

Lattice Boltzmann Algorithms for Complex Fluids and Complex Flows

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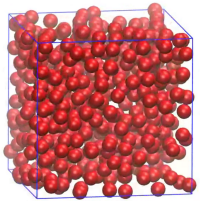
Fluids at different scales

Microscopic

single molecules

Newton's equations

(Molecular Dynamics)

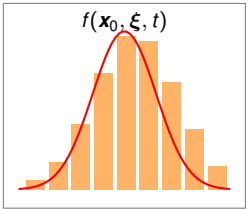


Mesoscopic

probability density

$f(\boldsymbol{x}, \boldsymbol{\xi}, t)$

(Kinetic theory)



Macroscopic

fields ρ, $\boldsymbol{u}$, T

Navier-Stokes

(Continuum)





High Performance Computing in Life Sciences, Engineering, and Physics
2015–2019



Simulation in multiscale physical and biological systems
2018–2022

AQTIVATE

Advanced computing, quantum algorithms, and data-driven approaches for science, technology and engineering
2023–2027







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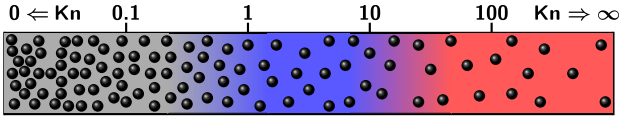
From a Mesoscopic to a Continuum description

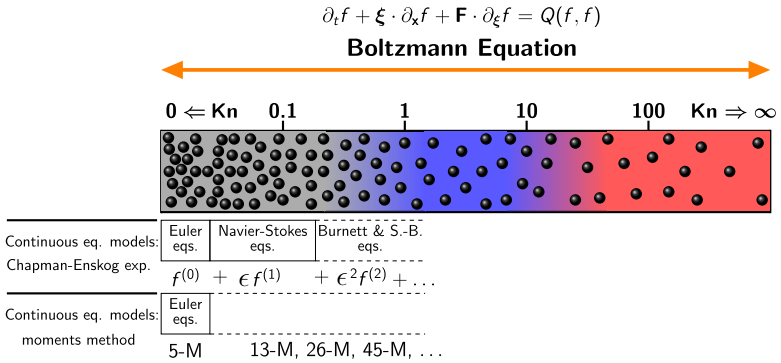
$$\partial_t f + \boldsymbol{\xi} \cdot \partial_{\mathbf{x}} f + \mathbf{F} \cdot \partial_{\boldsymbol{\xi}} f = Q(f, f)$$

Boltzmann Equation



$$\mathrm{Kn} = \frac{\lambda}{\mathrm{L}} = \frac{\text{mean free path}}{\text{system size}}$$

From a Mesoscopic to a Continuum description



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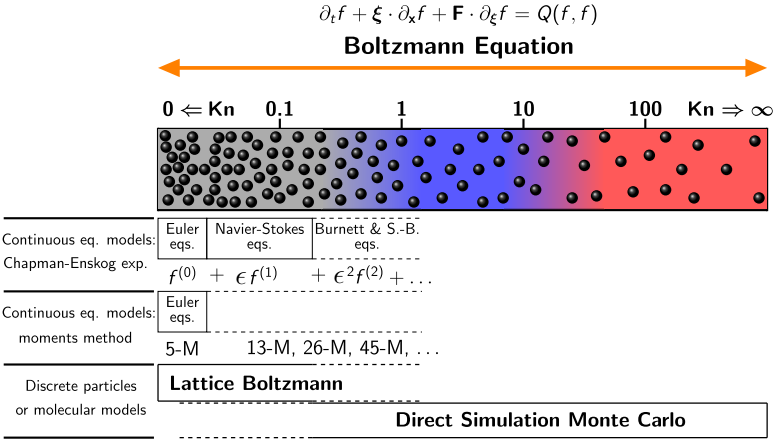
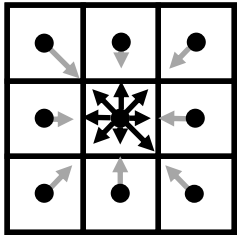


$$\mathrm{Kn} = \frac{\lambda}{\mathrm{L}} = \frac{\text{mean free path}}{\text{system size}}$$

Lattice Boltzmann Method

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = \Omega(f_i)$$



- Computationally efficient fluid dynamics method for solving complex fluid flows.
- Second order approximation of the **Navier-Stokes** equations.
- A set of virtual particles called **populations** arranged at the edges of a discrete regular mesh.
- Particles only have a finite number of velocity directions:

$$\boldsymbol{v} \rightarrow \{\boldsymbol{c}_i, i = 1, \ldots, q\}$$

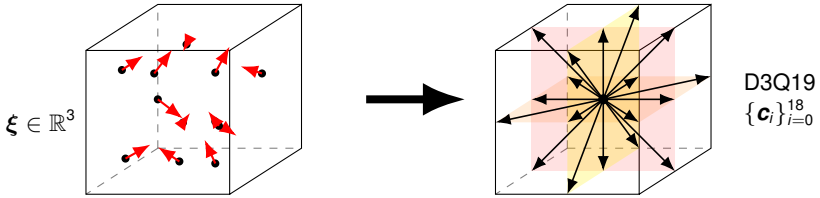
From the Continuum to the Lattice

Replace $\boldsymbol{\xi} \in \mathbb{R}^{\mathrm{D}}$ with a (small) set of velocities $\boldsymbol{c_i}$ such that:

- $\boldsymbol{c_i}$ connects two sites in a Cartesian grid (perfect streaming)
- The moments we need are preserved exactly:

$$\rho = \int f \, \mathrm{d}\boldsymbol{\xi} = \sum_i f_i, \qquad \rho \boldsymbol{u} = \int f \, \boldsymbol{\xi} \, \mathrm{d}\boldsymbol{\xi} = \sum_i f_i \, \boldsymbol{c_i}, \qquad \dots$$

- Mathematically: a **Gauss-Hermite quadrature** in velocity space



Computational Scheme

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta t, t + \Delta t) = f_i(\boldsymbol{x}, t) + \Omega_i\big(\boldsymbol{f}(\boldsymbol{x}, t)\big), \qquad i = 1, \ldots, q$$

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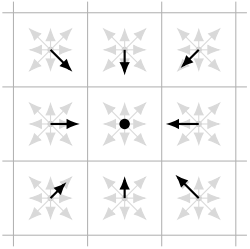
1. Streaming: exact, linear, non-local

$$f_i^{\mathrm{pre}}(\boldsymbol{x}, t) = f_i(\boldsymbol{x} - \boldsymbol{c}_i \Delta t, t)$$



gather from neighbours

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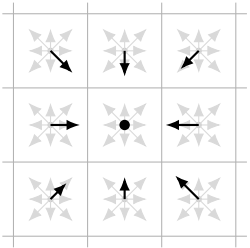

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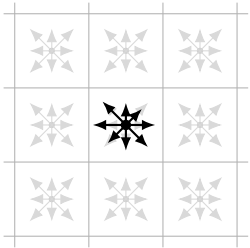

$\boldsymbol{f}^{\mathrm{pre}}$ at the node

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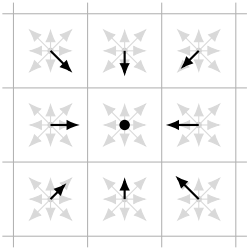

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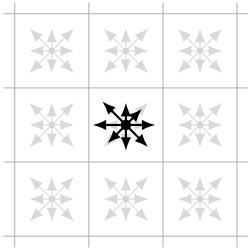
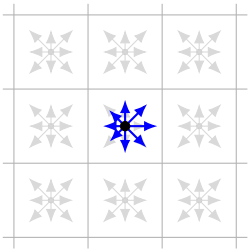


$\boldsymbol{f}^{\mathrm{pre}}$ at the node

2. Collision: non-linear, local

$$f_i(\boldsymbol{x}, t + \Delta t) = f_i^{\mathrm{pre}} + \Omega_i\big(\boldsymbol{f}^{\mathrm{pre}}\big)$$



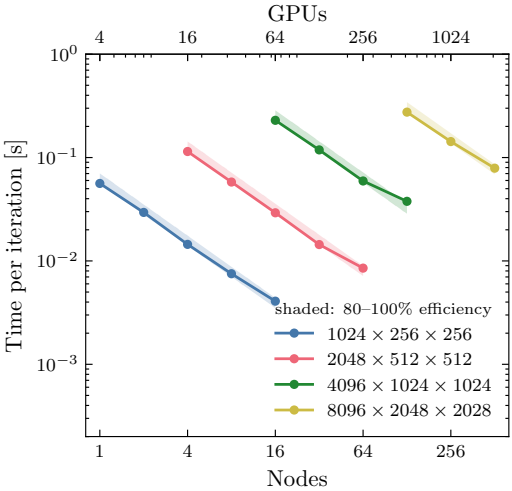
relax towards equilibrium

Why is LBM so well suited to HPC?

- **Regular grid**, nearest-neighbour interactions
- **Collision is local**: embarrassingly parallel
- **Streaming is just memory copy**
- Few flops per byte: performance is bound by **memory bandwidth**

Example: LBM for 3D pool boiling

- JUPITER (JSC): up to 512 nodes, 2048 GPUs
- Grids up to $\sim 3.4 \times 10^{10}$ sites
- $\sim 4 \times 10^{11}$ lattice updates/s



A zoo of collision operators

Operator	Idea	Reference
LBGK	single relaxation time	Qian et al. (1992)
TRT	two rates: even / odd moments	Ginzburg (2005)
MRT	one rate per (raw) moment	d'Humières (1992)
Cascaded / central moments	relax in the frame moving with the fluid	Geier et al. (2006)
Cumulant	relax cumulants (Galilean invariant)	Geier et al. (2015)
Regularized	filter non-hydrodynamic modes before colliding	Latt, Chopard (2006)
Entropic	enforce an H-theorem at each step	Karlin et al. (1999, 2014)

Trade-off between **stability**, **accuracy**, **cost**, and **physics you can tune**.

Review: Coreixas, Chopard, Latt, PRE 100 (2019)

BGK: the simplest collision

$$\Omega_i = -\frac{1}{\tau}\left(f_i - f_i^{\mathrm{eq}}\right)$$

Equilibrium: Hermite expansion of the Maxwell-Boltzmann distribution

$$f_i^{\mathrm{eq}} = w_i \rho \left[1 + \frac{\boldsymbol{u}\cdot\boldsymbol{c}_i}{c_s^2} + \frac{(\boldsymbol{u}\cdot\boldsymbol{c}_i)^2}{2c_s^4} - \frac{|\boldsymbol{u}|^2}{2c_s^2}\right]$$

Viscosity from the relaxation time:

$$\nu = c_s^2\left(\tau - \frac{1}{2}\right)\Delta t$$

Pros

- Simple, cheap
- Good enough for broad range of flows

Limitations

- Everything relaxes at the **same** rate: fixed Prandtl number ($\mathrm{Pr} = 1$)
- Unstable as $\tau \to 1/2$:
- No H-theorem guaranteed

Bhatnagar, Gross, Krook, Phys. Rev. 94, 511 (1954); Qian, d'Humières, Lallemand, EPL 17, 479 (1992)

Multiple relaxation times

$$\boldsymbol{\Omega}^{\mathrm{MRT}} = -\boldsymbol{M}^{-1}\boldsymbol{S}\boldsymbol{M}\left(\boldsymbol{f} - \boldsymbol{f}^{\mathrm{eq}}\right)$$

- $\boldsymbol{M}$: change of basis to **moments**
  $\boldsymbol{m} = \boldsymbol{M}\boldsymbol{f} = (\rho, \rho u_x, \rho u_y, \Pi_{xx}, \Pi_{xy}, \dots)$
- $\boldsymbol{S}$: relaxation matrix, one rate per moment
- Conserved moments: rate 0
- Stress moments: rates set shear & bulk viscosity
- Higher ("ghost") moments: free, tune for stability

Each mode decays at its own rate

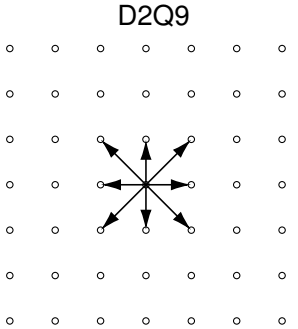
$$\boldsymbol{S} = \begin{pmatrix} 0 & & & & & \\ & \ddots & & & & \\ & & \omega_\nu & & & \\ & & & \omega_\zeta & & \\ & & & & \ddots & \end{pmatrix}$$

d'Humières (1992); Lallemand, Luo, PRE 61 (2000)

Higher-order kinetic models: a way beyond Navier-Stokes

- Expand f^{eq} in Hermite polynomials up to order N
- Larger N = more d.o.f. $\Rightarrow$ more velocities
- Equilibrium moments up to order N are **exact**

N	**Lattice**	**Exact moments**	**Physics**
2	D2Q9	$\rho,\ \rho\boldsymbol{u},\ \Pi_{\alpha\beta}$	isothermal, $\mathrm{Ma} \ll 1$



Shan, Yuan, Chen, JFM 550 (2006); Philippi et al., PRE 73, 056702 (2006)

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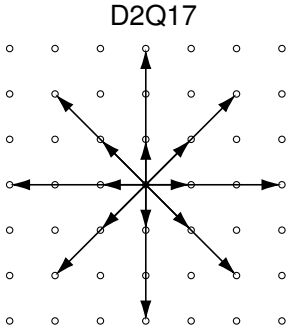

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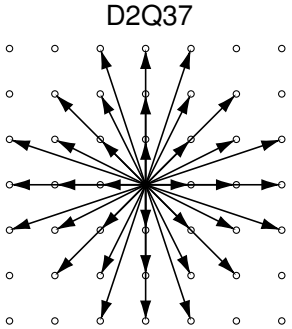
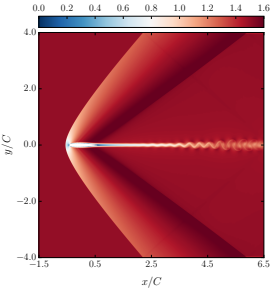
3	D2Q17	$+\ Q_{\alpha\beta\gamma}$	no $\mathcal{O}(\mathrm{Ma}^3)$ error, thermal
4	D2Q37	$+\ R_{\alpha\beta\gamma\delta}$	compressible, NS-Fourier
> 4	off-lattice	higher orders	beyond NS: rarefied



Shan, Yuan, Chen, JFM 550 (2006); Philippi et al., PRE 73, 056702 (2006)

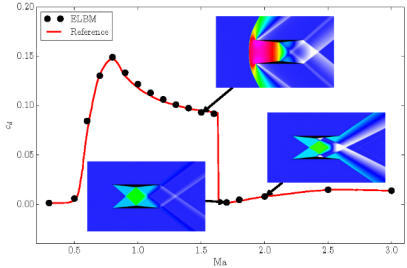
Where plain LBM struggles (1): compressible flows at high Mach

Problem: plain LBM (D2Q9, D3Q19) is built for weakly compressible, isothermal flows: $\mathrm{Ma} \lesssim 0.3$, no shocks



Supersonic airfoil, $\mathrm{Ma} = 1.5$

Latt et al., Phil. Trans. R. Soc. A 378, 20190559 (2020)



Busemann biplane: drag from subsonic to $\mathrm{Ma} = 3$, one entropic LBM

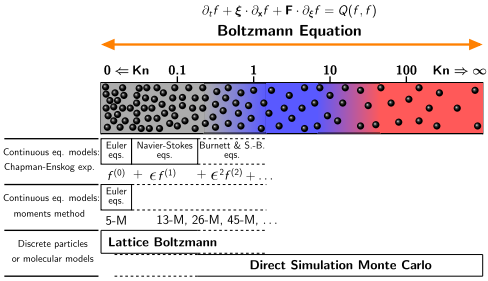
Frapolli, Chikatamarla, Karlin, Entropy 22, 370 (2020)

Way out: **high-order** lattices and equilibria, shifted lattices, particles on demand $\Rightarrow$ supersonic flows

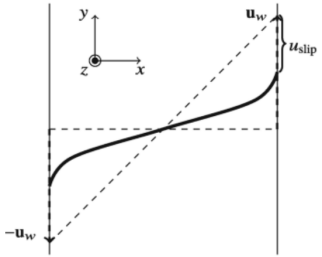
Frapolli et al., PRL 117 (2016); Dorschner et al., PRL 121 (2018); Hosseini et al., Comput. Fluids 259 (2023)

Where plain LBM struggles (2): rarefied gases

Problem: when the mean free path is not small ($\mathrm{Kn} \gtrsim 0.01$), Navier-Stokes, and plain LBM with it, fails



Micro/nano devices, vacuum, re-entry, ...



Couette flow. Dashed: Navier-Stokes, linear, no slip.

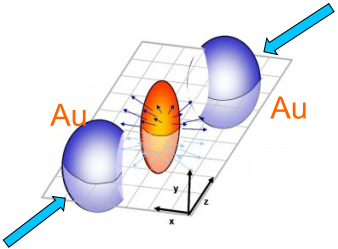
Solid: rarefied gas, slip u_{slip} and Knudsen layer.

Way out: **high-order** quadratures $\Rightarrow$ LBM as a discrete-velocity Boltzmann solver

Shan, Yuan, Chen, JFM 550 (2006); Ambruş, Sofonea, J. Comput. Sci. 17 (2016)

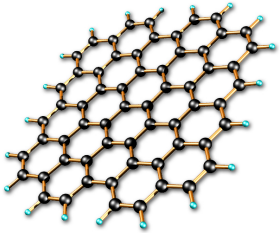
Pushing it further: relativistic dissipative fluids

- Same recipe, high-order models applied to the relativistic Boltzmann equation.
- Support for several relativistic regimes: bridges from ultra-relativistic regime down to classic fluids.



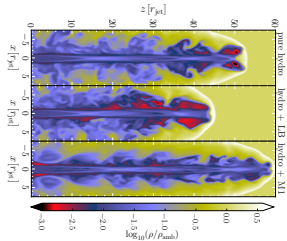
Quark-gluon plasma

Gabbana et al., Phys. Rep. 863 (2020)



Electrons in graphene

Gabbana et al., PRL 121, 236602 (2018)



Relativistic jets: radiative transport

Weih, Gabbana et al., MNRAS 498, 3374 (2020)

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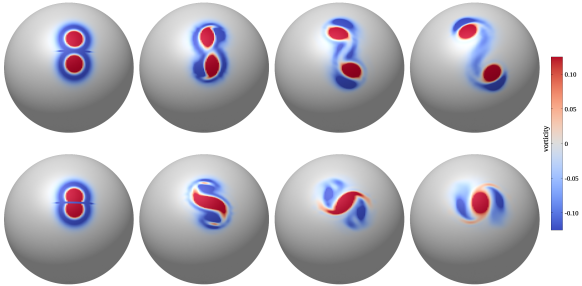
Ambruş, Gabbana, Simeoni, Succi, Tripiccione, Nat. Comput. Sci. 2 (2022)

Fluids on curved manifolds

Vielbein lattice Boltzmann

- A **vielbein** (local orthonormal frame) encodes the geometry
- Velocity space stays **Cartesian** $\Rightarrow$ standard quadratures still work
- Geometry enters as **inertial forces** that keep particles on the manifold
- Forces computed by projection on Hermite polynomials



Co-rotating vortex pairs on a sphere

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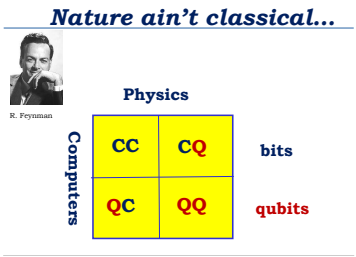
Ambruş, Bellantoni, Busuioc, Gabbana, Toschi, Phys. Rev. Fluids 10, 124901 (2025)

LBM goes Quantum



Succi, Itani, Sreenivasan, Steijl, EPL 144, 10001 (2023)

Quantum physics with lattice Boltzmann (CQ)

- The Dirac equation is a discrete kinetic equation: stream + "collide" (mass term)
- Schrödinger emerges as its "hydrodynamic" limit
- Dirac fluids: electrons in graphene

Succi, Benzi, Physica D 69, 327 (1993)

Lattice Boltzmann on quantum computers (QC)

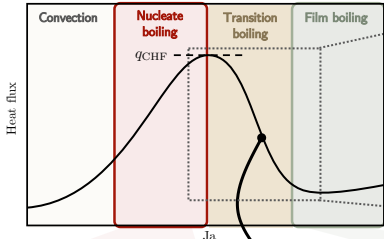
- n qubits store 2^n populations
- **streaming** is a permutation $\Rightarrow$ a quantum walk
- **Collision**: non-linear, dissipative $\Rightarrow$ not unitary

Budinski, Quantum Inf. Process. 20, 57 (2021); Itani, Succi, arXiv:2111.11327; Succi et al., EPL 144, 10001 (2023)

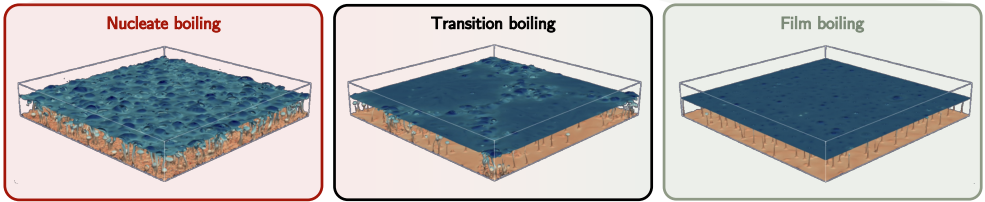
Example of Application #1

Hysteresis in Transition Boiling

Boiling regimes



- Heat flux vs wall superheat (Jakob number Ja)
- **Nucleate**: bubbles, efficient cooling, up to the critical heat flux q_{CHF}
- **Film**: a vapour layer insulates the wall
- **Transition**: unstable branch in between



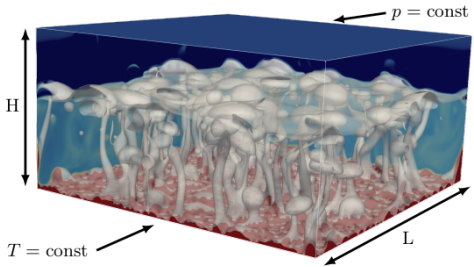
Gabbana, de Wit, Fei, Wang, Livescu, Toschi, arXiv:2509.14042 (2025)

Hysteresis in transition boiling

The heat flux at a given superheat depends on whether it is reached by **heating** (from nucleate) or by **cooling** (rewetting from film)

- Observed by Witte & Lienhard (1982), confirmed by other groups
- Other studies report no hysteresis
- Discrepancies blamed on transients, surface impurities, geometry, contact angle

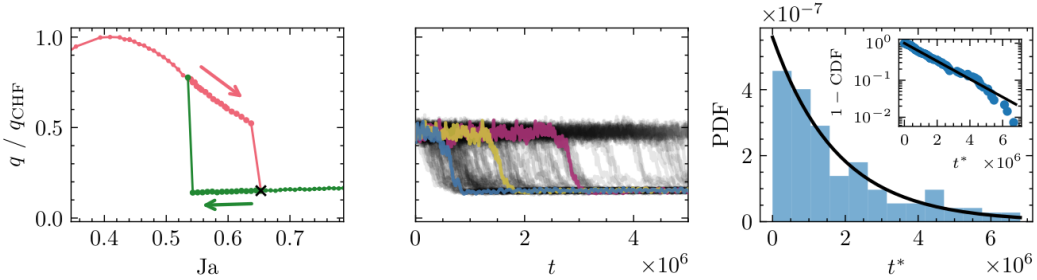
Intrinsic physics, or an artifact of the surface?



Large-scale 3D pool boiling under **idealized** conditions: flat isothermal wall, no impurities or defects.

Gabbana, de Wit, Fei, Wang, Livescu, Toschi, arXiv:2509.14042 (2025)

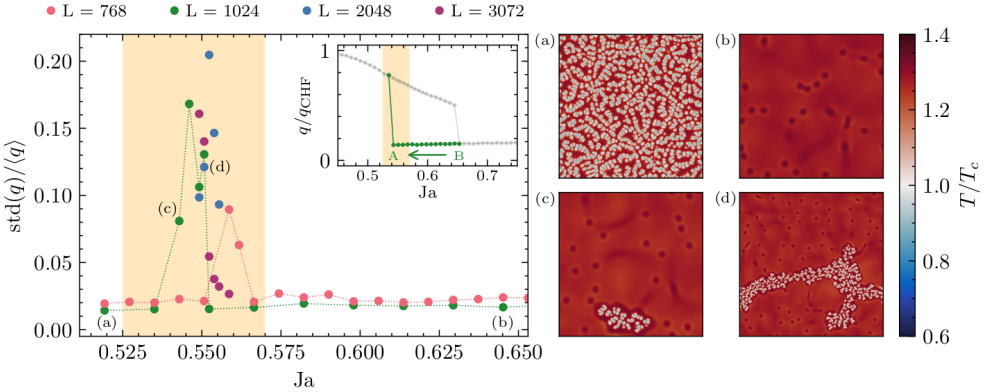
Heating: from nucleate to film boiling



- **Memoryless**: the switch is sharp and stochastic (exponential waiting times), driven by interfacial events
- **One way**: nucleate always turns into film boiling; the reverse never happens at the same Ja

Gabbana, de Wit, Fei, Wang, Livescu, Toschi, arXiv:2509.14042 (2025)

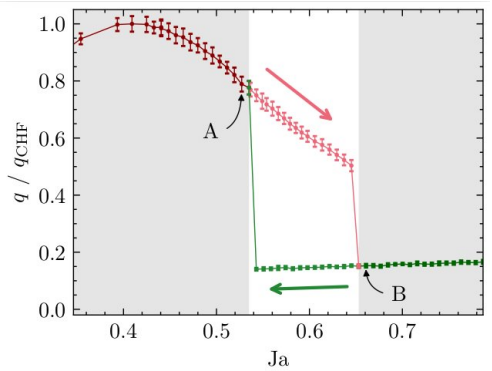
Cooling: from film to nucleate boiling



- Film and nucleate regions **coexist** on the wall: long-lived metastable states
- Filament-like patches are stabilized by convection rolls and delay rewetting

Gabbana, de Wit, Fei, Wang, Livescu, Toschi, arXiv:2509.14042 (2025)

Hysteresis in transition boiling: take-home



- Hysteresis is **intrinsic and hydrodynamic**: it appears even on a flat, clean, isothermal wall
- The loop is strongly **asymmetric**:
  heating is abrupt and memoryless,
  cooling goes through long-lived coexistence
- Coexistence is stabilized by the large-scale flow

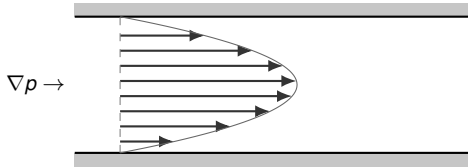
Gabbana, de Wit, Fei, Wang, Livescu, Toschi, arXiv:2509.14042 (2025)

Example of Application #2

Lattice Boltzmann for Odd Fluids

What is odd viscosity?

Ordinary fluid



Viscosity = friction between neighbouring fluid layers sliding at different speeds (shear)

$\Rightarrow$ it slows the flow down and **dissipates** energy: parabolic profile

Avron, J. Stat. Phys. 92, 543 (1998); Fruchart, Scheibner, Vitelli, Annu. Rev. Condens. Matter Phys. 14 (2023)

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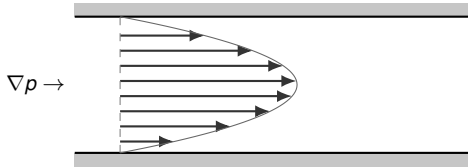
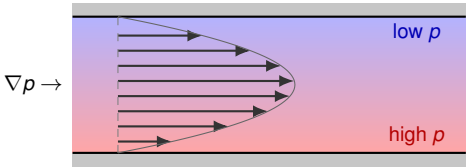


With odd (Hall) viscosity



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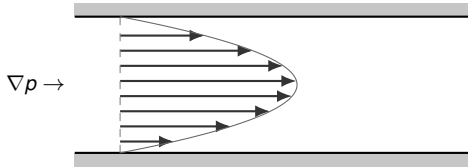
The same shear also pushes **sideways**, at 90°

$\Rightarrow$ same velocity profile, but a **pressure difference across** the channel; no dissipation

Avron, J. Stat. Phys. 92, 543 (1998); Fruchart, Scheibner, Vitelli, Annu. Rev. Condens. Matter Phys. 14 (2023)

What is odd viscosity?

Ordinary fluid



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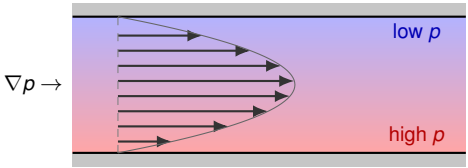

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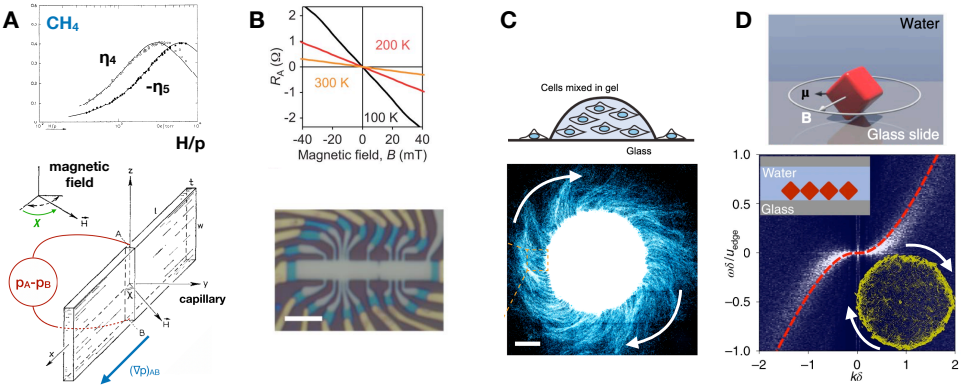
Like the **Hall effect**: current along a wire in a magnetic field $\Rightarrow$ voltage across it.
Needs a fluid that breaks **mirror** and **time-reversal** symmetry: spinning particles, magnetic fields, ...

Avron, J. Stat. Phys. 92, 543 (1998); Fruchart, Scheibner, Vitelli, Annu. Rev. Condens. Matter Phys. 14 (2023)

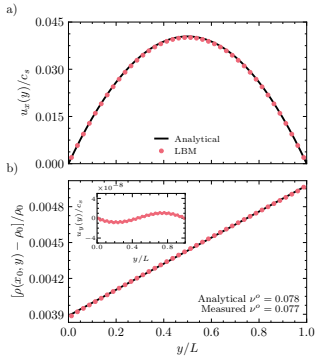
Where does odd viscosity show up?



Can we simulate odd fluids efficiently, at high Reynolds number, with boundaries?

Figure from Fruchart, Scheibner, Vitelli, Annu. Rev. Condens. Matter Phys. 14 (2023)

Odd lattice Boltzmann



(a) velocity: unchanged;

(b) density across the channel

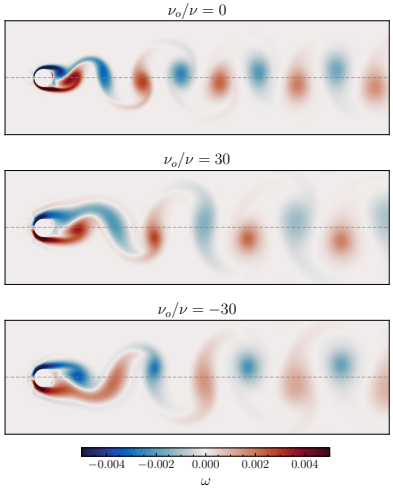
Couple the two shear moments $\Pi_2 = \frac{1}{2}(\Pi_{xx} - \Pi_{yy})$ and $\Pi_3 = \Pi_{xy}$ with an **antisymmetric** block in the MRT relaxation matrix:

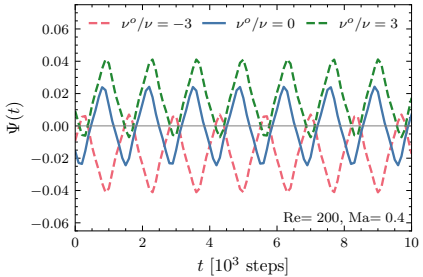
$$\boldsymbol{S}_2^o = \begin{pmatrix} \omega_\zeta & 0 & 0 \\ 0 & \omega_\nu & -\omega_o \\ 0 & \omega_o & \omega_\nu \end{pmatrix}$$

- Odd viscosity emerges from the **kinetic relaxation**, not added as an extra macroscopic stress
- Retains all properties and advantadges of plain LBM.

Eren, Gabbana, Touzo, Fruchart, Vitelli, *in preparation*

Odd von Kármán vortex street





Enstrophy of the two vortex rows: $E_\pm = \sum_{\omega \gtrless 0} \omega^2$,

$$\Psi = \frac{E_+ - E_-}{E_+ + E_-}$$

- Odd viscosity **breaks the mirror symmetry** of the wake: flipping ν^o gives the mirror image
- Ψ oscillates around a **non-zero mean**: one vortex row is stronger; the shedding frequency is almost unchanged

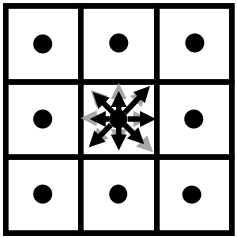
Eren, Gabbana, Touzo, Fruchart, Vitelli, *in preparation*

Example of Application #3

Lattice Boltzmann meets Machine Learning

Learn novel collision operators from data?

$$f_i^{\text{post}} = \Omega_{\text{NN}}(f_i^{\text{pre}})$$



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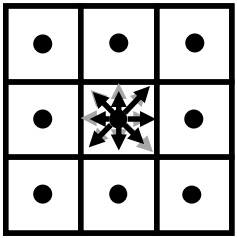


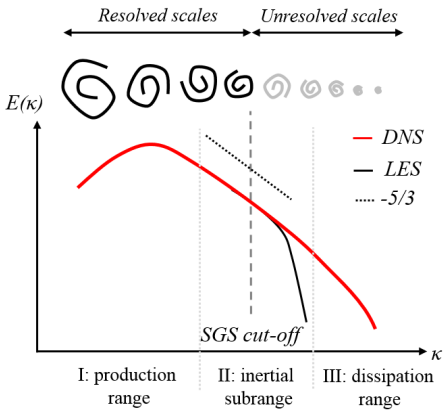
A first exercise: learning the BGK collision operator

Key ingredients:

- Hard contraints for conservation of mass and momentum
- Ensure preservation of symmetries

Corbetta, A., Gabbana, A., Gyrya, V., Livescu, D., Prins, J., Toschi, F.
Eur. Phys. J. E, 46 3 (2023)

Application: turbulence on coarse grids



Energy spectrum

Why turbulence needs modeling

- Energy cascades from the large scale L down to the dissipative (Kolmogorov) scale η
- $L/\eta \sim \mathrm{Re}^{3/4} \Rightarrow$ a full simulation (DNS) needs $N \sim \mathrm{Re}^{9/4}$ grid points in 3D
- Aircraft, atmosphere: $\mathrm{Re} \sim 10^7$–$10^9 \Rightarrow$ out of reach

Large Eddy Simulation

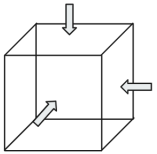
- Resolve the large scales, **model** the effect of the unresolved (subgrid) ones
- Example, Smagorinsky: extra **eddy viscosity** $\nu_t = (C_s\Delta)^2|\bar{S}|$
- In LBM it enters the collision: $\tau_{\mathrm{eff}} = (\nu + \nu_t)/c_s^2 + 1/2$ $\Rightarrow$ a subgrid model is a modified collision operator

Smagorinsky, Mon. Weather Rev. 91, 99 (1963); Pope, Turbulent Flows (2000)

Learning a subgrid model from DNS for HIT

Fully resolved simulation of homogeneous isotropic turbulence (HIT)

- Periodic grid of size 128^3
- Reynolds number: $6 \cdot 10^3$ ($Re_\lambda \approx 77$)
- Plain model unstable on grids of size 64^3, 32^3

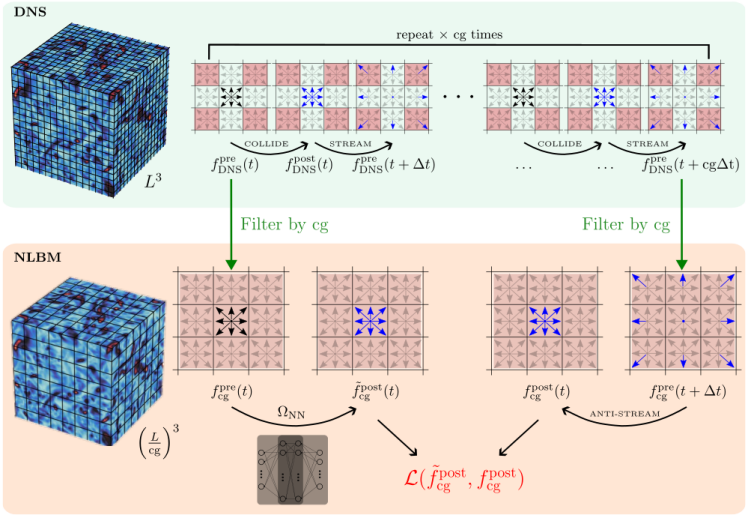


$$\begin{cases} F_x \sim sin(y) \\ F_y \sim sin(z) \\ F_z \sim sin(x) \end{cases}$$

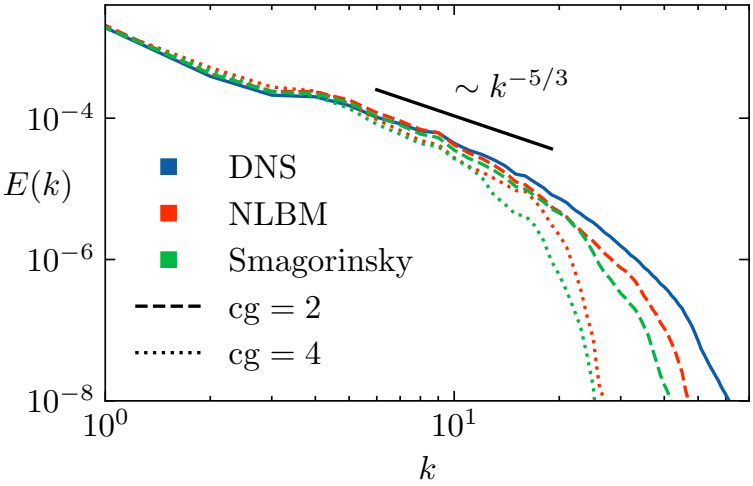
Can a neural network correct the collision to account for the unresolved scales?

$$\tilde{f}_i^{\mathrm{post}} = f_i^{\mathrm{pre}} + \frac{1}{\tau}\left((f_i^{\mathrm{eq}} - f_i^{\mathrm{pre}}) + \Omega^{\mathrm{NN}}(f_i^{\mathrm{pre}})\right)$$

Generating training data



Energy Spectrum



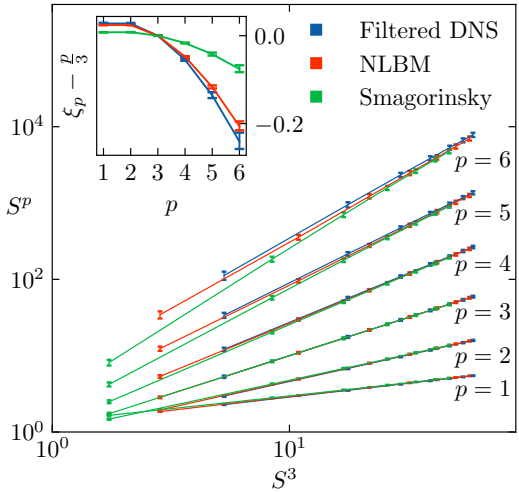
Beyond the spectrum: intermittency

- Structure functions of order p:

$$S^p(\ell) = \left\langle |\Delta \boldsymbol{u}(\ell)|^p \right\rangle \sim \ell^{\xi_p}$$

- Kolmogorov (1941): $\xi_p = p/3$
- Real turbulence deviates (**intermittency**)
- The learned model reproduces the deviations

Ortali, Gabbana, Demo, Rozza, Toschi,
Phys. Rev. Research 7, 013202 (2025)



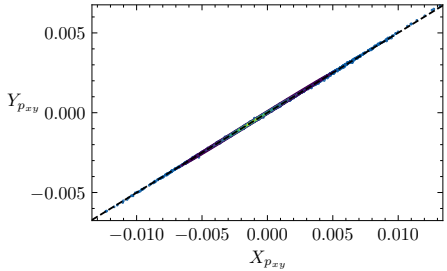
Interpretability: what did the network learn?

The network acts **only on the collision** $\Rightarrow$ project its action on moments and compare with BGK:

$\boldsymbol{X} = \boldsymbol{M}\left(\boldsymbol{f}^{\mathrm{eq}} - \boldsymbol{f}^{\mathrm{pre}}\right)$ (distance from equilibrium) $\qquad$ $\boldsymbol{Y} = \boldsymbol{M}\left(\boldsymbol{f}^{\mathrm{post}} - \boldsymbol{f}^{\mathrm{pre}}\right)$ (change made by the collision)

BGK: a straight line with slope $1/\tau$ (black dotted)

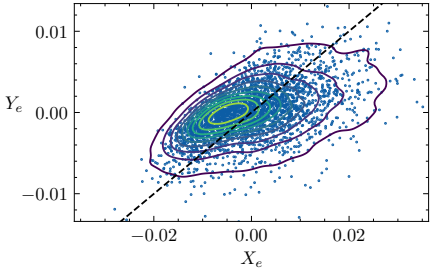
Shear stress p_{xy}



Linear: $\tau_{\mathrm{eff}} \approx 0.5023 > \tau = 0.5008$

$\Rightarrow$ the network learned an **eddy viscosity**

Energy e

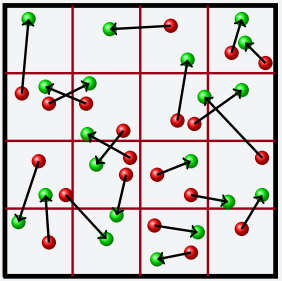


Strongly non-linear:

not a simple bulk-viscosity correction

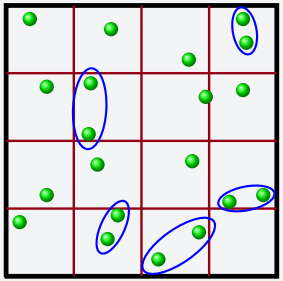
Ongoing: rarefied gases from particle simulations

Direct Simulation Monte Carlo (DSMC)



Deterministic ballistic motion

+

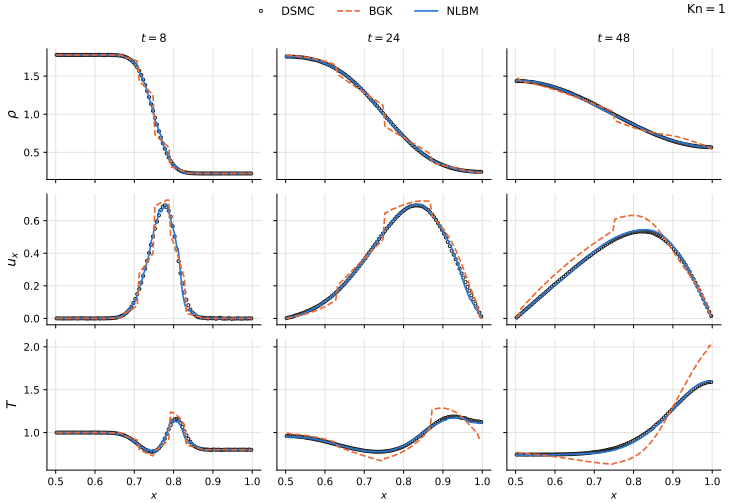


Stochastic binary collisions

DSMC is accurate at large Kn, but noisy and expensive.

Learn a collision operator from DSMC data, use it in a cheap LBM

Rarefied shock tube ($\mathrm{Kn} = 1$)



- Reference: particle simulation (DSMC)
- **BGK** LBM: spurious kinks, wrong temperature at late times
- **NLBM**: same LBM, collision operator learned from DSMC data
- NLBM follows DSMC through the whole evolution

proof of concept, preliminary

Summary

- **LBM**: by now a well established computationally efficient computational fluid dynamics method based on a minimal kinetic model.
- **The collision operator** sets the physics
- **High-order models** a way beyond Navier-Stokes with many applications: high Mach, rarefied, relativistic flows ...
- **Neural collision operators**: work once symmetries and conservation laws are built in $\rightarrow$ stable subgrid models for turbulence, surrogates for rarefied gases.



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Exascale, quantum computing and machine learning for innovation in sciences

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In memory of Lele



“ E’ facile, forse anche possibile ”

It is easy, maybe it is even possible!



Lattice Boltzmann Algorithms for Complex Fluids and Complex Flows

Alessandro Gabbana

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AQTIVATE Conference - Larnaca - September 30, 2026