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The Influence of Forcing Schemes on the Diffusion Properties in Pseudopotential-based Lattice Boltzmann Models for Multicomponents Flows

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Fundamentals

$$f_i^k(\boldsymbol{x} + \delta_t \boldsymbol{e}_i, t + \delta_t) = f_i^k - \frac{1}{\tau}\left(f_i^k - f_i^{k,\mathrm{eq}}\right) + S_i^k \quad \Longleftrightarrow \quad F_\alpha^k = -G\psi_k c_s^2 \sum_{\bar{k}} \partial_\alpha \psi_{\bar{k}}$$

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Chapman Enskog

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Chapman Enskog

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_\alpha}\rho u_{m,\alpha} = 0 + \mathcal{O}(\dots)$$

$$\frac{\partial}{\partial t}\rho u_{m,\alpha} + \frac{\partial}{\partial x_\beta}\rho u_{m,\alpha} u_{m,\beta} = -\frac{\partial}{\partial x_\beta}P_{\alpha\beta} + \frac{\partial}{\partial x_\beta}\left[\mu_m\left(\frac{\partial}{\partial x_\beta}u_{m,\alpha} + \frac{\partial}{\partial x_\alpha}u_{m,\beta}\right)\right] + \mathcal{O}(\dots)$$

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$$\frac{\partial}{\partial t}\rho_k + \frac{\partial}{\partial x_\alpha}\rho_k u_{m,\alpha} = -\frac{\partial}{\partial x_\alpha}\underbrace{\rho_k\left(u_{c,\alpha}^k - u_{m,\alpha}\right)}_{j_\alpha} = -\frac{\partial}{\partial x_\alpha} D \frac{\partial}{\partial x_\alpha}\rho_k$$

Fundamentals

$$f_i^k(\boldsymbol{x} + \delta_t \boldsymbol{e}_i, t + \delta_t) = f_i^k - \frac{1}{\tau}\left(f_i^k - f_i^{k,\mathrm{eq}}\right) + S_i^k \quad \Longleftrightarrow \quad F_\alpha^k = -G\psi_k c_s^2 \sum_{\bar{k}} \partial_\alpha \psi_{\bar{k}}$$

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$$\frac{\partial}{\partial t}\rho_k + \frac{\partial}{\partial x_\alpha}\rho_k u_{c,\alpha}^k = 0$$

Fundamentals

To this day, only the influence of the forcing scheme on the continuity and momentum equation was analysed but not its impact on the advection-diffusion equation in multicomponent systems.

$$\frac{\partial}{\partial t}\rho + \frac{\partial}{\partial x_\alpha}\rho u_{m,\alpha} = 0 + \mathcal{O}(\dots)$$

$$\frac{\partial}{\partial t}\rho u_{m,\alpha} + \frac{\partial}{\partial x_\beta}\rho u_{m,\alpha} u_{m,\beta} = -\frac{\partial}{\partial x_\beta}P_{\alpha\beta} + \frac{\partial}{\partial x_\beta}\left[\mu_m\left(\frac{\partial}{\partial x_\beta}u_{m,\alpha} + \frac{\partial}{\partial x_\alpha}u_{m,\beta}\right)\right] + \mathcal{O}(\dots)$$

$$\frac{\partial}{\partial t}\rho_k + \frac{\partial}{\partial x_\alpha}\rho_k u_{m,\alpha} = -\frac{\partial}{\partial x_\alpha}\underbrace{\rho_k\left(u_{c,\alpha}^k - u_{m,\alpha}\right)}_{j_\alpha} = -\frac{\partial}{\partial x_\alpha}D\frac{\partial}{\partial x_\alpha}\rho_k$$

$$\frac{\partial}{\partial t}\rho_k + \frac{\partial}{\partial x_\alpha}\rho_k u_{c,\alpha}^k = 0$$

Diffusion

Performing a Chapman-Enskog analysis for the pseudopotential-based multicomponent model for both the standard „Shan-Forcing“[1] and the improved „He-Forcing“[2] leads to the following diffusion coefficients

$$D^{\text{Shan}} = c_s^2 \left[G\tau(c_1\psi_1'\psi_2 + c_2\psi_2'\psi_1) - \left(\tau - \frac{1}{2}\right)\right]$$

$$D^{\text{He}} = c_s^2 \left(\tau - \frac{1}{2}\right)[G(c_1\psi_1'\psi_2 + c_2\psi_2'\psi_1) - 1]$$

→ The diffusion coefficient D changes with the forcing scheme!

[1] Shan, X.; Doolen, G. D.: J. Stat. Phys. 81 (1), 379-393 (1995)
[2] He, X.; Shan, X.; Doolen, G. D.: Phys. Rev. E 57 (R), R13 (1998)

How to get the critical value of G?

Phase separation occurs when D becomes negative

$$D^{\mathrm{Shan}} = c_s^2 \left[G\tau(c_1 \psi_1' \psi_2 + c_2 \psi_2' \psi_1) - \left(\tau - \frac{1}{2}\right) \right]$$

→ Set the diffusivity to zero, solve for G

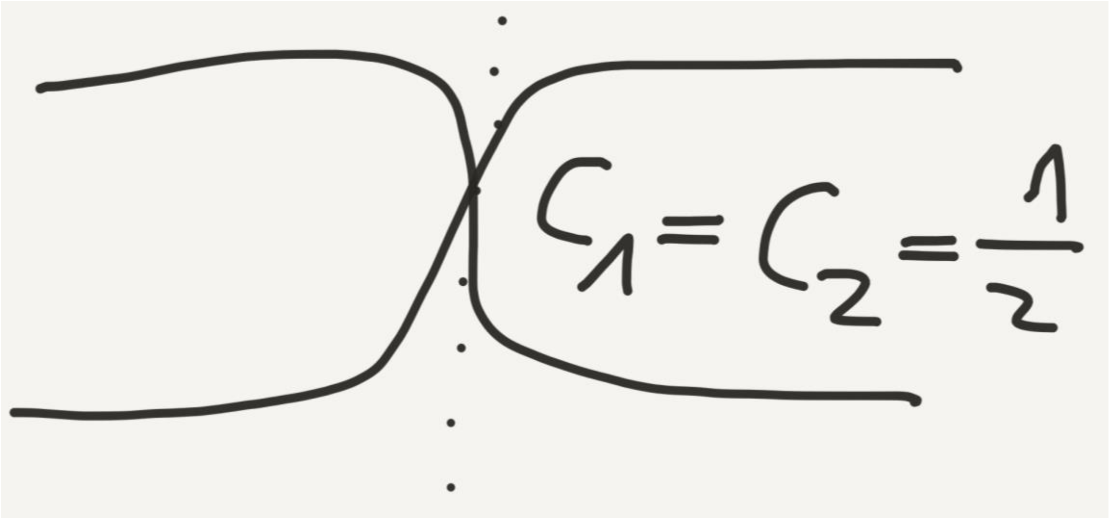
How to get the critical value of G?

Phase separation occurs when D becomes negative

$$D^{\mathrm{Shan}} = c_s^2 \left[G\tau(c_1\psi_1'\psi_2 + c_2\psi_2'\psi_1) - \left(\tau - \frac{1}{2}\right)\right]$$

→ Set the diffusivity to zero, solve for G
→ **Evaluate expression in the interface**, where F_α^k is the largest

$$\rho_{\mathrm{Int}} = \frac{\rho_1^{\mathrm{bulk}} + \rho_1^{\mathrm{dis}}}{2} = \frac{\rho_2^{\mathrm{bulk}} + \rho_2^{\mathrm{dis}}}{2}$$



How to get the critical value of G?

$$G_{\text{crit}}^{\text{Shan}} = \frac{\tau - \frac{1}{2}}{\tau[\psi'(\rho_{\text{Int}})\psi(\rho_{\text{Int}})]}$$

$$G_{\text{crit}}^{\text{He}} = \frac{1}{[\psi'(\rho_{\text{Int}})\psi(\rho_{\text{Int}})]}$$

$\tau = 1$

$$G_{\text{crit}}^{\text{Shan}} = \frac{1}{2[\psi'(\rho_{\text{Int}})\psi(\rho_{\text{Int}})]}$$

$$G_{\text{crit}}^{\text{He}} = \frac{1}{[\psi'(\rho_{\text{Int}})\psi(\rho_{\text{Int}})]}$$

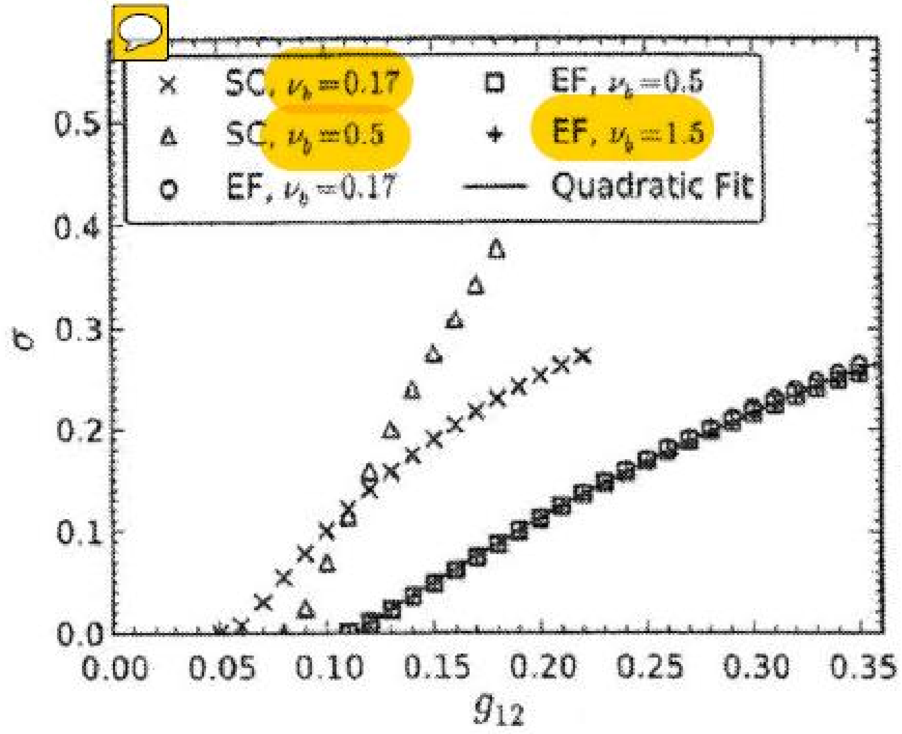
→ The critical value of G is shifted by a factor 2 for $\tau = 1$

→ Additionally, if $\psi = \rho$, $G_{\text{crit}}^{\text{Shan}}$ reduces to the well-known expression[1]

$$G_{\text{crit}}^{\text{Shan}} = \frac{1}{\rho_1^{\text{bulk}} + \rho_1^{\text{dis}}}$$

[1] Huang, H; Thorne, D. T.; Schaap, M. G.; Sukop, M. C.: Phys. Rev. E 76, 066701 (2007)

Factor 2

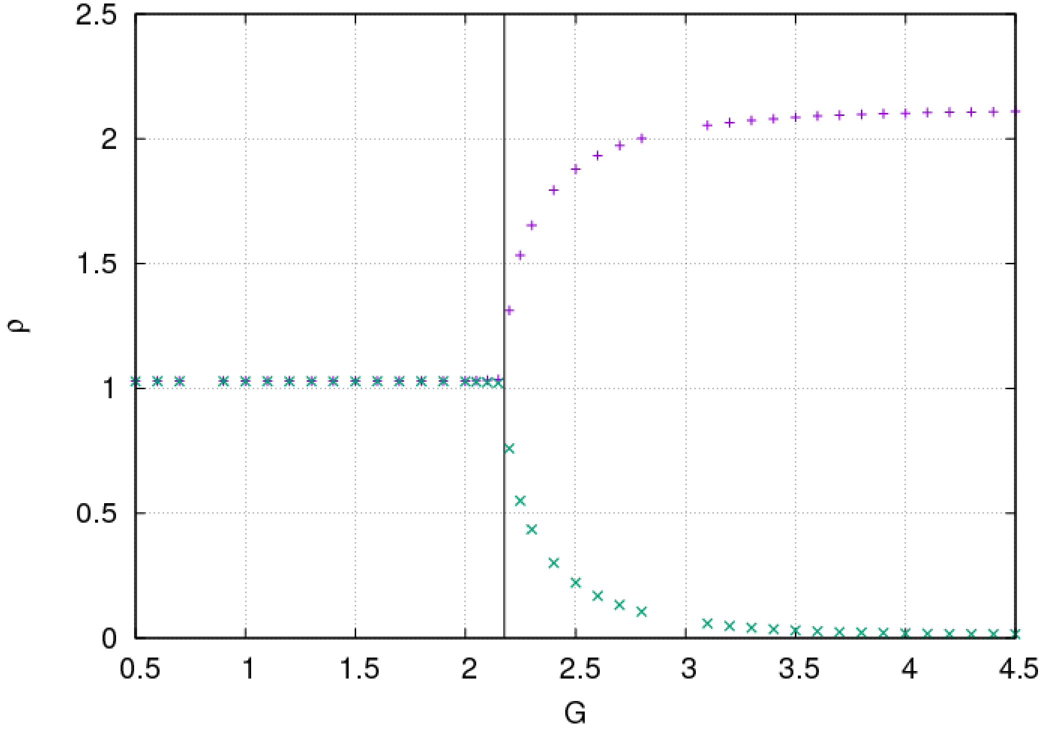


→ Factor two was already visible in initial publication[1]

[1] Porter, M. L.; Coon, E. T.; Kang, Q.; Moulton, J. D.; Carey, J. W.: Phys. Rev. E 86, 036701 (2012)

Critical Point

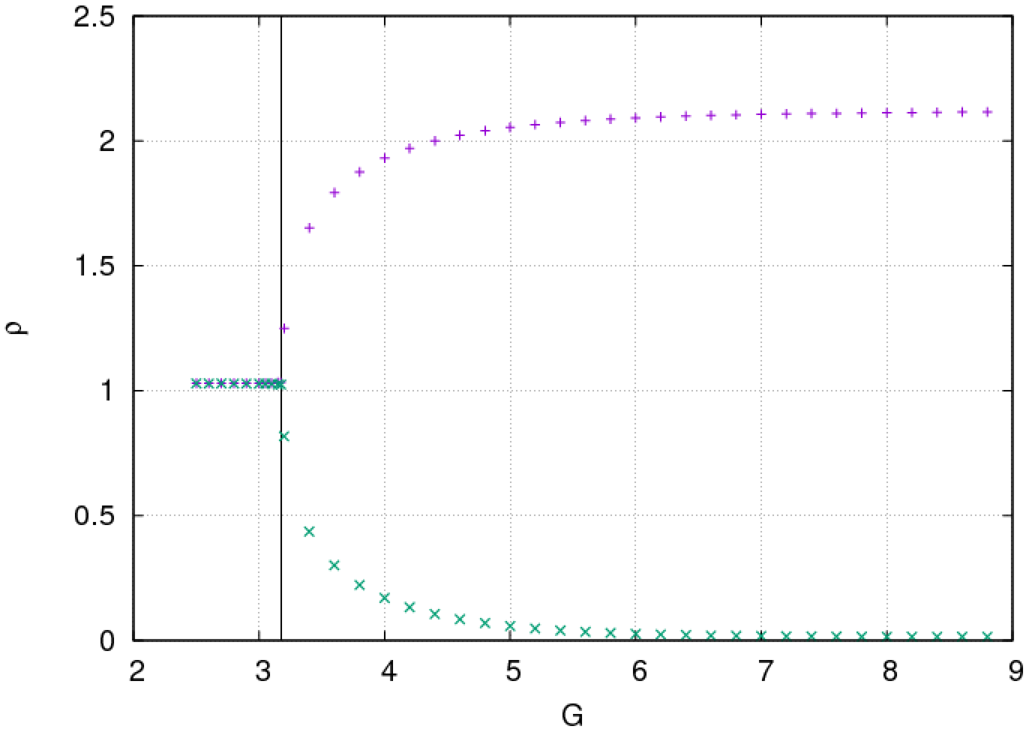
Measure ρ_1^{bulk} and ρ_1^{dis} in static droplet simulation for various G



$$\psi_k = 1 - e^{-\rho_k}$$

Critical Point

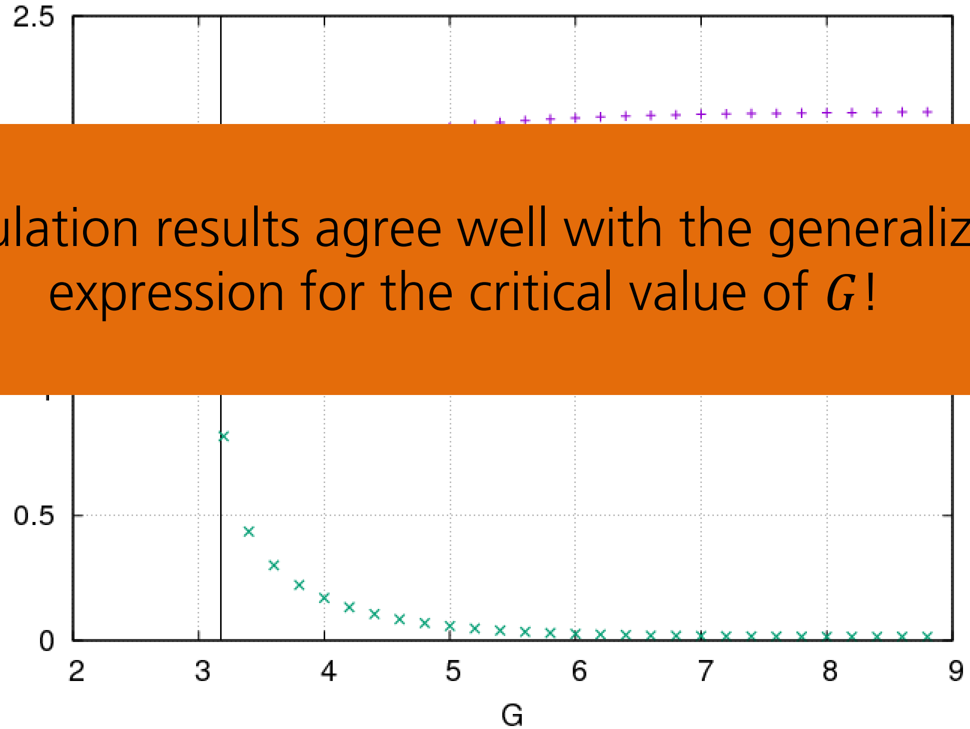
Measure ρ_1^{bulk} and ρ_1^{dis} in static droplet simulation for various G



$$\psi_k = \frac{2}{\pi} \tan^{-1} \rho_k$$

Critical Point

Measure ρ_1^{bulk} and ρ_1^{dis} in static droplet simulation for various G

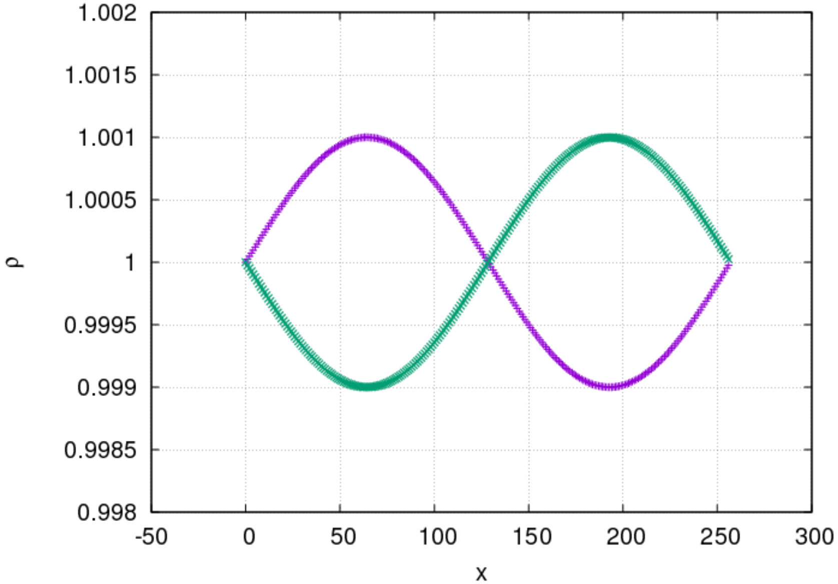


Simulation results agree well with the generalized expression for the critical value of G!

$$\psi_k = \frac{2}{\pi}\tan^{-1}\rho_k$$

Diffusion

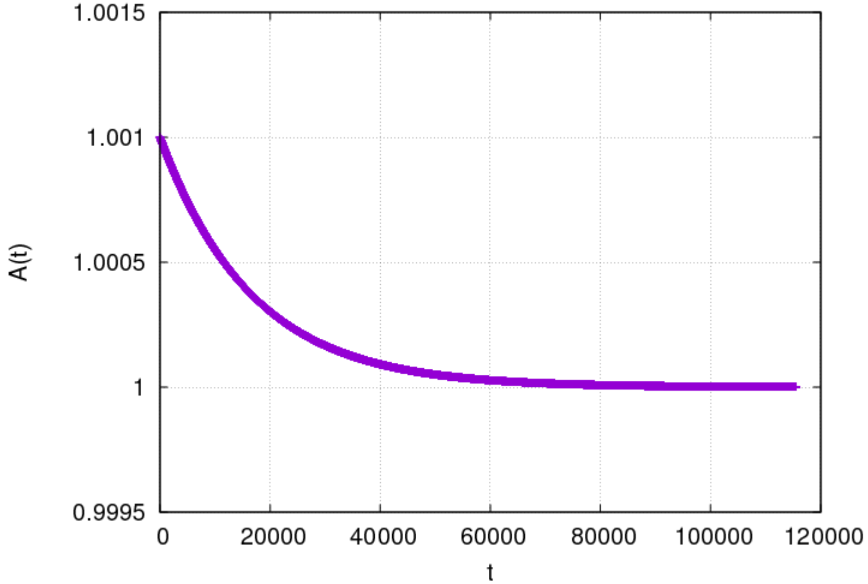
Measure diffusion in a $1D$ decaying sinusoidal concentration wave



Initial density distribution

$$\rho_1 = \rho_{\text{mean}}[1 + \delta \sin(kx)]$$

$$\rho_2 = \rho_{\text{mean}}[1 - \delta \sin(kx)]$$



Amplitude decay

Analytical Diffusion Coefficient

- $\rho_1 = \rho_{\mathrm{mean}}[1 + \delta \sin(kx)]$
- $\rho_2 = \rho_{\mathrm{mean}}[1 - \delta \sin(kx)]$
- $\tau = 1$
- $\psi = \rho$
- $\delta \to \mathrm{small}$

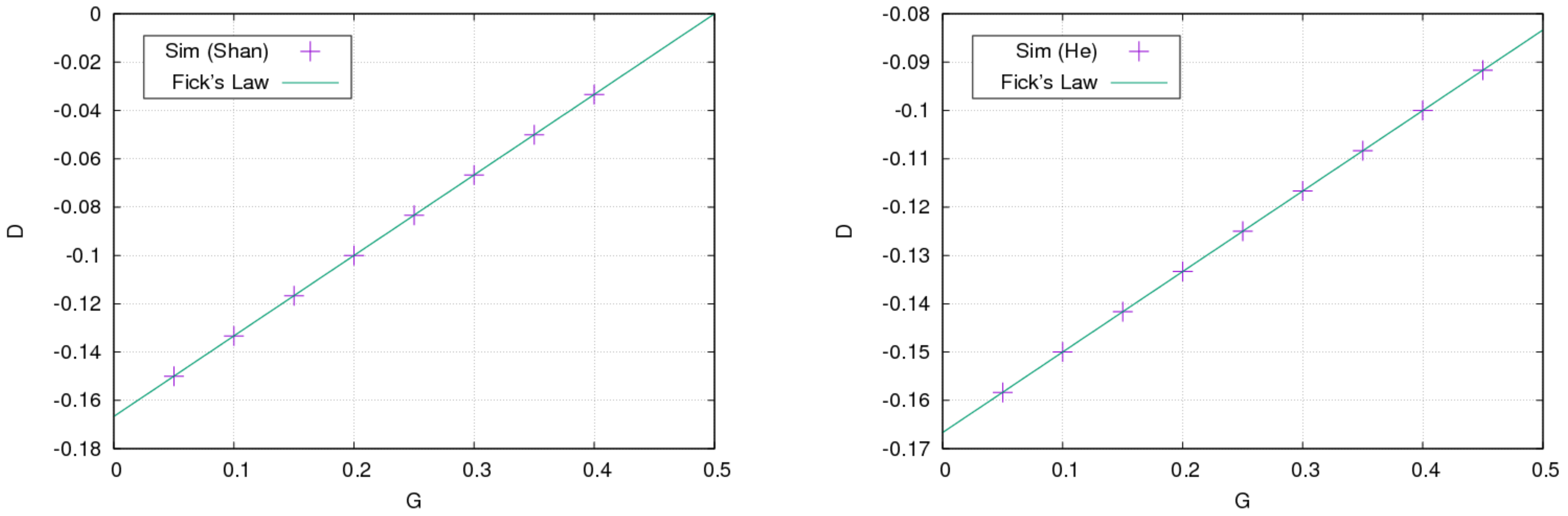
$$\Downarrow$$

$$D^{\mathrm{Shan}} = c_s^2 \left[G\tau(c_1\psi_1'\psi_2 + c_2\psi_2'\psi_1) - \left(\tau - \frac{1}{2}\right)\right]$$

$$\Downarrow$$

$$D^{\mathrm{Shan}} = c_s^2 \left[G\rho_{\mathrm{mean}} - \frac{1}{2}\right]$$

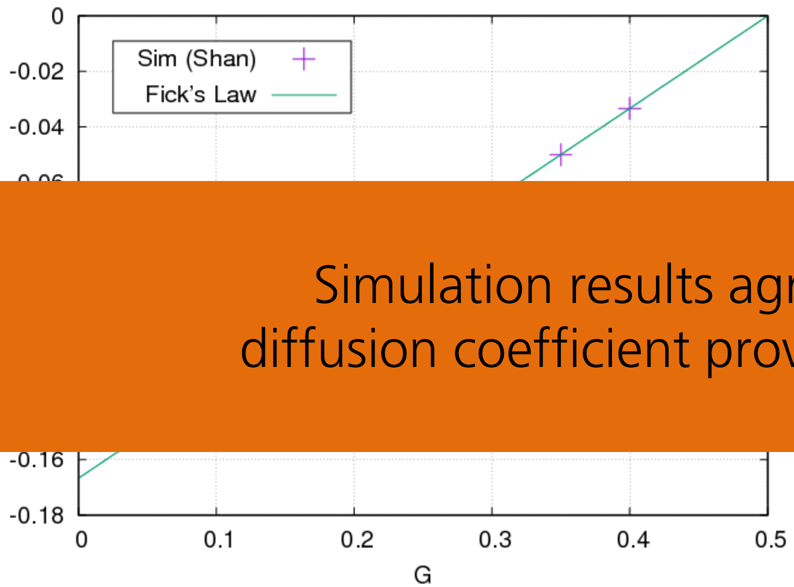
Diffusion (Shan vs. He)

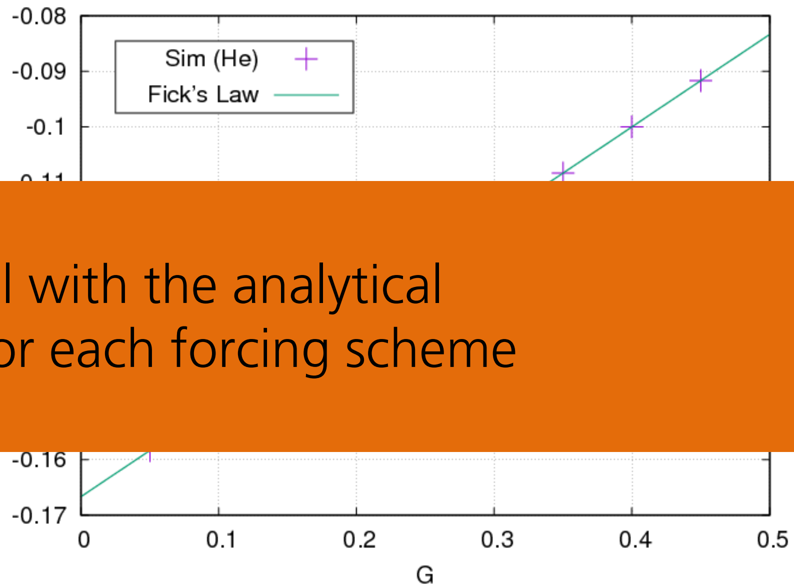


Solve Fick's Law to obtain the numerical diffusion:

$$D = \frac{\rho_k \left(u^c_{k,x} - u_{m,x}\right)}{\partial_x \rho_k}$$

Diffusion (Shan vs. He)





Simulation results agree well with the analytical diffusion coefficient provided for each forcing scheme

Solve Fick's Law to obtain the numerical diffusion:

$$D = \frac{\rho_k \left(u^c_{k,x} - u_{m,x}\right)}{\partial_x \rho_k}$$

Comparing $|u_s|$

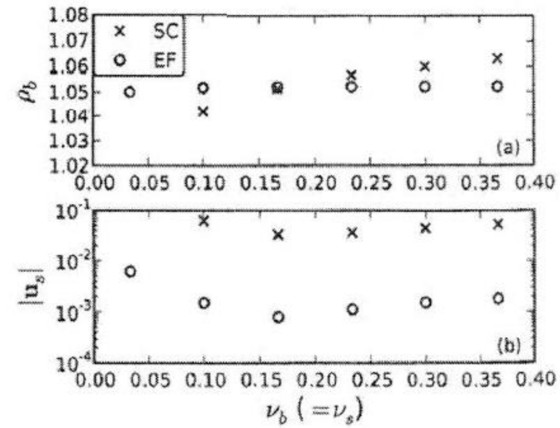
Spurious velocities should be compared for equal

$$G_{\text{red}} = \frac{G}{G_{\text{crit}}}$$

If the comparison was done for the same value of G, the surface tension and the interface thickness would be different for different forcing schemes!

suspending fluids, respectively. First we compare simulation results between the two models for 2D static bubbles, in which the kinematic viscosity ratio is 1 and ν_b has values from 0.03 to 0.37. The radius of the bubble is $R = 24$ and it is placed within a suspending fluid domain of 62×62 lattice sites. The interaction strength between components is $g_{12} = g_{21} = 0.17$, which produces sufficient phase separation. In addition, we used the SRT formulation and set the isotropy order to 4 to be consistent with the original formulation of the SC model. Figure 1 compares the bubble density ρ_b and the maximum magnitude of the spurious currents $|\mathbf{u}_s|$ obtained from the SC and EF models. The SC model results in a bubble density that is dependent on the chosen viscosity, whereas the EF model results in a bubble density that is independent of viscosity. In addition, the spurious currents are reduced by almost two orders of magnitude with the EF model. Overall, Fig. 1 shows considerable improvement with the EF model as compared to the SC model for static bubbles with a kinematic viscosity ratio of 1.

Next we consider static bubble simulations for kinematic viscosity ratios greater than 1. With the SC model we obtained stable results up to $\nu_b/\nu_s = 5$. This is consistent with



[1] Porter, M. L.; Coon, E. T.; Kang, Q.; Moulton, J. D.; Carey, J. W.: Phys. Rev. E 86, 036701 (2012)

Summary

- It was shown that **forcing schemes change the diffusion properties** in pseudopotential-based lattice Boltzmann models for multicomponent flows

- Since G is part of e.g. formulas for a priori **estimation of contact angle** estimation, they **have to be adjusted** if the forcing scheme changes. The same holds for previously determined estimates for the **surface tension**.

- Due to the change in diffusion as well as surface tension, **proper comparisons** of e.g. spurious velocities should be done for equal G_{red} but not for equal G

→ Using **a different forcing scheme** in multicomponent simulations not only eliminates error terms in the Navier-Stokes Equations, but also **changes fundamental physics** in the **macroscopic advection-diffusion equation**.