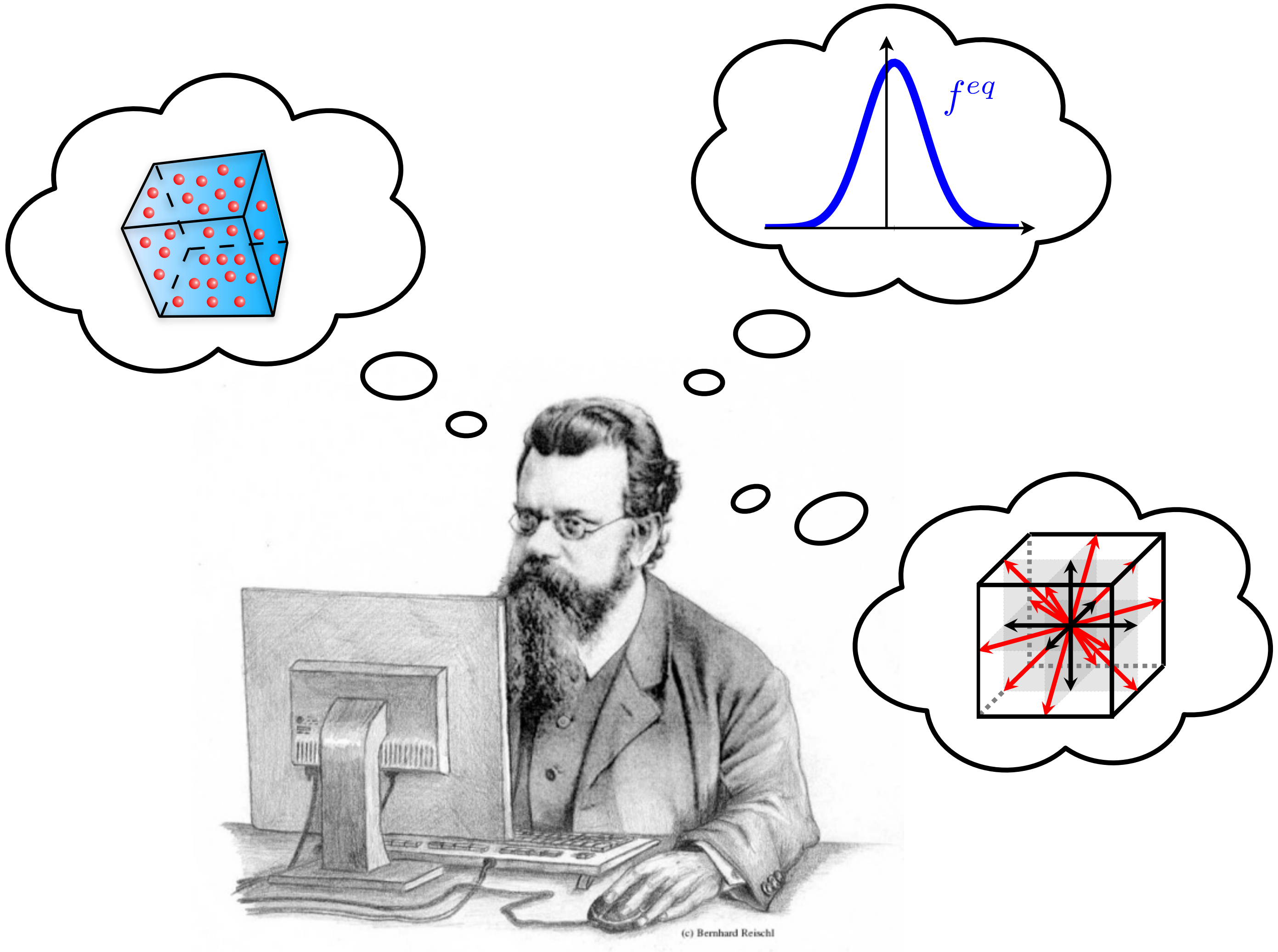

UNIVERSITY OF GENEVA

FACULTY OF SCIENCE
Computer Science Dept

PALABOS

PALABOS SUMMER SCHOOL
Recap on collision models in Palabos

Christophe Coreixas

Collision models in a nutshell

BGK
Linear relaxation towards equilibrium

MRT
Relaxation in a moment space

Regularization
Filter out high-order contributions

Entropic
Enforce a particular H-theorem

Subgrid models
Mimic properties of turbulence

Numerous variants

- Moment spaces (raw, Hermite, central, central Hermite, cumulant)
- Orthogonality of moment space
- Number and values of extra relaxation times (TRT, AllOne, etc)
- Standard, recursive and hybrid computation of non-equilibrium contributions
- H-functional and entropic formalism
- Smago (static and dyn), WALE, SISM, ADM, etc

Collision models in Palabos

isoThermalDynamics.h & .hh
thermalDynamics.h & .hh

BGK
Linear relaxation towards equilibrium

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Relaxation in a moment space

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Filter out high-order contributions

Entropic
Enforce a particular H-theorem

Subgrid models
Mimic properties of turbulence

Quasi-incompressible	*Weakly compressible*	*Fully compressible*
QuasiIncBGKdynamics (2nd) ConstRhoBGKdynamics (2nd) IncBGKdynamics (2nd)	BGKdynamics (2nd) CompleteBGKdynamics (comp)	ThermalBGKdynamics (4th)
IsoThermalBulkDynamics		*ThermalBulkDynamics*

Collision models in Palabos

isoThermalDynamics.h & .hh
mrtDynamics.h & .hh
trtDynamics.h & .hh

BGK
Linear relaxation towards equilibrium

MRT
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Filter out high-order contributions

Entropic
Enforce a particular H-theorem

Subgrid models
Mimic properties of turbulence

Quasi-incompressible	***Weakly compressible***	***Fully compressible***
IncTRTdynamics (2nd) IncMRTdynamics (2nd)	Ma1TRTdynamics (1st) TRTdynamics (2nd) MRTdynamics (2nd) etc	No formulation available

IsoThermalBulkDynamics (Quasi-incompressible and Weakly compressible)

ThermalBulkDynamics (Fully compressible)

There are other TRT models available but they differ from Ginzburg's approach!

Collision models in Palabos

isoThermalDynamics.h & .hh
thermalDynamics.h & .hh

BGK
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Regularization
Filter out high-order contributions

Entropic
Enforce a particular H-theorem

Subgrid models
Mimic properties of turbulence

Quasi-incompressible ***Weakly compressible*** ***Fully compressible***

IncRegularizedBGKdynamics (2nd)	RegularizedBGKdynamics (2nd) CompleteRegularizedBGKdynamics (comp) etc	ThermalRLBdynamics (4th)

IsoThermalBulkDynamics ***ThermalBulkDynamics***

Collision models in Palabos

BGK
Linear relaxation towards equilibrium

MRT
Relaxation in a moment space

Regularization
Filter out high-order contributions

entropicDynamics.h & .hh
kbcDynamics.h & .hh

Entropic
Enforce a particular H-theorem

Subgrid models
Mimic properties of turbulence

Quasi-incompressible	*Weakly compressible*	*Fully compressible*
No formulation available	EntropicDynamics (2nd, Newton-Raphson) KBCDynamics (2nd, D2Q9-RM only)	No formulation available

IsoThermalBulkDynamics (quasi-incompressible and weakly compressible)

ThermalBulkDynamics (fully compressible)

Collision models in Palabos

BGK
Linear relaxation towards equilibrium

MRT
Relaxation in a moment space

Regularization
Filter out high-order contributions

Entropic
Enforce a particular H-theorem

smagorinskyDynamics.h & .hh
dynamicSmagorinskyDynamics.h & .hh

Subgrid models
Mimic properties of turbulence

Quasi-incompressible

SmagorinskyIncBGKdynamics (2nd)
ConsistentSmagorinskyIncMRTdynamics (2nd)
etc

Weakly compressible

SmagorinskyBGKdynamics (2nd)
SmagorinskyMRTdynamics (2nd)
ConsistentSgsBGKdynamics (2nd)
etc

IsoThermalBulkDynamics

Fully compressible

No formulation available

ThermalBulkDynamics

It is usually a smarter move to rely on composite dynamics to account for sgs, instead of writing new dynamics !

Common misconception

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0 \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p \boldsymbol{\delta}) = \boxed{\nabla \cdot \boldsymbol{\Pi}} \\ \partial_t (\rho E) + \nabla \cdot ([\rho E + p]\, \mathbf{u}) = \boxed{\nabla \cdot (\lambda \nabla T) + \nabla \cdot (\boldsymbol{\Pi} \cdot \mathbf{u})} \end{cases}$$

Chapman-Enskog

$$\begin{cases} \partial_t (M_0^{eq}) + \nabla \cdot (M_1^{eq}) = 0 \\ \partial_t (M_1^{eq}) + \nabla \cdot (M_2^{eq}) \propto \boxed{\partial_t (M_2^{eq}) + \nabla \cdot (M_3^{eq})} \\ \partial_t (M_{\mathrm{Tr}2}^{eq}) + \nabla \cdot (M_{\mathrm{Tr}3}^{eq}) \propto \boxed{\partial_t (M_{\mathrm{Tr}3}^{eq}) + \nabla \cdot (M_{\mathrm{Tr}4}^{eq})} \end{cases}$$

Common misconception

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + p\boldsymbol{\delta}) = \boxed{\nabla \cdot \Pi}$$

For the same equilibrium,
different collision models DO NOT change the physics
but only the numerics

$$\partial_t (M^{eq}_{\mathrm{Tr}2}) + \nabla \cdot (M^{eq}_{\mathrm{Tr}3}) \propto \boxed{\partial_t (M^{eq}_{\mathrm{Tr}3}) + \nabla \cdot (M^{eq}_{\mathrm{Tr}4})}$$

Collision models in Palabos

BGK
Linear relaxation towards equilibrium

MRT
Relaxation in a moment space

Regularization
Filter out high-order contributions

comprehensiveIsoThermalDynamics.h & .hh

Entropic
Enforce a particular H-theorem

Subgrid models
Mimic properties of turbulence

To avoid issues due to different equilibria, a unified framework is now available in Palabos to compare all kinds of collision models with D2Q9, D3Q19 and D3Q27 lattices (https://gitlab.com/unigespc/palabos/-/tags/v2.3.0)

QUESTIONS ?

Unified formalism in a nutshell (D2Q9)

✤ **Example: Collision in the raw moment (RM) space**

$$M_{pq} = \sum_i \xi_{ix}^{p} \xi_{iy}^{q} f_i$$

$$M_{00}^* = M_{00} = M_{00}^{eq} = \rho$$
$$M_{10}^* = M_{10} = M_{10}^{eq} = \rho u_x$$
$$M_{01}^* = M_{01} = M_{01}^{eq} = \rho u_y$$

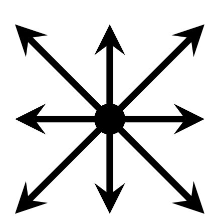
conservation rules

$$M_{20}^* = M_{20}^{eq} + (1-\omega_\nu) M_{20}^{neq}$$
$$M_{02}^* = M_{02}^{eq} + (1-\omega_\nu) M_{02}^{neq}$$
$$M_{11}^* = M_{11}^{eq} + (1-\omega_\nu) M_{11}^{neq}$$

shear + acoustics

$$M_{21}^* = M_{21}^{eq} + (1-\omega_3) M_{21}^{neq}$$
$$M_{12}^* = M_{12}^{eq} + (1-\omega_3) M_{12}^{neq}$$
$$M_{22}^* = M_{22}^{eq} + (1-\omega_4) M_{22}^{neq}$$

high-order (ghost)



D2Q9

Direct control on physics/numerics through post-collision RMs

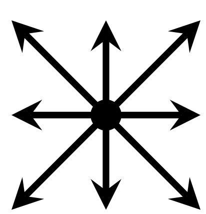
Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.

Unified formalism in a nutshell (D2Q9)

✤ **Example: Collision in the raw moment (RM) space**

$$M_{pq} = \sum_i \xi_{ix}^{p} \xi_{iy}^{q} f_i$$

$$\begin{aligned}
M_{00}^{*} &= M_{00} = M_{00}^{eq} = \rho \\
M_{10}^{*} &= M_{10} = M_{10}^{eq} = \rho u_x \\
M_{01}^{*} &= M_{01} = M_{01}^{eq} = \rho u_y \\
M_{20}^{*} &= M_{20}^{eq} + (1 - \boxed{\omega_\nu}) M_{20}^{neq} \\
M_{02}^{*} &= M_{02}^{eq} + (1 - \boxed{\omega_\nu}) M_{02}^{neq} \\
M_{11}^{*} &= M_{11}^{eq} + (1 - \boxed{\omega_\nu}) M_{11}^{neq} \\
M_{21}^{*} &= M_{21}^{eq} + (1 - \boxed{\omega_3}) M_{21}^{neq} \\
M_{12}^{*} &= M_{12}^{eq} + (1 - \boxed{\omega_3}) M_{12}^{neq} \\
M_{22}^{*} &= M_{22}^{eq} + (1 - \boxed{\omega_4}) M_{22}^{neq}
\end{aligned}$$



D2Q9

MRT, entropic and subgrid models

At the moment, it is only possible through composite dynamics for this framework

Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.

Unified formalism in a nutshell (D2Q9)

✤ Example: Collision in the raw moment (RM) space

$$M_{pq} = \sum_i \xi_{ix}^p \xi_{iy}^q f_i$$

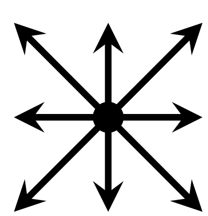
Efficient formulation (velocity space)

$$f_{(0,0)}^{*,\mathrm{RM}} = M_{00}^* - (M_{20}^* + M_{02}^*) + M_{22}^*$$

$$f_{(\sigma,0)}^{*,\mathrm{RM}} = \frac{1}{2}\left(\sigma M_{10}^* + M_{20}^* - \sigma M_{12}^* - M_{22}^*\right)$$

$$f_{(0,\lambda)}^{*,\mathrm{RM}} = \frac{1}{2}\left(\lambda M_{01}^* + M_{02}^* - \lambda M_{21}^* - M_{22}^*\right)$$

$$f_{(\sigma,\lambda)}^{*,\mathrm{RM}} = \frac{1}{4}\left(\sigma\lambda M_{11}^* + \sigma M_{12}^* + \lambda M_{21}^* + M_{22}^*\right)$$



D2Q9

$$M_{00}^* = M_{00} = M_{00}^{eq} = \rho$$

$$M_{10}^* = M_{10} = M_{10}^{eq} = \rho u_x$$

$$M_{01}^* = M_{01} = M_{01}^{eq} = \rho u_y$$

$$M_{20}^* = M_{20}^{eq} + (1-\omega_\nu) M_{20}^{neq}$$

$$M_{02}^* = M_{02}^{eq} + (1-\omega_\nu) M_{02}^{neq}$$

$$M_{11}^* = M_{11}^{eq} + (1-\omega_\nu) M_{11}^{neq}$$

$$M_{21}^* = M_{21}^{eq} + (1-\omega_3) M_{21}^{neq}$$

$$M_{12}^* = M_{12}^{eq} + (1-\omega_3) M_{12}^{neq}$$

$$M_{22}^* = M_{22}^{eq} + (1-\omega_4) M_{22}^{neq}$$

MRT, entropic and subgrid models

Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.

Unified formalism in a nutshell (D2Q9)

✤ Generalization to other moment spaces

Hermite (HM)			A_{pq} $H_{pq}(\boldsymbol{\xi}_i)$	$\longrightarrow$	M_{pq} $\boldsymbol{\xi}_i$
Central (CM)			$\widetilde{M}_{pq}$ $\boldsymbol{\xi}_i - \boldsymbol{u}$	$\longrightarrow$	M_{pq} $\boldsymbol{\xi}_i$
Cumulant (K)	K_{pq} $\boldsymbol{\xi}_i - \boldsymbol{u}$	$\longrightarrow$	$\widetilde{M}_{pq}$ $\boldsymbol{\xi}_i - \boldsymbol{u}$	$\longrightarrow$	M_{pq} $\boldsymbol{\xi}_i$
Central Hermite (CHM)	$\widetilde{A}_{pq}$ $H_{pq}(\boldsymbol{\xi}_i - \boldsymbol{u})$	$\longrightarrow$	A_{pq} $H_{pq}(\boldsymbol{\xi}_i)$	$\longrightarrow$	M_{pq} $\boldsymbol{\xi}_i$

Stability increase at relatively low cost (CPU time increases up to x2)

Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.
Latt et al., Cross-platform programming model for many-core lattice Boltzmann simulations, PLoS One, 2021.

Unified formalism in a nutshell (D2Q9)

✤ Discarding non-equilibrium moments: Standard regularisation (REG-HM)

HM $\quad \boxed{\begin{array}{c} A_{pq} \\ H_{pq}(\boldsymbol{\xi}_i) \end{array}} \longrightarrow \boxed{\begin{array}{c} M_{pq} \\ \boldsymbol{\xi}_i \end{array}}$

$$
\begin{aligned}
A^*_{00} &= \rho, \\
A^*_{10} &= \rho u_x \\
A^*_{01} &= \rho u_y \\
A^*_{11} &= A^{eq}_{11} + (1-\omega_\nu)A^{neq}_{11} \\
A^*_{20} &= A^{eq}_{20} + (1-\omega_\nu)A^{neq}_{20} \\
A^*_{02} &= A^{eq}_{02} + (1-\omega_\nu)A^{neq}_{02} \\
A^*_{21} &= A^{eq}_{21} + (1-\omega_3)A^{neq}_{21} \\
A^*_{12} &= A^{eq}_{12} + (1-\omega_3)A^{neq}_{12} \\
A^*_{22} &= A^{eq}_{22} + (1-\omega_4)A^{neq}_{22}
\end{aligned}
$$

$$
\begin{aligned}
A^{neq}_{20} &= \textstyle\sum_i (f_i - f_i^{eq})H_{20} \\
A^{neq}_{02} &= \textstyle\sum_i (f_i - f_i^{eq})H_{02} \\
A^{neq}_{11} &= \textstyle\sum_i (f_i - f_i^{eq})H_{11} \\
A^{neq}_{21} &= u_y A^{neq}_{20} + 2u_x A^{neq}_{11} \\
A^{neq}_{12} &= u_x A^{neq}_{02} + 2u_y A^{neq}_{11} \\
A^{neq}_{22} &= u_y^2 A^{neq}_{20} + u_x^2 A^{neq}_{02} + 4u_x u_y A^{neq}_{11}
\end{aligned}
$$

Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.
Latt & Chopard, Lattice Boltzmann Method with Regularized Pre-collision Distribution Functions, MCS, 2006.

Unified formalism in a nutshell (D2Q9)

✤ **Discarding non-equilibrium moments: Standard regularisation (REG-HM)**

HM $\quad \boxed{\begin{array}{c} A_{pq} \\ H_{pq}(\boldsymbol{\xi}_i) \end{array}} \longrightarrow \boxed{\begin{array}{c} M_{pq} \\ \boldsymbol{\xi}_i \end{array}}$

$$
\begin{aligned}
A^*_{00} &= \rho, \\
A^*_{10} &= \rho u_x \\
A^*_{01} &= \rho u_y \\
A^*_{11} &= A^{eq}_{11} + (1 - \omega_\nu) A^{neq}_{11} \\
A^*_{20} &= A^{eq}_{20} + (1 - \omega_\nu) A^{neq}_{20} \\
A^*_{02} &= A^{eq}_{02} + (1 - \omega_\nu) A^{neq}_{02} \\
A^*_{21} &= A^{eq}_{21} + (1 - \boxed{\omega_3}) A^{neq}_{21} \\
A^*_{12} &= A^{eq}_{12} + (1 - \boxed{\omega_3}) A^{neq}_{12} \\
A^*_{22} &= A^{eq}_{22} + (1 - \boxed{\omega_4}) A^{neq}_{22}
\end{aligned}
$$

$= 1$

regularisation of high-order HMs

$$
\begin{aligned}
A^{neq}_{20} &= \textstyle\sum_i (f_i - f_i^{eq}) H_{20} \\
A^{neq}_{02} &= \textstyle\sum_i (f_i - f_i^{eq}) H_{02} \\
A^{neq}_{11} &= \textstyle\sum_i (f_i - f_i^{eq}) H_{11} \\
\cancel{A^{neq}_{21}} &\cancel{= u_y A^{neq}_{20} + 2 u_x A^{neq}_{11}} \\
\cancel{A^{neq}_{12}} &\cancel{= u_x A^{neq}_{02} + 2 u_y A^{neq}_{11}} \\
\cancel{A^{neq}_{22}} &\cancel{= u_y^2 A^{neq}_{20} + u_x^2 A^{neq}_{02} + 4 u_x u_y A^{neq}_{11}}
\end{aligned}
$$

Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.
Latt & Chopard, Lattice Boltzmann Method with Regularized Pre-collision Distribution Functions, MCS, 2006.

Unified formalism in a nutshell (D2Q9)

✤ **Discarding non-equilibrium moments: Standard regularisation (REG-HM)**

HM $\quad A_{pq} \quad H_{pq}(\xi_i) \longrightarrow M_{pq} \quad \xi_i$

Discarding non-equilibrium contributions
is a common trick to improve stability
(cf double shear layer hands-on)

$$A^*_{21} = A^{eq}_{21} + (1 - \boxed{\omega_3})A^{neq}_{21}$$
$$A^*_{12} = A^{eq}_{12} + (1 - \boxed{\omega_3})A^{neq}_{12}$$
$$A^*_{22} = A^{eq}_{22} + (1 - \boxed{\omega_4})A^{neq}_{22}$$
$$= 1$$

$$\cancel{A^{neq}_{21} = u_y A^{neq}_{20} + 2u_x A^{neq}_{11}}$$
$$\cancel{A^{neq}_{12} = u_x A^{neq}_{02} + 2u_y A^{neq}_{11}}$$
$$\cancel{A^{neq}_{22} = u_y^2 A^{neq}_{20} + u_x^2 A^{neq}_{02} + 4u_x u_y A^{neq}_{11}}$$

regularisation of high-order HMs

Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.
Latt & Chopard, Lattice Boltzmann Method with Regularized Pre-collision Distribution Functions, MCS, 2006.

Unified formalism in a nutshell (D2Q9)

✤ Keeping all non-equilibrium moments: Recursive regularization (RR)

HM $\quad \begin{matrix} A_{pq} \\ H_{pq}(\boldsymbol{\xi}_i) \end{matrix} \longrightarrow \begin{matrix} M_{pq} \\ \boldsymbol{\xi}_i \end{matrix}$

$$
\begin{aligned}
A^*_{00} &= \rho, \\
A^*_{10} &= \rho u_x \\
A^*_{01} &= \rho u_y \\
A^*_{11} &= A^{eq}_{11} + (1-\omega_\nu) A^{neq}_{11} \\
A^*_{20} &= A^{eq}_{20} + (1-\omega_\nu) A^{neq}_{20} \\
A^*_{02} &= A^{eq}_{02} + (1-\omega_\nu) A^{neq}_{02} \\
A^*_{21} &= A^{eq}_{21} + (1-\omega_3) A^{neq}_{21} \\
A^*_{12} &= A^{eq}_{12} + (1-\omega_3) A^{neq}_{12} \\
A^*_{22} &= A^{eq}_{22} + (1-\omega_4) A^{neq}_{22}
\end{aligned}
$$

$$
\begin{aligned}
A^{neq}_{20} &= \textstyle\sum_i (f_i - f_i^{eq}) H_{20} \\
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A^{neq}_{11} &= \textstyle\sum_i (f_i - f_i^{eq}) H_{11} \\
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A^{neq}_{22} &= u_y^2 A^{neq}_{20} + u_x^2 A^{neq}_{02} + 4u_x u_y A^{neq}_{11}
\end{aligned}
$$

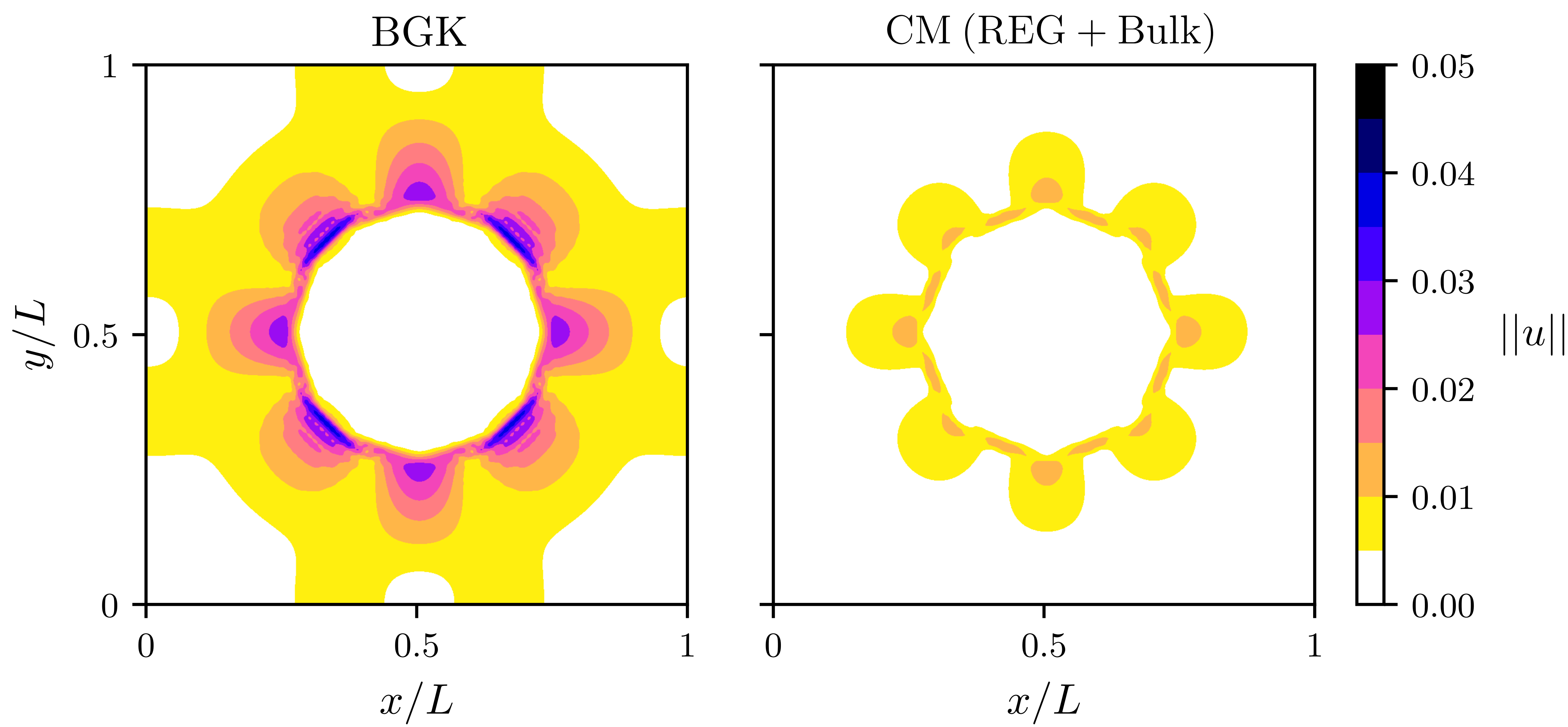
$$\omega_3 = \omega_4 = \omega_\nu \longrightarrow \text{SRT-RR} \equiv \text{REG-CHM}$$

Coreixas et al., Comprehensive comparison of collision models in the lattice Boltzmann framework: Theoretical investigations, PRE, 2019.
Coreixas et al., Impact of collision models on the physical properties and the stability of lattice Boltzmann methods, PTRSA, 2020.
Malaspinas, Increasing stability and accuracy of the lattice Boltzmann scheme: Recursivity and regularization, arXiv:1505.06900, 2015.
Chen et al., Filtered lattice Boltzmann collision formulation enforcing isotropy and Galilean invariance, PS, 2020.

QUESTIONS ?

Data processor, composite dynamics and collision models

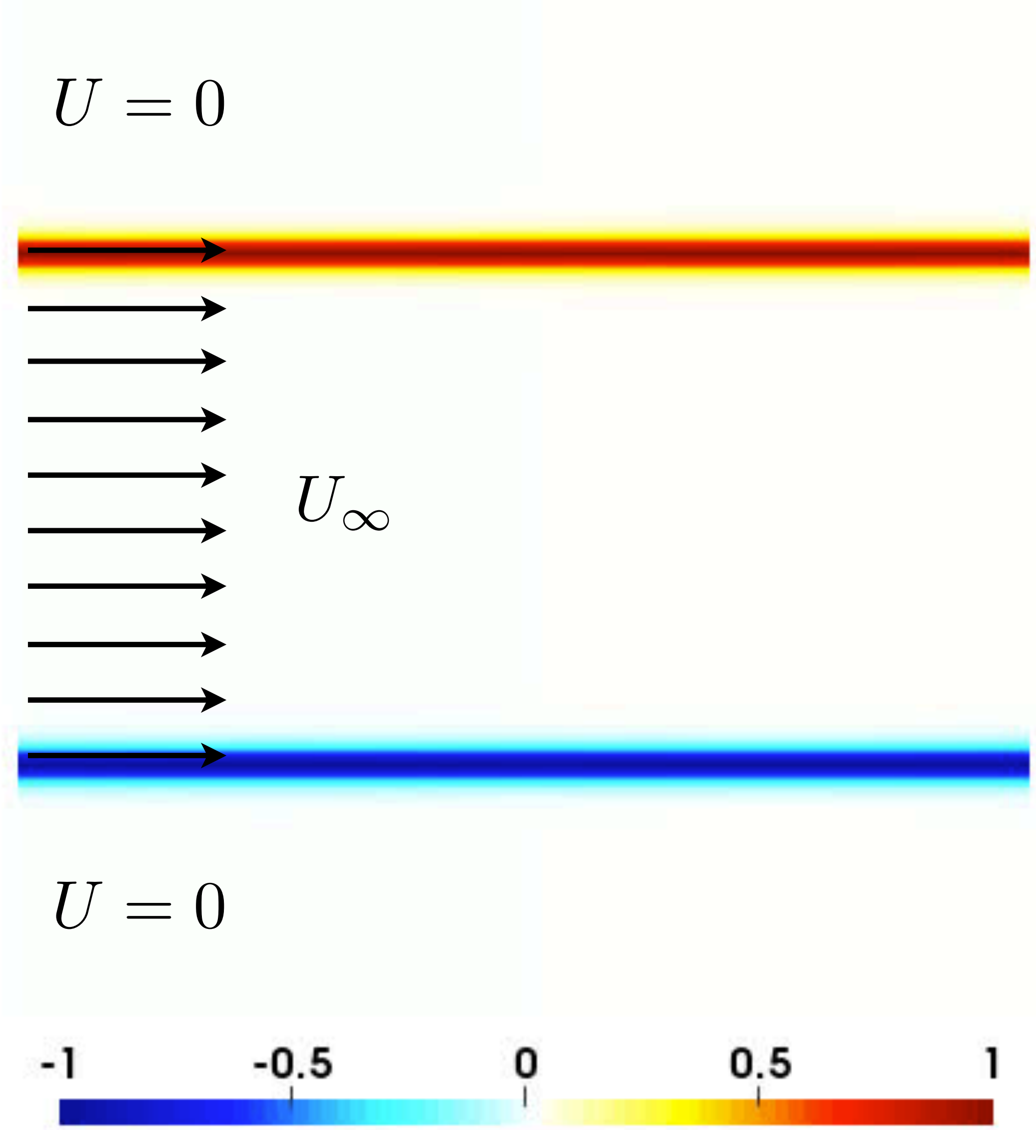
✤ **Static bubble: coupling Shan-Chen SCMP model with Guo's forcing method, and reducing spurious currents with more advanced collision models**



Shan & Chen. Lattice Boltzmann model for simulating flows with multiple phases and components, PRE, 1993.
Guo et al., Discrete lattice effects on the forcing term in the lattice Boltzmann method, PRE, 2002.
De Rosis & Coreixas, Multiphysics flow simulations using D3Q19 lattice Boltzmann methods based on central moments, PoF, 2020.

Data processor, composite dynamics and collision models

- Double shear layer: impact of collision model and relaxation parameters

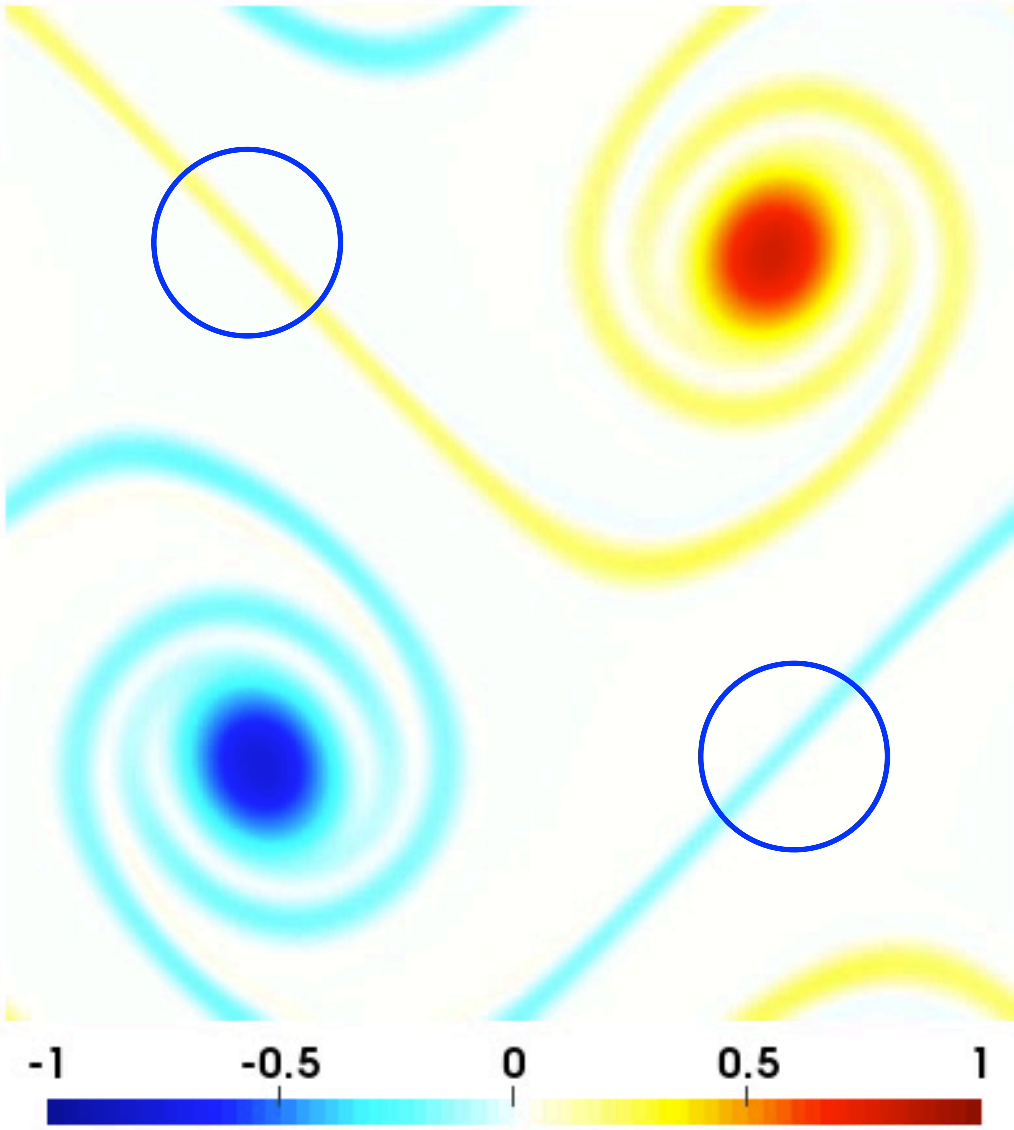


Normalized vorticity

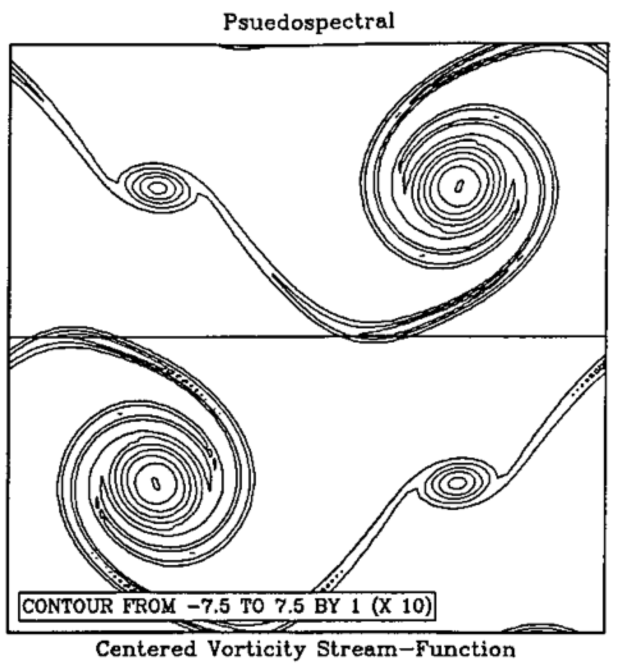
Brown & Minion. Performance of Under-resolved Two-Dimensional Incompressible Flow Simulations JCP, 1995.
Minion & Brown. Performance of Under-resolved Two-Dimensional Incompressible Flow Simulations, II JCP, 1997.

Data processor, composite dynamics and collision models

✤ Double shear layer: impact of collision model and relaxation parameters



Normalized vorticity



- First step to evaluate the robustness
- Spurious vortices allow to « see » dispersion errors

Brown & Minion. Performance of Under-resolved Two-Dimensional Incompressible Flow Simulations JCP, 1995.
Minion & Brown. Performance of Under-resolved Two-Dimensional Incompressible Flow Simulations, II JCP, 1997.

Thank you for your attention!
Questions?