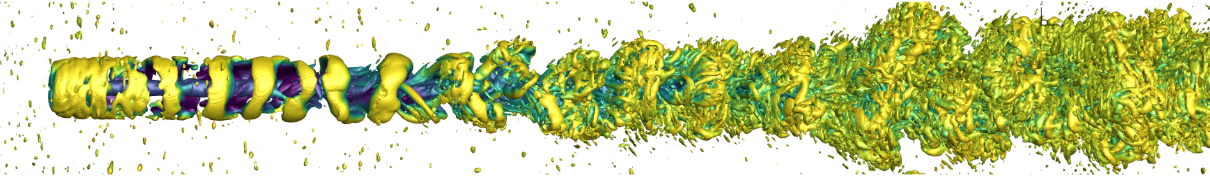
Controlling inflow boundary conditions in a lattice Boltzmann LES model for urban flows



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Motivation

Evaluate LBM as a scalable LES framework for real-world flows.

- Equinor project: Assess LBM for wind turbine wake simulations.
- UrbanAIR EU project: Explore data assimilation for LES.
- Open-source LBM implementation: `https://www.github.com/geirev/LBM`.

Maxwell-Boltzmann distribution function

A gas with constant temperature and no external forcing equilibrates to the

Maxwell-Boltzmann equilibrium distribution

$$f(\mathbf{w}) \quad \rightarrow \quad f^{\mathrm{eq}}(\mathbf{w}) = n\left(\frac{m}{2\pi\, k\, T}\right)^{3/2} \exp\left(-\frac{m\,(\mathbf{w}-\mathbf{v})^2}{2\, k\, T}\right) \tag{1}$$

- Here $f(\mathbf{w})$ is the probability density of the particle velocities.
- Macroscopic variables are moments of $f(\mathbf{w})$.
- In the absence of forcing, the solution relaxes toward this state.
- LBM evolves discrete distributions that are close to this equilibrium.
- Average particle velocity in air is 470 m/s.

Boltzmann equation

The probability density $f(\mathbf{w})$ evolves according to

Boltzmann equation (BGK approximation)

$$\frac{\partial f}{\partial t} + \mathbf{w} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{X}}{m} \cdot \frac{\partial f}{\partial \mathbf{w}} = \tau^{-1}(f^{\mathrm{eq}} - f) \tag{2}$$

- Collision term models relaxation toward equilibrium.
- Valid in the hydrodynamic limit (mean free path $\ll$ system size).
- Mean free path in air: $6.8 \cdot 10^{-8}$ m.
- Moments of this equation recover the Navier–Stokes equations.
- LBM solves a discrete, low-Mach approximation of this equation.

3'rd Order Hermite expansion

Represent $f(\mathbf{r}, \mathbf{w}, t)$ using a 3rd-order Hermite expansion in velocity

$$f(\mathbf{w}, \mathbf{r}, t) = e^{-\mathbf{w}^T \mathbf{w}/2} \Big[a^{(0)}(\mathbf{r}, t) + a_i^{(1)}(\mathbf{r}, t) \, H_i^{(1)}(\mathbf{w}) + \tfrac{1}{2} a_{ij}^{(2)}(\mathbf{r}, t) \, H_{ij}^{(2)}(\mathbf{w}) + \tfrac{1}{6} a_{ijk}^{(3)}(\mathbf{r}, t) \, H_{ijk}^{(3)}(\mathbf{w}) \Big] \tag{3}$$

$$= \omega(\mathbf{w}) \, p(\mathbf{w}, \mathbf{r}, t). \tag{4}$$

- Second-order truncation captures the macroscopic NS variables and stress tensor.
- Third-order term is needed for stability in high-Reynolds-number flows.

Macroscopic variables by Gauss–Hermite quadrature

Velocity moments become discrete sums

$$\int \phi(\mathbf{w})\, f(\mathbf{r},\mathbf{w},t)\, d\mathbf{w} \approx \int \phi(\mathbf{w})\, \omega(\mathbf{w})\, p(\mathbf{r},\mathbf{w},t)\, d\mathbf{w} \tag{5}$$

$$= \sum_{l=1}^{Q} w_l\, \phi(\mathbf{c}_l)\, p(\mathbf{r},\mathbf{c}_l,t) = \sum_{l=1}^{Q} \phi(\mathbf{c}_l)\, f_l(\mathbf{r},t) \tag{6}$$

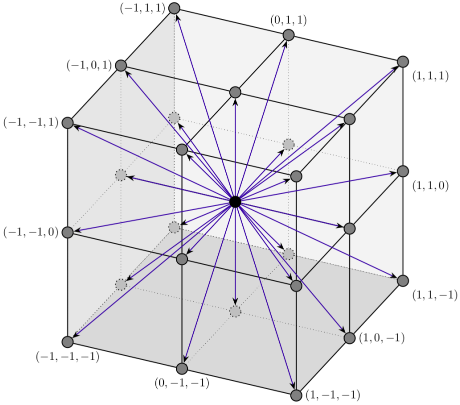
when defining discrete populations

$$f_l(\mathbf{r},t) = w_l\, p(\mathbf{r},\mathbf{c}_l,t) = w_l \frac{f(\mathbf{r},\mathbf{c}_l,t)}{\omega(\mathbf{c}_l)} \tag{7}$$

- Velocity moments (up to quadrature order) are evaluated exactly using discrete velocities $\mathbf{c}_l$.

LBM discretization in 3D (D3Q27)

- Discrete velocities $\mathbf{c}_l$ arise from Gauss–Hermite quadrature.
- At each grid point (i, j, k), we store populations $f_l(i, j, k)$ for $l = 1, \ldots, 27$.
- f_l represents the population moving with velocity $\mathbf{c}_l$.
- Choice of lattice units: $\Delta x = \Delta t = 1$
  - $\mathbf{c}_l \in \{-1, 0, 1\}$
  - Exact streaming to neighboring nodes in one timestep
- Advection is exact in lattice units!
- D3Q27 better than D3Q19 for high-Re flows



Macroscopic variables

Density

$$\rho(\mathbf{r}, t) = \sum_l f_l(\mathbf{r}, t) \tag{8}$$

Fluid velocity

$$\mathbf{v}(\mathbf{r}, t) = \frac{1}{\rho} \sum_l \mathbf{c}_l \, f_l(\mathbf{r}, t) \tag{9}$$

Isothermal equation of state

$$p(\mathbf{r}, t) = c_s^2 \, \rho(\mathbf{r}, t), \qquad c_s^2 = \frac{1}{3} \tag{10}$$

Collision step and non-equilibrium

Decompose the distribution:

$$f_l = f_l^{\mathrm{eq}} + f_l^{\mathrm{neq}}. \tag{11}$$

- Collision (BGK relaxation)

$$f_l^* = f_l - \frac{1}{\tau}(f_l - f_l^{\mathrm{eq}}) + F_l \tag{12}$$

$$= f_l^{\mathrm{eq}} + \left(1 - \frac{1}{\tau}\right) f_l^{\mathrm{neq}} + F_l. \tag{13}$$

- Regularization

$$f_l^{\mathrm{neq}} \longrightarrow \mathcal{R}\left(f_l^{\mathrm{neq}}\right) \tag{14}$$

removes high-order (non-hydrodynamic) components that can lead to instabilities

Streaming step

- Exact advection of populations

$$f_l(t + \Delta t, \mathbf{x}) = f_l^*(t, \mathbf{x} - \mathbf{c}_l \Delta t) \tag{15}$$

- Due to $\Delta x = \Delta t = 1$:
  - particles move exactly to neighboring nodes
  - no interpolation or numerical diffusion

Implementation specifics

- Numerical method
  - D3Q27 velocity discretization
  - 3rd-order regularized BGK collision operator (Jacob et al., 2018)
  - Forcing scheme (Kupershtokh et al., 2009)
- Turbulence modeling
  - Vreman's Smagorinsky-type SGS model (Vreman, 2004)
- Boundary conditions
  - Closed, periodic, and inflow–outflow boundaries
  - Bounce-back scheme for solid objects
  - Turbulent inflow via smooth pseudo-random perturbations
- Wind-turbine forcing
  - Uses actuator-line method (ALM) by Sørensen and Shen (2002).
- Implementation
  - NVIDIA CUDA Fortran with GPU + MPI parallelization

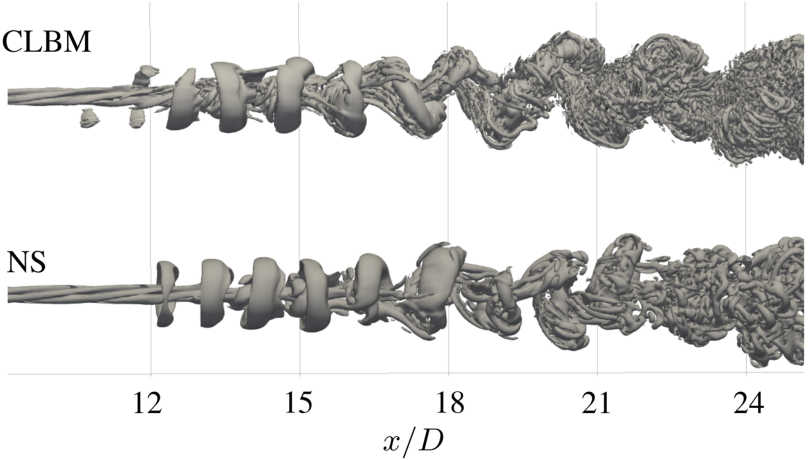
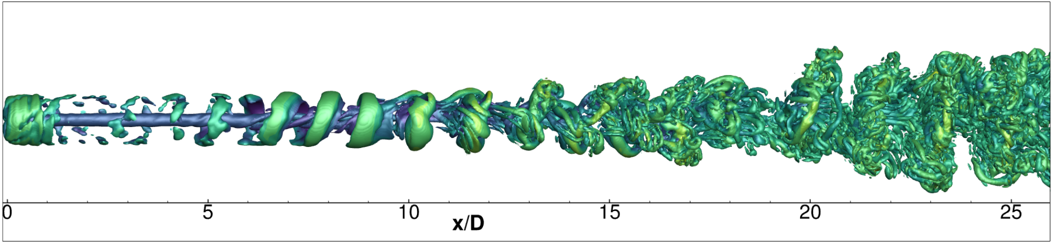


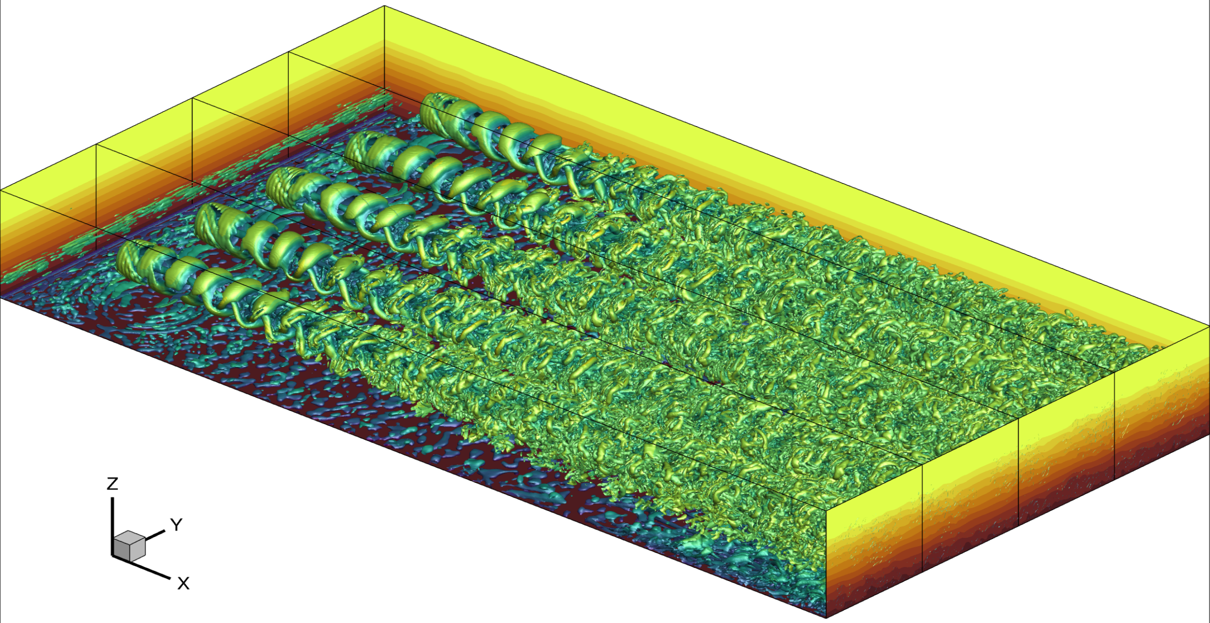
Figure 11. Rendering of the instantaneous contours of the Q criterion ($Q = 0.0005$) in the far wake with the CLBM and NS with $\Delta x = D/32$.

Q-criterion plot

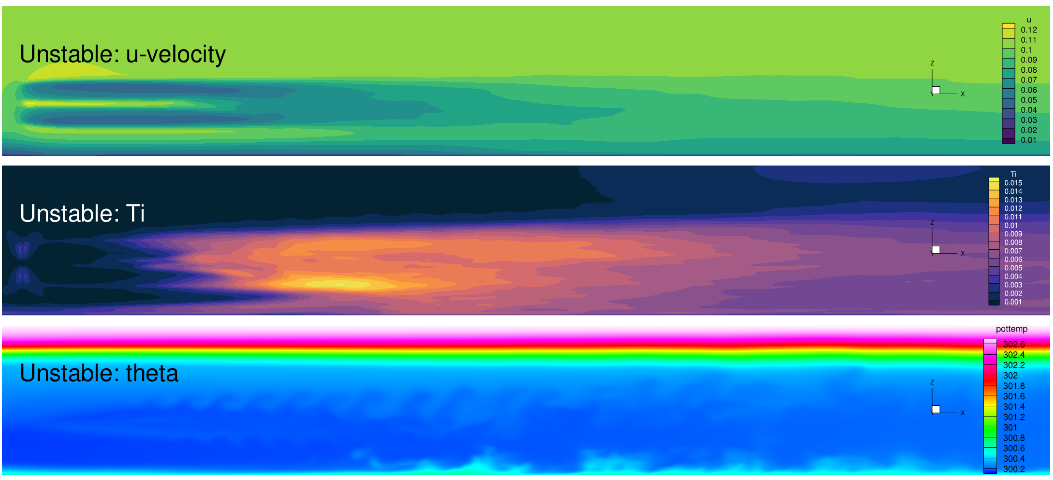
- Rich small-scale structures in the wake
- Low numerical dissipation preserves vortical structures
- Exact streaming avoids artificial diffusion
- D3Q27 + regularization improves isotropy and stability



von Kármán vortex street


Z
Y
X

Unstable atmospheric boundary layer



UrbanAIR: Motivation

- High fidelity city-LES (4 m res)
- Model wind and temperature
- Uncertain inflow conditions from meteo (1 km res)
- **Improve inflow conditions by data assimilation**
- Observations are wind measurements in the city

Flow through a city

Flow through a city

Time varying inflow

UrbanAIR: Experiment

- Estimate **uncertain inflow wind speed and direction**.
- Interior observations collected at **four locations within the city**.
- Measurements available every **60 s** with **2% relative observation error**.
- Recursive data assimilation with **5-,10-, or 20-minute assimilation windows**.
- **4-step ESMDA** for updating the inflow forcing.
- Prior inflow from **AR(2) simulations continued from the previous window**.

Simulating the prior ensemble

Generate a **continuous and smooth prior ensemble** for the next DA window.

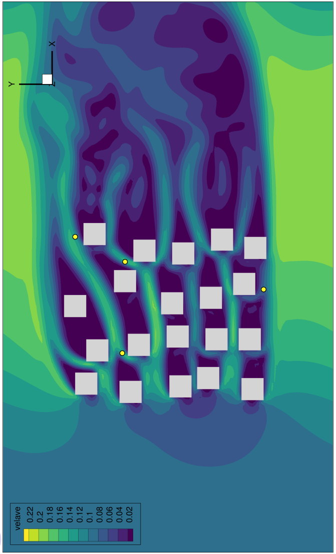
The prior ensemble for the next assimilation window is

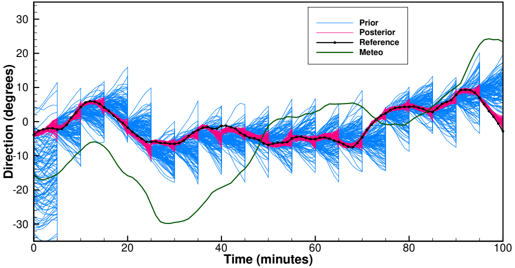
$$X_j(t_k) = (1 - \alpha_k)\,\text{meteo}(t_k) + \alpha_k\,\overline{X} + \sigma z_j(t_k), \tag{16}$$

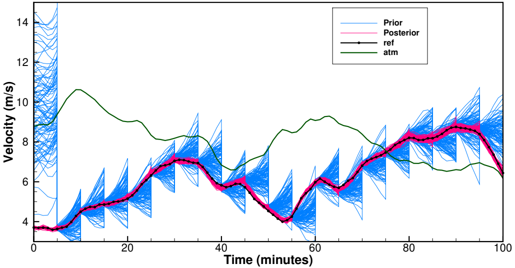
with a relaxation towards the atmospheric prediction determined by

$$\alpha_k = \exp\left[-\left(\frac{k\Delta t}{l_{\mathrm{corr}}}\right)^2\right]. \tag{17}$$

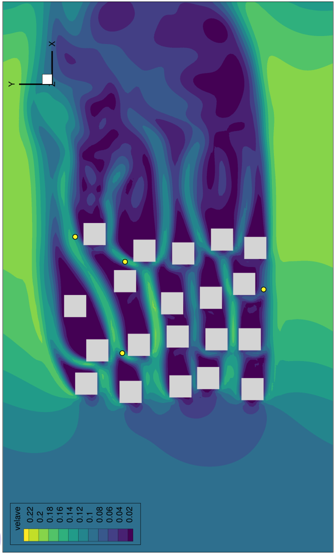
Estimating inflow conditions, ESMDA-4

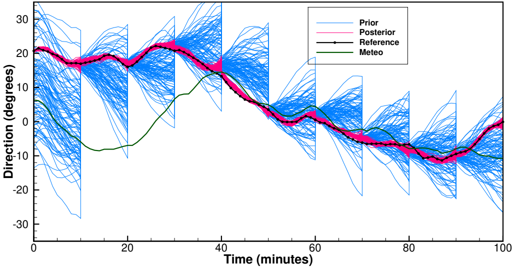


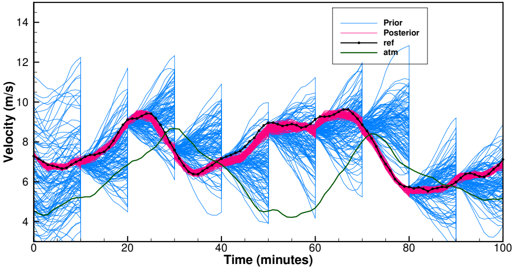




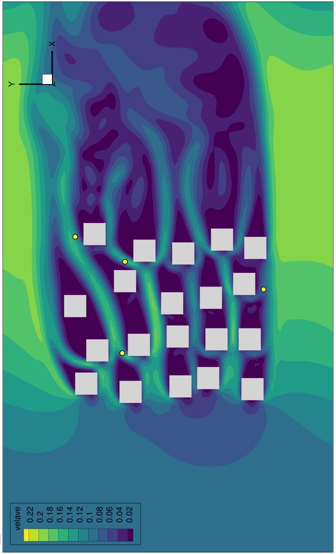
Estimating inflow conditions, ESMDA-4

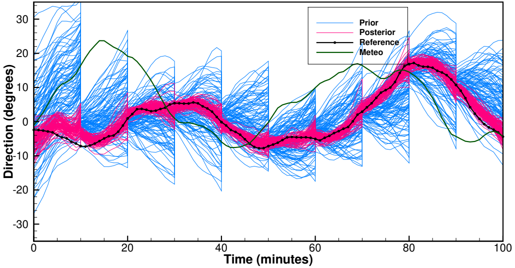


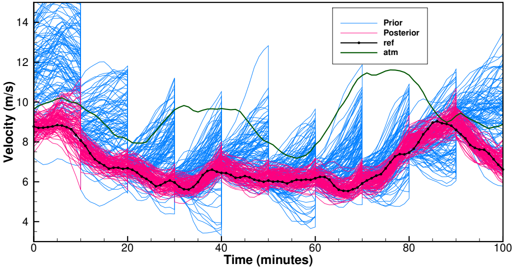




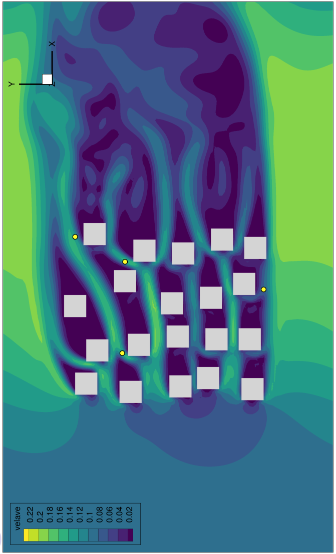
Estimating inflow conditions, ES

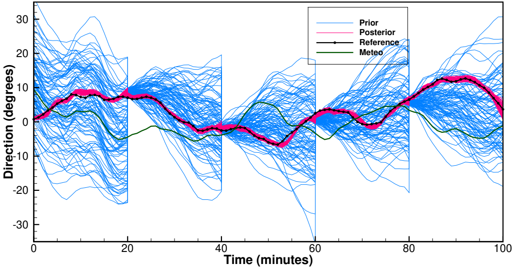


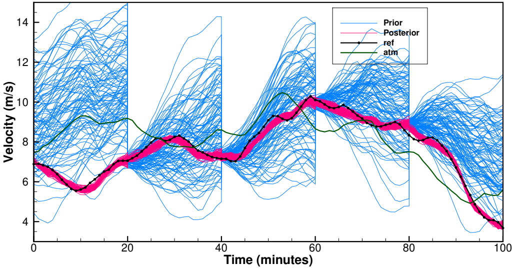




Estimating inflow conditions, ESMDA-4





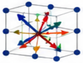


Summary

- **LBM is a competitive framework for high-Reynolds-number LES:**
  - D3Q27 lattice and 3rd-order Hermite expansion improve stability for turbulent flows.
  - Regularization removes non-hydrodynamic higher-order components.
  - Stability with BGK simplicity (Jacob et al., 2018).
  - Explicit advection and local operations are highly GPU-friendly.
- **Open-source LES framework:**
  - Model buoyancy forcing by advecting potential temperature.
  - Vreman subgrid-scale model (Vreman, 2004).
  - Efficient GPU implementation (CUDA Fortran + MPI).
  - Validated for wind-turbine wake simulations.
  - Open-source code: `https://www.github.com/geirev/LBM`.
- **Practical framework for continuous updating of urban flows:**
  - We can continuously update uncertain inflow conditions using internal wind observations.
  - Next step: realistic urban-scale applications.

LATTICE BOLTZMANN METHOD: DERIVATION & PROPERTIES

From the Boltzmann equation to a discrete, efficient and robust fluid solver



1. ORIGIN: FROM STATISTICAL MECHANICS TO BOLTZMANN

Statistical mechanics

A dilute gas of many particles is described by the s-particle distribution function $F_s(\mathbf{r}_1, \mathbf{v}_1, \ldots, \mathbf{r}_s, \mathbf{v}_s, t)$.

Liouville's theorem

Conservation of probability in 6Ns-dimensional phase space:

$$\frac{df_s}{dt} = 0$$

BBGKY hierarchy

Leads to an infinite hierarchy of equations for reduced distributions $f^{(s)}$.

Boltzmann equation (assumptions)

Molecular chaos (Stosszahlansatz) and binary, short-range collisions $\Rightarrow$ closed equation for the one-particle distribution $f(\mathbf{r}, \mathbf{v}, t)$:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f = \Omega(f)$$

f: particle distribution function
$\mathbf{r}$: position, $\mathbf{v}$: velocity, t: time
$\mathbf{F}$: external force (e.g., gravity)

2. HERMITE EXPANSION

Factorize the distribution

$$f(\mathbf{r}, \mathbf{v}, t) = \omega(\mathbf{v})\ p(\mathbf{r}, \mathbf{v}, t)$$

$$\omega(\mathbf{v}) = \exp\left(-\frac{\mathbf{v}^{\mathrm{T}}\mathbf{v}}{2c_s^2}\right)$$

$\omega(\mathbf{v})$: Gaussian weight
(c_s: lattice sound speed)

$p(\mathbf{r}, \mathbf{v}, t)$: polynomial in $\mathbf{v}$ (Hermite expansion)

$$p(\mathbf{r}, \mathbf{v}, t) = \sum_{n=0}^{N} \frac{1}{n!} a^{(n)}(\mathbf{r}, t) : \mathbf{H}^{(n)}(\mathbf{v})$$

$\mathbf{H}^{(n)}$: n-th order Hermite tensors

Truncate at order N
(e.g., $N = 2$ for NS, $N = 3$ for improved stability)

3. GAUSS–HERMITE QUADRATURE

Discretize velocity space

$$\int_{RD} \omega(\mathbf{v})\ q(\mathbf{v})\ d\mathbf{v} \approx \sum_{l=1}^{Q} w_l\ q(\mathbf{c}_l)$$

$(\mathbf{c}_l, w_l)$: abscissas (discrete velocities) and weights of Gauss–Hermite quadrature

Exact for all polynomials $q(\mathbf{v})$ up to degree $2M - 1$
(M: order of the quadrature)

4. DISCRETE POPULATIONS

Define f_l on a lattice

$$f_l(\mathbf{r}, t) = w_l\ p(\mathbf{r}, \mathbf{c}_l, t) = w_l \frac{f(\mathbf{r}, \mathbf{c}_l, t)}{\omega(\mathbf{c}_l)}$$

$\mathbf{c}_l$: discrete velocities (stencil)

w_l: quadrature weights

Q: number of discrete velocities

5. MOMENTS AS DISCRETE SUMS

Macroscopic fields

$$\int \phi(\mathbf{v})\ f(\mathbf{r}, \mathbf{v}, t)\ d\mathbf{v} \approx \sum_{l=1}^{Q} \phi(\mathbf{c}_l)\ f_l(\mathbf{r}, t)$$

Examples:

- $\rho = \sum_l f_l$ (density)
- $\rho\mathbf{u} = \sum_l f_l\, \mathbf{c}_l$ (momentum)
- $\mathbf{\Pi} = \sum_l f_l\, \mathbf{c}_l\, \mathbf{c}_l$ (stress tensor)

(. . . higher moments similarly)

KEY PROPERTIES

RECOVERS NAVIER–STOKES

Second-order truncation is sufficient to recover the Navier–Stokes equations. Third-order improves stability at high Reynolds numbers.

MOMENT CONSERVATION

Mass and momentum are exactly conserved by the collision operator. Higher-order moments are accurate up to the quadrature order.

ISOTROPY

Discrete velocities and weights are chosen to preserve isotropy of tensors up to a given order, ensuring correct macroscopic behavior.

SIMPLE & LOCAL

Streaming and collision are local operations. No global solves. Ideal for parallel computing.

NATURAL BOUNDARIES

Bounce-back and other schemes are simple to implement and robust.

ALGORITHM

Two-step update:
1) Collision (relaxation)
2) Streaming (advection)

TYPICAL LBM MODEL (BGK) WITH REGULARIZATION

Collision (relaxation) with regularization:

$$f_l^*(\mathbf{r}, t) = f_l(\mathbf{r}, t) - \frac{1}{\tau}\left[f_l(\mathbf{r}, t) - f_l^{eq}(\mathbf{r}, t)\right]$$

Regularize the non-equilibrium part:

$$f_l^{neq} = f_l - f_l^{eq} \Rightarrow f_l^{neq,reg} = \mathcal{R}\left(f_l^{neq}\right)$$

$\mathcal{R}(\cdot)$: projection onto the space spanned by Hermite polynomials up to order N; removes components not represented by the truncated expansion.

Streaming (advection):

$$f_l(\mathbf{r} + \mathbf{c}_l \Delta t, t + \Delta t) = f_l^*(\mathbf{r}, t)$$

Macroscopic relations (from moments):

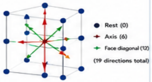
- $\rho = \sum_l f_l$
- $\rho\mathbf{u} = \sum_l f_l\, \mathbf{c}_l$
- $\mathbf{\Pi} = \sum_l f_l\, \mathbf{c}_l\, \mathbf{c}_l$

(. . . higher moments similarly)

$c_s^2 = \frac{1}{D}$ (lattice sound speed)
$\nu = c_s^2 \left(\tau - \frac{1}{2}\right) \Delta t$ (kinematic viscosity)

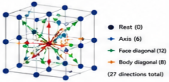
DISCRETE VELOCITY SETS (EXAMPLES)

D3Q19 (3D)



$Q = 19$ directions
2nd-order isotropy

D3Q27 (3D)



$Q = 27$ directions
3rd-order isotropy

KEY TAKEAWAYS

- LBM follows rigorously from the Boltzmann equation.
- Hermite expansion + Gauss–Hermite quadrature enable exact moments up to a chosen order.
- Second order $\Rightarrow$ Navier–Stokes level.
- Third order $\Rightarrow$ improved stability.
- Regularization of f^{neq} suppresses non-hydrodynamic modes and enhances stability.
- Simple, local, parallel, and naturally suited for complex geometries.

PHYSICALLY CONSISTENT | **NUMERICALLY EFFICIENT** | **HIGHLY PARALLEL** | **ROBUST & VERSATILE**

Thank you!

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