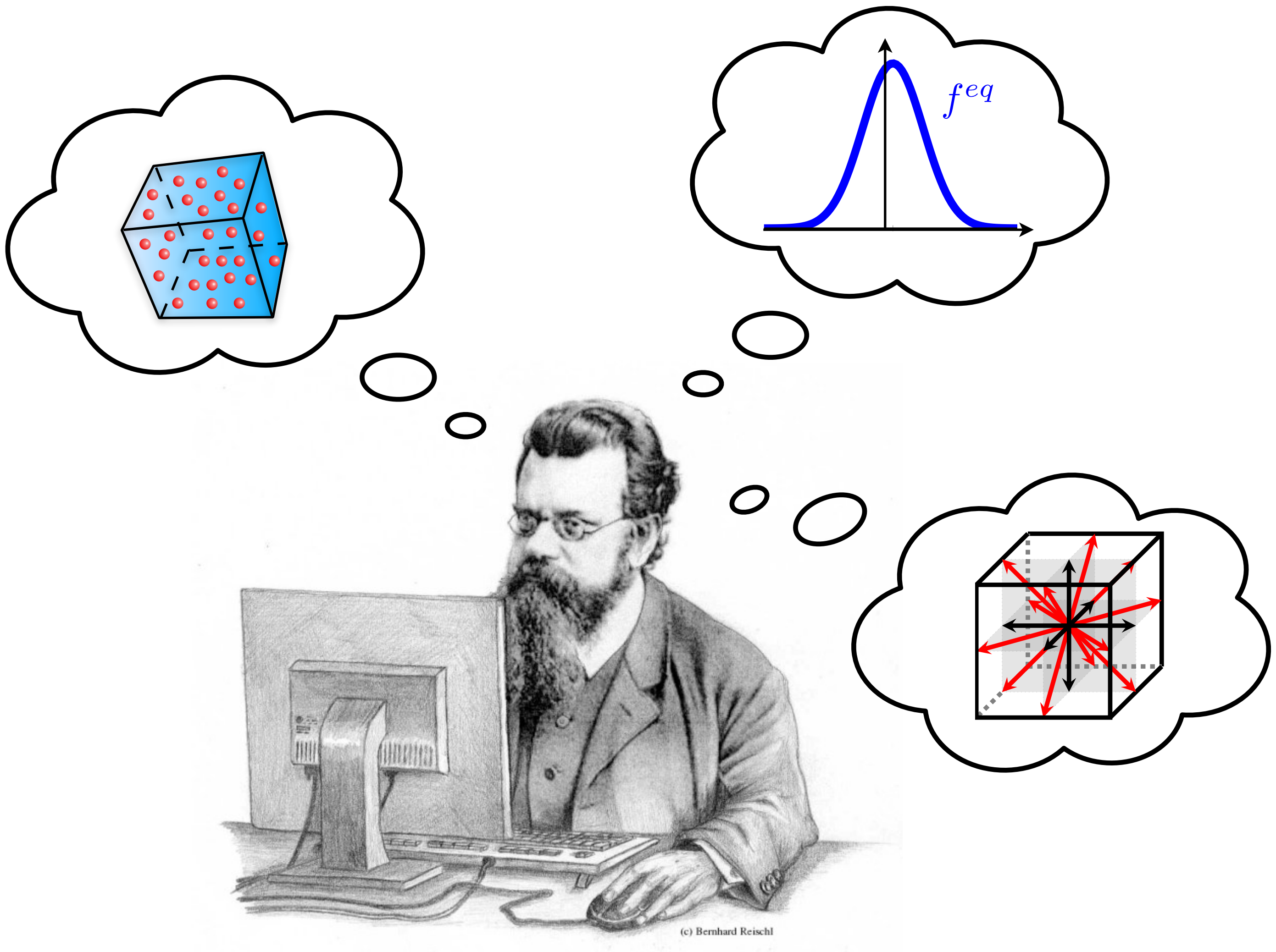


UNIVERSITY OF GENEVA
FACULTY OF SCIENCE
Computer Science Dept

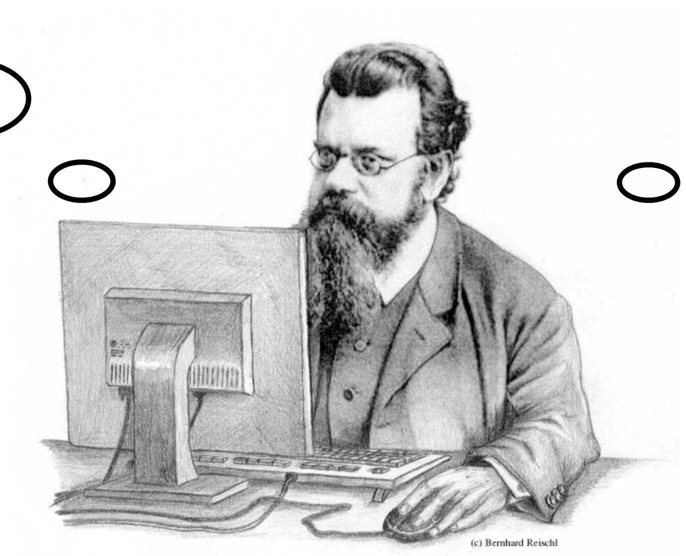
Compressible lattice Boltzmann methods
Overview and recent advances (Part 2)

Christophe Coreixas

Outline (previously)

How do we design LBMs ?

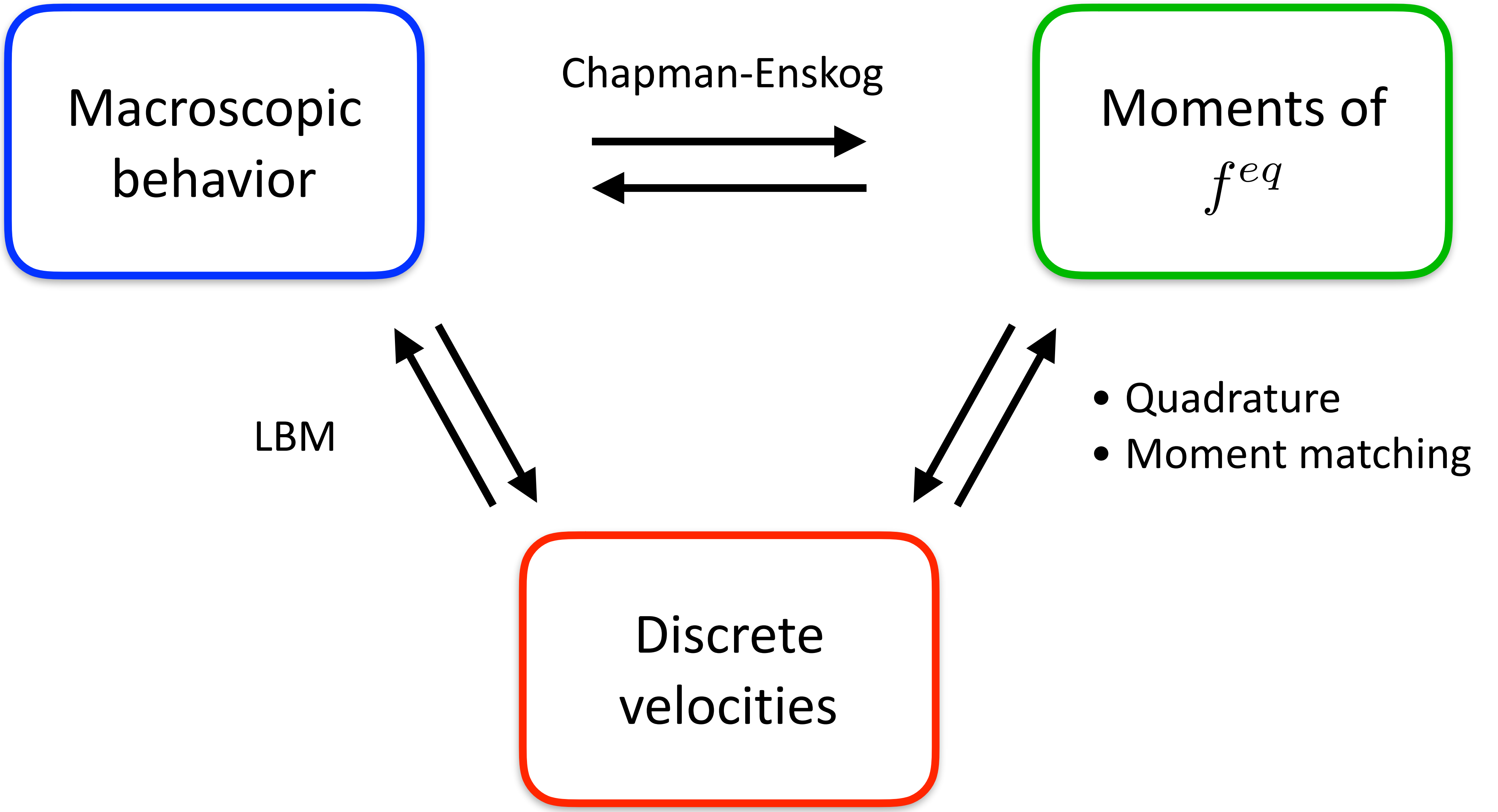
Two-equation models



Quadrature free LBMs

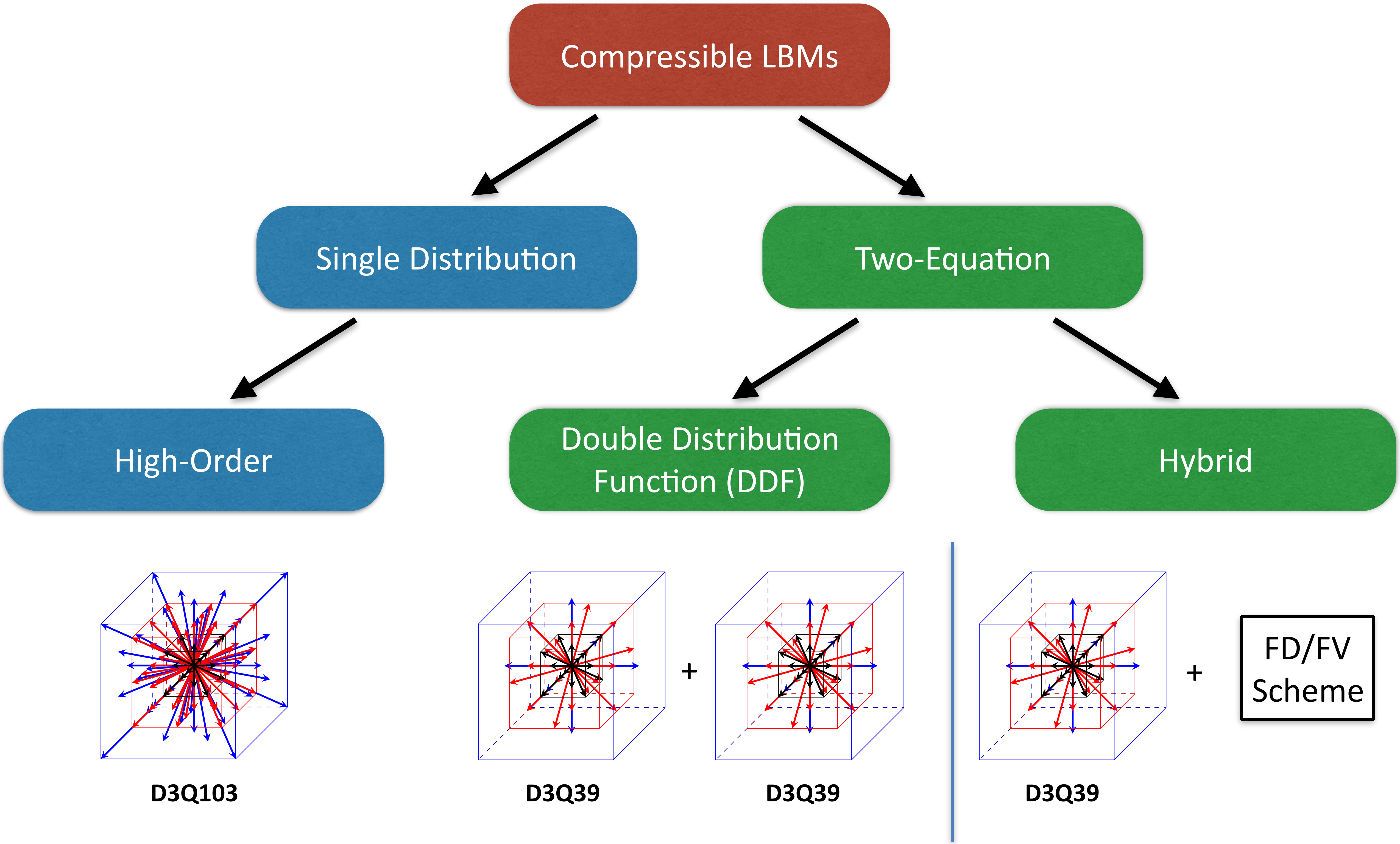
Adaptive lattices

How do we design LBMs?

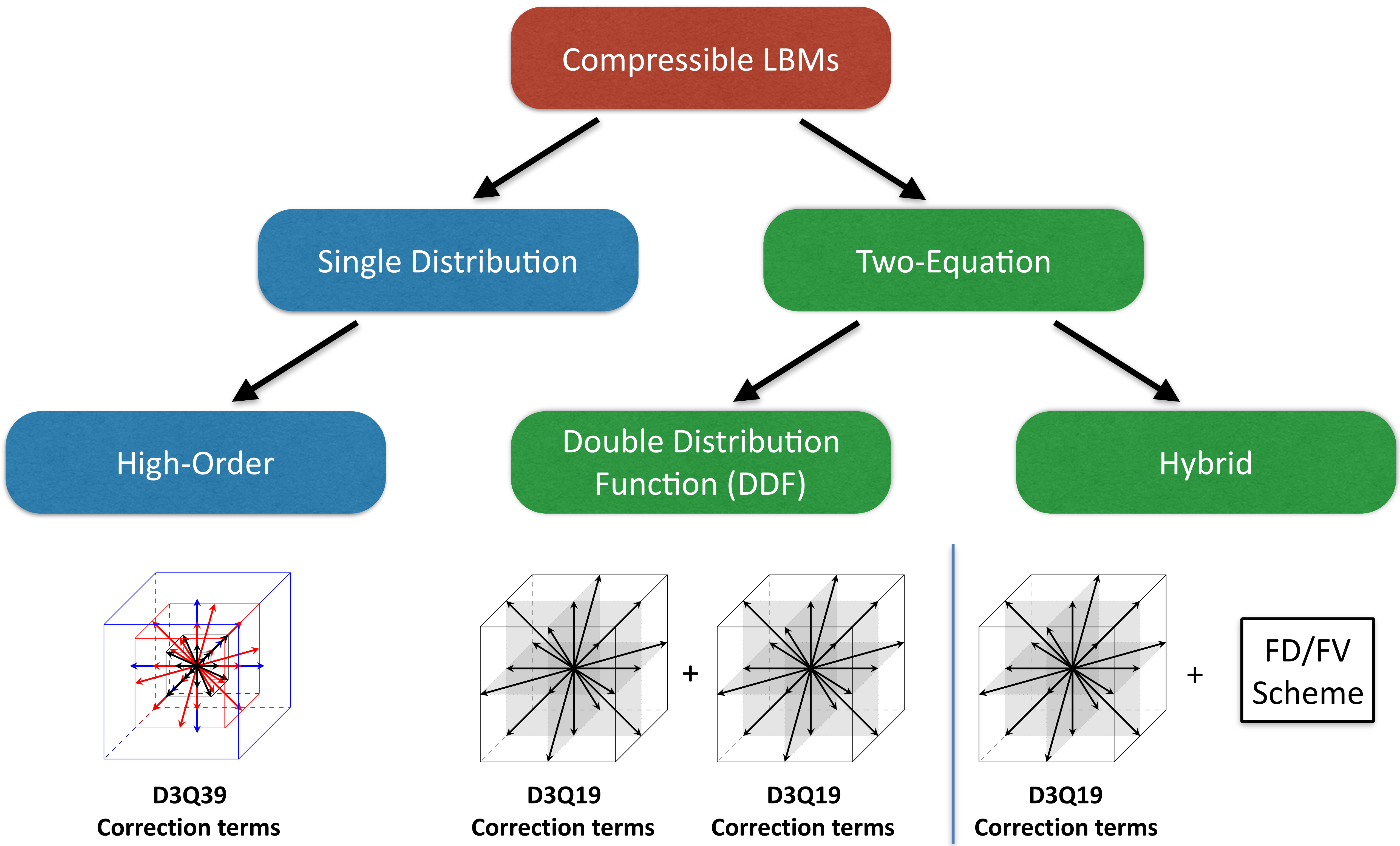


Of course, you also need (at least) **two relaxation times** to correctly impose the **Reynolds** and **Prandtl** numbers!

CPU Time and Memory Reduction Strategy



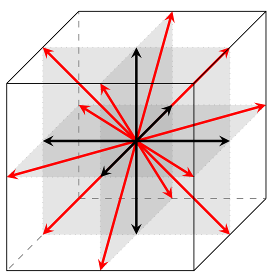
CPU Time and Memory Reduction Strategy



This is in agreement with PowerFLOW's methodology

Convection

$(\rho, \mathbf{u})$



D3Q19

FD or FV discretization of the energy equation

$p = \rho r T$

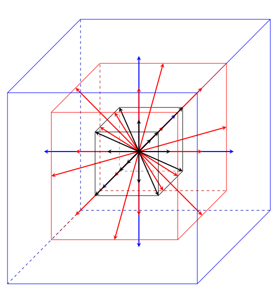
Ideal Gas EOS

High-subsonic LBM [1]

- D3Q19 + Mach correction
- **Entropy** equation
- Limitation: **Mach < 0.9**

Convection

$(\rho, \mathbf{u})$



D3Q39

FD or FV discretization of the energy equation

$p = \rho r T$

Ideal Gas EOS

Supersonic LBM [2]

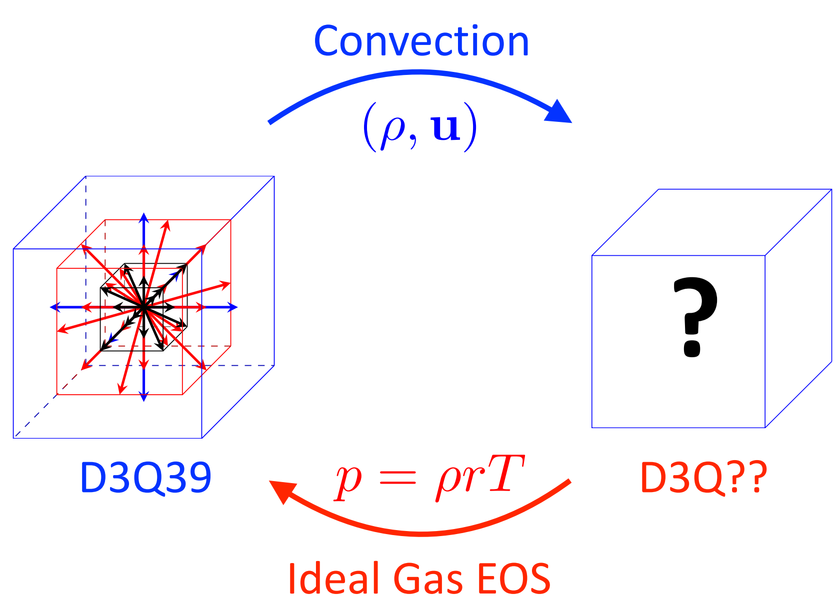
- D3Q39
- **Entropy** equation
- Limitation: **Mach < 2**

[1] **Casalino et al.**, Towards lattice-boltzmann prediction of turbofan engine noise. AIAA Paper, **2014-3101.**
[2] **Fares *et al.***, Validation of a Lattice-Boltzmann Approach for Transonic and Supersonic Flow Simulations, AIAA Paper, **2014-0952.**

PowerFLOW is coming back to DDF-LBMs due to conservation issues of the entropy formulation…

Lattice-Boltzmann Very Large Eddy Simulations of Fluidic Thrust Vectoring in a Converging/Diverging Nozzle

Avinash Jammalamadaka *, Gregory Laskowski †, Yanbing Li‡
James Kopriva §, Pradeep Gopalakrishnan ¶, Raoyang Zhang ‖, and Hudong Chen **
Dassault Systemes SIMULIA Corp, Waltham, MA, 02451, U.S.A.



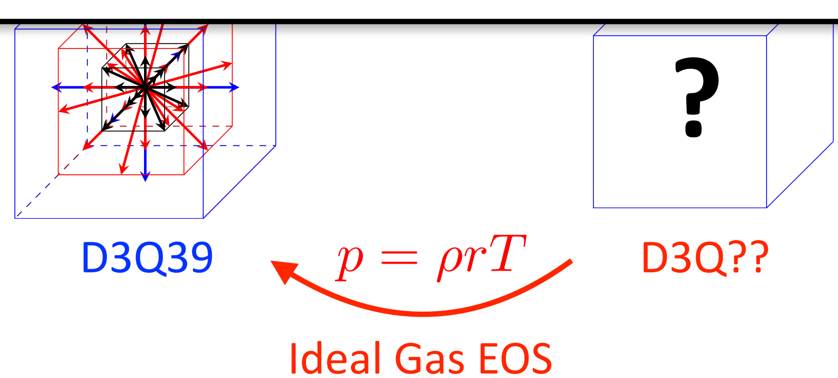
Regularized collision models

PowerFLOW is coming back to DDF-LBMs due to conservation issues of the entropy formulation…

Lattice-Boltzmann Very Large Eddy Simulations of Fluidic Thrust Vectoring in a Converging/Diverging Nozzle

Avinash Jammalamadaka *, Gregory Laskowski †, Yanbing Li‡

All these models rely on:
(1) analytical equilibria, and (2) static lattices



Regularized collision models

Outline (today)

How do we design LBMs ?

Two-equation models

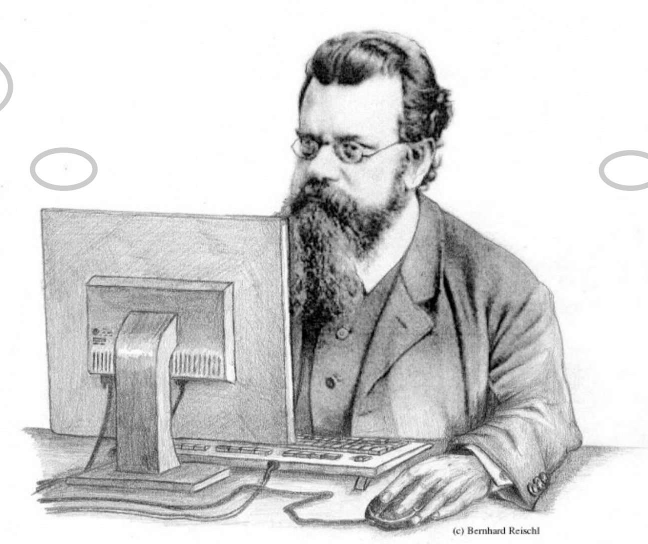
Quadrature free LBMs

Adaptive lattices

Outline

How do we design LBMs ?

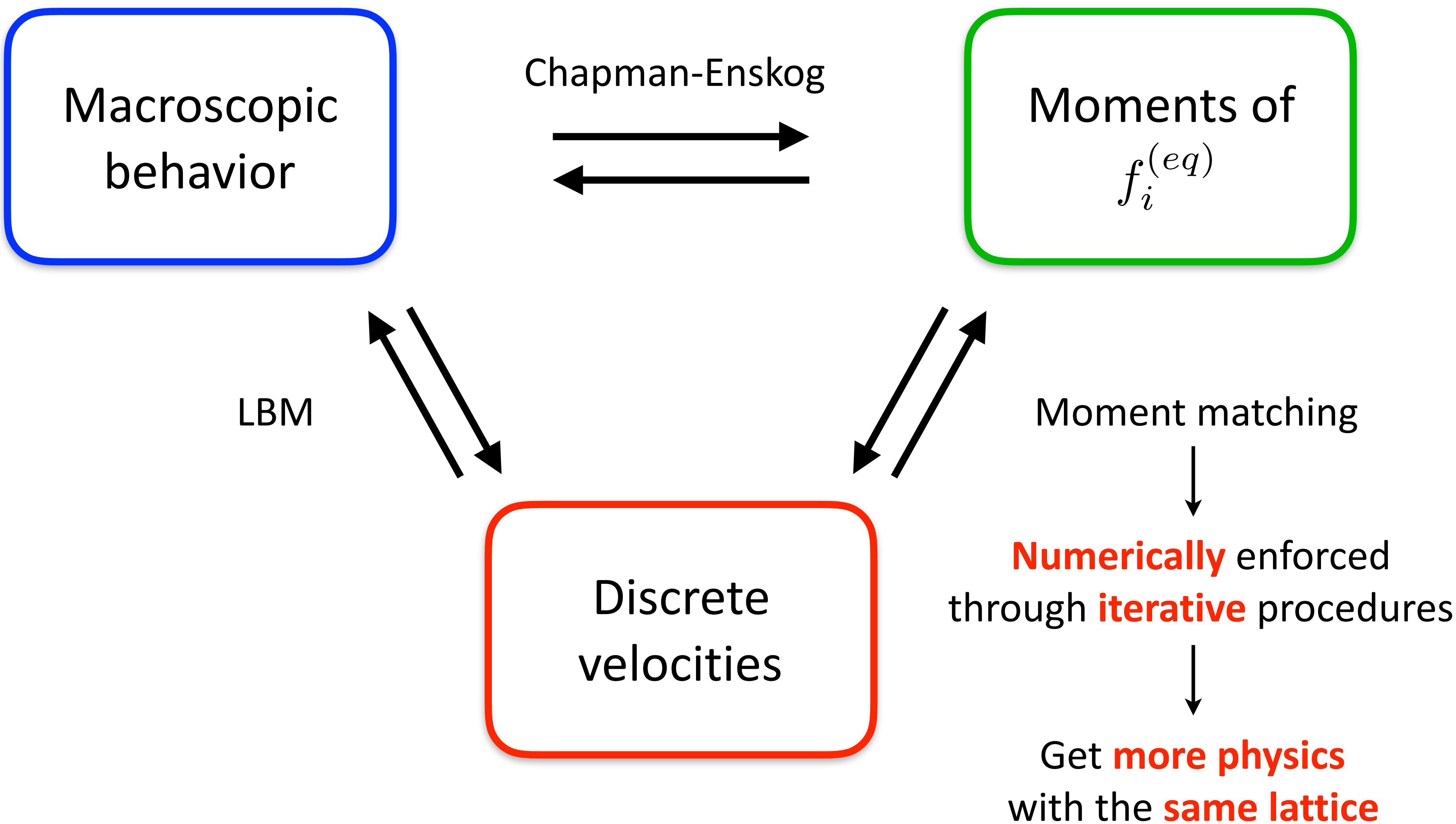
Two-equation models



Quadrature free LBMs

Adaptive lattices

Numerical equilibria for quadrature free LBMs



What are numerical equilibria?

- Equilibria (e.g., with an exponential form) which are computed iteratively

$$f_i^{eq} = \rho \exp[-(1 + \sum_n \boldsymbol{\lambda}_{M_n^{eq}} : \boldsymbol{\xi}_i^n)]$$

- Lagrange multipliers $\boldsymbol{\lambda}_{M_n^{eq}}$ are returned by a root-finding solver that imposes a number of constraints (usually mass, momentum and energy)

$$G_n = \sum_i f_i^{eq} \boldsymbol{\xi}_i^n - M_n^{eq} = 0$$

- The number of constraints is related to the targeted physics

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

What are numerical equilibria?

- **Equilibria (e.g., with an exponential form) which are computed iteratively**

$$f_i^{eq} = \rho\, \exp[-(1 + \sum_n \boldsymbol{\lambda}_{M_n^{eq}} : \boldsymbol{\xi}_i^n)]$$

Is it new?...

- **The number of constraints is related to the targeted physics**

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

Origin of numerical equilibria

Concept introduced in the 1990s/2000s for the simulation of

1. Supersonic flows using lattice gas cellular automata (LGCA)

PHYSICA D

Physica D 69 (1993) 333–344
North-Holland

SDI: 0167-2789(93)E0221-V

Supersonic lattice gases:
Restoration of Galilean invariance
by nonlinear resonance effects

Paul J. Kornreich and John Scalo
Department of Astronomy, University of Texas, Austin, TX 78712, USA

Received 28 June 1992
Accepted 11 June 1993
Communicated by E. Jen

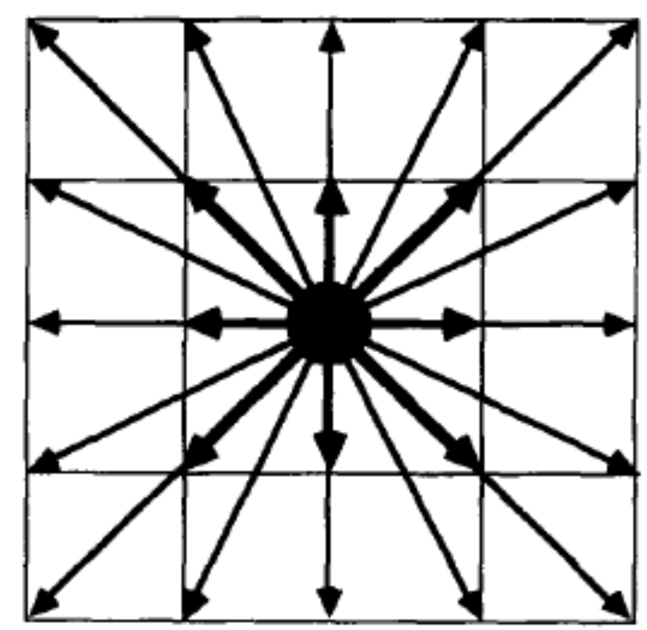


Fig. 1. Possible velocities at a lattice site of the Sq25 model. The dark circle at center represents the rest particle.

Origin of numerical equilibria

Concept introduced in the 1990s/2000s for the simulation of

1. Supersonic flows using lattice gas cellular automata (LGCA)
2. Hypersonic rarefied gas flows using discrete velocity models (DVMs)

Numerical analysis of Levermore's moment system.

Patrick Le Tallec *, Jean Philippe Perlat †

Thème 4 — Simulation et optimisation
de systèmes complexes
Projet M3N

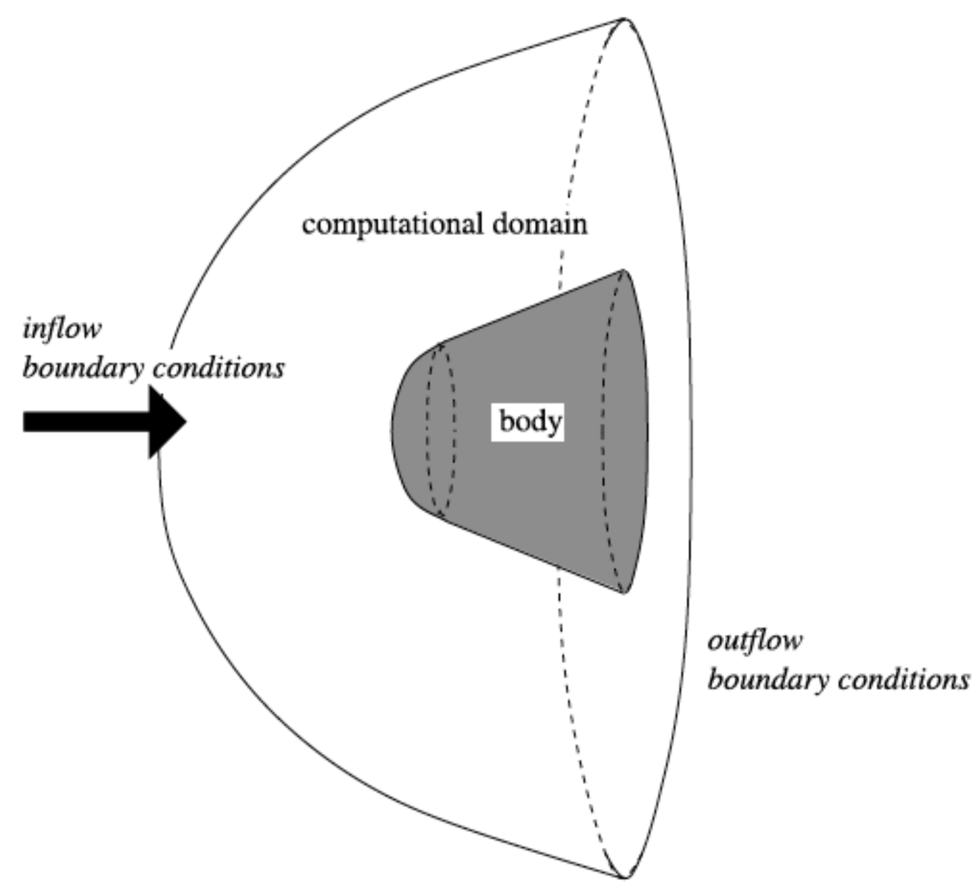
Rapport de recherche n° 3124 — Mars 1997 — 33 pages

DISCRETE VELOCITY MODEL AND IMPLICIT SCHEME FOR THE BGK EQUATION OF RAREFIED GAS DYNAMICS

LUC MIEUSSENS*
Mathématiques Appliquées de Bordeaux, Université Bordeaux I,
33405 Talence Cedex, France
and
CEA-CESTA (DEV/SIS), BP2 33114 Le Barp, France

Communicated by P. Degond
Received 2 October 1998
Revised 17 February 1999

C. Baranger et al. / Journal of Computational Physics 257 (2014) 572–593



Atmospheric re-entry simulations

Sets of constraints and macroscopic behavior

✤ **Standard 5-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq} \boldsymbol{\xi}_i - \rho \boldsymbol{u} = 0 \qquad G_{\mathrm{Tr2}} = \sum_i f_i^{eq} \xi_i^2 - 2\rho E = 0$$

✤ **Requires large lattices to compensate for numerous errors (more than 100…)**

$$\partial_t (M_0^{eq}) + \nabla \cdot (M_1^{eq}) = 0$$

$$\partial_t (M_1^{eq}) + \nabla \cdot (M_2^{eq}) \propto \partial_t (M_2^{eq}) + \nabla \cdot (M_3^{eq})$$

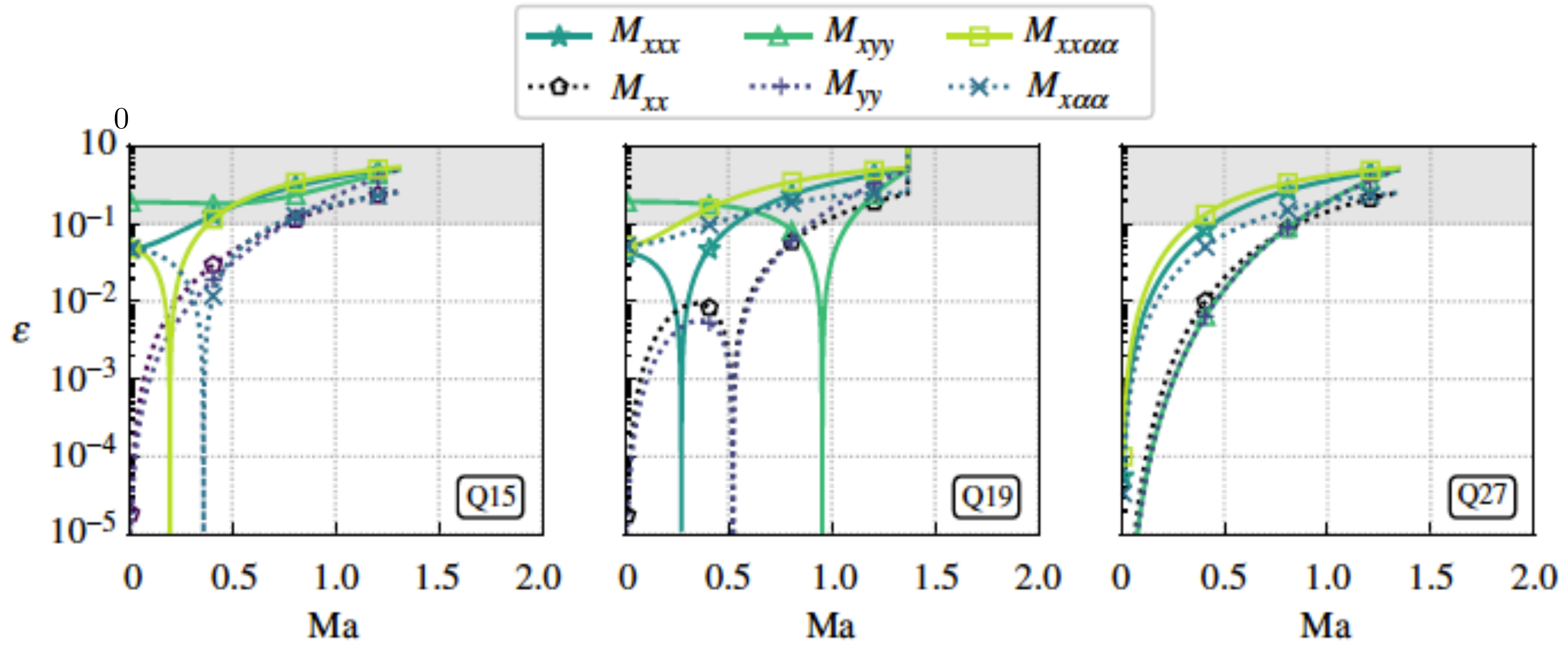
$$\partial_t (M_{\mathrm{Tr2}}^{eq}) + \nabla \cdot (M_{\mathrm{Tr3}}^{eq}) \propto \partial_t (M_{\mathrm{Tr3}}^{eq}) + \nabla \cdot (M_{\mathrm{Tr4}}^{eq})$$

Convective | Diffusive

Sets of constraints and macroscopic behavior

✤ **Standard 5-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq} \boldsymbol{\xi}_i - \rho \boldsymbol{u} = 0 \qquad G_{\mathrm{Tr}2} = \sum_i f_i^{eq} \xi_i^2 - 2\rho E = 0$$

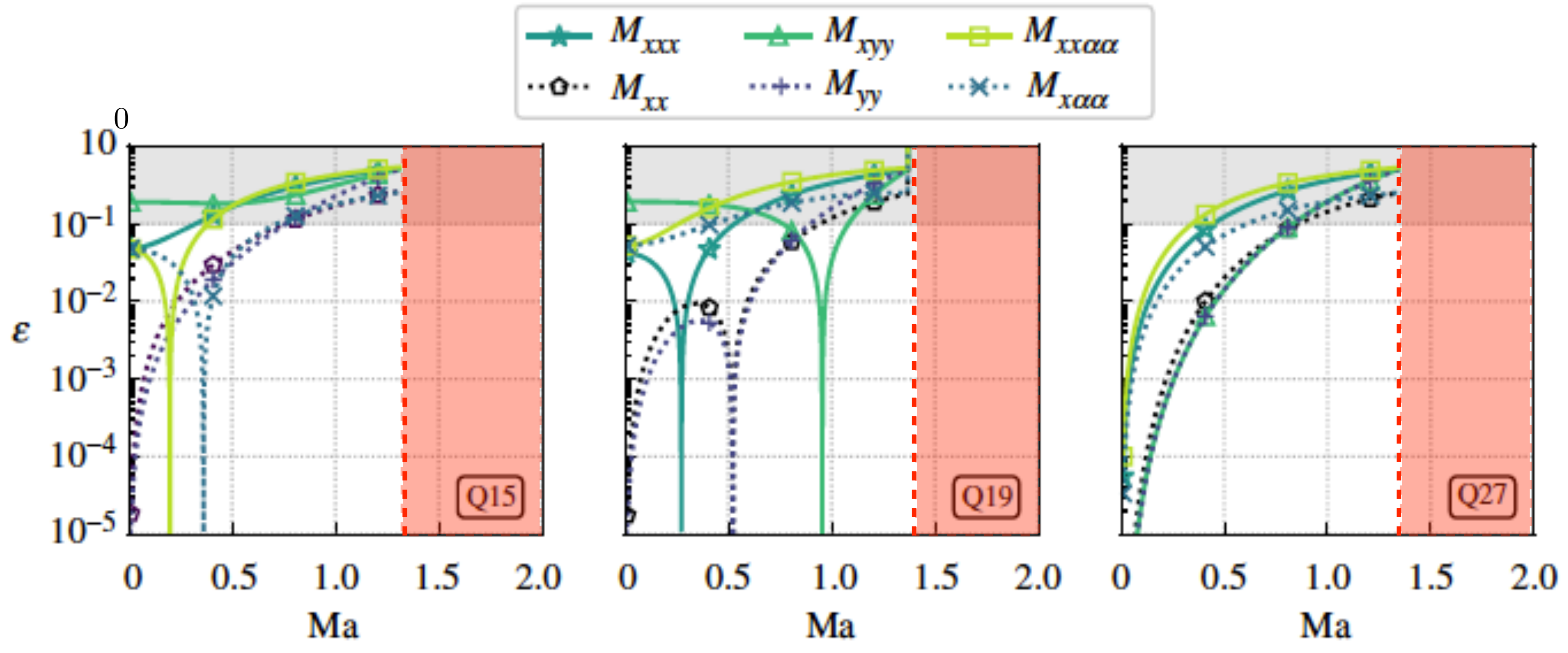


$$\varepsilon = \frac{|M_{pqr}^{\mathrm{MB}} - M_{pqr}^{\mathrm{eq}}|}{M_{pqr}^{\mathrm{MB}}}$$

Sets of constraints and macroscopic behavior

✤ **Standard 5-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq}\boldsymbol{\xi}_i - \rho\boldsymbol{u} = 0 \qquad G_{\mathrm{Tr}2} = \sum_i f_i^{eq}\xi_i^2 - 2\rho E = 0$$



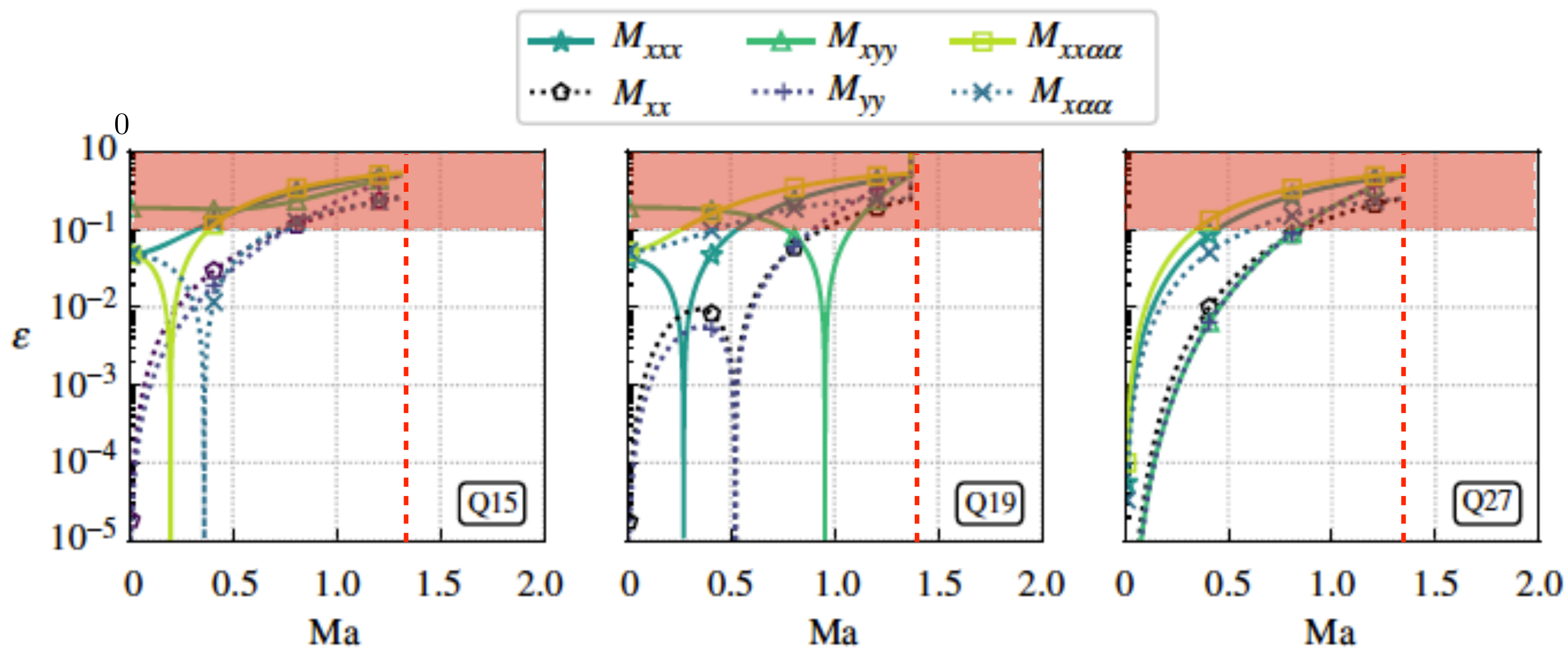
Stability: NOK

$$\varepsilon = \frac{|M_{pqr}^{\mathrm{MB}} - M_{pqr}^{\mathrm{eq}}|}{M_{pqr}^{\mathrm{MB}}}$$

Sets of constraints and macroscopic behavior

✤ **Standard 5-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq}\boldsymbol{\xi}_i - \rho\boldsymbol{u} = 0 \qquad G_{\mathrm{Tr}2} = \sum_i f_i^{eq}\xi_i^2 - 2\rho E = 0$$



Stability: NOK

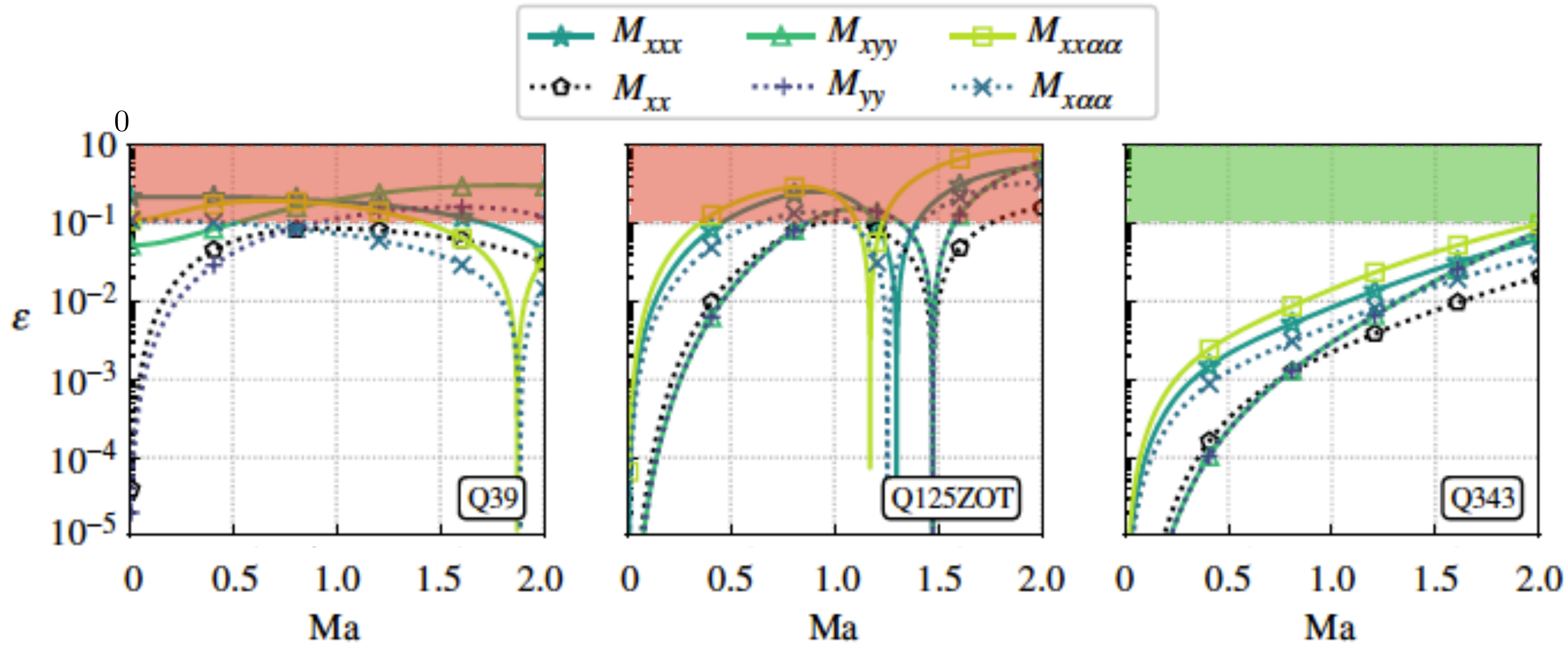
Accuracy: NOK

$$\varepsilon = \frac{|M_{pqr}^{\mathrm{MB}} - M_{pqr}^{\mathrm{eq}}|}{M_{pqr}^{\mathrm{MB}}}$$

Sets of constraints and macroscopic behavior

✤ **Standard 5-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq} \boldsymbol{\xi}_i - \rho \boldsymbol{u} = 0 \qquad G_{\mathrm{Tr}2} = \sum_i f_i^{eq} \xi_i^2 - 2\rho E = 0$$



Stability: OK

Accuracy:

NOK (Q39, Q125)

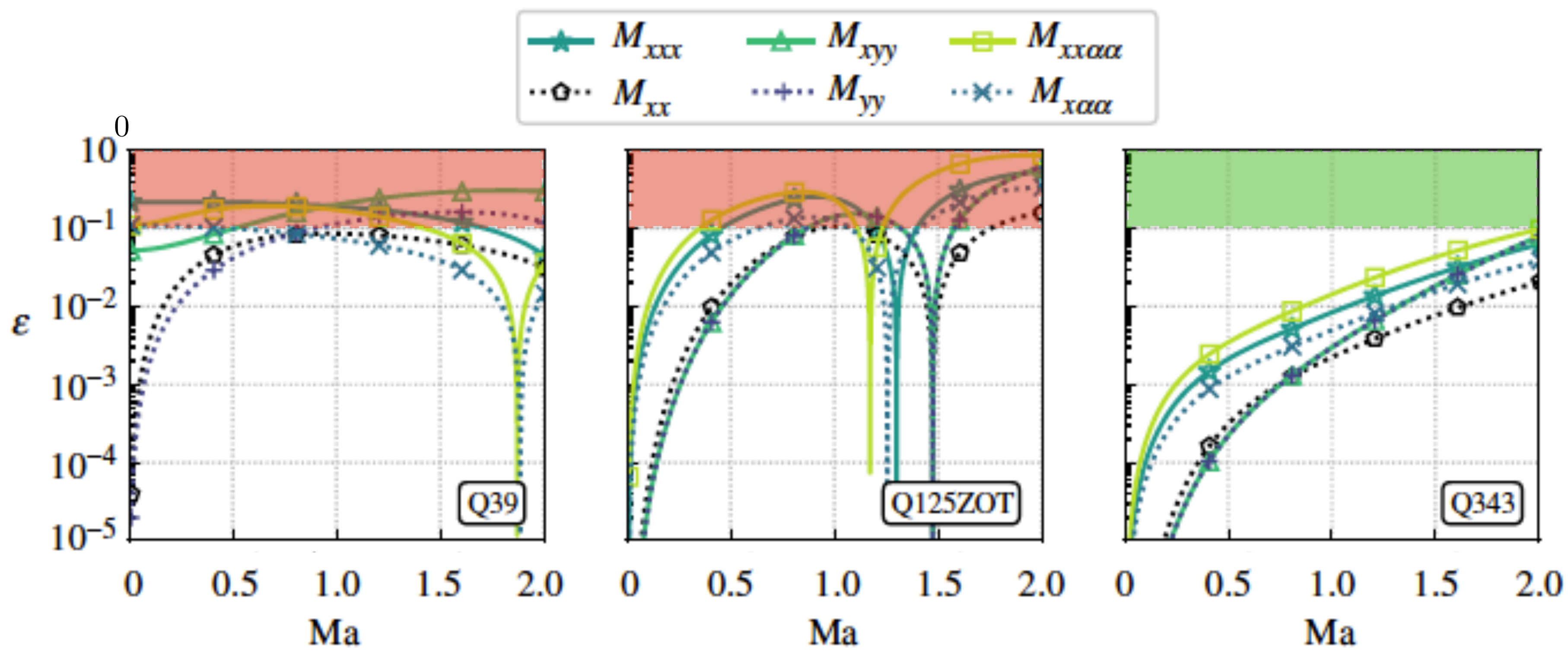
OK (Q343)

$$\varepsilon = \frac{\left|M_{pqr}^{\mathrm{MB}} - M_{pqr}^{\mathrm{eq}}\right|}{M_{pqr}^{\mathrm{MB}}}$$

Sets of constraints and macroscopic behavior

✤ **Standard 5-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq} \boldsymbol{\xi}_i - \rho \boldsymbol{u} = 0 \qquad G_{\mathrm{Tr}2} = \sum_i f_i^{eq} \xi_i^2 - 2\rho E = 0$$



Stability: OK

Accuracy:

NOK (Q39, Q125)

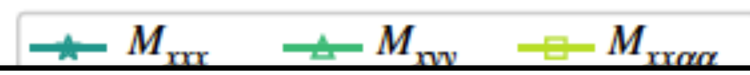
OK (Q343)

✤ **Requires large lattices to compensate for numerous errors (cf Frapolli's model)**

Sets of constraints and macroscopic behavior

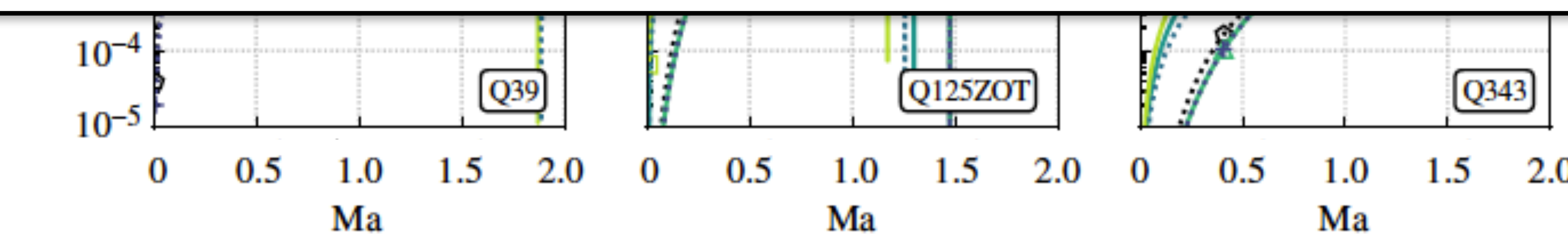
✤ **Standard 5-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq} \boldsymbol{\xi}_i - \rho \boldsymbol{u} = 0 \qquad G_{\mathrm{Tr}2} = \sum_i f_i^{eq} \xi_i^2 - 2\rho E = 0$$



Can we get the correct physics at a lower cost?…

Yes!… if you put more effort on the equilibrium instead of the lattice



OK (Q343)

✤ **Requires large lattices to compensate for numerous errors (cf Frapolli's model)**

Sets of constraints and macroscopic behavior

✤ **Full 26-moment approach**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq}\boldsymbol{\xi}_i - \rho\boldsymbol{u} = 0$$

$$G_2 = \sum_i f_i^{eq}\boldsymbol{\xi}_i^2 - \rho(\boldsymbol{u}^2 + T\boldsymbol{\delta}) = 0 \qquad G_3 = \sum_i f_i^{eq}\boldsymbol{\xi}_i^3 - \rho(\boldsymbol{u}^3 + T\boldsymbol{u}\boldsymbol{\delta}) = 0$$

$$G_{\mathrm{Tr}4} = \sum_i f_i^{eq}\xi_i^2\boldsymbol{\xi}_i^2 - 2\rho[(E+2T)\boldsymbol{u}^2 + (E+T)T\boldsymbol{\delta}] = 0$$

✤ **Exact behavior at the cost of robustness (convergence issues…)**

$$\partial_t(M_0^{eq}) + \nabla\cdot(M_1^{eq}) = 0$$

$$\partial_t(M_1^{eq}) + \nabla\cdot(M_2^{eq}) \propto \partial_t(M_2^{eq}) + \nabla\cdot(M_3^{eq})$$

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

Convective | Diffusive

Sets of constraints and macroscopic behavior

✤ **Full 26-moment approach**

$G_0 = \sum_i f_i^{eq} - \rho = 0$

$G_1 = \sum_i f_i^{eq} \boldsymbol{\xi}_i - \rho \boldsymbol{u} = 0$

$G_2 = \sum_i f_i^{eq} \boldsymbol{\xi}_i^2 - \rho(\boldsymbol{u}^2 + T\boldsymbol{\delta}) = 0$

$G_3 = \sum_i f_i^{eq} \boldsymbol{\xi}_i^3 - \rho(\boldsymbol{u}^3 + T\boldsymbol{u}\boldsymbol{\delta}) = 0$

One needs to find the proper balance between accuracy, efficiency and robustness

$$\partial_t(M_0^{eq}) + \nabla\cdot(M_1^{eq}) = 0$$

$$\partial_t(M_1^{eq}) + \nabla\cdot(M_2^{eq}) \propto \partial_t(M_2^{eq}) + \nabla\cdot(M_3^{eq})$$

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

Convective | Diffusive

Sets of constraints and macroscopic behavior

✤ **Pragmatic 13-moment approach (simplification of Le Tallec and Perlat)**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq}\boldsymbol{\xi}_i - \rho\boldsymbol{u} = 0$$

$$G_2 = \sum_i f_i^{eq}\boldsymbol{\xi}_i^2 - \rho(\boldsymbol{u}^2 + T\boldsymbol{\delta}) = 0 \qquad G_{\mathrm{Tr}3} = \sum_i f_i^{eq}\xi_i^2\boldsymbol{\xi}_i - 2\rho(E+T)\boldsymbol{u} = 0$$

✤ **Exact convective behavior and reduced diffusive errors (good trade-off)**

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

Convective — Diffusive

Le Tallec and Perlat, *Numerical Analysis of Levermore's Moment System INRIA,* **1997**

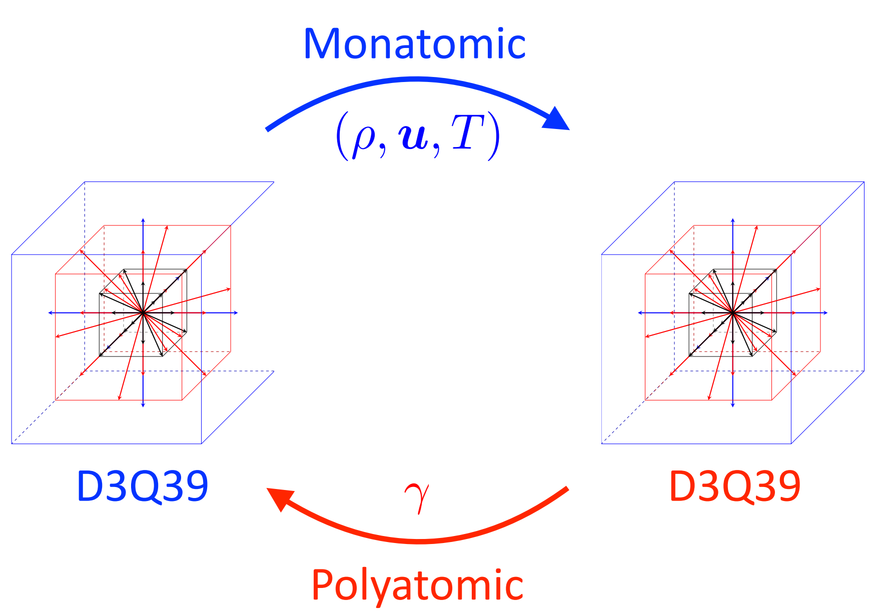
Sets of constraints and macroscopic behavior

✤ **Pragmatic 13-moment approach (simplification of Le Tallec and Perlat)**

$$G_0 = \sum_i f_i^{eq} - \rho = 0 \qquad G_1 = \sum_i f_i^{eq}\boldsymbol{\xi}_i - \rho\boldsymbol{u} = 0$$

$$G_2 = \sum_i f_i^{eq}\boldsymbol{\xi}_i^2 - \rho(\boldsymbol{u}^2 + T\boldsymbol{\delta}) = 0 \qquad G_{\mathrm{Tr}3} = \sum_i f_i^{eq}\xi_i^2\boldsymbol{\xi}_i - 2\rho(E+T)\boldsymbol{u} = 0$$

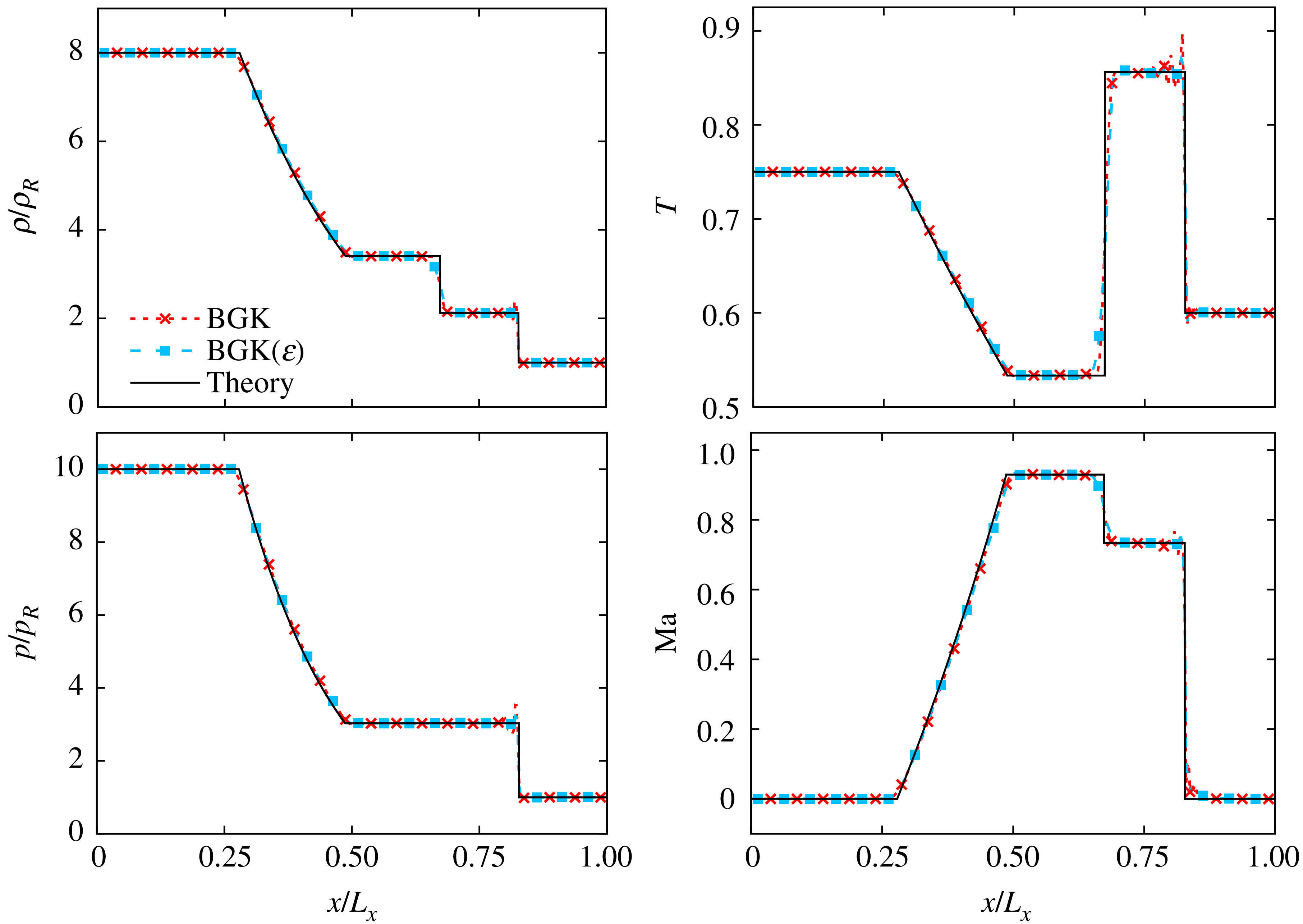
✤ **It is sufficient to work with 39 velocities (as in PowerFLOW software)**



Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

Results - Sod Shock Tube

✤ Inviscid Sod shock tube using 400 points



- Good robustness even using the BGK operator
- Kinetic sensor allows for **inviscid** simulations

$$\epsilon = \frac{1}{V}\sum_{i=0}^{V-1}\frac{|f_i - f_i^{\mathrm{eq}}|}{f_i^{\mathrm{eq}}}$$

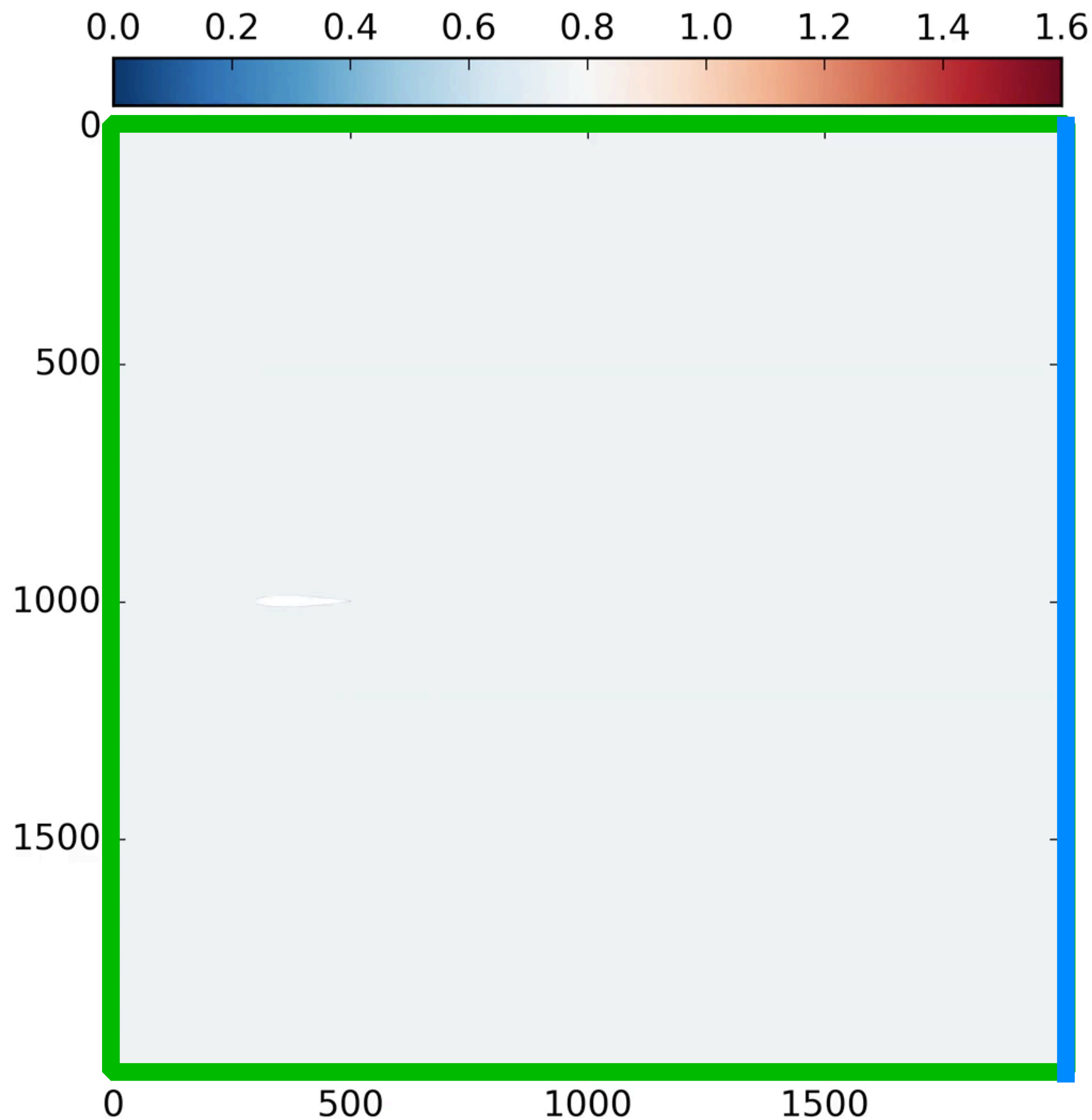
↑

Thanks to
Florian De Vuyst's
for this idea!

Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

Results - 2D NACA0012

✤ **Mach number field**



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Results - 2D NACA0012

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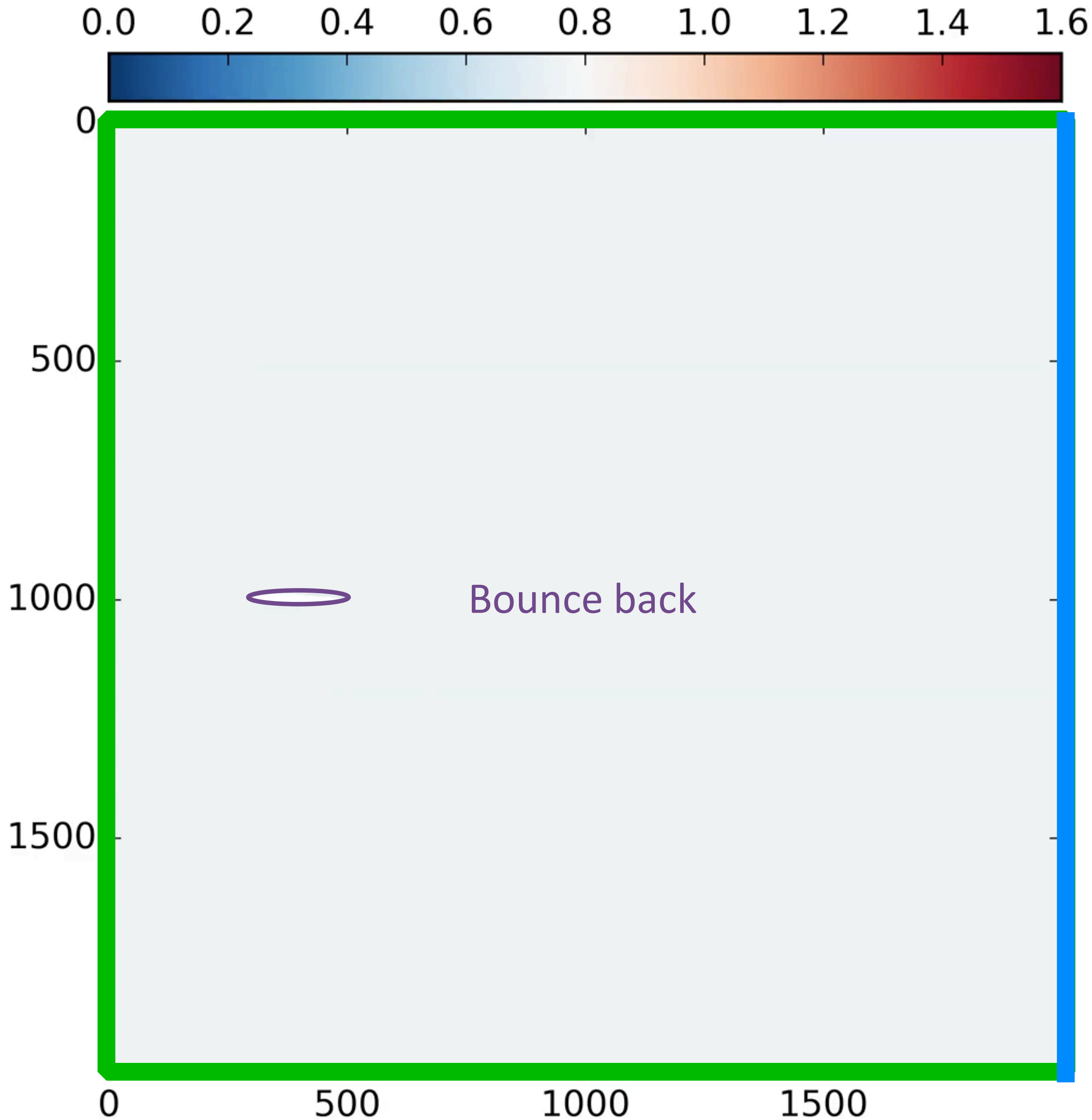

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Results - 2D NACA0012

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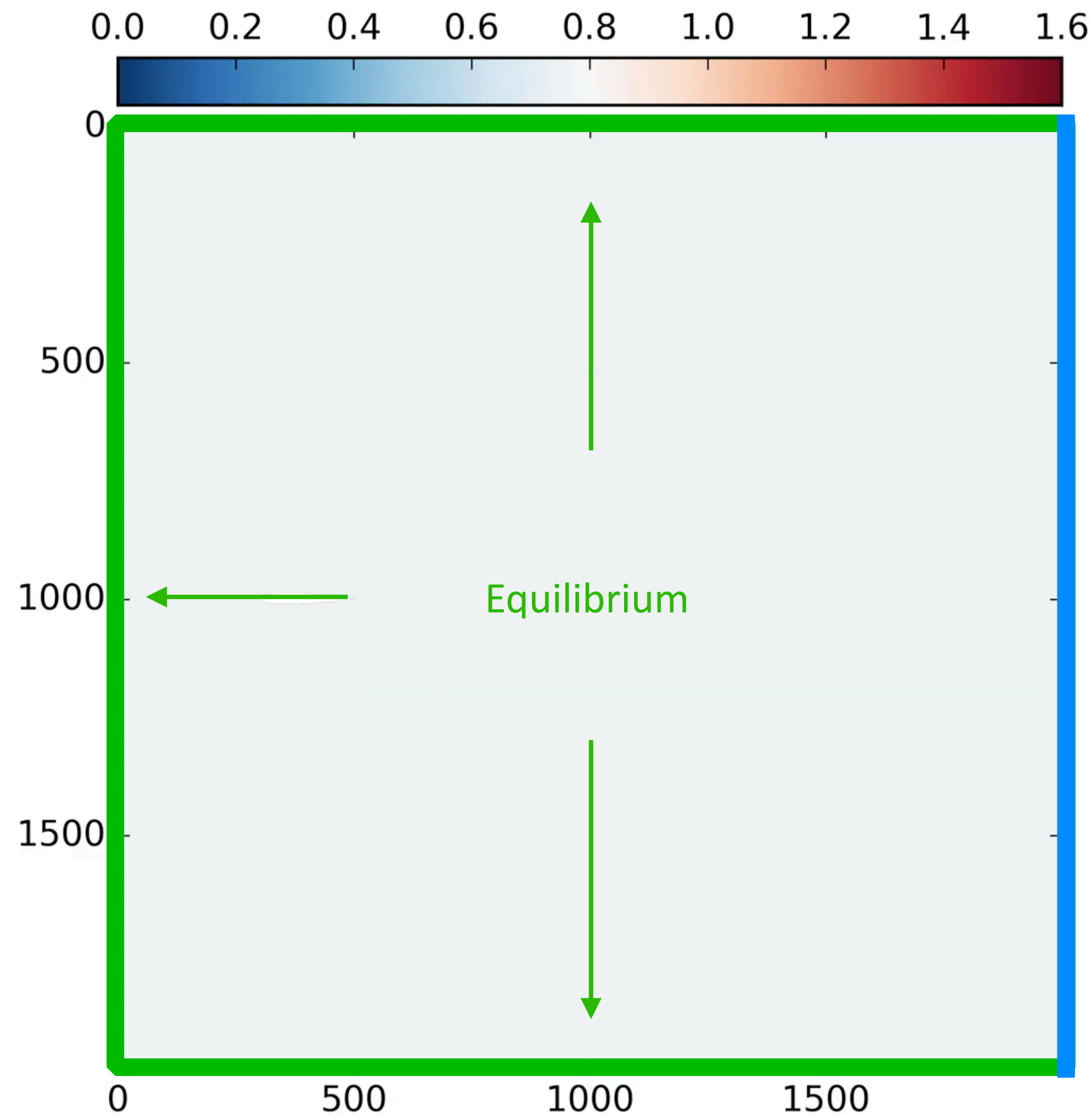

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Results - 2D NACA0012

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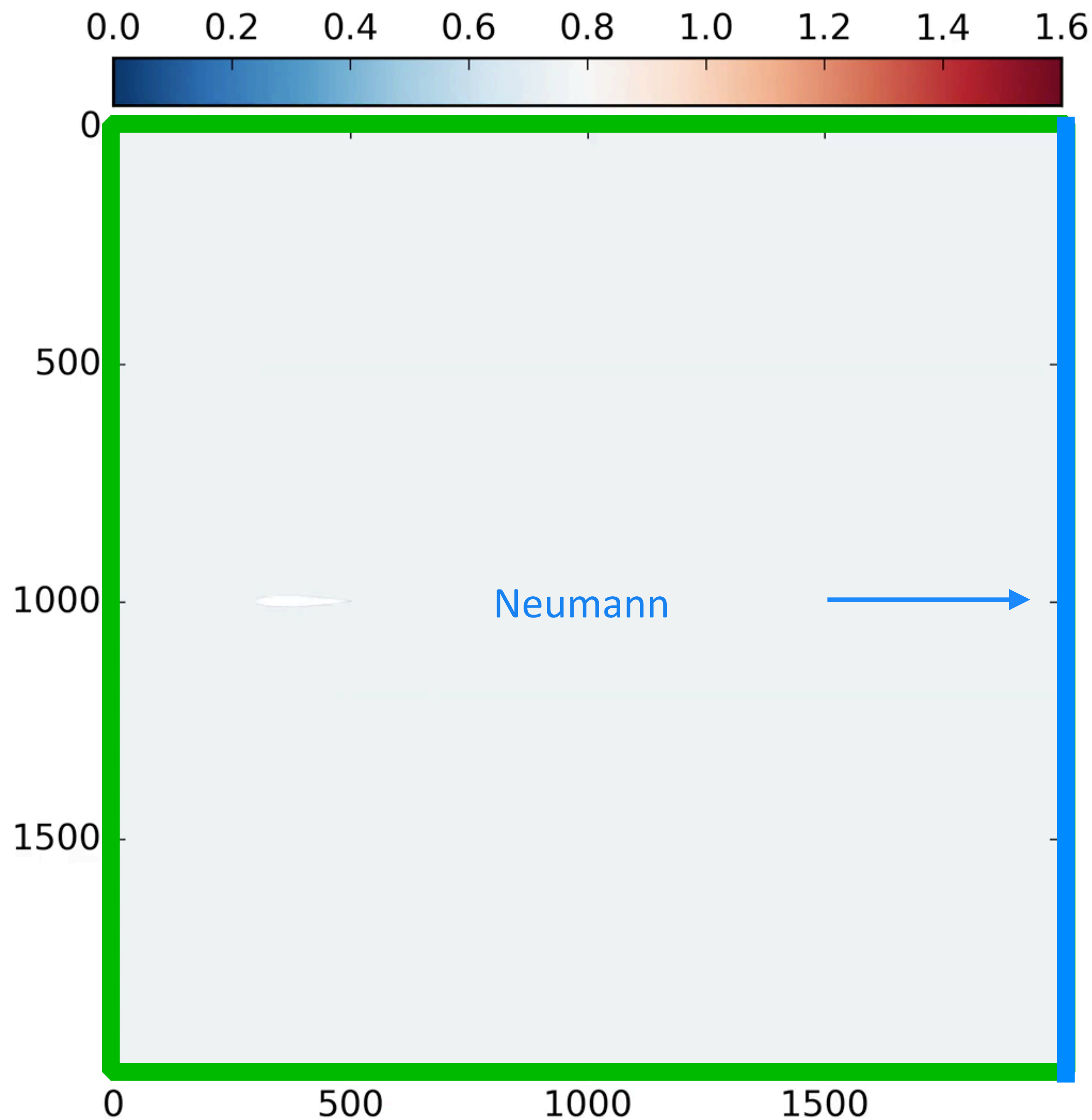

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Results - 2D NACA0012

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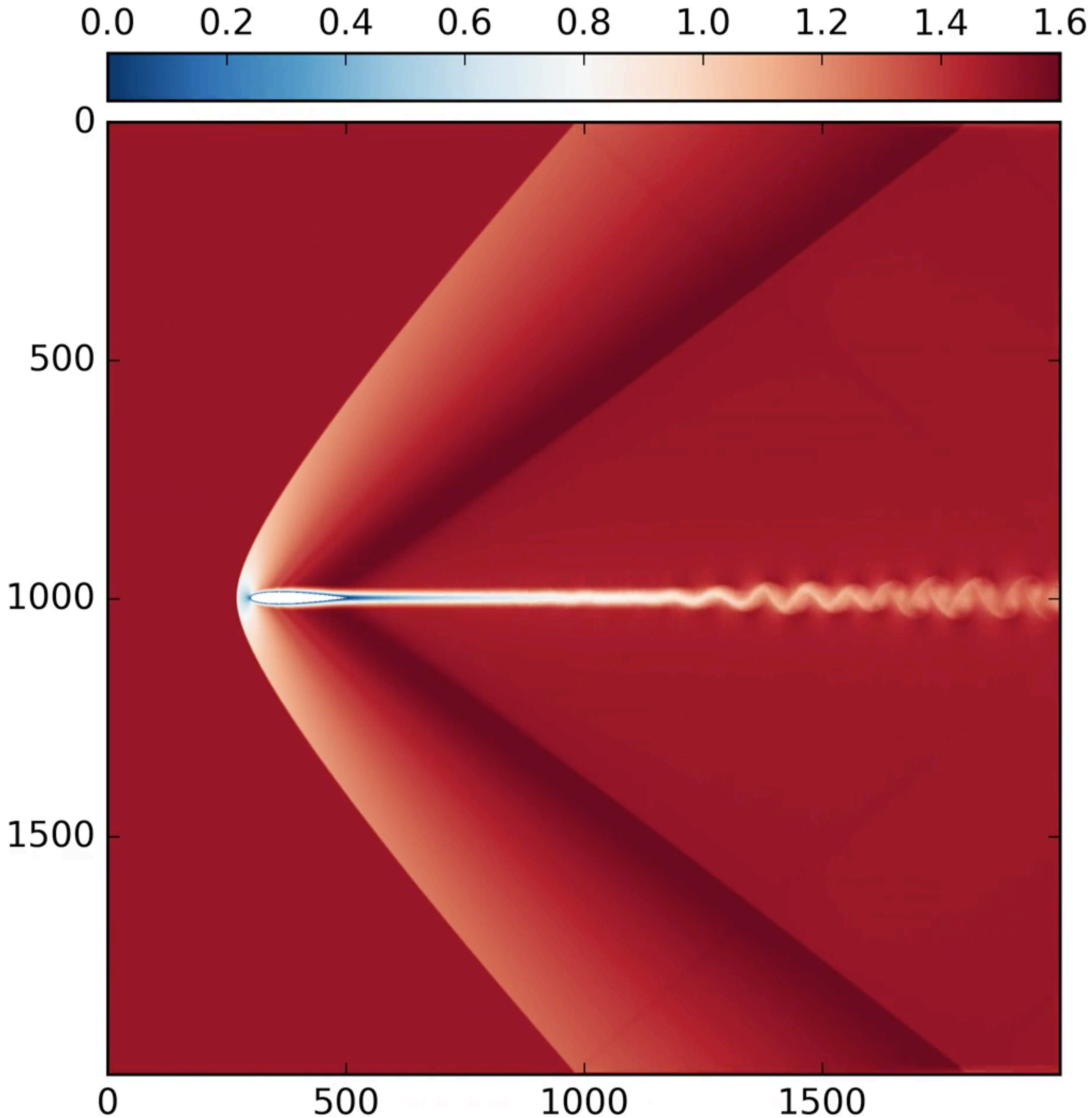
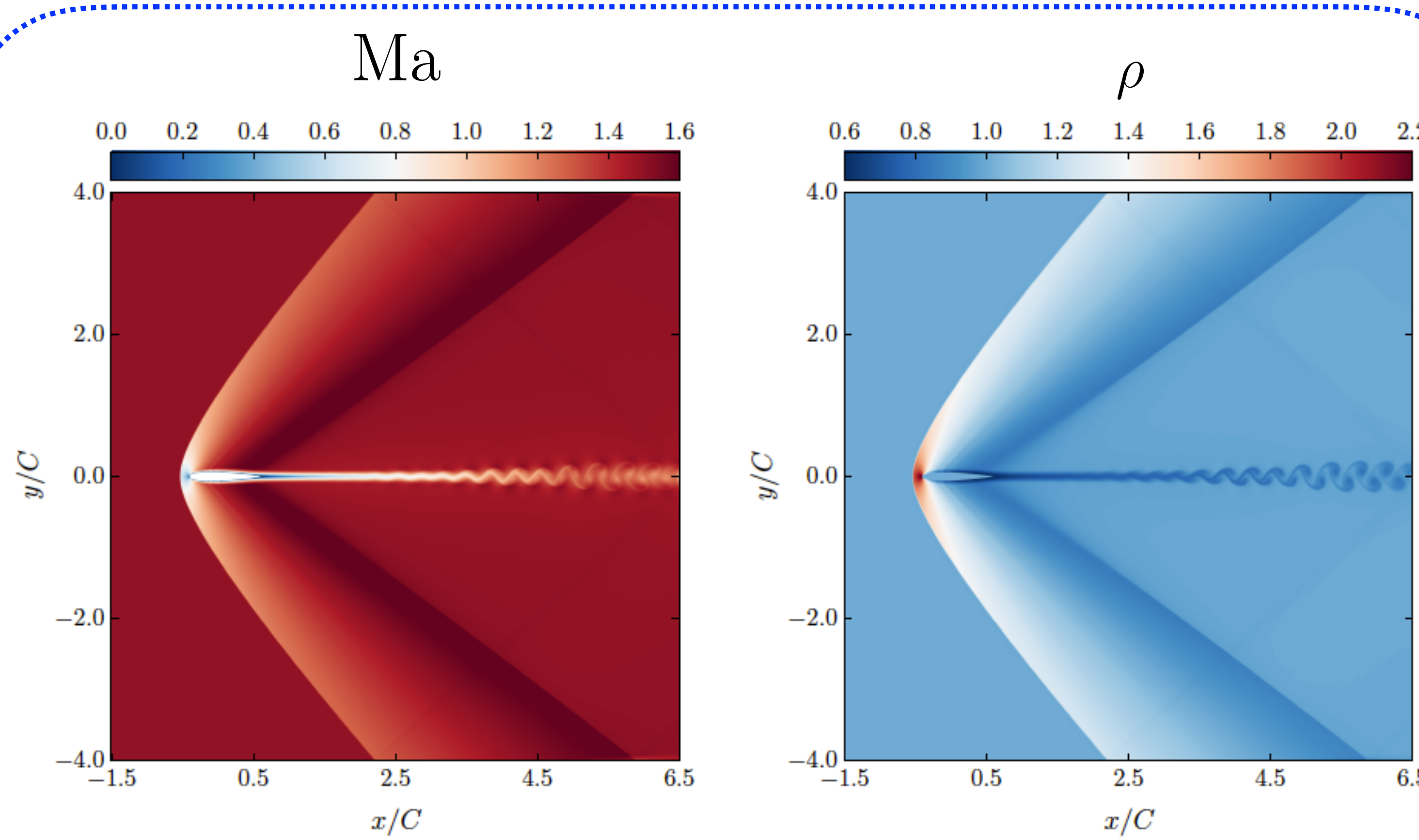


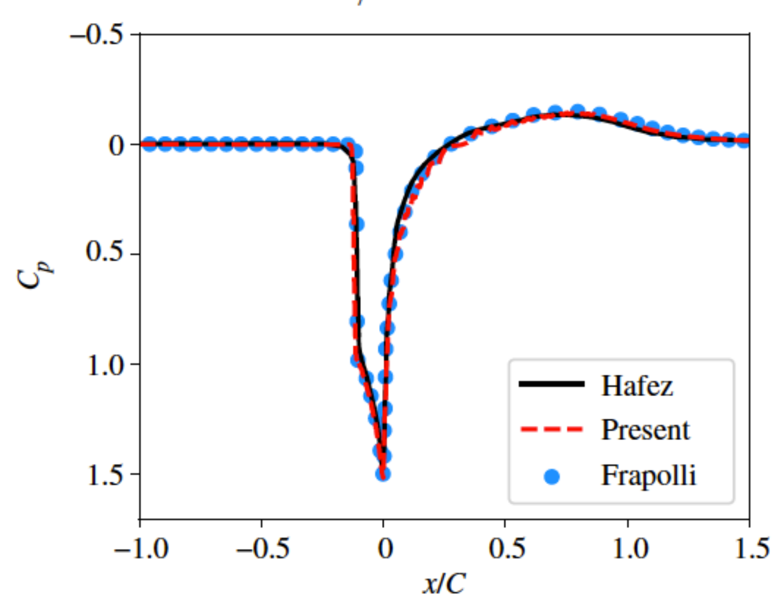
- **Surprisingly**, all BCs have a **good** behavior
- **Only the BB** leads to **spurious** oscillations

Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

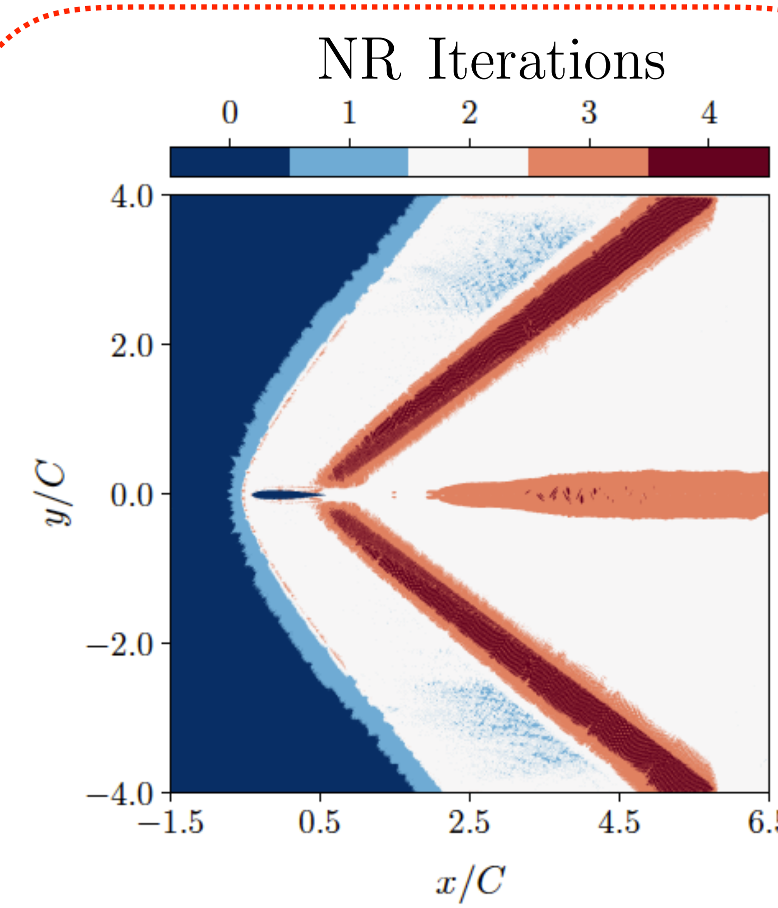
Results - 2D NACA0012

✤ **High-Reynolds number flow past a 2D airfoil: [8C, 8C, 1] with C=350 points**





- Good accuracy
- Speedup ~ 100

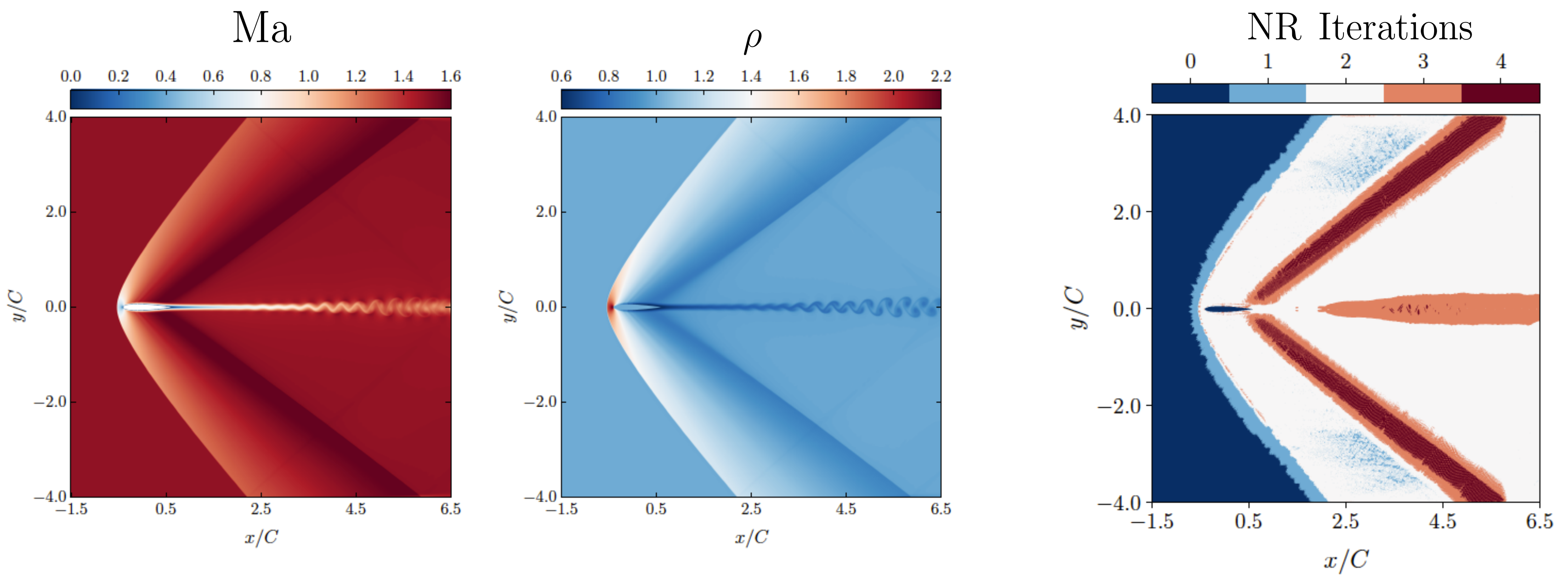


- Fast convergence ~ 2 ite
- Faster in smooth regions

Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

Results - 2D NACA0012

✤ **High-Reynolds number flow past a 2D airfoil: [8C, 8C, 1] with C=350 points**



Hardware	i7-8700 (3.2 GHz)	GTX 1080 Ti	RTX 2080 Ti	Volta 100	Ampere 100
MLUPS	0.67	12	17	30	~ 60
μs/pt/it	1.49	0.083	0.059	0.033	~ 0.016

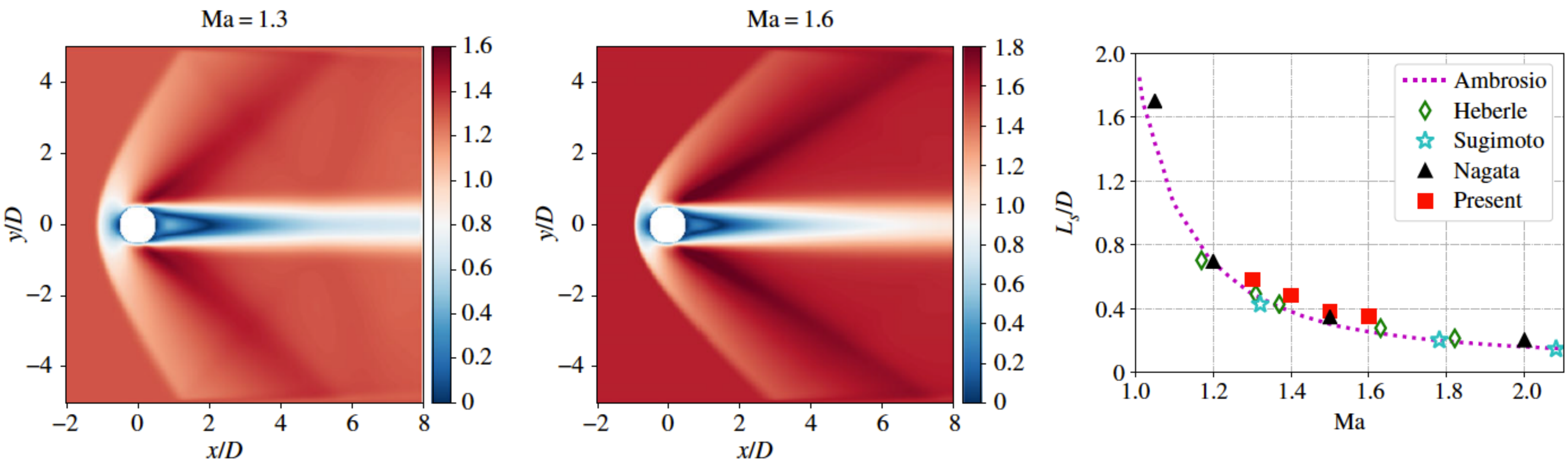
Median of performance evaluated every 100 iterations (C=256)

GPUs allow for a good speedup (10-100)!

Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

Results - 3D behavior

✤ **Low-Reynolds number flow past a sphere: [10D, 10D, 10D] with D=30 points**



- The main features are well captured
- Shock stand-off distances are in agreement with experiments, models and simulations

Latt et al., Efficient supersonic flow simulations using lattice Boltzmann methods based on numerical equilibria
Phil. Trans. R. Soc. A, **2020**, 378, 20190559

Outline

How do we design LBMs?

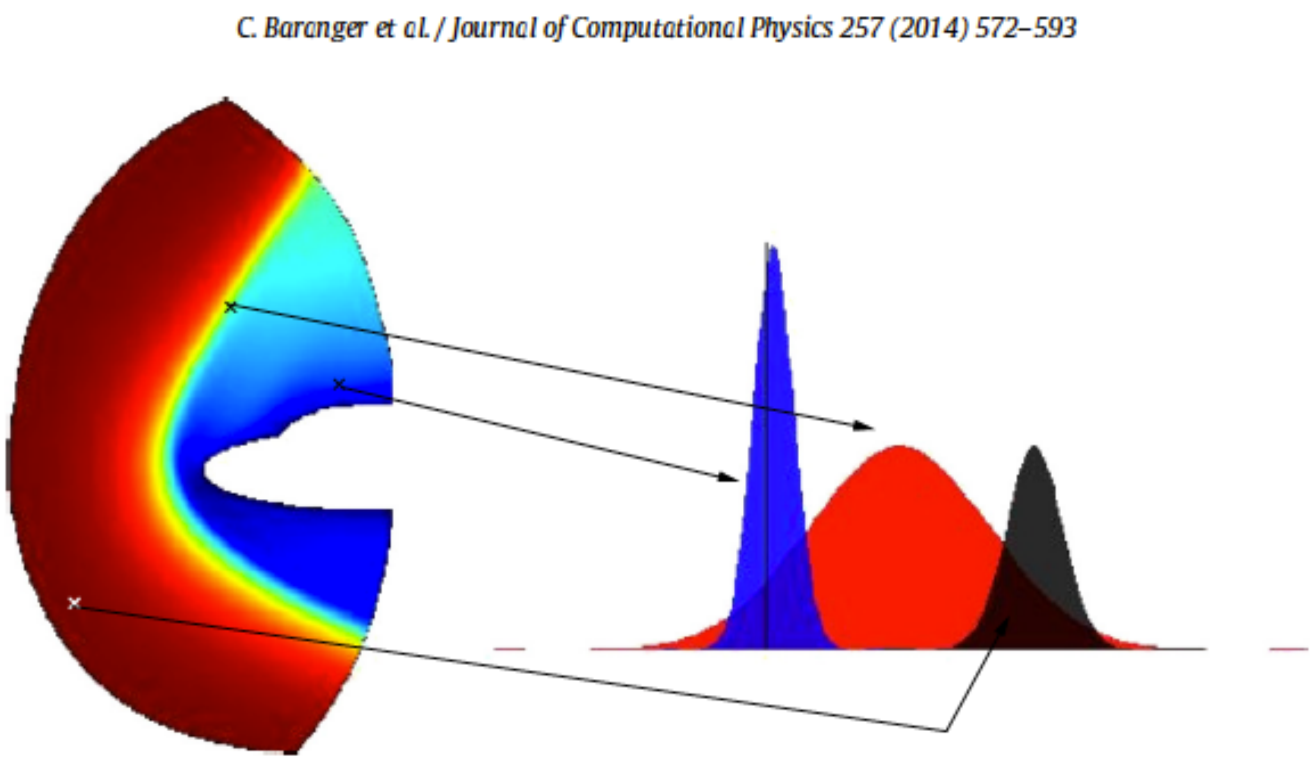
Two-equation models

Quadrature free LBMs

Adaptive lattices

Link between physics and velocity discretization

Idea: Velocity distribution functions have different shapes depending on the local flow conditions



Typical flow conditions during atmospheric re-entry

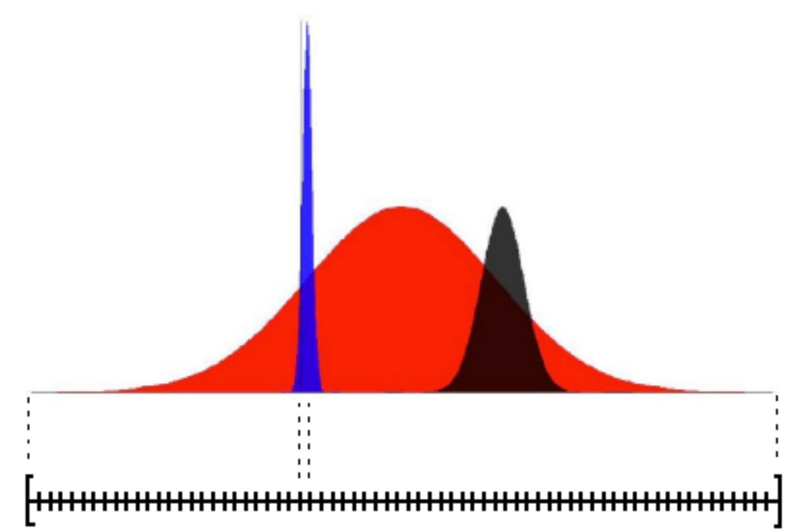
<u>Best practices (DVMs)</u>

Mieussens, Math. Models Methods Appl. Sci., 2000, 10, 1121-1149

$$\min_{\mathcal{K}} v_k^{(i)} \leq u^{(i)} \leq \max_{\mathcal{K}} v_k^{(i)}, \quad i = 1, \ldots, D$$

$$\frac{1}{DR} \min_{\mathcal{K}} |v_k - u|^2 \leq T \leq \frac{1}{DR} \max_{\mathcal{K}} |v_k - u|^2$$

Static manner to ensure good properties



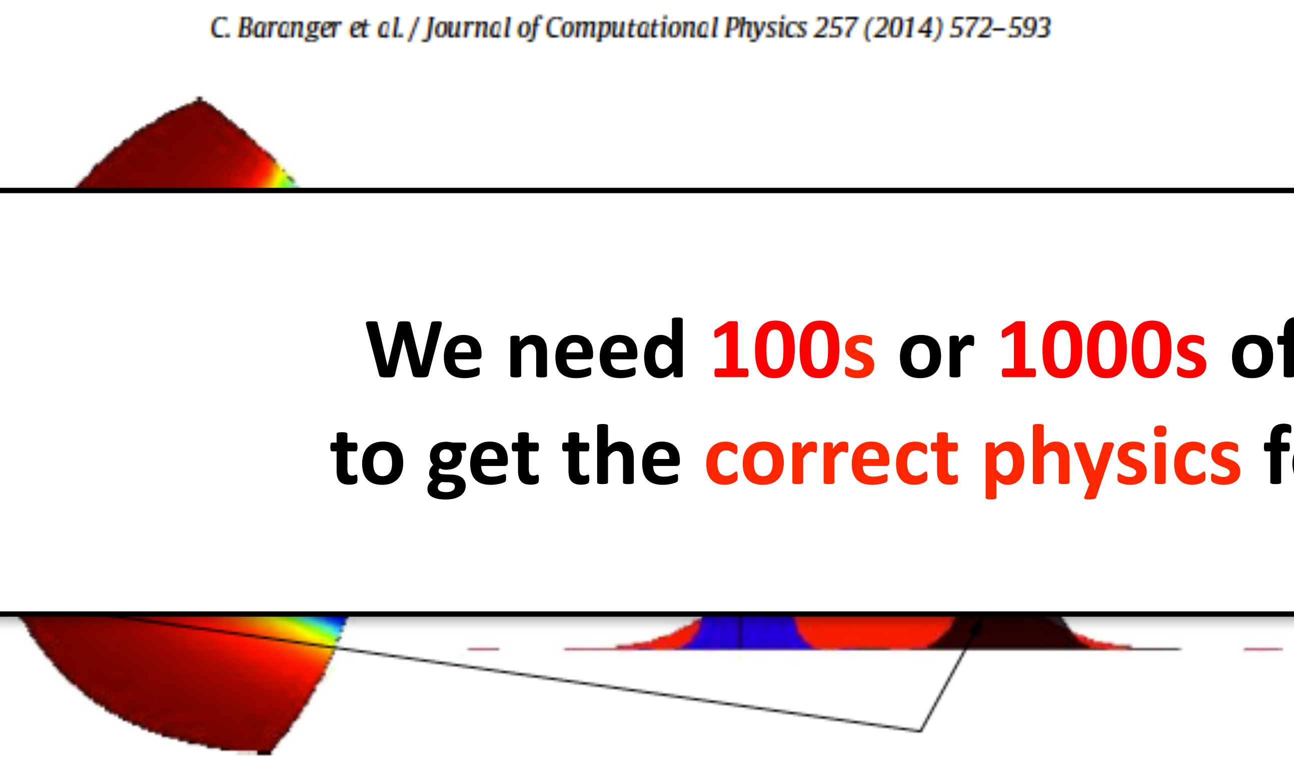
Link between physics and velocity discretization

Idea: Velocity distribution functions have different shapes depending on the local flow conditions

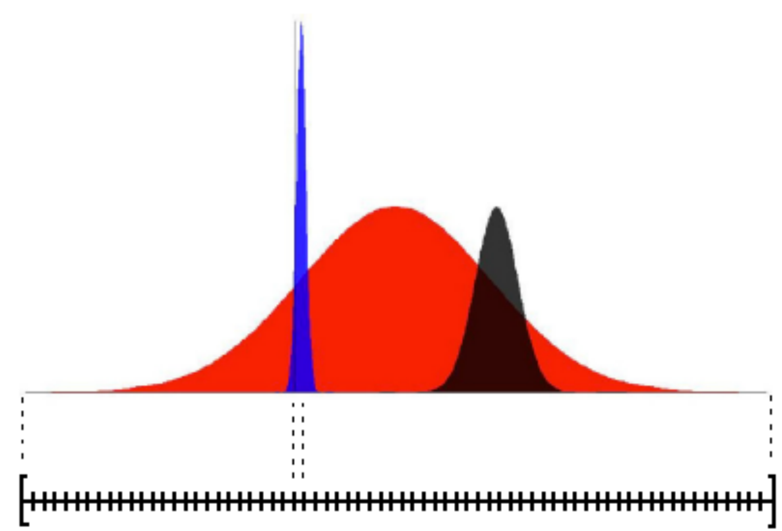
<u>Best practices (DVMs)</u>

Mieussens, Math. Models Methods Appl. Sci., 2000, 10, 1121-1149

We need 100s or 1000s of discrete velocities
to get the correct physics for large variations…

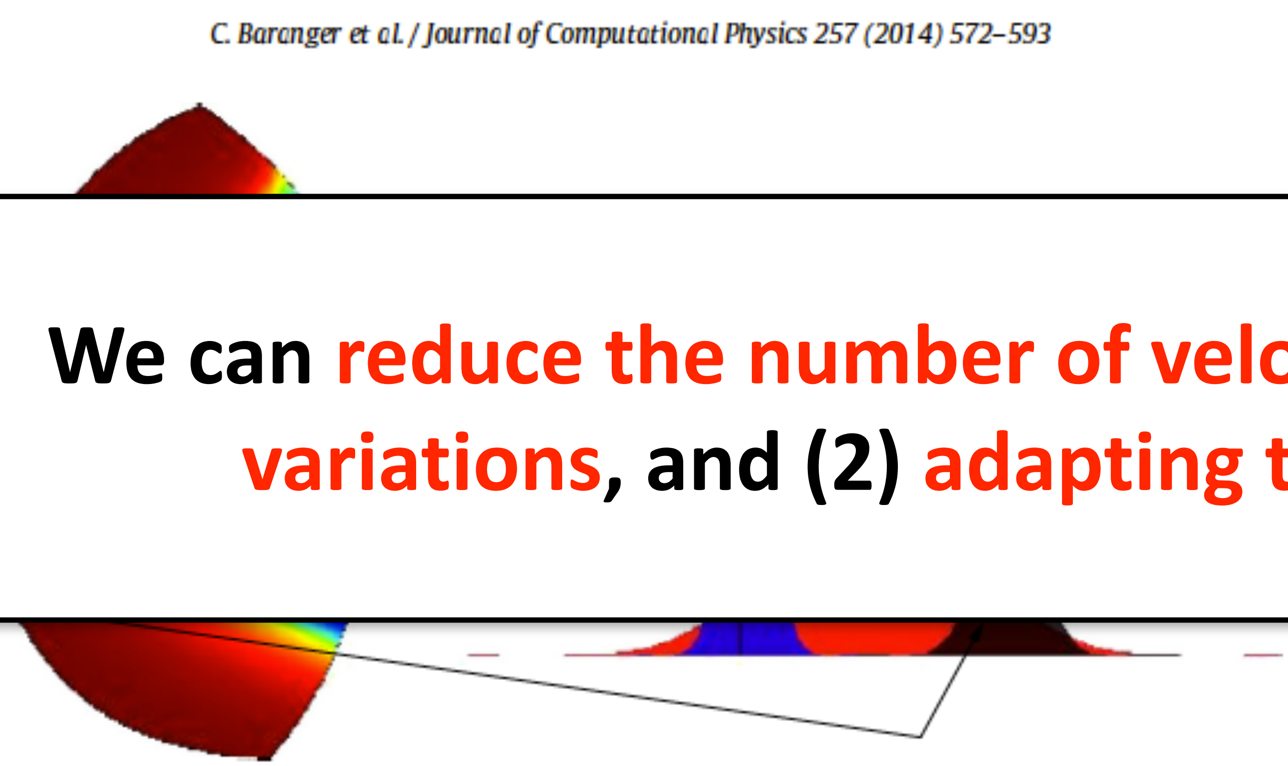


Typical flow conditions during atmospheric re-entry



Link between physics and velocity discretization

Idea: Velocity distribution functions have different shapes depending on the local flow conditions

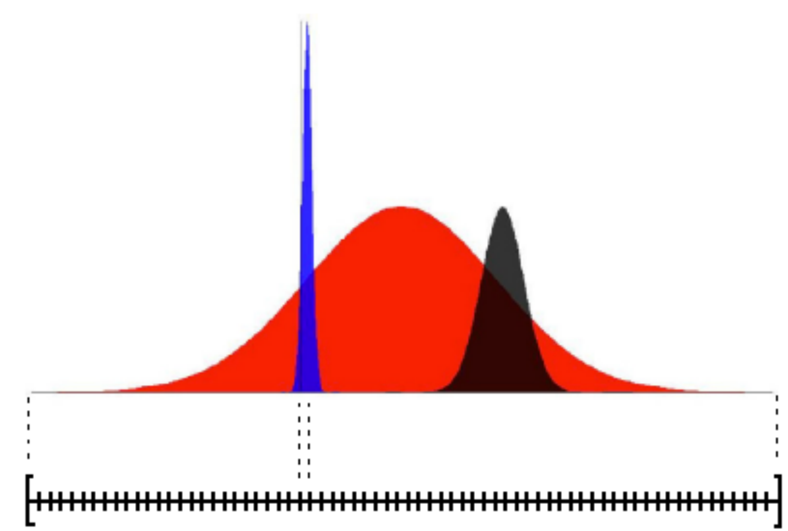


Best practices (DVMs)

Mieussens, Math. Models Methods Appl. Sci., 2000, 10, 1121-1149

We can reduce the number of velocities by (1) looking at local variations, and (2) adapting the lattice accordingly!

Typical flow conditions during atmospheric re-entry



Increased efficiency through adaptive velocities

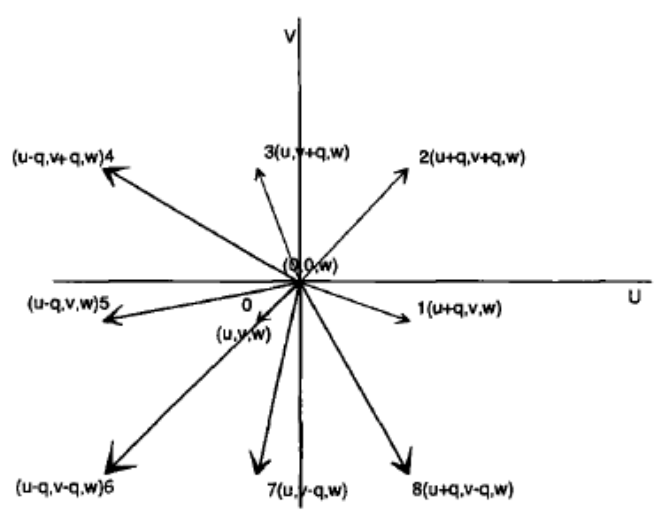
Concept introduced in the 1990s/2000s for the simulation of supersonic flows

1. DVMs

An Euler Solver Based on Locally Adaptive Discrete Velocities

B. T. Nadiga[1]

Received October 12, 1994



D3Q27 formulation

A THERMAL LBGK MODEL FOR LARGE DENSITY AND TEMPERATURE DIFFERENCES

JIAN HUANG, FENG XU, MICHEL VALLIÈRES, DA HSUAN FENG
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YUE-HONG QIAN
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BRUCE FRYXELL
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E-mail: fryxell@neutrino.gsfc.nasa.gov

MIKE R. STRAYER
Physics Division, Oak Ridge National Laboratory
Oak Ridge, TN 37831, USA
E-mail: strayermr@ornl.gov

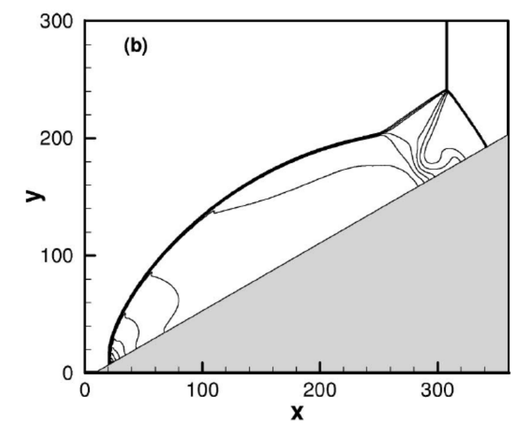
Received 31 October 1996
Revised 6 March 1997

$$\{\mathbf{v_i}\} = \left\{\mathbf{u} + \sqrt{\frac{\varsigma e}{e_0}}\mathbf{C_i}\right\}$$

Increased efficiency through adaptive velocities

Concept introduced in the 1990s/2000s for the simulation of supersonic flows

1. DVMs
2. LBMs

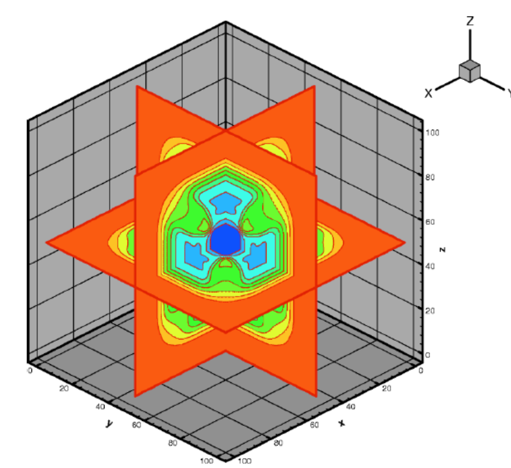


Euler

PHYSICAL REVIEW E VOLUME 58, NUMBER 6 DECEMBER 1998

Lattice-Boltzmann models for high speed flows

Chenghai Sun
State Key Laboratory of Tribology, Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China
(Received 17 December 1997; revised manuscript received 22 May 1998)

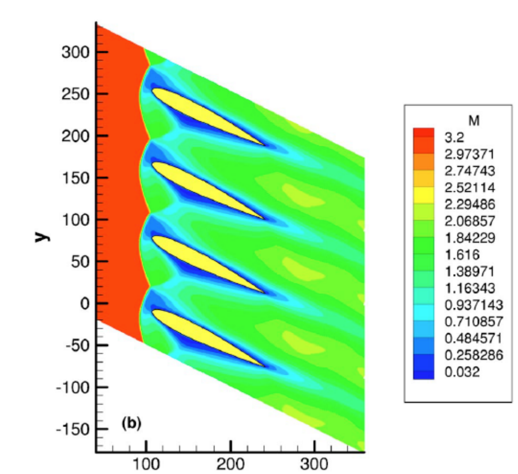


Euler

PHYSICAL REVIEW E VOLUME 61, NUMBER 3 MARCH 2000

Adaptive lattice Boltzmann model for compressible flows: Viscous and conductive properties

Chenghai Sun
State Key Laboratory of Tribology, Department of Engineering Mechanics, Tsinghua University, Beijing 100084, People's Republic of China
(Received 9 July 1999; revised manuscript received 24 September 1999)



NSF

PHYSICAL REVIEW E 68, 016303 (2003)

Three-dimensional lattice Boltzmann model for compressible flows

Chenghai Sun* and Andrew T. Hsu†
Department of Mechanical Engineering, Indiana University-Purdue University, Indianapolis, Indiana 46202-5132, USA
(Received 4 December 2001; revised manuscript received 18 December 2002; published 11 July 2003)

Static shift of velocity discretizations

Shifted lattices are the rule for DVMs but exceptions for LBMs

Lattice Kinetic Theory in a Comoving Galilean Reference Frame

N. Frapolli,[*] S. S. Chikatamarla,[†] and I. V. Karlin[‡]
Department of Mechanical and Process Engineering, ETH Zurich, 8092 Zurich, Switzerland
(Received 25 April 2016; published 30 June 2016)

Lattice Boltzmann model for compressible flows on standard lattices: Variable Prandtl number and adiabatic exponent

Mohammad Hossein Saadat,[*] Fabian Bösch,[†] and Ilya V. Karlin[‡]
Department of Mechanical and Process Engineering, ETH Zurich, 8092 Zurich, Switzerland
(Received 2 July 2018; published 18 January 2019)

Application of DVMs' best practices to LBMs

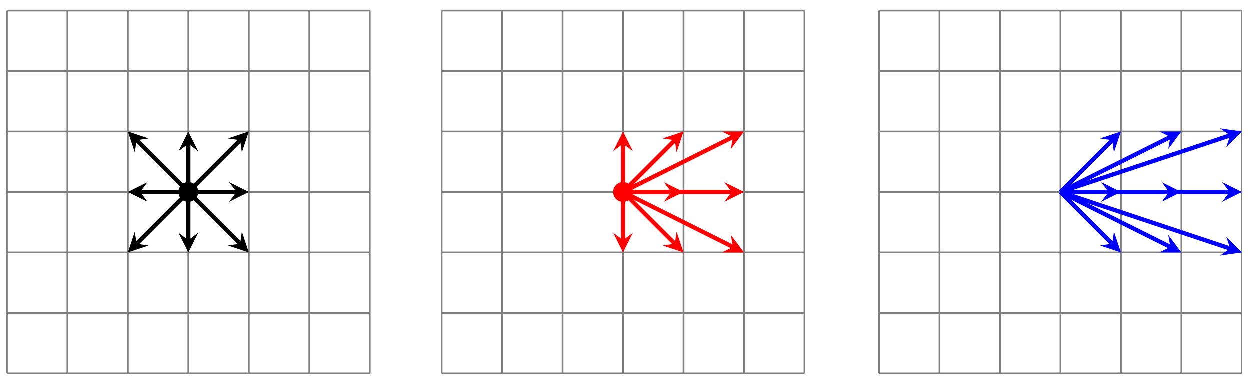
Extensive analysis of the lattice Boltzmann method on shifted stencils

S. A. Hosseini,[1,2,3] C. Coreixas,[4] N. Darabiha,[2] and D. Thévenin[1]
[1]*Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg "Otto von Guericke," D-39106 Magdeburg, Germany*
[2]*Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay, 91192 Gif-sur-Yvette Cedex, France*
[3]*International Max Planck Research School (IMPRS) for Advanced Methods in Process and Systems Engineering, Magdeburg, Germany*
[4]*Department of Computer Science, University of Geneva, 1204 Geneva, Switzerland*
(Received 21 September 2019; published 4 December 2019)

Understanding their impact on LBMs (macroscopic and numerical errors)

Static shift of velocity discretizations

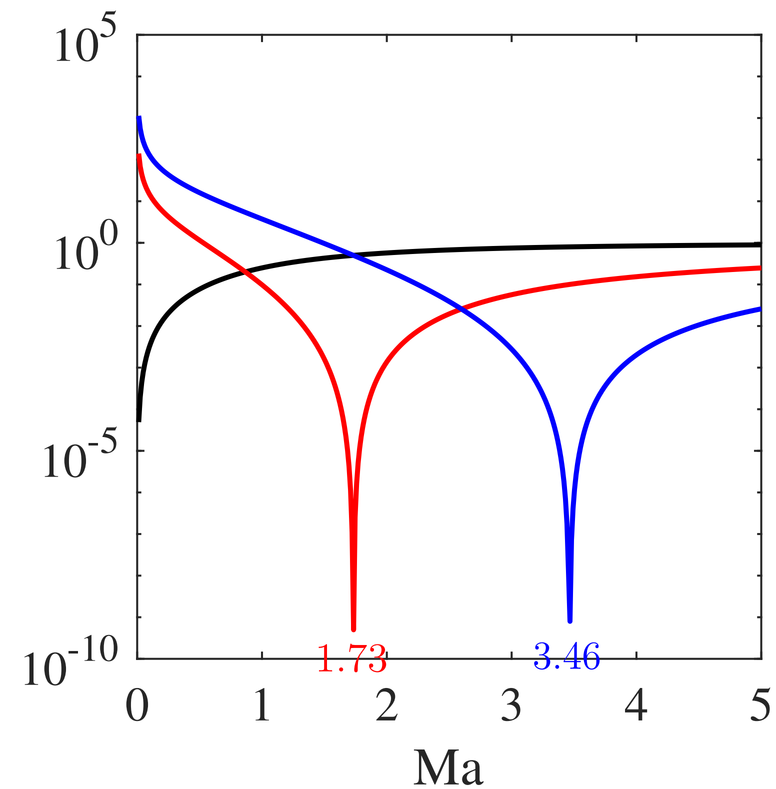
Shifted lattices shift the physical properties…



$\boldsymbol{U} = (0,0)$, $\mathrm{Ma}^{opt} = 0$

$\boldsymbol{U} = (1,0)$, $\mathrm{Ma}^{opt} = 1/c_s \approx 1.73$

$\boldsymbol{U} = (2,0)$, $\mathrm{Ma}^{opt} = 2/c_s \approx 3.46$



$$\epsilon = \frac{|a^{(3)}_{\mathrm{MB}} - a^{(3)}_{\mathrm{eq}}|}{a^{(3)}_{\mathrm{MB}}}$$

Extensive analysis of the lattice Boltzmann method on shifted stencils

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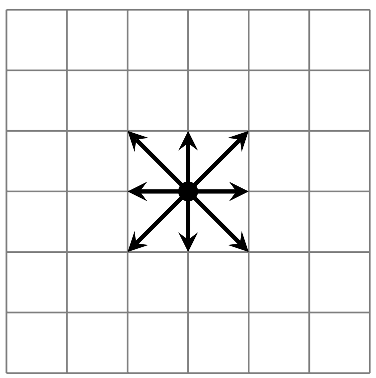
(Received 21 September 2019; published 4 December 2019)

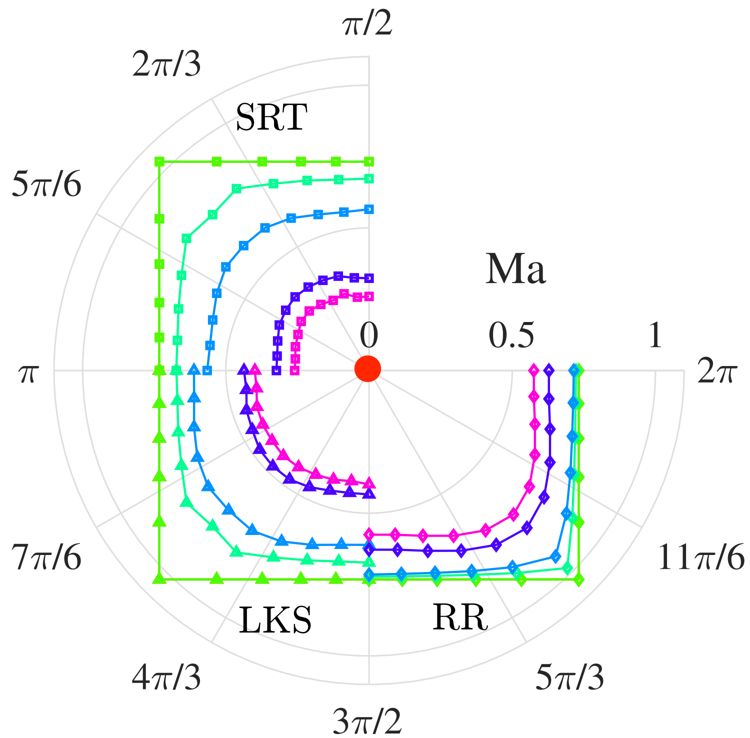
Understanding their impact on LBMs (**macroscopic** and numerical errors)

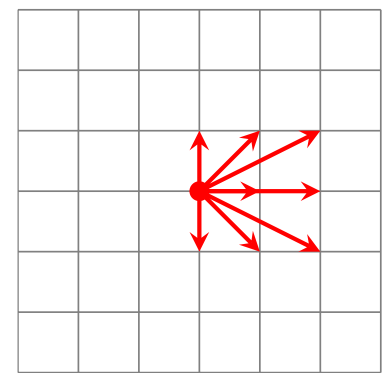
Static shift of velocity discretizations

Shifted lattices shift the physical properties… and the numerical ones!

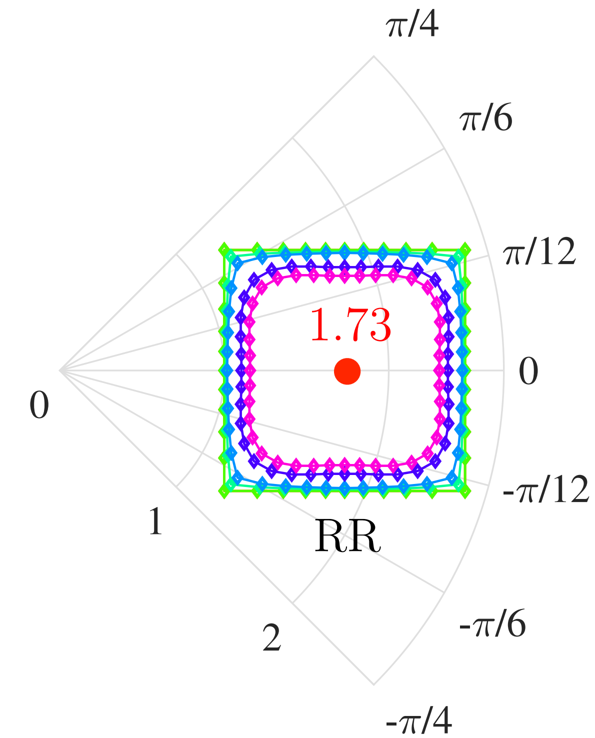


$\boldsymbol{U} = (0,0)$
$\mathrm{Ma}^{opt} = 0$





$\boldsymbol{U} = (1,0)$
$\mathrm{Ma}^{opt} = 1/c_s$
≈ 1.73



Extensive analysis of the lattice Boltzmann method on shifted stencils

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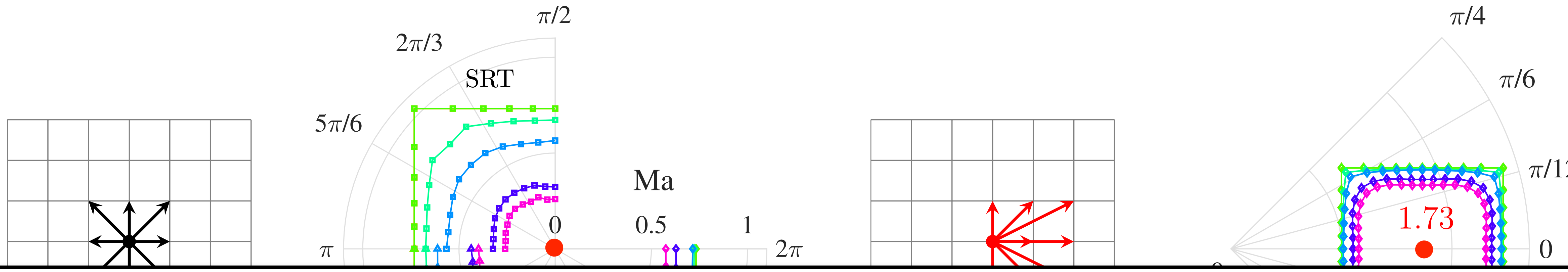
(Received 21 September 2019; published 4 December 2019)

Understanding their impact on LBMs (macroscopic and **numerical** errors)

Static shift of velocity discretizations

Shifted lattices shift the physical properties… and the numerical ones!



Optimal accuracy and stability by adjusting the lattice to local macroscopic conditions!

Extensive analysis of the lattice Boltzmann method on shifted stencils

S. A. Hosseini,[1,2,3] C. Coreixas,[4] N. Darabiha,[2] and D. Thévenin[1]

[1] *Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg "Otto von Guericke," D-39106 Magdeburg, Germany*
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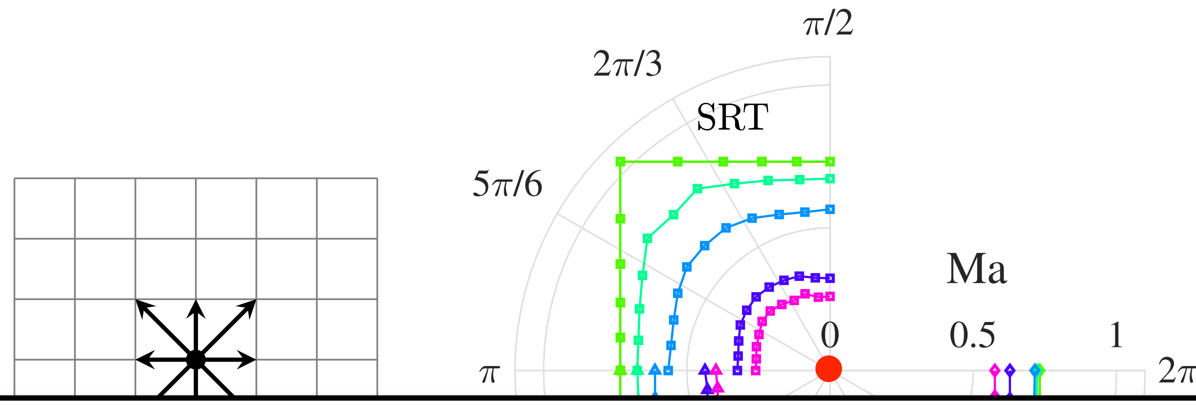
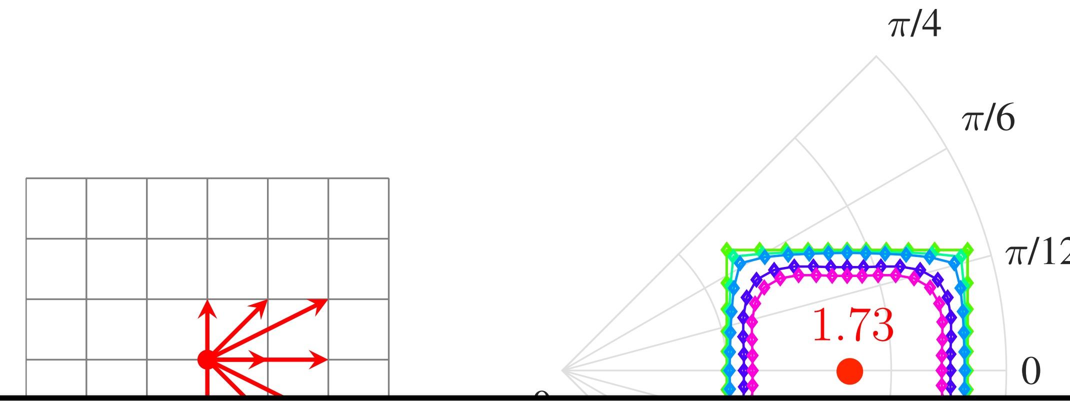
(Received 21 September 2019; published 4 December 2019)

Understanding their impact on LBMs (macroscopic and **numerical** errors)

Static shift of velocity discretizations

Shifted lattices shift the physical properties… and the numerical ones!





I'll upload a code on RG for people to play with it (convected vortex simulation)

Extensive analysis of the lattice Boltzmann method on shifted stencils

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[3]*International Max Planck Research School (IMPRS) for Advanced Methods in Process and Systems Engineering, Magdeburg, Germany*
[4]*Department of Computer Science, University of Geneva, 1204 Geneva, Switzerland*

(Received 21 September 2019; published 4 December 2019)

Understanding their impact on LBMs (macroscopic and **numerical** errors)

Overview and recent developments

Several authors are reviving the concept of adaptive LBMs, and propose alternative ways to reconstruct missing information

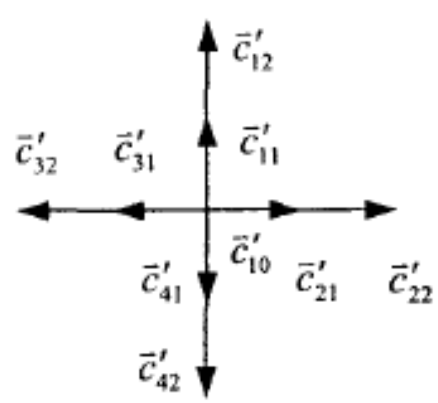
- Sun, Hsu et al. (end 1990s - beg 2000s)

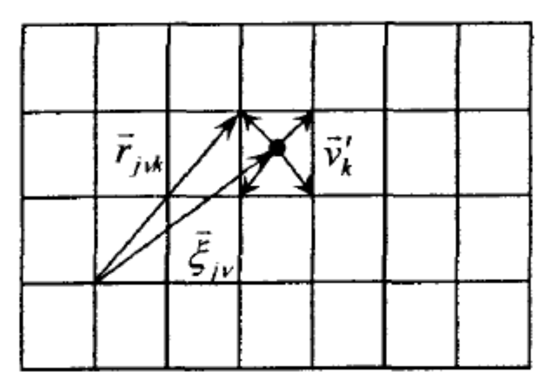
  1 - Redistribution of macros during streaming

  2 - Pragmatic reconstruction

  f_i^{eq} + correction terms (viscous effects)

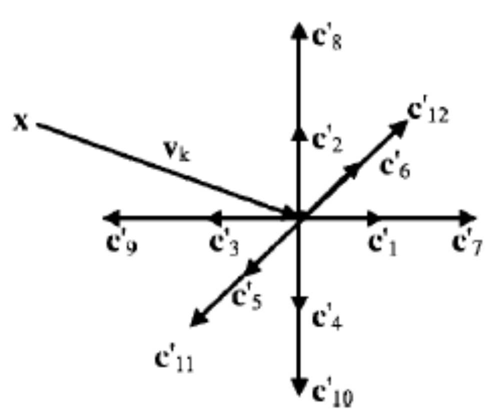
D2Q8

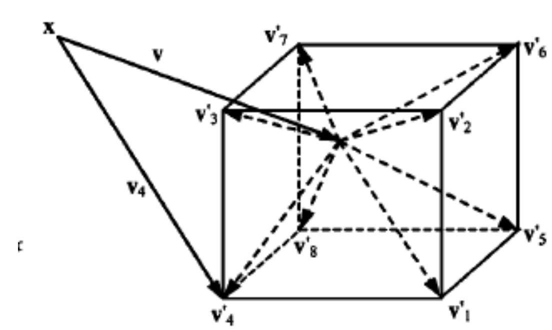




4x8=32
« virtual »
velocities

D3Q12





8x12=96
« virtual »
velocities

Overview and recent developments

Several authors are reviving the concept of adaptive LBMs, and propose alternative ways to reconstruct missing information

- <u>Sun, Hsu et al. (end 1990s - beg 2000s)</u>

  1 - Redistribution of macros during streaming

  2 - Pragmatic reconstruction

  f_i^{eq} + correction terms (viscous effects)

+ Efficient reconstruction of missing populations
+ No interpolation (parallel efficiency + conservativity)
- Complex partitioned streaming (but local)
- Requires correction terms (viscous)

A Review of Lattice Boltzmann Models for Compressible Flows

A.T. Hsu[a], T. Yang[a], I. Lopez[b], and A. Ecer[a]

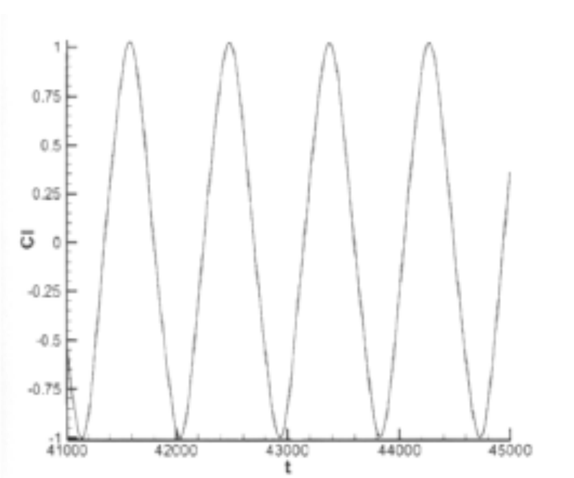


Figure 4. Lift coefficient on circular cylinder

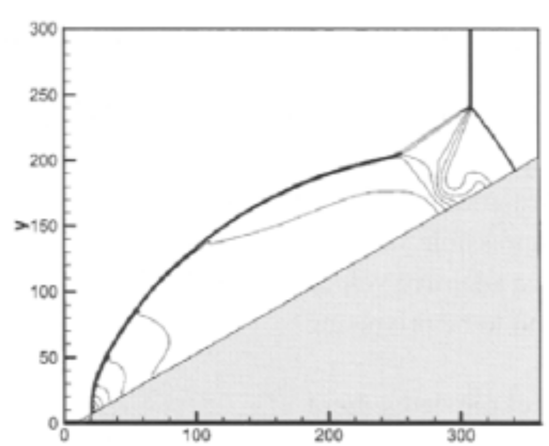


Figure 5. Mach 10 shock reflection

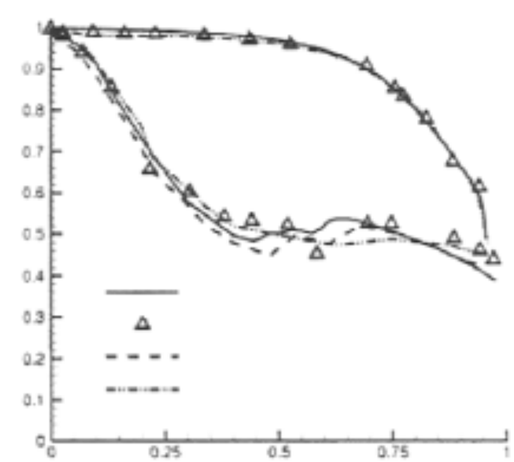


Figure 6. Pressure distribution on cascade blades

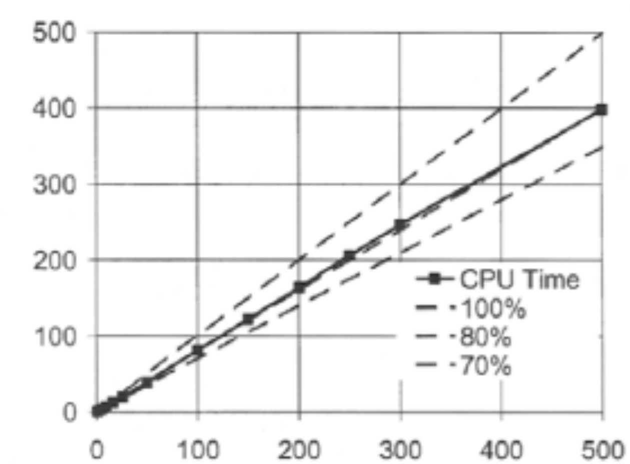


Figure 7 Parallel efficiency of LBM

Hsu et al., A Review of Lattice Boltzmann Models for Compressible Flows, *Parallel Computational Fluid Dynamics*, **2004**.

Overview and recent developments

Several authors are reviving the concept of adaptive LBMs, and propose alternative ways to reconstruct missing information

- Sun, Hsu et al. (end 1990s - beg 2000s)

  1 - Redistribution of macros during streaming

  2 - Pragmatic reconstruction

  f_i^{eq} + correction terms (viscous effects)

- Dorschner et al. (2018)

  1 - Third-order Lagrange interpolation

  2 - Predictor-corrector

  3 - Full reconstruction (moment space)

+ No correction terms
- Space interpolation (loss of parallel efficiency)
- Predictor-corrector step
- Requires the computation of all moments
- Restricted to tensor-product-based lattices (Q27, Q125, etc)
- Severe conservation issues depending on the interpolation

Overview and recent developments

Several authors are reviving the concept of adaptive LBMs, and propose alternative ways to reconstruct missing information

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- Restricted to tensor-product-based lattices (Q27, Q125, etc)
- Severe conservation issues depending on the interpolation

Andrey Zakirov, Boris Korneev,
Vadim Levchenko, Anastasia Perepelkina

On the conservativity
of the Particles-on-Demand method
for the solution of the Discrete
Boltzmann Equation

← **In-depth investigation of this alternative adaptive LBM (named 'Particles on Demand')**

Overview and recent developments

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  2 - Pragmatic reconstruction

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- Requires the computation of all moments

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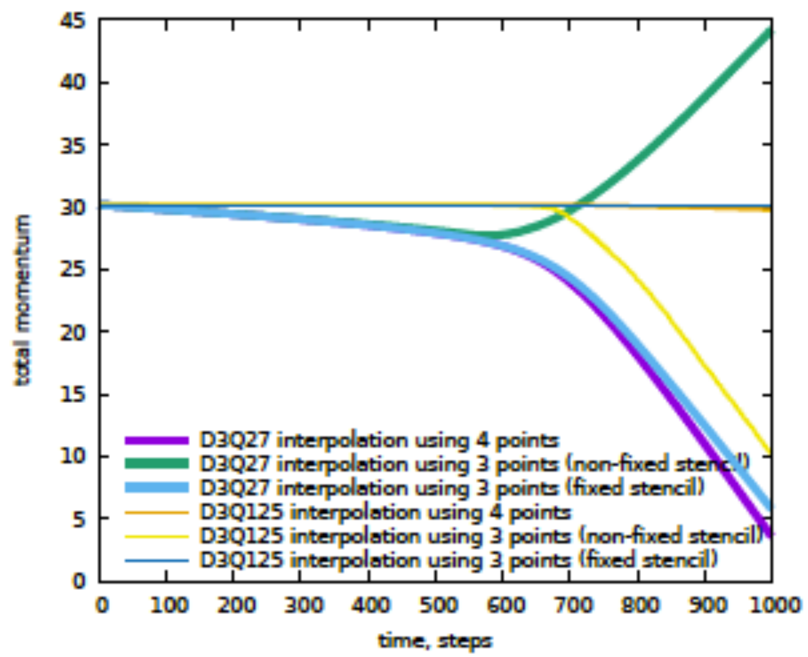
- Severe conservation issues depending on the interpolation



←

In-depth investigation of this alternative adaptive LBM (named 'Particles on Demand')

27 interpolation points and at least 100 velocities are required in 3D

Overview and recent developments

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  2 - Pragmatic reconstruction

  f_i^{eq} + correction terms (viscous effects)

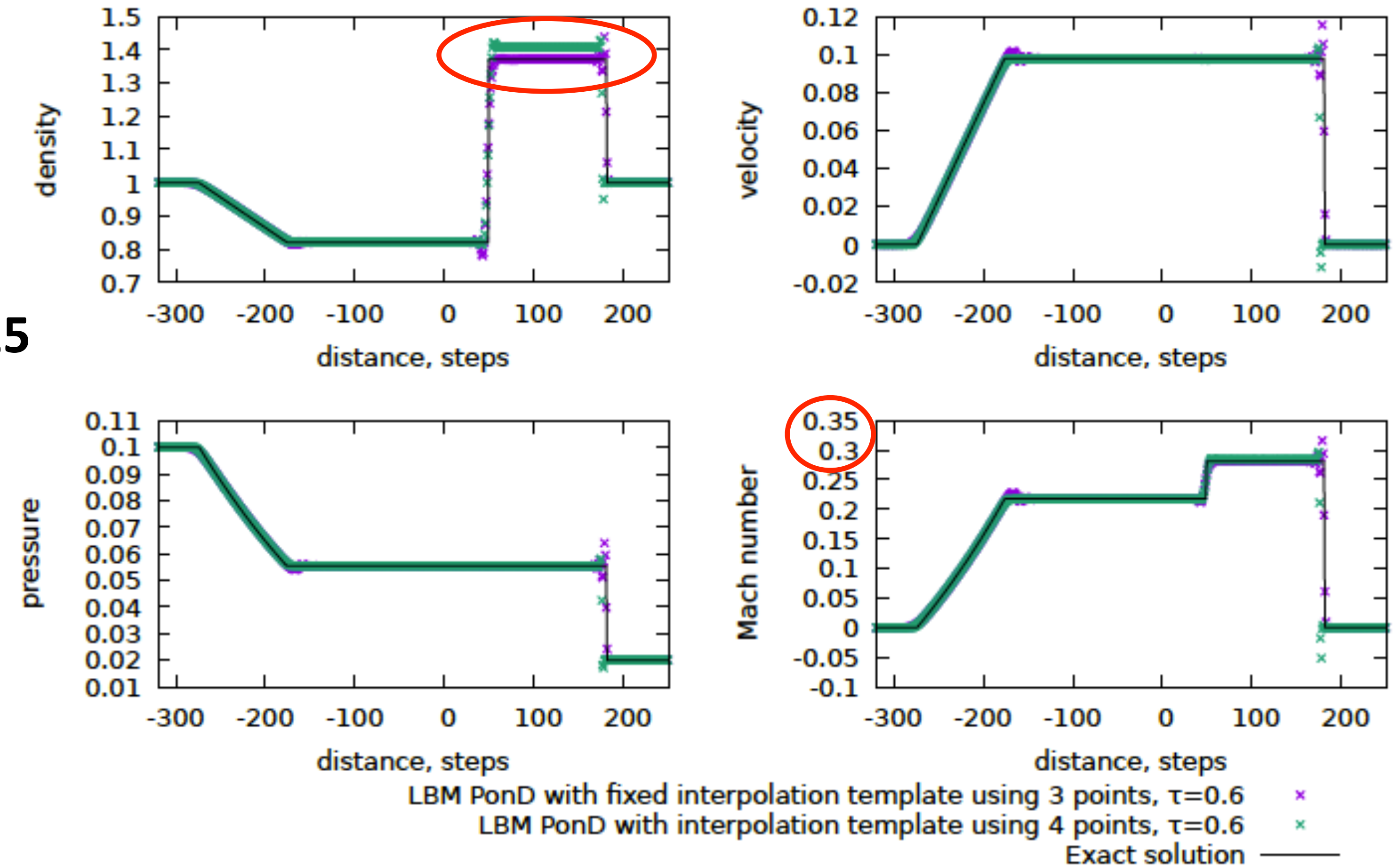
- Dorschner et al. (2018)

  1 - Third-order Lagrange interpolation

  2 - Predictor-corrector

  3 - Full reconstruction (moment space)

D3Q125



If this problem is not taken seriously, **conservation issues** are encountered even at **low Mach number** conditions…

↓

Need to **adopt a conservative numerical scheme**, as done with DVMs for hypersonic flow simulations…

Overview and recent developments

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  2 - Pragmatic reconstruction

  f_i^{eq} + correction terms (viscous effects)

- Dorschner et al. (2018)

  1 - Third-order Lagrange interpolation

  2 - Predictor-corrector

  3 - Full reconstruction (moment space)

- Zipunova et al. (2020)

  1 - Third-order Lagrange interpolation

  2 - Predictor-corrector

  3 - Regularized reconstruction

  $f_i^{eq} + \boxed{f_i^{neq}}$ ← Hermite expansion

Reg-PonD is supposed to be more efficient

https://www.youtube.com/watch?v=FfpjSu7G594&list=PLmp2AWh1L6AoFETV5ZNhFtbU1vbX0fSOC&index=11

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  2 - Pragmatic reconstruction

  f_i^{eq} + correction terms (viscous effects)

- Dorschner et al. (2018)

  1 - Third-order Lagrange interpolation

  2 - Predictor-corrector

  3 - Full reconstruction (moment space)

- Coreixas and Latt (2020)

  1 - Interpolation free

  2 - Predictor-corrector not required

  3 - Regularized reconstruction

  $f_i^{eq} + \boxed{f_i^{neq}}$ ← Grad's formulation (or CE expansion)

- Zipunova et al. (2020)

  1 - Third-order Lagrange interpolation

  2 - Predictor-corrector

  3 - Regularized reconstruction

  $f_i^{eq} + \boxed{f_i^{neq}}$ ← Hermite expansion

To obtain an efficient scheme, we should avoid modifications proposed for PonD, i.e., interpolation + full reconstruction

Overview and recent developments

Several authors are reviving the concept of adaptive LBMs, and propose alternative ways to reconstruct missing information

- Coreixas and Latt (2020)

  1 - Interpolation free

  2 - Predictor-corrector not required

  3 - Regularized reconstruction

$$f_i^{eq} + \boxed{f_i^{neq}}$$ ← Grad's formulation (or CE expansion)

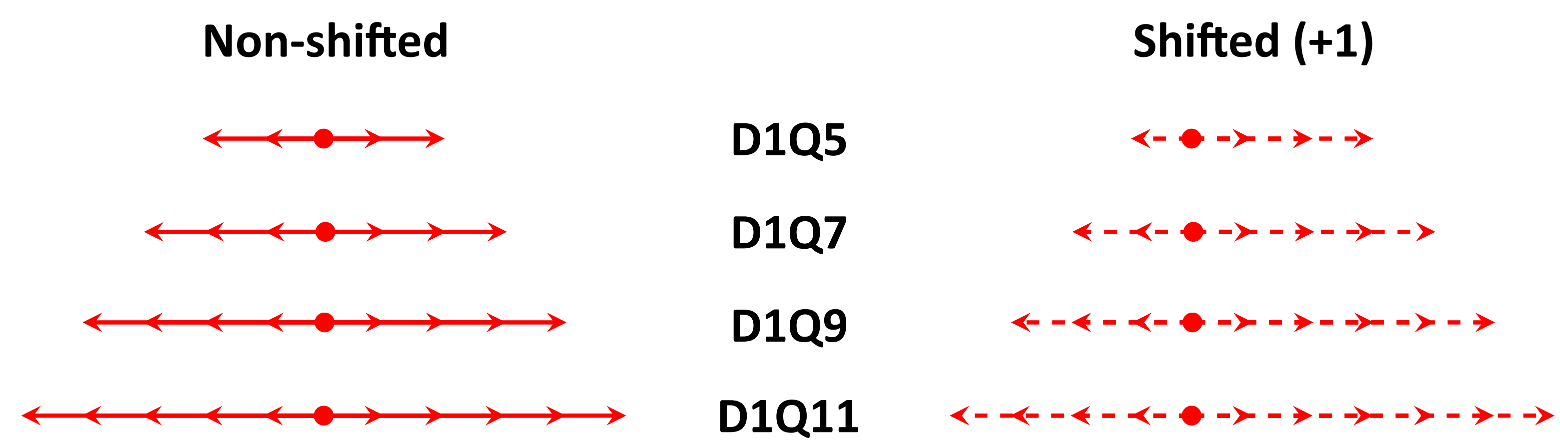
To obtain an efficient scheme, we should avoid modifications proposed for PonD, i.e., interpolation + full reconstruction

Coreixas and Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *PoF*, **2020**.

Stability condition to dynamically shift the lattice

LSA of 1D models with an analytical equilibrium (integer-value shift)

To get rid of interpolations



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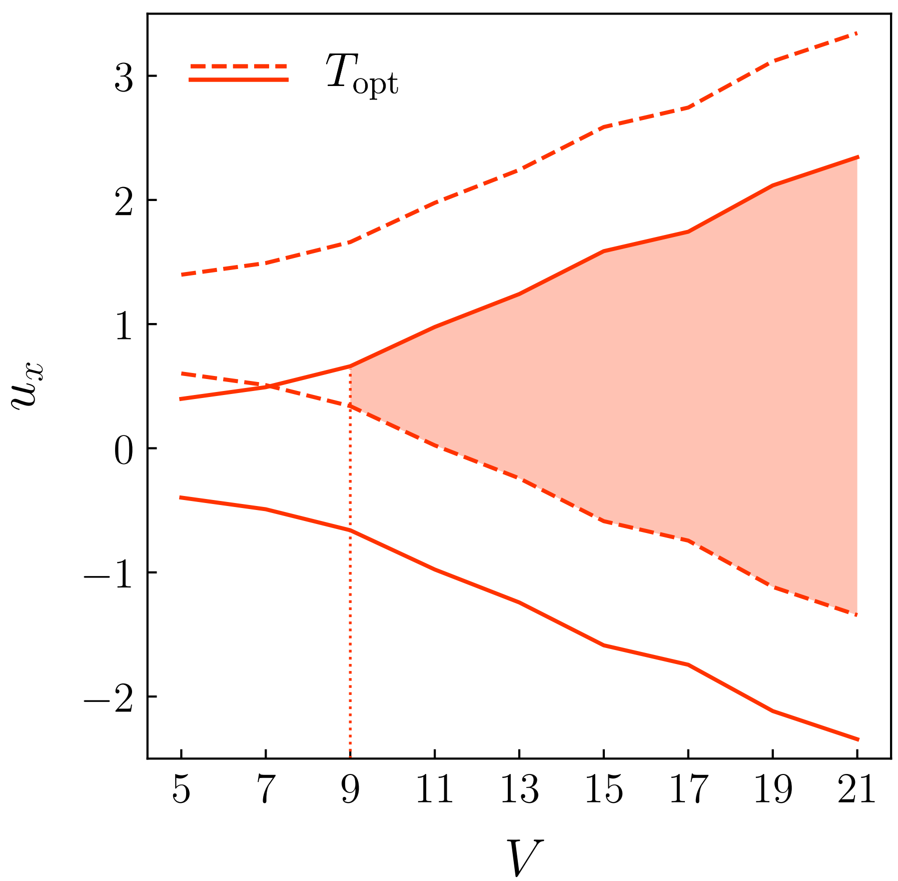

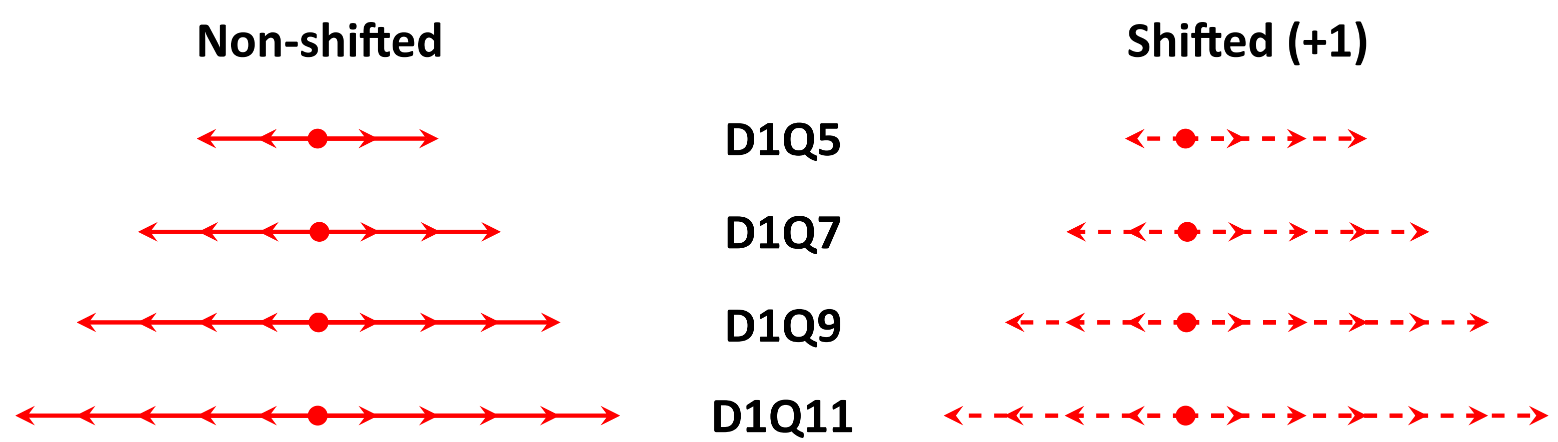

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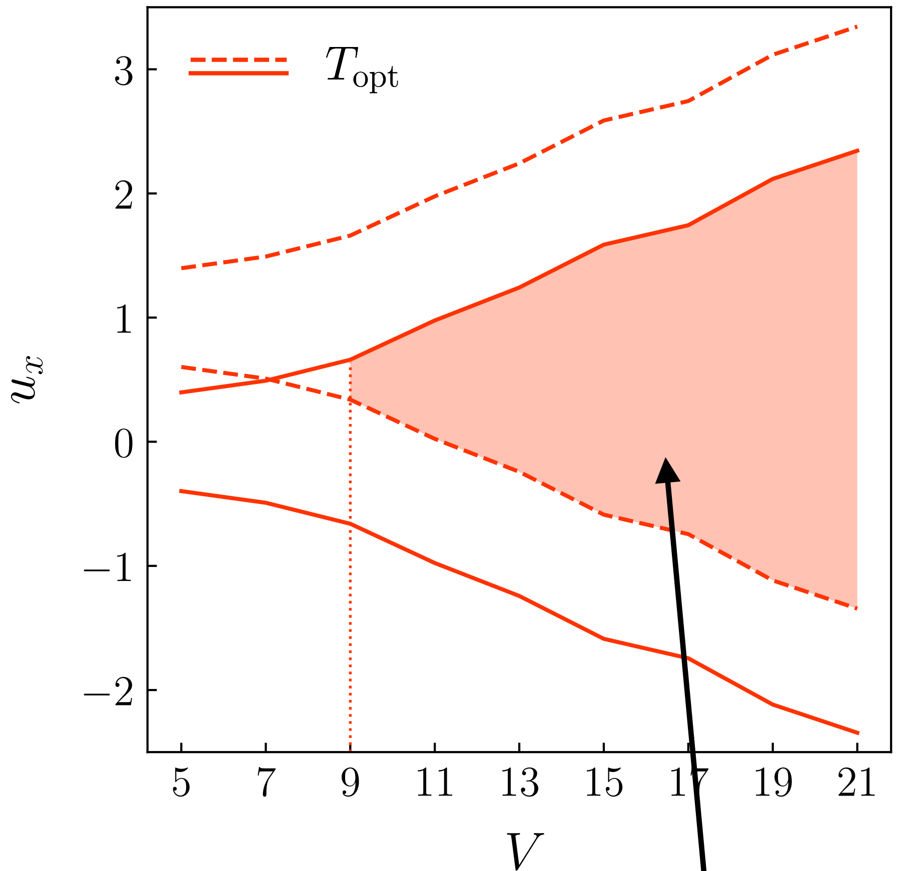
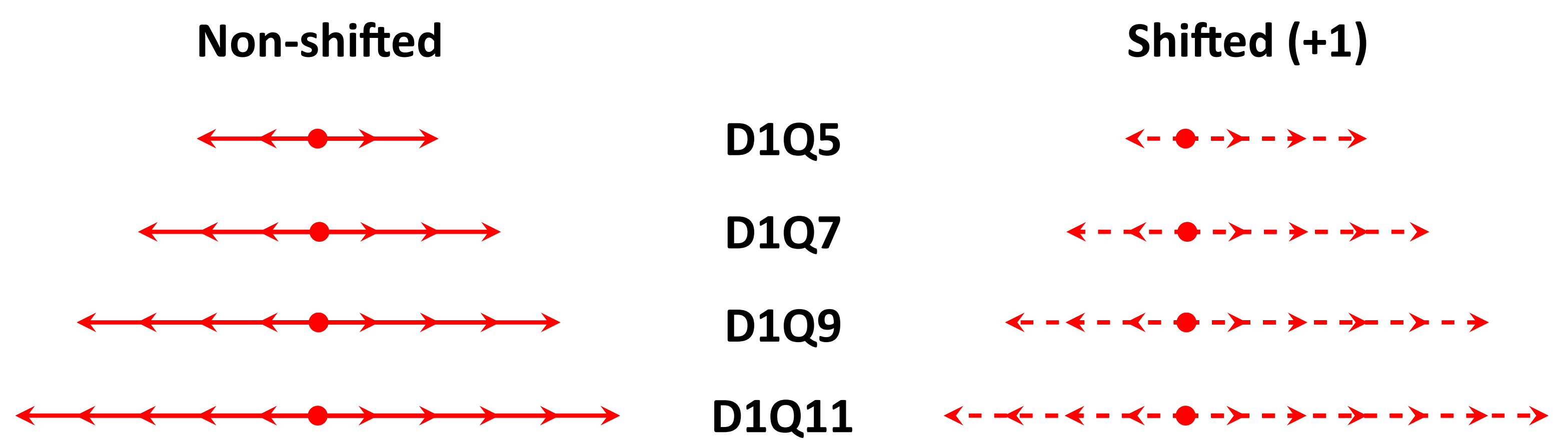




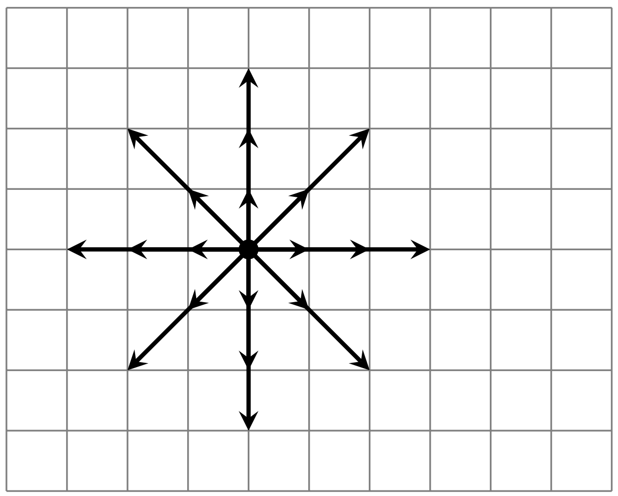
Stability domains must overlap!... but it only happens for D1Q9, D1Q11, etc...
LBMs based on analytical equilibria cannot be used to design an efficient model when the shift is based on integer values!

Coreixas and Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *PoF*, **2020**.

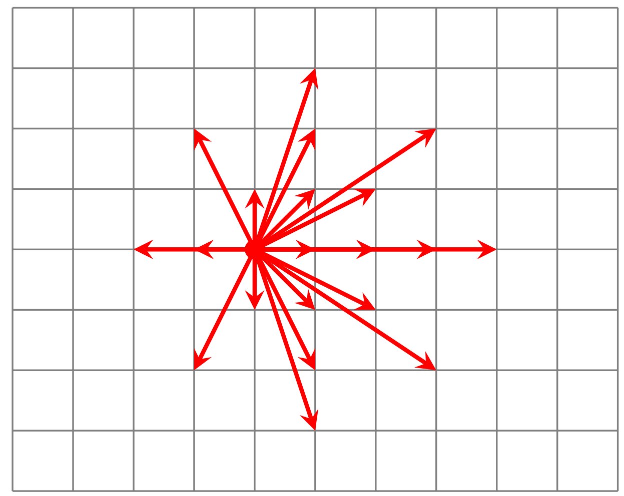
Stability condition to dynamically shift the lattice

What about LBMs based on numerical equilibria?

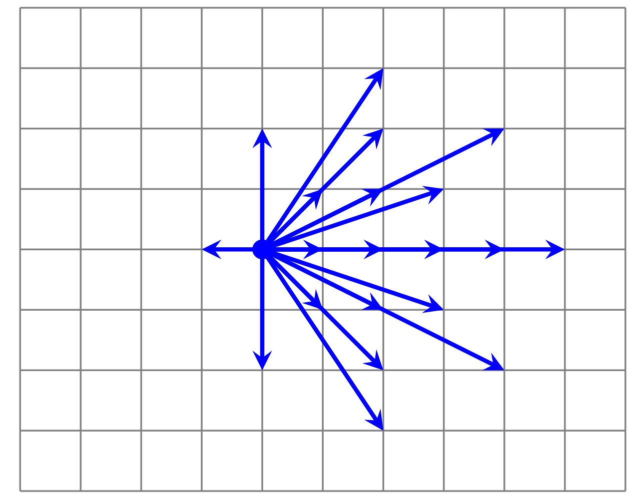
D2Q21 (Ux=0)



D2Q21 (Ux=1)

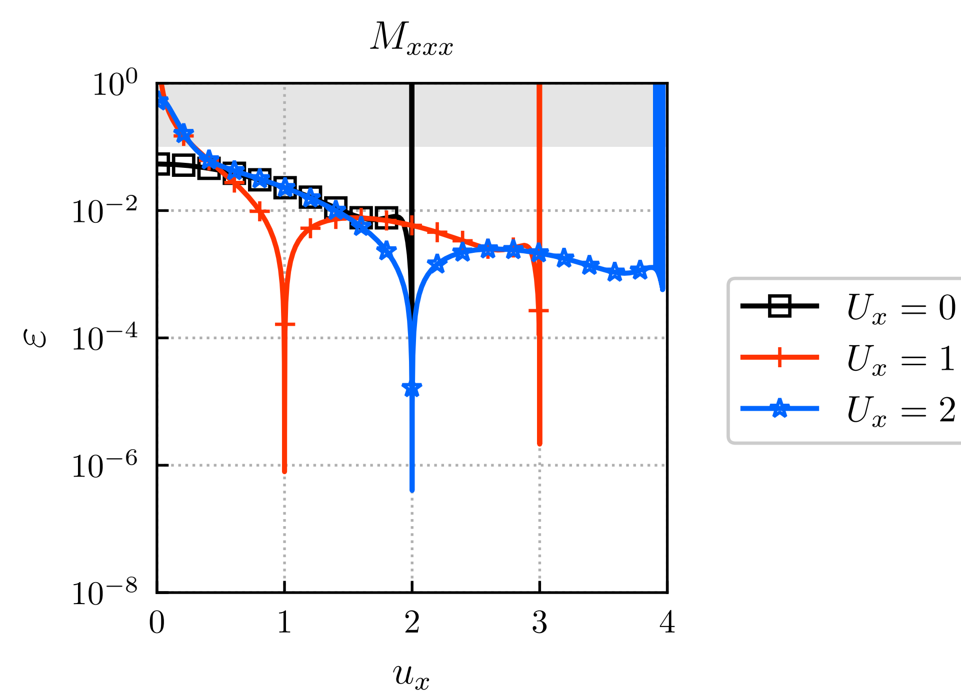


D2Q21 (Ux=2)



Impose all convective moments (10 in 2D)

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



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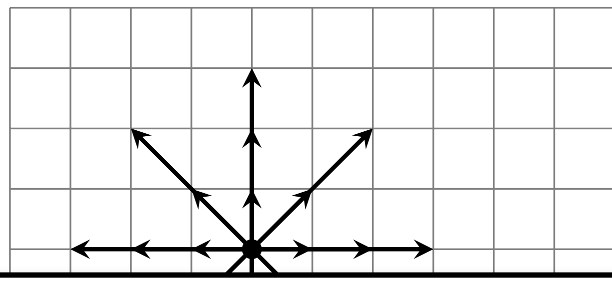
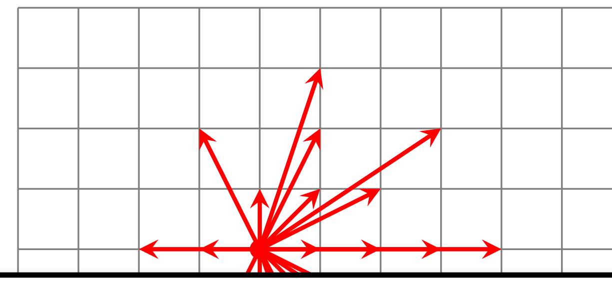
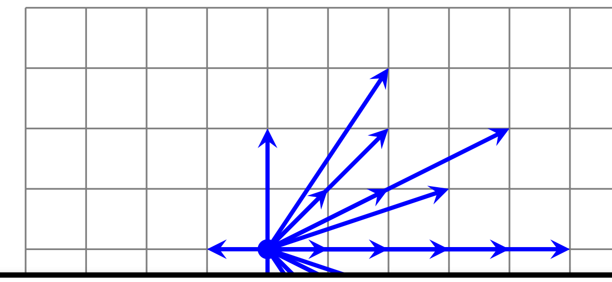


D2Q21 (Ux=1)



D2Q21 (Ux=2)



We can use compact lattices (2D version of PowerFLOW's D3Q39) thanks to numerical equilibria

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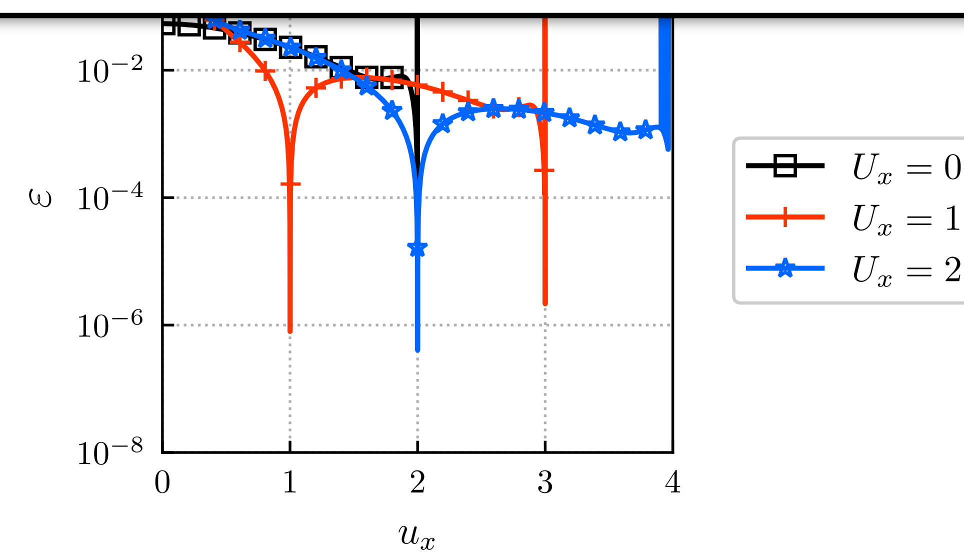
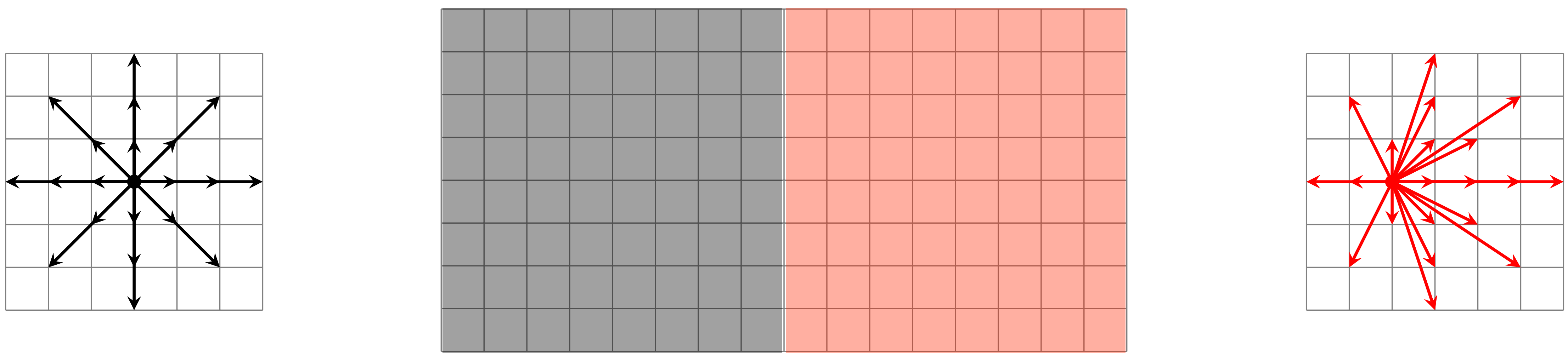


Coreixas and Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *PoF*, **2020**.

Reconstruction strategy

Dynamic domain decomposition based on macroscopic quantities (u and/or T)

$-0.5 < u_x \leqslant 0.5$ $\quad$ $0.5 \leqslant u_x < 1.5$



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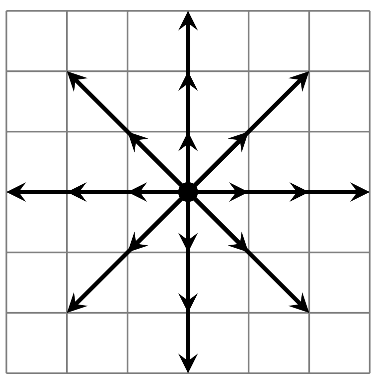

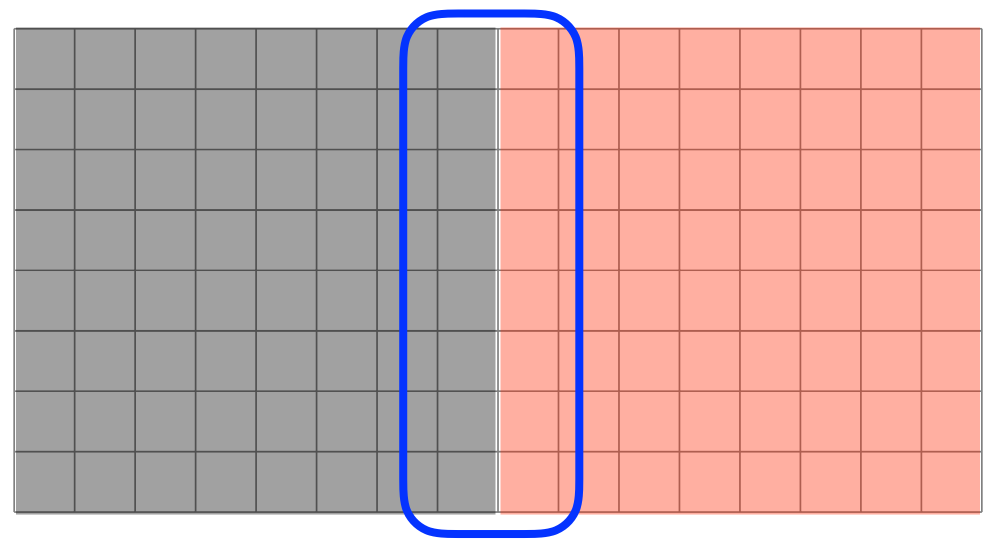

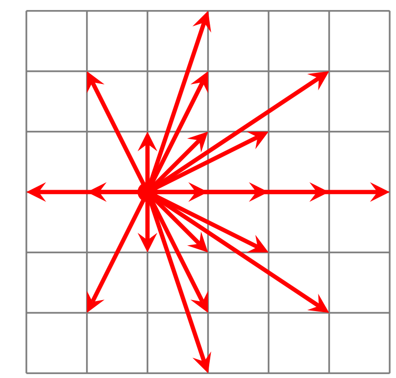

How do we compute missing populations at the interface?

$$h_i^* = h_i^{eq} + (1 - 1/\tau_h) h_i^{neq}$$

analytical or numerical

Chapman-Enskog

$$h_i^{neq} \approx h_i^{(1),\mathrm{CE}} = -\tau_h [\partial_t h_i^{eq} + \xi_{i\alpha} \partial_\alpha h_i^{eq}]$$

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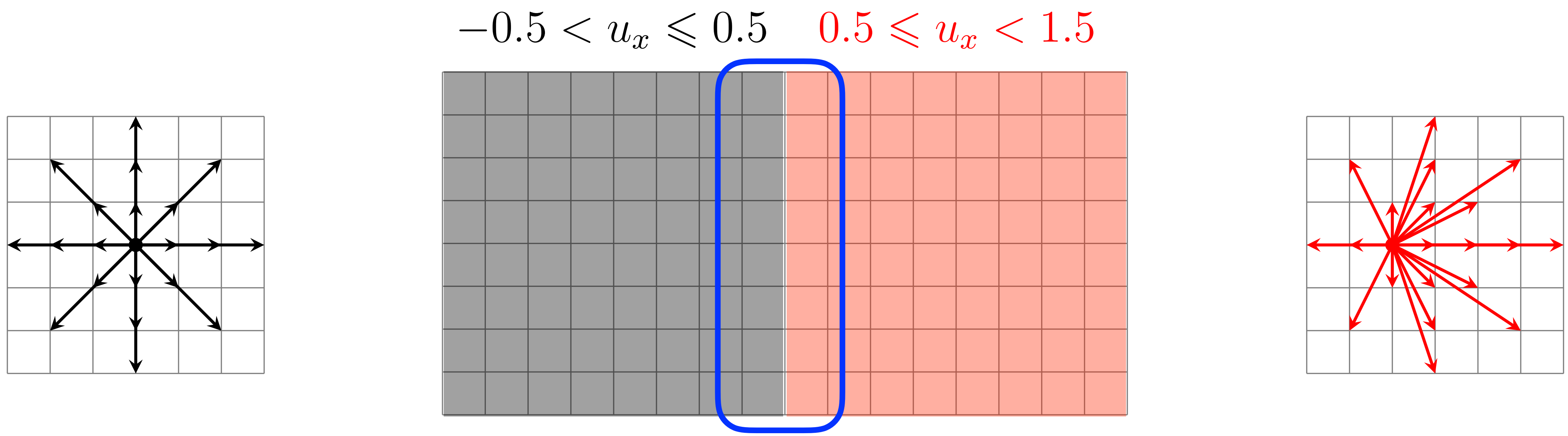

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Grad's formulation of populations

$$h_i^{neq} \approx h_i^{(1),\mathrm{Grad}} = h_i^{eq}(1 + \phi_h)$$

velocity and temperature gradients

Coreixas and Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *PoF*, **2020**.

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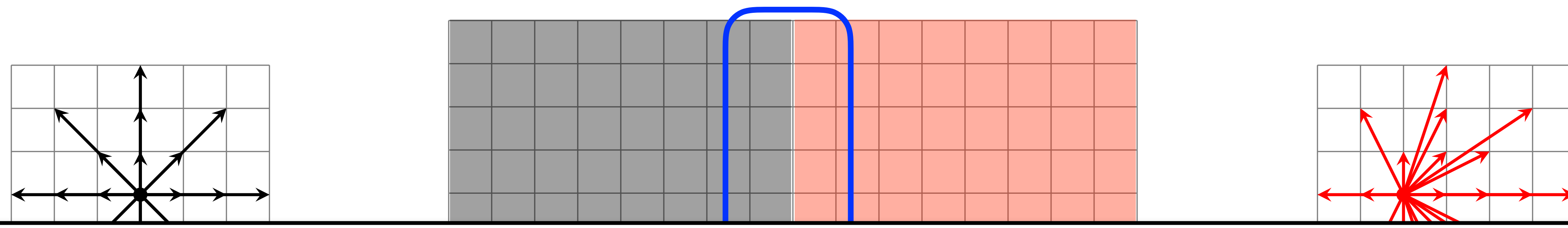

Interpolation-free reconstruction strategy
that can be coupled with all equilibria (analytical/numerical)

$$h_i^* = h_i^{eq} + (1 - 1/\tau_h) h_i^{neq}$$

analytical or numerical

Grad's formulation of populations

$$h_i^{neq} \approx h_i^{(1),\mathrm{Grad}} = h_i^{eq}(1 + \phi_h)$$

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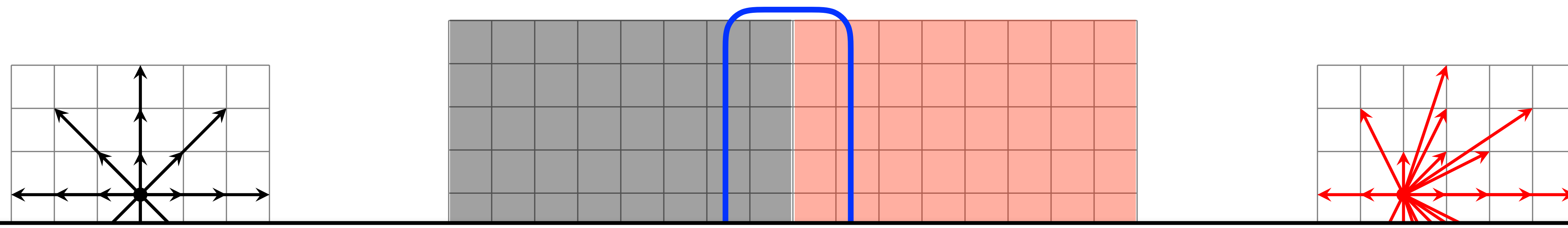

It will further be applied to initial and boundary conditions

$$h_i^* = h_i^{eq} + (1 - 1/\tau_h)h_i^{neq}$$

analytical or numerical

Grad's formulation of populations

$$h_i^{neq} \approx h_i^{(1),\text{Grad}} = h_i^{eq}(1 + \phi_h)$$

velocity and temperature gradients

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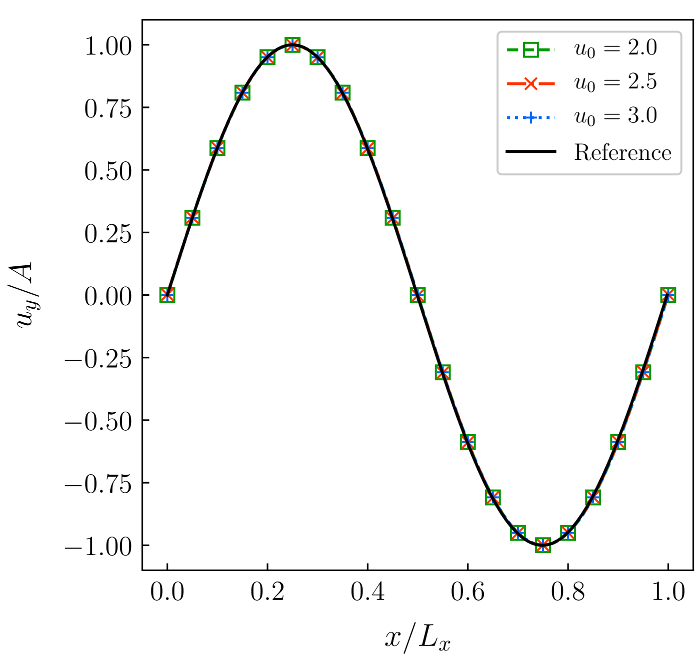
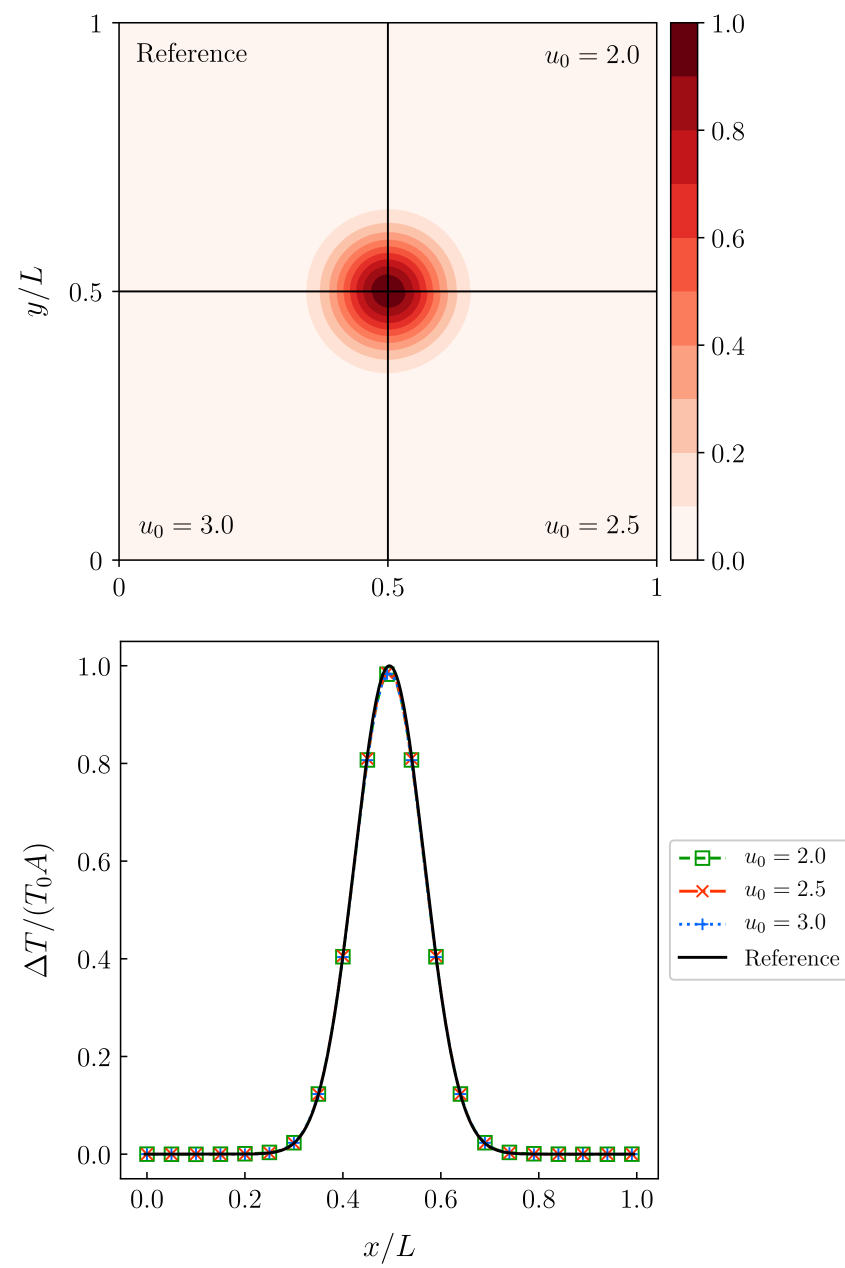
Accuracy of interpolation-free formulation

Propagation of waves (inviscid conditions and L=100 points)

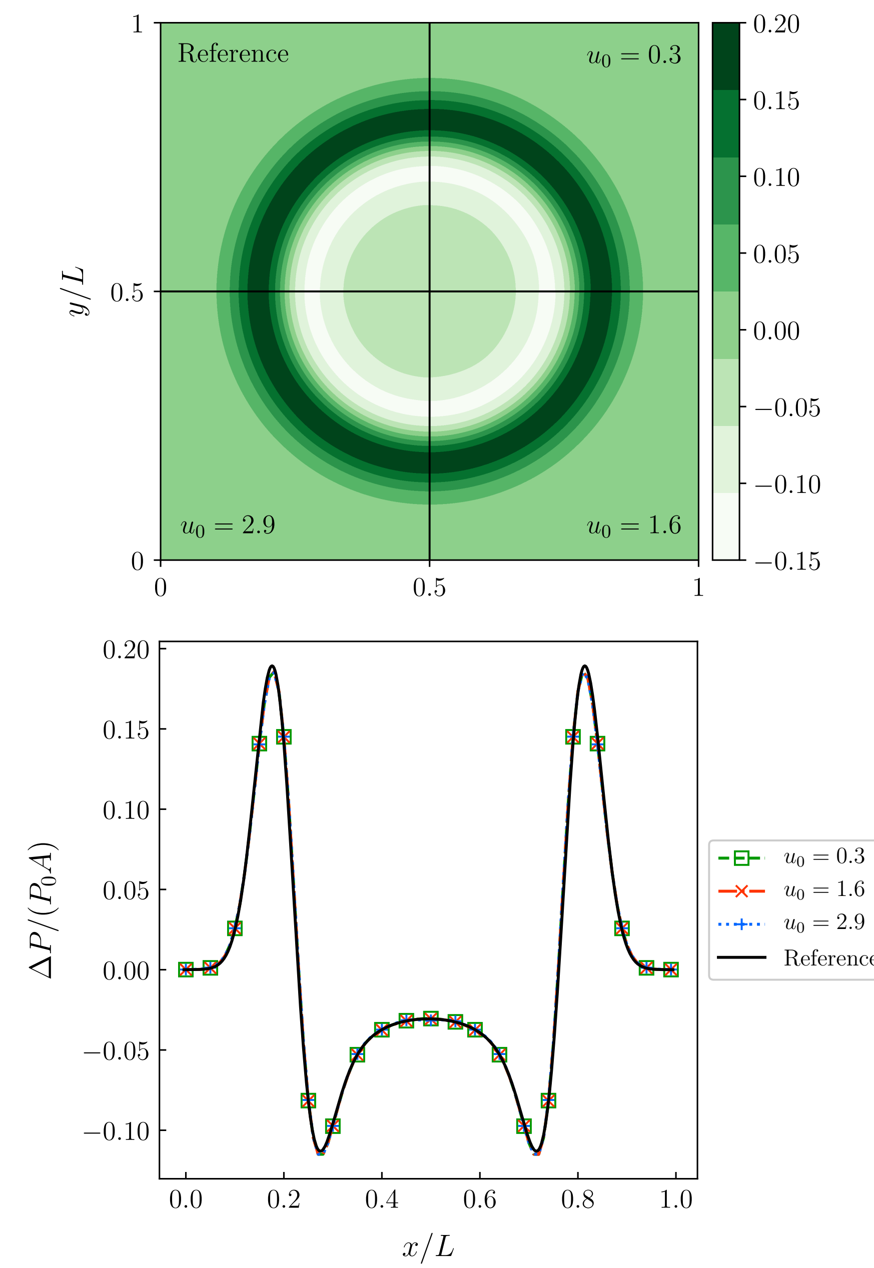
1D shear



2D entropic



2D acoustic

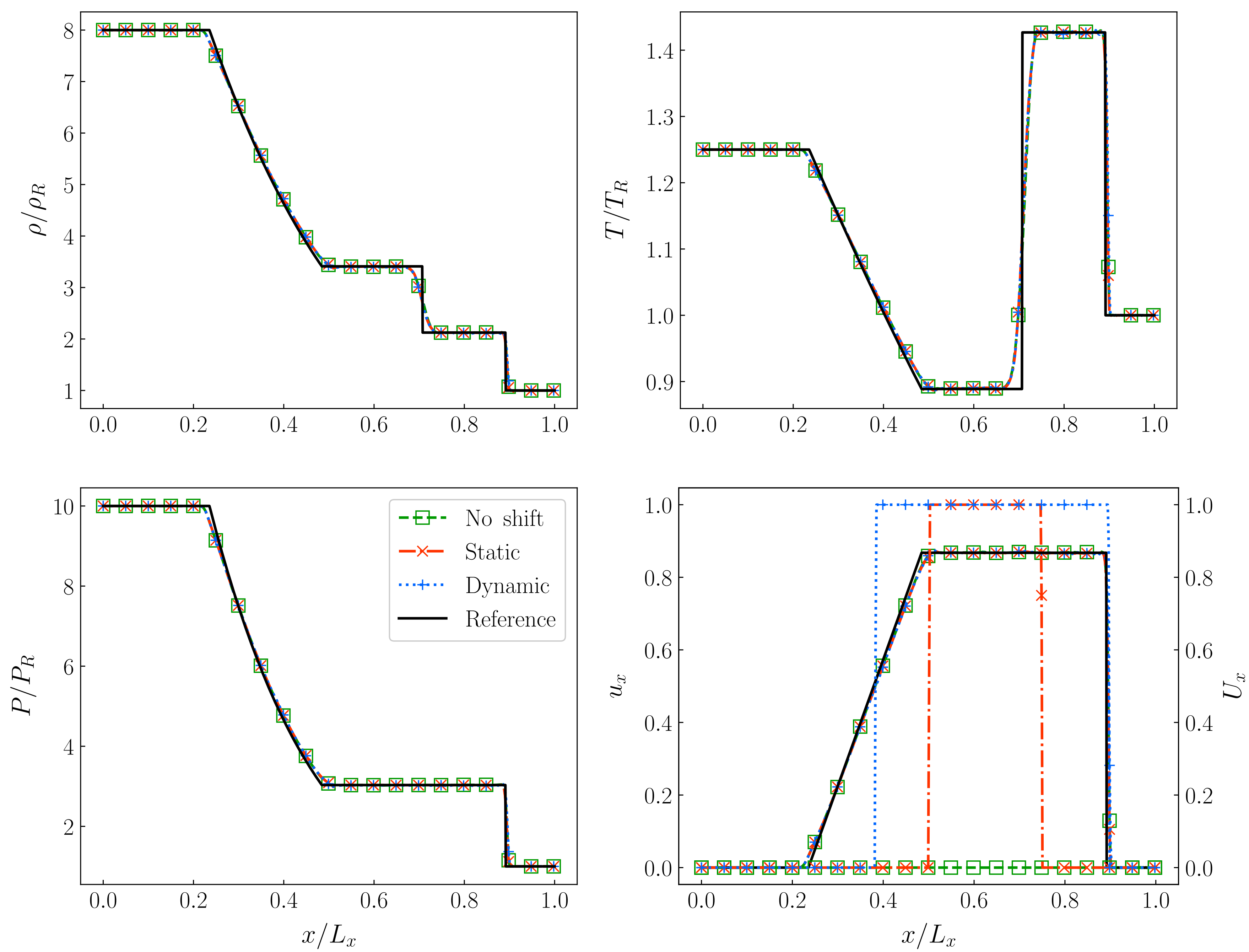


Low dissipation and dispersion errors

Coreixas and Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *PoF*, **2020**.

Accuracy of interpolation-free formulation

1D Riemann problem (L=500 points)

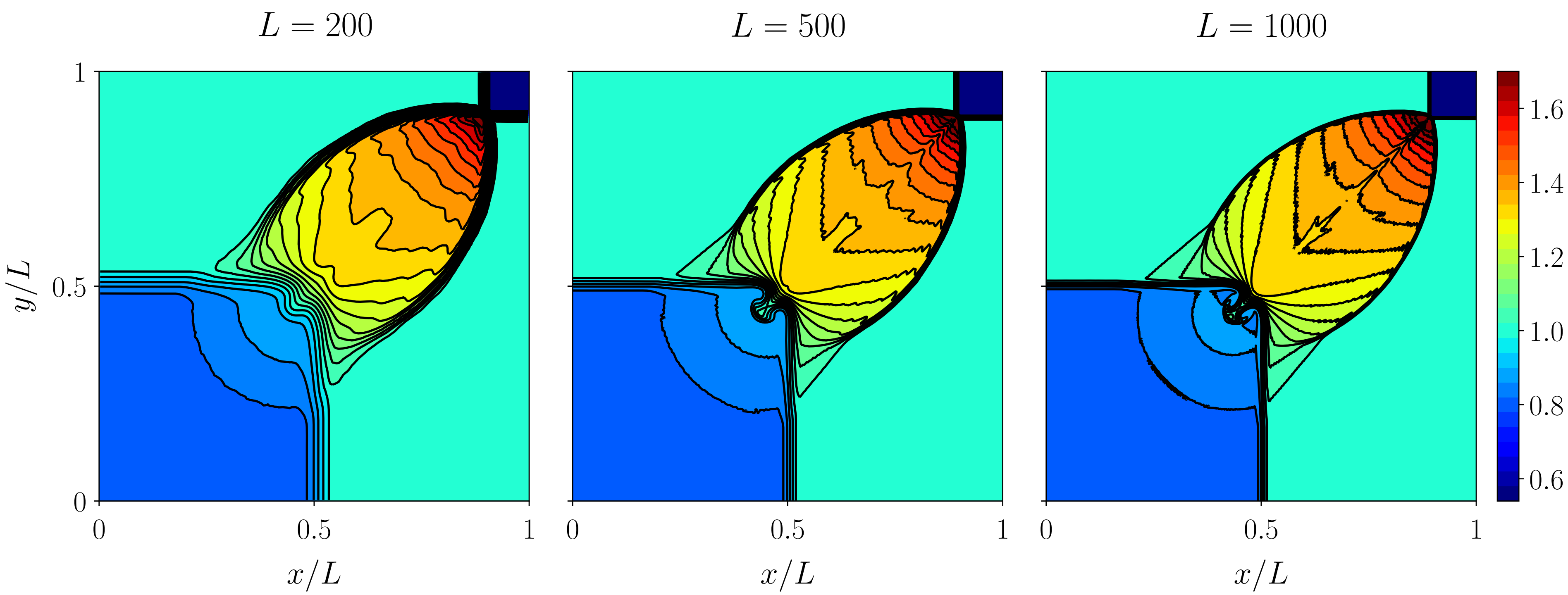


- All methods perform **very well**
- **No issue** with BCs
- Kinetic sensor allows for **inviscid** simulations
- Contact discontinuity is **over-dissipated**
- Interface is **following** the shock and rarefaction wave

Coreixas and Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *PoF*, **2020**.

Accuracy of interpolation-free formulation

2D Riemann problem (L points in each direction)



- Main features are **properly recovered** (symmetry, « mushroom », complex pattern)
- The kinetic sensor allows for **inviscid** simulations but it is **too dissipative**
- The kinetic sensor **would benefit from fine tuning** (e.g., based on wave types)

Astoul et al., Analysis and reduction of spurious noise generated at grid refinement interfaces with the lattice Boltzmann method, *JCP*, **2020.**

Coreixas and Latt, Compressible lattice Boltzmann methods with adaptive velocity stencils: An interpolation-free formulation, *PoF*, **2020**.

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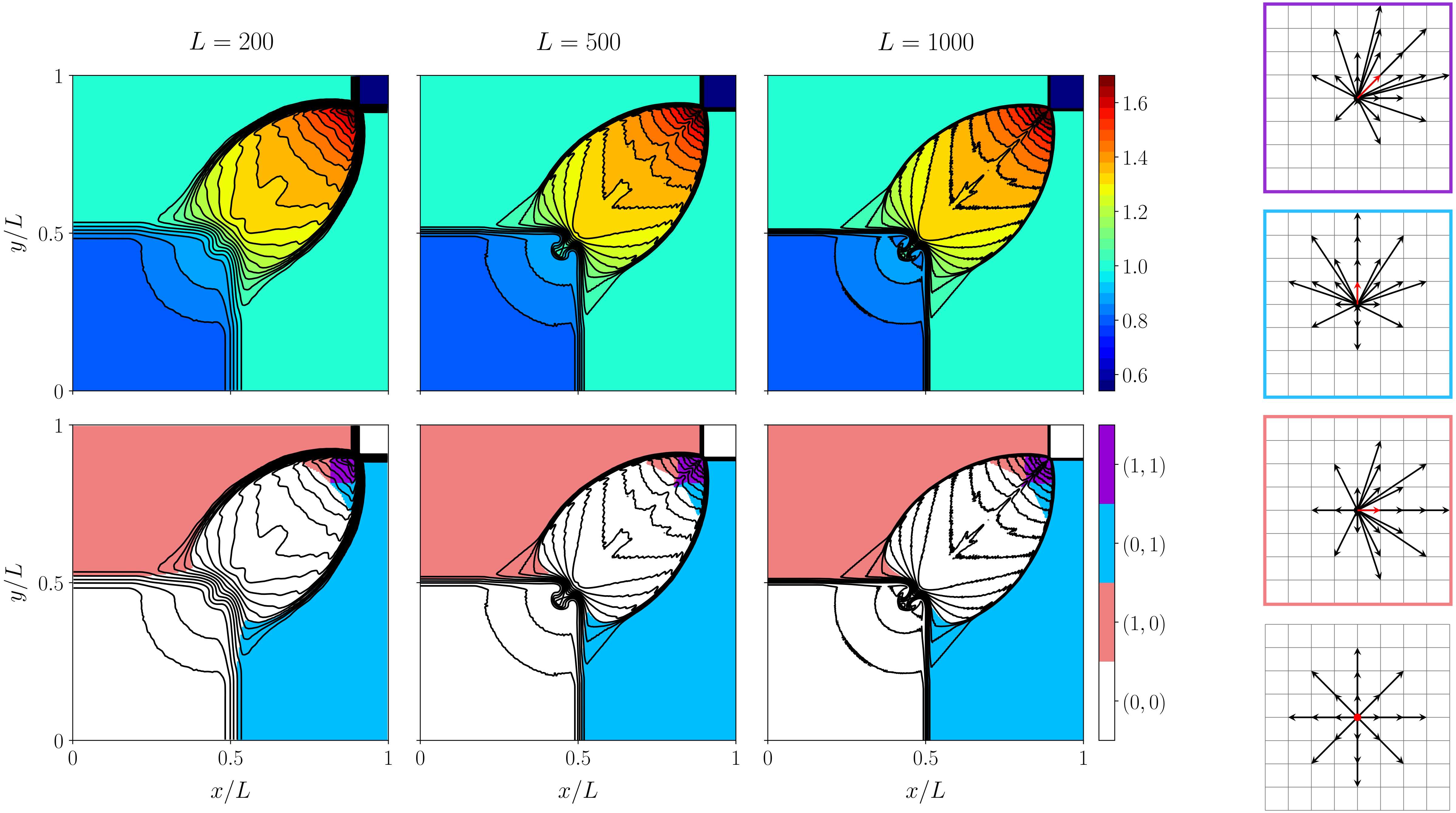

The lattice **self-adapts** to all main features

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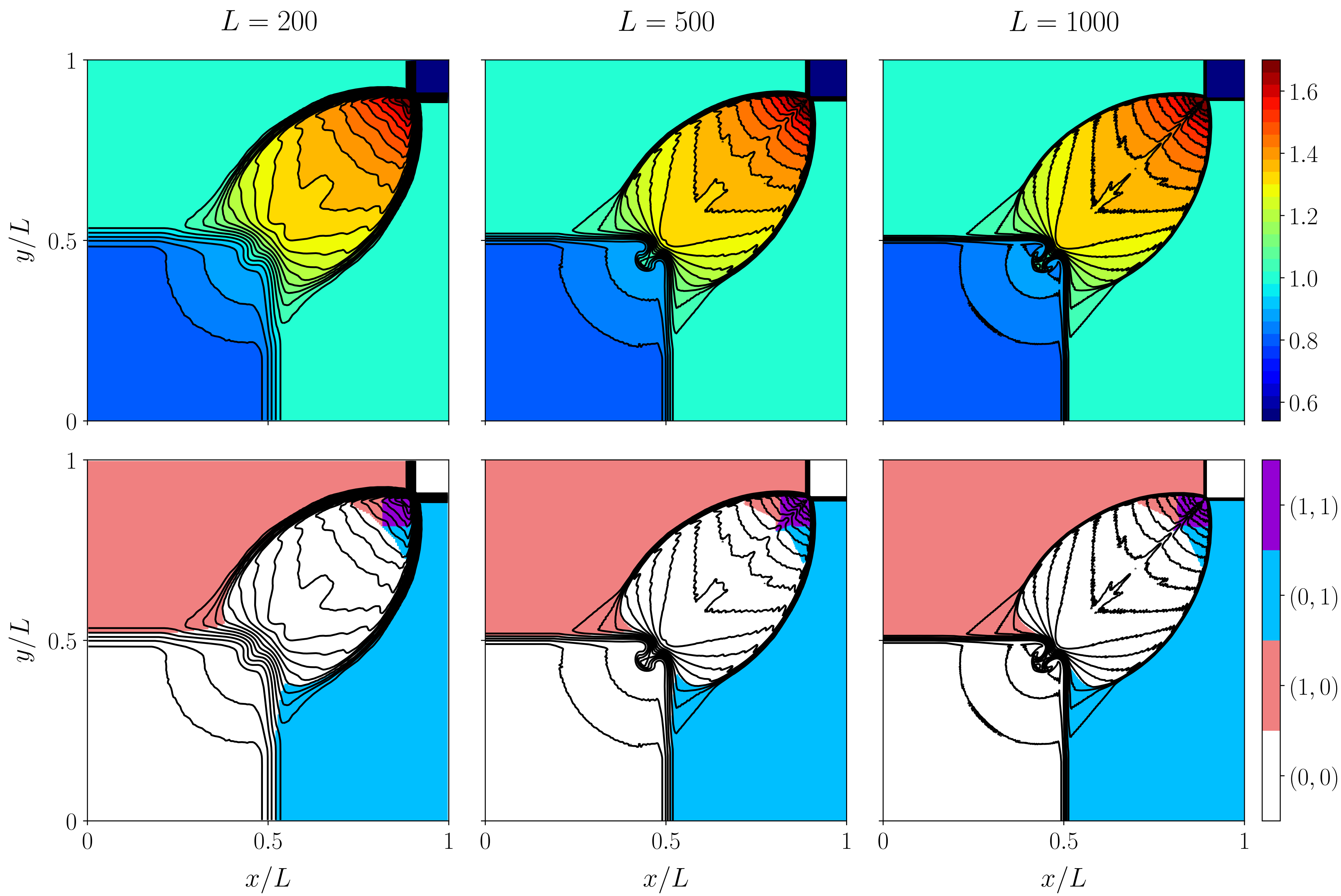

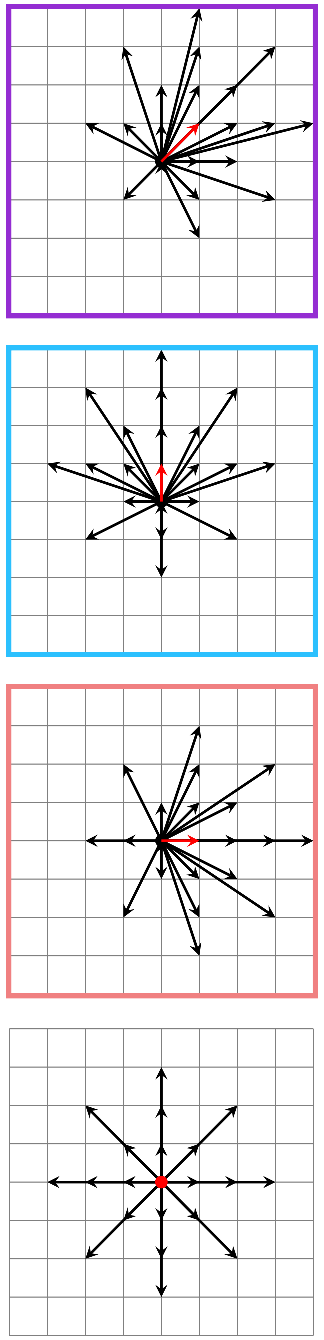

All of this is very promising!

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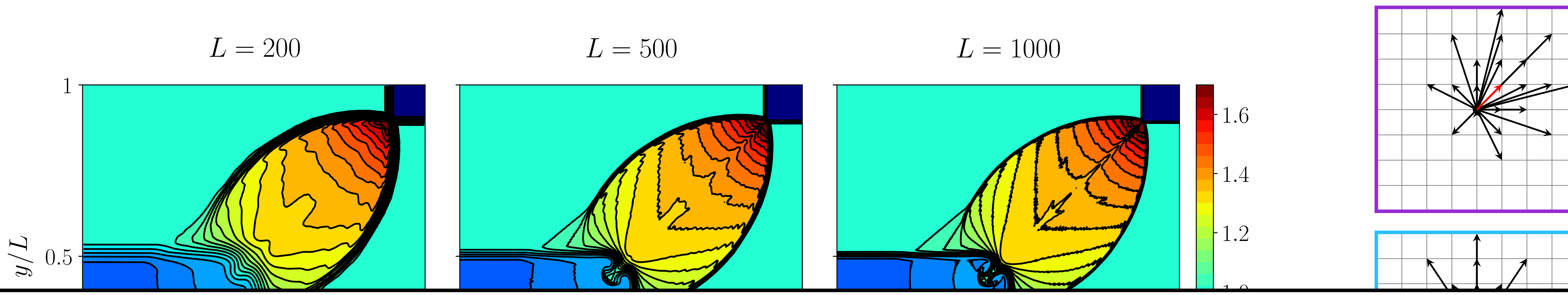
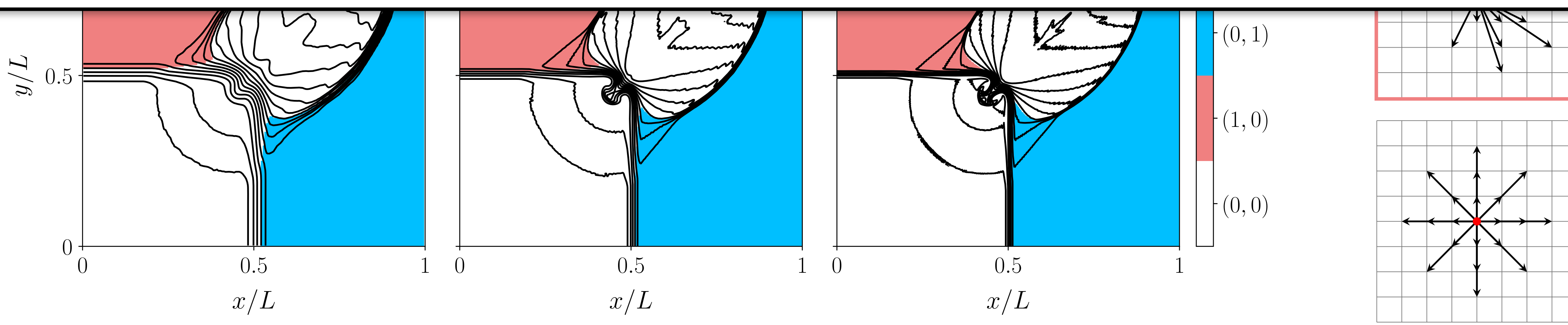


What's next?



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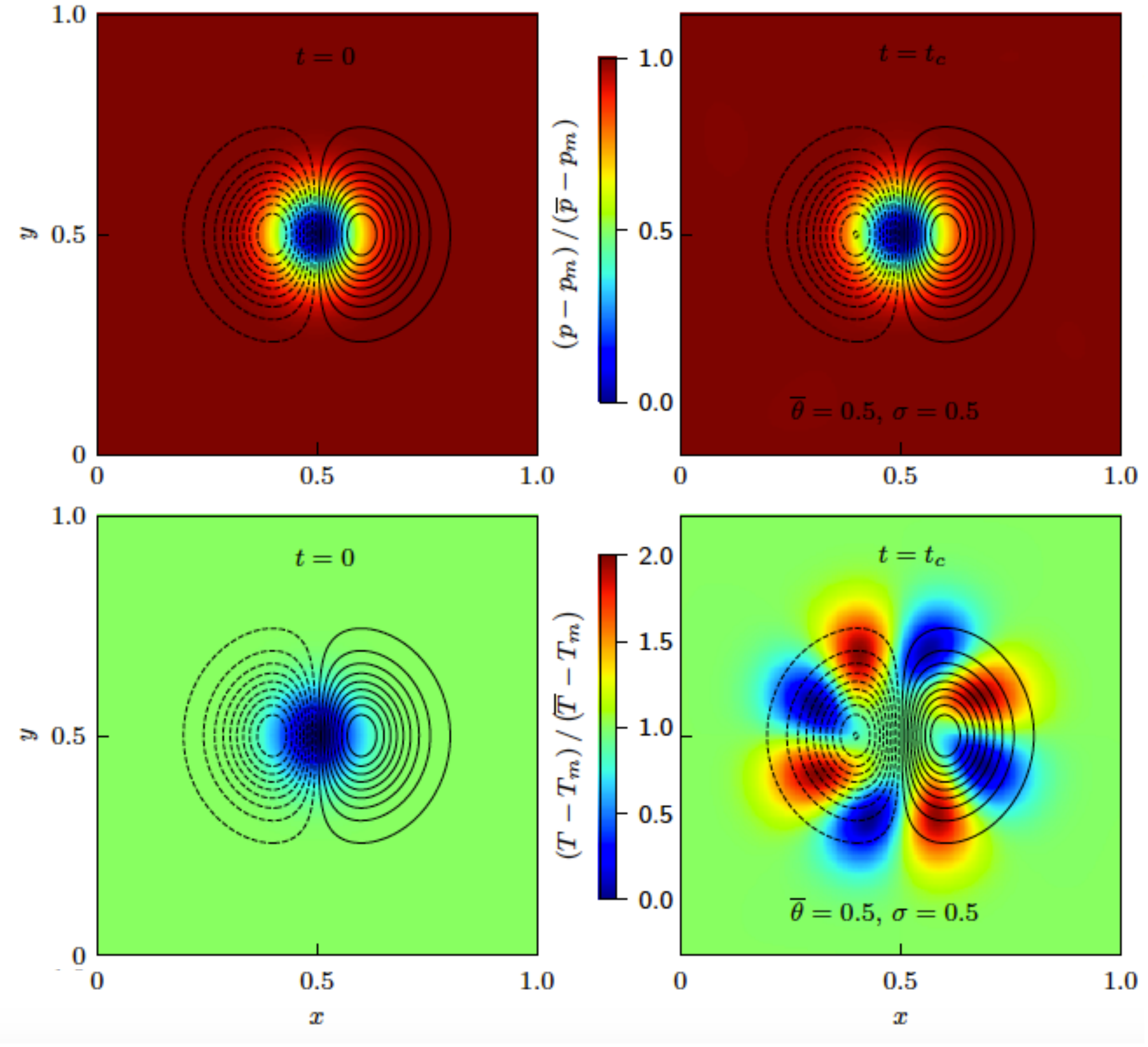
On-going investigations

Mode transfer: Hybrid LBMs…



Usually, either **pressure** or **velocity** fields of the convected vortex are plotted in papers…

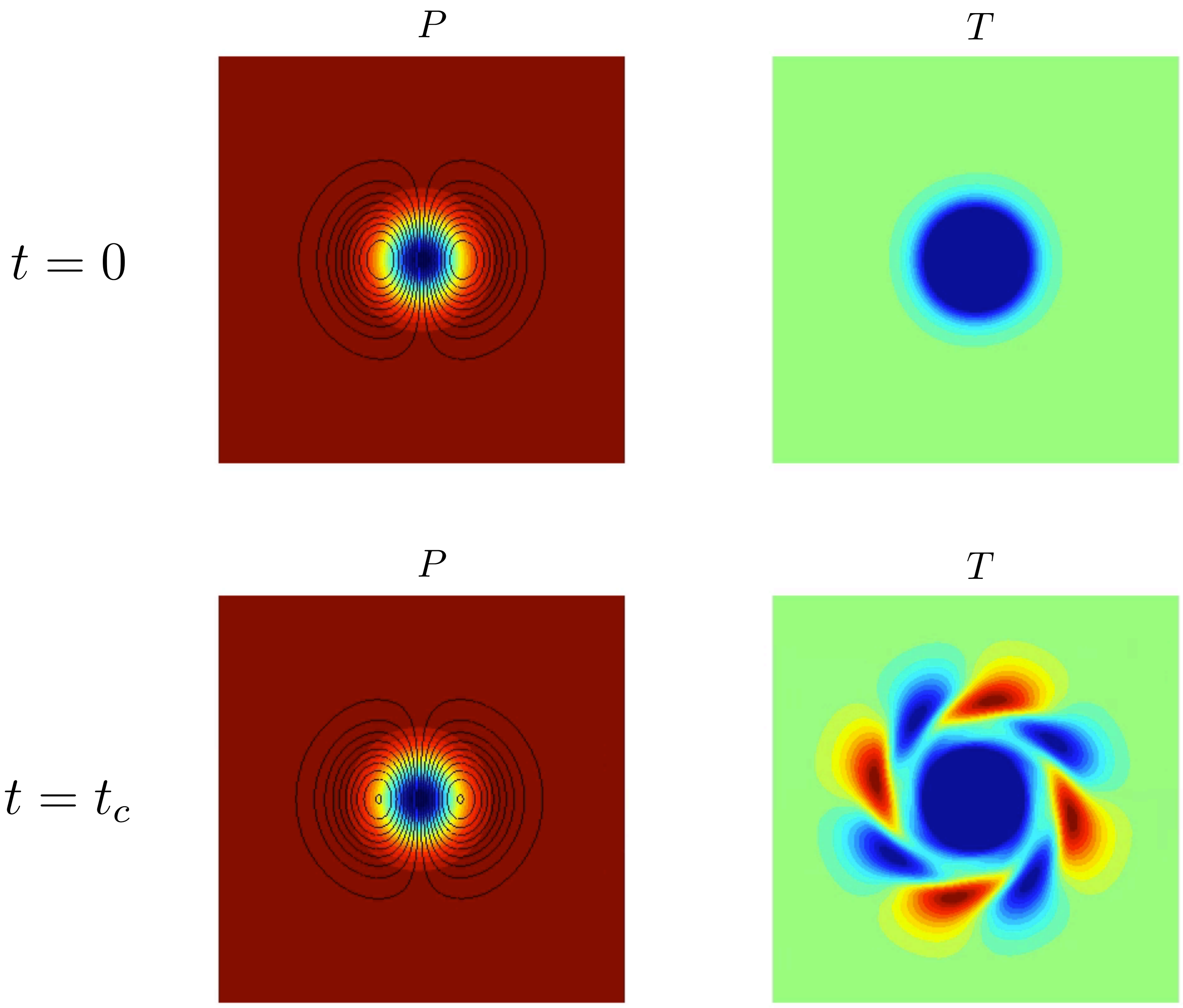
↓

and this might hide **spurious transfers** between vorticity and **temperature**!

Renard et al., A linear stability analysis of compressible hybrid lattice Boltzmann methods, *arXiv*, **2020.**

On-going investigations

Mode transfer: Hybrid LBMs… but not only! $M_a = 0.1$ $M_v = 0.05$ $\tau = 10^{-5}$



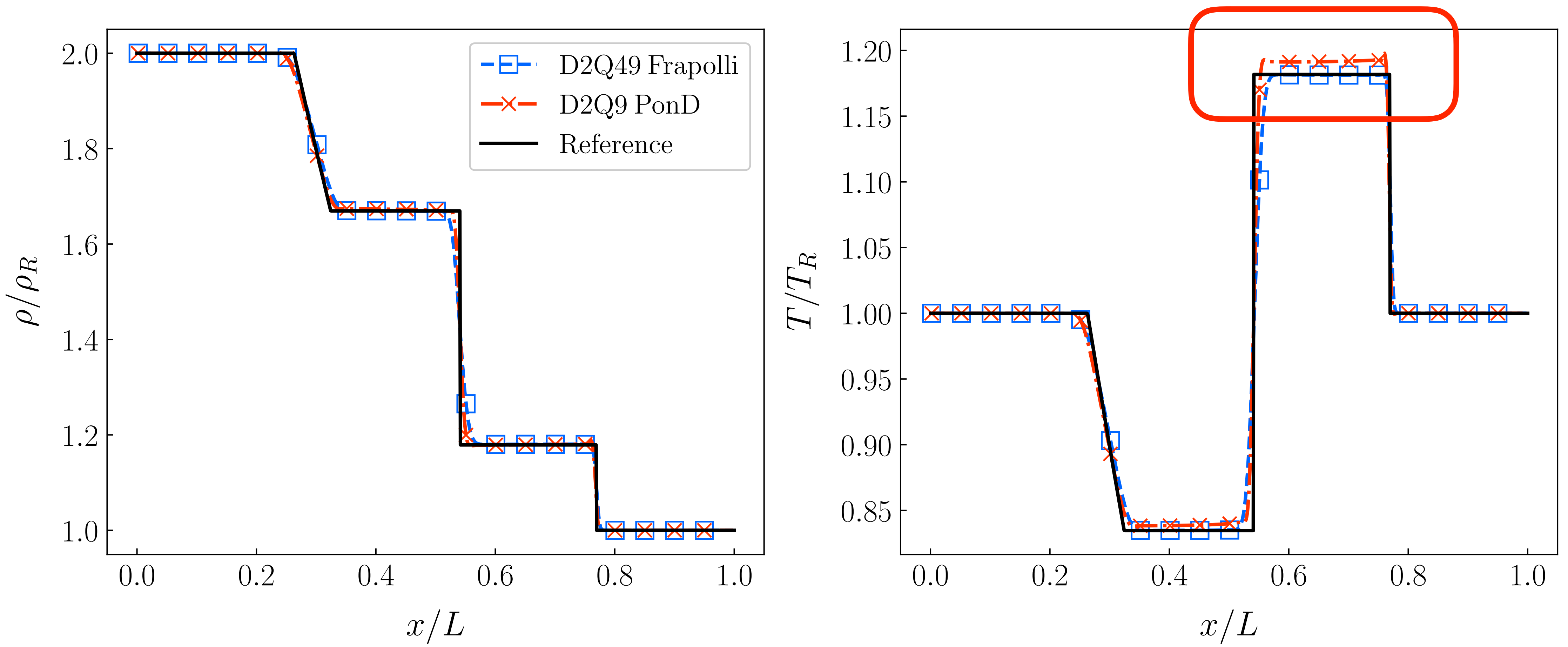
PonD (D2Q9) also have mode transfer issues!…

What about other adaptive LBMs?

Dorschner, Bösch and Karlin, Particles on Demand for Kinetic Theory, *PRL*, **2018**

On-going investigations

Preliminary comparison of some compressible LBMs (no shock sensor)



$L = 500$
$\tau = 0.7$

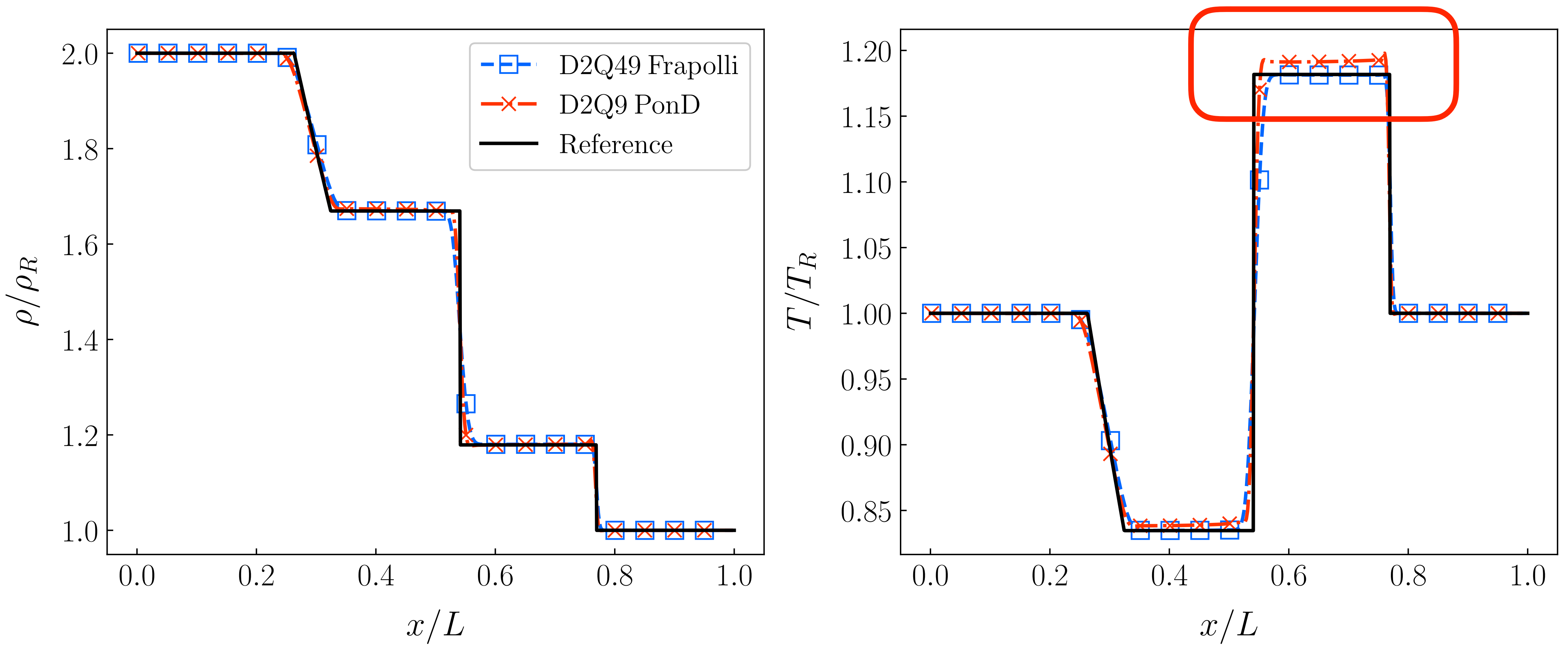
$\rho_L/\rho_R = 2$
$P_L/P_R = 2$

Solver	Navier-Stokes 3D	Frapolli D2Q49	PonD D2Q9
MLUPS	$0.1 - 1.0$	~ 0.14	~ 0.13
μs/pt/it	$1 - 10$	~ 7.1	~ 7.7

High variability depending on the numerical scheme

On-going investigations

Preliminary comparison of some compressible LBMs (no shock sensor)



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i7-10700K CPU @ 3.80GHz (perfo based on 1 core)

On-going investigations

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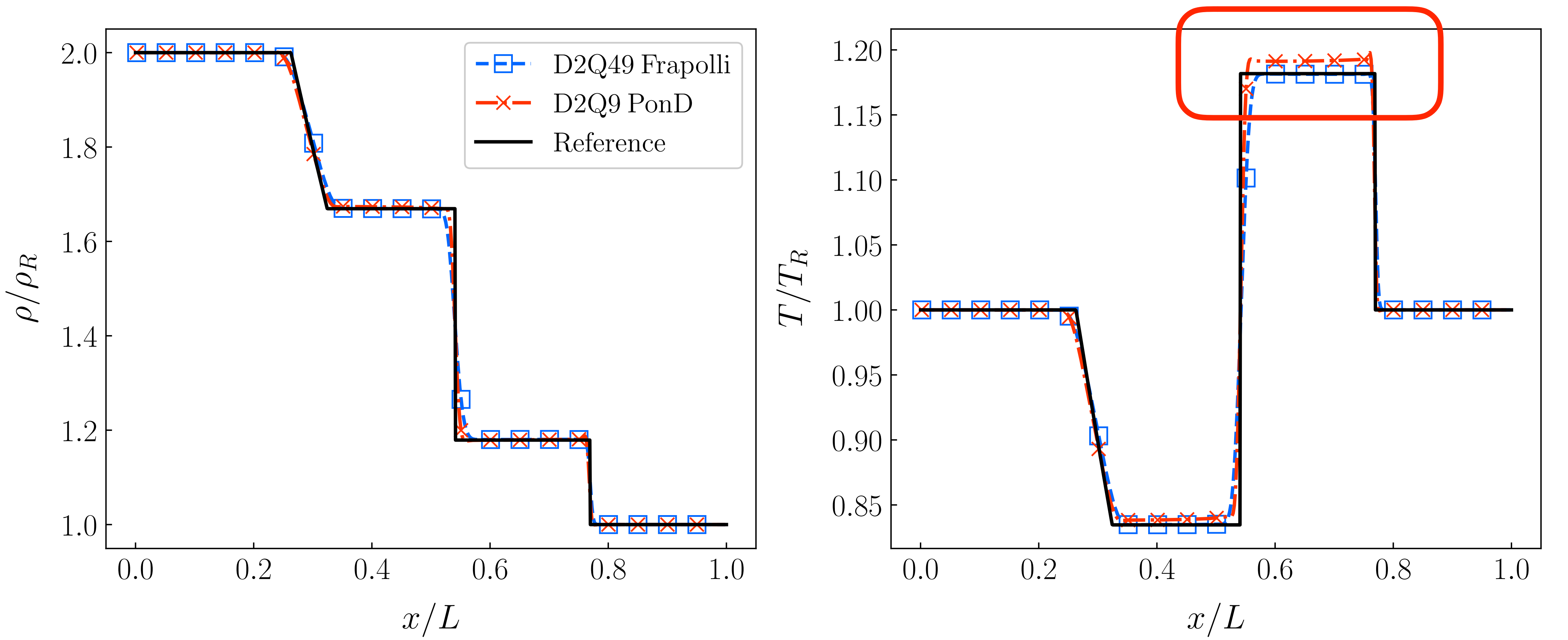

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In addition to having conservation issues, PonD (D2Q9) performance is similar to Frapolli's model (4-moment-based D2Q49) and 3D Navier-Stokes solvers!

On-going investigations

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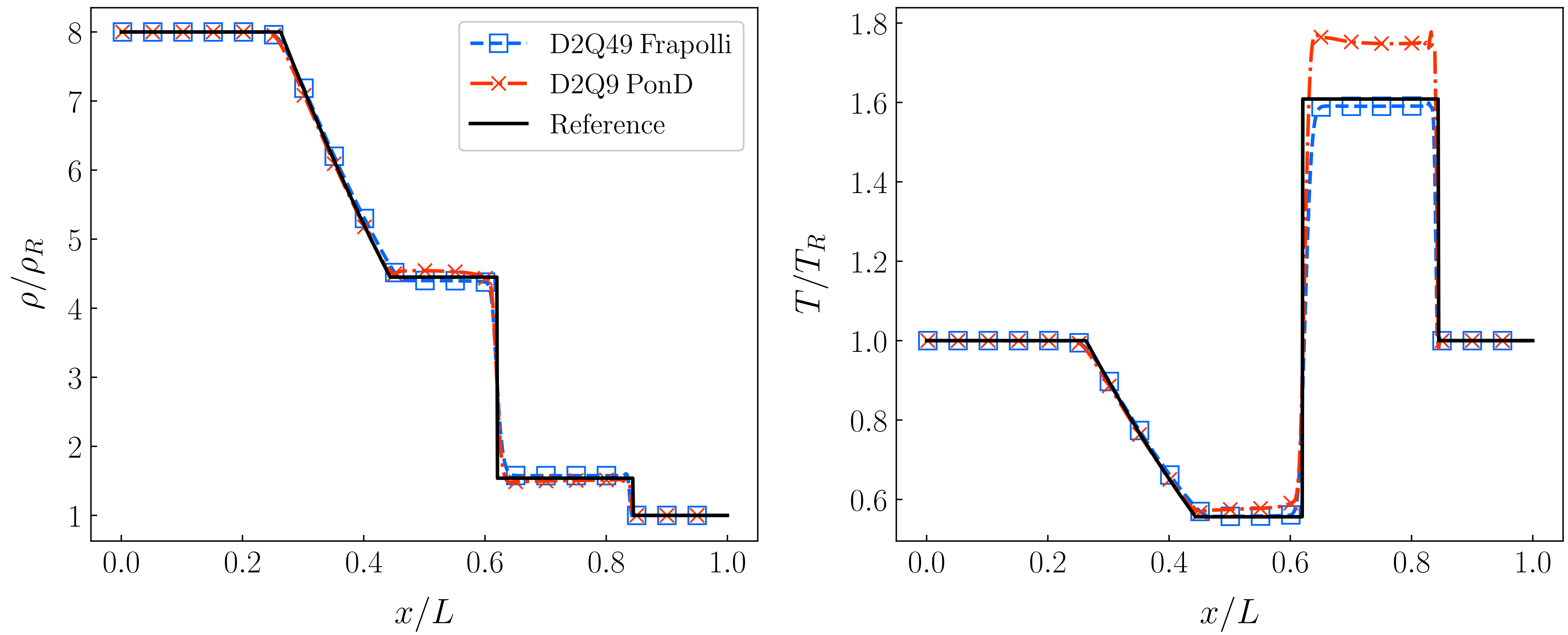


$L = 500$
$\tau = 0.7$

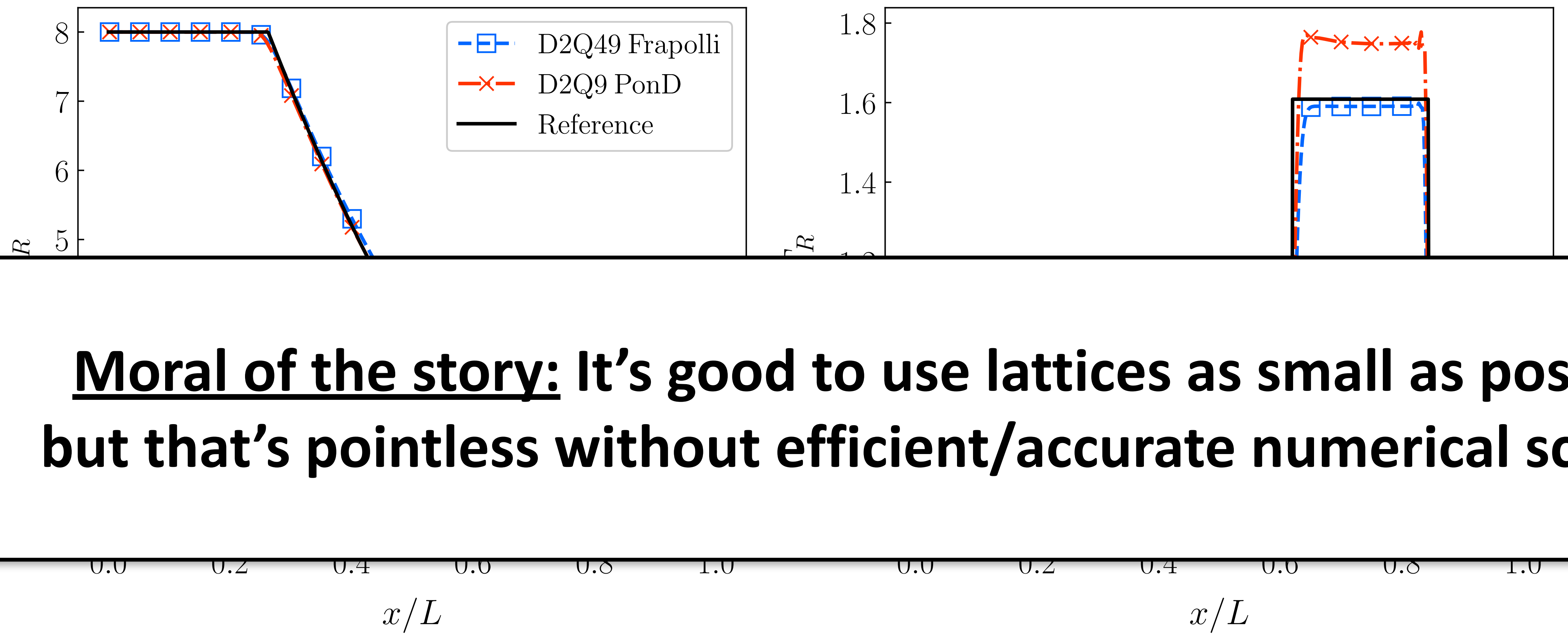
$\rho_L/\rho_R = 8$
$P_L/P_R = 8$

Solver	Navier-Stokes 3D	Frapolli D2Q49	PonD D2Q9
MLUPS	$0.1 - 1.0$	~ 0.13	~ 0.05
μs/pt/it	$1 - 10$	~ 7.7	~ 20

Performance and conservation issues are worsen when increasing ratios…

On-going investigations

Preliminary comparison of some compressible LBMs (no shock sensor)



$L = 500$
$\tau = 0.7$

Moral of the story: It's good to use lattices as small as possible… but that's pointless without efficient/accurate numerical schemes!

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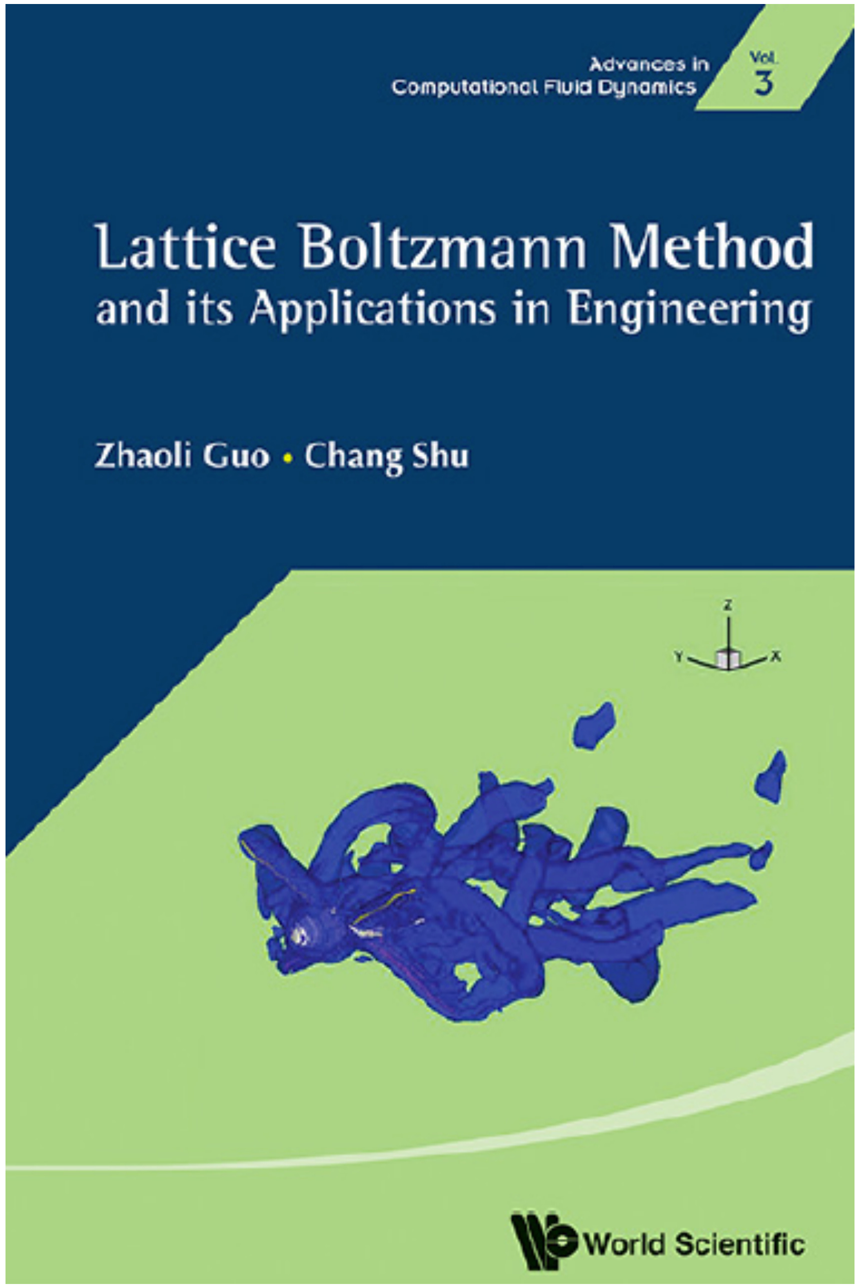
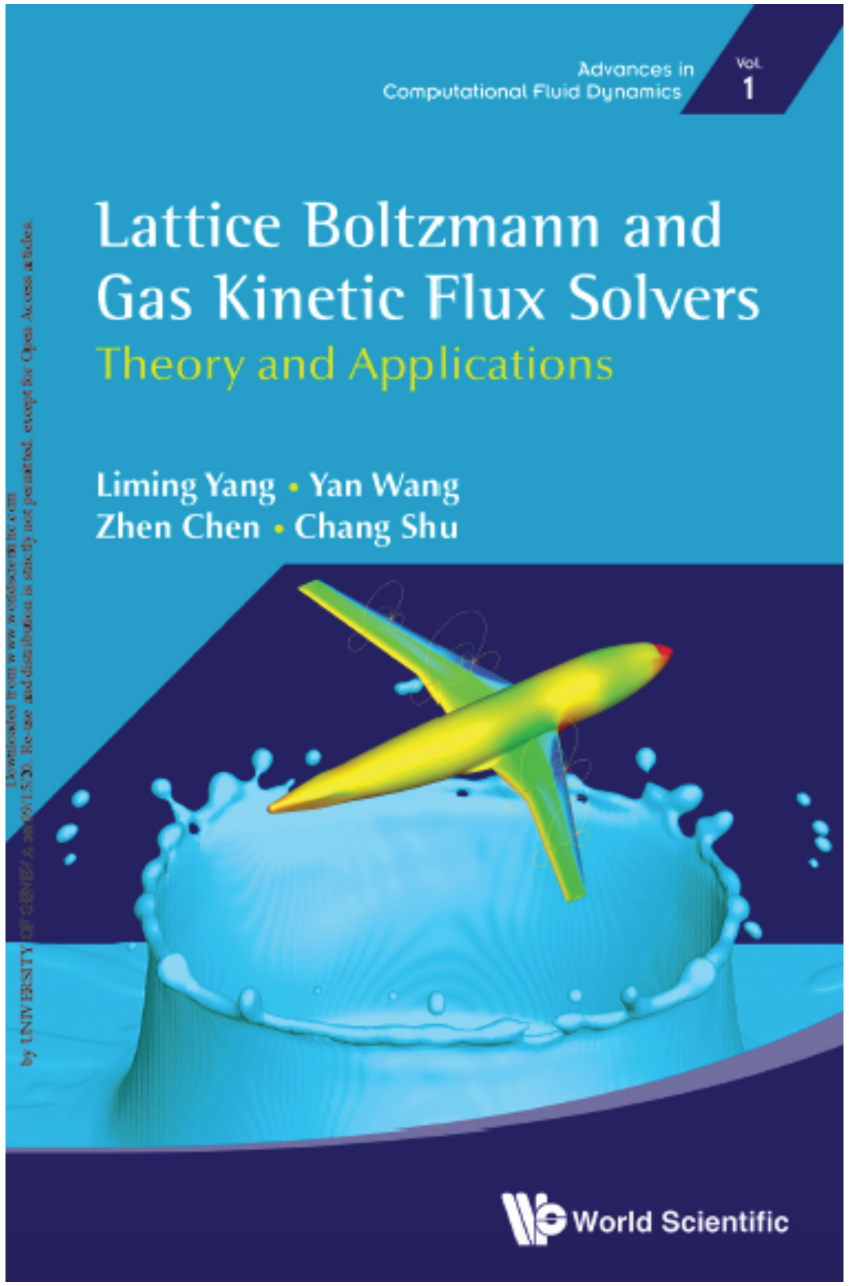
Further reading



Guo & Shu, *Lattice Boltzmann Method and Its Applications in Engineering*, World Scientific, **2013.**



Yang et al., *Lattice Boltzmann and Gas Kinetic Flux Solvers*, World Scientific, **2020.**

- Other types of equilibria (circular, spherical, etc)
- Other numerical discretizations (TVD, IMEX, etc)
- Lattice Boltzmann / gas kinetic flux solvers
- Go and check papers about DUGKS and DBM (not shown here)

Thank you for your attention!
Questions?