The lattice Boltzmann equation: background and boundary conditions

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Lattice Boltzmann perspectives

The first LBE review article tells us that [Succi, Benzi, Higuera 1991]

> *“The LBE...does not result from the discretisation of any partial differential equation!"*

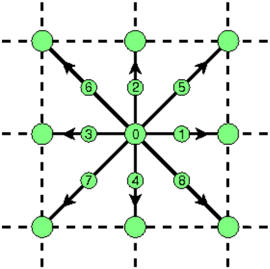
The “second generation" of LB is derived from “purely microscopic considerations" and approximates the continuous Boltzmann equation [Chen and Doolen 1998 (which has about 2500 citations!)]

This may suggest that the LBE can go “beyond" Navier-Stokes, *e.g* capture the Knudsen layer in the transition regime - a view also held in the most recent review article [Aidun and Clausen 2010]

The standard (D2Q9) lattice Boltzmann equation

This equation:

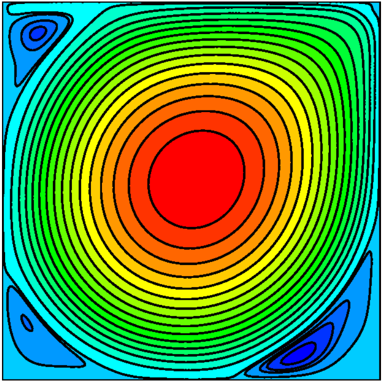
$$\bar{f}_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t)-\bar{f}_i(\mathbf{x}, t) = \Omega(\mathbf{x}, t)$$



is used to solve these equations:

$$\begin{aligned} \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) &= -\nabla P + \mu\nabla^2\mathbf{u} \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned}$$

Lid-driven cavity flow: Re=7500



Roll-up of shear waves

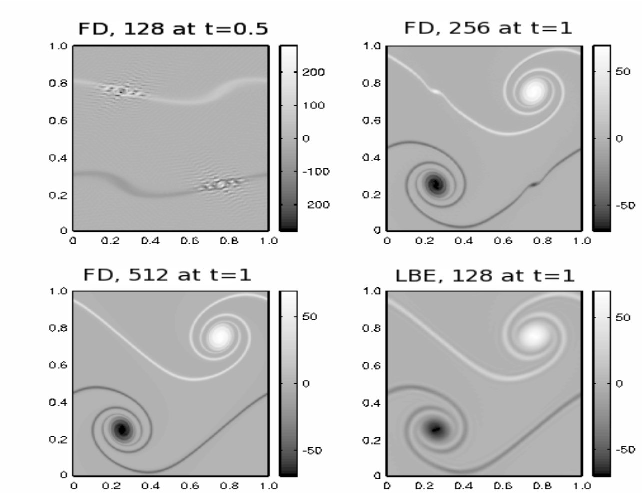
Roll-up of shear layers in Minion & Brown [1997] test problem,

$$u_x = \begin{cases} \tanh(\kappa(y - 1/4)), & y \le 1/2, \\ \tanh(\kappa(3/4 - y)), & y > 1/2, \end{cases}$$

$$u_y = \delta \sin(2\pi(x + 1/4)).$$

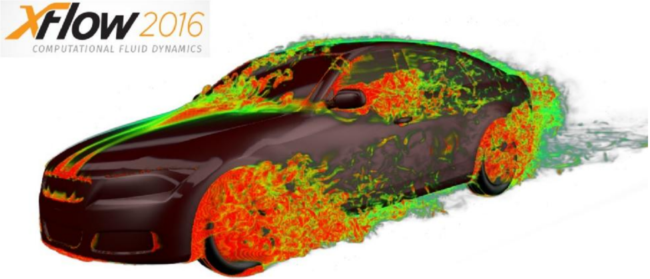
Roll-up of Shear wave with LBE

Re $= 30,000$, $\kappa = 80$ and $\delta = 0.05$



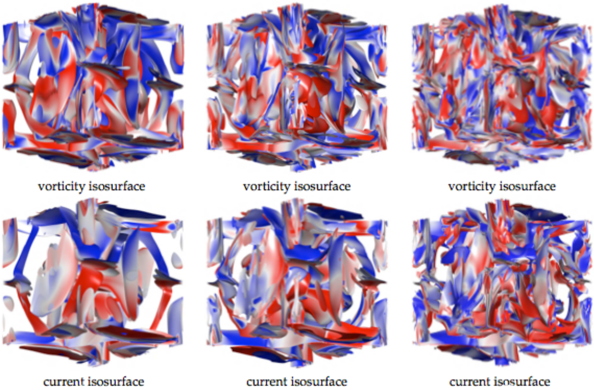
On GPU: 600 MLUPS

Used in the automotive industry



Courtesy of Xflow [www.xflowcfd.com]

LBE for MHD Turbulence

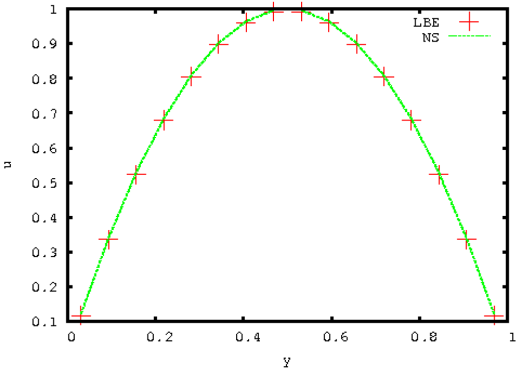


1800^3 grid points,Superlinear scaling, 9.1 TFlops/s

Vahala *et al*, Commun. Comput. Phys, 4 (2008), 624-646

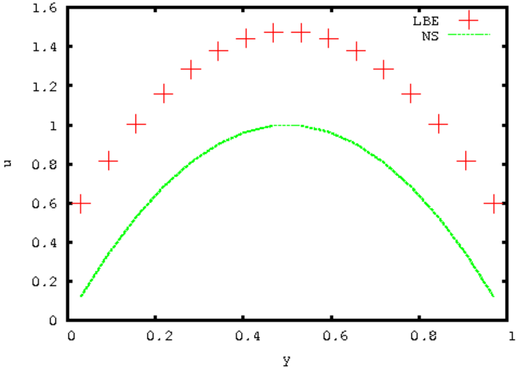
Velocity profile: Poiseuille flow, $Re = 100$

Using bounce–back boundary conditions, we appear to get an accurate solution at moderate Re numbers . . .



Velocity profile: Poiseuille flow

...but not at smaller Reynolds numbers



- This is not Knudsen slip He *et al.* [1997]
- We should be able to get the *exact* solution
- More sophisticated boundary conditions can be used ...

Overview

Derivation of the lattice Boltzmann equation

- From kinetic theory to hydrodynamics
- Matching moments: from continuous to discrete kinetic theory
- From discrete Boltzmann to lattice Boltzmann (PDEs to numerics)

Exact solutions of the D2Q9 LBE

- Boundary conditions
- Velocity field
- Deviatoric stress
- Implications for numerical stability

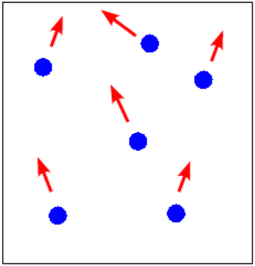
Summary

The kinetic theory of gases

The Navier-Stokes equations for a Newtonian fluid can be derived from Boltzmann's equation for a monotomic gas

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega(f)$$

where $f = f(\mathbf{x}, \mathbf{c}, t)$ is the distribution function of particles at $\mathbf{x}$ and t with velocity $\mathbf{c}$:



$\Omega(f)$ is Boltzmann's binary collision operator.

Hydrodynamics from moments

Hydrodynamic quantities are moments of the distribution function f:

$$\begin{aligned}
\rho(\mathbf{x}, t) &= \int f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \\
\mathbf{u}(\mathbf{x}, t) &= \frac{1}{\rho} \int \mathbf{c} f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}, \\
\theta(\mathbf{x}, t) &= \frac{1}{3\rho} \int |\mathbf{c} - \mathbf{u}|^2 f(\mathbf{x}, \mathbf{c}, t) d\mathbf{c}.
\end{aligned}$$

The collision operator $\Omega(f)$ drives f back to the Maxwell-Boltzmann distribution

$$f^{(0)} = \frac{\rho}{(2\theta\pi)^{3/2}} \exp\left(-\frac{|\mathbf{c} - \mathbf{u}|^2}{2\theta}\right).$$

From kinetic theory to fluid dynamics

Recall Boltzmann's equation

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = \Omega(f)$$

Assume f relaxes towards $f^{(0)}$ with a single relaxation time τ:

$$\frac{\partial f}{\partial t} + \mathbf{c} \cdot \nabla f = -\frac{1}{\tau} \left(f - f^{(0)} \right)$$

The zeroth and first moments of the Boltzmann equation give exact conservation laws:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{\Pi} = 0$$

Evolution of the momentum flux

The momentum flux $\mathbf{\Pi}$ is given by another moment

$$\mathbf{\Pi} = \int f\mathbf{c}\mathbf{c}d\mathbf{c}, \quad \text{and} \quad \mathbf{\Pi}^{(0)} = \int f^{(0)}\mathbf{c}\mathbf{c}d\mathbf{c}.$$

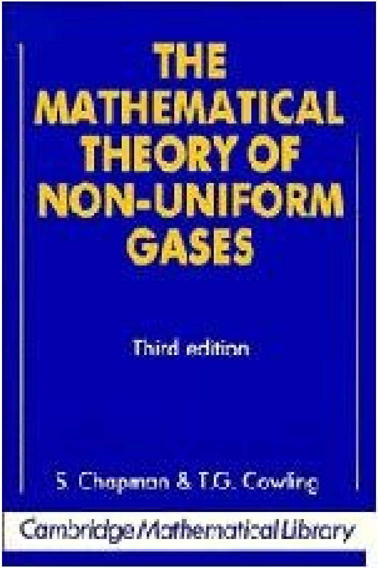
$\mathbf{\Pi}$ is *not* conserved by collisions. It evolves according to

$$\frac{\partial \mathbf{\Pi}}{\partial t} + \nabla \cdot \boldsymbol{Q} = -\frac{1}{\tau}\left(\mathbf{\Pi} - \mathbf{\Pi}^{(0)}\right),$$

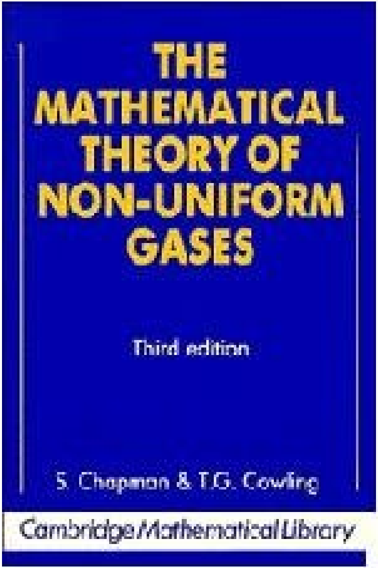
where

$$\mathbf{\Pi}^{(0)} = \rho\mathbf{u}\mathbf{u} + \rho\theta\mathbf{I}, \quad \text{and} \quad \boldsymbol{Q} = \int f\mathbf{c}\mathbf{c}\mathbf{c}d\mathbf{c}.$$

Hydrodynamics follow by exploiting $\tau \ll T$.



S. Chapman and T.G Cowling (1970)

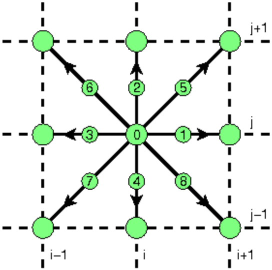


"Reading this book is like chewing glass [S. Chapman]"

Discrete kinetic theory

Look to simplify Boltzmann's equation without losing the properties needed to recover the Navier-Stokes equation.

Discetise the velocity space such that $\mathbf{c}$ is confined to a set $\mathbf{c}_0, \mathbf{c}_1, \ldots, \mathbf{c}_9$:



Instead of $f(\mathbf{x}, \mathbf{c}, t)$ we have $f_i(\mathbf{x}, t)$.

The discrete Boltzmann equation

The Boltzmann equation with discrete velocities is

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right)$$

We now supply the equilibrium function, for example

$$f_i^{(0)} = W_i \rho \left(1 + \frac{1}{\theta}\mathbf{u}\cdot\mathbf{c}_i + \frac{1}{2\theta^2}(\mathbf{u}\cdot\mathbf{c}_i)^2 - \frac{1}{2\theta}|\mathbf{u}|^2\right)$$

The previous integrals are now replaced by summations:

$$\begin{aligned}
\rho &= \sum_i f_i = \sum_i f_i^{(0)}, \\
\rho\mathbf{u} &= \sum_i f_i \mathbf{c}_i = \sum_i f_i^{(0)} \mathbf{c}_i \\
\mathbf{\Pi}^{(0)} &= \sum_i f_i^{(0)} \mathbf{c}_i \mathbf{c}_i = \rho\mathbf{u}\mathbf{u} + \theta\rho\mathbf{I}.
\end{aligned}$$

Moment equations

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right)$$

Taking the zeroth, first, and second moments of the discrete Boltzmann equation give

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &+ \nabla \cdot (\rho \mathbf{u}) = 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} &+ \nabla \cdot \mathbf{\Pi} = 0, \\
\frac{\partial \mathbf{\Pi}}{\partial t} &+ \nabla \cdot \boldsymbol{Q} = -\frac{1}{\tau}\left(\mathbf{\Pi} - \mathbf{\Pi}^{(0)}\right)
\end{aligned}$$

Note that we did exactly the same for the continuum Boltzmann equation.

Chapman-Enskog expansion

Hydrodynamics now follows from seeking solutions to

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right)$$

that vary slowly compared with the timescale τ.

We assume f_i is close to equilibrium and expand:

$$f_i = f_i^{(0)} + \tau f_i^{(1)} + \tau^2 f_i^{(2)} + \dots$$

Or, equivalently,

$$\mathbf{\Pi} = \mathbf{\Pi}^{(0)} + \tau\mathbf{\Pi}^{(1)} + \tau^2\mathbf{\Pi}^{(2)} \dots, \quad \boldsymbol{Q} = \boldsymbol{Q}^{(0)} + \tau\boldsymbol{Q}^{(1)} + \tau^2\boldsymbol{Q}^{(2)} \dots$$

Also expand the temporal derivative:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \tau\frac{\partial}{\partial t_1} \dots$$

Hydrodynamics from moments

Substituting these expansions into the moment equations and truncating at $\mathcal{O}(1)$ we obtain

$$\begin{aligned}
\frac{\partial \rho}{\partial t_0} &+ \nabla \cdot (\rho \mathbf{u}) = 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t_0} &+ \nabla \cdot \mathbf{\Pi}^{(0)} = 0, \\
\frac{\partial \mathbf{\Pi}^{(0)}}{\partial t_0} &+ \nabla \cdot \boldsymbol{Q}^{(0)} = -\mathbf{\Pi}^{(1)}
\end{aligned}$$

The first two equations coincide with the compressible Euler equations if we choose

$$\mathbf{\Pi}^{(0)} = \rho \theta \mathbf{I} + \rho \mathbf{u}\mathbf{u}$$

Calculating the viscous stress tensor

For the Navier-Stokes equation we need to compute the first correction $\mathbf{\Pi}^{(1)}$ to the momentum flux.

$$\frac{\partial \mathbf{\Pi}^{(0)}}{\partial t_0} + \nabla \cdot \boldsymbol{Q}^{(0)} = -\mathbf{\Pi}^{(1)}.$$

Given $\mathbf{\Pi}^{(0)} = \rho\theta\mathbf{I} + \rho\mathbf{u}\mathbf{u}$ we find (after a messy calculation)

$$\begin{aligned}
\partial_{t_0} \Pi^{(0)}_{\beta\gamma} &= -\theta\delta_{\beta\gamma}\partial_\alpha(\rho u_\alpha) - \theta u_\beta \partial_\gamma \rho - \theta u_\gamma \partial_\beta \rho - \partial_\alpha(\rho u_\alpha u_\beta u_\gamma), \\
\partial_\alpha Q^{(0)}_{\alpha\beta\gamma} &= \theta\delta_{\beta\gamma}\partial_\alpha(\rho u_\alpha) + \theta\partial_\beta(\rho u_\gamma) + \theta\partial_\gamma(\rho u_\beta)
\end{aligned}$$

Assembling the Navier-Stokes equations

The viscous stress is then found to be

$$\mathbf{\Pi}^{(1)} = -\rho\theta\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) + \mathcal{O}(Ma^3),$$

where $Ma = |\mathbf{u}|/c_s$ is the Mach number ($c_s = \sqrt{\theta}$).

We have obtained the (compressible) Navier-Stokes equations

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{u}) = 0, \quad \partial_t(\rho\mathbf{u}) + \nabla\cdot\left(\mathbf{\Pi}^{(0)} + \tau\mathbf{\Pi}^{(1)}\right) = 0,$$

where the dynamic viscosity $\mu = \tau\rho\theta$.

From discrete Boltzmann to lattice Boltzmann

Integrating the discrete Boltzmann equation

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = \Omega_i(f)$$

along a characteristic for time Δt gives

$$f_i(x + c_i \Delta t, t + \Delta t) - f_i(x, t) = \int_0^{\Delta t} \Omega_i(x + c_i s, t + s)\, ds,$$

Approximating the integral by the trapezium rule yields

$$\begin{aligned} f_i(x+c_i\Delta t, t+\Delta t) - f_i(x, t) &= \frac{\Delta t}{2}\Big(\Omega_i(x+c_i\Delta t, t+\Delta t) \\ &+ \Omega_i(x, t)\Big) + O\left(\Delta t^3\right). \end{aligned}$$

This is an implicit system.

Change of Variables

To obtain a second order explicit LBE at time $t + \Delta t$ define

$$\bar{f}_i(x,t) = f_i(x,t) + \frac{\Delta t}{2\tau}\left(f_i(x,t) - f_i^{(0)}(x,t)\right).$$

The new algorithm is

$$\bar{f}_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) - \bar{f}_i(\mathbf{x},t) = -\frac{\Delta t}{\tau + \Delta t/2}\left(\bar{f}_i(\mathbf{x},t) - f_i^{(0)}(\mathbf{x},t)\right)$$

This could have also been obtained by Strang splitting Dellar [2011]

A quick note on forcing

A body force R_i in the discrete Boltzmann equation

$$\frac{\partial f_i}{\partial t} + \mathbf{c}_i \cdot \nabla f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right) + R_i$$

should have the following moments:

$$\sum_i R_i = 0, \quad \sum_i R_i \mathbf{c}_i = \boldsymbol{F}, \quad \sum_i R_i \mathbf{c}_i \mathbf{c}_i = \boldsymbol{F}\mathbf{u} + \mathbf{u}\boldsymbol{F}$$

and implemented as

$$\begin{aligned} &\bar{f}_i(x + c_i \Delta t \ , \ t + \Delta t) - \bar{f}_i(x, t) \\ &\qquad = \ -\frac{\Delta t}{\tau + \Delta t/2} \ \left(\bar{f}_i(x,t) - f_i^{(0)}(x,t)\right) + \frac{\tau \Delta t}{\tau + \Delta t/2} \ R_i(x,t) \end{aligned}$$

Analytic solution of the LBE

$$\bar{f}_i(x + c_i\Delta t\ ,\ t + \Delta t) - \bar{f}_i(x,t)$$
$$= \ -\frac{\Delta t}{\tau + \Delta t/2}\ \left(\bar{f}_i(x,t) - f_i^{(0)}(x,t)\right) + \frac{\tau\Delta t}{\tau + \Delta t/2}\ R_i(x,t)$$

Consider flows satisfying

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial t} = 0, \quad \boldsymbol{F} = (\rho G, 0)$$

Walls located at $j = 1$ and $j = n$

Let $\bar{f}_i^j$ denote the the distribution function $\bar{f}_i$ at node j; similarly for u_j and v_j. Then ...

$$
\begin{aligned}
\bar{f}_0^j &= \frac{4\rho}{9}\left(1-\frac{3}{2}\left(u_j^2+v_j^2\right)\right),\\
\bar{f}_1^j &= \frac{\rho}{9}\left(1+3u_j+3u_j^2-\frac{3v_j^2}{2}\right)+\frac{\tau\rho G}{3}\left(2u_j+1\right),\\
\bar{f}_2^j &= \frac{\rho}{9(\tau+1/2)}\left(1+3v_{j-1}+2v_{j-1}^2-\frac{3u_{j-1}^2}{2}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_2^{j-1},\\
\bar{f}_3^j &= \frac{\rho}{9}\left(1-3u_j+3u_j^2-\frac{3v_j^2}{2}\right)+\frac{\tau\rho G}{3}\left(2u_j-1\right),\\
\bar{f}_4^j &= \frac{\rho}{9(\tau+1/2)}\left(1-3v_{j+1}+3v_{j+1}^2-\frac{3u_{j+1}^2}{2}\right)-\frac{\tau-1/2}{\tau+1/2}\bar{f}_4^{j+1},\\
\bar{f}_5^j &= \frac{\rho}{36(\tau+1/2)}\left(1+3u_{j-1}+3v_{j-1}+3u_{j-1}^2+3v_{j-1}^2+9u_{j-1}v_{j-1}\right)\\
&+ \frac{\tau\rho G}{12(\tau+1/2)}\left(1+2u_{j-1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_5^{j-1},
\end{aligned}
$$

$$
\begin{aligned}
\bar{f}_6^j &= \frac{\rho}{36(\tau+1/2)}\left(1-3u_{j-1}+3v_{j-1}+3u_{j-1}^2+3v_{j-1}^2-9u_{j-1}v_{j-1}\right) \\
&- \frac{\tau\rho G}{12(\tau+1/2)}\left(1-2u_{j-1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_6^{j-1}, \\
\bar{f}_7^j &= \frac{\rho}{36(\tau+1/2)}\left(1-3u_{j+1}-3v_{j+1}+3u_{j+1}^2+3v_{j+1}^2+9u_{j+1}v_{j+1}\right) \\
&- \frac{\tau\rho G}{12(\tau+1/2)}\left(1-2u_{j+1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_7^{j+1}, \\
\bar{f}_8^j &= \frac{\rho}{36(\tau+1/2)}\left(1+3u_{j+1}-3v_{j+1}+3u_{j+1}^2+3v_{j+1}^2-9u_{j+1}v_{j+1}\right) \\
&+ \frac{\tau\rho G}{12(\tau+1/2)}\left(1+2u_{j+1}\right)+\frac{\tau-1/2}{\tau+1/2}\bar{f}_8^{j+1},
\end{aligned}
$$

Poiseuille flow

This recurrence relation reduces to

$$\frac{u_{j+1}v_{j+1} - u_{j-1}v_{j-1}}{2} = \nu\left(u_{j+1} + u_{j-1} - 2u_j\right) + G,$$

This is the second order finite–difference form of the incompressible Navier–Stokes equations with a constant body force:

$$\frac{\partial(uv)}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2} + G$$

Solution of the difference equation

$$\frac{u_{j+1}v_{j+1} - u_{j-1}v_{j-1}}{2} = \nu\left(u_{j+1} + u_{j-1} - 2u_j\right) + G$$

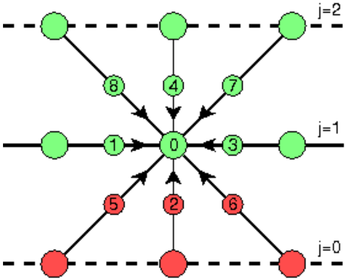
We can show ρ is constant and $v_j = 0$

The solution to this second order difference equation is

$$u_j = \frac{4U_c}{(n-1)^2}(j-1)(n-j) + U_s, \quad j = 1, 2, \ldots, n$$

where $U_c = H^2 G/8\nu$ is the centre-line velocity and $H = (n-1)$ is the channel height.

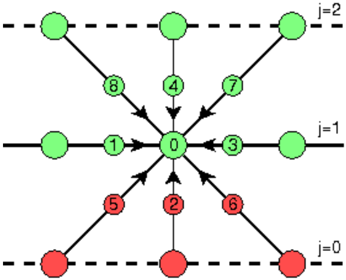
Numerical slip for bounce–back



If we use bounce–back boundary conditions, we find the numerical slip to be He *et al.* [1997]

$$U_s = \frac{48\nu^2 - 1}{n^2} U_c$$

Moments at a wall



$$\begin{aligned}
\rho &= f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 + f_8, \\
\rho u_x &= f_1 - f_3 + f_5 - f_6 - f_7 + f_8, \\
\rho u_y &= f_2 - f_4 + f_5 + f_6 - f_7 - f_8.
\end{aligned}$$

Moment-based boundary conditions

THE PLAN:

Formulate the boundary conditions in the moment basis, and then transform them into into boundary conditions for the distribution functions Bennett [2010].

Moments	Combination of unknowns
ρ, ρu_y, Π_{yy}	$f_2 + f_5 + f_6$
ρu_x, Π_{xy}, Q_{xyy}	$f_5 - f_6$
Π_{xx}, Q_{xxy}, R_{xxyy}	$f_5 + f_6$

We can pick one constraint from each group. A natural choice is

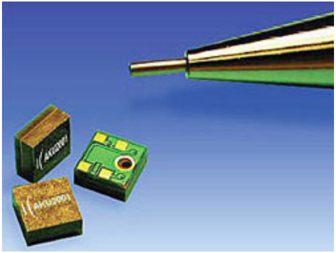
$$
\begin{aligned}
\rho u_y &= 0, \\
\rho u_x &= \rho u_{slip}, \\
\Pi_{xx} &= \theta\rho + \rho u_{slip}^2 \implies \quad \frac{\partial u_{slip}}{\partial x} = 0.
\end{aligned}
$$

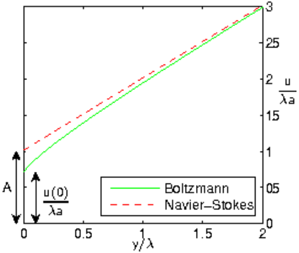
It really is quite simple

For no-slip, these conditions translate into

$$\begin{aligned}
\bar{f}_2 &= \bar{f}_1 + \bar{f}_3 + \bar{f}_4 + 2\left(\bar{f}_7 + \bar{f}_8\right) - \frac{\rho}{3}, \\
\bar{f}_5 &= -\bar{f}_1 - \bar{f}_8 + \frac{\rho}{6}, \\
\bar{f}_6 &= -\bar{f}_3 - \bar{f}_7 + \frac{\rho}{6},
\end{aligned}$$

Flow in a microchannel





No slip	Slip flow	Transition	Molecular
$Kn \lesssim 10^{-3}$	$10^{-3} \lesssim Kn \lesssim 10^{-1}$	$10^{-1} \lesssim Kn \lesssim 10$	$Kn \gtrsim 10$

In shear flow the LBE reduces to a linear second–order recurrence relation $\Longrightarrow$ linear or parabolic profiles at *all Kn*

But we can capture flow in the bulk from with slip conditions

Maxwell–Navier boundary condition

Wall boundary conditions:

$$u_{slip} = \sigma KnH \partial_y u|_{wall}\,, \quad \sigma = (2-\sigma_a)/\sigma_a.$$

These can be expressed in terms of moments:

$$\begin{aligned}
\bar{f}_2 &= \bar{f}_1 + \bar{f}_3 + \bar{f}_4 + 2\left(\bar{f}_7 + \bar{f}_8\right) - \left(P - \rho u_{slip}^2\right),\\
\bar{f}_5 &= -\bar{f}_1 - \bar{f}_8 + (P + \rho u_{slip}^2 + \rho u_{slip})/2,\\
\bar{f}_6 &= -\bar{f}_3 - \bar{f}_7 + (P + \rho u_{slip}^2 - \rho u_{slip})/2,
\end{aligned}$$

and since $\Pi_{xy}|_{wall} = \frac{2\tau\bar{\Pi}_{xy}|_{wall}}{(2\tau+\Delta t)} = \mu\partial_y u|_{wall}$,

$$u_{slip} = -\frac{6\left(-\bar{f}_1 + \bar{f}_3 + 2\bar{f}_7 - 2\bar{f}_8\right)}{\rho(2\tau + 1 + 6KnH)}.$$

Flow in a microchannel: asymptotic solution

We consider a viscous fluid in a channel with an aspect ratio $\delta = L/H \ll 1$.

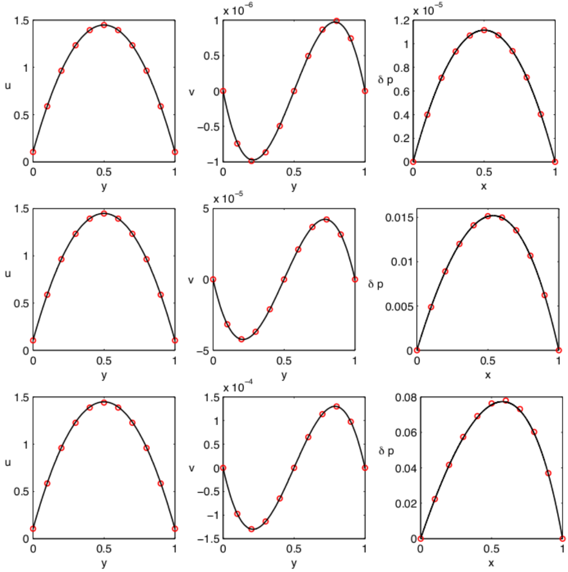
The relevant dimensionless numbers are

$$Re = \frac{\rho_o U_o H}{\mu}, \quad Ma = \frac{U_o}{\sqrt{\gamma RT}}, \quad Kn = \sqrt{\frac{\pi\gamma}{2}} \frac{Ma}{Re}$$

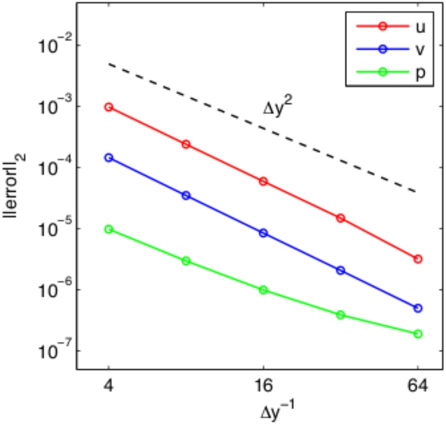
An expansion in δ yields the leading–order solution

$$\begin{aligned} u(x,y) &= -\frac{\epsilon Re}{8Ma^2} p' \left(1 - 4y^2 + 4\sigma \frac{Kn}{p}\right) \\ v(x,y) &= \frac{\epsilon^2 Re}{8pMa^2} \left[\frac{1}{2}(p^2)'' \left(1 - \frac{4}{3}y^2\right) + 4\sigma Kn p''\right] \\ P(x) &= \sqrt{(6Kn)^2 + (1+12Kn)x + \theta(\theta + 12Kn)(1-x)} - 6Kn \end{aligned}$$

Flow in a microchannel: $Kn = 0.1$

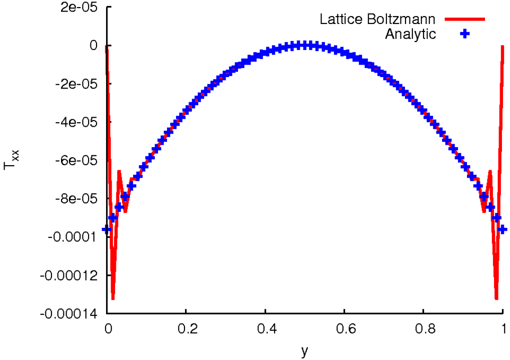


Convergence



Deviatoric stress in Poiseuille flow, $Re = 100$

For Newtonian fluids: $T_{xx} \propto \partial u / \partial x = 0$
From BGK: $T_{xx} = -2\mu\tau(\partial u / \partial y)^2$



"Analytic" is the exact solution from the continuous BGK Boltzmann equation

Analysis of the stress field

We use the same ideas to solve the LBE stress field:

$$\begin{aligned} \Pi_{yy} &= \frac{\rho}{3}, \\ \Pi_{xy} &= -\nu\rho\frac{u_{j+1} - u_{j-1}}{2} \end{aligned}$$

These agree with the components of the Newtonian deviatoric stress

Deviatoric stress

The T_{xx}^j component of $\mathbf{T}$ is more interesting

$$
\begin{aligned}
&3\left(4\tau^2-1\right)\left(T_{xx}^{j+1}-2T_{xx}^j+T_{xx}^{j-1}\right)-12T_{xx}^j= \\
&\quad 4\tau^2\rho\left(u_{j-1}^2-2u_j^2+u_{j+1}^2\right)-16\tau^3\rho G\left(u_{j+1}+u_{j-1}-2u_j\right) \\
&\quad +6\tau\rho G\left(u_{j+1}+u_{j-1}+2u_j\right).
\end{aligned}
$$

The homogenous solution is

$$T_{xx}^j = Am^j + Bm^{-j},$$

where A and B are constants and

$$m = \frac{2\tau+1}{2\tau-1}.$$

Deviatoric stress solution

The particular integral is

$$T_{xx}^{j(PI)} = -2\mu\tau \left(u'\right)^2 + O(Ma^3)$$

Recall the Navier–Stokes boundary condition

$$\Pi_{xx} = \Pi_{xx}^{(0)} \implies T_{xx} = 0$$

Hence

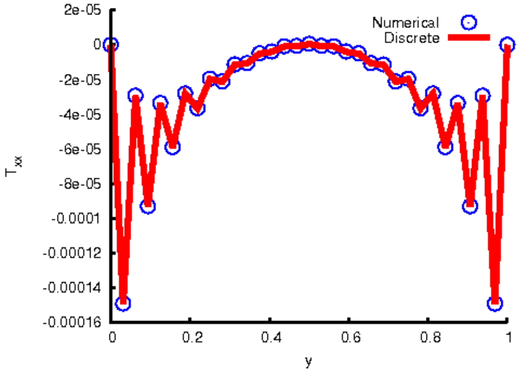
$$\begin{aligned} A &= \frac{m^{n-1} - 1}{m\left(m^{2n-2} - 1\right)} T^W, \\ B &= \frac{m^n\left(m^{n-1} - 1\right)}{m^{2n-2} - 1} T^W, \end{aligned}$$

where T^W is the particular integral evaluated at the wall.

Inconsistency

The stress with Navier-Stokes boundary conditions is

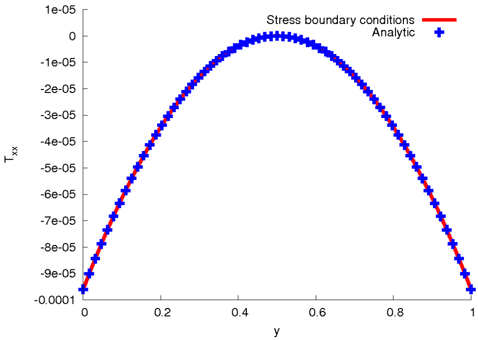
$$T_{xx}^{j} = \left(\frac{m^{n-1}-1}{m\left(m^{2n-2}-1\right)}\right) T^{W} m^{j} + \left(\frac{Tm^{n}\left(m^{n-1}-1\right)}{m^{2n-2}-1}\right) T^{W} m^{-j}$$
$$- \quad 2\mu\tau\left(u'\right)^{2} + 3G^{2}(1+4\tau^{2})$$



Stress boundary conditions

A consistent boundary condition for the stress is

$$\begin{aligned}\overline{\Pi}_{xx} &= \frac{\rho}{3} - \frac{2\tau + \Delta t}{2\tau} T_{xx}, \\ &= \frac{\rho}{3} + \frac{12\tau}{\rho\,(2\tau + \Delta t)} \overline{\Pi}_{xy}^2\end{aligned}$$



Finite difference interpretation

Solving the lattice Boltzmann recurrence equation

$$
\begin{aligned}
3\left(4\tau^2-1\right)\left(T_{xx}^{j+1}-2T_{xx}^{j}+T_{xx}^{j-1}\right) &- 12T_{xx}^{j} \\
&= 4\tau^2\rho\left(u_{j-1}^2-2u_j^2+u_{j+1}^2\right) \\
&- 16\tau^3\rho G\left(u_{j+1}+u_{j-1}-2u_j\right) \\
&+ 6\tau\rho G\left(u_{j+1}+u_{j-1}+2u_j\right)
\end{aligned}
$$

$\tau^2 = 1/4 \implies$ no recurrence in non–conserved moments

$\tau^2 = 1/6 \implies$ Lele's compact finite difference scheme [Lele 92]

Two relaxation time LBE

Relax odd and even moments at different rates:

$$\begin{aligned}
\bar{f}_i(\mathbf{x}+\mathbf{c}_i, t+\Delta t) = \bar{f}_i(\mathbf{x}, t) \quad &- \quad \frac{1}{\tau^+ + 1/2}\left[\frac{1}{2}\left(\bar{f}_i + \bar{f}_k\right) - f_i^{(0+)}\right] \\
&- \quad \frac{1}{\tau^- + 1/2}\left[\frac{1}{2}\left(\bar{f}_i - \bar{f}_k\right) - f_i^{(0-)}\right]
\end{aligned}$$

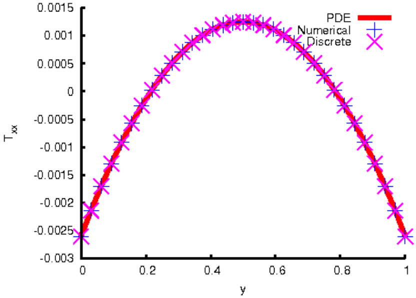
Solving the recurrence yields

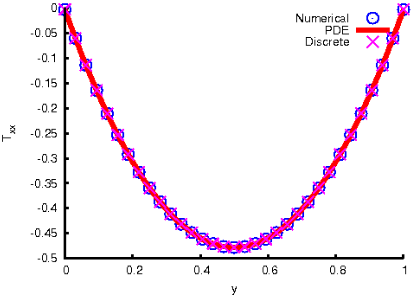
$$\begin{aligned}
3(4\Lambda - 1)\left(T_{xx}^{j+1} - 2T_{xx}^{j} + T_{xx}^{j-1}\right) \quad &- \quad 12T_{xx}^{j} \\
&= \quad 4\Lambda\rho\left(u_{j-1}^2 - 2u_j^2 + u_{j+1}^2\right) \\
&- \quad 16\Lambda\tau\rho G\left(u_{j+1} + u_{j-1} - 2u_j\right) \\
&+ \quad 6\tau\rho G\left(u_{j+1} + u_{j-1} + 2u_j\right)
\end{aligned}$$

where $\Lambda = \tau^+\tau^-$

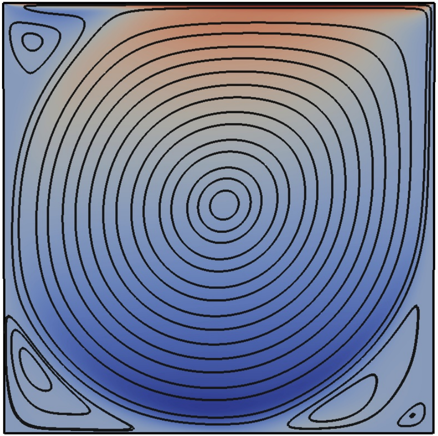
TRT results, $\Lambda = 1/4$

$$T_{xx} = 2\tau^+ \mu u u'' - \frac{2\Lambda}{3}\left(u u'' + (u')^2\right)$$





Lid-driven cavity flow: $Re = 7500$



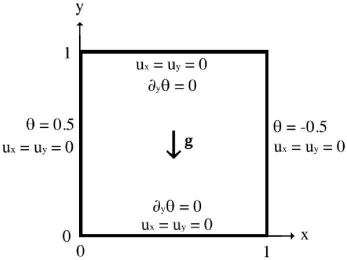
Lid-driven cavity flow: the numbers

	Primary		
Re $= 400$			
Present $\Lambda = 1/4$	0.1139	0.5547	0.6055
Ghia *et al.*	0.1139	0.5547	0.6055
Sahin and Owens	0.1139	0.5536	0.6075
Re $= 1000$			
Present $\Lambda = 1/4$	0.1189	0.5313	0.5664
Ghia *et al.*	0.1179	0.5313	0.5625
Sahin and Owens	0.1188	0.5335	0.5639
Botella *et al.*	0.1189	0.4692	0.5652
Re $= 7500$			
Present $\Lambda = 1/4$	0.1226	0.5117	0.5352
Ghia *et al.*	0.1200	0.5117	0.5322
Sahin and Owens	0.1223	0.5134	0.5376

Note: Second order convergence of L_2 error norm for global velocity and pressure fields

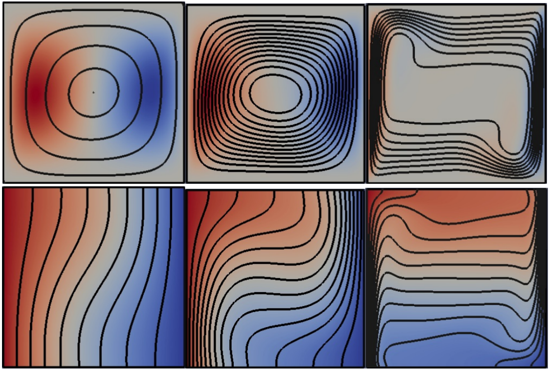
Natural Convection

Flow is driven by density variation



$$
\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla P + Pr \nabla^2 \mathbf{u} + Ra Pr \mathbf{g}, \\
\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta &= \nabla^2 \theta,
\end{aligned}
$$

Streamfunction and Temperature plots



Contours of flow fields for convection in a square cavity. From left to right, $Ra = 1000$, $Ra = 10000$, $Ra = 1000000$

Nusselt numbers

Ra	Study	*Nu*
10^3	Present	1.1178
	de Vahl Davis	1.118
10^6	Present	8.8249
	Le Quere	8.8252
	de Vahl Davis	8.800
10^8	Present	30.23339
	Le Quere	30.225

Work with moments

Summary

The kinetic formulation yields a linear, constant coefficient hyperbolic system where all nonlinearities are confined to algebraic source terms.

The linear differential operators may be discretised exactly by integrating along their characteristics, while the hydrodynamic equations with their nonlinear convection terms are recovered by seeking slowly varying solutions to the kinetic equations

Nonlinearity is local, non-locality is linear Sauro Succi

The LBE in its standard form does NOT capture kinetic effects in the velocity field but more subtle effects manifest themselves in the stress at $O(\tau^2)$

Analytic solutions of the LBE for simple flows gives insight into its numerical and physical characteristics

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Knudsen boundary layers??