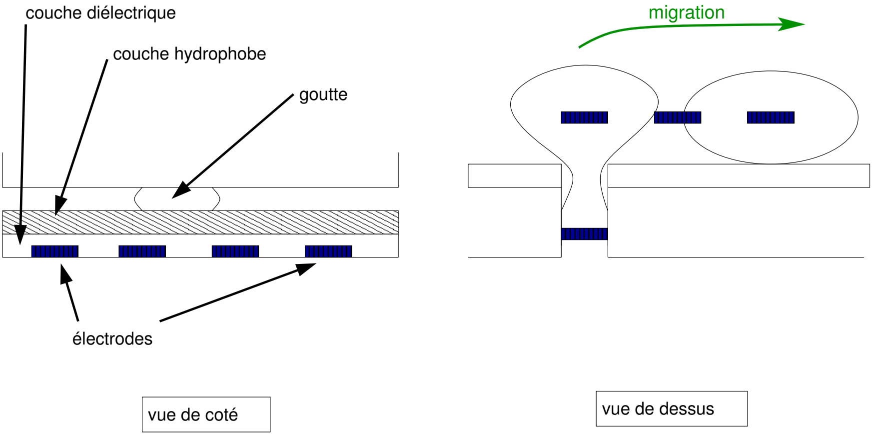


Ho C-M, Huang P-H, Yang JM, Lee G-B, Tai Y-C. *Active flow control by micro systems.* Kluwer Academic Pub., 1999. p. 195-202.

- Electrohydrodynamics : electrowetting on dielectric ▸ Next

- Droplet sorting via laser ▸ Next

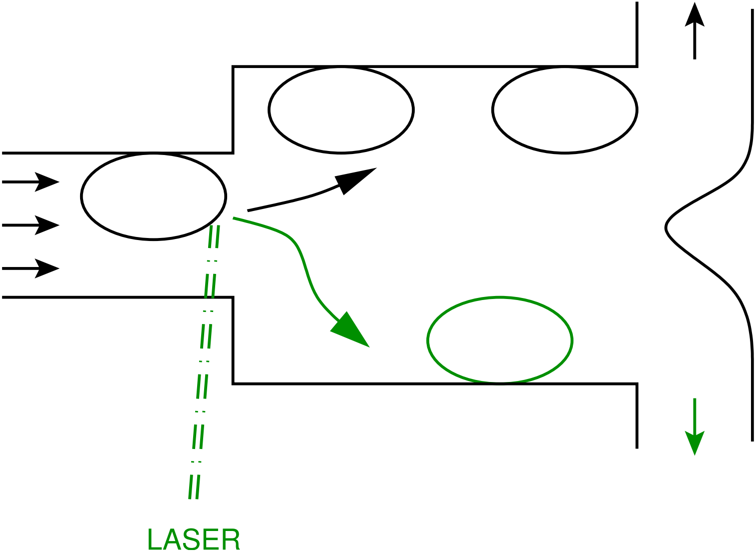
Flow control – electrowetting



O. Raccurt *et al.*, Euromech Coll. 472, Sep 6-8, 2005, Grenoble. See also : Lee *et al.*. Sensors & Actuators A 95 (2002) 259–268

Rk : existence of **triple line** → boundary condition ? **Coming up next ...**

Flow control – laser



C. N. Baroud, Euromech Coll. 472, Sep 6-8, 2005, Grenoble

Physics at microscale

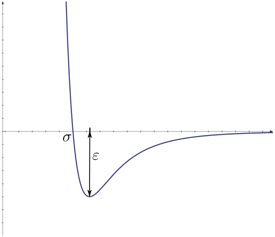
In the next slides, we describe a bit of Physics at the scale of “molecules” and “scaling laws” in this “world”

Forces of microscopic origin
Small molecules in vacuum

As an approximation model, we can assume that essential features of the simplest molecular interaction are :

- strong hard-sphere repulsion
- weaker interaction at some larger distances

→ typically approximated with a Lennard-Jones potential :



$$V(r) = 4\varepsilon\left(\left(\frac{\varsigma}{r}\right)^{12} - \left(\frac{\varsigma}{r}\right)^{6}\right)$$

$$F(r) = -\frac{dV}{dr}(r) \quad \underset{+\infty}{\overset{r}{\sim}} \quad \frac{1}{r^7}$$

Rk : valid for both neutral and polar molecules in vacuum

Conclusion : ranges of forces between molecules do not exceed a few nanometers, in these cases [Israelachvili, 1991]

Forces of microscopic origin

In a solvent...

... **Small molecules** interact within a few nanometers
$\leftarrow$ numerous phenomena including hydrogen bonds and hydration forces in water

... **Bigger molecules $\sim$ 10 nm** :

- more “actors” in the interaction game
- possibility of shape change (conformation)

  Ex : hydro-phobic/philic forces (not described by Lenn-J.)

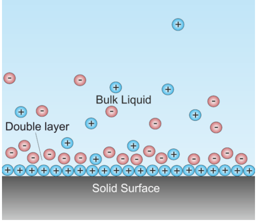
  Ex : conformation entropy $\Rightarrow$ defines associated forces

Roughly :
ranges of interaction forces $\sim \mathcal{O}$(size of the molecule) $\sim$ 10 nm

Forces of microscopic origin...

... between surfaces

- Quantum forces
- van der Waals forces
  - for plane-molecule systems : $\sim 1/r^5$
  - for plane-plane systems : $\sim 1/r^3$



- **Electrostatic forces** : dielectric immersed in an electrolyte → surface charges appears ; **Debye-Huckel double layer**
- among others

Typically :

- ranges of interaction forces $\gg$ as in the molec.-molec. case
- in practice, ranges not exceed 100 nm
- → in "real" microfluidics, they can be ignored
- → but below 100 nm, they need to be accounted for

A first introduction of “molecules lengths”

For **liquids & gases** :

- **size of molecules** := equilibrium radius of Lennard Jones

  $$r = 2^{\frac{1}{6}}\varsigma$$

  Ex : for simple molecules, $r \sim 10^{-10}$ m
- **mean molecular spacing** d : if n is molecule density

  $$d = n^{-\frac{1}{3}}$$

  - Liquids : $d \sim r$
  - Gases : $r \ll d$, typically $d \approx 3.10^{-9}$ m

For gases the meaningful length is the **mean free path** λ
:= mean distance travelled by a molecule between 2 collisions

$$\lambda = \frac{1}{\sqrt{2}\pi r^2 n}, \qquad \text{typically } \lambda \approx 10 \text{ or } 100.10^{-9} m$$

Miniaturisation & counter-intuitive phenomena

Scaling laws = variation of a physical quantity vs characteristic length of the system

Quantity	Scaling	μscale Weight
van der Waals force	l^{-7}	**+++**
Time	l^0	↑
Capillary force	l^1	|
Thermal conduction	l^1	|
Electrostatic force	l^2	|
Volume	l^3	|
Mass	l^3	|
Gravity force	l^3	**- - -**

Ex : *Gerris*' water walk

$\leftarrow$ capillary $\gg$ gravity f.

Warning : scaling laws can be too "rough" and lead to wrong evaluation of preponderant effects. Need to be careful and to consider the "full" physical laws instead.

Electro - statics/magnetics in small systems

- Dielectric breakdown is retarded.
  A gas subjected to intense electric field $\rightarrow$ ionisation $\rightarrow$ plasma, if E greater than a critical E_c.
  In μsystems : rarefaction $\nearrow$ $\Rightarrow$ breakdown less probable $\Rightarrow$ E_c $\nearrow$

- Parallel-plate capacitors : if a force is used to displace one of the plate (scaling law l^3), it is negligible vs electrostatic force (scaling law l^2). This is useful for sudden impacts detection with accelerometers (cf. airbags previous. mentioned).

- For electromagnetic systems expertise was developed and it seems possible to obtain quite high magnetic fields at μscale (see e.g. works at CEA-LETI and around).

Mechanics and Thermics in small systems

- Mechanics : possibility to build resonating beams but thermal noise became preponderant as we miniaturise
- Thermics : volumetric heat sources easily thermalized by conduction (if Fourier's law applies).
- Evaporation of microdroplets is very fast

Outline

Gases : from microscopic description to hydrodynamic limits

A bit of kinetic theory

We want to model a gas as a set of n identical particles in interaction (no mixture, non relativistic, non quantum), in a space $\mathbb{R}^N$ ($N = 3$). Typically, $n \sim 10^{20}$

Assumption – description is given by x_i (position) and v_i (speed) of each particle → huge phase space $\left(\mathbb{R}^N_x \times \mathbb{R}^N_v\right)^n$

First (ambitious) step – **Microscopic model** – $(x_i, v_i)_{i=1,n}$, known at $t = 0$; apply Newton's law with known interaction forces → well-posed problem, one can theoretically determine evolution of particles. But practically intractable ...

Next step – replace it by simpler **macroscopic models** : kinetic or hydrodynamic (see later)

Kinetic model state of the gas is represented by a probability density $f(t, x, v)$ such that at time t, $f(t, x, v)\, dx\, dv =$ density of particles in volume $dx\, dv$ around (x, v).
Depending on interaction, derive various kinetic equations : Vlasov, Boltzmann, etc

A bit of kinetic theory – Evolution of f

- forgetting interaction : particles move on a straight line at constant speed :

$$\frac{\partial f}{\partial t} + v.\nabla_x f = 0 \qquad \text{or} \qquad \frac{\partial f}{\partial t} + v.\nabla_x f + F(x).\nabla_v f = 0$$

if a macroscopic force $F(x)$ applies on particles.

- **Interactions** – Assumptions : **binary collisions** (dilute gas, interaction with more than 2 particles neglected), **localized** in space and time, **elastic** (moment. and kin. energy preserved), microreversible (time), *Boltzmann chaos* (speeds of 2 collid. part. uncorrelated before collision). $\Rightarrow \exists$ a quadratic collision operator which models effect of interactions on f :

$$\begin{aligned}\left.\frac{\partial f}{\partial t}\right|_{collisions}(t,x,v) &= Q(f,f)(t,x,v)\\ &= \int_{\mathbb{R}^N} dv_\star \int_{\mathcal{S}^{N-1}} d\sigma \quad B(v-v_\star,\sigma)(f' f'_\star - f\, f_\star)\end{aligned}$$

where B is the **Boltzmann collision kernel**. **To sum up :**

A bit of kinetic theory – Boltzmann equations :

$$\frac{\partial f}{\partial t} + v.\nabla_x f = Q(f,f) \qquad \text{or} \qquad \frac{\partial f}{\partial t} + v.\nabla_x f + F(x).\nabla_v f = Q(f,f)$$

There are a lot of collisions kernels. Let us mention two which are explicit :

- **“hard-sphere”** – particles bounce each other like billiard balls

$$B(v - v_\star, \sigma) = K\,|\langle v - v_\star, \sigma\rangle|, \quad K > 0$$

- Coulomb interaction – with $\phi(r) = 1/r$ as interaction potential

$$B(v - v_\star, \sigma) = \frac{1}{|v - v_\star|^3\ \sin^4(\theta/2)}$$

where θ is the deviation angle of the collision.

Rk : “hard-sphere” is the only kernel for which rigorous hydrodynamic limits are derived

▸ Next

Boltzmann equations – Observables

One of the ideas of kinetic approach is that all measurable **macroscopic quantities** can be expressed in terms of f : at t and x given,

- local density ρ :

$$\rho = \int_{\mathbb{R}^N} f(t, x, v)\, dv,$$

- local macroscopic velocity u :

$$\rho u = \int_{\mathbb{R}^N} f(t, x, v) v\, dv,$$

- local temperature T :

$$\rho |u|^2 + N \rho T = \int_{\mathbb{R}^N} f(t, x, v)\, |v|^2\, dv.$$

These quantities are involved when writing **macroscopic hydrodynamic models** such as Navier-Stokes, Euler, Stokes...

Boltzmann equations – some properties

- For $f : v \in \mathbb{R}^N \to f(v)$, with ad hoc integrability properties.

If $\zeta \in \{1, v_j, |v|^2\}, j = 1, N$: $\displaystyle\int_{\mathbb{R}^N} Q(f,f)\,\zeta(v)\,dv = 0.$

This implies **local conservation laws** :

$$\frac{\partial}{\partial t}\left(\int f\zeta dv\right) + \nabla_x \left(\int f\zeta v dv\right) = 0.$$

- Another important property : $\displaystyle\int_{\mathbb{R}^N} Q(f,f)\log f\;dv = -D(f),\;(\clubsuit)$

$$D(f) := \frac{1}{4}\int_{\mathbb{R}^N\times\mathbb{R}^N\times\mathcal{S}^{N-1}} (f' f'_\star - f\,f_\star)\;\log\frac{f' f'_\star}{f\,f_\star}\;B\,dv\,dv_\star\,d\sigma \geq 0$$

$$(\clubsuit) \Rightarrow \frac{\partial}{\partial t}\left(\int f\log f\;dv\right) + \nabla_x\left(\int (f\log f)v\;dv\right) = -D(f) \leq 0.$$

$$\Rightarrow H(f) := \int f\log f\,dx\,dv, \quad \frac{d}{dt}H(f(t,.,.)) = -\int_{\mathbb{R}^N} D(f(t,x,.))dx \leq 0,$$

is the **H-Theorem of Boltzmann**, D being “entropy dissipation”

Boltzmann equations – some properties (cont'd)

Consequences on the macroscopic quantities :

$$\frac{\partial \rho}{\partial t} + \nabla_x . (\rho u) = 0 \tag{1}$$

Each molecule has its velocity v and $c = v - u$ is called random velocity and such that $\langle c \rangle = 0$.

Flow momentum $m_{ij} := \int_{\mathbb{R}^3} v_i v_j f dv$, rewritten $m_{ij} = \rho u_i u_j + p_{ij}$

$$\text{with } p_{ij} = \int_{\mathbb{R}^3} c_i c_j f dv, (i, j = 1, 2, 3)$$

It reads

$$\frac{\partial \rho u}{\partial t} + \nabla_x . (\rho u \otimes u + \mathbf{p}) = 0 \tag{2}$$

And so on (energy equation, etc). **Rk :** about "closure" *à la* Euler

Boltzmann equations – Boundary conditions

Interactions between particles and walls : many choices

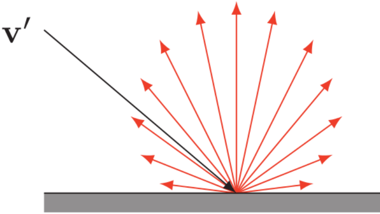
- **Specular reflection** : $\mathcal{R}v = v - 2(v.n(x))\, n(x)$, where $n(x)$ is outward unit normal at x (⇔ to optics' Snell-Descartes law) :

$$f(x, \mathcal{R}v) = f(x, v). \qquad \text{(not really realistic)}$$

- **Bounce-back condition** : simple but more relevant in some cases $f(x, -v) = f(x, v)$.
- **Maxwellian diffusion** : $f(x, v) = \rho^-(x)\, \mathcal{M}_w(v), v.n(x) > 0$

where $\rho^-(x) = \int_{v.n<0} f(x, v)|v.n|\, dv$ and $\mathcal{M}_w(v)$ is a given Gaussian distribution depending on the wall :

$$\mathcal{M}_w(v) = \frac{e^{-\frac{|v|^2}{2T_w}}}{(2\pi)^{\frac{N-1}{2}}\ T_w^{\frac{N+1}{2}}}$$



- **Convex combin.** of spec/diff, **Cercignani-Lampis** model, etc

Boltzmann equations – Variants

Many. To name a few :

- relativistic, quantum, linear, diffusive, energy dissipating
- **model equations** :
  - **BGK model** : Boltzmann tricky operator is replaced by the simplistic $M^f - f$, where M^f is the Maxwellian distribution with the same local ρ, u, T than f ▸ Next
  - Kac model : a 1D toy-model
- discrete-velocity models (including numerical perspectives)
- Of note, one of the assumptions which lead to Boltzmann equations is “localized interaction” ; some works were done on this “delocalization” of collisions.

Boltzmann equations – Physical validity

Realistic description of

- dilute atmosphere : aeronautics at high altitude, plasmas
- at low densities, Navier-Stokes not accurate :
  cf “Knudsen’s paradox” in his 1909 experimental paper
  but good agreement with Boltzmann
- study of boundary layers (Knudsen layer, Sone sublayer...)

The Knudsen number

Let us go back to the classical : $\frac{\partial f}{\partial t} + v.\nabla_x f = Q(f,f)$

Consider for typical scales : time τ, length L and velocity ν. One can show :

$$\frac{\partial f}{\partial t} \sim \frac{f}{\tau}, \qquad v.\nabla_x f \sim \frac{\nu}{L} f, \qquad Q(f,f) \sim n\nu\varsigma^2 f \sim \frac{\nu}{\lambda} f$$

where n : density of molecules, ς : molecular diameter (or range of interaction potential) and λ : mean free path

Def : nondimensional **Knudsen number,** $Kn = \frac{\lambda}{L}$

Nondimensional form of the Boltzmann equation :

$$\frac{\partial f}{\partial t} + v.\nabla_x f = \frac{1}{Kn} Q(f,f) \tag{3}$$

Suggests two asymptotics :

- $Kn \to 0$ (continuum or hydrodynamic)
- $Kn \to +\infty$ (free-molecular)

> *“Le livre de M. Boltzmann sur les Principes de la Mécanique nous incite à établir et à discuter du point de vue mathématique d’une manière complète et rigoureuse les méthodes basées sur l’idée de passage à la limite, et qui de la conception atomique nous conduisent aux lois du mouvement des continua.”*

D. Hilbert (1900), *Sur les problèmes futurs des mathématiques* (trad. L. Laugel), Comptes rendus du 2me congrès international des mathématiciens, Gauthier-Villars, 1902.

Continuum limit – Hilbert's 6^{th} problem

Kinetic description (though simplified w.r. to microscopic descr.) is still complex and expansive.

Practically, it is often better to replace a kinetic model by a macroscopic description such an hydrodynamic model (Navier-Stokes' like)

Theoretical underlying justification of such "simplification" is the **local thermodynamical equilibrium hypothesis**.

Def : $f(x,v)$ is a **local equilibrium for the Boltzmann equation** if

$$Q(f,f)=0.$$

$(\clubsuit) \Rightarrow f' f'_\star = f\, f_\star,\ a.a.\ x, v, v_\star \Rightarrow$ (Boltzmann)

$$f(x,v)=M_{\rho,u,T}(x,v):=\rho(x)\,\frac{e^{-\frac{|v-u(x)|^2}{2T(x)}}}{(2\pi\ T(x))^{\frac{N}{2}}}$$

So called local Maxwellian $M_{\rho,u,T}$ maximizes the entropy $-H(f)$, which explains so called *local equilibrium*.

Continuum limit – Hilbert's 6^{th} problem – Cont'd

This concept leads to the idea : a distribution f is close to a local equilibrium in a regime where collisions are very frequent $\Leftrightarrow$ when Kn is small

Deriving an hydrodynamic limit of Boltzmann equation thus consists in ;

- proving a kind of local thermodynamical equilibrium when $Kn \to 0$
- deduce limit equations for the macroscopic quantities associated to f : ρ, u, etc

This was a part of the Hilbert's 6^{th} problem : can we derive rigorously the continuum equation of fluid mechanics from Newton laws ? To this end, he proposed to prove :

Microscop. Newton eqs $\rightarrow$ Boltzmann eqs $\rightarrow$ Hydrodyn. eqs

"instead of" : Microscop. Newton eqs $\rightarrow$ Hydrodyn. eqs

Rk : perfect gas law limitation for Bo. $\rightarrow$ Hy. : less general

Continuum limit – Hilbert's 6^{th} problem – Cont'd

In other words, continuum limit consists in passing :

from a Boltzmann model of dilute gas, on microscopic scales of space ($\sim \lambda$) and time ($\sim$ mean time between collisions)

to an hydrodynamic model on macroscopic scales of time and space (*à la* Batchelor)

This scaling modification is *not innocent* : depending on the choice, one can derive various limits.

Continuum limit – an example

Contract time and space by ε (think *Kn*), preserve speed ; the new distribution function (not a prob. density) is

$$t \rightsquigarrow \frac{t}{\varepsilon}, \quad x \rightsquigarrow \frac{x}{\varepsilon}, \quad v \rightsquigarrow v; \qquad f_\varepsilon(t,x,v) = f\left(\frac{t}{\varepsilon}, \frac{x}{\varepsilon}, v\right).$$

If f solution of Boltzmann, then f_ε solves the rescaled Boltz. eq

$$\frac{\partial f_\varepsilon}{\partial t} + v.\nabla_x f_\varepsilon = \frac{1}{\varepsilon}\, Q(f_\varepsilon, f_\varepsilon) \quad \text{and the macrosc. quant. verify}$$

$$\frac{\partial \rho_\varepsilon}{\partial t} + \nabla_x.\left(\rho_\varepsilon u_\varepsilon\right) = 0$$

$$\frac{\partial \rho_\varepsilon u_\varepsilon}{\partial t} + \nabla_x.\left(\int_{\mathbb{R}^N} f_\varepsilon v \otimes v \, dv\right) = 0$$

$$\frac{\partial}{\partial t}\left(\rho_\varepsilon |u_\varepsilon|^2 + N\rho_\varepsilon T_\varepsilon\right) + \nabla_x.\left(\int_{\mathbb{R}^N} f_\varepsilon\, |v|^2 v \, dv\right) = 0$$

...

Continuum limit – an example – Cont'd

Assumption of local thermo. equilibrium allows to close this system when $\varepsilon \to 0$, formally (I_N : identity matrix) :

$$\frac{\partial \rho}{\partial t} + \nabla_x . (\rho u) = 0$$

$$\frac{\partial \rho u}{\partial t} + \nabla_x . (\rho u \otimes u + \rho T I_N) = 0$$

$$\frac{\partial}{\partial t}\left(\rho |u|^2 + N\rho T\right) + \nabla_x . \left(\rho\, |u|^2 u\ + (N+2)\rho T u\right) = 0$$

which is the compressible Euler system with the law of perfect gas : $p = \rho T$.

Other scalings can lead to Navier-Stokes, giving a "kinetic" interpretation of viscosity.

Continuum limit – Overview of expansions

- **Hilbert** himself (1912, Math. Ann.) ; look for f as ($\varepsilon = Kn$) :

$$f(t,x,v;\varepsilon) \;=\; \sum_{n=0}^{\infty} \varepsilon^n f_n(t,x,v)$$

and identifying coefficients of various powers of ε, get systems of equations for f_0, $f_0 + \varepsilon f_1$, $f_0 + \varepsilon f_1 + \varepsilon^2 f_2$, ...

- **Chapman-Enskog** expansion is a variant of Hilbert where f_n depend on
  - the macroscopic quantities $\rho(t,x;\varepsilon),\; u(t,x;\varepsilon),\; T(t,x;\varepsilon)$ associated to f_ε ;
  - and v.

Both approaches allow to formally recover Euler and Navier-Stokes (compressible or incompressible)

But they are not necessarily convergent, and they can only represent very special kind of solutions.

Continuum limit – expansions – Cont'd

A more "robust" approach is the **moment method of Grad**

The idea is to write, for ε fixed, equations verified by $\int_{\mathbb{R}^N} f(t,x,v) v_1^{\alpha_1} ... v_N^{\alpha_N}$, including the usual macroscopic quantities, ρ, ρu, $\rho(|u|^2 + NT)$ subject to the local conservation laws.

Then the key point is to close these equations in the limit $\varepsilon \to 0$ with a law based on the local thermo. equilibrium. This law needs to be justified properly.

To sum up : rigorous limits can be proved as long as hydrodynamic solutions are smooth

Continuum limit – Last (but not least) comments

- Surprises can happen with formal asymptotics... leading to wrong hydrodynamic model, as *e.g.* shown by Sone and coworkers (so called “ghost effects”). See also, more generally, all their numerous works on these associated asymptotic theories.

- Results on the “Micro → Boltzmann” asymptotics, cf Lanford (1975, Springer) and extension by Illner & Pulverenti (C.M.P., 1986 and 1989)

- Results on the “Boltzmann → Hydro” asymptotics, see in particular Bardos, Golse & Levermore (1989, 1991, 1993), Golse & Saint-Raymond (2001, 2009)

- Results on the asymptotic “Micro → Hydro”, see Varadhan and collaborators

Free-molecular regime

It is the opposite limit : $Kn \to \infty$

In this case, Boltzmann equation reduce to a transport equation (no collision between molecules)

Interesting situations are thus flows with bodies ; study momentum and energy exchanged between molecules and the solid body

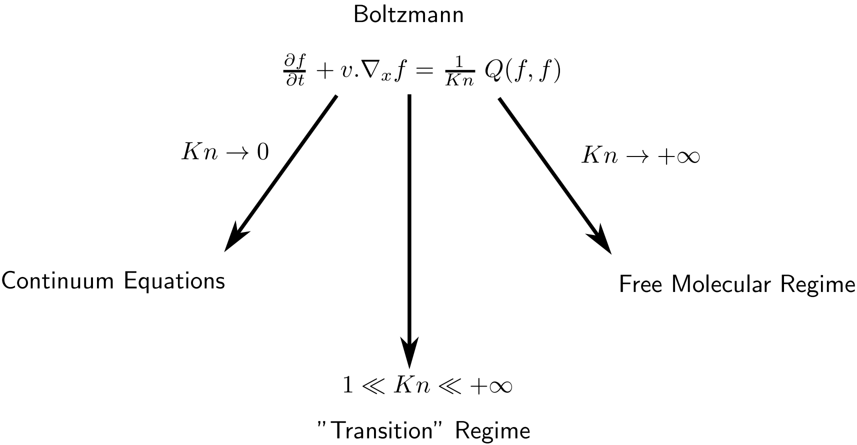
Hence the dynamics depends crucially on the boundary condition model adopted and on the body geometry (convex or not, etc)

We will not talk more on that and redirect to the literature for more details.

A summary (1)

Model equation / description

Newton → Liouville → Boltzmann→ Hydrodynamic



Boltzmann

$$\frac{\partial f}{\partial t} + v.\nabla_x f = \frac{1}{Kn}\, Q(f,f)$$

$Kn \to 0$

Continuum Equations

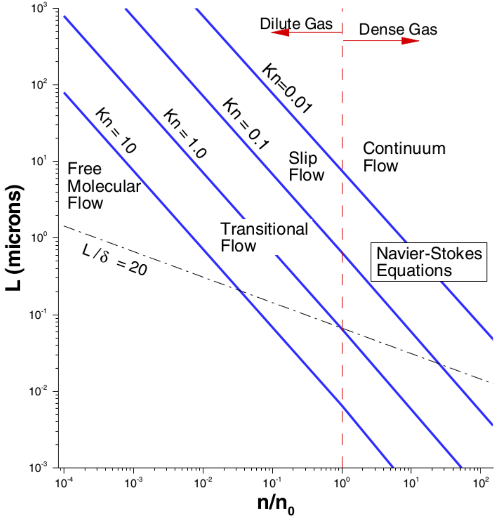
$Kn \to +\infty$

Free Molecular Regime

$1 \ll Kn \ll +\infty$

"Transition" Regime

A summary (2)



Karniadakis et al, 2005

L : characteristic length ; n/n_0 : number density normalized with corresp atmosph. cond.. *Kn* regimes based on air at isothermal conditions at T = 273 K. Statistical fluctuations significant below the line $L/\delta = 20$.

Gases : numerical methods

Direct Simulation Monte Carlo : DSMC

Pioneered by G. Bird in the ’60-’70.

DSMC uses typically 10^6 of "simulated particles" ($<$ real nb)

Space discretized in similar cells ($\Delta x \propto \lambda$)

Idea : decouple molecular motion and intermolecular collisions
$\Rightarrow \Delta t <$ mean collision time

It is a probabilistic approach ($\neq$ deterministic MD simulation)

Four main steps, during a time interval Δt :

1. motion of particles
2. indexing and cross-referencing of particles
3. simulation of collisions
4. sampling of macroscopic quant. of the flow

DSMC : step 1

- move particles
- some particles will collide ($\Delta t < \Delta t_c$) ...
- some will go out of cells, boundaries, etc
- enforce boundary conditions here, with conservation laws, instead of velocity distribution function (à la Boltzmann)
- $\rightarrow$ can add a bit more of physics (chemical reaction, radiation, etc) without changing the global DSMC procedure. Price to pay : need to know the accommodation coefficients at the boundaries

DSMC : step 2

- index and track particles
- to know in which cell they are and detect collisions
- From the implementation point of view, data structure and algorithms must be efficient to handle a huge number of particles

DSMC : step 3

- **simulation of collisions** : probabilistic
- During Δt, only collisions between particles belonging to the same cell are considered
- Each collision considered as a random event with some probability
- In every cell, pairs of colliding particles are randomly sampled and associated pre-collisional velocities are transformed in post-collisional ones
- Example of collision model : the No-Time-Counter (NTC) (cf Bird 1994)

DSMC : step 4 and Loops

- compute macroscopic quantities :
- by averaging on each cell

Loops : in time and/or in "realizations”

- for steady flows : average samples after reaching steady
- for unsteady flows : iterate (steps 1–4 + time) to obtain the required number of realizations and then take average of all runs

♣ DSMC method is still subject to evolutions/transformations.
See *e.g.* Gallis et al. JCP 228 (2009) 4532-4548

DSMC : pitfalls

DSMC is the only possible way to high Knudsen number rarefied flows, in complex geometry. Many things done.

However, caution must be taken :

- Cell size : no larger than (local mean free path)/3
- Time step : no larger than (local mean free time)
- Boundary condition : in/out-flow in pipe can be tricky
- Slow “convergence” : error $\propto \sqrt{n}$, $n =$nbr of particles to be compared with continuum models ($\Rightarrow$ to be adopted if $Kn < 0.1$)

In particular, for gas microflows

- large statistical noise & long time to reach steady states : due to higher orders of magnitude difference between speeds of particles and macr. speed (slow in μfl.)
- not always easy to have a good modelling of the wall-boundary conditions

Direct resolution of Boltzmann equations

These numerical simulations are very expensive

Generally done in simple geometry (pipes) and with simplified versions of the equations like BGK.

Hard sphere + Maxwellian molecular model

Some works on **fast spectral methods** to decrease CPU time : Mouhot & Pareschi. Math. of Comput. 75(256) 2006. Wu et al. JCP 250 (2013)

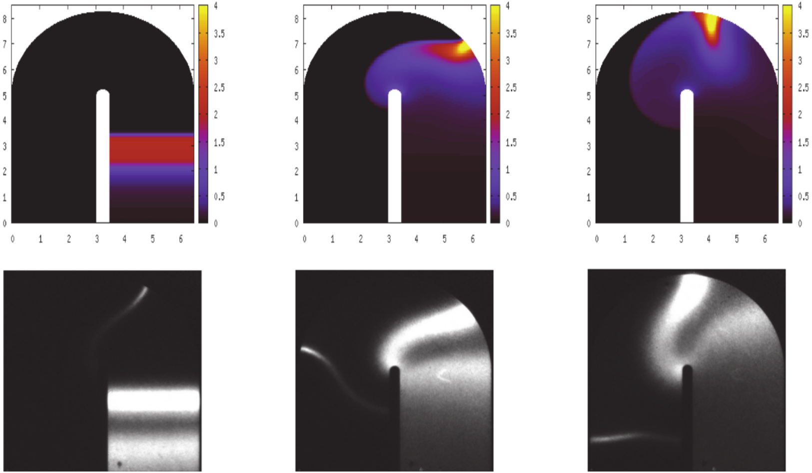
More generally, see recent review by Di Marco-Pareschi : Acta Numerica 2014

E.g., extension to **complex geometries** : see e.g. F. Filbet, C. Yang. Journal of Computational Physics 245 (2013) 43-61 and

...

Direct resol. of Boltzmann eq. - Complex geom

... Filbet-Yang. Kinetic models for Chemotaxis. SIAM JSC 36(3) 2014

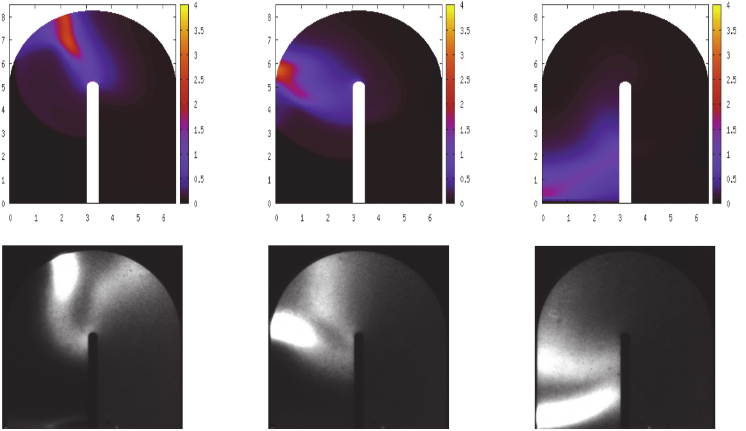


(a) (b) (c)

FIG. 7. *Test 5: Numerical simulations (top) and experiments on* E. coli *(bottom): time evolution of the cell density* (a) $t = 7.5\ \bar{t}$, (b) $t = 18.5\ \bar{t}$, *and* (c) $t = 23\ \bar{t}$ *in seconds.*

Direct resol. of Boltzmann eq. - Complex geom

... Filbet-Yang. Kinetic models for Chemotaxis. SIAM JSC 36(3) 2014



(d) (e) (f)

FIG. 8. *Test 5: Numerical simulations (top) and experiments on* E. coli *(bottom): time evolution of the cell density* (d) $t = 28\ \bar{t}$, (e) $t = 34.5\ \bar{t}$, *and* (f) $t = 46.5\ \bar{t}$ *in seconds.*

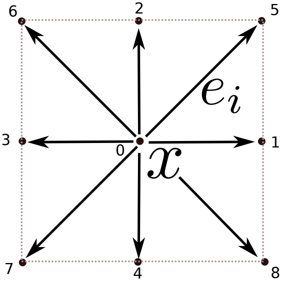
See also Dechristé-Mieussens, preprint 2015.

Lattice–Boltzmann Method (LBM) - LBGK version

BGK simplification of collision term + discretization of Boltzmann on a finite set of velocities :

$$f_i(x + e_i \Delta t, t + \Delta t) - f_i(x,t) = \frac{1}{\tau}\left[\mathcal{M}_i^f(\rho, u) - f_i(x,t)\right]$$

Discrete velocities : $e_0 = 0$, $e_1 = (1;0)$, $e_2 = (0;1)$, etc



D2Q9 lattice

Relax. time τ

$$\rho = \sum_i f_i$$

$$\rho u = \sum_i e_i f_i$$

Lattice–Boltzmann Method (LBM) - LBGK version

Algorithm :

1. Streaming step

$$\tilde{f}_i(x,t) = f_i(x + e_i, t)$$

2. Collision step

Compute moments $\rho, \rho u$

Compute equilibirum function : $\mathcal{M}_i^f(\rho, u)$

Advance in time :

$$f_i(x, t+\Delta t) = \tilde{f}_i(x,t) + \frac{1}{\tau}\left[\mathcal{M}_i^f(\rho,u) - \tilde{f}_i(x,t)\right]$$

Used in a vast amount of applications (mixture, phase change) and interesting on new computational architecture (GPU).

Outline

Overview

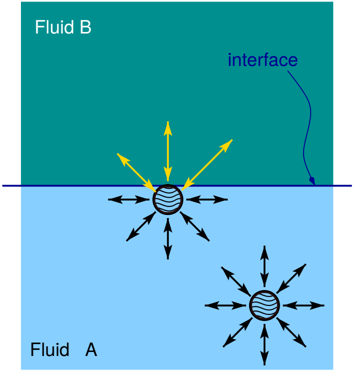
For liquids, classical continuum models (Stokes (++), Navier - Stokes(+)) can be used down to a scale smaller than for gases.

The key point is that, thanks to “scaling laws”, preponderant forces are not the “usual suspects”. Typically, gravity can be neglected but surface tension is crucial.

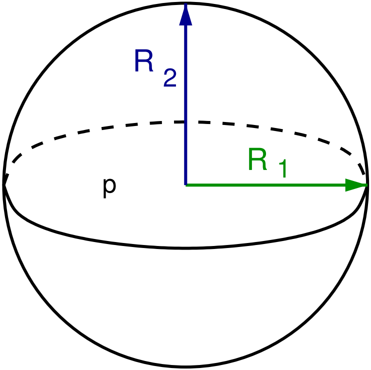
The “no-slip” boundary condition may be changed to Navier BC.

If we go to so tiny domains that Continuum hypothesis breaks down, need to switch to “atomistic” methods, e.g. Molecular Dynamics.

Overview – Capillary effects



Origin of surface tension
= capillary force



Laplace's law

$$[p] = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

At μ-scale : surface effects $\gg$ volume effects

Overview – Capillarity, Young's law

Young's law :

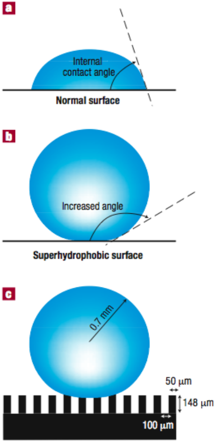
$$\gamma_{LV} \cos\theta = \gamma_{SV} - \gamma_{LS}$$

Wetting regimes :

- $0 < \theta < 90^o$: partially wetting ...
- ... hydrophilic
- $\theta > 90^o$: non-wetting ...
- ... hydrophobic
- $\theta = 0^o$: complete wetting

Perspectives :

- Role on slippage ▸ Next
- Microfluidics of droplets ▸ Next



From Quéré ; Nature Mat. (2002) →

Liquids : numerical methods

Molecular Dynamics (MD) method

Compute trajectories of atoms of a system, knowing interaction force fields

$\Rightarrow$ Simulations over small volumes ($\sim (100nm)^3$) and small time intervals (several tens 10^{-9}s)

Usually not appropriate for gas flow (see instead DSMC)

One can distinguish between :

- Equilibrium MD (EMD)
- Nonequilibrium MD (NEMD)

Molecular Dynamics (MD) method

Model system : N particles and Newton's law

$$m_i \frac{d^2 r_i}{dt^2} = F_i$$

Solved until system's properties reach steady state, in the framework of Equilibrium MD.

MD method – main steps

☐ **Initialisation** : initial position and velocities assigned to particles, compatible with the simulated structure. Ex : Maxwellian

Then loop, for each time step :

☐ **Force computation** : (most time consuming) interaction between particles ; depends on the choice of intermolecular potential, see ▸ Next

☐ **Integration of equations of motion** : in time, with finite difference schemes such as Verlet

$$r^{n+1} = 2r^{n} - r^{n-1} + \Delta t^{2}\, a(t) \;+\; \mathcal{O}(\Delta t^{4})$$

or others : leap-frog, Velocity Verlet, etc

☐ **Statistics and storage** : compute temperature, pressure, volume, etc and store them together with r and v.

MD method – intermolecular potentials

Key point. Potential energy V of a N-particles system

$$V = \sum_i V_1(r_i) + \sum_i \sum_{j>i} V_2(r_i, r_j) + \sum_i \sum_{j>i} \sum_{k>j>i} V_3(r_i, r_j, r_k) + \dots$$

- V_1 : external fields
- $V_i, i \geq 2$: particles interactions (pairs, triplets, etc)
- typical : truncation after the second term
- i.e. three-body and higher order interactions neglected

MD method – Pairwise intermolecular potentials

Potential	$V(r) =$	Parameters
Square-well	$\begin{cases} \infty, & r \leq \varsigma \\ -\varepsilon, & \varsigma < r \leq \lambda\varsigma \\ 0, & r > \lambda\varsigma \end{cases}$	ς, ε
Yukawa	$\begin{cases} \infty, & r \leq \varsigma \\ -\frac{\varepsilon\varsigma}{r} e^{-z(\frac{r}{\varsigma}-1)}, & r > \varsigma \end{cases}$	$\varsigma, \varepsilon, z$
Lennard-Jonnes	$4\varepsilon \left[\left(\frac{\varsigma}{r}\right)^{12} - \left(\frac{\varsigma}{r}\right)^{6} \right]$	ς, ε
Buckingham	$V(r) = Ae^{-Br} - \frac{C_6}{r^6}$	A, B, C_6
Coulomb	$V(r) = \frac{1}{4\pi\varepsilon_r\varepsilon_0} \frac{q_1 q_2}{r}$	q_1, q_2, ε_r
WCA	$\begin{cases} 4\varepsilon \left[\left(\frac{\varsigma}{r}\right)^{12} - \left(\frac{\varsigma}{r}\right)^{6} \right] - V_{LJ}(r_c), & r \leq r_c \\ 0, & r > r_c \end{cases}$	$\varsigma, \varepsilon, r_c$

Ref : Karniadakis, Beskok, Aluru (Springer, 2005)

Rk : in some cases, they are not sufficient. Need to introduce three-body potential (e.g. Tersoff potential)

MD method – Effective computation of potentials

♣ **Short range interactions.** Generally : neighbour particles list and “cutoff” outside this region. The list needs to be updated at each time step due to particle motion : lot of algos available.

♣ **Long range interactions.** Much more difficult. (Trade off between artefacts and comput. cost.) Let us consider *Coulomb potential* (& periodic BC). Again, several methods available, including

- Ewald summation
- Particle Mesh Ewald (PME)
- Fast Multipole Method (FMM)

MD method – Thermostats

Necessity to control temperature during simulation (equilibration drift, force truncation drift, integration errors, external or friction forces heating, etc)

♣ **Berendsen Thermostat.** Deviation from the system temperature T_0 corrected following :

$$\frac{dT}{dt} = \frac{T_0 - T}{\tau}, \qquad \text{time constant } \tau$$

♣ **Nose-Hoover Thermostat.** Equation of motion modified

$$\frac{d^2 r_i}{dt^2} = \frac{F_i}{m_i} - \xi \frac{dr_i}{dt}, \qquad \text{and} \qquad \frac{d\xi}{dt} = \frac{T - T_0}{Q}$$

ξ : "heat bath" parameter ; constant Q : strength of coupling

MD method – Thermostats

Thermostat	Key concept	Suitability/Application
Berendsen	1st order kinetic-based weak coupling	Easy implementation & computationally inexpensive
Nose-Hoover	Extended Lagrangian	Most rigorous implementation of the NVT ensemble
Andersen	Stochastic collision	Suitable for the thermal coupling of atomistic and continuum domains ; also for DPD

Ref : Karniadakis, Beskok, Aluru (Springer, 2005)

MD method – Statistics

♣ **Density profiles.** $\rho_i = \langle n_i / VOL(i) \rangle_s$, in cell i with n_i atoms, averaged over s steps.

♣ **Velocity profiles.** Same spirit as above

$$u_i = \frac{\sum_{k=1}^{s} \sum_{j=1}^{n_{k,i}} v_{k,i}^{j}}{\sum_{k=1}^{s} n_{k,i}}$$

Rk : steady state vs transient.

♣ **Diffusion coefficient.** Einstein relationship

$$D = \frac{1}{6} \lim_{t \to \infty} \frac{\langle [r(t_0 + t) - r(t_0)]^2 \rangle}{t}$$

MD method – Statistics

Idem, based on MD quantities r_i, v_i and interaction forces, one can approximate :

♣ **Stress tensor.** Irving-Kirkwood expression

♣ **Shear viscosity.** Using Green-Kubo formula, in the Equilibrium case (EMD). Other algorithms for NEMD : e.g. Sllod algorithm. Such computations are rather expensive.

♣ **Sources of errors.**

- errors in equilibrium averages : actually, realizations are not completely independent

MD method – Issues

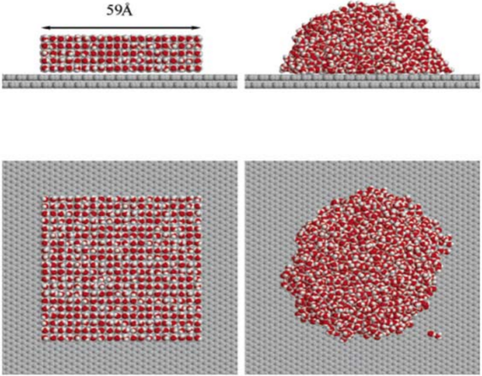
♣ Time step. A fraction of the period of the highest-frequency motion in the system. An option to check that Δt is sufficiently small : run an EMD simul. without temperature coupling and check whether fluctuation of total energy of the system is less than 5% of the total en.

♣ *Boundary conditions*. Most common : periodic. Take care of images and long-range interactions. – *Cut-Off*. See previously.

♣ Storage. Usually only trajectories, and not at each time steps. But for some statistics, each time step is needed $\Rightarrow$ trade off between storage and CPU/accuracy on these variables (use "on the fly" computation to save storage)

♣ Trade off between finer cells and number of particles per cell : discretisation error vs statistical error

Molecular Dynamics (MD) – an illustration



Contact angle of water on graphite surface (119×118 $\dot{A}$) at $t = 0$ and 0.2 *ns*. By Petros Koumoutsakos.

Molecular Dynamics (MD) method

Some (open-source) softwares : GROMACS, AMBER, CHARMM, etc

Dissipative Particle Dynamics (DPD)

Combines features of MD and Lattice Boltzmann methods

Hoogerburgge & Koelman, 1992 : improve LBM on some aspects and capture scales larger than MD ones.

In DPD : a “particle” $\equiv$ molecular clusters (coarse-grained)

Motion/interaction with prescribed, velocity dependent forces :

1. repulsive conservative force ($\rightarrow$ “homogenize” particles locations)
2. dissipative force ($\rightarrow$ “viscous” resistance between fluid zones)
3. stochastic force ($\rightarrow$ a way to represent “what is lost” through coarse graining)

Dissipative Particle Dynamics (DPD)

(1) and (2) implement a thermostat → achieve thermal equilibrium

Amplitude of forces dictated by fluctuation-dissipation theorem → ensures thermodynamic equilibrium has a canonical distribution

DPD conserves mass and momentum.

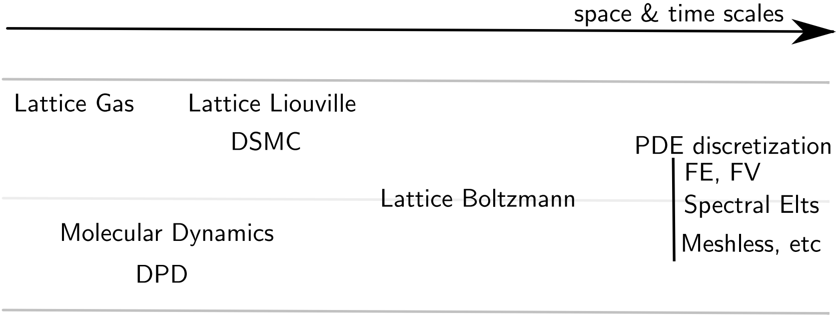
See Karniadakis et al. (Springer, 2005) for more details.

A summary (3) ... of parts 2 and 3

Model equation / description

Newton → Liouville → Boltzmann → Hydrodynamic

Numerical methods



space & time scales

Lattice Gas

Lattice Liouville

DSMC

Molecular Dynamics

DPD

Lattice Boltzmann

PDE discretization

- FE, FV
- Spectral Elts
- Meshless, etc

Outline

1. Overview
2. Gases
3. Liquids
4. **Wall laws for liquids**
5. Droplets in microfluidics
6. Level Set

An overview on wall laws for liquids,

following Tabeling (2004) and Bocquet & Barrat (2007).

See also Lauga, Brenner & Stone (2007).

The question :

Is there any slippage at the wall for liquids ?

Usually, we are taught at school that “u=0”.

But, soon, problems arise ...

- motion of a triple line
- gas (slippage already described by Maxwell 1879), Navier - Stokes + Slip B.C. via *Kn* expansions
- Superhydrophobic surfaces
- Non-Newtonian liquids : polymers

Heuristic approach

If "wetting" situation applies : balance of forces $\rightarrow$

- Close to the wall : a molecule is attracted to the solid by the van der Waals forces
  - a : size of the molecules
  - ϵ : surface energy by unit surface $\Rightarrow F_v \sim \epsilon a$

- Hydrodynamic shear which attracts the molecule
  - S : shear
  - μ : dynamical viscosity of fluid $\Rightarrow F_s \sim \mu a^2 S$

allows to write the condition, for a molecule to be attracted by the flow : $S > S_c = \frac{\epsilon}{\mu a}$

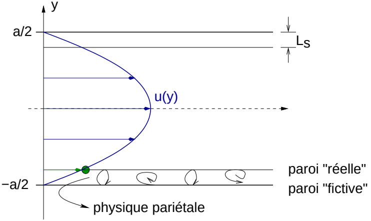
In other words : if shear is $> Sc$ in the fluid, slippage may occur. Ex : water on plastic, $S_c = 10^{10} Hz$

The slip length approach

Introduction of the Navier (or Robin) boundary condition :

y : normal direction
u : tangential wall speed
L_s : so called “slip length”

$$u = L_s \left(\frac{\partial u}{\partial y} \right)$$



Lauga *et al.* 2007 (→)

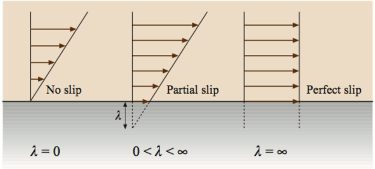


Fig. 19.1 Interpretation of the (Maxwell–Navier) slip length λ

The slip length approach

Usually, in hydrodynamics, shear $\ll S_c \Rightarrow L_s \sim 10^{-9}m$

Rk : such law leads to a decreased pressure drop and this was used to study experimentally the slip phenomena (Pfahler et al., ASME 32 (1991) ; Giordani - Cheng, J. Phys Condens. Matter 13 (2001)). Of note, in these experiments :

- really small channels
- tricky experiments due to leaks upstream
- $L_s \sim 50nm$

More generally, slippage **question open** since some experiments (in the '90 – '00) using Navier law showed also that $L_s \sim 10^{-6}m$ and numerical simulation at the same time where in agreement with the heuristic approach ($L_s \sim 10^{-9}m$).

Some experimental studies :

wall speed measurements

- Pit et al. PRL 85 (2000) : wetting fluid $L_s \sim 200.10^{-9} m$ and increasing with the wetting angle, up to $L_s \sim 10^{-6} m$

> *“For hexadecane flowing on a hydrocarbo/lyophobic smooth surface, **we give what we think to be the first direct experimental evidence of noticeable slip at the wall**. We show that the surface roughness and the strength of the fluid-surface interactions both act on wall slip, in antagonist ways.”*

- Tretheway - Meinhart, LPF 14(3) 2002 : $L_s \sim 1\mu m$ with an error of $450nm$ (hydrophobic case) ; hydrophilic case : slip $<$ measure error

The nanofilm of Pierre-Gilles de Gennes

On Fluid/Wall Slippage. P. G. de Gennes. Langmuir 2002 18 (9), 3413-3414

Definition of the slip length and characterisation : k, coefficient of surface friction, σ, shear stress inducing a speed v_s at the wall surface $\Rightarrow \sigma = kv_s$

On the other hand, shear stress in the fluid (of viscosity η) is given by : $\sigma = \eta \left| \frac{\partial v(z)}{\partial z} \right|$.

Then : slip length $L_s = \frac{\eta}{k}$. Usually, one expects $L_s \sim$ “molecular diameter” but “exotic” things were shown experimentally or numerically.

The nanofilm of Pierre-Gilles de Gennes

An hypothesis is then introduced by de Gennes : there exists a nanometric gaseous film at solid–liquid interface. Physical origins may be of 2 types (to be clarified) :

- non-wetting case : bubbles are created at the wall to reduce the system energy. If we use the thermal fluctuations to estimate the size of the bubbles, this leads to an estimation of the molecular size

- presence of external gas dissolved in the liquid, up to metastable concentrations

Rk : such hypothesis of the existence of such a layer of nano-bubbles seems to be shown experimentally (Tyrel & Attard, PRL 88 2001).

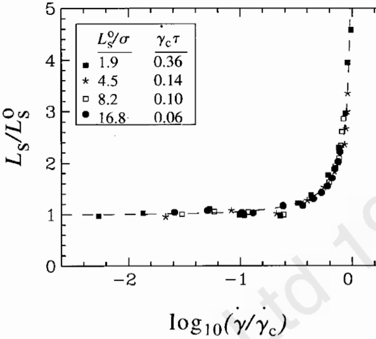
Assuming a high Kn in the gas : $L_s \sim \frac{viscosity}{thermal\ speed} \sim 10^{-6} m$

Some numerical simulations

Thompson & Troian, Nature 389 (1997)

MD simulations (with truncated Lenn- Jones potential and a Couette flow). Proposed general law :

$$L_s = L_0\left(1 - \frac{S}{S_c}\right)^{-\frac{1}{2}}$$



Of note, very difficult to obtain S_c experimentally (cf. Freeman Scholar lecture of Gad el Hak). This law $\Rightarrow L_s \sim 10^{-9} m$

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)

Influence of wetting properties on hydrodynamic boundary conditions at a fluid-solid interface.

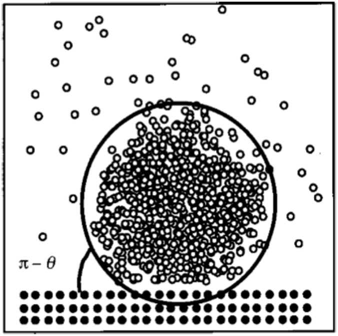
One can give a simple description of liquid films, not too thin (i.e. width $>$ 10 – 20 atom size) : use a macroscopic hydrodyn. equation with bulk coefficients and slip BC.

But studies (experim. or numer.) leading to such results where in the case of **total wetting**.

Here, they look a fluid film forced to penetrate a thin pore, in a situation of **partial wetting** ($\gamma_{LS} + \gamma_{LV} > \gamma_{SV}$) $\equiv$ droplet in equilibrium on a substrate ▸ Next :
one can write Young's law $\gamma_{LV} \cos\theta = \gamma_{SV} - \gamma_{LS}$.

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)



partial wetting

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)

Ingredients :

• Lennard-Jones interactions – ϵ : interaction energy, σ : molecular diameter, similar for all molecules ; it is c_{ij} which allows to adjust the surface energies between molecules

$$v_{ij}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - c_{ij}\left(\frac{\sigma}{r}\right)^{6}\right]$$

• Substrate : fixed atoms on a FCC lattice

• The fluid is more cohesive than a usual L-J (since $c_{FF} = 1.2$ instead of 1). Fluid - Substrate interaction : $c_{FS} = 0.5 \to 1$

• Geometry : 2 parallel plates. Code : constant temperature + Hoover's Thermostat on the velocity orthogonal to the flow only

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)

Ingredients :

- One can estimate roughly the angle as a function of c_{FS} : $\cos\theta = -1 + 2\rho_s c_{FS}/\rho_F c_{FF}$. But one can also compute them using results of simul. : $(c_{FS};\theta)$: $(0.5; 137^o) \rightarrow (0.9; 99^o)$

- Definition/Convention in their paper : non-wetting case when $\theta > 90^o$. **Rk :** In such case, if we want fluid to enter pore (cf. above), a supplementary pressure is needed : $P_0 = 2(\gamma_{LS} - \gamma_{SV})/h$.

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)

Simulations :

• Static case : when P_0 is high, one retrieves density profile of the usual wetting case.

• Couette & Poiseuille flows : slippage is clearly visible and fitting by Navier's law gives

$$\left.\frac{\partial u}{\partial z}\right|_{z=z_w} = \frac{1}{L_s}\, u|_{z=z_w}$$

They found a z_w in the fluid at $\sim$ 1 atomic distance (σ) from the solid wall and $L_s \sim$ several dozens of σ when $\theta \to 150^o$, i.e. nonwetting case.

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)

Physical theory :

- Using Green-Kubo formula for the slipping length and successive simplifying hypothesis, they derive (σ : molecular diameter, $D_{q_{\|}}$: collective diffusion coefficient, η : shear viscosity, ρ_c : density at the first layer) :

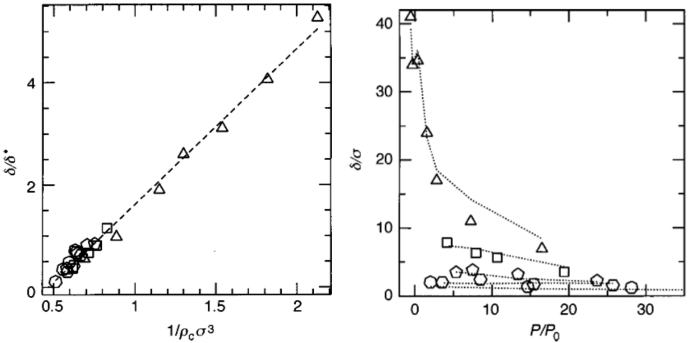
$$\frac{L_s}{\sigma} \sim \frac{D^*_{q_{\|}}}{S_1(q_{\|}) c^2_{FS} \rho_c \sigma^3} \text{ with } D^*_{q_{\|}} = \frac{D_{q_{\|}}}{D_0} \text{ and } D_0 = \frac{k_B T}{3\pi\eta\sigma},$$

where all involved quantities can be post-treated from the MD simulation. Indeed, it appears this law is in agreement with previous simulations ▸ Next :

$$\frac{L_s}{\sigma} = \alpha \frac{D^*_{q_{\|}}}{S_1(q_{\|}) c^2_{FS} \rho_c \sigma^3} \left(1 - \frac{\rho_c}{\rho_{shift}}\right) \text{ with } \alpha = 3.04 \text{ and } \frac{1}{\rho_{shift}} = 0.47$$

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)



Fits of L_s vs Wetting properties of Fluid on Substrate

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)

Physical theory : consequences

- if c_{FS} is fixed (fluid-solid interaction) : L_s decreases with the structuration of fluid in the first layer close to the wall $\Rightarrow$ L_s small in a fluid s.t. pressure is high (which is what is observed experimentally)

- if ρ_c is fixed (mean density of the fluid in the zone close to the wall) : if (pressure $\nearrow$)-and-($c_{FS} \searrow \Leftrightarrow$ non-wetting $\nearrow$) then L_s strongly increases (even if structuration is strong). This is not intuitive *a priori*.

In addition, one can expect that if $\theta = \pi$ (i.e. idealized perfect slip) then $L_s = +\infty$.

Some numerical simulations

Barrat & Bocquet, Farad. Disc. 112, 119-127 (1999)

Slip length is proportional to the wetting angle.

Role of rugosity

Cottin-Bizone et al. Nature Material, Vol 2 (Apr. 2003)

Experiments mentioned :

- Zhu & Granick, PRL 88, 106102 (2002) : rugosity decrease slippage
- Watanabe et al. JFM 381, 225–238 (1999) : high slippage observed on various rugosities

They explore these facts with the same simulation tool as Barrat & Boquet (FD, 1999)

First, recall non rough wall : with $c_{FS} = 0.5 \Leftrightarrow \theta = 137^o$, they find $L_S \sim 20 - 25\sigma \sim 10 - 25nm$.

Then : "square dot" wall roughness and 2 situations ▸ Next

Role of rugosity

Cottin-Bizone et al. Nature Material, Vol 2 (Apr. 2003)

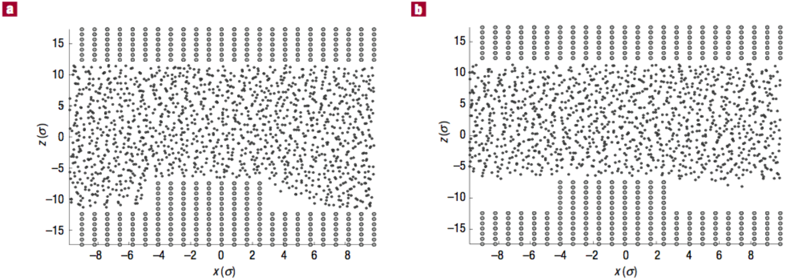


Figure 3 Flow patterns under different conditions. a, Transverse view of the atomic configuration in the wetted situation. Atoms belonging to the liquid and solid are represented by points and round dots, respectively. The liquid occupies nearly all the available volume. **b,** A composite interface is formed under low-pressure.

Fully wetted (Left) and Partially wetted (Right)

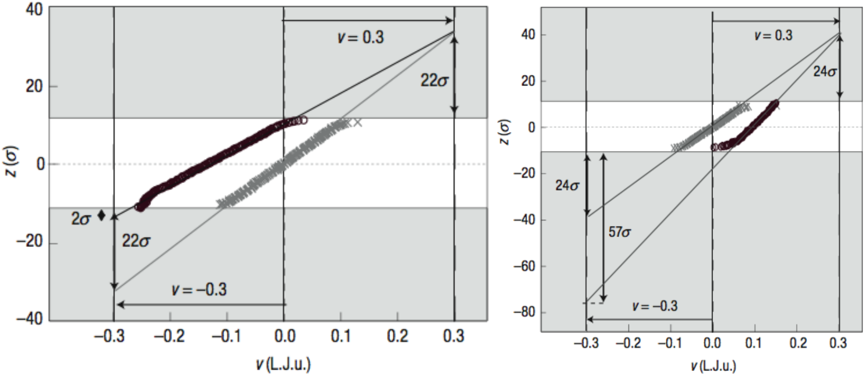
Role of rugosity

Cottin-Bizone et al. Nature Material, Vol 2 (Apr. 2003)

- Case “fully wetted” (a) : no modification of L_s on the upper wall (compared to non-rough case) but **decrease** of L_s on the lower (rough) wall to 2σ at the trough of rugosity (or 7σ at the crest of rugosity). See ▸ Next–Left
- Case “partially wetted” (b) : no modification of L_s on the upper wall (compared to non-rough case) but **increase** of L_s on the lower (rough) wall to 57σ (instead of 24 for the flat wall). See ▸ Next–Right

Role of rugosity

Cottin-Bizone et al. Nature Material, Vol 2 (Apr. 2003)



Gray crosses (flat wall) ; Black circles (rough wall). **Left :** Case (a) High pressure / Wetted. **Right :** Case (b) Low pressure / Composite.

Role of rugosity

Cottin-Bizone et al. Nature Material, Vol 2 (Apr. 2003)

- Qualitatively, increase of L_s due to absence of friction in the trough of the rugosity $\Leftrightarrow$ Boundary condition : null stress at the wall. Rugosity favouring gaseous lubrication $\Rightarrow L_s \nearrow$

- As for the wettability, roughness modifies flow properties at the wall. They think that differences between the 2 articles mentioned come from different wettability conditions. They also mention the nanofilm of de Gennes : they can't prove its existence but if it exists $\Rightarrow L_s \nearrow$.

- Dewetting : present on patterned surfaces from nm to μm scale $\Rightarrow$ friction reduction expected for patterns from nm to μm scale. But this effect expected to be stronger for nm patterns. **Perspective : use this for low flow resistance in small channels.**

Toward a clearer view

Bocquet & Barrat. Soft matter, 3, 685-693 (2007)

Thanks to a study at various scales

☐ A look at molecular scale and plane interface. À la de Gennes : $L_s = \eta/\kappa$: slip length is the ratio of a “bulk property” and an “interface” prop. κ depends on intermolecular interaction (non/wetting). $L_s \sim 1 - 50.10^{-9} m$

☐ A look at “mesoscopic” scale : when surface is structured (wettability or roughness patterns at this intermediate scale). Molecular details are “homogenized” in a position dependent $L_s(x)$. L_s can be inferred by the surface pattern scale and the surface area of the dewetted part.

Toward a clearer view

Bocquet & Barrat. Soft matter, 3, 685-693 (2007)

☐ Naturally, the knowledge/control of surface state at each of these scales $\Rightarrow$ control of flow properties of the complex surfaces we are able to build at $< 1\mu$m.

☐ In brief, if one knows exactly properties at these 2 levels, slipping for simple liquids is relatively well understood theoretically and experimentally.

A remark

Interpretation of MD results and continuum limit is not a trivial point.

See Brenner & Ganesan (Phys. Rev. E 61, 6879-6897 (2000)) : scale separation between MD and C

Boundary condition in the Continuum limit should come asymptotically as a matching between

- inner limit of the outer system (continuum)
- outer limit of the inner system (molecular)

This needs to be taken into account when slip lengths are determined.

Wall laws - A mathematical viewpoint,

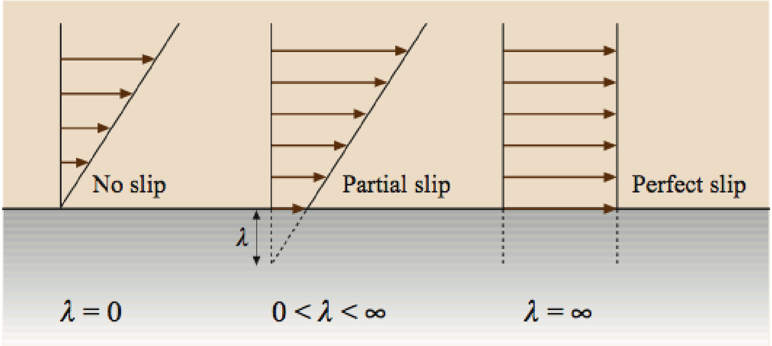
following David Gerard-Varet et al.

Wall laws - A mathematical viewpoint

Reminder

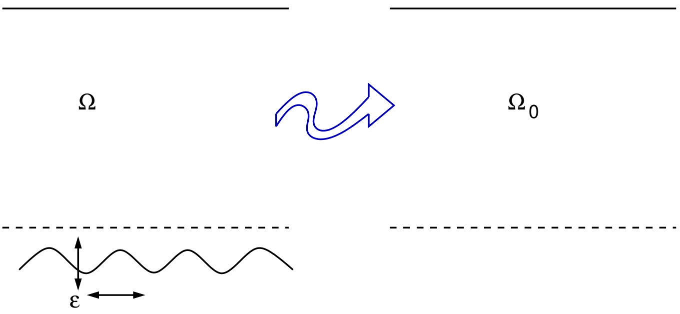
Normal component : $\vec{u}.\vec{n}_\Omega = 0$ and **Tangential component** :

- no-slip : $\vec{u}.\vec{\tau}_\Omega = 0$
- perfect slip : $\frac{\partial(\vec{u}.\vec{\tau}_\Omega)}{\partial \vec{n}_\Omega} = 0$
- Navier slip : $\vec{u}.\vec{\tau}_\Omega = L_s \frac{\partial(\vec{u}.\vec{\tau}_\Omega)}{\partial \vec{n}_\Omega}$



Wall laws - A mathematical viewpoint

Homogenization of rugosities :
apparent ($L_s(x)$) vs effective ($L_{s_{eff}}$)



NS + BC on $\partial\Omega$

NS + BC* on $\partial\Omega_0$

Wall laws - A mathematical viewpoint

Context : inspired by previously described physical aspects

we know actual **surfaces are not straight** but rough.

May roughness induce an "homogenized" slip at $\partial\Omega_0$?

Can this be proved rigorously ?

+ Computational viewpoint : often impracticable to mesh

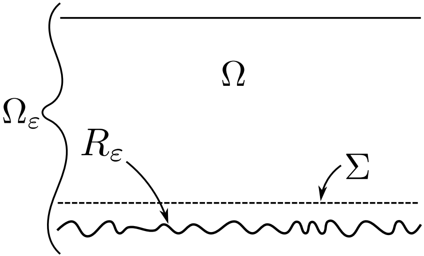
the domain at the precision of the roughness $\Rightarrow$

flat domain with equivalent bound. cond. is highly desirable.

Wall laws - A mathematical viewpoint

The problem

$$R_\varepsilon = \{x = (x_1, x_2), 0 > x_2 > \varepsilon\omega(x_1/\varepsilon)\}$$



Problem (NS_ε) :

$$\begin{cases} u.\nabla u - \Delta u + \nabla p = 0, \\ \nabla.u = 0, x \in \Omega_\varepsilon \\ u|_{\partial\Omega_\varepsilon} = 0, \quad \int_\sigma u_1 = \phi \end{cases}$$

with σ, vertic. cross-sect.,

and $\phi > 0$, imposed flux.

when $\varepsilon \to 0$, what is the approx of u_ε by a sol. of NS in Ω ?

Wall laws - A mathematical viewpoint

Order 0

$u_\varepsilon \approx u_P$, sol of NS with wall law $u|_\Sigma = 0$ (Poiseuille flow),

namely $u_P = u_P(x_2) = (6\phi x_2(1 - x_2); 0)^t$.

Theorem : For sufficiently small ϕ and ε, (NS_ε) has a unique solution $u_\varepsilon \in H^1_{uloc}(\Omega_\varepsilon)$, s.t.

$$\|u_\varepsilon - u_P\|_{H^1_{uloc}(\Omega_\varepsilon)} \leq C\sqrt{\varepsilon},$$

$$\|u_\varepsilon - u_P\|_{L^2_{uloc}(\Omega_\varepsilon)} \leq C\varepsilon.$$

Wall laws - A mathematical viewpoint
Order 1

Previously : no slip $\Rightarrow$ $\mathcal{O}(\varepsilon)$ approx in L^2 but there is better :

$u_\varepsilon \approx u_P + 6\phi\varepsilon(\alpha; 0)^t + o(\varepsilon)$, in L^2 and this approx. is the sol of

NS with Navier B.C. : $u_1|_\Sigma = \varepsilon\alpha\, \partial_2 u_1|_\Sigma$ and $u_2|_\Sigma = 0$.

Wall laws - A mathematical viewpoint

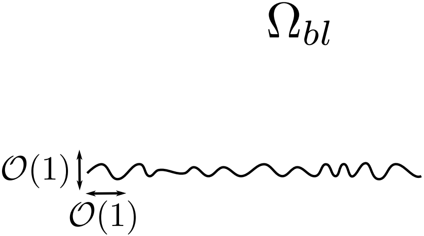
Order 1 – How ?

Comes from a boundary layer corrector v s.t. (size-ε zoom)

$$\Omega_{bl} := \{y_2 > \omega(y_1)\}$$

Problem (BL) :

$$\begin{cases} -\Delta v + \nabla p = 0, \\ \nabla . v = 0, y \in \Omega_{bl} \\ v|_{\partial\Omega_{bl}} = (-\omega(y_1),\ 0)^t \end{cases}$$



$\exists\ \alpha,\ \ v \longrightarrow v^\infty = (\alpha,\ 0)^t$, as $y_2 \to +\infty$ and $u_\varepsilon \approx u_P + 6\phi\varepsilon v(\frac{x}{\varepsilon})$

This can be proved rigorously for rather general random ω.

Basson & G-V. CPAM (2008), D.G-V. CMP (2009), G-V. & Masmoudi CMP (2010)

Wall laws - A mathematical viewpoint

What is the nature of slip ?

Does rugosity improve slip ?

Rk : α depends on the position of Σ.

Previously : Σ was **above** the rugosity.

Prop : (Bucur-Dalibard-G-V, 2012). Assume $< \omega >= 0$. Consider all rugosities $\omega \in W^{1,\infty}(\mathbb{T})$. Maximum slip coefficient is achieved for flat surface !

$\Longrightarrow$ Rugosity does not improve slip. Slip is apparent.

Wall laws - A mathematical viewpoint

Blending slip and no slip

Reminder : previously, we always had homogeneous scaling

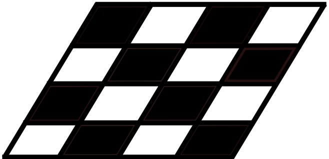
$$\varepsilon \updownarrow \quad \underset{\varepsilon}{\longleftrightarrow}$$

$\Longrightarrow$ Analysis with more general scaling would be interesting

Inspired by functionalized surfaces (Cottin-Bizonne et al. 2012)

flat boundary but with **pure slip** and **no-slip** zones patterns :

Patches



Riblets

Wall laws - A mathematical viewpoint

Blending slip and no slip

Let ϕ^{ε} be the volume fraction of no-slip

One can show (Bonnivard, Dalibard, Gerad-Varet, M3AS 2014) :

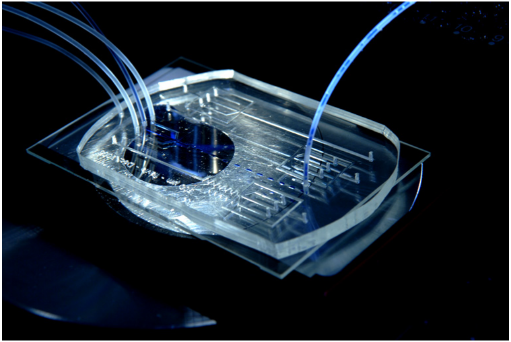
Patches ...	Riblets ...	Then limit cond.
If $\phi^{\varepsilon} \gg \varepsilon^2$	If $\phi^{\varepsilon} \gg \exp(-c/\varepsilon)$	Dirichlet
If $\phi^{\varepsilon} \ll \varepsilon^2$	If $\phi^{\varepsilon} \ll \exp(-c/\varepsilon)$	Pure slip
If $\phi^{\varepsilon} \sim \varepsilon^2$	If $\phi^{\varepsilon} \sim \exp(-c/\varepsilon)$	Navier

Summary :

- significant slip possible but relative area of no-slip zone needs to be very small (unrealistic ?)
- riblets are less efficient in improving slip

Outline

Microchannels to handle fluids



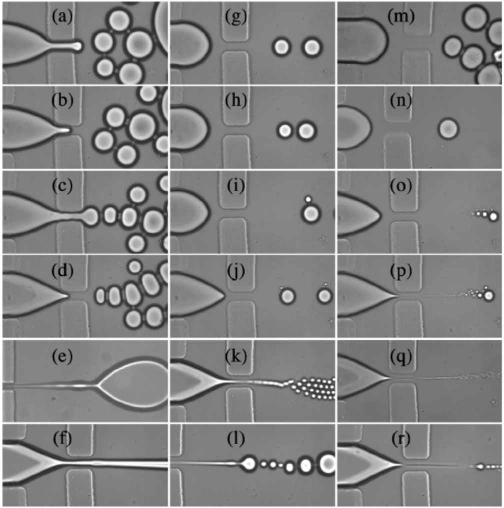
Tiny volumes : nanolitres

Otherwise stated, pictures of this section courtesy LOF (Bordeaux) :

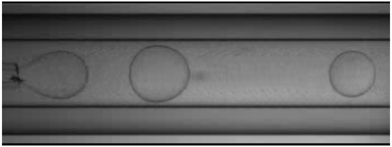
A. Colin, G. Cristobal, P. Guillot.

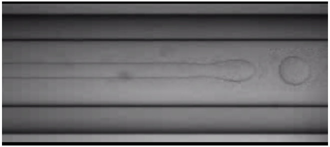
Droplet creation

Anna et al., 2003 – “Flow focusing” and various regimes

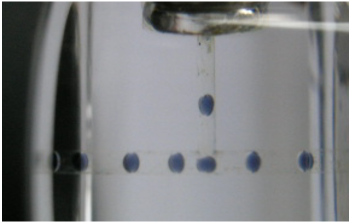


Droplet creation - Axisymetric

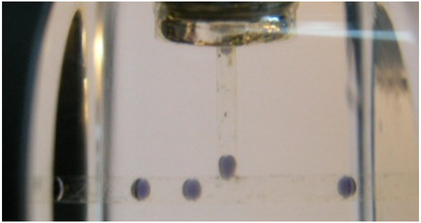




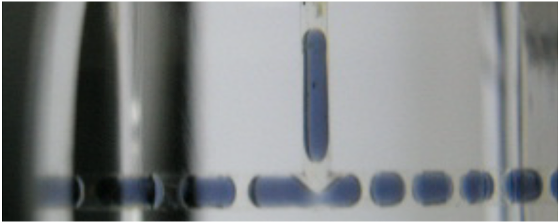
Droplet creation - Routing



Regular



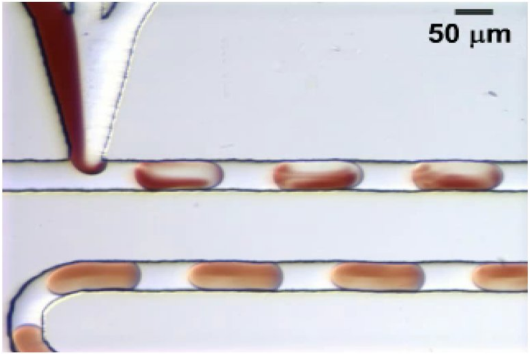
"Weird"



Topological change

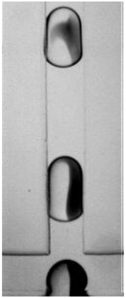
Droplet Usage

Song and Ismagilov, 2003 – Fast chemical Kinetic : 10^{-3} s

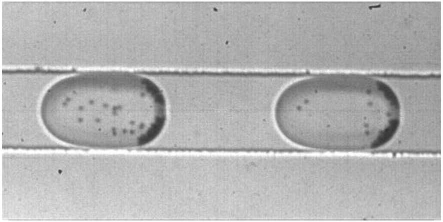


Rk : getting things homogeneous in the droplet

Droplet mixing : 2 examples of tracing



Diffusion +
Mixing



Tracers

Modelling

Hypothesis

- Fluids :
  - immiscible
  - viscous
  - newtonian
  - homogeneous
- incompressible & isothermal flow
- zero-thickness interface
- negligible gravity
- constant surface tension

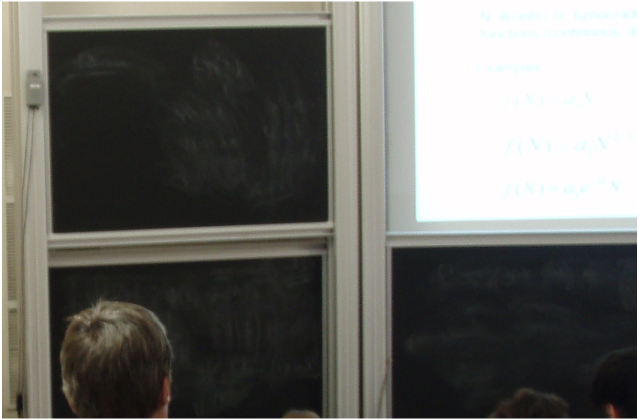
Usual features in Microfluidics

- Low Reynolds, laminarity
- Interfaces with stationary shape

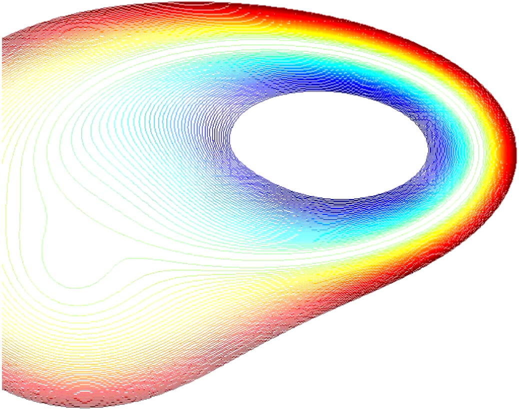
Outline

1. Overview
2. Gases
3. Liquids
4. Wall laws for liquids
5. Droplets in microfluidics
6. **Level Set**

Methods for moving interfaces



Level Set tools - Redistanciation



$$\phi_t + sgn(\phi_0)[\|\nabla\phi\| - 1] = 0 \text{ and } \phi(t = 0, x) = \phi_0(x)$$

Numerical results

Model & LS formulation

Flow resolution ...

$$(\mathcal{NS})\left\{\begin{array}{rl} \rho\,(\partial_t u + u.\nabla u) - div(2\eta D u) + \nabla p & = \sigma\;\kappa\;\delta(\phi)\;n \\ div(u) & = 0 \\ + \quad \text{B.C.} & \end{array}\right.$$

... coupled with a **Level Set method** ...

$$(\mathcal{T})\left\{\begin{array}{ll} \phi_t + u\,.\,\nabla\phi & = 0 \\ \quad + \quad \text{B.C.} & + \quad \text{I.C.} \end{array}\right.$$

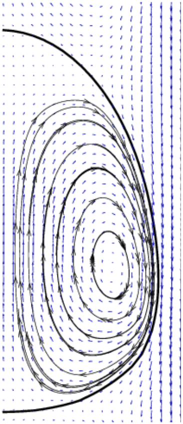
$$\eta(\phi) \quad = \quad \eta_1 + (\eta_2 - \eta_1)H(\phi)$$

Discretization of $(\mathcal{NS})$:

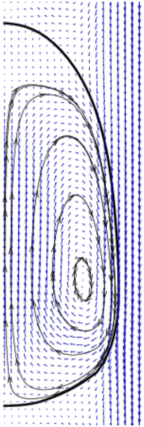
☐ Time : implicit except surface tension (standard approach)

Various mixing regimes : confined droplets 1/2

Small



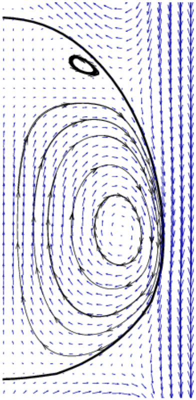
Big

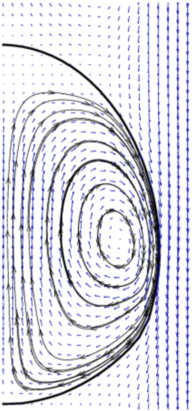


Various mixing regimes : confined droplets 2/2

Small : switch of η

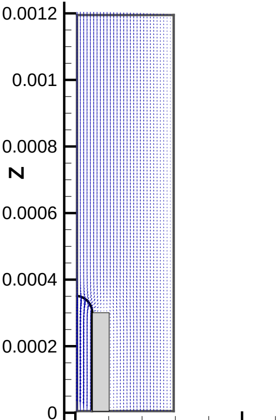
Small : more contrasted η



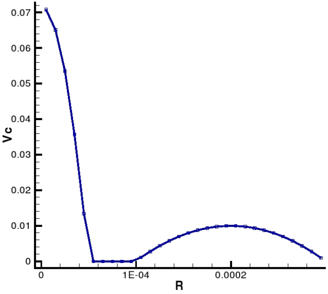


Droplets Creation in coaxial tubes 1/3

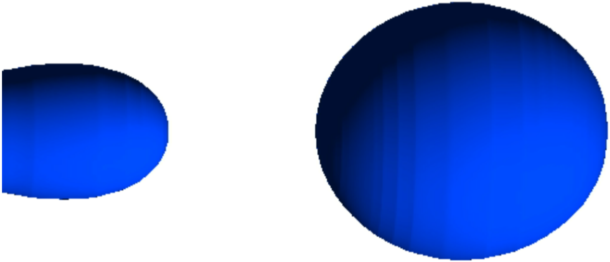
Geometry



Injection

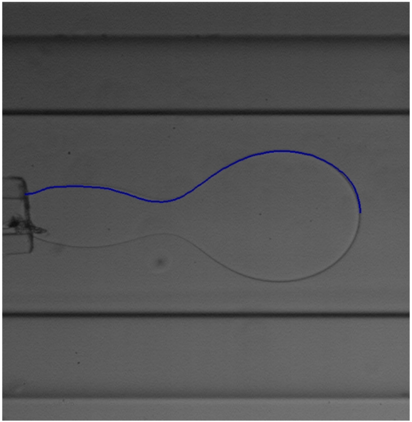


Droplets Creation in coaxial tubes 2/3



Droplets Creation in coaxial tubes 3/3

Qualitative comparison between experiments and simulations



Numerical difficulties

- Stability condition : discr. of surface tension

See Galusinski-P.V., JCP 227(12), pp. 6140-6164, 2008 :

On stability condition for bifluid flows with surface tension : application to microfluidics

- Boundary conditions : outflow with surface tension ?

Perspectives (among others)

- more general forces at interface, equilibrium shapes of vesicles

  e.g. Cottet-Maitre-Milcent (2004, 2006, 2007, 2009)

- fluid-structure interaction (cf C. Grandmont lecture)
- cell motility on substrate
- from newtonian to non-newtonian rheologies

References

These notes rely heavily on the following refs. The reader is highly encouraged to explore them for thorough details.

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