A Very Brief Introduction into Kinetic Equations of Gas Dynamics

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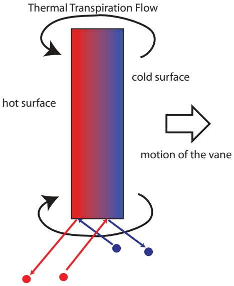
Introduction

Crookes Radiometer

Thermal transpiration is an effect observed in **rarefied gas** when molecules can travel large distances before colliding ("cold" molecules reaching "hot" wall regions and vice versa)



At each point we have several low-interacting steams. This is different from the classical continuum mechanics where the fluid is fully described by density, velocity and temperature at each point.

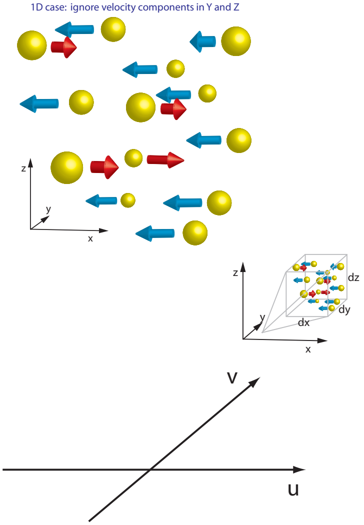
In fact, thermal transpiration is a **non-continuum** effect.

Kinetic Description of Gas

Gas consists of particles that most of the time do not interact.

Each particle is associated with a velocity and a position.

The state of gas is described using the *molecular velocity distribution function* $f(t, \vec{x}, \vec{v})$ defined by the property that $f(t, \vec{x}, \vec{v})dxdv$ gives the number of molecules contained in a box of size $dx \times dv$ at point $(\vec{x}, \vec{v})$ of the physical space.



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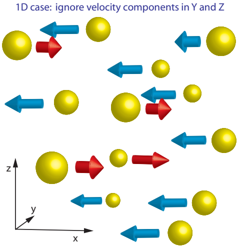

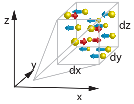

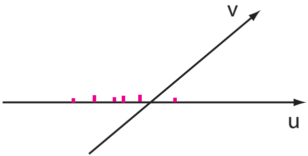

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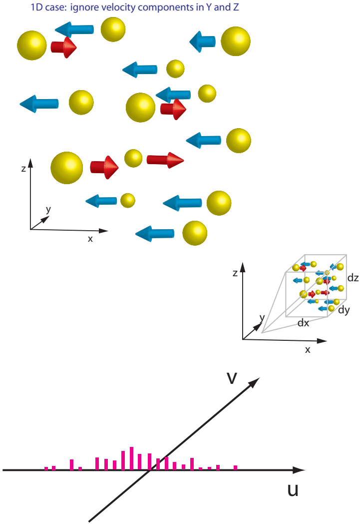

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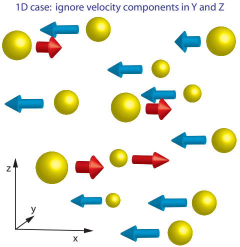

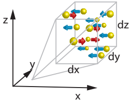

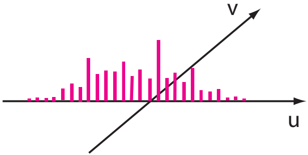

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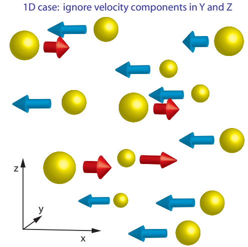

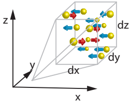

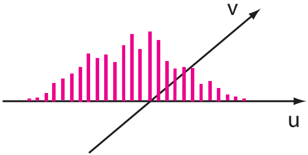

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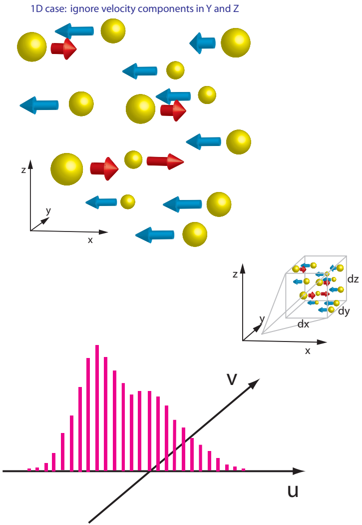

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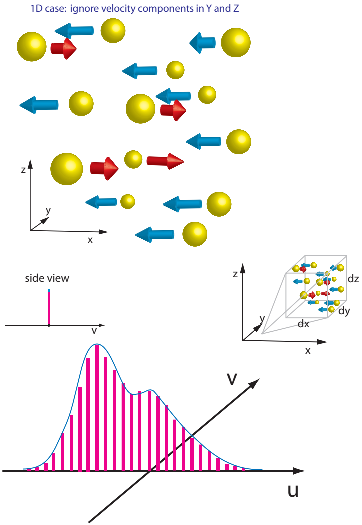


Macroscopic Quantities

How is the velocity distribution function related to properties of the gas that we experience on the daily basis? E.g., hot or cold wind? Air compression?

The observable quantities, known as **macroscopic quantities** or **moments** are computed from the velocity distribution function by integration.

$$n(t,\vec{x}) = \int f(t,\vec{x},\vec{v})dv \quad \text{(density)}$$

$$n(t,\vec{x})\vec{u}(t,\vec{x}) = \int \vec{v} f(t,\vec{x},\vec{v})dv \quad \text{(bulk velocity)}$$

$$n(t,\vec{x})T(t,\vec{x}) = \frac{1}{3R}\int |\vec{v}-\vec{u}|^2 f(t,\vec{x},\vec{v})dv \quad \text{(temperature)}$$

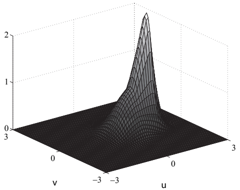
also,

$$\mathbb{T}(t,\vec{x}) = \frac{1}{3}\int (\vec{v}-\vec{u})(\vec{v}-\vec{u})^T f(t,\vec{x},\vec{v})dv \quad \text{(stress tensor)}$$

$$\mathcal{E}(t,\vec{x}) = \int \vec{v}\frac{|\vec{v}|^2}{2} f(t,\vec{x},\vec{v})dv \quad \text{(energy flux)}$$

Continuum vs. Non-Continuum

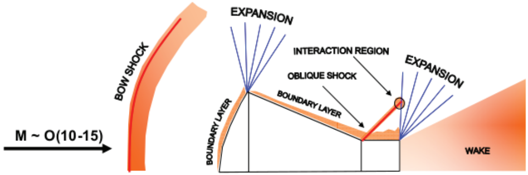
As molecules collide and exchange energy, their velocity distribution approaches the Maxwellian distribution



$$f_M(\vec{v}) = n(2\pi RT)^{-3/2} \exp\left(-\frac{|\vec{v}-\vec{u}|^2}{2RT}\right)$$

The gas is **at continuum** (at a point in space) if its v. d. f. is Maxwellian.

Continuum gas is governed by **Euler equations**, near continuum by **Navier-Stokes equations**. Non-continuum - **Kinetic equations** or **Extended hydrodynamics**.



Regions of non-continuum flow. Pic: A. Wood

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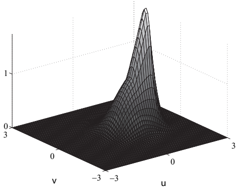

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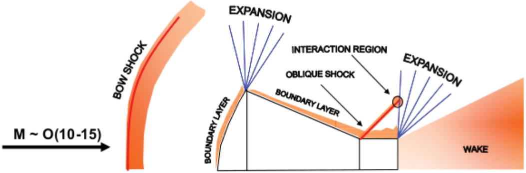

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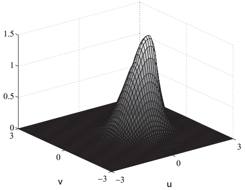

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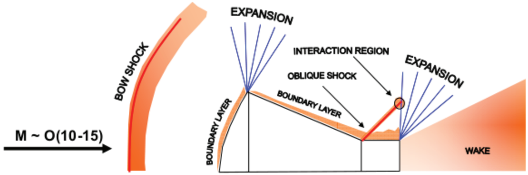

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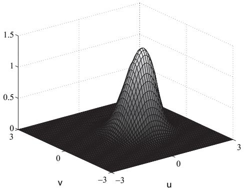

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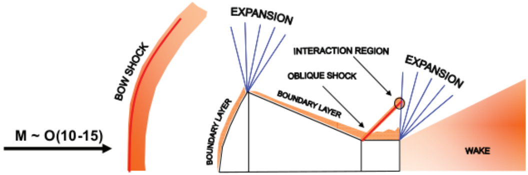

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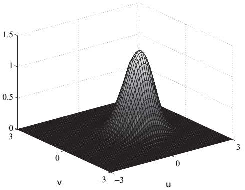

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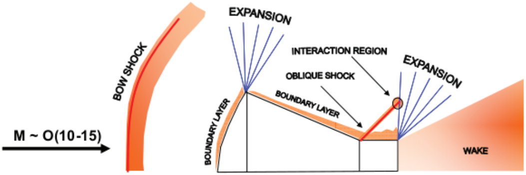

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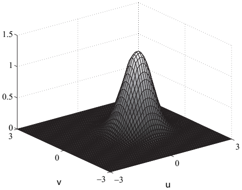

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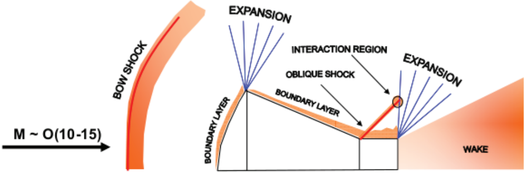

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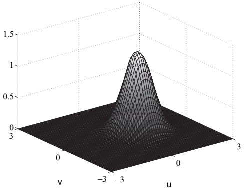

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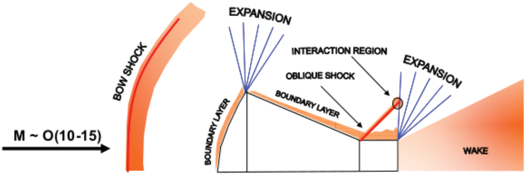

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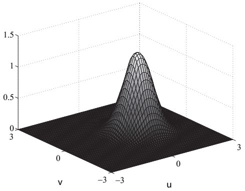

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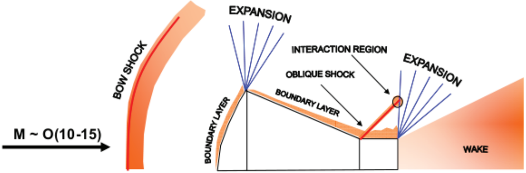

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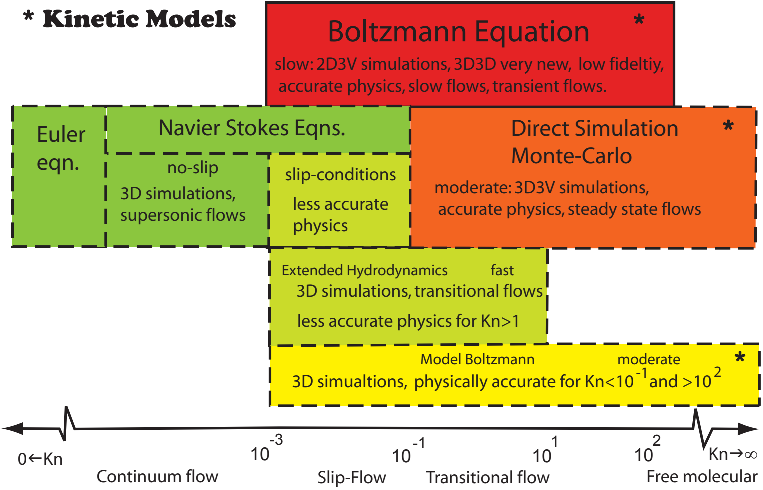
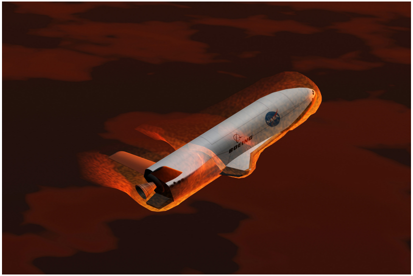
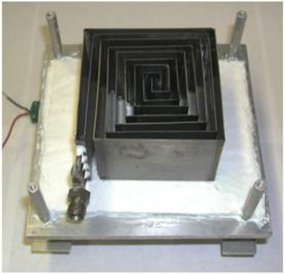
A Map of CFD Models for Different Flow Regimes

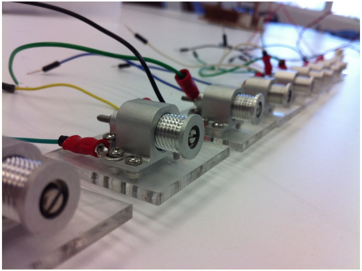


$\mathrm{Kn} = \lambda/L$; λ - mean free molecular path; L - characteristic length scale of the flow.

Applications of Non-Continuum Gas Flows







Picture credit: USAF, NASA, Dr. Muntz, USC, Dr. Keidar, GWU

The Kundsen Number

Traditionally, Knudsen number is used to determine if the gas is at continuum.

$$\mathrm{Kn} = \frac{\lambda}{L},$$

where λ is the mean free moleculuar path and L is the characteristic lengthscale of the flow.

Altitude	n, 1/m^3	λ, m	τ, sec
0	10^{25}	10^{-7}	10^{-9}
100 km	10^{19}	10^{-3}	10^{-5}
300 km	10^{15}	10^{3}	1

Table: Number density of molecules, *n*, **mean free path**, λ, and **mean time between collisions**, τ, for air at different altitudes

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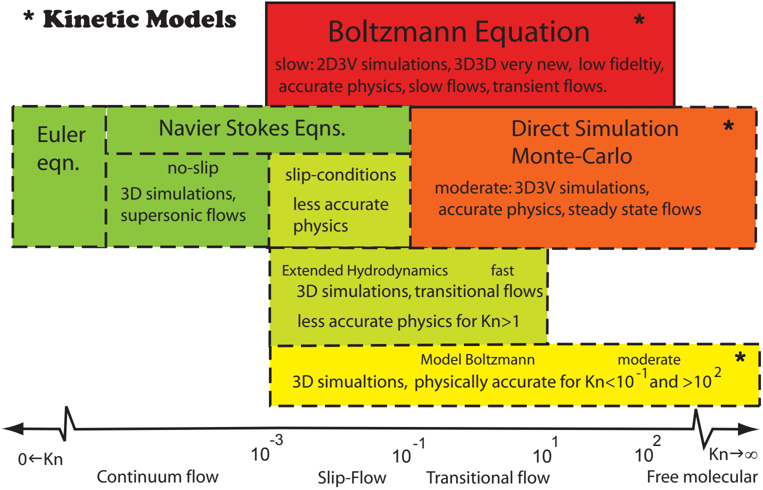


$\mathrm{Kn} = \lambda/L$; λ - mean free molecular path; L - characteristic lengthscale of the flow.

The dynamics of gas is given the Boltzmann equation:

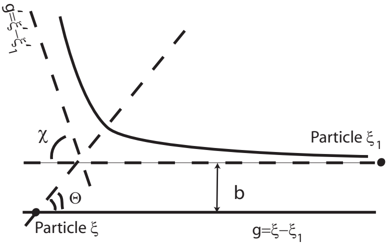
$$\frac{\partial}{\partial t} f(t,\vec{x},\vec{v}) + \vec{v}\cdot\vec{\nabla}_x f(t,\vec{x},\vec{v}) = Q(f,f),$$

where (no external forces, binary collisions, single species)

$$Q(f,f) = \int_{R^3}\int_0^{2\pi}\int_0^{b_0} (f' f_1' - f f_1)|g| b\, db\, d\varepsilon\, dv_1$$

Where $f = (t,\vec{x},\vec{v})$, $f = (t,\vec{x},\vec{v}_1)$, $f' = (t,\vec{x},\vec{v}')$, and $\vec{v}$ and $\vec{v}_1$ are pre-collisional and $\vec{v}'$ and $\vec{v}_1'$ are post collisional velocities.

Five dimensional integration requires $O(n^5)$ operations at each point of six dimensional phase space where n is the number of D.O.F. in one dimension.



Generalizations of the Boltzmann Equation

The evolution of the velocity distribution function is governed by the Boltzmann equation (no external forces, binary collisions, single species):

$$\frac{\partial}{\partial t} f(t, \vec{x}, \vec{v}) + \vec{v} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{v}) = Q[f](t, \vec{x}, \vec{v}),$$

where $Q[f](t, \vec{x}, \vec{v})$ is an operator modeling molecular collisions.

Challenges: high dimensionality, slow evaluation of the collision operator.

Multiple species, internal energies, external forces:

$$\frac{\partial}{\partial t} f_i(t, \vec{x}, \vec{v}) + \vec{v} \cdot \vec{\nabla}_x f_i(t, \vec{x}, \vec{v}) + \frac{1}{m_i} \vec{F}_i \cdot \vec{\nabla}_v f_i(t, \vec{x}, \vec{v}) = \sum_{ij} Q[f_i, f_j](t, \vec{x}, \vec{v}),$$

where $Q[f_i, f_j](t, \vec{x}, \vec{v})$ models collisions between two species.

Add: large numbers of species, differences of molecular masses, differences in time scales for collision.

However, an efficient solution of single species will advance methods for more general model as well.

$$\frac{\partial}{\partial t} f(t,\vec{x},\vec{v}) + \vec{v}\cdot\vec{\nabla}_x f(t,\vec{x},\vec{v}) + \frac{1}{m}\vec{F}\cdot\vec{\nabla}_v f(t,\vec{x},\vec{v}) = Q[f](t,\vec{x},\vec{v})$$

High dimensionality: if one uses m spatial points and n velocity point in one spatial or velocity dimensions, discretization of left side requires $O(m^3 n^3)$ memory units and $O(m^3 n^3)$ operations for one explicit time step. Continuum-kinetic hybrid codes can reduce m.

High cost of evaluating

$$Q[f](t,\vec{x},\vec{v}) = \int_{R^3}\int_0^{2\pi}\int_0^{b_0} (f' f_1' - f f_1)|g|b\, db\, d\varepsilon\, dv_1$$

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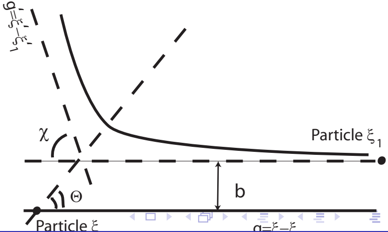
Evaluation requires $O(n^8)$ operations.

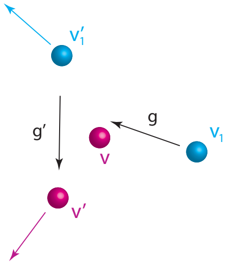


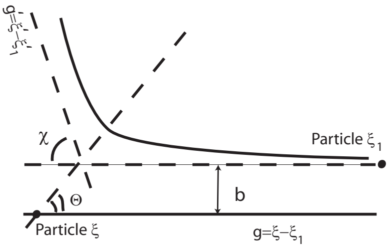
Molecular Collisions

As molecules collide, the gas velocity distribution function $f(t, \vec{x}, \vec{v})$ changes.

Velocities of molecules before and after the collision are different.

It is fairly straightforward to track the changes caused by collisions.





Physics of Collisions

Let velocities $\vec{v}$ and $\vec{v}_1$ be pre-collisional and $\vec{v}'$ and $\vec{v}_1'$ be post-collisional. Conservation laws

$$m\vec{v} + m\vec{v}_1 = m\vec{v}' + m\vec{v}_1'$$

$$m\|\vec{v}\|^2 + m\|\vec{v}_1\|^2 = m\|\vec{v}'\|^2 + m\|\vec{v}_1'\|^2$$

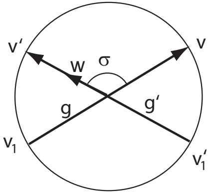
$$\|\vec{v} - \vec{v}_1\| = \|\vec{v}' - \vec{v}_1'\|$$

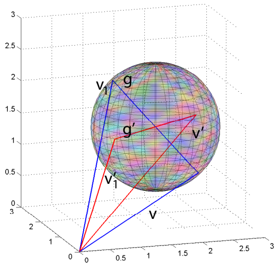
Pairs $\vec{v}$, $\vec{v}_1$ and $\vec{v}'$, $\vec{v}_1'$ make diameters on the collision sphere. It is convenient to write

$$\vec{v}' = \frac{\vec{v} + \vec{v}_1}{2} + \vec{w}\frac{\|\vec{g}\|}{2}, \quad \vec{v}_1' = \frac{\vec{v} + \vec{v}_1}{2} - \vec{w}\frac{\|\vec{g}\|}{2},$$

where $\vec{w}$ parametrizes the rotation of $\vec{g} = \vec{v} - \vec{v}_1$, $\vec{w}$ depends on impact parameters and physics of interaction.

Shift $\vec{\xi}$ in collision sphere: If $\vec{v} \to \vec{v} + \vec{\xi}$ and $\vec{v}_1 \to \vec{v}_1 + \vec{\xi}$, then $\vec{v}' \to \vec{v}' + \vec{\xi}$, $\vec{v}_1' \to \vec{v}_1' + \vec{\xi}$.



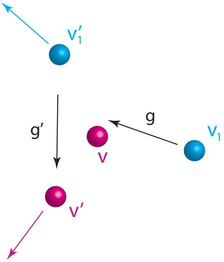


Computing Loss of Molecules with Velocity $\vec{v}$

A loss of molecule with velocity $\vec{v}$ happens when another molecule hits it and both change velocity.

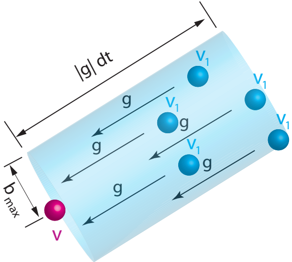
$$\vec{v}' = \frac{\vec{v}+\vec{v}_1}{2} + \vec{w}\frac{\|\vec{g}\|}{2}, \quad \vec{v}_1' = \frac{\vec{v}+\vec{v}_1}{2} - \vec{w}\frac{\|\vec{g}\|}{2},$$

where $\vec{w}$ parametrizes the rotation of $\vec{g} = \vec{v} - \vec{v}_1$.

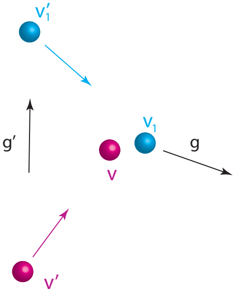


The total loss of molecules is given by the probability of such collision during time dt:

$$dQ^- = dt\, f(\vec{v}) \int_{R^3} \int_0^{2\pi} \int_0^{b_{max}} f(\vec{v}_1)|g|b\, db\, d\varepsilon\, dv_1$$
$$= dt\, f(\vec{v})\pi b_{max}^2 \int_{R^3} f(\vec{v}_1)|g| dv_1$$

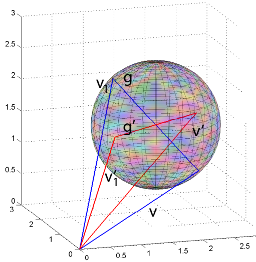


A gain of molecule with velocity $\vec{v}$ happens when two molecules collide with just the right velocities so that one of them has velocity $\vec{v}$ after the collision.



$$\vec{v}' = \frac{\vec{v}+\vec{v}_1}{2} + \vec{w}\frac{\|\vec{g}\|}{2}, \quad \vec{v}_1' = \frac{\vec{v}+\vec{v}_1}{2} - \vec{w}\frac{\|\vec{g}\|}{2},$$

where $\vec{w}$ parametrizes the rotation of $\vec{g} = \vec{v} - \vec{v}_1$.



The total gain of molecules is given by the probability of such collision during time dt:

$$dQ^{+} = dt \int_{R^3} \int_0^{2\pi} \int_0^{b_{max}} f(\vec{v}')f(\vec{v}_1')|g|b\,db\,d\varepsilon\,dv_1$$

The Boltzmann Equation

Evolution of the v.d.f. $f(t, \vec{x}, \vec{v})$ is governed by the Boltzmann eq.:

$$\frac{\partial}{\partial t} f(t, \vec{x}, \vec{v}) + \vec{v} \cdot \vec{\nabla}_x f(t, \vec{x}, \vec{v}) = Q[f](t, \vec{x}, \vec{v}),$$

where

$$Q[f](t, \vec{v}) = \int_{R^3} \int_0^{2\pi} \int_0^{b_0} (f(\vec{v}')f(\vec{v}_1') - f(\vec{v})f(\vec{v}_1))|g|b\, db\, d\varepsilon\, dv_1$$

- Need high fidelity methods, i.e., high values of n! The largest n in 0D is 64, in 2D and 3D are about 32.
- Scalability Challenges: CPU Time and Memory!
- Direct evaluation takes $O(n^8)$ operations and $O(n^3)$ memory. Need more efficient methods: $O(n^6)$, $O(n \log n)$ operations, even faster?
- Memory constraints become important for $O(n^6)$ methods.

Evaluation of the Boltzmann Collision Operator

$$e^{x+y} = e^x e^y$$

Exponentials, including complex exponentials are very attractive to discretize the collision operator.

$O(N^2)$, $O(N^2 \log N)$: Pareschi and Perthame (1996), Pareschi and Russo (2000), Bobylev and Rjasanov (1999) ($O(N^{2/3}$, Maxwell), Ibragimov and Rjasanov (2002), Kirsch and Rjasanov (2007), Gamba and Tharkabhushanam (2009, 2010), Haack and Gamba (2012) ($b(\theta, \varepsilon)|g|^\gamma$). All methods use Fourier Basis functions or the Fourier Transform. Potentials: HS, VHS, VSS, $\sigma = B \sin^\alpha(\theta)|g|^\gamma$.

$O(MN \log N)$: Mohout and Pareschi (2006); Filbet, Mouhot, and Pareschi (2006); Wu, White, Scanlon, Reese, and Zhang (2013) (extended to L-J and more); Gamba, Haack and Hu (2014)

2D: Filbet and Russo (2003); Liu, Xu, Sun, and Cai (2014) (UGKS);

Internal Energy/ Polyatomic: Munafo, Haack, Gamba, and Magin (2012); Liu, Yu, Xu and Zhong (2014) (UGKS);

Numerical Solution of the Boltzmann Equation.

Fast Stochastic Integration: $O(P)$ operations and $O(n^3)$ memory. Tcheremissine (2003,2006), Morris, Varghese, and Goldstein (2008,2011), Arslanbekov, Kolobov, and Frolova (2013) (UFS);

Discontinuous Galerkin Discretizations $O(n^8)$. Aristov (2001), Aristov and Zabelok (2002), Majorana (2011), Alekseenko and Josyula (2013), Gamba and Zhang (2014);

There methods can be made $O(n^6)$ and $O(Mn^3)$, $M < n^3$: Alekseenko, Nguyen and Wood (2018), Alekseenko and Limbacher (2018).

Key: Convolution form of the collision operator

$$Q[f](t,\vec{u}-\vec{\xi}) = \int_{R^3}\int_0^{2\pi}\int_0^{b_0} (f(\vec{u}'-\vec{\xi})f(\vec{u}_1'-\vec{\xi}) - f(\vec{u}-\vec{\xi})f(\vec{u}_1-\vec{\xi}))|g|b\,db\,d\varepsilon\,dv_1$$

Other Galerkin Methods. Grohs, Hiptmair and Pintarelli (2015), Gamba and Rjasanow (2017)