DSMC AND KINETIC THEORY FAR FROM EQUILIBRIUM: A STIMULATING DIALOGUE

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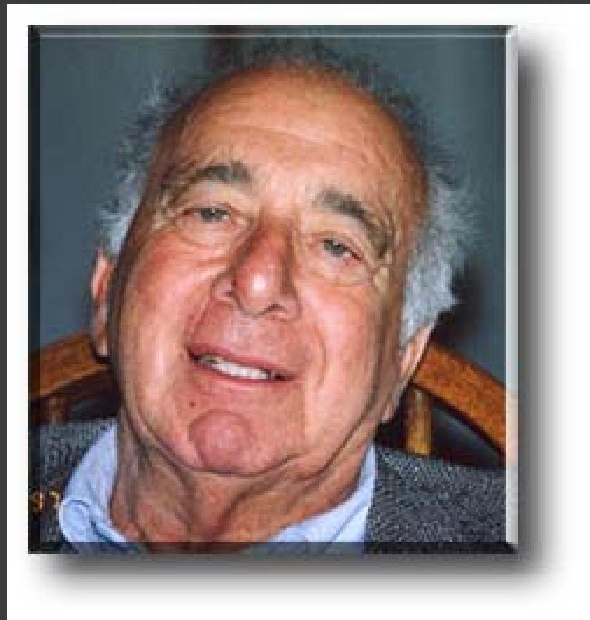

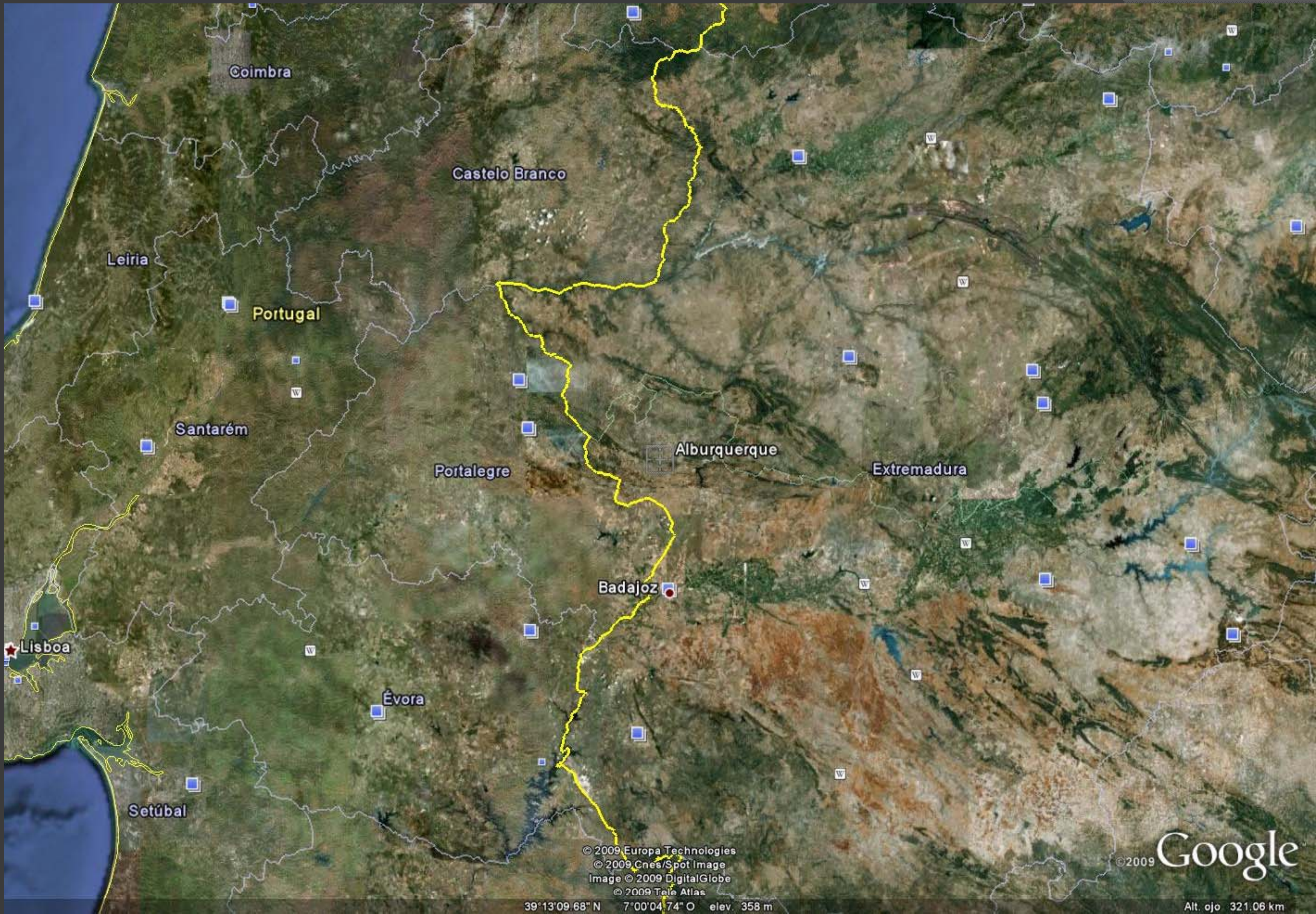
Coimbra
Castelo Branco
Leiria
Portugal
Santarém
Alburquerque
Extremadura
Portalegre
Badajoz
Lisboa
Évora
Setúbal
© 2009 Europa Technologies
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© 2009 Tele Atlas
39°13'09.68" N 7°00'04.74" O elev. 358 m
©2009 Google
Alt. ojo 321.06 km

History [edit]

Early settlers [edit]

The city was founded in 1706 as the Spanish colonial outpost of *Ranchos de Alburquerque*[citation needed]; present-day Albuquerque retains much of the Spanish cultural and historical heritage.

Albuquerque was a farming community and strategically located military outpost along the Camino Real. The town of Alburquerque was built in the traditional Spanish village pattern: a central plaza surrounded by government buildings, homes, and a church. This central plaza area has been preserved and is open to the public as a museum, cultural area, and center of commerce. It is referred to as "Old Town Albuquerque" or simply "Old Town." "Old Town" was sometimes referred to as "La Placita" ("little plaza" in Spanish).

The village was named by the provincial governor Don Francisco Cuervo y Valdes in honour of Don Francisco Fernández de la Cueva, viceroy of New Spain from 1653 to 1660. One of de la Cueva's aristocratic titles was Duke of Alburquerque, referring to the Spanish town of Alburquerque.

The Alburquerque family name dates from pre-12th century Iberia (Spain and Portugal) and is habitational in nature (*de Alburquerque* = from Alburquerque). The Spanish village of Alburquerque is within the Badajoz province of Extremadura region, and located just fifteen miles (24 km) from the Portuguese border. Cork trees dominate the landscape and Alburquerque is a center of the Spanish cork industry.[5] Over the years, this region has been alternately under both Spanish and Portuguese rule. It is interesting to note that the name of the New Mexico city of Albuquerque follows the Portuguese spelling with only one 'r'. Historically, the land around Alburquerque was invaded and settled by the Moors (711 AD) and the Romans (218 BC) before them. Thus, the word Alburquerque may be rooted in the Arabic (Moorish) 'Abu al-Qurq', which means "father of the cork oak", or "land of the cork oak" (the land as father - fatherland). Alternately, it may be Latin (Roman) in origin and from 'albus quercus' or "white oak" (the wood of the cork oak is white after the bark has been removed). The seal of the Spanish village of Alburquerque is a white oak tree, framed by a shield, topped by a crown.[6]

During the Civil War Albuquerque was occupied in February 1862 by Confederate troops under General Henry Hopkins Sibley, who soon afterwards advanced with his main body into northern New Mexico. During his retreat from Union troops into Texas he made a stand on April 8, 1862 at Albuquerque and fought the Battle of Albuquerque against a detachment of Union soldiers commanded by Colonel Edward range led to few casualties.

When the Atchison, Topeka and Santa Fe Railroad arrived in 1880, it bypassed the Plaza, locating the passenger depot and railyards about 2 miles (3 km) east in what quickly became known as New Albuqu crime rate, gunman Milt Yarberry was appointed the town's first Marshal that same year. New Albuquerque was incorporated as a town in 1885, with Henry N. Jaffa its first mayor, and incorporated as a city ir community until the 1920s when it was absorbed by the City of Albuquerque. Albuquerque High School, the city's first public high school, was established in 1879.

Early 20th Century

New Albuquerque quickly became a tidy southwestern town which by 1900 boasted a population of 8,000 inhabitants and all the modern amenities including an electric street railway connecting Old Town, Ne the recently established UNM campus on the East Mesa. In 1902 the famous Alvarado Hotel was built adjacent to the new passenger depot and remained a symbol of the city until it was torn down in 1970 tc for a parking lot. In 2002, the Alvarado Transportation Center was built on the site in a manner resembling the old landmark. The large metro station functions as the downtown headquarters for the city's transi and serves as an intermodal hub for local buses, Greyhound buses, Amtrak passenger trains, and the Rail Runner commuter rail line.

New Mexico's dry climate brought many tuberculosis patients to the city in search of a cure during the early 1900s, and several sanitaria sprang up on the West Mesa to serve them. Presbyterian Hospital an Hospital, two of the largest hospitals in the Southwest, had their beginnings during this period. Influential New Deal-era governor Clyde Tingley and famed southwestern architect John Gaw Meem were among to New Mexico by tuberculosis.

Decades of growth

In June 2007, Albuquerque was listed as the 6th fastest growing city in America by CNN and the US Census Bureau.[4]

The first travelers on Route 66 appeared in Albuquerque in 1926, and before long, dozens of motels, restaurants, and gift shops had sprung up along the roadside to city on a north-south alignment along Fourth Street, but in 1937 it was realigned along Central Avenue, a more direct east-west route. The intersection of Fourth and the city for decades. The majority of the surviving structures from the Route 66 era are on Central, though there are also some on Fourth. Signs between Bernalillo a historical highway markers denoting it as *Pre-1937 Route 66*.

The establishment of Kirtland Air Force Base in 1939, Sandia Base in the early 1940s, and Sandia National Laboratories in 1949, would make Albuquerque a key pl continued to expand outward onto the West Mesa, reaching a population of 201,189 by 1960. In 1990 it was 384,736 and in 2007 it was 518,271.

DSMC

is an extremely powerful, efficient, reliable, and flexible tool for studying *rarefied* gas flows (extensions accounting for non-ideal gases have been proposed).

Is there any need for analytical or semi-analytical solutions?

Do we actually need a dialogue between

DSMC

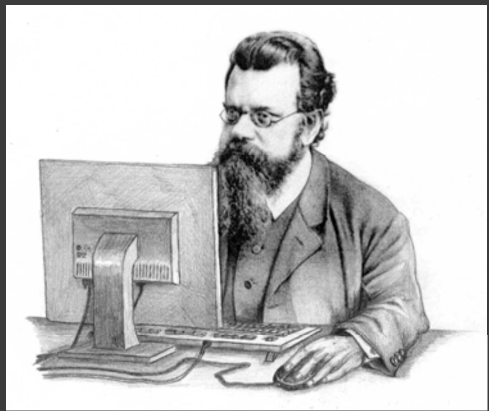
and

kinetic theory solutions

(Cartoon by Bernhard Reischl, University of Vienna)

?

Yes!



Kinetic theory solutions

Realistic?

Accurate?

DSMC

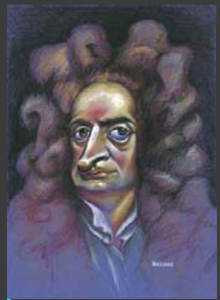
Outline

- Hydrodynamics beyond Navier-Stokes
- Boltzmann equation. Maxwell molecules
- Some solvable states:
  - Planar Fourier flow
  - Planar Fourier flow with gravity
  - Planar Couette flow
  - Force-driven Poiseuille flow
  - Uniform shear and longitudinal flows
- Conclusions

Classical hydrodynamics: Navier-Stokes constitutive equations

Claude-Louis Navier
(1785-1836)

$$\mathbf{q} = -\kappa_{\mathrm{NS}} \nabla T$$



George Gabriel Stokes
(1819-1903)

$$P_{ij} = p\delta_{ij} - \eta_{\mathrm{NS}} \left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3} \nabla \cdot \mathbf{u} \delta_{ij} \right)$$

$$\boxed{\mathrm{Kn} \lesssim 0.1}$$

The Knudsen number

Martin Hans Christian Knudsen (1871–1949)

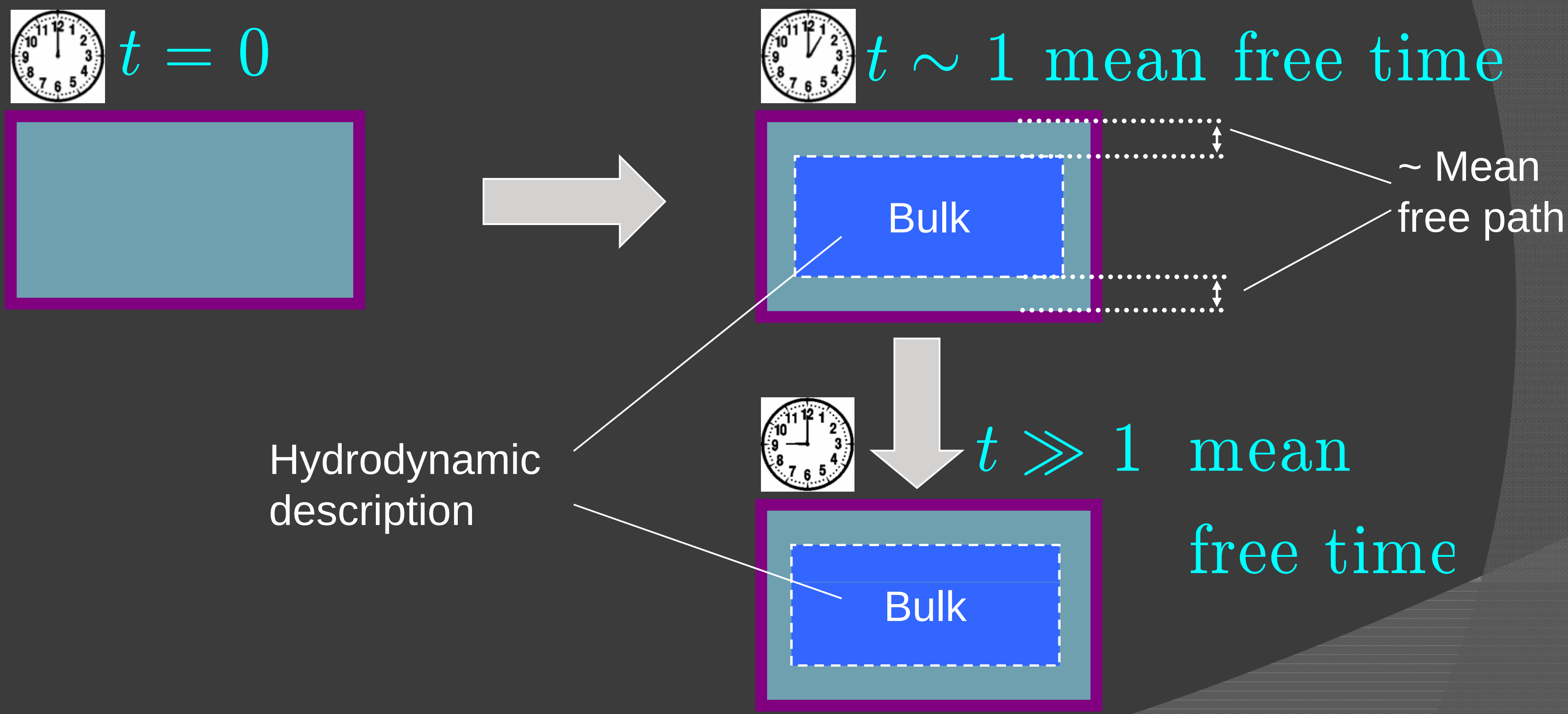
$$\mathrm{Kn} = \frac{\textit{mean free path } (\delta)}{\textit{characteristic distance } (L)}$$

Characteristic distance?
Two types of Knudsen numbers:

$$\textit{characteristic distance} = \begin{cases} \textit{system size } (L_s) \\ \textit{gradient length scale } (L_\nabla) \end{cases}$$

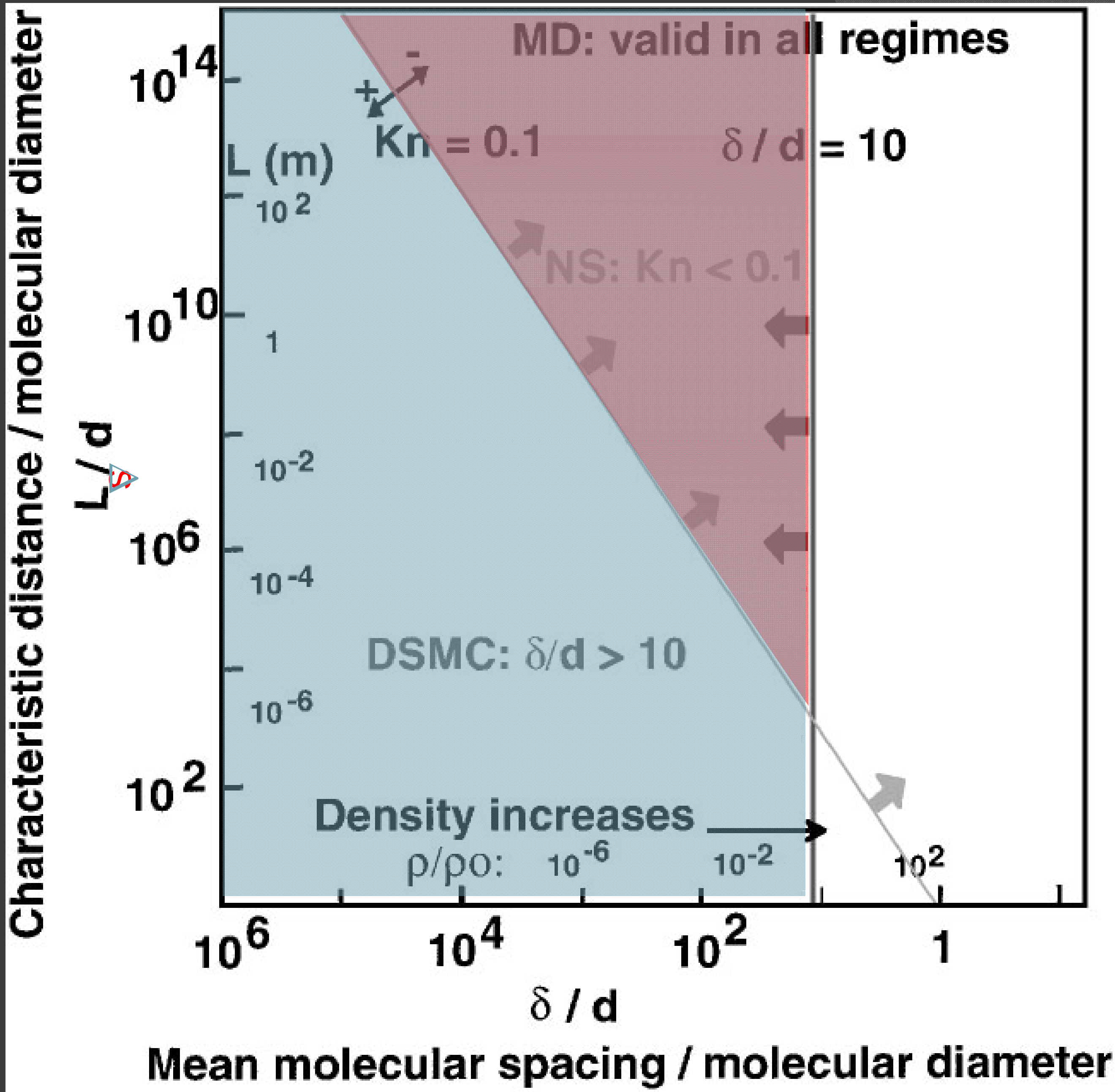
If $L_s \gg \delta \sim L_\nabla$, a *bulk* region exists with hydrodynamics beyond NS

"Aging" to hydrodynamics (whether NS or not)

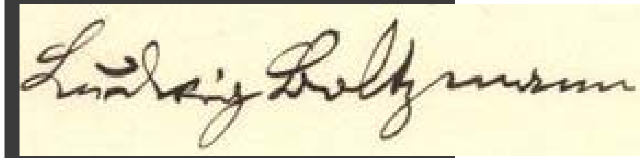


DIRECT SIMULATION MONTE CARLO: Recent Advances and Applications
E.S. Oran, C.K. Oh, and B.Z. Cybyk

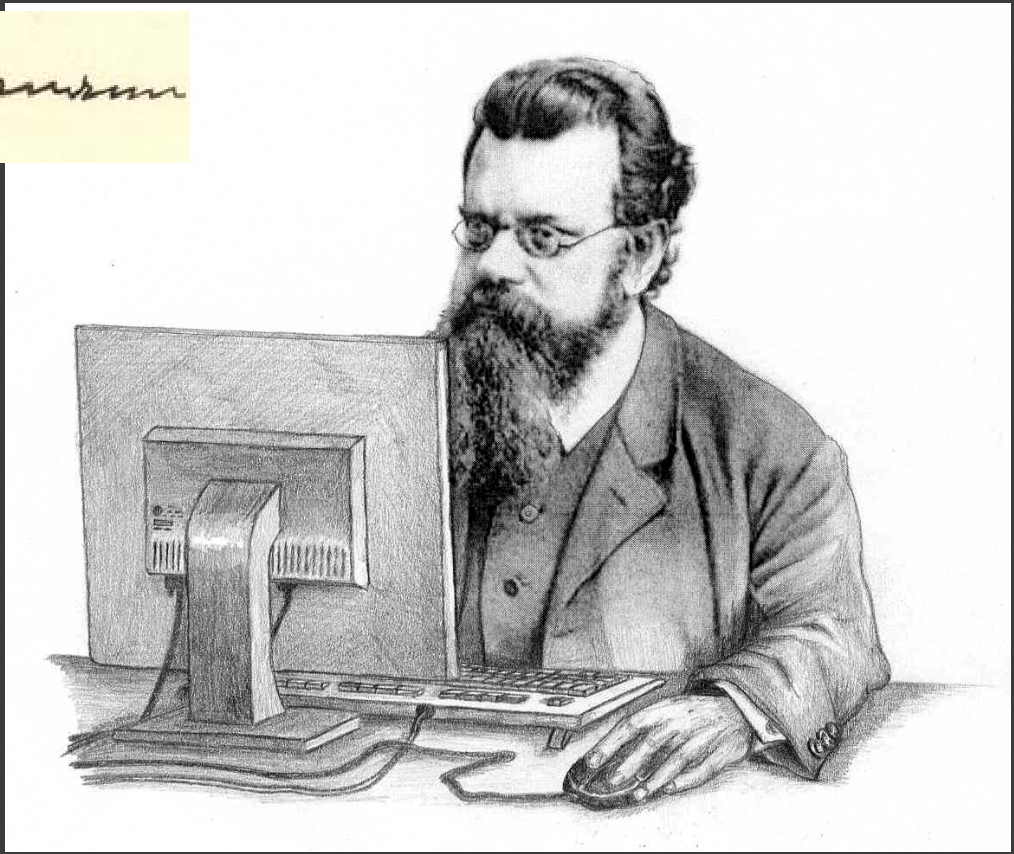
Annu. Rev. Fluid Mech. 1998. 30:403–41



The Boltzmann equation



(1844-1906)



(Cartoon by Bernhard Reischl, University of Vienna)

Weak form of the Boltzmann equation

$$\underbrace{\Psi(\mathbf{r},t) = \int d\mathbf{v}\,\psi(\mathbf{v}) f(\mathbf{r},\mathbf{v};t)}_{\text{Density of } \psi(\mathbf{v})} \Rightarrow \boxed{\frac{\partial \Psi}{\partial t} + \nabla\cdot\mathbf{\Phi}_\psi = \sigma_\psi^{(F)} + J_\psi}$$

$$\underbrace{\mathbf{\Phi}_\psi = \int d\mathbf{v}\,\mathbf{v}\psi(\mathbf{v}) f(\mathbf{v}),}_{\text{Flux}} \qquad \underbrace{\sigma_\psi^{(F)} = \int d\mathbf{v}\,\frac{\partial \psi}{\partial \mathbf{v}}\cdot\frac{\mathbf{F}}{m} f(\mathbf{v})}_{\text{Source: external force}}$$

$$\underbrace{\begin{aligned} J_\psi &= \int d\mathbf{v}\,\psi(\mathbf{v}) J[\mathbf{v}|f,f] \\ &= \frac{1}{4}\int d\mathbf{v}\int d\mathbf{v}_1 \int d\Omega\, gB(g,\chi)\left[\psi(\mathbf{v}) + \psi(\mathbf{v}_1) - \psi(\mathbf{v}') - \psi(\mathbf{v}_1')\right] \\ &\quad \times f(\mathbf{v}) f(\mathbf{v}_1) \end{aligned}}_{\text{Source: collisions}}$$

Hierarchy of moment equations

$$\frac{\partial \Psi}{\partial t} + \nabla \cdot \mathbf{\Phi}_\psi = \sigma_\psi^{(F)} + J_\psi$$

$\psi(\mathbf{v})$ = polynomial of degree $k \Rightarrow \Psi$ = velocity moment of degree k

$\sigma_\psi^{(F)}$ = velocity moment of degree $k-1$, if $\mathbf{F} \neq \mathbf{F}(\mathbf{v})$

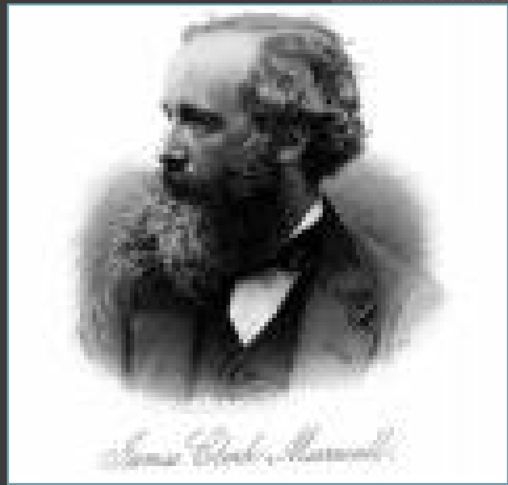
$\mathbf{\Phi}_\psi$ = velocity moment of degree $\boxed{k+1}$

J_ψ = bilinear combination of velocity moments of any degree

Maxwell molecules

On the Dynamical Theory of Gases
Phil. Trans. Roy. Soc. (London) **157**, 49-88 (1867)

In the present paper I propose to consider the molecules of a gas, not as elastic spheres of definite radius, but as small bodies or groups of smaller molecules repelling one another with a force whose direction always passes very nearly through the centres of gravity of the molecules, and whose magnitude is represented very nearly by some function of the distance of the centres of gravity.



(1831-1879)

I have made this modification of the theory in consequence of the results of my experiments on the viscosity of air at different temperatures, and I have deduced from these experiments that the repulsion is inversely as the *fifth* power of the distance.

I have found by experiment that the coefficient of viscosity in a given gas is independent of the density, and proportional to the absolute temperature, so that if ET be the viscosity, $ET \propto p/\rho$.

Maxwell molecules

$$\phi(r) \sim r^{-4} \Rightarrow gB(g,\chi) = \mathcal{B}(\chi)$$

True Maxwell potential (inverse power law, IPL):

$$\mathcal{B}(\chi) \propto \frac{\beta}{\sin\chi}\left|\frac{d\beta}{d\chi}\right|, \quad \chi(\beta) = \pi - 2\int_0^{\beta_0} d\beta' \left[1 - \beta'^2 - \frac{1}{2}\left(\frac{\beta'}{\beta}\right)^4\right]^{-1/2}$$

Variable soft-sphere (VSS) model: $\mathcal{B}(\chi) = \cos^{2(\alpha-1)}\frac{\chi}{2}, \quad \alpha = 2.13986$

Variable hard-sphere (VHS) model: $\mathcal{B}(\chi) = \text{const}, \quad \alpha = 1$

Properties of the collisional moments in Maxwell models

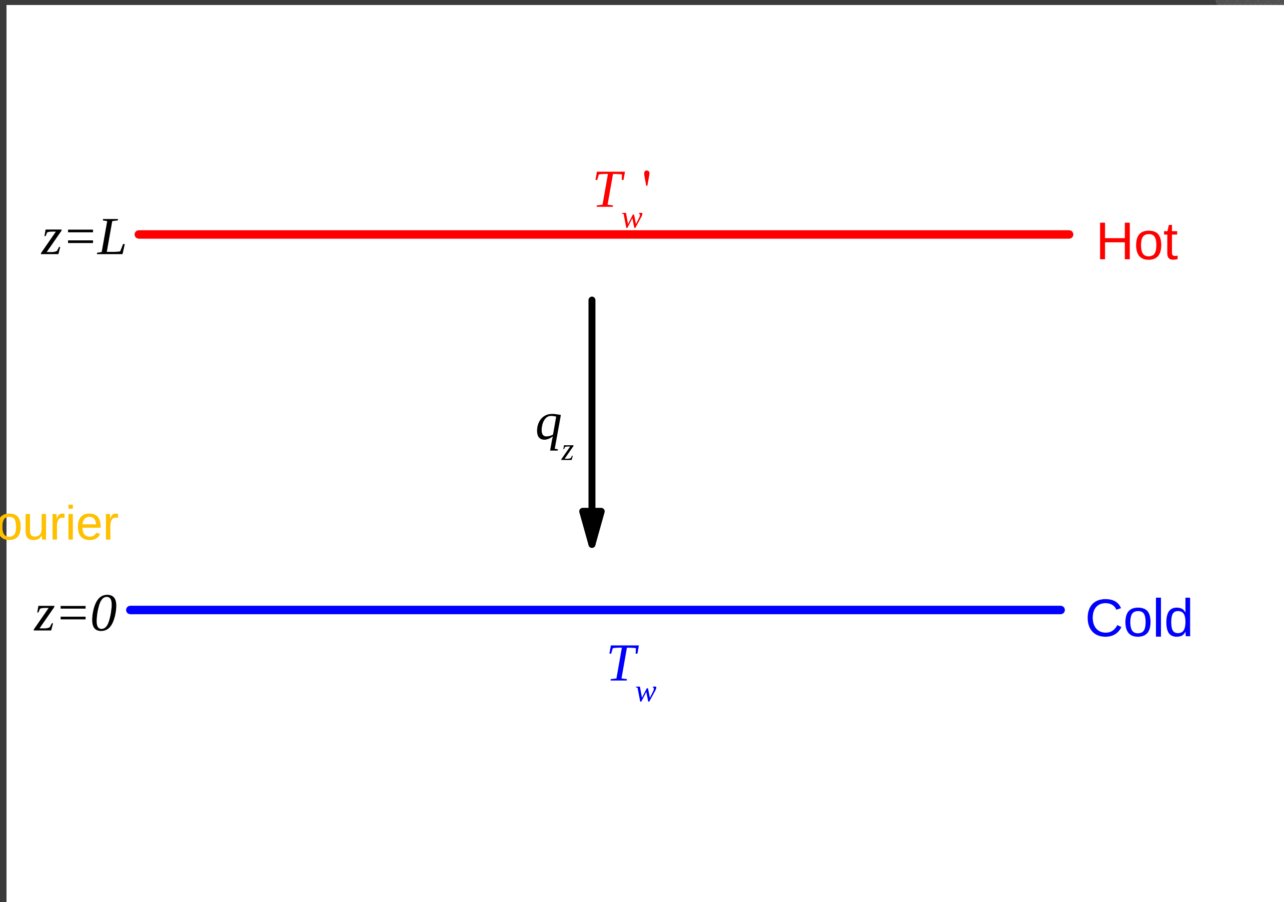
$$\text{If } \psi(\mathbf{v}) = \text{polynomial of degree } k$$

$$\text{then}$$

$$J_\psi = \text{bilinear combination of velocity moments of degree equal to or smaller than } k$$

1. Steady planar Fourier flow

Jean-Baptiste Joseph Fourier
(1768-1830)



Asmolov, Makashev, and Nosik (1979) proved that an exact solution of the (nonlinear) Boltzmann equation for Maxwell molecules exists with

$$p = nk_B T = \mathrm{const}$$

$$\mathbf{u} = \mathbf{0}$$

$$\frac{\partial}{\partial z} T \frac{\partial T}{\partial z} = 0 \Rightarrow T(z) = \sqrt{A + Bz}$$

Dimensionless quantities

(Local) Knudsen number:

$$\boxed{\epsilon = \frac{4\kappa_{\mathrm{NS}}}{5nk_B\sqrt{2k_BT/m}}\frac{\partial \ln T}{\partial z}} = \frac{\delta}{L_\nabla}$$

Reduced distribution function:

$$\phi(\mathbf{c};\epsilon) = \frac{1}{n(z)}\left[\frac{2k_BT(z)}{m}\right]^{3/2} f(z,\mathbf{v}), \quad \mathbf{c} = (m/2k_BT)^{1/2}\,\mathbf{v} \quad \text{“Normal” solution}$$

Reduced moments:

$$M_{r\ell}(\epsilon) = \int d\mathbf{c}\, c^{2r} c_z^{\ell} \phi(\mathbf{c};\epsilon)$$

Hierarchy of moment equations

$$\frac{\epsilon}{2}\left(2r+\ell-1-\epsilon\frac{\partial}{\partial\epsilon}\right)M_{r,\ell+1}(\epsilon) = \frac{n}{\lambda_{11}}\int d\mathbf{c}\, c^{2r} c_z^{\ell} J[\mathbf{c}|\phi(\epsilon),\phi(\epsilon)] \equiv J_{r\ell}(\epsilon)$$

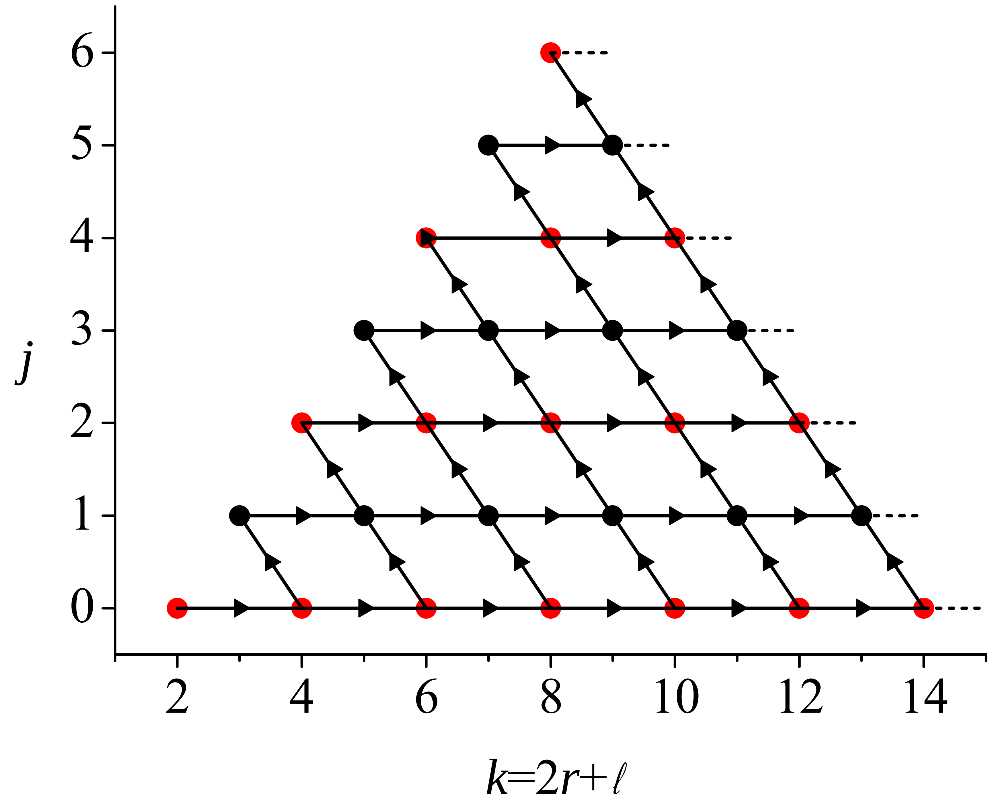
The hierarchy admits a solution whereby the moments $M_{r\ell}(\epsilon)$ are *polynomials* in ϵ of degree $2r+\ell-2$ and parity ℓ:

$$M_{r\ell}(\epsilon) = \sum_{j=0}^{2r+\ell-2} \mu_j^{(r\ell)}\epsilon^j, \quad \mu_j^{(r\ell)} = 0 \text{ if } j+\ell = \text{odd}$$

Both sides of the hierarchy are polynomials of degree $2r+\ell-2$. Equating the coefficients of both sides allows one to get $\mu_j^{(r\ell)}$ recursively

A.S. , Cont. Mech. Thermod., in press (2009)

Sketch of the sequence followed in the recursive determination of the coefficients $\mu_j^{(r\ell)}$



First few moments

$$k = 2r + \ell = 2 : \begin{cases} M_{10} = \frac{3}{2} \\ M_{02} = \frac{1}{2} \Rightarrow P_{xx} = P_{yy} = P_{zz} = nk_B T \end{cases}$$

Fourier's law

$$k = 2r + \ell = 3 : \begin{cases} M_{11} = -\frac{5}{4}\epsilon \Rightarrow \boxed{q_z = -\kappa_{\mathrm{NS}} \dfrac{\partial T}{\partial z}} \\ M_{03} = -\frac{3}{4}\epsilon \Rightarrow \langle v_z^3 \rangle = 3\langle v_x^2 v_z \rangle = \frac{3}{5}\langle v^2 v_z \rangle \end{cases}$$

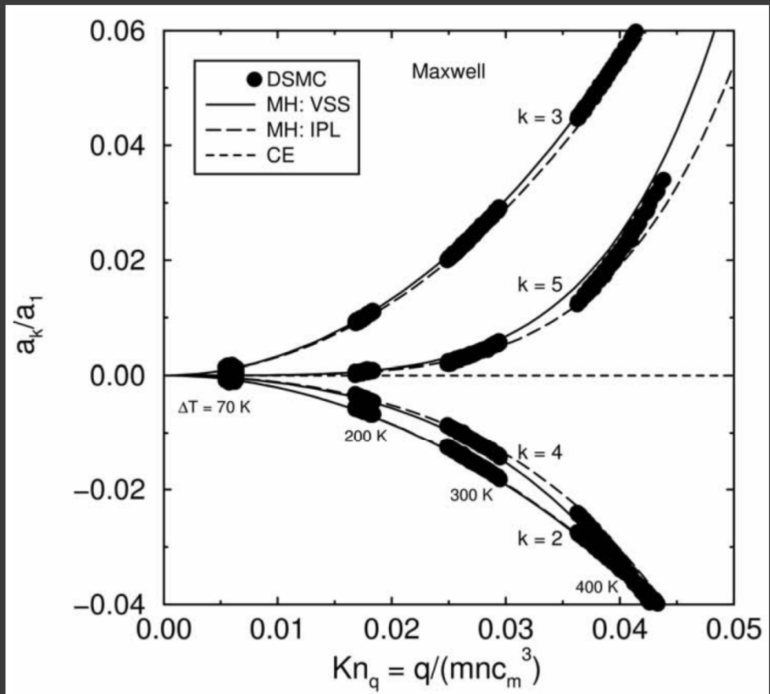
First few moments

$$k = 2r + \ell = 4 : \begin{cases} M_{20} = \frac{15}{4} + \frac{35}{4}\epsilon^2 \\ M_{12} = \frac{5}{4} + \frac{17}{4}\epsilon^2 \\ M_{04} = \frac{3}{4} + \frac{81}{28}\epsilon^2 \end{cases}$$

$$k = 2r + \ell = 5 : \begin{cases} M_{21} = -\frac{35}{4}\epsilon - \left(\frac{1163}{36} + \frac{7}{\lambdabar_{22}}\right)\epsilon^3 \\ M_{13} = -\frac{21}{4}\epsilon - \left[\frac{1163}{60} + \frac{21}{5\lambdabar_{22}} + \frac{27}{10\lambdabar_{13}}\left(\frac{8}{7} + \frac{1}{\lambdabar_{22}}\right)\right]\epsilon^3 \\ M_{05} = -\frac{15}{4}\epsilon - \frac{9}{2}\left[\frac{1163}{378} + \frac{2}{3\lambdabar_{22}} + \frac{2}{3\lambdabar_{13}}\left(\frac{8}{7} + \frac{1}{\lambdabar_{22}}\right)\right]\epsilon^3 \end{cases}$$

Benchmark for DSMC simulations

$$\frac{a_k(\epsilon)}{a_1(\epsilon)} \equiv \frac{15\sqrt{\pi}}{8}\sum_{r=1}^{k}\frac{(-1)^{r-1}k!}{r!(k-r)!(r+3/2)!}\frac{M_{r1}(\epsilon)}{M_{11}(\epsilon)}$$
$$= \text{Polynomial of degree } 2k-2$$



Gallis et al., Phys. Fluids **18**, 017104 (2006)

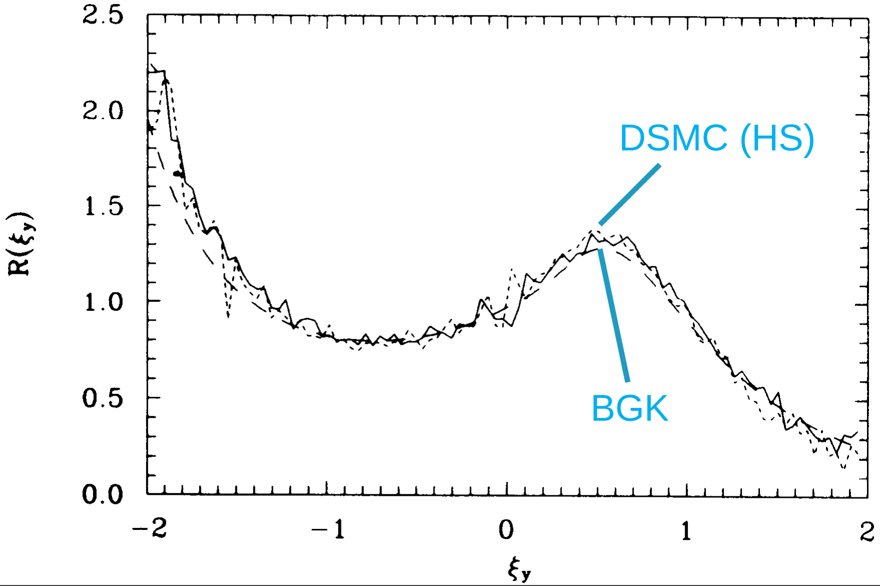
BGK description (arbitrary potentials)

- Same qualitative results for moments.
- Full velocity distribution function $\phi(\mathbf{c};\epsilon)$.
- Divergence of the (CE) expansion of $\phi(\mathbf{c};\epsilon)$ in powers of ϵ.

$$\phi(\mathbf{c};\epsilon) = \frac{\pi^{-3/2}}{\epsilon|c_z|}\int_0^\infty dt\,\Theta\left((1-t)\mathrm{sgn}(c_z)\right)t^{-5/2}e^{-c^2/t+(t-1)/\epsilon c_z}$$

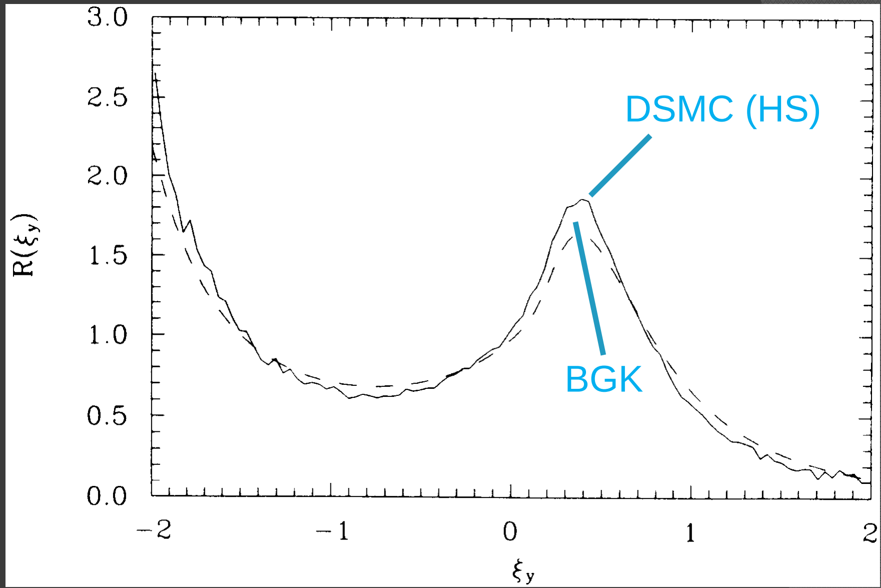
Montanero et al., Phys. Rev. E **49**, 367 (1994)

$\phi(c_z)/\phi_{\rm LE}(c_z)$



$\epsilon = 0.334$

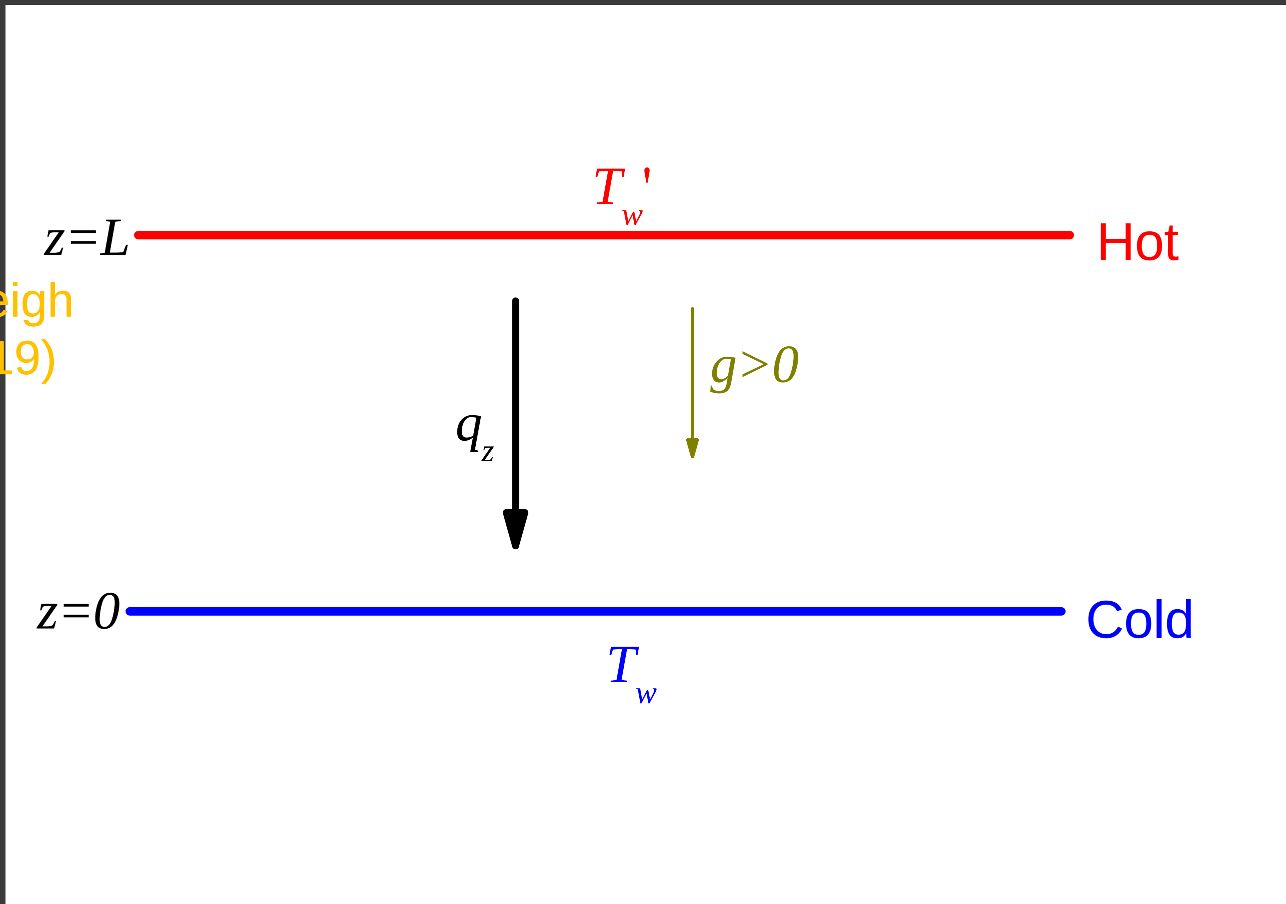
$\phi(c_z)/\phi_{\rm LE}(c_z)$



$\epsilon = 0.68$

2. Steady planar Fourier flow with *gravity* (Rayleigh-Bénard-like flow)

Lord Rayleigh
(1842-1919)



Henri Bénard
(1874-1939)

Perturbation analysis

Tij, Garzó, and A.S., Phys. Rev. E **56**, 6729 (1997)

$$\underbrace{\gamma \equiv \left(\frac{2m\kappa_{\mathrm{NS}}}{5nk_B^2 T}\right)^2 g\,\frac{\partial \ln T}{\partial z}}_{\text{akin to the Rayleigh number}}, \qquad \mathrm{Ra} \sim |\gamma| \left(\frac{L_s}{\delta}\right)^4$$

$$|\gamma| \ll 1, \qquad M_{r\ell} = \underbrace{\boxed{M_{r\ell}^{(0)}}}_{\text{Pure Fourier flow}} + M_{r\ell}^{(1)}\gamma + M_{r\ell}^{(2)}\gamma^2 + \cdots$$

Corrections to Navier-Stokes

$$\gamma \equiv \left(\frac{2m\kappa_{\mathrm{NS}}}{5nk_B^2 T}\right)^2 g\frac{\partial \ln T}{\partial z}$$

$$\frac{\partial p}{\partial z} = -\rho g + \mathcal{O}(\gamma^3), \qquad \frac{P_{zz} - p}{p} = \frac{128}{45}\gamma^2 + \mathcal{O}(\gamma^3)$$

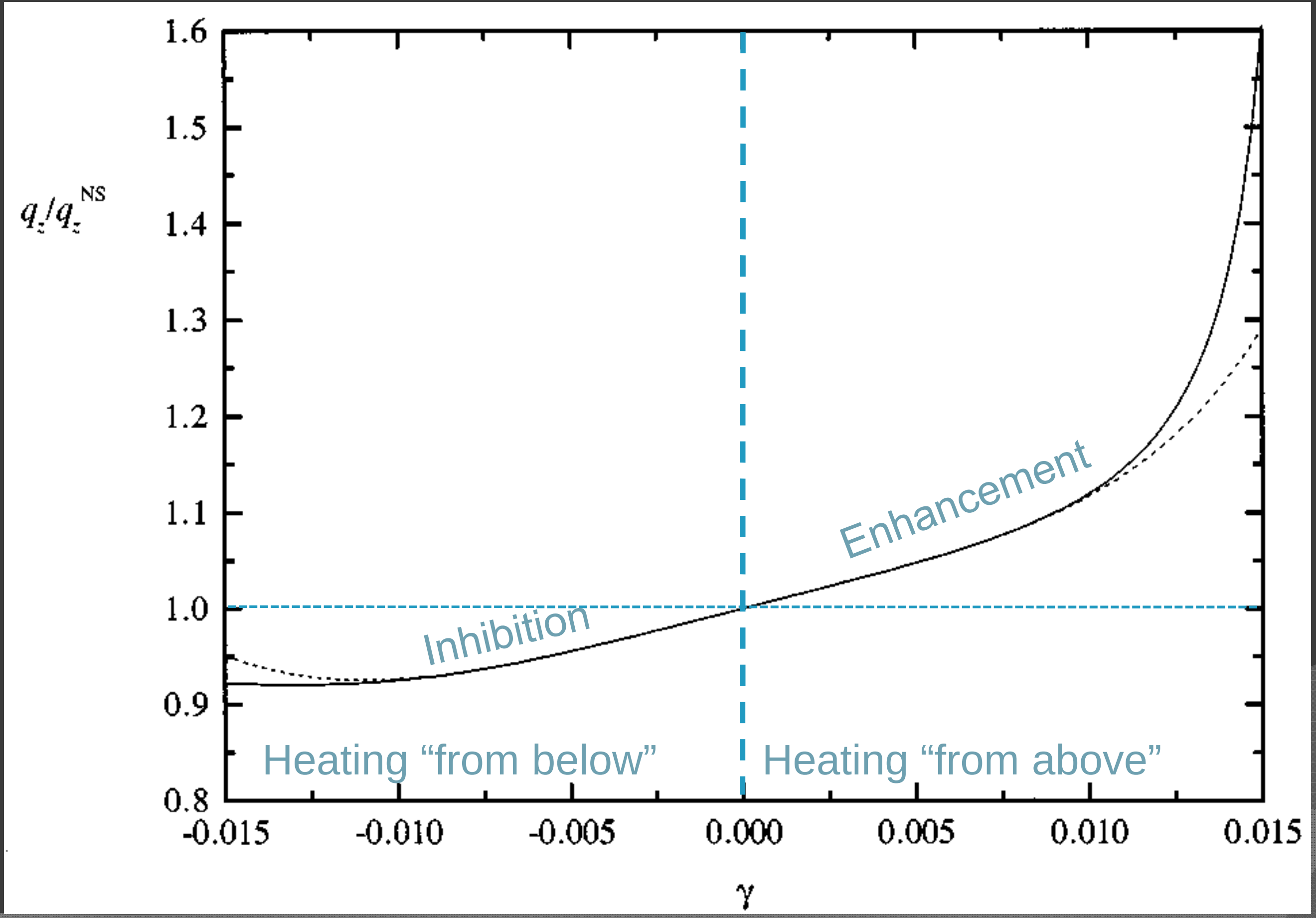
$$\frac{\partial}{\partial z} T \frac{\partial T}{\partial z} = -130\,\frac{n^2 k_B^2 T^5}{m\kappa_{\mathrm{NS}}^2}\gamma^2 + \mathcal{O}(\gamma^3)$$

$$q_z = q_z^{\mathrm{NS}}\left[1 + \frac{46}{5}\gamma + \mathcal{O}(\gamma^2)\right]$$

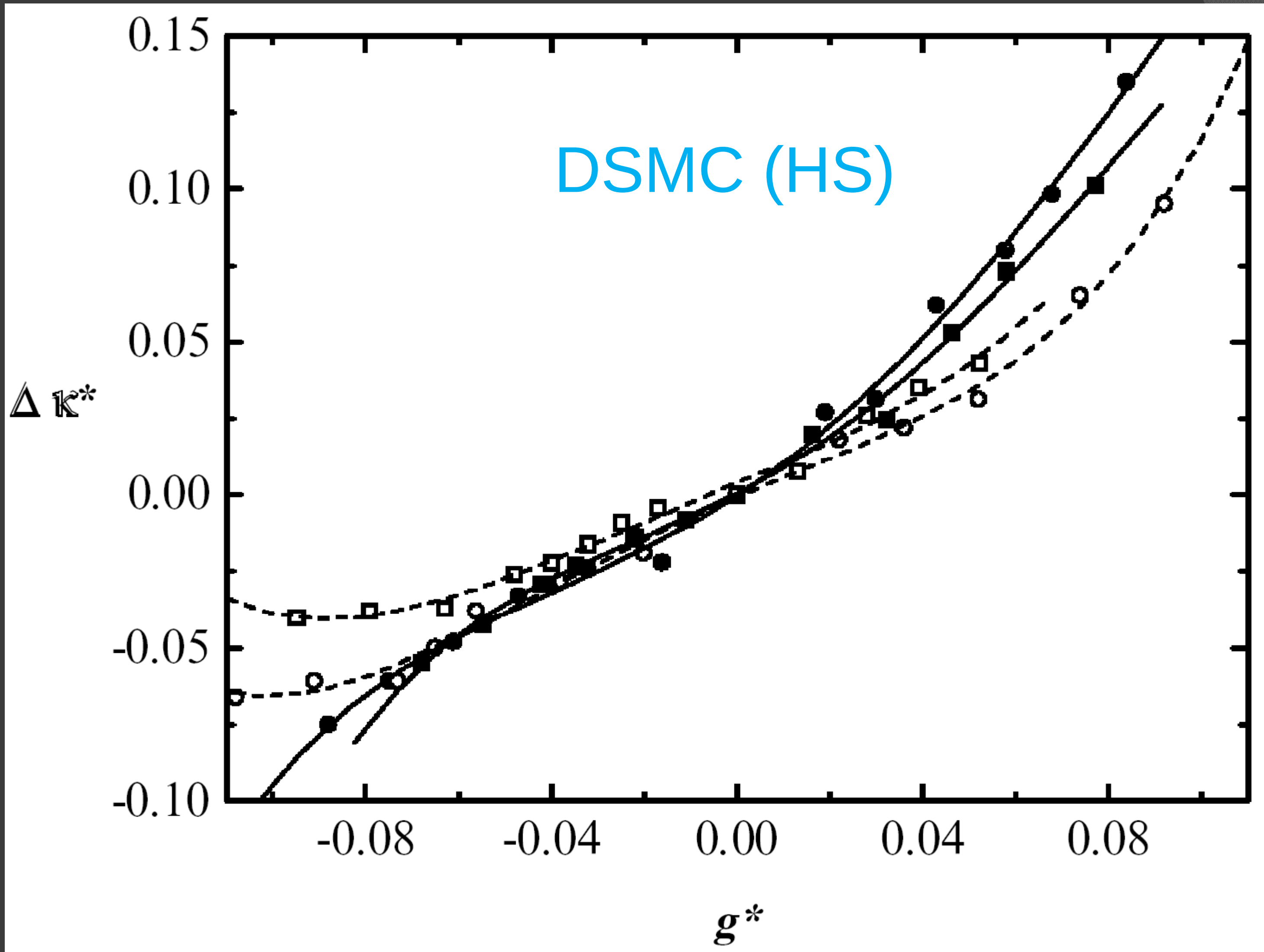
$$\frac{\langle v_z^3\rangle}{\langle v^2 v_z\rangle} = \frac{3}{5}\left[1 + \frac{64}{105}\gamma + \mathcal{O}(\gamma^2)\right]$$

Corrections to Navier-Stokes

$$\gamma \equiv \left(\frac{2m\kappa_{\mathrm{NS}}}{5nk_B^2 T}\right)^2 g\frac{\partial \ln T}{\partial z}$$



Tahiri, Tij, and A.S., Mol. Phys. **98**, 239 (2000)

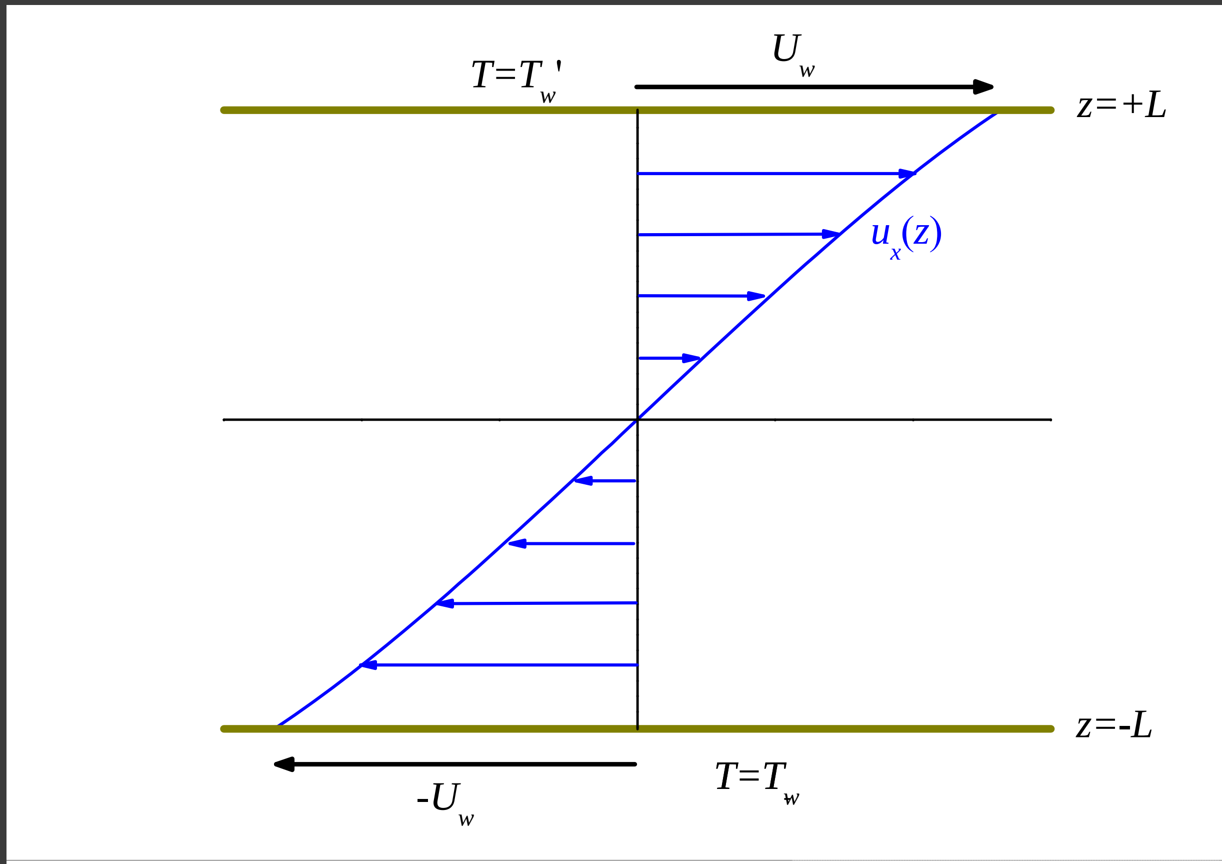


BGK description

- Same qualitative results.
- Moments up to order γ^6.
- Divergence of the expansion in powers of γ.

3. Steady planar Couette flow

Maurice Couette
(1858-1943)



Makashev and Nosik (1981) proved that an exact solution of the (nonlinear) Boltzmann equation for Maxwell molecules exists with

$$p = nk_B T = \text{const}$$

$$\boxed{a = \frac{\eta_{\text{NS}}}{p}\frac{\partial u_x}{\partial z}} = \text{const} \qquad \text{(2nd Knudsen number)}$$

$$\frac{\partial}{\partial z} T \frac{\partial T}{\partial z} = -\frac{15 n^2 (k_B T)^3}{4 m \kappa_{\text{NS}}^2} a^2 \boxed{\theta(a)} = \text{const}$$

NS: $\theta(a)=1$

Dimensionless quantities

Knudsen numbers:

$$\boxed{\epsilon = \frac{4\kappa_{\rm NS}}{5nk_B\sqrt{2k_BT/m}}\frac{\partial \ln T}{\partial z}} \quad \text{(local)}, \qquad \boxed{a = \frac{\eta_{\rm NS}}{p}\frac{\partial u_x}{\partial z}} \quad \text{(global)}$$

Reduced distribution function:

$$\phi(\mathbf{c};\epsilon,a) = \frac{1}{n(z)}\left[\frac{2k_BT(z)}{m}\right]^{3/2} f(z,\mathbf{v}) \qquad \text{“Normal” solution (Bulk)}$$

Reduced moments:

$$M_{r\ell h}(\epsilon,a) = \int d\mathbf{c}\, c^{2r} c_z^{\ell-h} c_x^h \phi(\mathbf{c};\epsilon,a)$$

Hierarchy of moment equations

$$\left[\frac{\epsilon}{2}\left(2r+\ell-1-\epsilon\frac{\partial}{\partial\epsilon}\right)-\frac{6}{5}a^2\theta(a)\frac{\partial}{\partial\epsilon}\right]M_{r,\ell+1,h}+\frac{3}{2}a\left(2rM_{r-1,\ell+2,h+1}+hM_{r,\ell,h-1}\right)$$

$$=\frac{n}{\lambda_{11}}\int d\mathbf{c}\, c^{2r}c_z^{\ell-h}c_x^h J[\mathbf{c}|\phi(\epsilon,a),\phi(\epsilon,a)]\equiv J_{r\ell h}(\epsilon,a)$$

The hierarchy admits a solution whereby the moments $M_{r\ell h}(\epsilon,a)$ are *polynomials* in ϵ of degree $2r+\ell-2$ and parity ℓ:

$$M_{r\ell h}(\epsilon,a)=\sum_{j=0}^{2r+\ell-2}\mu_j^{(r\ell h)}(a)\epsilon^j,\quad \mu_j^{(r\ell h)}(a)=0 \text{ if } j+\ell=\text{odd}$$

Corrections to Navier-Stokes

$$a = \frac{\eta_{\mathrm{NS}}}{p} \frac{\partial u_x}{\partial z}$$

$$q_z = -\kappa_{\mathrm{NS}} \kappa^*(a) \frac{\partial T}{\partial z}, \quad P_{xz} = -\eta_{\mathrm{NS}} \eta^*(a) \frac{\partial u_x}{\partial z}, \quad \eta^*(a) = \theta(a) \kappa^*(a)$$

$$q_x = \kappa_{\mathrm{NS}} \Phi(a) \frac{\partial T}{\partial z}$$

$$\frac{P_{xx} - P_{zz}}{p} = \Delta_1(a), \quad \frac{P_{yy} - P_{zz}}{p} = \Delta_2(a)$$

NS: $\kappa^* = \eta^* = \theta = 1, \quad \Phi = \Delta_1 = \Delta_2 = 0$

Perturbation analysis

Tij and A.S., Phys. Fluids **7**, 2857 (1995)

$$\kappa^*(a) = 1 - \left(\frac{1091}{150} - \frac{6\lambda_{04}}{1225}\right) a^2 + \mathcal{O}(a^4)$$

$$\eta^*(a) = 1 - \frac{149}{45} a^2 + \mathcal{O}(a^4)$$

$$\theta(a) = 1 + \left(\frac{1783}{450} - \frac{6\lambda_{04}}{1225}\right) a^2 + \mathcal{O}(a^4)$$

super-Burnett

$$\Phi(a) = \frac{7}{2} a + \mathcal{O}(a^3)$$

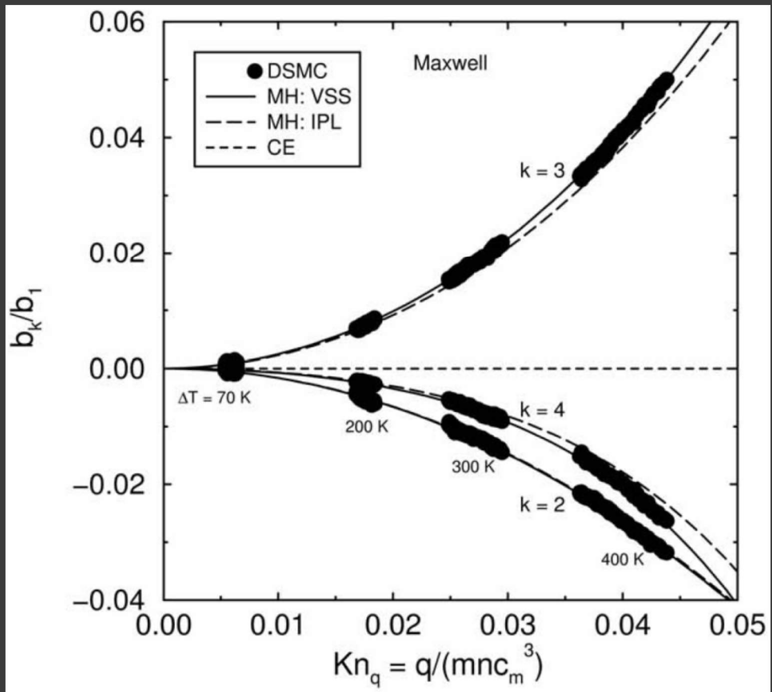
$$\Delta_1(a) = \frac{14}{5} a^2 + \mathcal{O}(a^4), \quad \Delta_2(a) = \frac{4}{5} a^2 + \mathcal{O}(a^4)$$

Burnett

Benchmark for DSMC simulations

$$\frac{b_k(\epsilon)}{b_1(\epsilon)} \equiv \lim_{a\to 0} \frac{15\sqrt{\pi}}{8} \sum_{r=1}^{k} \frac{(-1)^{r-1}(k-1)!}{(r-1)!(k-r)!(r+3/2)!} \frac{M_{r-1,2,1}(\epsilon,a)}{M_{021}(\epsilon,a)}$$

$$= \text{Polynomial of degree } 2k-2$$

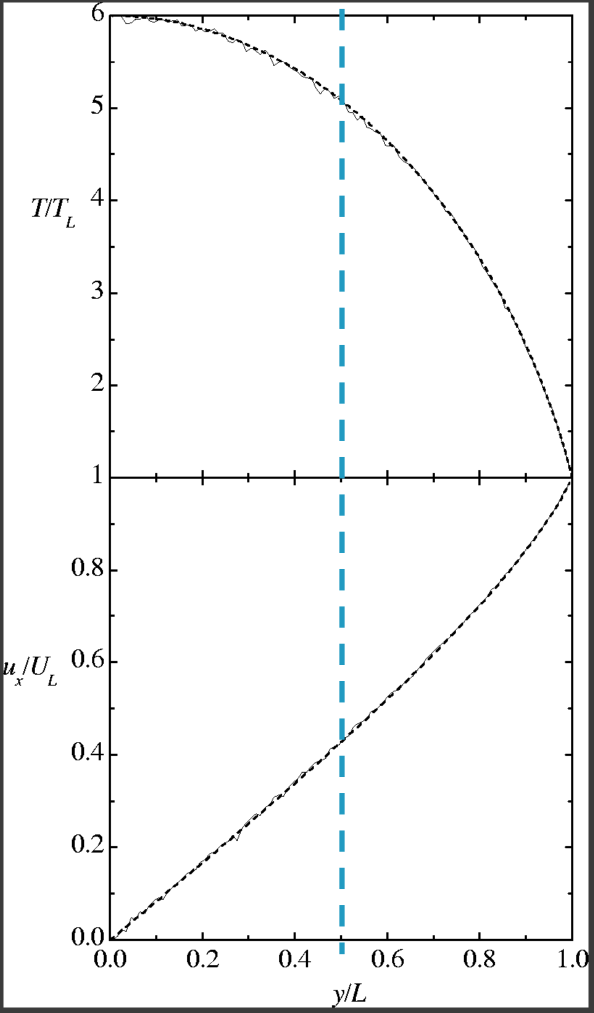


Gallis et al., Phys. Fluids **18**, 017104 (2006)

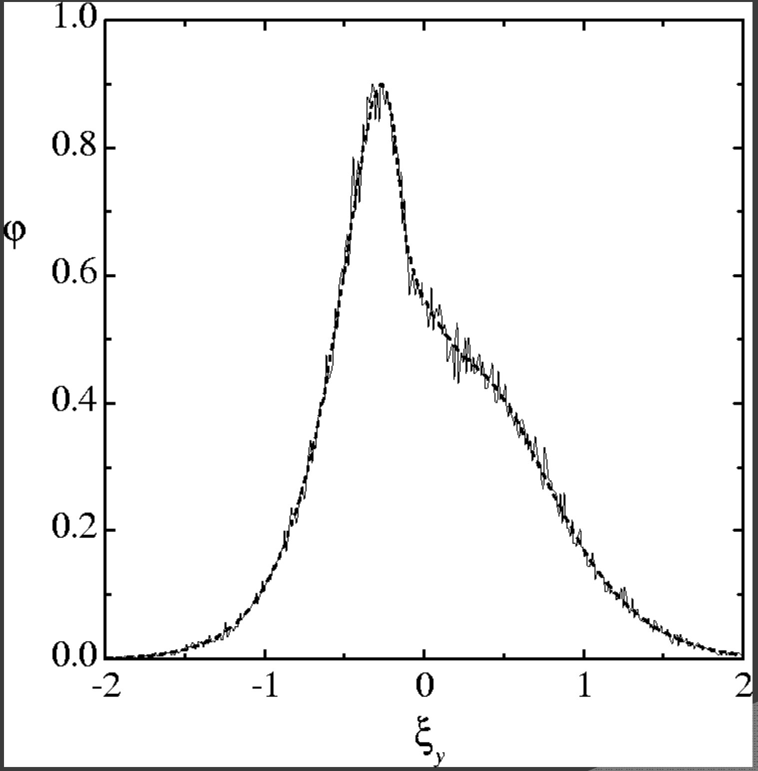
BGK description (arbitrary potentials)

- Same qualitative results for moments.
- Explicit expressions for $\kappa^*(a)$, $\eta^*(a)$, $\theta(a)$, $\Phi(a)$, $\Delta_1(a)$, and $\Delta_2(a)$.
- Full velocity distribution function $\phi(\mathbf{c};\epsilon,a)$.
- Divergence of the expansion in powers of a.
- Influence of gravity analyzed.

Montanero, A.S., and Garzó, Phys. Fluids **11**, 3060 (2000)



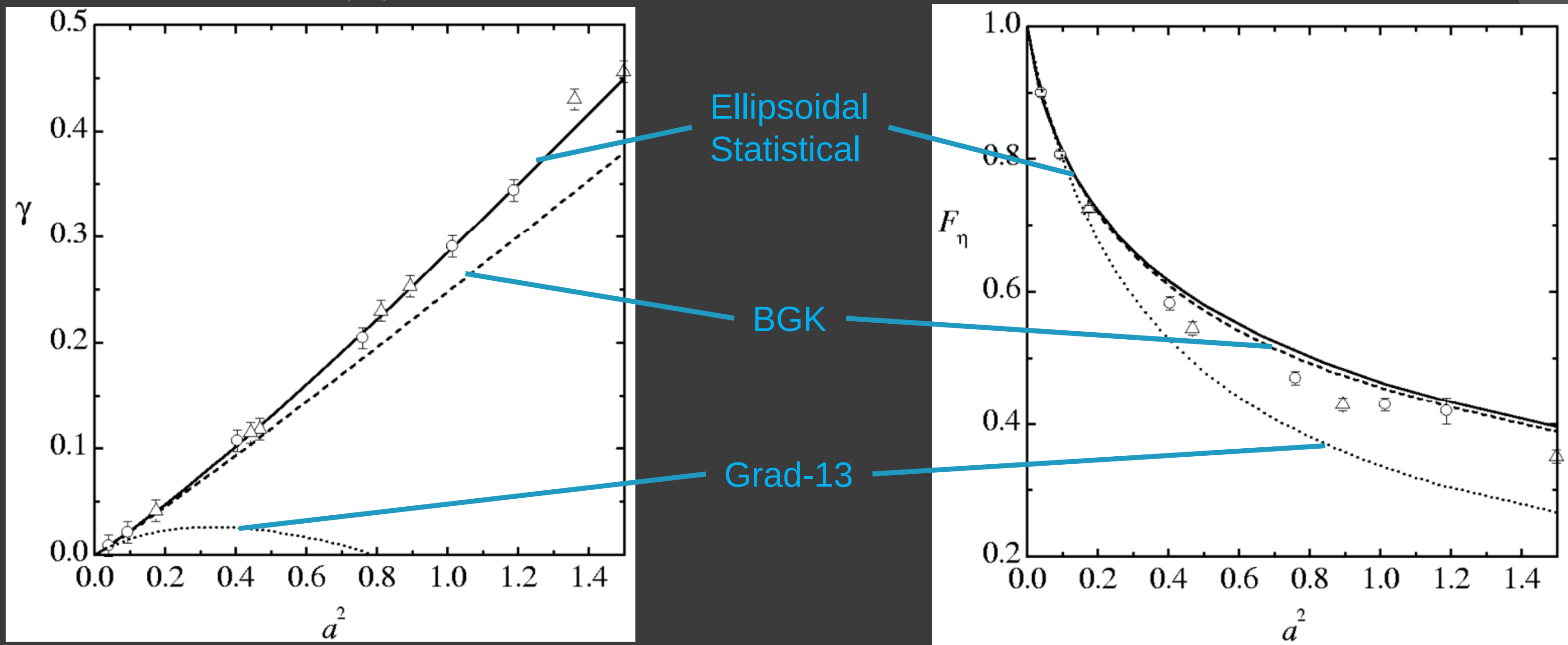
Test of DSMC:
DSMC (BGK) vs exact solution (BGK)



$\text{HS} : a = 1, \epsilon = -0.60$

Montanero, A.S., and Garzó, Phys. Fluids **11**, 3060 (2000)

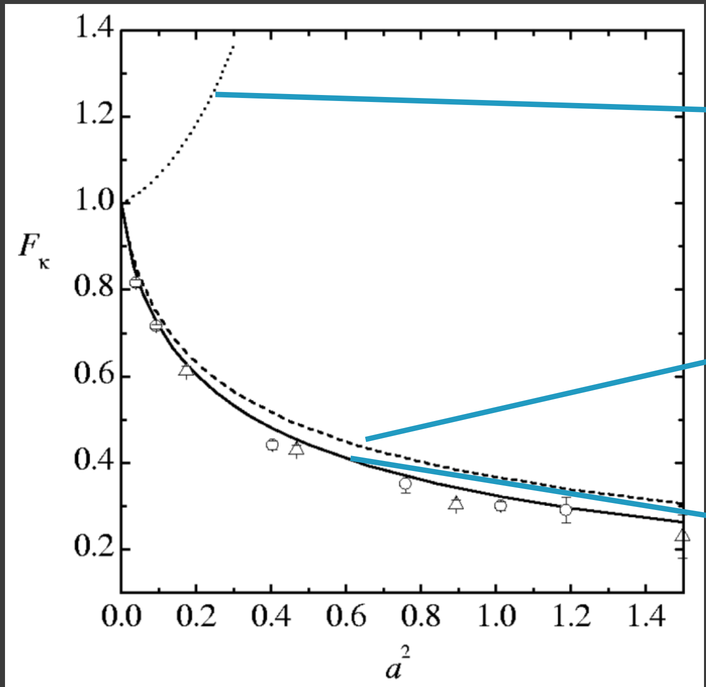
$a^2\theta(a)$ $\eta^*(a)$



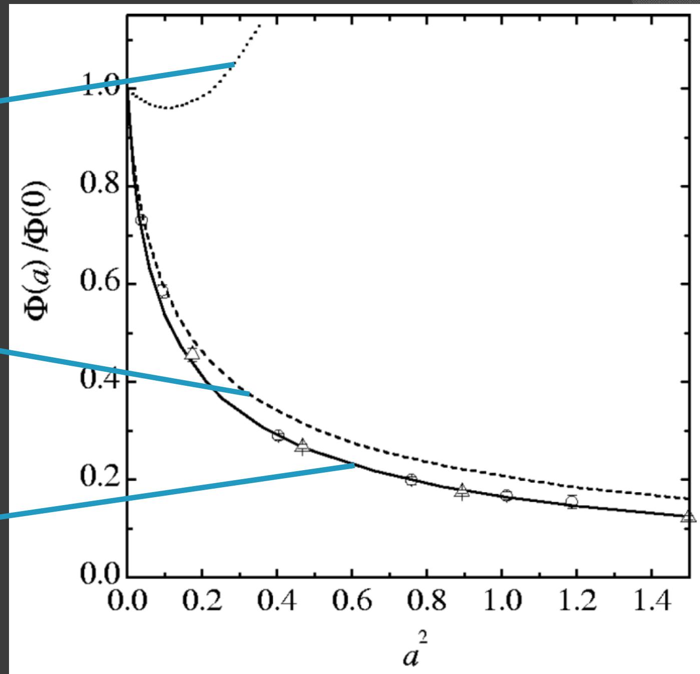
$$\text{DSMC}\begin{cases}\circ:\ \text{Maxwell}\\ \triangle:\ \text{HS}\end{cases}$$

Montanero, A.S., and Garzó, Phys. Fluids **11**, 3060 (2000)

$\kappa^*(a)$



$\Phi(a)/a$



Grad-13

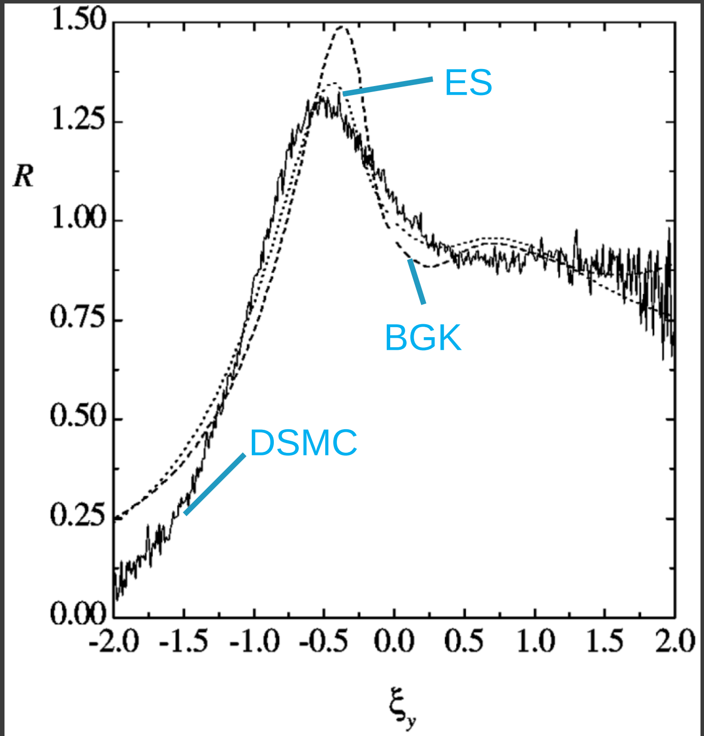
BGK

Ellipsoidal Statistical

$$\text{DSMC}\begin{cases}\circ\text{: Maxwell}\\ \triangle\text{: HS}\end{cases}$$

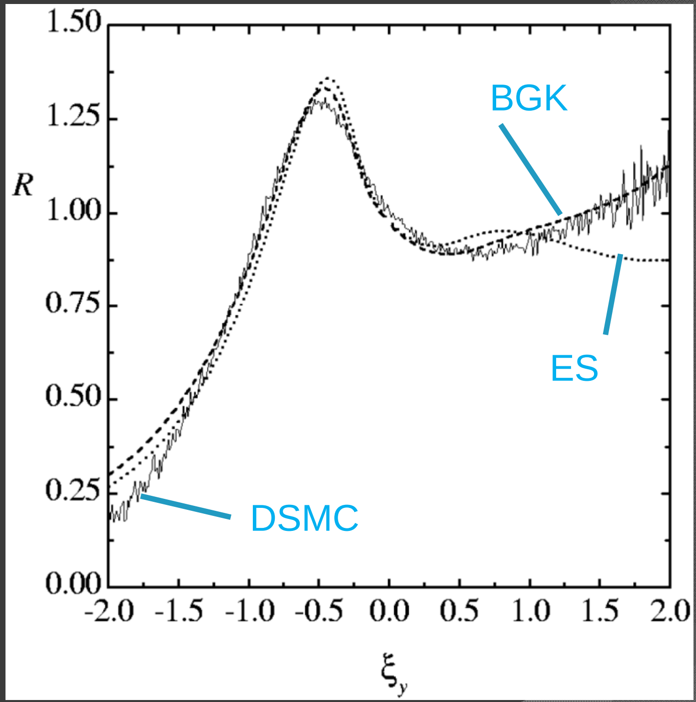
Montanero, A.S., and Garzó, Phys. Fluids **11**, 3060 (2000)

$\phi(c_z)/\phi_{\mathrm{LE}}(c_z)$



$\text{Maxwell}: a = 0.636, \epsilon = -0.272$

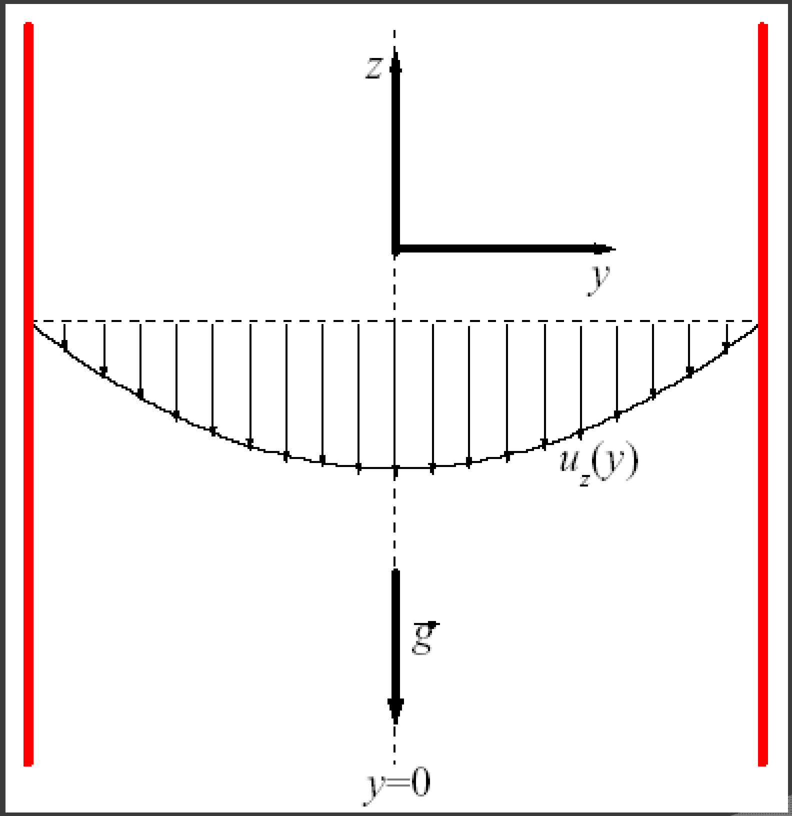
$\phi(c_z)/\phi_{\mathrm{LE}}(c_z)$



$\text{HS}: a = 0.419, \epsilon = -0.195$

4. Force-driven Poiseuille flow

Jean-Louis-Marie Poiseuille
(1797-1869)



NAVIER-STOKES (NEWTONIAN) DESCRIPTION

$$P_{xx} = P_{yy} = P_{zz} = p$$ Equal normal stresses

$$P_{yz} = -\eta \frac{\partial u_z}{\partial y}$$ Newton's law

$$q_y = -\kappa \frac{\partial T}{\partial y}$$ Fourier's law

$$q_z = 0$$ No longitudinal heat flux

$$p(y) = p_0 = \text{const}$$

$$u_z(y) = u_0 + \frac{\rho_0 g}{2\eta_0} y^2 + \mathcal{O}(g^3)$$

$$T(y) = T_0 - \frac{\rho_0^2 g^2}{12\eta_0 \kappa_0} y^4 + \mathcal{O}(g^4)$$

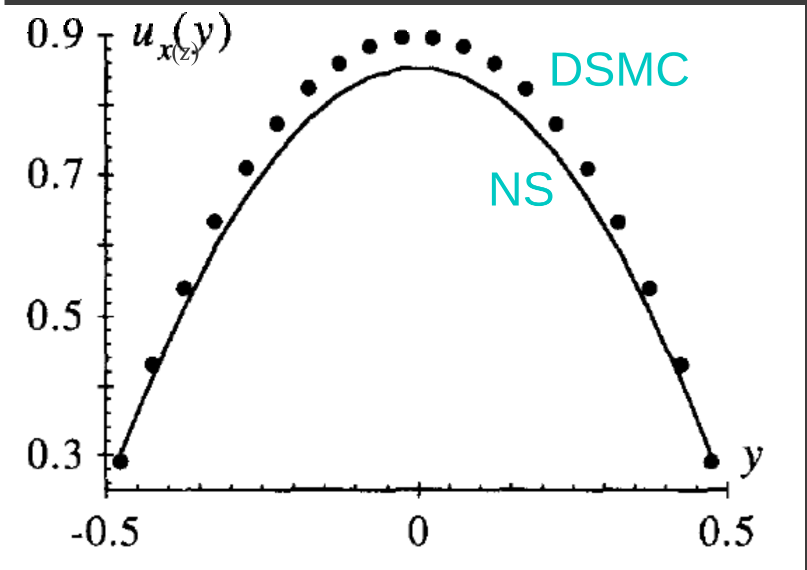
Temperature is *maximal* at the central layer (y=0)

Do NS predictions agree with computer simulations?

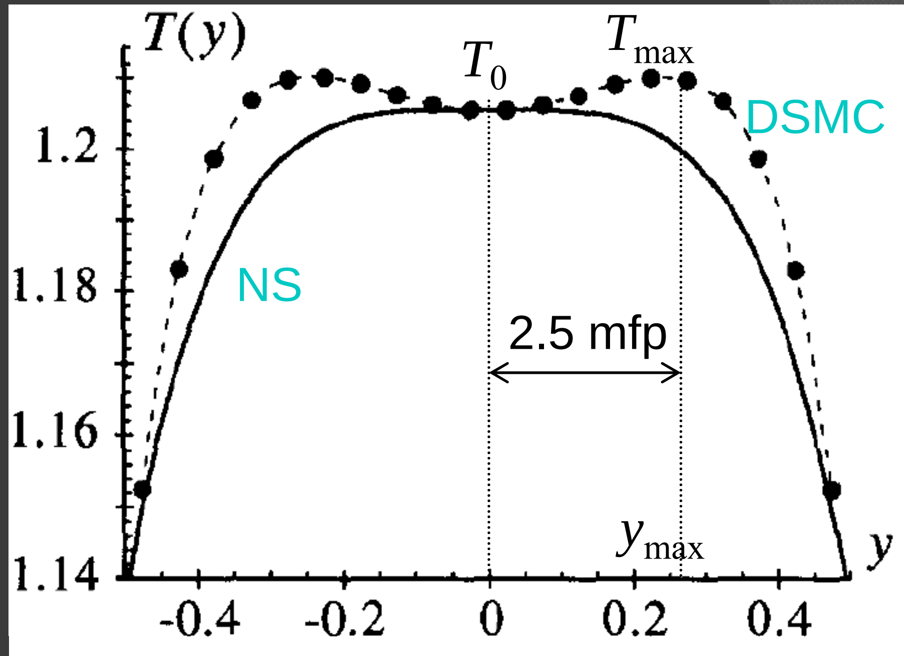
On the validity of hydrodynamics in plane Poiseuille flows

M. Malek Mansour[a,*], F. Baras[a], Alejandro L. Garcia[b,1]

Physica A 240 (1997) 255–267



but ...



A Burnett-order effect?

PHYSICAL REVIEW E VOLUME 60, NUMBER 4 OCTOBER 1999

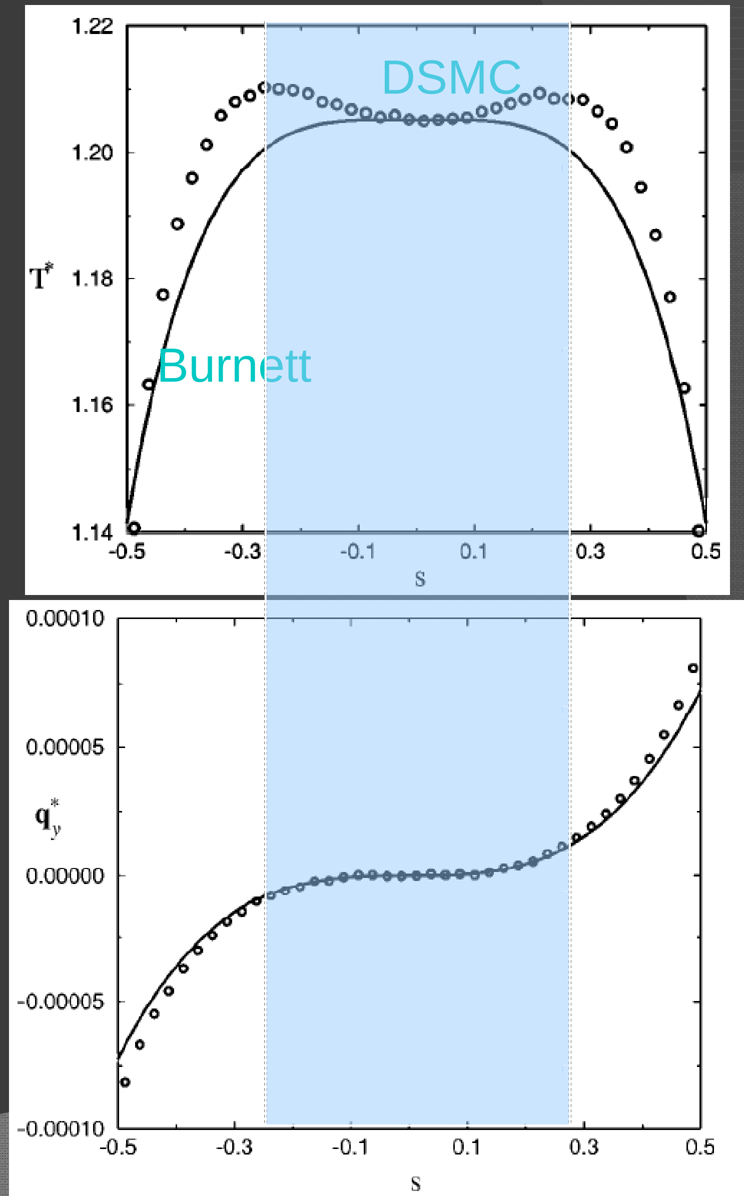
Burnett description for plane Poiseuille flow

F. J. Uribe Alejandro L. Garcia*

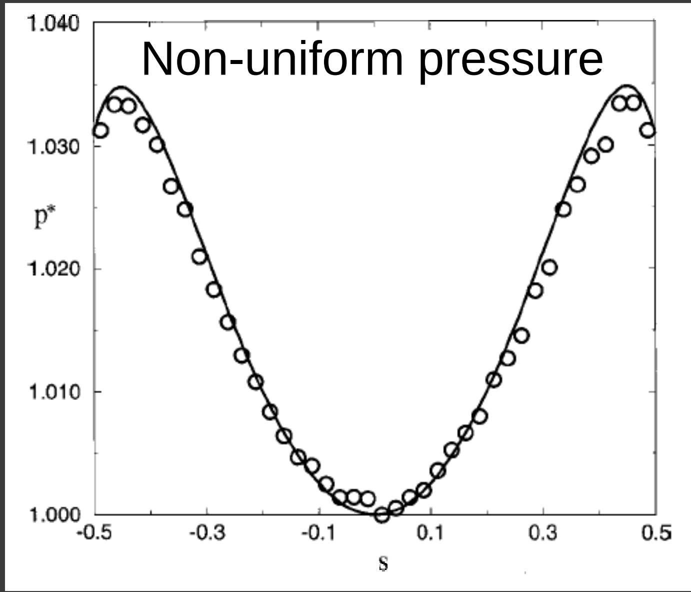
In the slab $y<|y_{\max}|$,

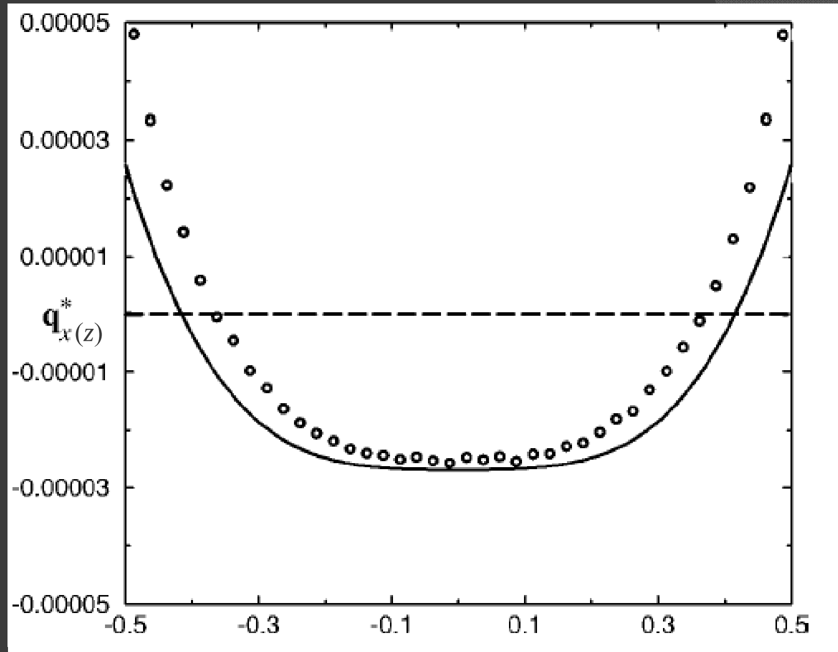
$$\boxed{\mathrm{sgn}\, q_y = \mathrm{sgn}\, \partial T/\partial y}$$

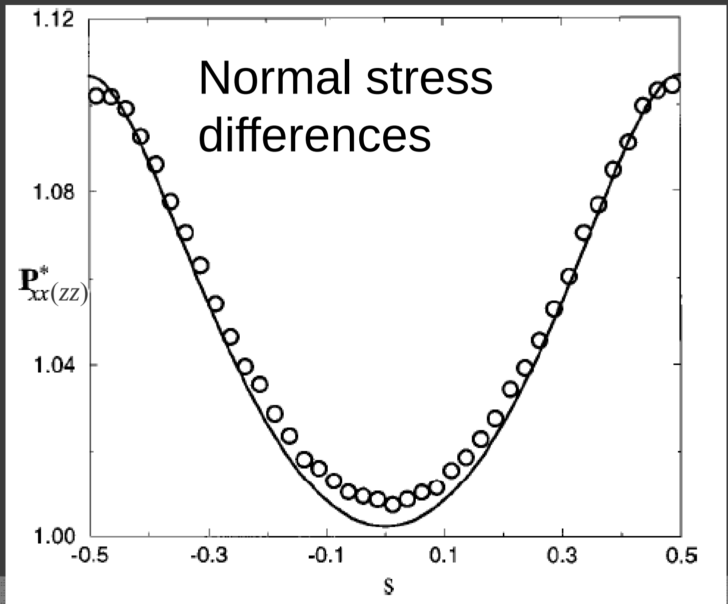
Heat flows from the colder to the hotter layers!!



Other Non-Newtonian properties







Longitudinal component of the heat flux (but no longitudinal thermal gradient!)

Hierarchy of moment equations

$$M_{k_1,k_2,k_3}(y;g) = \int d\mathbf{v}\, v_x^{k_1} v_y^{k_2} [v_z - u_z(y,g)]^{k_3} f(y,\mathbf{v};g)$$

$$\frac{\partial}{\partial y} M_{k_1,k_2+1,k_3} + k_3 \left(\frac{\partial u_z}{\partial y} M_{k_1,k_2+1,k_3-1} + g M_{k_1,k_2,k_3-1} \right) = J_{k_1,k_2,k_3}$$

Perturbation analysis

Tij, Sabanne, and A.S., Phys. Fluids **10**, 1021 (1998)

$$M_{\vec{k}}(y;g) = \underbrace{M_{\vec{k}}^{(0)}}_{\text{Equilibrium moments (at } y=0)} + \sum_{j=1}^{\infty} M_{\vec{k}}^{(j)}(y) g^j$$

$$M_{\vec{k}}^{(1)}(y) = \text{Linear function of } y$$

$$M_{\vec{k}}^{(j)}(y) = \text{Polynomial in } y \text{ of degree } 2j, \quad j \geq 2$$

Results to order g^2: Hydrodynamic fields

$$u_z(y) = u_0 + \frac{\rho_0 g}{2\eta_0} y^2 + \mathcal{O}(g^3)$$

$$p(y) = p_0 \left[1 + C_p \left(\frac{mg}{T_0} \right)^2 y^2 \right] + \mathcal{O}(g^4)$$

$$T(y) = T_0 \left[1 - \frac{\rho_0^2 g^2}{12\eta_0 \kappa_0 T_0} y^4 + C_T \left(\frac{mg}{T_0} \right)^2 y^2 \right] + \mathcal{O}(g^4)$$

Results to order g^2: Hydrodynamic fluxes

$$P_{zz}(y) = p_0 \left[1 + \frac{7}{3} C_p \left(\frac{mg}{T_0} \right)^2 y^2 + C_{zz} \frac{\rho_0 \eta_0^2 g^2}{p_0^3} \right] + \mathcal{O}(g^4)$$

$$P_{yy} = p_0 \left(1 - C_{yy} \frac{\rho_0 \eta_0^2 g^2}{p_0^3} \right) + \mathcal{O}(g^4)$$

$$P_{yz}(y) = -\rho_0 g y \left[1 + \frac{\rho_0^2 g^2}{60 \eta_0 \kappa_0 T_0} y^4 + \frac{C_p - C_T}{3} \left(\frac{mg}{T_0} \right)^2 y^2 \right] + \mathcal{O}(g^5)$$

$$q_y(y) = \frac{\rho_0^2 g^2}{3\eta_0} y^3 + \mathcal{O}(g^4), \quad q_z(y) = C_q m g \kappa_0 + \mathcal{O}(g^3)$$

Numerical values of the coefficients (gravity-driven Poiseuille flow)

Coefficient	Quantity	NS	Burnett[a]	13-moment[b]	R13-moment[c]	19-moment[d]	BGK[e]	Exact
C_p	p	0	1.2	1.2	1.2	1.2	1.2	1.2
C_T	T	0	0	0.56	0.9295	1.04	0.76	1.0153
C_{zz}	P_{zz}	0	0	0	3.413	?	13.12	6.4777
C_{yy}	P_{yy}	0	0	0	3.36	?	12.24	6.2602
C_q	q_z	0	0.4	0.4	0.4	0.4	0.4	0.4

[a] Uribe & Garcia (1999)
[b] Risso & Cordero (1998)
[c] Taheri, Struchtrup & Torrilhon (2008)
[d] Hess & Malek Mansour (1999)
[e] Tij & A.S. (1994)

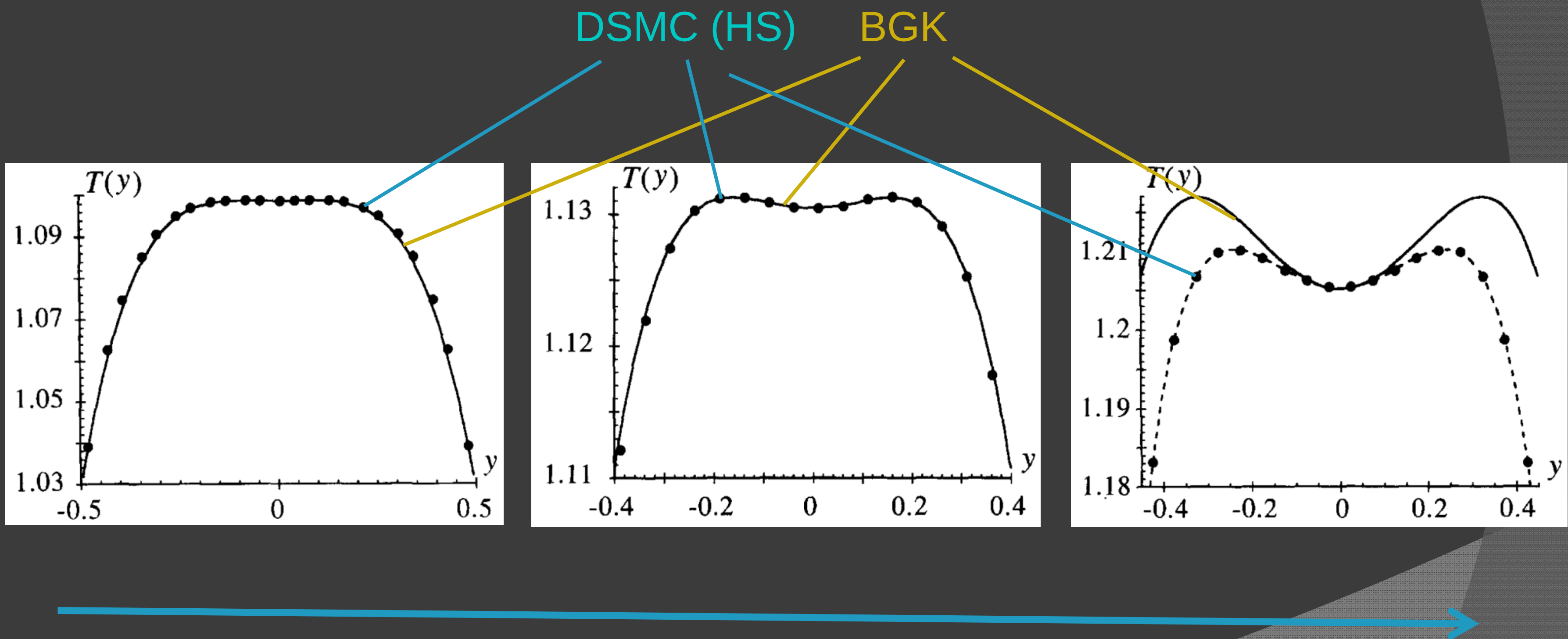
BGK description

- Same qualitative results.
- Hydrodynamic fields up to order g^5.
- Velocity distribution function up to order g^3.
- Divergence of the expansion in powers of g.
- Exact non-perturbative solution for a special value of g.

On the validity of hydrodynamics in plane Poiseuille flows

M. Malek Mansour[a,*], F. Baras[a], Alejandro L. Garcia[b,1]

Physica A 240 (1997) 255–267



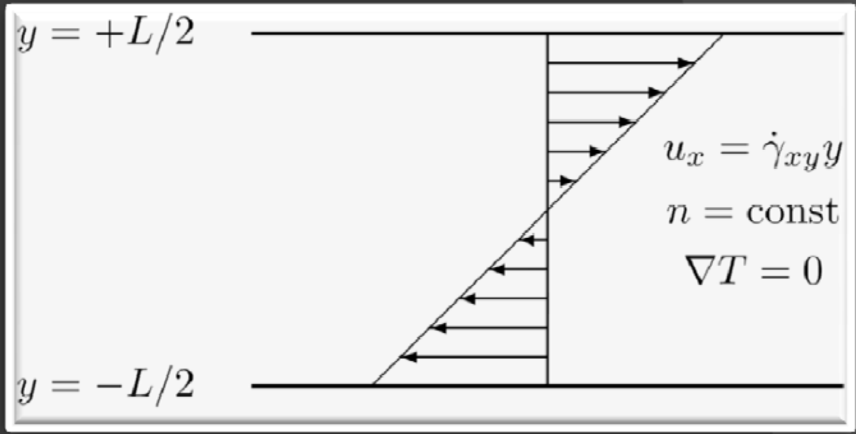
Increasing g

5. Other (quasi-uniform) states

Uniform Shear Flow

$$n(t) = n(0)$$

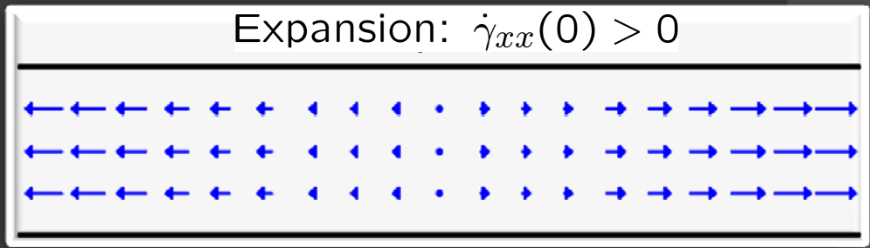
$$\dot{\gamma}_{xy}(t) = \dot{\gamma}_{xy}(0)$$

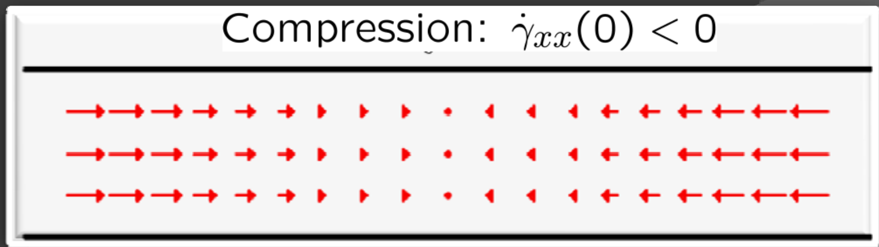


Uniform Longitudinal Flow

$$n(t) = \frac{n(0)}{1 + \dot{\gamma}_{xx}(0)t}$$

$$\dot{\gamma}_{xx}(t) = \frac{\dot{\gamma}_{xx}(0)}{1 + \dot{\gamma}_{xx}(0)t}$$





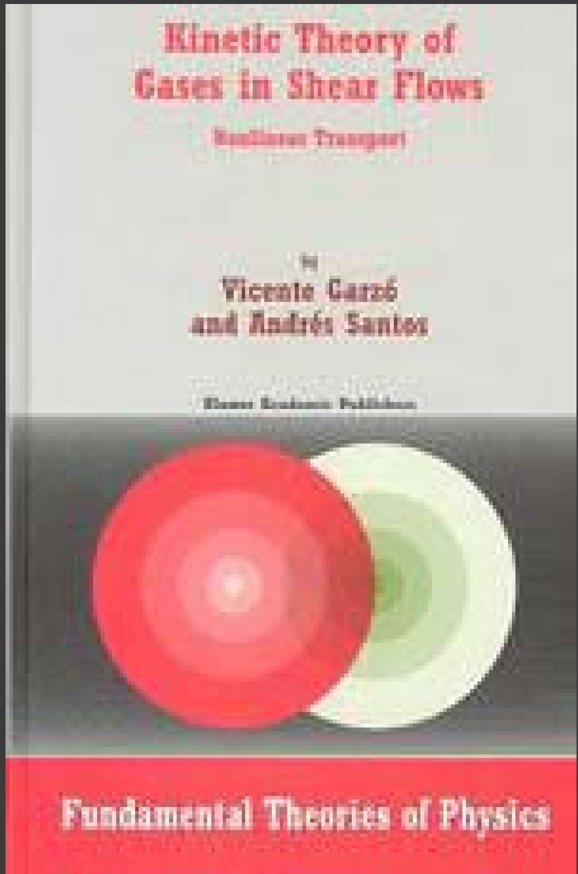
In both cases,

- Exact rheological functions for *arbitrary* values (*non-perturbative* solution) of the corresponding Knudsen number.
- Divergence of the fourth-degree moments beyond a *critical* shear rate.
- Algebraic high-velocity decay of the velocity distribution function: Finite number of convergent moments.

Conclusions

- Dialogue between DSMC and theoretical results for non-Newtonian hydrodynamics benefits both sides:
- Assessment of the validity of the theoretical approach, usually derived under simplifying assumptions (bulk, Maxwell particles, kinetic models, …).
- Benchmarks to test the accuracy of DSMC under stringent conditions.

More details about shear flows (including mixtures, BGK model description, …)



(Kluwer/Springer, 2003)

Acknowlegments (in alphabetical order):

- J. Javier Brey, Universidad de Sevilla, Spain
- James. W. Dufty, University of Florida, USA
- Vicente Garzó, Universidad de Extremadura, Spain
- José María Montanero, Universidad de Extremadura, Spain
- Mohamed Tij, Université Moulay Ismaïl, Morocco

THANKS FOR YOUR ATTENTION!