Lecture 1: On fluids, molecules and probabilities

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1 Introduction

Computational fluid dynamics (CFD) is commonly associated to continuum mechanics, which surely offers an economic and powerful representation of the physics of fluids. However, the picture is deeper and broader than that; in fact modern science is increasingly concerned with flowing matter at micro and nanoscales, where the atomistic/molecular nature of the materials is fully exposed. This is why modern CFD must be informed on all three levels above.

In this lecture we provide an introduction to the three main descriptions of matter: the Macroscopic (Ma) level of continuum fields, the microscopic (Mi) level of atoms and molecules and the mesoscopic (Me) level of probability distribution functions. For completeness, we also mention the quantum level, which lies underneath the atomistic ones, although this course shall not discuss moving matter below the classical atomistic scales.

Which one of three levels is most apt to the solution of a given problem depends on the nature of the problem itself; in general continuum mechanics holds at macroscopic scales, say micrometers upwards, but no general rule exists; sometimes the continuum picture can be brought down to nearly nanometer scales. Conversely, under conditions of strong non-equilibrium, say large gradients in the flow configuration, the continuum picture can break down at micrometric scales, well above the atomistic ones. This is where the mesoscopic description becomes essential.

So the main take-home message is: there’s more to fluid dynamics than continuum mechanics.

2 The four level hierarchy

The quantitative description of matter relies on two main pillars: continuum and atomistic mechanics. In the former, matter is described by a set of space-filling continuum fields, such as the fluid density and temperature, or the strain of an elastic solid. In the latter, matter is explicitly represented for what it really is, namely a a collection of individual microconstituents, namely atoms and molecules. We shall generically refer to fields and particles, respectively. The giants here are Navier, Stokes and Newton.

These two basic descriptions also reflect into two major paradigms of applied and computational math, namely partial and ordinary differential
However, statistical physics and most notably kinetic theory inform us that there is a third intermediate level, where matter is described by probability rules. This is the ground of Boltzmann’s kinetic theory.

At an even more fundamental level, matter is described by the law of quantum mechanics, but this is beyond the scope of this course.

3 Macroscopic Level: Continuum Fields, Navier-Stokes

This the (allegedly) most economical representation: just a few space-time dependent fields: (density, pressure, velocity, temperature) instead of zillions (Avogadro $= 6 \times 10^{23}$) molecules! The field interactions are conceptually simple, as they are dictated by general symmetries (translations, rotations) and associated conservation laws (mass-momentum-energy). The mathematics is also deceivingly simple, the basic equations of fluids, known as Navier-Stokes equations, are basically mass conservation and momentum conservation, i.e. Newton’s law, as applied to a finite volume of fluid, supplemented with an assumption of linearity between the applied stress and the resulting strain.

Three main actors on stage: Pressure, Inertia and Dissipation (PID) and two independent dimensionless groups, Reynolds number $= I/D$, Mach number $= I/P$.

The Mach number is defined as the flow versus the sound speed:

$$Ma = U/c_s,$$

and reflects the compressibility of the fluid: sound waves usually carry density perturbations across the fluid (stone-in-the-pond). High Mach number flows host shock waves and abrupt density changes which raise a significant challenge to the modeler.

The Reynolds number is defined as:

$$Re = UL/\nu,$$

where $L$ is the macroscale of the problem (the size of the macroscopic object) and $\nu$ the kinematic viscosity of the fluid (length square/time). The Reynolds number can also be recast as $Re = U/U_d$, where $U_d = \nu/L$ is the diffusive speed, i.e. the speed at which momentum is transmitted across the
fluid. Amazingly, for most common fluids in daily life, this number is exceedingly high, an ordinary car would feature \( Re \sim 10^7 \) (ten millions), an airplane \( Re = 10^8 \), and megascopic flows, say the ones met in meteorology and environmental/planetary science can easily go into the tens of billions. Current computers can reach up to \( Re \sim 10^4 \) at most.

This opens up a major Pandora’s box of complexity, going by the name of \textit{Turbulence}.

Given the structure of the Navier-Stokes equations, it is readily appreciated that the Reynolds number measures the strength of non-linearity versus dissipation, i.e. \( u \nabla u \), versus \( \nu \Delta u \).

Thus, in the language of theoretical physics, fluid dynamics is a strongly non-linear self-interacting field theory. Indeed, turbulence is often quoted as the last open problem of classical (Newtonian) physics.

Finally, there is a third major dimensionless group, the Knudsen number, measuring dissipation over pressure, or more precisely

\[
Kn = \frac{\nu}{csL}
\]

It can be readily shown (see Lecture on kinetic theory of fluids), that this is also the ratio between the molecular mean free path, i.e. the distance travelled by a molecule before bumping into another molecule, versus a typical macroscopic scale. It is also readily shown that \( Kn = Ma/Re \), also known as vo Karman relation.

\textit{Fluid dynamics, i.e. collective behavior, holds in the limit of zero Knudsen number.}

4 Microscopic Level, Atoms and Molecules (Newton)

This the reign of Newtonian mechanics: molecular trajectories evolving under the effect of interatomic potentials. A huge (Avogadro-like) number of Newton equations for the particle positions and momenta \( \{ \vec{r}_i, \vec{p}_i \}, i = 1, N \).

These are ”simple” ODE’s, but far too many to be viable and useful, totally unwieldy for macroscopic purposes. Nevertheless they are key for fluids at the nanoscale and the corresponding computational technique, Molecular Dynamics (MD), plays a pivotal role in modern computational physics. As of today, MD can track about a billion molecules for a time-stretch of hundreds
of nanoseconds. This level makes the object of other courses and it will be only occasionally referred to in the present course.

5 Mesoscopic Level, Probability Distributions (Boltzmann)

At intermediate scales, say microns, there are many fluid phenomena which are "too small" for the continuum and "too large" for the atomistic description. This is intermediate ground of kinetic theory, the branch of theoretical physics founded by Ludwig Boltzmann.

Kinetic theory replaces deterministic trajectories with the probability of finding a molecule at a given position in space at a given time with a given molecular velocity. This is the so-called Boltzmann probability distribution function, defined by:

$$\Delta N = f(\vec{r}, \vec{v}; t) \Delta \vec{r} \Delta \vec{v}$$

where $\Delta N$ is the (average) number of molecules in a volume $\Delta \vec{r}$ of configuration space and $\Delta \vec{v}$ in velocity space.

This is a single field living in six-dimensional phase-space (three dimensions in ordinary space and three in velocity space). This much less information than atomistic and much more than continuum.

Central quantities in kinetic theory are as follows.

Mean-free-path $\lambda$: the distance traveled by any two molecules before colliding.

Cross section $\sigma$: the effective size (area) presented by a molecule to a colliding partner. It depends strictly on the interatomic potential and tends to increase with the range of such potential, to the point of becoming formally infinite for long-range interactions, say $1/r$ Coulomb or gravitational ones. Under these circumstances Boltzmann’s kinetic theory needs deep revisions, leading to different types of kinetic equations, known as Fokker-Planck kinetic equations.

Collision frequency $\gamma = n \sigma v_{th} \equiv v_{th}/\lambda$: the inverse time scale between two collisions. Here, $n$ is the number density (molecules per unit volume) and $v_{th} \sim \sqrt{k_B T/m}$ is the thermal speed, $m$ being the atomic mass of the molecule and $k_B$ Boltzmann’s constant.
All bear a statistical meaning, as they refer to a representative molecule, collecting the cumulative behavior of a large ensemble of real molecules.

The cornerstone of kinetic theory is Boltzmann’s kinetic equation, which is a complicated integro-differential equation leaving in six-dimensional phase space: The BE is a continuity equation in phase space:

$$\frac{df}{dt} = \partial_t f + \vec{v} \cdot \nabla _r f + \vec{a} \cdot \nabla _v f = C \equiv G - L$$

The lhs (Streaming) is a mirror of Newtonian mechanics, the rhs describes the interparticle collisions (Collide) in terms of gain and loss processes.

Major dimensionless parameter: Knudsen number=mean free path/device length,

$$Kn = \lambda / L$$

The Knudsen number controls the transition from kinetic theory to continuum fluid mechanics, which takes place in the limit $$Kn \to 0$$. Central to this transition is the notion of local equilibrium. This is the shape of the distribution function which is left unchanged by collisions (gain=loss):

$$C(f^{eq}) = 0$$

It can be shown that the local equilibrium is universal and takes the form of a local Maxwell-Boltzmann distribution, i.e. a gaussian centered about the local flow speed $$u(x; t)$$ and width equal to the thermal speed $$v_{th}(x; t)$$.

The solution of the Boltzmann equation is very demanding, best computational practice reaching up to $$32^6$$ grid points (one billion degrees of freedom). However, for mere fluid dynamic purposes it lends itself to drastic and yet realistic simplifications which give rise to very efficient computational methods (Lattice Boltzmann).

6 Kinetic theory of dense gases

A central assumption of Boltzmann’s kinetic theory is that collisions are binary, i.e. n-body encounters with $$n > 1$$ are exponentially rare. This is true only in dilute gases, where the size of the molecules is much shorter than their interparticle distance. For dense fluids, or fluids with long-range
interactions, the picture is quite different: each particle constantly interacts with many others, so that collisions are best treated as a diffusion in velocity space. This is described by the so-called Fokker-Planck equation.

The underlying particle picture is known as Langevin stochastic particle dynamics, basically Newton equations enriched with dissipative drag and random noise.

Modern generalizations of the Langevin dynamics give rise to very interesting mesoscale computational methods (Dissipative Particle Dynamics).

7 Walking across the MiMeMA hierarchy

How do we connect the three levels?

This is the so called coarse-graining procedure: how to eliminate irrelevant degrees of freedom when proceeding bottom-up, from micro to Macro. Central to coarse-graining is a clear appreciation of the length (time) scales involved at the various levels.

Lengthscales, in ascending order:

1. De Broglie length, \( \lambda_b = \frac{\hbar}{mv_{th}} \)
2. Range of microscopic potential, \( r_0 \)
3. Effective size of the molecule, \( s \sim \sqrt{\sigma} \)
4. Intermolecular mean distance, \( n = d^{-1/3} \)
5. Mean-free path, \( \lambda = \frac{1}{n\sigma} \)
6. Coherence length of the field, \( \Lambda \)
7. Macroscopic length of the device, \( L \)

All lengths above have been defined, except the coherence length. This is basically the shortest dynamically active scale in the fluid. This is not a material property of the fluid but a statistical property of the flow and is generally a decreasing function of the Reynolds number, \( \Lambda \sim \frac{L}{Re^\alpha} \), where \( 0 < \alpha < 1 \) is a scaling exponent, typically \( 3/4 \) in three dimensional turbulence.

The ordering depends on the fluid: dilute, dense, quantum, classical.
A major dimensionless number is the diluteness parameter, defined as:

$$\tilde{n} = ns^3$$

Given that, by definition $nd^3 = 1$, we also have:

$$\tilde{n} = (s/d)^3$$

namely the volume occupied by the molecule within the total volume of the system $N s^3/V$, $V = N d^3$ being the total volume occupied by $N$ particles.

The regime $\tilde{n} \ll 1$ denotes *dilute gases*, whereas $\tilde{n} \sim 1$ is typical of dense fluid and liquids.

Note that, based on the definition of $s = \sqrt{\sigma}$ and of the mean-free path, we also have:

$$\tilde{n} = s/\lambda$$

and

$$d/\lambda = \tilde{n}^{2/3}$$

Thus in a dilute gas with short-range interactions, the scale hierarchy is:

$$r_0 \sim s < d < \lambda < \Lambda < L$$

whereas in a dense gas or liquid:

$$r_0 \sim s \sim d < \lambda < \Lambda < L$$

For long-range interactions the situation is more involved since $s$ is in principle divergent. This means that molecules are constantly interacting and the mean free path is virtually zero. This is a very different physical situation which does not lend itself to a straightforward application of Boltzmann’s kinetic theory.

Fluids with $s/\lambda > 1$ are sometimes called *strongly interacting*, as they move freely over a distance shorter than their own size.

Finally, since we are dealing with classical fluids, it is understood that $\lambda_B < r_0$ always holds.

# 8 Micro to Meso

The transition micro-to-meso is formally achieved by counting the number of molecules around a given spatial location $r$ at time $t$. For instance, density
is constructed as:

\[ f(r, v; t) = \sum_{i=1}^{\mathcal{N}} <\delta(r-r_i(t))\delta(v-v_i(t))> \]

In the above, brackets denote averages over many trajectories with different initial conditions and same macroscopic conditions (pressure, temperature and so on). This is called \textit{ensemble-averaging}. In practice, the singular delta function is replaced by proper weighting functions extending over a small but finite volume of the fluid (basically the size of the molecule).

\section{Meso to Macro}

The transition meso-to-macro is formally achieved by taking averages over molecular velocities (moments). For instance, once it is accepted that a Boltzmann distribution can be defined for the system, the fluid density is computed as:

\[ \rho(r; t) = m \int f(r, v; t)dv \]

and likewise the fluid current

\[ \rho u(r; t) = m \int v f(r, v; t)dv \]

and kinetic energy

\[ \rho e(r; t) = m \int \frac{v^2}{2} f(r, v; t)dv \]

It can be shown that the kinetic moments obey an open hierarchy of equations which must be truncated by means of some physically-informed approximation. Typically, Weak departure from local equilibrium, which amounts to assume that the statistical distribution is never too far from a local Maxwell distribution. It can be shown that this is precisely the physical meaning of the limit \( Kn \rightarrow 0 \). Thus, fluid dynamics alwas deals with quasi-Maxwell distributions; major departures from this distribution \textit{cannot} be described by the Navier-Stokes equations.
10 Micro to Macro

Formally, one can go direct from micro to macro without transiting through the meso level, i.e.

\[
\rho(r; t) = m < \sum_{i=1}^{N} \delta(r - r_i(t)) >, \quad \rho u(r; t) = m < \sum_{i=1}^{N} v_i(t) \delta(r - r_i(t)) >
\]

Being a much longer jump, the conditions controlling convergence to macroscopic behavior are more restrictive. In fact, such convergence can be rigorously proved only for a very limited class of interacting potentials.

11 Computational paradigms

The continuum picture is in principle the most economical, as it involves the least number of degrees of freedom, namely a few fields, density, velocity, pressure, functions of space and time. As mentioned above, molecular dynamics is simply unviable for scales above some tens/hundreds nanometers and tens of microseconds. However the macro degrees of freedom interact in a highly non-linear (inertia) and non-local (pressure) fashion, hence the solution of the Navier-Stokes equations proves exceedingly hard.

New numerical methods are in ceaseless demand, and we shall see a good share of these methods during this course (deep coverage would required a full course for each of these methods!).

The mesoscopic level, properly designed, can achieve the optimum between the two worlds, i.e. approach a (global ?) minimum in complexity landscape. That is the beyond-continuum part of the Course.

12 Summary

There is more to the physics of fluids than continuum mechanics. We shall learn how to navigate across the three-level hierarchy and choose the best method tailored to the given problem. This is most important in modern science, where fluid dynamics is increasingly interfaced with allied disciplines, material science, chemistry, biology and soft matter in general.
(Everything flows)
(Heraclitus)

A pervasive presence across virtually ALL human endeavours!

Modeling Matter in Motion
(fluids across scales)

What is a fluid?

Shape changing (gas, liquids)
Modeling Matter in Motion
(fluids across scales)

Why are fluids important?

Pervasive!

Statistical Mechanics

The art of building bridges from micro to MACRO
The Four Levels

**MACRO**

Continuum Fields
\[ \frac{\partial u}{\partial t} + (u \cdot \nabla) u = - \frac{\nabla P}{\rho} + \nu \Delta u \]

Probability distributions
\[ \frac{\partial f}{\partial t} + (v \cdot \nabla) f = - \frac{1}{\tau} (f - f^{eq}) \]

Particles (atoms/molecules)
\[ \frac{d^2 r_i}{dt^2} = - \sum_{j>i} \nabla V_{ij} \]

**MESO**

Complex Fields
\[ i\hbar \frac{\partial \Psi}{\partial t} = H \Psi \]

**MICRO**

Wash out *irrelevant* details (tube/baby problem)

**QUANTUM**

MACRO: Navier-Stokes

(L. Navier, 1785-1836)](L. Navier, 1785-1836)

(G. Stokes, 1819-1903)
Continuum Fluids

Mass-Momentum-Energy Conservation:

\[ \rho = \frac{M}{V} = \frac{N_m}{V} \]

\[ M \ddot{a} = \vec{F} \]

The Navier-Stokes equations of continuum fluid mechanics are a statement of mass-momentum-energy conservation in a "small" volume of fluid.

Mass Flux

\[ \Delta (\rho \Delta \Delta y \Delta z) \]

\[ \Delta (\rho u_x y z) = [(\rho u_x)_{\text{in}} - (\rho u_x)_{\text{out}}] \Delta y \Delta z + \ldots \]

\[ \frac{\partial \rho}{\partial t} = \frac{\partial (\rho u_x)}{\partial x} + \frac{\partial (\rho u_y)}{\partial y} + \frac{\partial (\rho u_z)}{\partial z} \]
Momentum Flux

\[
\begin{align*}
\frac{\Delta p}{\Delta t} & = \left[ \rho u_x \Delta x \Delta y \right] \Delta x \Delta y + \left[ \rho u_z u_x \right] \Delta x \Delta y + \text{Gain} - \text{Loss} \\
\frac{\partial (\rho u_x)}{\partial t} & = \frac{\partial (\rho u_x)}{\partial z} + \text{Gain} - \text{Loss}
\end{align*}
\]

Momentum Flux & viscosity

\[
\begin{align*}
\frac{\Delta p}{\Delta t} & = \left[ \rho u_x \Delta x \Delta y \right] \Delta x \Delta y + \left[ \rho u_z u_x \right] \Delta x \Delta y + \text{Gain} - \text{Loss} \\
\frac{\partial (\rho u_x)}{\partial t} & = \frac{\partial (\rho u_x)}{\partial z} + \text{Gain} - \text{Loss}
\end{align*}
\]

Collisions conserve mass-mom-energy but change momflux!

Momentum freely enters the fluid via \( u_x \), until a collision occurs. Momentum does not change, but flux of momentum does. If collisions are infinitely frequent, this information cannot diffuse within the fluid: ZERO DIFFUSIVITY. The same is true for a collision with the wall. Momentum is dissipated but if collisions are infinitely frequent, this info does not diffuse within the fluid: NO DISSIPATION.
The Navier-Stokes equations

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

\[ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + \mathbf{P}) = \mathbf{f} \]

\[ \mathbf{P} = p \mathbf{I} - \mathbf{\sigma} \]

\[ p = f(\rho, T) \]

\[ \mathbf{\sigma} = \lambda (\nabla \cdot \mathbf{u}) \mathbf{I} + \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] \]

Equation of State
(Ideal/Nonideal)

Stress-Strain Constitutive Relation
(Newtonian/Non-Newtonian)

Three actors on stage

PID = Pressure/Inertia/Dissipation

\[ \nabla p / \rho \]

Ma

Kn

u\nabla u

Re

\[ \nu \Delta u \]
**Dimensionless groups: Mach number**

Mach number (inertia/pressure ~ compressibility)

\[
Ma^2 = \frac{\nabla (\rho uu)}{\nabla p} \approx \frac{U^2}{c_s^2}
\]

\[Ma = 0.8\]

**Dimensionless groups: Reynolds**

Mach number (inertia/dissipation ~ Turbulence)

\[
Re = \frac{\nabla (\rho uu)}{\nu \partial u/\partial u} \approx \frac{UL}{\nu}
\]

\[Re \approx 10^7\]
Dimensionless groups: Knudsen

Knudsen number: Dissipation/sqrt(Pressure*Inertia)

\[ Kn = \frac{Ma}{Re} \]

\[ Kn = \frac{\lambda}{L} \quad \text{(micro)} \]

\[ Kn \approx 10^7 \]

The NSE’s look innocent but they are not!
**Turbulence: why is Reynolds so large?**

\[
\text{Re} = \frac{u \Delta u}{v \Delta u} = \frac{UL}{v}
\]

\[
\text{Re} = \frac{UL}{\nu} = \frac{UL}{c_s \lambda} \approx \text{Ma} \approx Kn^{-1}
\]

\[
\text{Re}(L) \approx \# \text{Collisions} \_ \text{size} = L
\]

\[
\lambda_{\text{up}} \approx 0.1 \mu m
\]

\[
L = 10 m \quad \text{Re} \approx 10^8
\]

**Going micro and nano**

The NSE’s break down at small distances and/or under strong gradients
Continuum Breakdown

Exposing Molecular Individualism:

Small size: 30 water molecules/nm cube
Visible light ~ 100 nm cube ~ 30 millions

Strong changes: molecular mean-free-path
(interfaces, shocks ....)

Loss of collective behavior: bunch of molecules, NOT a fluid!!!
MICRO (Particles)

Isaac Newton (1642 – 1727)

Molecular Dynamics

\[ m \frac{d^2 r_j}{dt^2} = -\sum_{i \neq j}^{N} \nabla_j V_{ij} + \sum_{k \neq j}^{N^2} \nabla_{ij} V_{ik} + \ldots \]
Molecular Dynamics

Avogadro’s syndrome:

Too many molecules!

1 cc air contains ca $10^{21}$ molecules

Current bar of MD simulations: 100 nm x 1 ms

ANTON: MD world record

20 microsecond/day on 25K atom water-protein system; Compare to D(100) ns/day
Mesoscale: soft matter flows

Internal structure: weakly broken universality

Beyond Navier-Stokes

Generalized Navier-Stokes

Two strategies:

Molecular Dynamics

Standard attitude: Stick as much as possible to the continuum formalism via generalizations of NSE. When untenable: jump to MD.

New attitude: Kinetic theory of fluids

Mesoscale Methods!
Microfluids: droplets

\[ \dot{\rho} \vec{u} + \nabla \cdot (\rho \vec{u} \vec{u}) + \tilde{P} + \tilde{P}_{\text{surf}} = 0 \]
**MESO (Probability)**

Ludwig Boltzmann (1844-1906)

Kinetic Theory: half particles and half fields = *fieldicles*
Boltzmann: Probability Distribution Function

\[ \Delta N = f(\vec{r}, \vec{v}; t) \Delta \vec{r} \Delta \vec{v} \]

*f lives in a 6-dimensional world (phase-space)*

Kinetic theory

\[ f(\vec{r}, \vec{v}; t) \Delta \vec{r} \Delta \vec{v} = \Delta N \]

Continuity in phase-space:

\[ \partial_t f + \vec{v} \cdot \nabla f + \left( \frac{\vec{F}}{m} \right) \cdot \nabla_v f = C(f, f) \]

\[ \frac{d\vec{r}}{dt} = \vec{v} \quad \quad \frac{d\vec{v}}{dt} = \vec{F} \]

Mean Representative Molecule
**Binary collisions: Dilute gases**

\[ C(f, f') = \int [f(1', 2') - f(1, 2)] g \sigma(g, \Omega) dgd\Omega d\vec{v}_1 \]

\[ g = |\vec{v}_2 - \vec{v}_1| \]

**Microscopic invariants: mass/momentum/energy**

Collision invariants

\[ m'_1 + m'_2 = m_1 + m_2 \]
\[ m'_1 \vec{V}_1 + m'_2 \vec{V}_2 = m_1 \vec{V}_1 + m_2 \vec{V}_2 \]
\[ m'_1 \vec{V}_1^2 + m'_2 \vec{V}_2^2 = m_1 \vec{V}_1^2 + m_2 \vec{V}_2^2 \]

Collision variants

\[ m'_1 \vec{V}_1 \vec{V}_1' + m'_2 \vec{V}_2 \vec{V}_2' \neq m_1 \vec{V}_1 \vec{V}_1' + m_2 \vec{V}_2 \vec{V}_2' \]
Non-equilibrium and transport phenomena

Collisions drive the system to a UNIVERSAL local equilibrium: Maxwell-Boltzmann

**Weak departure from local equilibrium (herd effect)**

\[ f = f^{eq} + f^{neq} \]

\[ Kn = \left| \frac{f^{neq}}{f^{eq}} \right| \ll 1 \]

Order params:
- \( n = n(r, t) \)
- \( u = u(r, t) \)
- \( T = T(r, t) \)

**Viscosity = Momentum-flux diffusivity**

\[ \frac{F_x}{A} = -\nabla_y (\rho u_x) \]
Boltzmann to NSE: Smooth changes

Macro field

\[ \lambda \]

\[ Kn \equiv \frac{\lambda}{L} \ll 1 \]

Transport in dilute media far from local equilibrium

- Neutron transport
- Gamma rays transport
- Shuttle re-entry
- Electron flows
- Traffic flows
Dense Fluids: Liquids

\[ d = \left( \frac{1}{n} \right)^{1/3} \]

\[ \sigma = k s^2 \]

\[ \lambda \approx \frac{1}{(n \sigma)} \]

Liquid

\[ \tilde{n} \equiv \left( \frac{s}{d} \right)^3 = \left( \frac{s}{\lambda} \right) \approx 1 \]

Meso: Stochastic dynamics

Dense fluids, liquids

\[ \frac{dx}{dt} = v \]

\[ \frac{dv}{dt} = -\gamma v + f(x) / m + \xi \]

\[ <\xi> = 0 \]

\[ <\xi(t)\xi(t')> = \frac{kT}{m} \delta(t-t') \]

Include correlations!
Noise and dissipation

P. Langevin (1872-1946)
Connecting the three levels

**Newton to Boltzmann:**
Molecular size $\ll$ intermolecular distance,
Small granularity, $s/d<1$

**Newton to Langevin:**
Molecular size $\approx$ intermolecular distance,
$s/d\approx 1$
Each molecule sees many others molecules

**Boltzmann/Langevin to Navier-Stokes:**
Weak gradients, pdf close to Maxwell local equilibrium: Small mean free path: $Kn<<1$

Due to MME micro-conservation laws Maxwell equilibria hold for both gases and liquids:
UNIVERSALITY of Navier-Stokes!

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Navier  Stokes

$Kn \to 0$

Langevin

$\tilde{n} \to 1$

Boltzmann

$\tilde{n} \to 0$

Newton

All routes take to Navier-Stokes!
Entry Computers

**Macro-Continuum:**
Most economical, least degrees of freedom, but
STRONGLY NONLINEAR!

**Micro-Molecular:**
Simpler equations, but TOO MANY!

**Meso-Probability distributions:**
Intermediate, excellent on parallel computers, best compromise?

Summary

1. There is more to the physics of fluids than continuum fluid mechanics

2. The three levels micro-meso-Macro are fully exposed by modern fluid-dynamics (micro-nanotech, soft matter, biology)

3. Statistical physics provides the conceptual tools to investigate flows across scales

4. Modern CFD must gracefully integrate methods from ALL 3 levels!

5. Mesoscale methods highly suited to modern parallel computers
Assignments

1. Derive the von Karman relation

2. Compute the Reynolds number for an ordinary kitchen faucet

3. Estimate the mean free path of air molecules in standard conditions