MA621L-Mathematical Modelling

Model-7 : From a Balloon to the Boltzmann Equation: Kinetic Theory and the BGK Model

Panchatcharam Mariappan[1]

[1]Associate Professor
Department of Mathematics and Statistics
IIT Tirupati, Tirupati

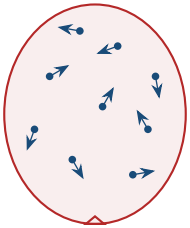
November 11, 2026



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Kinetic Theory of Gases: Why Does a Balloon Push Back?

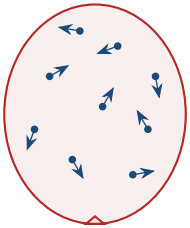
Blowing Up a Balloon



Question

You blow into a balloon and it grows. Nothing solid is inside. What pushes the rubber outward?

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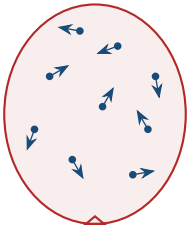


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The air: a huge number of tiny molecules, flying in all directions and hitting the rubber again and again.

Each hit is a tiny push. Billions of hits per second, added up, feel like a steady push on every part of the wall: the **pressure**.

How Many Molecules? How Fast?



Question

Guess: how many air molecules are in a one-litre balloon, and how fast do they move?

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Guess: how many air molecules are in a one-litre balloon, and how fast do they move?

- At room conditions there are about 2.5×10^{25} molecules per m^3, so about 2.5×10^{22} in one litre.
- They move at about 500 m/s, faster than a passenger jet.
- Each one collides with another about every 10^{-10} s, after flying only about 70 nm.

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Can we write Newton's law for every molecule and solve it?

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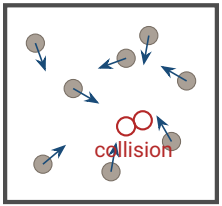


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No: 10^{22} equations, with unknown starting values. We need a different description, one that counts molecules instead of following them.

A Room Full of Bouncing Balls

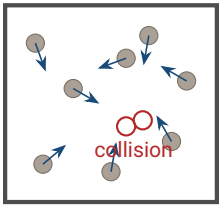


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A Room Full of Bouncing Balls



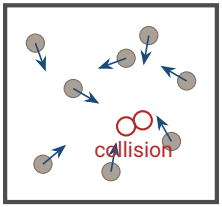
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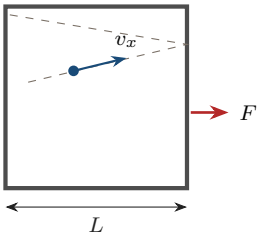
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Keep these three effects in mind: they will become the three terms of the Boltzmann equation.

Pressure from Collisions: One Molecule



One molecule of mass m flies inside a cube side L with velocity component v_x towards the right wall.

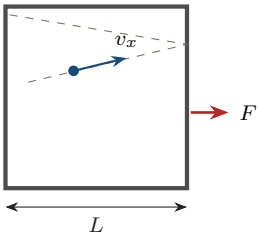
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Average force $=$ momentum change per unit time:

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- Each bounce reverses v_x: momentum change $2mv_x$.
- Between two hits on the same wall it travels $2L$: time $2L/v_x$.

Pressure from Collisions: All Molecules



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Question

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Pressure of a gas

$$\boxed{p = \tfrac{1}{3}\,n\,m\,\langle v^2\rangle}$$

More molecules, or faster molecules, give a larger pressure.

What Is Temperature?



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Temperature measures the average kinetic energy of the molecules.

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Faster than the speed of sound in air (340 m/s), as it should be: sound is carried by these molecules.

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Why does a balloon shrink when you put it in a refrigerator?
Colder air means slower molecules, smaller $\langle v^2 \rangle$, lower pressure: the rubber pulls the balloon smaller.

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Where else does the behaviour of many colliding molecules matter?

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- Air flowing over an aircraft wing, and the inflation of a car's airbag.
- Weather prediction: the atmosphere is a gas.
- Engines and refrigerators: gases being compressed and expanded.
- A spacecraft re-entering the thin upper atmosphere.
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For some of these, ordinary fluid equations work; for others they fail. Kinetic theory explains both.



Counting Molecules: the Distribution Function

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Distribution function $f(\boldsymbol{x}, \boldsymbol{v}, t)$

$f(\boldsymbol{x}, \boldsymbol{v}, t)\, d\boldsymbol{x}\, d\boldsymbol{v} =$ amount of gas in a small box $d\boldsymbol{x}$ around $\boldsymbol{x}$, with velocity in $d\boldsymbol{v}$ around $\boldsymbol{v}$.

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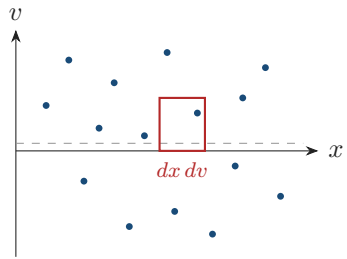
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f is a *density*: it lives in a six-dimensional space of positions and velocities, called **phase space**. Here we measure the amount in mass, so integrating f over velocities gives the mass density.

Phase Space, Pictured

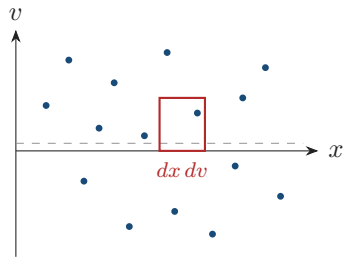


Each dot is one molecule: its position x and its velocity v (one dimension of each, for the picture).

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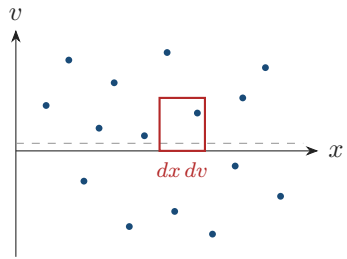
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A molecule moving right ($v > 0$) is above the axis; one moving left is below.

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If we know f, how do we get the density of the gas at x?

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In the phase-space picture: count all the dots above and below a point x, along the vertical line.

Momentum and Energy from f



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Weight each velocity by $\boldsymbol{v}$, or by $\frac{1}{2}|\boldsymbol{v}|^2$:

$$\rho \boldsymbol{U} = \int_{\mathbb{R}^3} \boldsymbol{v}\, f\, d\boldsymbol{v}, \qquad E = \int_{\mathbb{R}^3} \frac{|\boldsymbol{v}|^2}{2}\, f\, d\boldsymbol{v}.$$

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These integrals are called the **moments** of f. The fluid quantities we know (density, velocity, energy) are moments of the molecular list.



How Does the List Change? The Boltzmann Equation

Effect 1: Molecules Move



Question

No forces, no collisions. Molecules at x with velocity v: where are they after a short time dt?

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At $\boldsymbol{x} + \boldsymbol{v}\,dt$, still with velocity $\boldsymbol{v}$. So the list is simply carried along:

$$f(\boldsymbol{x} + \boldsymbol{v}\,dt,\ \boldsymbol{v},\ t + dt) = f(\boldsymbol{x}, \boldsymbol{v}, t).$$

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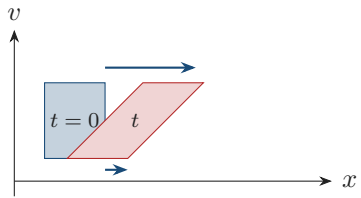
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Expand the left side to first order in dt. What equation do you get?

$$f + \frac{\partial f}{\partial t}\,dt + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f\,dt = f \quad \Longrightarrow \quad \frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = 0.$$

The **advection term** $\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f$: change of f because molecules move through space.

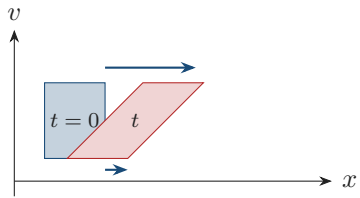
Free Flight in Phase Space



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A block of molecules starts in the blue square. What shape is it at a later time?

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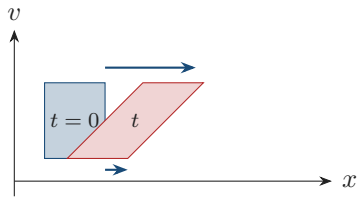


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The exact solution is $f(\boldsymbol{x}, \boldsymbol{v}, t) = f_0(\boldsymbol{x} - \boldsymbol{v}t, \boldsymbol{v})$: each molecule just keeps flying. Check it by substitution.

Effect 2: Forces Change Velocities



Question

Now a force gives every molecule an acceleration a (for example gravity). What changes in the argument?

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In time dt the velocity also changes, from $\boldsymbol{v}$ to $\boldsymbol{v} + \boldsymbol{a}\,dt$:

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Expanding again:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \boldsymbol{a} \cdot \nabla_{\boldsymbol{v}} f = 0.$$

The **force term** $\boldsymbol{a} \cdot \nabla_{\boldsymbol{v}} f$: change of f because forces push molecules to new velocities.

Effect 3: Collisions



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The Boltzmann equation (1872)

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- left side: molecules moving and being pushed by forces;
- right side: molecules being scattered by collisions.

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$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \iint \left[f(\boldsymbol{v}')f(\boldsymbol{v}_1') - f(\boldsymbol{v})f(\boldsymbol{v}_1)\right] g\,\sigma(g,\Omega)\,d\Omega\,d\boldsymbol{v}_1$$

- $\boldsymbol{v}, \boldsymbol{v}_1$: velocities before, $\boldsymbol{v}', \boldsymbol{v}_1'$: after the collision;
- $g = |\boldsymbol{v} - \boldsymbol{v}_1|$: relative speed; σ: probability of scattering into the solid angle Ω.

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Look at the collision integral. What makes it difficult to work with?

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- It is **quadratic** in f: the products ff make the equation nonlinear.
- It is a **five-dimensional integral** (three for $\boldsymbol{v}_1$, two for the angle Ω), to be computed at every point $\boldsymbol{x}$ and every velocity $\boldsymbol{v}$.
- It needs the scattering law σ, which depends on how molecules interact.

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So we ask: what does the collision term *do*, overall? If we knew that, perhaps a simpler formula would do the same job.

What Collisions Never Change



Question

In a collision between two molecules, which quantities are the same before and after?

What Collisions Never Change



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Remember these three conditions: later they will turn the Boltzmann equation into the equations of fluid flow.

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$$\ln f(\boldsymbol{v}') + \ln f(\boldsymbol{v}_1') = \ln f(\boldsymbol{v}) + \ln f(\boldsymbol{v}_1).$$

So $\ln f$ is conserved in every collision, like mass, momentum and energy. It must be a combination of them:

$$\ln f = a + \boldsymbol{b} \cdot \boldsymbol{v} - c\,|\boldsymbol{v}|^2.$$

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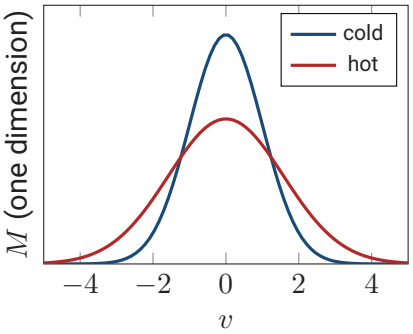
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So $\ln f$ is conserved in every collision, like mass, momentum and energy. It must be a combination of them:

$$\ln f = a + \boldsymbol{b} \cdot \boldsymbol{v} - c\,|\boldsymbol{v}|^2.$$

So f is a Gaussian in $\boldsymbol{v}$: the **Maxwellian** distribution.

The Maxwellian Distribution



Choosing the constants so that the moments are $\rho, \boldsymbol{U}, T$:

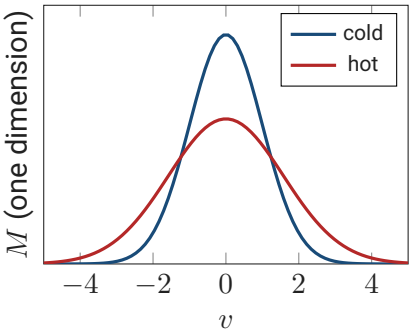
$$M = \frac{\rho}{(2\pi RT)^{3/2}} \exp\Big(- \frac{|\boldsymbol{v} - \boldsymbol{U}|^2}{2RT} \Big)$$

(R: gas constant per unit mass).

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What happens to the curve when the gas gets hotter?

It becomes lower and wider: more fast molecules, the same total amount.

Why Does Every Gas End Up Maxwellian?



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Start a gas with any strange velocity distribution. Why does it always relax to M, and never move away from it?

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Boltzmann's **H-theorem**: for a uniform gas, the quantity

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can only decrease in time, and it stops decreasing exactly when $f = M$.

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Collisions act in one direction only: they drive the gas towards equilibrium. This is the arrow of time, appearing from the mechanics of colliding molecules.



A Simpler Collision Term: the BGK Model

The BGK Idea



We know what collisions do overall: they push f towards the Maxwellian M, and they conserve mass, momentum, and energy.

Question

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Make the rate of change proportional to the distance from equilibrium:

BGK collision model (Bhatnagar, Gross and Krook, 1954)

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- τ: the **relaxation time**, roughly the average time between collisions.
- M: the local Maxwellian, built from the local density, velocity and temperature of the gas.

Is the Sign Right?



Question

At some velocity, there are more molecules than in equilibrium: $f > M$.
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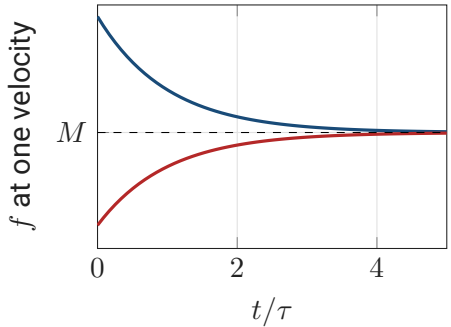
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Warning

Writing the term as $(f - M)/\tau$ reverses the sign: f would run away from equilibrium. Always check the sign with this argument.

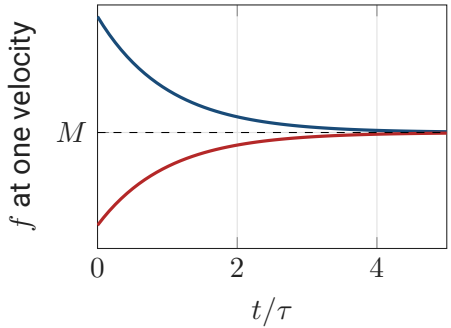
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Question

In a uniform gas with no forces, $\frac{df}{dt} = \frac{M - f}{\tau}$, with M fixed. Solve it.

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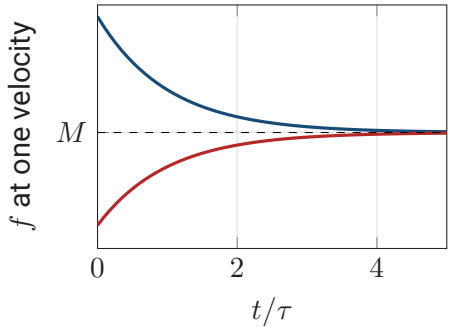


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After a few times τ, the gas is Maxwellian. For air at room conditions $\tau \approx 10^{-10}$ s: equilibrium is reached almost instantly.

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Question

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Only if M is built from the moments of f itself: the same ρ, $\boldsymbol{U}$ and T. Then

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So M is not a fixed function: it changes whenever f changes. This makes the BGK equation **nonlinear**, even though it looks linear in f.

The Boltzmann–BGK Equation

With no external forces, the Boltzmann equation with the BGK collision term is

Boltzmann–BGK equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = \frac{1}{\tau}(M - f), \qquad f(\boldsymbol{x}, \boldsymbol{v}, 0) = f_0(\boldsymbol{x}, \boldsymbol{v}),$$

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with $\boldsymbol{x}, \boldsymbol{v} \in \mathbb{R}^3$ and $\rho(\boldsymbol{x}, t) \in \mathbb{R}$, $\boldsymbol{U}(\boldsymbol{x}, t) \in \mathbb{R}^3$, $T(\boldsymbol{x}, t) \in \mathbb{R}$.

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From f itself, through its moments: next slide.

From f to Density, Velocity and Temperature



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$$\rho = \int_{\mathbb{R}^3} f \, d\boldsymbol{v}, \qquad \boldsymbol{U} = \frac{1}{\rho} \int_{\mathbb{R}^3} \boldsymbol{v} \, f \, d\boldsymbol{v}, \qquad E = \int_{\mathbb{R}^3} \frac{|\boldsymbol{v}|^2}{2} \, f \, d\boldsymbol{v}.$$

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$$E = \tfrac{1}{2}\rho|\boldsymbol{U}|^2 + \rho e, \qquad e = \tfrac{3}{2}RT.$$

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So

$$T = \frac{2}{3R}\Big(\frac{E}{\rho} - \frac{|\boldsymbol{U}|^2}{2}\Big).$$

The loop is closed: $f \to (\rho, \boldsymbol{U}, T) \to M \to$ new f.



From Molecules to Fluids

From BGK to the Continuity Equation



Question

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$$\frac{\partial}{\partial t}\int f\,d\boldsymbol{v} + \nabla_{\boldsymbol{x}} \cdot \int \boldsymbol{v}\, f\,d\boldsymbol{v} = \frac{1}{\tau}\int (M - f)\,d\boldsymbol{v}.$$

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The continuity equation of fluid dynamics, derived from molecules.
Multiplying first by $\boldsymbol{v}$ or by $\frac{1}{2}|\boldsymbol{v}|^2$ gives the momentum and energy equations in the same way.

When Is a Gas a Fluid?



Question

A molecule flies a distance λ (the mean free path) between collisions. When can we ignore individual molecules and treat the gas as a smooth fluid?

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Flow	λ	L	Kn
air in a room	70 nm	1 m	10^{-7}: fluid
gas in a micro-channel	70 nm	$1\ \mu$m	0.07: in between
spacecraft at 100 km altitude	~ 10 cm	1 m	0.1: in between
satellite in orbit	km	1 m	$\gg 1$: free molecules

Frequent Collisions Give Fluid Equations



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$f \approx M$: the gas is in local equilibrium everywhere. Taking moments then gives the **Euler equations** of gas dynamics.

The first correction (the Chapman–Enskog expansion, $f = M + \tau f_1 + \dots$) gives the **Navier–Stokes equations**, with

$$\mu = \tau\, p \qquad \text{(viscosity from the BGK model).}$$

Checking with Real Air

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The viscosity of air, something we feel and measure, is set by how often its molecules collide.

Where Is the BGK Model Used?



Question

Why would anyone use a kinetic equation when the Navier–Stokes equations exist?

Where Is the BGK Model Used?



Question

Why would anyone use a kinetic equation when the Navier–Stokes equations exist?

- To **derive** the Navier–Stokes equations from molecular physics, and know when they hold.
- For **rarefied gases**, where Kn is not small: spacecraft re-entry, the upper atmosphere.
- For gas flows in **micro- and nanoscale devices**.
- As the basis of a numerical method, the **lattice Boltzmann method** (LBM), which solves a discrete BGK equation on a grid.

Where Does the BGK Model Fall Short?



Question

One relaxation time τ for everything. What could go wrong?

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One relaxation time τ for everything. What could go wrong?

- Real gases relax momentum and heat at different rates. BGK uses one τ for both, so it predicts a Prandtl number $\mathrm{Pr} = \mu c_p/\kappa = 1$; a monatomic gas has $\mathrm{Pr} \approx 2/3$. The ratio of viscosity to heat conduction is wrong.

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- Far from equilibrium (strong shock waves, rapid expansions, large temperature gradients) a single relaxation towards M misses details of the real collisions.

Remedies: models with corrected relaxation (ES-BGK, Shakhov), and multiple relaxation times (MRT) in the lattice Boltzmann method.

Back to the Balloon



Question

Explain the balloon again, this time with the model we built.

Back to the Balloon



Question

Explain the balloon again, this time with the model we built.

1. The air is described by a distribution $f(\boldsymbol{x}, \boldsymbol{v}, t)$ of molecular velocities.
2. Collisions keep f close to a Maxwellian, with $\tau \approx 10^{-10}$ s.
3. The moments of f give the density, the flow velocity and the temperature.
4. The pressure is the momentum carried to the wall by molecules: $p = \frac{1}{3} nm\langle v^2 \rangle = \rho RT$.
5. Blowing adds molecules and warmth, so the pressure rises and the rubber stretches until the forces balance.

Summary



Idea	Equation	Meaning
pressure from impacts	$p = \frac{1}{3} nm\langle v^2 \rangle$	momentum delivered to the wall
temperature	$\frac{1}{2} m\langle v^2 \rangle = \frac{3}{2} kT$	average kinetic energy
distribution function	$f(\boldsymbol{x}, \boldsymbol{v}, t)$	amount of gas in phase space
Boltzmann equation	$\partial_t f + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f + \boldsymbol{a} \cdot \nabla_{\boldsymbol{v}} f = C(f)$	motion, forces, collisions
equilibrium	$M \propto e^{-\lvert \boldsymbol{v} - \boldsymbol{U} \rvert^2 / 2RT}$	collisions balance
BGK model	$C(f) \approx (M - f)/\tau$	relaxation towards M
moments	$\rho,\ \rho \boldsymbol{U},\ E$	fluid quantities
fluid limit	$\tau \to 0$, $\mathrm{Kn} \ll 1$	Euler, Navier–Stokes ($\mu = \tau p$)

Exercises: Kinetic Theory



Exercise 1: Pressure from impacts

Repeat the one-molecule calculation for a molecule that hits the wall at an angle. Show that the result $p = \frac{1}{3} nm\langle v^2 \rangle$ does not change.

Exercise 2: Moments of the Maxwellian

Show that $\int M \, d\boldsymbol{v} = \rho$, $\int \boldsymbol{v} M \, d\boldsymbol{v} = \rho \boldsymbol{U}$ and $\int \frac{1}{2} |\boldsymbol{v}|^2 M \, d\boldsymbol{v} = \frac{1}{2} \rho |\boldsymbol{U}|^2 + \frac{3}{2} \rho R T$. (Use $\int e^{-x^2/2} dx = \sqrt{2\pi}$.)

Exercise 3: Free flight

Show that $f(\boldsymbol{x}, \boldsymbol{v}, t) = f_0(\boldsymbol{x} - \boldsymbol{v}t, \boldsymbol{v})$ solves $\partial_t f + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = 0$. Sketch it in phase space for an initial square.

Exercises: Kinetic Theory (contd.)



Exercise 4: Relaxation

Solve $df/dt = (M - f)/\tau$ for a uniform gas. How many times τ until f is within 1% of M? Evaluate for air.

Exercise 5: Momentum equation

Multiply the BGK equation by $\boldsymbol{v}$ and integrate over $\boldsymbol{v}$. Which momentum equation do you obtain when $f = M$?

Exercise 6: Knudsen numbers

The mean free path is about $\lambda = \mu/p\,\sqrt{\pi RT/2}$. Compute Kn for air in a $10\ \mu$m channel and around a 1 m object at 80 km altitude ($p \approx 1$ Pa).



Ledger and Classification

Kinetic Theory: Dym's Questions

Question	Kinetic model of a gas
Why?	Explain pressure and temperature from molecules; know when fluid equations hold.
Find?	The distribution $f(\boldsymbol{x}, \boldsymbol{v}, t)$, and from it ρ, $\boldsymbol{U}$, T, p.
Given?	Initial distribution f_0; gas constant R; relaxation time τ (or the scattering law σ).
How?	Boltzmann equation; BGK relaxation towards the local Maxwellian; moments.
Valid?	Moments conserve mass, momentum, energy; $\tau \to 0$ gives the Euler and Navier–Stokes equations.
Verified?	Ideal gas law; measured viscosity gives $\tau \approx 10^{-10}$ s; rarefied-gas experiments.

Kinetic Theory: Assumption Ledger



- A1: A dilute gas: molecules interact only in brief binary collisions.
- A2: Molecular chaos: the velocities of two colliding molecules are independent.
- A3: Collisions conserve mass, momentum and kinetic energy (elastic).
- A4: BGK: collisions are replaced by relaxation towards M with one relaxation time τ.
- A5: No external forces ($\boldsymbol{a} = 0$) in the BGK equation used here.
- A6: Monatomic gas: internal energy $e = \frac{3}{2}RT$, no rotation or vibration.

Velten SQM. S physical, natural; Q mechanistic (collisions) with a phenomenological closure (BGK), instationary, distributed in position and velocity; M continuous, a nonlinear integro-differential equation in seven variables $(\boldsymbol{x}, \boldsymbol{v}, t)$, deterministic for f though built on statistical reasoning.



Thank You