

Thermal fluctuations in a kinetic model for multicomponent fluids



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11 December 2015 @ SM&FT

Outline



Kinetic model — Introducing kinetic theory for isothermal binary mixtures

- Binary Boltzmann equation
- Non-ideal effects
- Thermal fluctuations

Technicalities — Sketching how to apply fluctuation-dissipation theorem

- Equilibrium correlations
- Noise correlations

Numerics — Checking theoretics with numerical simulations

- Homogeneous ideal mixture
- Homogeneous interacting mixture
- Non-homogeneous interacting mixture

Conclusions — Summarizing results



Kinetic model

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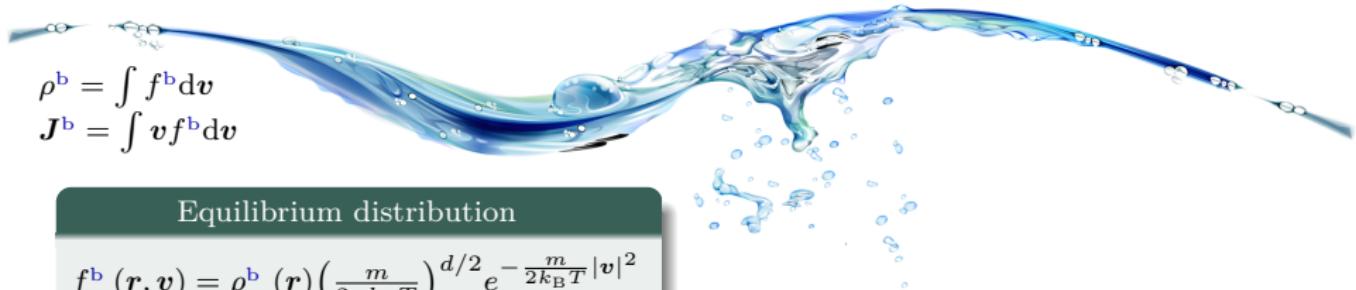
Binary Boltzmann equation

$$\partial_t f^{\text{b}} + \mathbf{v} \cdot \nabla f^{\text{b}} = \text{Coll}(f^{\text{b}}, f^{\text{g}})$$

$$\rho^{\text{b}} = \int f^{\text{b}} d\mathbf{v}$$

$$\mathbf{J}^{\text{b}} = \int \mathbf{v} f^{\text{b}} d\mathbf{v}$$

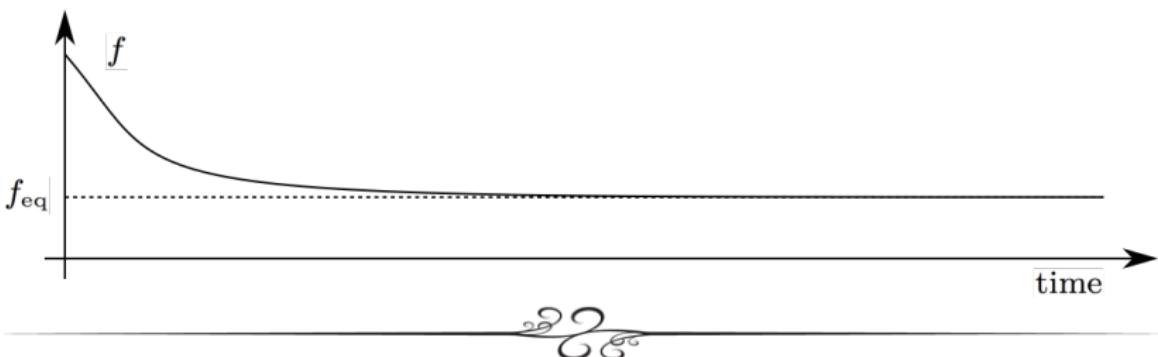
The probability of finding a blue, risp. green, particle at t in a phase space volume $d\omega = d\mathbf{r} d\mathbf{v}$ around (\mathbf{r}, \mathbf{v}) is $f^{\text{b}}(t, \mathbf{r}, \mathbf{v})d\omega$, risp. $f^{\text{g}}(t, \mathbf{r}, \mathbf{v})d\omega$.



Equilibrium distribution

$$f_{\text{eq}}^{\text{b}}(\mathbf{r}, \mathbf{v}) = \rho_{\text{eq}}^{\text{b}}(\mathbf{r}) \left(\frac{m}{2\pi k_B T} \right)^{d/2} e^{-\frac{m}{2k_B T} |\mathbf{v}|^2}$$

$$f^{\text{b}} \rightarrow f_{\text{eq}}^{\text{b}} \implies \nabla \rho_{\text{eq}}^{\text{b}} = \mathbf{0}$$



Non-ideal binary Boltzmann equation

$$\partial_t f^b + v \cdot \nabla f^b = \text{Coll}(f^b, f^g) - a^b \cdot \nabla_v f^b$$

$$\rho^b = \int f^b dv$$

$$J^b = \int v f^b dv$$

The body-force acceleration $a^b = a[\rho^g]$ exerted by a blue particle is assumed to depend on the green mass distribution.

Equilibrium distribution

$$f_{\text{eq}}^b(r, v) = \rho_{\text{eq}}^b(r) \left(\frac{m}{2\pi k_B T} \right)^{d/2} e^{-\frac{m}{2k_B T} |v|^2}$$

$$f^b \rightarrow f_{\text{eq}}^b \implies \nabla \rho_{\text{eq}}^b = \frac{m}{k_B T} \rho_{\text{eq}}^b a[\rho^g]$$



Non-ideal fluctuating binary Boltzmann equation

$$\partial_t f^{\text{b}} + \mathbf{v} \cdot \nabla f^{\text{b}} = \text{Coll}(f^{\text{b}}, f^{\text{g}}) - \mathbf{a}^{\text{b}} \cdot \nabla_{\mathbf{v}} f^{\text{b}} + \xi^{\text{b}}$$

$$\rho^{\text{b}} = \int f^{\text{b}} d\mathbf{v}$$

$$\mathbf{J}^{\text{b}} = \int \mathbf{v} f^{\text{b}} d\mathbf{v}$$

Equilibrium distribution

$$f_{\text{eq}}^{\text{b}}(\mathbf{r}, \mathbf{v}) = \rho_{\text{eq}}^{\text{b}}(\mathbf{r}) \left(\frac{m}{2\pi k_B T} \right)^{d/2} e^{-\frac{m}{2k_B T} |\mathbf{v}|^2}$$

$$\langle f^{\text{b}} \rangle \rightarrow f_{\text{eq}}^{\text{b}} \implies \nabla \rho_{\text{eq}}^{\text{b}} = \frac{m}{k_B T} \rho_{\text{eq}}^{\text{b}} \mathbf{a}[\rho_{\text{eq}}^{\text{g}}]$$

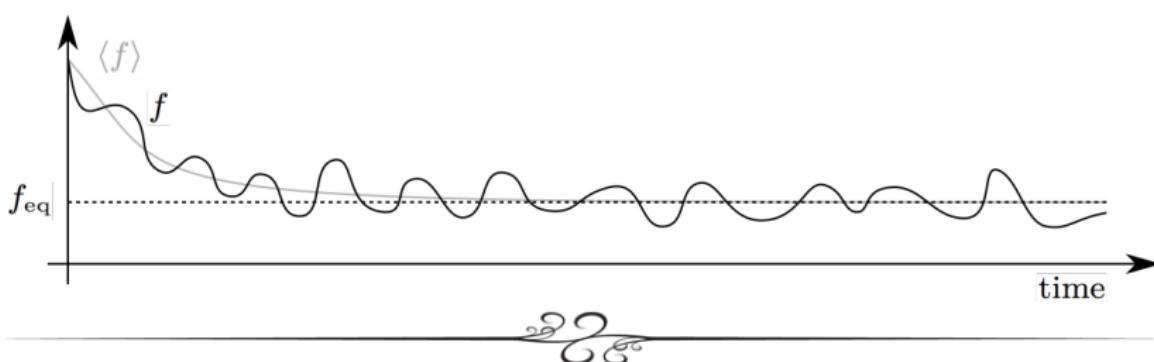
Averages over all possible trajectories $\langle \cdot \rangle$ are equivalent to canonical ensemble averages.



Brownian motion

$$\partial_t V = -\lambda V + \xi$$

$$\langle V^2 \rangle \rightarrow k_B T \implies \langle \xi^2 \rangle = 2\lambda k_B T$$



Multicomponent Boltzmann equation

$$\partial_t f^S + \mathbf{v} \cdot \nabla f^S = (\text{Coll}f)^S - \mathbf{a}^S \cdot \nabla_{\mathbf{v}} f^S + \xi^S$$

$$\rho^S = \int f^S d\mathbf{v}$$

$$\mathbf{J}^S = \int \mathbf{v} f^S d\mathbf{v}$$

Equilibrium distribution

$$f_{\text{eq}}^S(\mathbf{r}, \mathbf{v}) = \rho_{\text{eq}}^S(\mathbf{r}) \left(\frac{m}{2\pi k_B T} \right)^{d/2} e^{-\frac{m}{2k_B T} |\mathbf{v}|^2}$$

$$\langle f^S \rangle \rightarrow f_{\text{eq}}^S \implies \nabla \rho_{\text{eq}}^S = \frac{m}{k_B T} \rho_{\text{eq}}^S \mathbf{a}[\rho_{\text{eq}}]$$

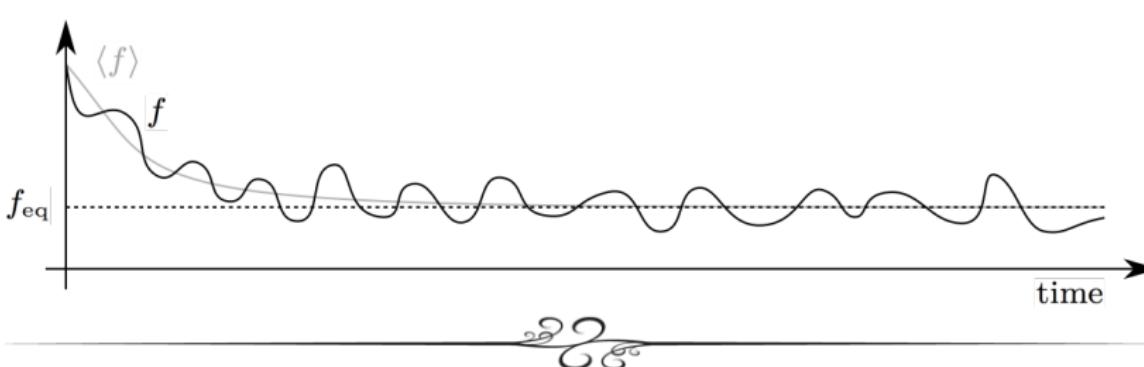
The Boltzmann distributions are labeled by the species index $S = \text{b, g, ...}$ and are collected in $f = (f^S)_{S=\text{b,g,...}}$.



Brownian motion

$$\partial_t V_i = -(LV)_i + \xi_i$$

$$\langle V_i V_j^* \rangle \rightarrow E_{ij} \implies \langle \xi_i \xi_j^* \rangle = (LE + EL)_{ij}$$



Multicomponent Boltzmann equation

$$\partial_t f^S + \mathbf{v} \cdot \nabla f^S = (\text{Coll}f)^S - \mathbf{a}^S \cdot \nabla_{\mathbf{v}} f^S + \xi^S$$

$$\rho^S = \int f^S d\mathbf{v}$$

$$\mathbf{J}^S = \int \mathbf{v} f^S d\mathbf{v}$$

Equilibrium distribution

$$f_{\text{eq}}^S(\mathbf{r}, \mathbf{v}) = \rho_{\text{eq}}^S(\mathbf{r}) \left(\frac{m}{2\pi k_B T} \right)^{d/2} e^{-\frac{m}{2k_B T} |\mathbf{v}|^2}$$

$$\langle f^S \rangle \rightarrow f_{\text{eq}}^S \implies \nabla \rho_{\text{eq}}^S = \frac{m}{k_B T} \rho_{\text{eq}}^S \mathbf{a}[\rho_{\text{eq}}]$$

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Brownian motion

$$\partial_t V_i = -(LV)_i + \xi_i$$

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Linearity: Collisional operator and self-generated forcing are non-linear functional of f \implies Small deviation from equilibrium

ODE: Non-ideal Boltzmann equation involves spatial and velocity gradient of f \implies Velocity moments and Fourier space





Technicalities

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Evolution equation for the velocity moments

$$\partial_t f_a^S + \nabla \cdot (v f^S)_a = (\text{Coll}_a f_a)^S - a^S \cdot (\Phi f^S)_a + \xi_a^S$$

$$\begin{aligned}\rho^S &= \int f^S dv = f_0^S \\ J^S &= \int v f^S dv = f_{1,\dots,d}^S \\ &\dots\end{aligned}$$

$$\begin{aligned}\xi_\rho^S &= \int \xi^S dv = \xi_0^S \\ \xi_J^S &= \int v \xi^S dv = \xi_{1,\dots,d}^S \\ &\dots\end{aligned}$$

Hermite transformation

$$f_a = \int H_a f dv \quad H_0 = 1 \quad H_{1,\dots,d} = v \quad \dots$$

Linear evolution equation for the velocity moments

$$\partial_t \delta f_a^S + \nabla \cdot (\mathbf{v} \delta f^S)_a = (\lambda_a \delta f_a)^S - \mathbf{a}[\rho_{\text{eq}}] \cdot (\Phi \delta f^S)_a - \delta \mathbf{a}^S \cdot (\Phi f_{\text{eq}}^S)_a + \xi_a^S$$



$$\begin{aligned}\delta \rho^S &= \int \delta f^S d\mathbf{v} = \delta f_0^S \\ \delta \mathbf{J}^S &= \int \mathbf{v} \delta f^S d\mathbf{v} = \delta f_{1,\dots,d}^S \\ &\dots\end{aligned}$$

$$\begin{aligned}\xi_\rho^S &= \int \xi^S d\mathbf{v} = \xi_0^S \\ \xi_{\mathbf{J}}^S &= \int \mathbf{v} \xi^S d\mathbf{v} = \xi_{1,\dots,d}^S \\ &\dots\end{aligned}$$

Hermite transformation

$$f_a = \int H_a f d\mathbf{v} \quad H_0 = 1 \quad H_{1,\dots,d} = \mathbf{v} \quad \dots$$

Small deviation from equilibrium

$$\delta f = f - f_{\text{eq}} \quad f_{\text{eq}} = \lim_{t \rightarrow \infty} \langle f \rangle$$

Linear evolution equation for the Fourier-transformed velocity moments

$$\partial_t \delta f_{a;\mathbf{k}}^S + i\mathbf{k} \cdot (\mathbf{v} \delta f_{\mathbf{k}}^S)_a = (\lambda_a \delta f_{a;\mathbf{k}})^S - (\mathbf{a}[\rho_{\text{eq}}] * (\Phi \delta f^S)_a)_{\mathbf{k}} - (\delta \mathbf{a}^S * (\Phi f_{\text{eq}}^S)_a)_{\mathbf{k}} + \xi_{a;\mathbf{k}}^S$$

$$\begin{aligned}\delta \rho_{\mathbf{k}}^S &= \int \delta f_{\mathbf{k}}^S d\mathbf{v} = \delta f_{0;\mathbf{k}}^S \\ \delta \mathbf{J}_{\mathbf{k}}^S &= \int \mathbf{v} \delta f_{\mathbf{k}}^S d\mathbf{v} = \delta f_{1,\dots,d;\mathbf{k}}^S \\ &\dots\end{aligned}$$

$$\begin{aligned}\xi_{\rho;\mathbf{k}}^S &= \int \xi_{\mathbf{k}}^S d\mathbf{v} = \xi_{0;\mathbf{k}}^S \\ \xi_{\mathbf{J};\mathbf{k}}^S &= \int \mathbf{v} \xi_{\mathbf{k}}^S d\mathbf{v} = \xi_{1,\dots,d;\mathbf{k}}^S \\ &\dots\end{aligned}$$

Hermite transformation

$$f_a = \int H_a f d\mathbf{v} \quad H_0 = 1 \quad H_{1,\dots,d} = \mathbf{v} \quad \dots$$

Small deviation from equilibrium

$$\delta f = f - f_{\text{eq}} \quad f_{\text{eq}} = \lim_{t \rightarrow \infty} \langle f \rangle$$

Fourier transformation

$$f_{\mathbf{k}} = \int e_{\mathbf{k}} f d\mathbf{r} \quad e_{\mathbf{k}} = \frac{1}{(2\pi)^{d/2}} e^{-i\mathbf{k} \cdot \mathbf{r}}$$

Linear evolution equation for the Fourier-transformed velocity moments

$$\partial_t \delta f_{a;\mathbf{k}}^{\text{b}} + i\mathbf{k} \cdot (\mathbf{v} \delta f_{\mathbf{k}}^{\text{b}})_a = (\lambda_a \delta f_{a;\mathbf{k}})^{\text{b}} - (\mathbf{a}[\rho_{\text{eq}}] * (\Phi \delta f_{\mathbf{k}}^{\text{b}})_a)_{\mathbf{k}} - (\delta \mathbf{a}^{\text{b}} * (\Phi f_{\text{eq}}^{\text{b}})_a)_{\mathbf{k}} + \xi_{a;\mathbf{k}}^{\text{b}}$$

$$\delta \rho_{\mathbf{k}}^{\text{b}} = \int \delta f_{\mathbf{k}}^{\text{b}} d\mathbf{v} = \delta f_{0;\mathbf{k}}^{\text{b}}$$

$$\delta \mathbf{J}_{\mathbf{k}}^{\text{b}} = \int \mathbf{v} \delta f_{\mathbf{k}}^{\text{b}} d\mathbf{v} = \delta f_{1,\dots,d;\mathbf{k}}^{\text{b}}$$

...

$$\xi_{\rho}^{\text{b}} = \int \xi^{\text{b}} d\mathbf{v} = \xi_0^{\text{b}}$$

$$\xi_{\mathbf{J}}^{\text{b}} = \int \mathbf{v} \xi^{\text{b}} d\mathbf{v} = \xi_{1,\dots,d}^{\text{b}}$$

...

Equilibrium correlations

$$\langle \delta \rho_{\mathbf{k}}^{\text{b}} \delta \rho_{-\mathbf{k}}^{\text{b}} \rangle = m \frac{\rho_{\mathbf{k}}^{\text{b}}}{1 - \rho_{\mathbf{k}}^{\text{b}} \rho_{-\mathbf{k}}^{\text{g}} \alpha_{\mathbf{k}}^2} \quad \langle \delta \rho_{\mathbf{k}}^{\text{b}} \delta \rho_{-\mathbf{k}}^{\text{g}} \rangle = -m \frac{\rho_{\mathbf{k}}^{\text{b}} \rho_{-\mathbf{k}}^{\text{g}} \alpha_{\mathbf{k}}}{1 - \rho_{\mathbf{k}}^{\text{b}} \rho_{-\mathbf{k}}^{\text{g}} \alpha_{\mathbf{k}}^2}$$

$$\langle \delta \mathbf{J}_{\mathbf{k}} \delta \mathbf{J}_{-\mathbf{k}} \rangle = k_B T (\rho^{\text{b}} + \rho^{\text{g}}) \mathbf{1} \quad (\mathbf{J} = \mathbf{J}^{\text{b}} + \mathbf{J}^{\text{g}}) \quad \dots$$

... self-consistently derived in the theory!

Noise correlations

$$\langle \xi_{\rho}^{\text{b}} \xi_{\rho}^{\text{b}} \rangle = \langle \xi_{\rho}^{\text{b}} \xi_{\rho}^{\text{g}} \rangle = 0 \quad \langle \xi_{\mathbf{J}}^{\text{b}} \xi_{\mathbf{J}}^{\text{b}} \rangle = -\langle \xi_{\mathbf{J}}^{\text{b}} \xi_{\mathbf{J}}^{\text{g}} \rangle = 2 \lambda k_B T \frac{\rho^{\text{b}} \rho^{\text{g}}}{\rho^{\text{b}} + \rho^{\text{g}}} \mathbf{1}$$

...

↑ stochastic diffusion fluxes (sdf) ↑



Numerics

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D. Belardinelli, M. Sbragaglia, L. Biferale, M. Gross & F. Varnik, *Phys. Rev. E* **91**, 023313



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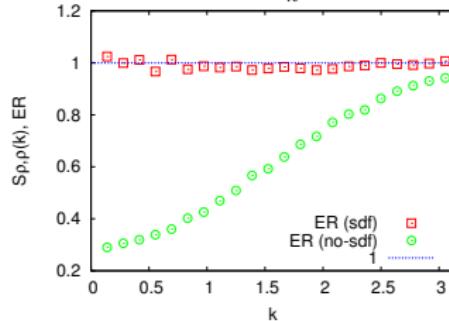
Binary lattice Boltzmann equation

$$f_\ell^{\text{b}}(t+1, \mathbf{r} + \mathbf{v}_\ell) = f_\ell^{\text{b}}(t, \mathbf{r}) + R_\ell(f^{\text{b}}, f^{\text{g}})$$

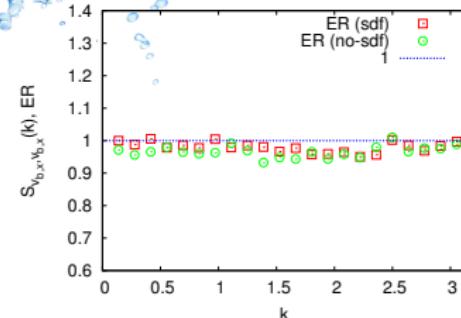
The probability of finding a blue, risp. green, particle at t in a unitary lattice cell around \mathbf{r} with velocity \mathbf{v}_ℓ is $f_\ell^{\text{b}}(t, \mathbf{r})$, risp. $f_\ell^{\text{g}}(t, \mathbf{r})$.



$$\langle \delta \rho_{\mathbf{k}}^{\text{b}} \delta \rho_{-\mathbf{k}}^{\text{b}} \rangle = m \frac{\rho^{\text{b}}}{1 - \rho^{\text{b}} \rho^{\text{g}} \alpha_k^2}$$



$$\langle \delta J_{\mathbf{k}} \delta J_{-\mathbf{k}} \rangle = k_B T (\rho^{\text{b}} + \rho^{\text{g}}) \mathbf{1}$$



Lattice mutual interaction

$$\mathbf{a}^{\text{b}}(\mathbf{r}) = \mathbf{a}[\rho^{\text{g}}](\mathbf{r}) = -G \sum_{\ell} w_{\ell} \mathbf{v}_{\ell} \rho^{\text{g}}(\mathbf{r} + \mathbf{v}_{\ell}) \quad \alpha_{\mathbf{k}} = G(1 - \frac{1}{6}|\mathbf{k}|^2)$$

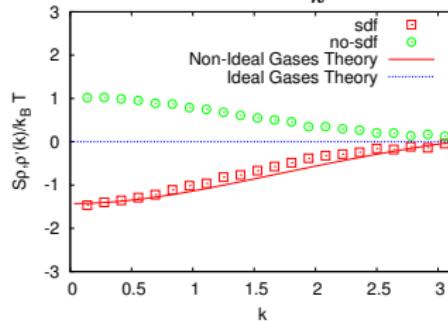
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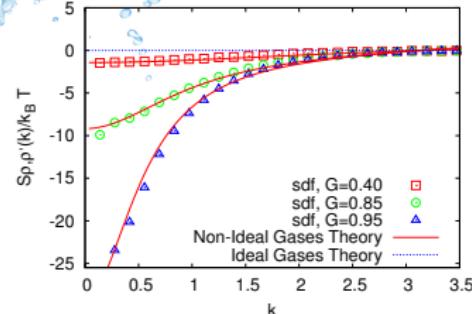
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$$\langle \delta \rho_{\mathbf{k}}^{\text{b}} \delta \rho_{-\mathbf{k}}^{\text{g}} \rangle = -m \frac{\rho^{\text{b}} \rho^{\text{g}} \alpha_{\mathbf{k}}}{1 - \rho^{\text{b}} \rho^{\text{g}} \alpha_{\mathbf{k}}^2}$$



$$\langle \delta \rho_{\mathbf{k}}^{\text{b}} \delta \rho_{-\mathbf{k}}^{\text{g}} \rangle = -m \frac{\rho^{\text{b}} \rho^{\text{g}} \alpha_{\mathbf{k}}}{1 - \rho^{\text{b}} \rho^{\text{g}} \alpha_{\mathbf{k}}^2}$$



Lattice mutual interaction

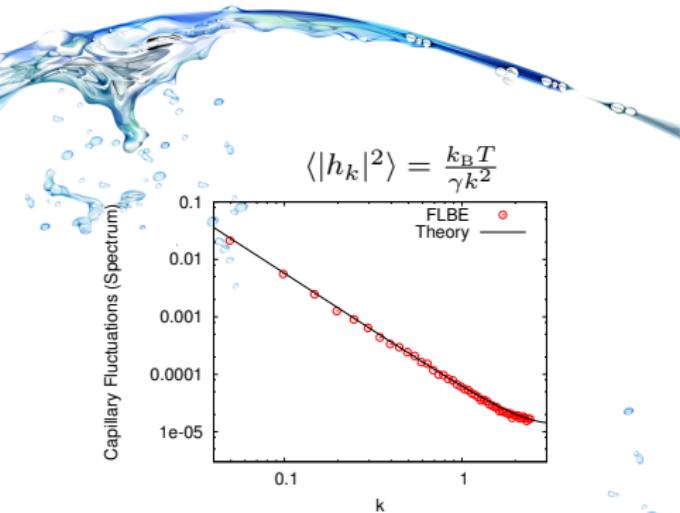
$$\mathbf{a}^{\text{b}}(\mathbf{r}) = \mathbf{a}[\rho^{\text{g}}](\mathbf{r}) = -G \sum_\ell w_\ell \mathbf{v}_\ell \rho^{\text{g}}(\mathbf{r} + \mathbf{v}_\ell) \quad \alpha_{\mathbf{k}} = G(1 - \frac{1}{6}|\mathbf{k}|^2)$$

Binary lattice Boltzmann equation

$$f_\ell^{\text{b}}(t+1, \mathbf{r} + \mathbf{v}_\ell) = f_\ell^{\text{b}}(t, \mathbf{r}) + R_\ell(f^{\text{b}}, f^{\text{g}})$$

The probability of finding a blue, risp. green, particle at t in a unitary lattice cell around \mathbf{r} with velocity \mathbf{v}_ℓ is $f_\ell^{\text{b}}(t, \mathbf{r})$, risp. $f_\ell^{\text{g}}(t, \mathbf{r})$.

$$P[h] \propto e^{-\frac{\gamma}{2k_B T} \int (\frac{dh}{dx})^2 dx}$$



Lattice mutual interaction

$$\mathbf{a}^{\text{b}}(\mathbf{r}) = \mathbf{a}[\rho^{\text{g}}](\mathbf{r}) = -G \sum_\ell w_\ell \mathbf{v}_\ell \rho^{\text{g}}(\mathbf{r} + \mathbf{v}_\ell) \quad \alpha_{\mathbf{k}} = G(1 - \frac{1}{6}|\mathbf{k}|^2)$$

Conclusions



Kinetic model — A non-ideal kinetic model for mixture has been successfully extended to incorporate the effects of thermal fluctuations

Technicalities — Application of fluctuation-dissipation theorem to derive the expression of both equilibrium and noise correlations directly at the kinetic level has allowed to go beyond hydrodynamics, by controlling thermalization of all the kinetic modes (velocity moments)

Numerics — Agreement between numerical simulations and theoretical expectations is very good for all wavevectors investigated in both homogeneous and non-homogeneous (phase separation) cases

Conclusions — Conclusion, thanks for your attention!

