# Cumulant-based LBM

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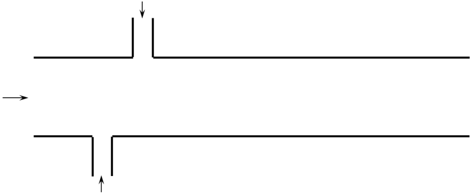
# Content

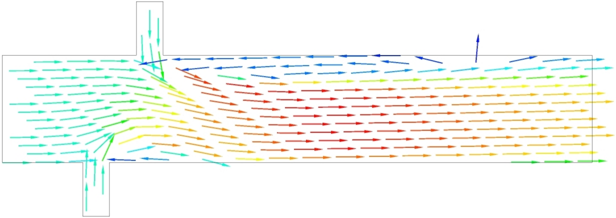
# Repetition: LBM and notation

# Computational Fluid Dynamics

- Numerical simulation of flows



- Calculation of the velocity field



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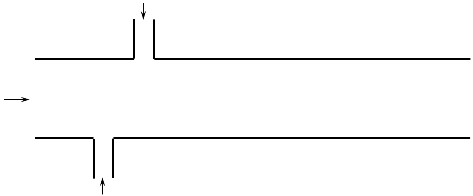

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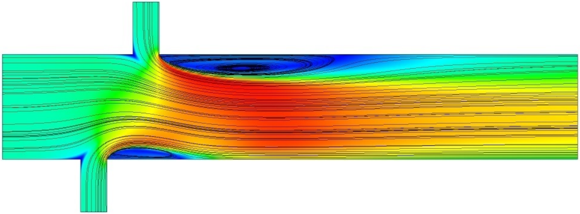
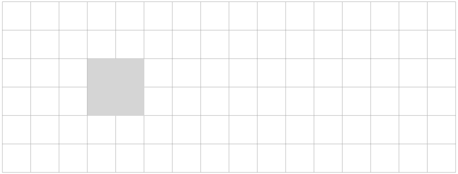
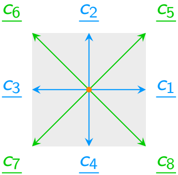


# Discretization

- In space

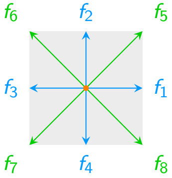


- In velocity (D2Q9-model)



# (Discrete) Boltzmann-equation

- Considering „probabilities of an encounter" $f_i$




- Derivation of a (discrete) transport-equation for the distributions $f_i$:

$$\frac{\partial f_i(t,\underline{x})}{\partial t} + \underline{c_i} \cdot \nabla_{\underline{x}} f_i(t,\underline{x}) = Q(f_i) \approx -\frac{1}{\tau_C} \cdot \left(f_i(t,\underline{x}) - f_i^{\text{eq}}(t,\underline{x})\right)$$

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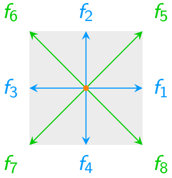


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# Equilibrium distributions $f_i^{\text{eq}}$

- Maxwell-distribution as „natural“velocity-distribution of an ideal gas:

$$M(\underline{\xi}, \rho, \underline{u}, T) = \rho \cdot \left(\frac{m}{2\pi\, k_B T}\right)^{3/2} \cdot \exp\left(-\frac{m\,|\underline{\xi} - \underline{u}|^2}{2 k_B T}\right)$$

- Taylor expansion up to second order $\underline{\xi} = \underline{c_i}$:

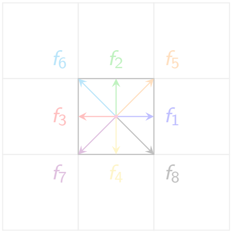
$$f_i^{\text{eq}} = \rho\,\omega_i \cdot \left(1 + \frac{3\,\underline{c_i} \cdot \underline{u}}{c^2} - \frac{3\,|u|^2}{2c^2} + \frac{1}{2}\,\frac{9}{c^4}\,\left(\underline{c_i} \cdot \underline{u}\right)^2\right)$$

# SRT-equation

- Discretization of the derivative by finite differences

$$f_i(t+\Delta t, \underline{x} + \underline{c_i}\Delta t) = f_i(t, \underline{x}) - \frac{1}{\tau} \cdot \left(f_i(t, \underline{x}) - f_i^{\mathrm{eq}}(t, \underline{x})\right)$$

- Interpretation as collision and streaming:



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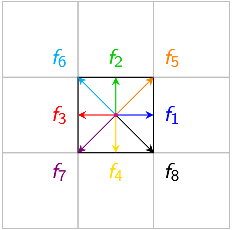


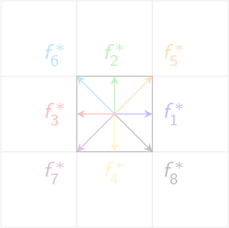

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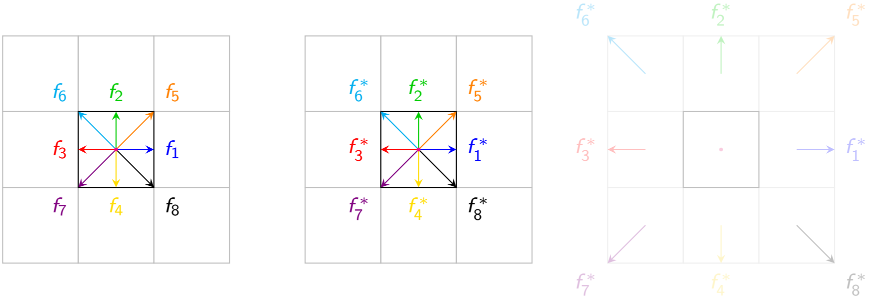

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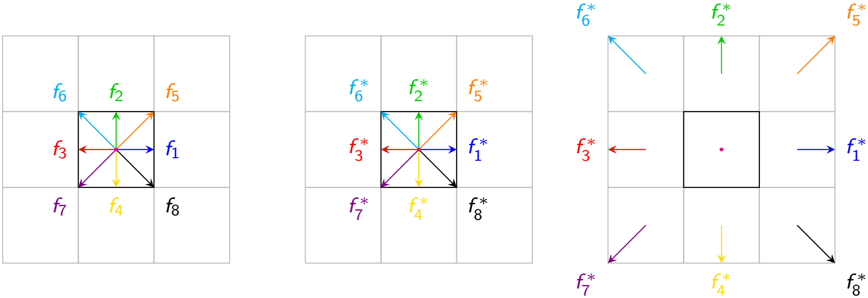
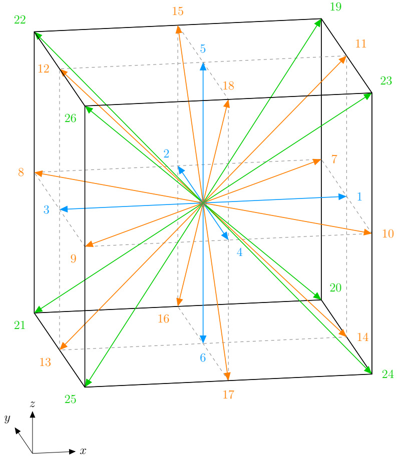


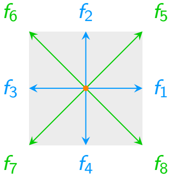
# In three dimensions

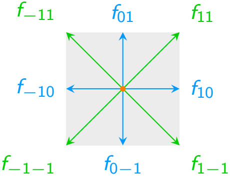
- Analogously in three dimensions (D3Q27-model)



# Notation

- Convenient notation by index-tupel:




$f_i \to f_{ij}$ with $i, j \in \{-1, 0, 1\}$

- Analogously in three dimensions: $f_i \to f_{ijk}$ with $i, j, k \in \{-1, 0, 1\}$

# MRT-model

# Basic idea of MRT (1)

- The SRT-equation reads:

$$f_i(t+\Delta t, \underline{x}+\underline{c_i}\Delta t) = f_i(t,\underline{x}) - \frac{1}{\tau} \cdot \left(f_i(t,\underline{x}) - f_i^{\mathrm{eq}}(t,\underline{x})\right)$$

- Idea: Mix the relaxation terms

$$f_i(t+\Delta t, \underline{x}+\underline{c_i}\Delta t) = f_i(t,\underline{x}) - \sum_{j=0}^{n_\mathcal{V}} \frac{1}{\tau_{ij}} \cdot \left(f_j(t,\underline{x}) - f_j^{\mathrm{eq}}(t,\underline{x})\right)$$

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- In matrix-vector-form

$$\begin{pmatrix} \vdots \\ f_i(t+\Delta t, \underline{x}+\underline{c_i}\Delta t) \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ f_i(t,\underline{x}) \\ \vdots \end{pmatrix} - S\cdot \begin{pmatrix} \vdots \\ (f_i(t,\underline{x}) - f_i^{\text{eq}}(t,\underline{x})) \\ \vdots \end{pmatrix}$$

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# Basic idea of MRT (2)

- In matrix-vector-form

$$f(t+\Delta t, \underline{x}+\underline{c_\times}\Delta t) = f(t,\underline{x}) - S\cdot(f(t,\underline{x}) - f^{\text{eq}}(t,\underline{x}))$$

- Diagonalize the matrix $S$:

$$f(t+\Delta t, \underline{x}+\underline{c_\times}\Delta t) = f(t,\underline{x}) - M^{-1}\widehat{S}\cdot(Mf(t,\underline{x}) - Mf^{\text{eq}}(t,\underline{x}))$$

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# Moments

## Definition: (Raw)-moments

For $\alpha, \beta, \gamma = 0, 1, 2, \ldots$ one defined the (raw)-moments of order $\alpha + \beta + \gamma$ as follows:

$$m_{\alpha\beta\gamma} = \sum_{i,j,k=-1}^{1} \left(\underline{c_{ijk}}\right)_x^{\alpha} \cdot \left(\underline{c_{ijk}}\right)_y^{\beta} \cdot \left(\underline{c_{ijk}}\right)_z^{\gamma} \cdot f_{ijk} = \sum_{i,j,k=-1}^{1} i^{\alpha} \cdot j^{\beta} \cdot k^{\gamma} \cdot f_{ijk}$$

- In matrix-vector-form (in 2D)

$$\begin{pmatrix} m_{00} \\ m_{10} \\ m_{01} \\ m_{20} \\ m_{02} \\ m_{11} \\ m_{21} \\ m_{12} \\ m_{22} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \end{pmatrix}$$

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# Interpretation of the moments

- The moments correspond to different physical quantities like:




  - $m_{00} = \sum_{i,j=-1}^{1} f_{ij} = \rho \quad \longrightarrow \quad$ density
  - $m_{10} = \sum_{i,j=-1}^{1} \left(\underline{c_{ij}}\right)_x \cdot f_{ij} = \rho \cdot \underline{u}_x \quad \longrightarrow \quad$ x-momentum
  - $m_{01} = \sum_{i,j=-1}^{1} \left(\underline{c_{ij}}\right)_y \cdot f_{ij} = \rho \cdot \underline{u}_y \quad \longrightarrow \quad$ y-momentum

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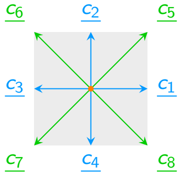


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- Some moments have to be combined for a reasonable interpretation
  - $m_{20} + m_{02} = \sum_{i,j=-1}^{1} \left( \left(\underline{c_{ij}}\right)_x^2 + \left(\underline{c_{ij}}\right)_y^2 \right) \cdot f_{ij} \sim E_{\text{kin}}$

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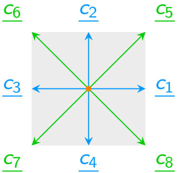


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# Moment-transformation

- The respective linear combination of matrix-lines yields the moment-transformationmatrix

$$\begin{pmatrix} M_0 \\ M_1 \\ M_2 \\ M_3 \\ M_4 \\ M_5 \\ M_6 \\ M_7 \\ M_8 \end{pmatrix} = \begin{pmatrix} m_{00} \\ m_{10} \\ m_{01} \\ m_{20}+m_{02} \\ m_{20}-m_{02} \\ m_{11} \\ m_{21} \\ m_{12} \\ m_{22} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 1 & 1 & 1 & 1 & 2 & 2 & 2 & 2 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \end{pmatrix}$$

- Further ***linear*** combinations of (raw)-moments are possible as for example row-wise orthogonalization.

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# Pro/Con MRT-model

- More „tuning-parameter“ $\omega_i$ as for SRT
- Better insight into the model by identification with physical quantities
- Linear transformations

- statistical dependencies among the moments ($\rightarrow$ dependencies between $\omega_i$)
- Physics gets lost by (wrong) variation of parameters. How to choose them?

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# Cumulant-based LBM

# Basic idea of cumulant-based LBM

- Goal: Find a transformation to ***statistically independent*** quantities $C_m$
- Mathematically this is described by a factorization of the probability-density

$$f_{ijk} = \prod_{m=0}^{n_{\mathcal{V}}} F_m(C_m)$$

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# Distributions

- Recall from measure theory: Lebesgue-space $L^2$:
  $L^2(\mathbb{R}) := \{f : \mathbb{R} \to \mathbb{R} \mid \int_{\mathbb{R}} |f(x)|^2 \, \mathrm{d}x < \infty\}$

- Consider the following functional

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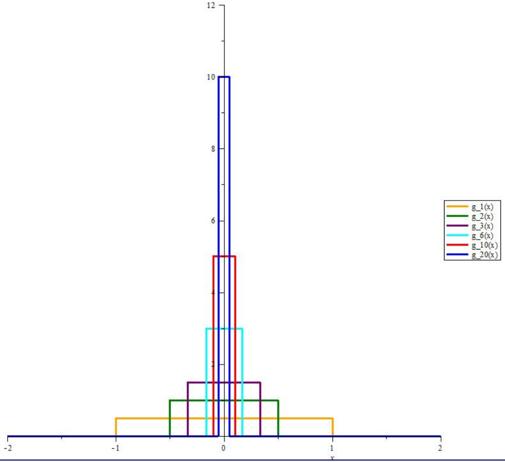
# Dirac-sequence

- Interprete the functions $g_n(x) = \frac{n}{2} \cdot \mathbb{1}_{\left[-\frac{1}{n}, \frac{1}{n}\right]}(x),\ n \in \mathbb{N}$ as functionals



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- For continuous functions $f$ there holds:

$$\int_{\mathbb{R}} g_n(x) \cdot f(x)\, \mathrm{d}x = \frac{n}{2} \cdot \int_{-\frac{1}{n}}^{\frac{1}{n}} f(x)\, \mathrm{d}x$$

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# Repetition: Fourier-transform

- The Fourier-transform of $f : \mathbb{R} \to \mathbb{C}$ is (modulo scaling) defined by:

$$\widehat{f}(\omega) = \mathcal{F}[f(x)](\omega) := \int_{\mathbb{R}} f(x) \cdot e^{-i\omega x} \, \mathrm{d}x$$

- $\widehat{f}(\omega)$ tells, how strong $e^{i\omega}$ is present in the frequency-spectrum of $f$

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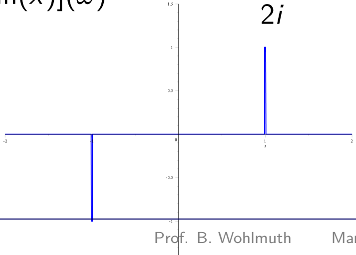
- Example: $\mathcal{F}[\sin(x)](\omega) \sim \dfrac{\delta(\omega-1) - \delta(\omega+1)}{2i}$



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- Instead of projection onto oscillations $\{e^{i\omega}\}_{\omega\in\mathbb{R}}$ one „projects“ onto damping-functions $\{e^{-s}\}_{s\in\mathbb{R}^+}$

$$F(s) := \mathcal{L}[f(x)](s) := \int_0^\infty f(x)\cdot e^{-sx}\,\mathrm{d}x$$

- Laplace-transformations of a few common functions:
  - $\mathcal{L}[x^n](s) = \frac{n!}{s^{n+1}}$
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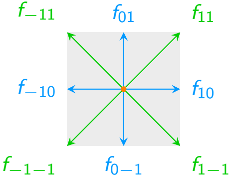
# Derivation of the cumulants (1) - „Analytization“

- Want to capture the discrete velocity-distributions analytically




- This can be done by the „peak-function“ $f(\underline{\xi})$:

$$f(\underline{\xi}) = f(\xi_x, \xi_y, \xi_z) = \sum_{i,j,k=-1}^{1} f_{ijk}\, \delta(ic - \xi_x)\, \delta(jc - \xi_y)\, \delta(kc - \xi_z)$$

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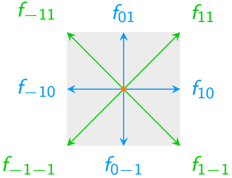


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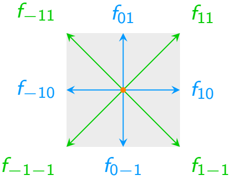


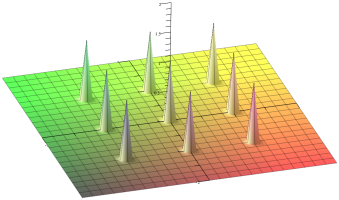

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# Derivation (3) - statistical independence

- Applying the statistical independence (which one aims to have) in the frequency space:

$$F(\Xi_x, \Xi_y, \Xi_z) = \prod_{m=0}^{n_{\mathcal{V}}} F_m(C_m)$$

- And using the logarithm

$$\ln\left(F(\Xi_x, \Xi_y, \Xi_z)\right) = \sum_{m=0}^{n_{\mathcal{V}}} \ln\left(F_m(C_m)\right)$$

# Derivation (4) - Taylor-expansion

- The multivariate Taylor-expansion of $\ln\left(F(\Xi_x, \Xi_y, \Xi_z)\right)$ around $\underline{\Xi} = 0$ is:

$$\ln(F(\Xi_x, \Xi_y, \Xi_z)) = \sum_{\alpha+\beta+\gamma \geq 0} \frac{1}{\alpha!\beta!\gamma!} \; \frac{\partial^{\alpha+\beta+\gamma}}{\partial \Xi_x^\alpha \; \partial \Xi_y^\beta \; \partial \Xi_z^\gamma} \ln(F(\Xi_x, \Xi_y, \Xi_z))\Big|_{\underline{\Xi}=0} \cdot \; \Xi_x^\alpha \, \Xi_y^\beta \, \Xi_z^\gamma$$

**Definition: Cumulants**

For $\alpha, \beta, \gamma = 0, 1, 2, \ldots$ one defines the cumulants of order $\alpha + \beta + \gamma$ as follows:

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# Efficient calculation via moments

- Conduct the Taylor-expansion ***without*** the logarithm:

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- Analogously consider the coefficients:

$$\left. \frac{\partial^{\alpha+\beta+\gamma}}{\partial \Xi_x^\alpha \, \partial \Xi_y^\beta \, \partial \Xi_z^\gamma} F(\Xi_x, \Xi_y, \Xi_z) \right|_{\underline{\Xi}=0}$$

# Where the magic happens

- Explicit calculation of these coefficients yields:

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# Cumulants vs. Moments

- The (raw)-moments were shown to be:

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# Cumulant-transformation (1)

- We conduct the idea on the example $c_{100}$:

$$c_{100} = c^{-(1+0+0)} \frac{\partial^1}{\partial \Xi_x^1 \ \partial \Xi_y^0 \ \partial \Xi_z^0} \ln(F(\Xi_x, \Xi_y, \Xi_z))\Big|_{\Xi=0}$$

$$= c^{-1} \frac{1}{F(0,0,0)} \cdot \frac{\partial^1}{\partial \Xi_x^1} F(\Xi_x, \Xi_y, \Xi_z)\Big|_{\Xi=0}$$

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$$c_{100} = c^{-(1+0+0)} \frac{\partial^1}{\partial \Xi_x^1 \, \partial \Xi_y^0 \, \partial \Xi_z^0} \ln(F(\Xi_x, \Xi_y, \Xi_z))\Big|_{\Xi=0}$$

$$= c^{-1} \frac{1}{F(0,0,0)} \cdot \frac{\partial^1}{\partial \Xi_x^1} F(\Xi_x, \Xi_y, \Xi_z)\Big|_{\Xi=0}$$

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# Cumulant-transformation (2)

- Analogous procedure for the remaining cumulants:

$$C_{100} = -m_{100} \qquad C_{010} = -m_{010} \qquad C_{001} = -m_{001}$$

$$C_{200} = m_{200} - \frac{1}{\rho} m_{100}^2 \qquad C_{020} = m_{020} - \frac{1}{\rho} m_{010}^2 \qquad C_{002} = m_{002} - \frac{1}{\rho} m_{001}^2$$

$$C_{110} = m_{110} - \frac{1}{\rho} m_{100} m_{010} \qquad C_{101} = m_{101} - \frac{1}{\rho} m_{100} m_{001} \qquad \ldots$$

$$C_{210} = -m_{210} - \frac{2}{\rho^2} m_{100}^2 m_{010} + \frac{2}{\rho} m_{110} m_{100} + \frac{1}{\rho} m_{200} m_{010}$$

$$\vdots$$

# Half-time score

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- Efficient transformation of equilibria
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- Apply the logarithm:

$$\ln(F^{\mathrm{eq}}(\underline{\Xi})) = \ln\left(\frac{\rho}{\rho_0}\right) - \Xi_x\, u_x - \Xi_y\, u_y - \Xi_z\, u_z + \frac{c_s^2}{2}\left(\Xi_x^2 + \Xi_y^2 + \Xi_z^2\right)$$

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# Cumulant equilibria

- Only a certain few cumulants have an equilibrium not equal 0:

$$
\begin{aligned}
c_{000}^{\mathrm{eq}} &= \ln(\rho/\rho_0) \\
c_{100}^{\mathrm{eq}} &= -c^{-1}u_x \\
c_{010}^{\mathrm{eq}} &= -c^{-1}u_y \\
c_{001}^{\mathrm{eq}} &= -c^{-1}u_z \\
c_{200}^{\mathrm{eq}} &= c^{-2}c_s^2 \\
c_{020}^{\mathrm{eq}} &= c^{-2}c_s^2 \\
c_{002}^{\mathrm{eq}} &= c^{-2}c_s^2
\end{aligned}
$$

- For all others, there holds: $c_{\alpha\beta\gamma}^{\mathrm{eq}} = 0$

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- Efficient transformation of equilibria ✓
- Choice of relaxation parameters $\omega_i$
- Inverse mapping $\mathfrak{C}^{-1}$

# Choice of relaxation parameters

- For the most cumulants the equilibrium is 0, hence one gets for example:

$$C^*_{222} = \omega_{10}\ (C_{222} - 0)$$

$$C^*_{110} = \omega_1\ C_{110}$$
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# Advantages of Cumulant-based LBM

- Better representation of physical processes due to statistical independence
- Equilibria of cumulants are almost all 0
- More (real) degrees of freedom than in classical MRT
- Gradual improvement of the method by asymptotic analysis and elimination of error-terms

# Synthesis of Navier-Stokes-equation

- By a Chapman-Enskog expansion one can derive the Navier-Stokes equations:

$$\nabla \cdot \underline{u} = 0$$
$$\frac{\partial \underline{u}}{\partial t} + (\underline{u} \cdot \nabla)\,\underline{u} = -\frac{1}{\rho}\,\nabla p + \underbrace{\frac{1}{3}\left(\frac{1}{\omega_1} - \frac{1}{2}\right)}_{=\nu}\,\Delta \underline{u} + \frac{f}{\rho}$$

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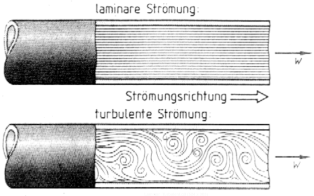
# Validation a.k.a. colorful pictures

# Turbulence measure

- The Reynolds-number is dimensionless parameter of a flow

$$\mathrm{Re} = \frac{U \cdot L}{\nu}$$

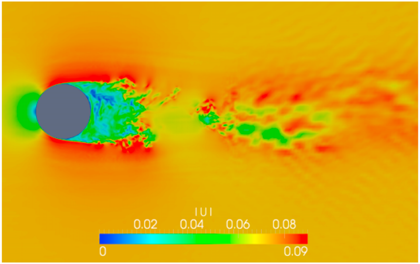
- At some specific threshold $\mathrm{Re}^*$ the laminar-turbulent transition starts



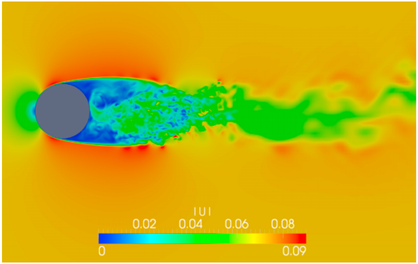

- Traditional LBM methods have problems with high Reynolds-numbers:

# Comparison: BGK $\leftrightarrow$ Kumulanten

- Comparison SRT- and cumulant-based LBM for a cylinder flow at Re $= 8000$



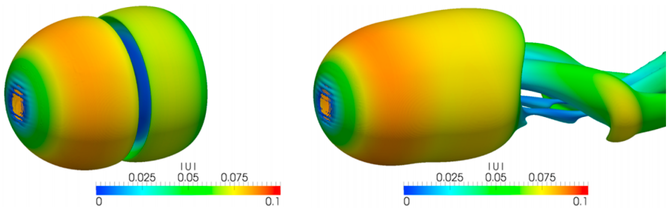

**a)** BGK-SRT-LBM (Picture source [5])




**b)** Cumulant-based LBM (Picture source [5])

# Turbulence resolution in 3D

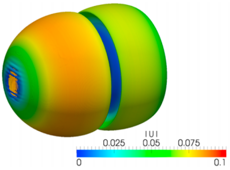
- Representation of (turbulence) vortices around a sphere flow:



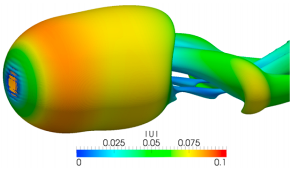

(a) $Re = 200$. (b) $Re = 400$.

(Picture source [5])

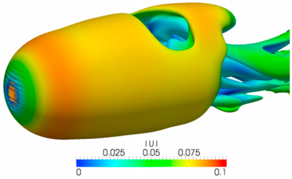
# Turbulence resolution in 3D



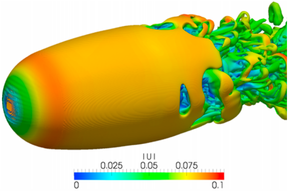

(a) $Re = 200$.




(b) $Re = 400$.



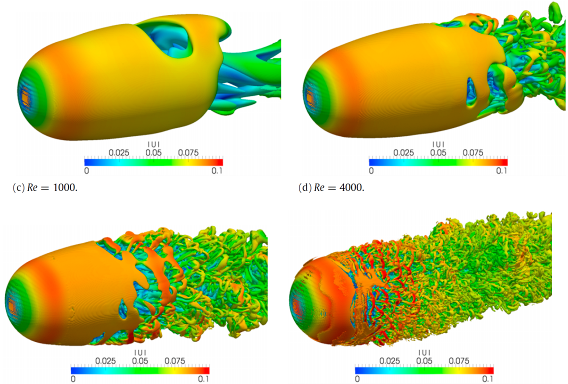

(c) $Re = 1000$.




(d) $Re = 4000$.

(Picture source [5])

# Turbulence resolution in 3D




(c) $Re = 1000$.

(d) $Re = 4000$.

(e) $Re = 10\,000$.

(f) $Re = 100\,000$.

(Picture source [5])

# The highlights

- MRT-like-method with nonlinear transformation to statistical independent quantities
- Mathematical methods:
  - Distributions as generalized functions (Analytization)
  - Laplace-transform
  - Comparison of Taylor-coefficients

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# Literature I

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