Stochastic Particle Approach for Non-Continuum Multiphase Flows: A Study on Inverted Temperature Gradient

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Motivation

Goal?

Accurate & efficient predictions of multiphase flows at large scales.

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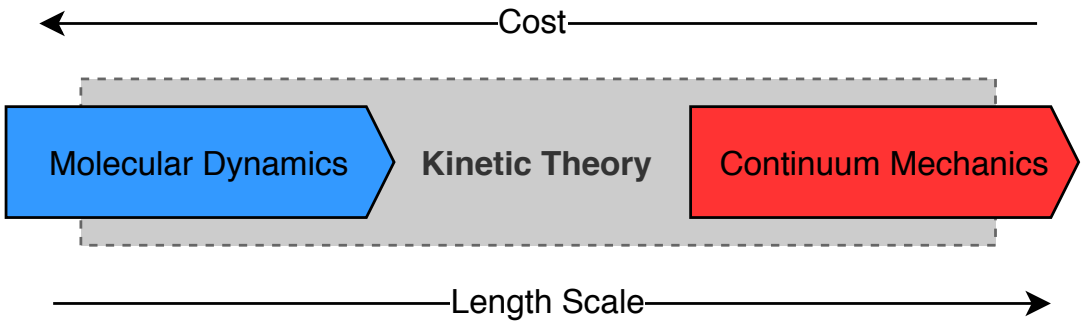
Methods	Non-equilibrium physics	No closure problem	No inter-phase problem	Large scale simulation	No noise
Continuum Mechanics	✗	✗	✗	✓	✓
Molecular Dynamics	✓	✓	✓	✗, cost=$\mathcal{O}(N^2_{\text{Mol.}})$	✗
Kinetic theory	✓	✓	✓	✓, cost=$\mathcal{O}(N^2_{\text{Particle}})$ → $\mathcal{O}(N_{\text{Particle}})$	✗

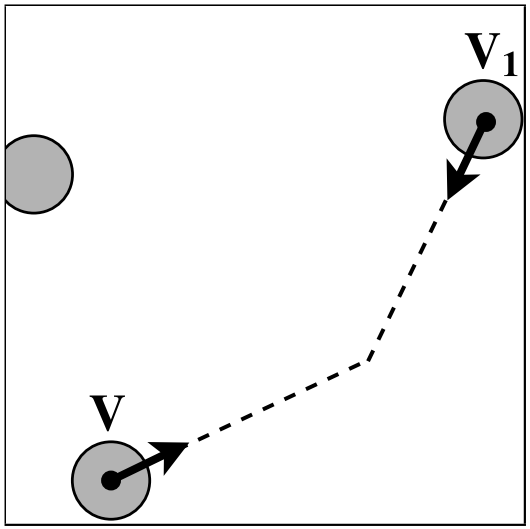


Applications?

- Fuel droplets [1].
- Molecular distillation. [2, 3, 4]
- Evaporation processes in the laser solid interaction [5].
- Sonoluminescence [6].

Dilute *.vs.* Dense Fluids

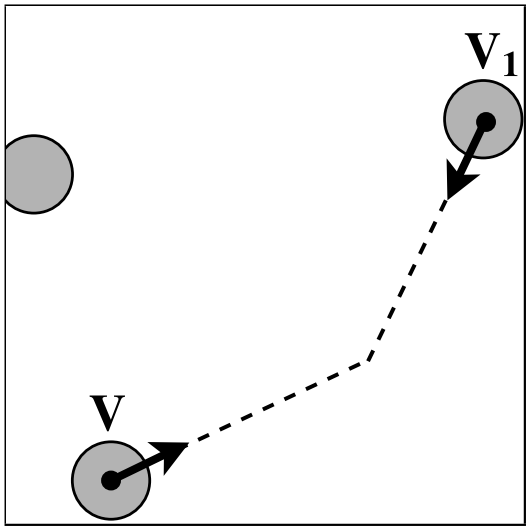
Dilute



Point particle:
Boltzmann collision operator

Dilute *.vs.* Dense Fluids

Dilute



Point particle:
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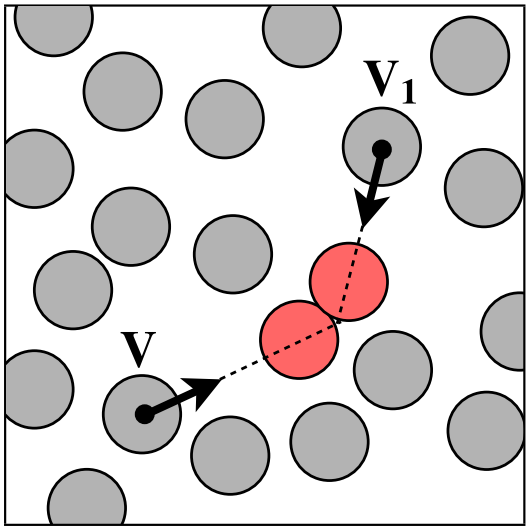
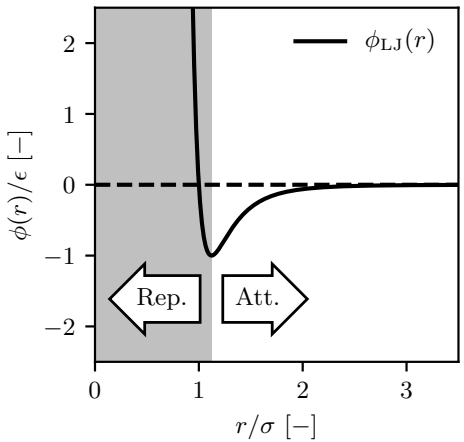
Dense



Particles with Sutherland potential:
Enskog collision operator
+ **attraction.**

Enskog-Vlasov equation

Evolution of velocity distribution function $\mathcal{F}(\boldsymbol{V}, \boldsymbol{x}, t)$ is described via



$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F} V_j)}{\partial x_j} - \underbrace{\xi_j \frac{\partial \mathcal{F}}{\partial V_j}}_{\textbf{Attraction}} = \underbrace{S^{\mathrm{Ensk}}(\mathcal{F})}_{\text{Repulsion}} \qquad (1.1)$$

where $\xi_i = \partial U / \partial x_i$ indicates inter-molecular attractive force and

$$U(\boldsymbol{x}) = \frac{1}{m} \int_{r:=|\boldsymbol{x}'-\boldsymbol{x}|>\sigma} \phi(r) n(\boldsymbol{x}') d^3 \boldsymbol{x}' \qquad (1.2)$$

with

$$\phi(r) = \epsilon \left(\frac{\sigma}{r} \right)^6 \qquad (1.3)$$

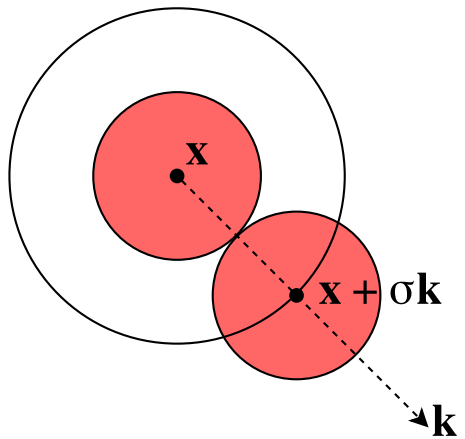
Enskog-Vlasov equation

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F} V_j)}{\partial x_j} - \underbrace{\xi_j \frac{\partial \mathcal{F}}{\partial V_j}}_{\text{Attraction}} = \underbrace{S^{\text{Ensk}}(\mathcal{F})}_{\textbf{Repulsion}} \qquad \text{(1.1 revisited)}$$

and collision operator accounts for repulsion, i.e.

$$S^{\text{Ensk}} = \int_{\mathbb{R}^3} \int_0^{2\pi} \int_0^{+\infty} \Big[Y(\boldsymbol{x} + \frac{1}{2}\sigma \hat{\boldsymbol{k}}) \mathcal{F}(\boldsymbol{V}^*, \boldsymbol{x}) \mathcal{F}(\boldsymbol{V}_1^*, \boldsymbol{x} + \sigma \hat{\boldsymbol{k}}) - Y(\boldsymbol{x} - \frac{1}{2}\sigma \hat{\boldsymbol{k}}) \mathcal{F}(\boldsymbol{V}, \boldsymbol{x}) \mathcal{F}(\boldsymbol{V}_1, \boldsymbol{x} - \sigma \hat{\boldsymbol{k}}) \Big] g \hat{b} d\hat{b} d\hat{\epsilon} d^3 \boldsymbol{V}_1. \qquad (1.4)$$

- $\hat{b}$, $\hat{\epsilon}$ and $\hat{\boldsymbol{k}}$ specify collision cross section.
- σ: effective diameter of particles.
- Y: pair correlation function.
- * : post-collision state.



Step 1: Enskog equation

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F} V_j)}{\partial x_j} - \underbrace{\xi_j \frac{\partial \mathcal{F}}{\partial V_j}}_{\textbf{Attraction}} \overset{0}{\nearrow} = \underbrace{S^{\text{Ensk}}(\mathcal{F})}_{\textbf{Repulsion}} \tag{1.5}$$

Approaches:

- Directly discretize $\mathcal{F}$ in $(\boldsymbol{x}, \boldsymbol{v}, t) \rightarrow$ high dimensionality!
- Solve for the moments $\rightarrow$ fast but needs further assumptions for $\mathcal{F}$!
- Evolve the samples of $\mathcal{F} \rightarrow$ efficient/accurate with stochastic noise ✓

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- Evolve the samples of $\mathcal{F} \rightarrow$ efficient/accurate with stochastic noise ✓
  - Resolving underlying jump process $\rightarrow$ exact but cost is of $\mathcal{O}(n^2)$!
  - Modeling with continuous process $\rightarrow$ reasonably accurate/efficient ✓

This motivates developing Fokker-Planck model for phase transition.

Review: Fokker-Planck model

Consider an Itô process

$$\begin{cases} d\boldsymbol{M} = \boldsymbol{A}dt + D d\boldsymbol{W} \text{ and} \\ d\boldsymbol{X} = \boldsymbol{M}dt \ , \end{cases} \tag{1.6}$$

where $\boldsymbol{W}$ is a Wiener process. Itô calculus provides us the equivalent Fokker-Planck equation[1]

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F} V_i)}{\partial x_i} = -\frac{\partial (\mathcal{F} A_i)}{\partial V_i} + \frac{1}{2}\frac{\partial^2}{\partial V_j \partial V_j}(D^2 \mathcal{F}). \tag{1.7}$$

Drift and diffusion

$\boldsymbol{A}$ and D are called drift and diffusion coefficients, respectively, and are set to give an approximation of a generic collision operator.

[1] see Gardiner (1996) [7].

Homogeneous relaxation rates of Enskog equation

- Re-writing Enskog operator

$$S^{\text{Ensk}} = Y(\boldsymbol{x}) S^{\text{Boltz}} + S_\phi \tag{1.8}$$

where S_ϕ includes all spatial dependency of $\mathcal{F}$ and Y in $\boldsymbol{x}$.

- Relaxation rates of shear stress and heat fluxes then become

$$\frac{\partial \pi_{ij}}{\partial t} = -Y \frac{p}{\mu^{\text{kin}}} \pi_{ij} \tag{1.9}$$

$$\text{and} \quad \frac{\partial q_i}{\partial t} = -Y \frac{2}{3} \frac{p}{\mu^{\text{kin}}} q_i \ . \tag{1.10}$$

- $\boldsymbol{A}$ and $\boldsymbol{D}$ can be approximated by a cubic FP model similar to treatment of Boltzmann operator[2].

[2] see Gorji *et al.* (2011) [8].

Taking velocity moment $\psi \in \{1, V_j, V_j V_j/2\}$ of expanded Enskog equation leads to

$$\int_{\mathbb{R}^3} \psi \left(\frac{\partial \mathcal{F}}{\partial t} + V_i \frac{\partial \mathcal{F}}{\partial x_i} \right) d^3 \boldsymbol{V} = -\frac{\partial \Psi_i^{\phi}}{\partial x_i}. \tag{1.11}$$

where $\boldsymbol{\Psi}^{\phi}$ is called collsional transfer. Ignoring higher order terms lead to

$$p^{\text{tot}} = (1 + nbY) nkT - w \frac{\partial U_k}{\partial x_k}, \tag{1.12}$$

$$\pi_{ij}^{\text{tot}} = (1 + 2nbY/5)\pi_{ij} - (5w/6) \frac{\partial U_{\langle i}}{\partial x_{j\rangle}} \tag{1.13}$$

and

$$q_i^{\text{tot}} = (1 + 3nbY/5) q_i - c_v w \frac{\partial T}{\partial x_i} \tag{1.14}$$

where $w = (nb)^2 Y \sqrt{mkT}/(\pi^{3/2}\sigma^2)$ is bulk viscosity.
Extra streaming in FP should account for dense effects.

Dense gas Fokker-Planck model (DFP)

- Collisional transfer promotes idea of extra streaming

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F} V_i)}{\partial x_i} = -\frac{\partial (\mathcal{F} A_i)}{\partial V_i} + \frac{1}{2} \frac{\partial^2 (D^2 \mathcal{F})}{\partial V_j \partial V_j} - \frac{\partial (\mathcal{F} \hat{A}_i)}{\partial x_i} \ . \qquad (1.15)$$

- What is $\hat{\boldsymbol{A}}$?
  $\hat{\boldsymbol{A}}$ is a spatial drift set to guarantee dense effects in the transport.
- A cubic model for $\hat{\boldsymbol{A}}$ was designed [9], i.e.

$$\hat{A}_i \ = \ \hat{c}_{ij} v_j' + \hat{\gamma}_i \left(v_j' v_j' - \frac{3kT}{m} \right) + \hat{\Lambda} \left(v_i' v_j' v_j' - \frac{2q_i}{\rho} \right) \ . \qquad (1.16)$$

Accuracy and efficiency of DFP: equilibrium pressure[3]

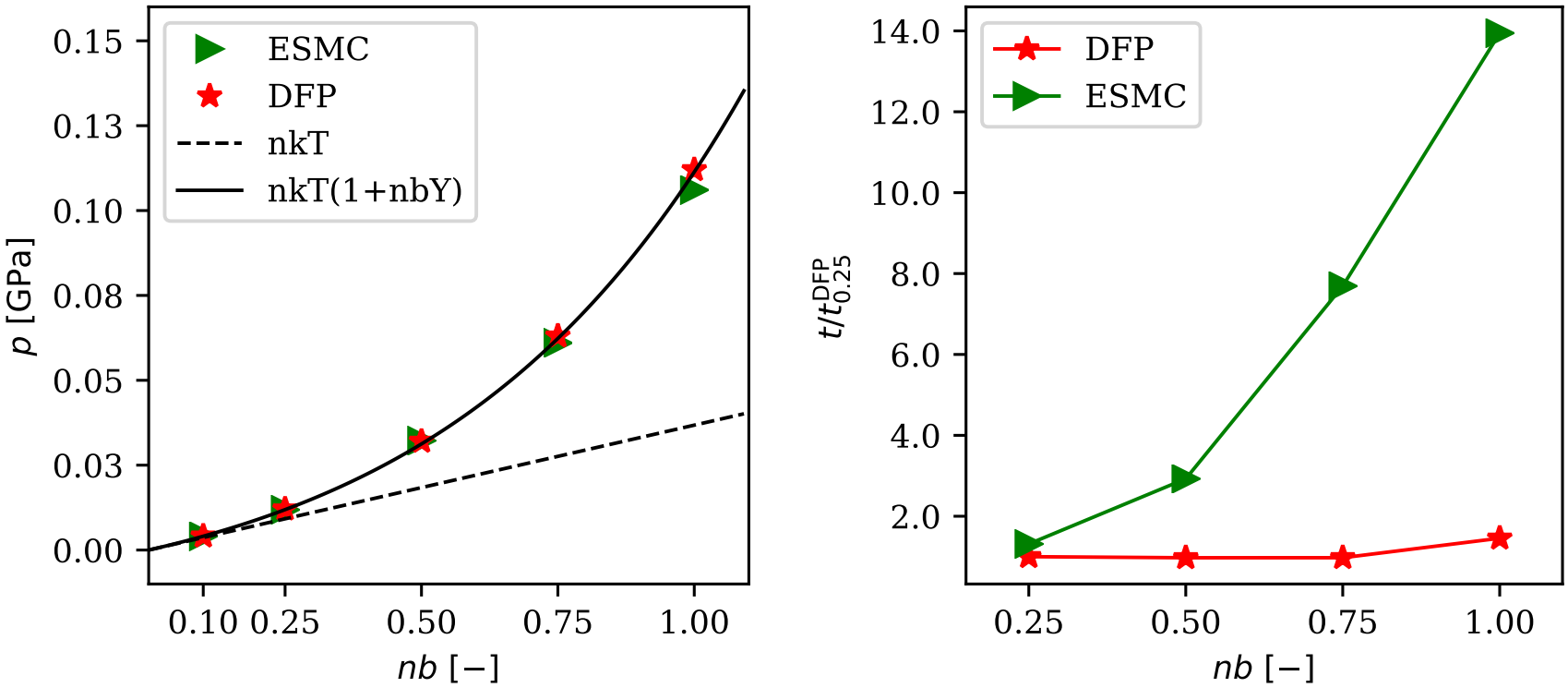
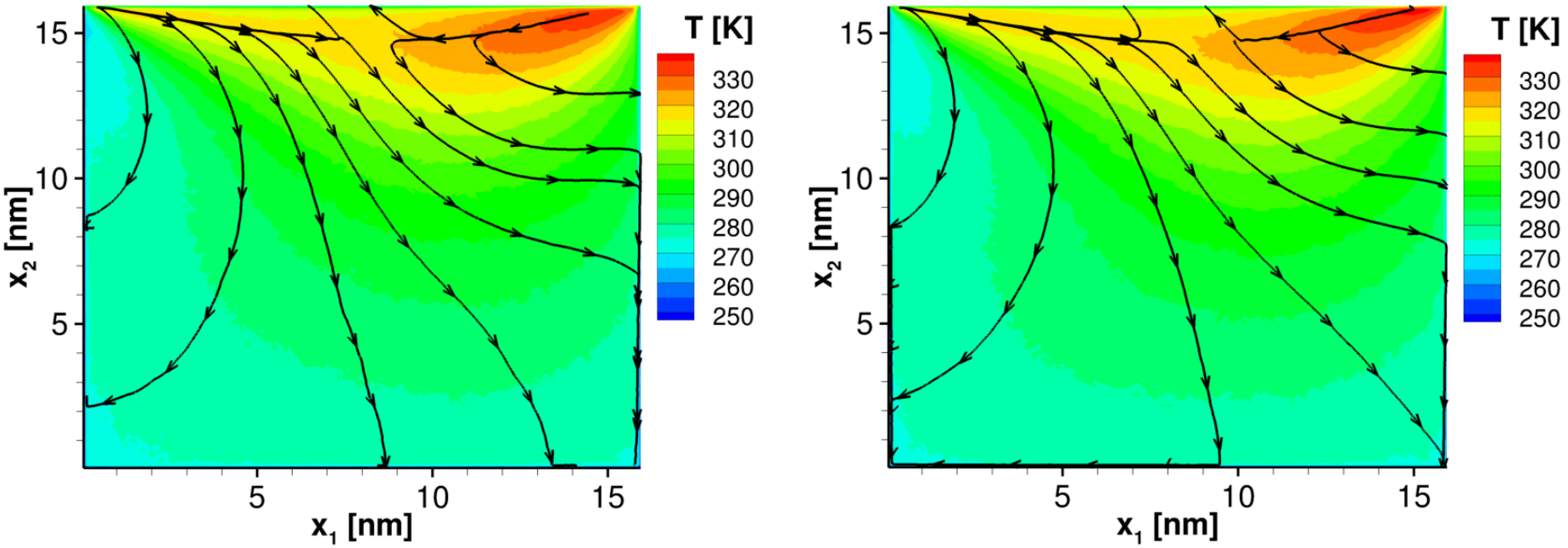


Figure 1: Equilibrium test case.

[3] see Sadr and Gorji (2017) [9]

Lid-driven cavity [4]



(a) DFP (b) ESMC

Figure 2: Temperature contours and heat fluxes of the lid-driven cavity flow at $\mathrm{Kn} = 0.1$, $nb = 0.1$ and $U_w = 300\ \mathrm{m/s}$.

[4] see Sadr and Gorji (2017) [9]

Step 2: Modelling long-range interaction

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F} V_j)}{\partial x_j} - \underbrace{\xi_j \frac{\partial \mathcal{F}}{\partial V_j}}_{\textbf{Attraction}} = \underbrace{S^{\text{Ensk}}(\mathcal{F})}_{\text{Repulsion}} \qquad \text{(1.1 revisited)}$$

where $\xi_i = \partial U / \partial x_i$ and

$$U(\boldsymbol{x}) = \frac{1}{m} \int_{r:=|\boldsymbol{x}'-\boldsymbol{x}|>\sigma} \phi(r) n(\boldsymbol{x}') d^3 \boldsymbol{x}' \qquad \text{(1.2 revisited)}$$

Approaches:

- Integrating with particles $\rightarrow$ acceptable resolution requires too many particles!
- Using quadrature rule $\rightarrow$ mesh refinement and cut-off are required!
- Convolution and density expansion $\rightarrow$ only includes local variation and higher order derivatives of density needs to be ignored!
- How about transforming the Vlasov integral to the solution of an elliptic PDE? ✓

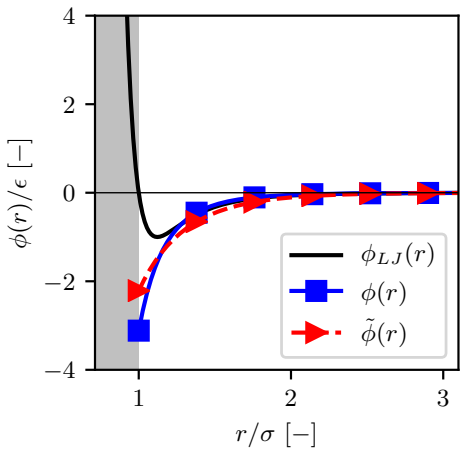
Screened-Poisson equation (SP), unbounded domain

Idea: Relating Vlasov integral

$$U(\boldsymbol{x}) = \int_{r>\sigma} \phi(r) n(\boldsymbol{x}') d^3\boldsymbol{x}' \tag{1.17}$$

to a Poisson-type PDE.

- Approximate ϕ by $\tilde{\phi}$ via minimizing $|\phi(r) - \tilde{\phi}(r)|$ for $r \in (\sigma, \infty)$



$$\phi(r) = \epsilon\left(\frac{\sigma}{r}\right)^6$$
$$\approx a\frac{e^{-\lambda r}}{4\pi r} = \underbrace{aG(r)}_{\tilde{\phi}(r)} \tag{1.18}$$

- $G(r)$ for $r > 0$ is the fundamental solution of the screened-Poisson PDE, i.e.

$$\left(\nabla^2 - \lambda^2\right) u(\boldsymbol{x}) \quad = \quad -n(\boldsymbol{x}), \qquad \forall \boldsymbol{x} \in \mathbb{R}^3. \tag{1.19}$$

Screened-Poisson equation (SP), unbounded domain

Rewrite the Vlasov integral as:

$$U(\boldsymbol{x}) = \underbrace{\int_{r>0} \phi(r) n(\boldsymbol{x}') d^3\boldsymbol{x}'}_{U_{r>0}} - \underbrace{\int_{r<\sigma} \phi(r) n(\boldsymbol{x}') d^3\boldsymbol{x}'}_{U_{r<\sigma}}. \tag{1.20}$$

- $U_{r<\sigma}$ can be solved analytically assuming density doesn't vary much within $r \in (0, \sigma) \rightarrow$ modelling decision.
- $U_{r>0}$ is the solution of unbounded screened-Poisson PDE, i.e.

$$\left(\nabla^2 - \lambda^2\right) u(\boldsymbol{x}) \quad = \quad -n(\boldsymbol{x}), \qquad \forall \boldsymbol{x} \in \mathbb{R}^3. \tag{1.21}$$

Challenge: we cannot solve the PDE numerically in $\mathbb{R}^3$.

SP on bounded domains

What we want is the solution of unbounded screened-Poisson

$$(\nabla^2 - \lambda^2)u(\boldsymbol{x}, t) = n(\boldsymbol{x}, t) \qquad (\forall \boldsymbol{x} \in \mathbb{R}^3), \tag{1.22}$$

only in some $\Omega \subset \mathbb{R}^3$. Consider the PDE

$$\begin{aligned} \left(\nabla^2 - \lambda^2\right)\psi(\boldsymbol{x}, t) &= n(\boldsymbol{x}, t) \qquad (\forall \boldsymbol{x} \in \Omega) \quad \text{and} & (1.23) \\ \psi(\boldsymbol{y}, t) &= g(\boldsymbol{y}, t) \qquad (\forall \boldsymbol{y} \in \partial\Omega). & (1.24) \end{aligned}$$

Uniqueness of screened-Poisson equation with Dirichlet BC implies

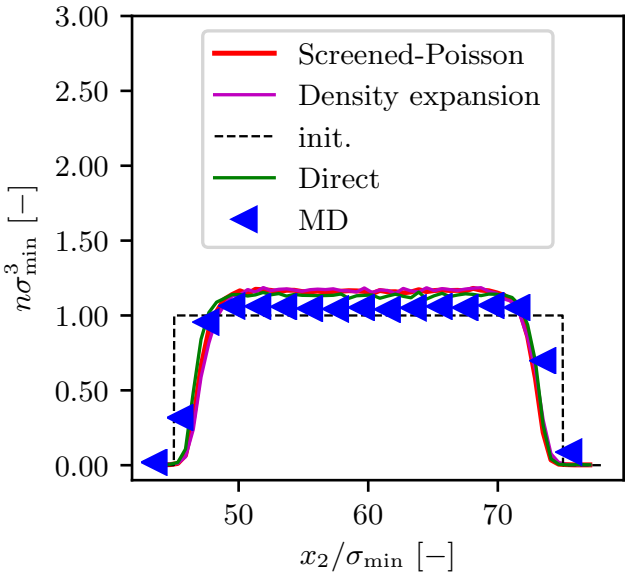
$$\psi(\boldsymbol{x}, t) = u(\boldsymbol{x}, t) \quad (\forall \boldsymbol{x} \in \Omega) \tag{1.25}$$

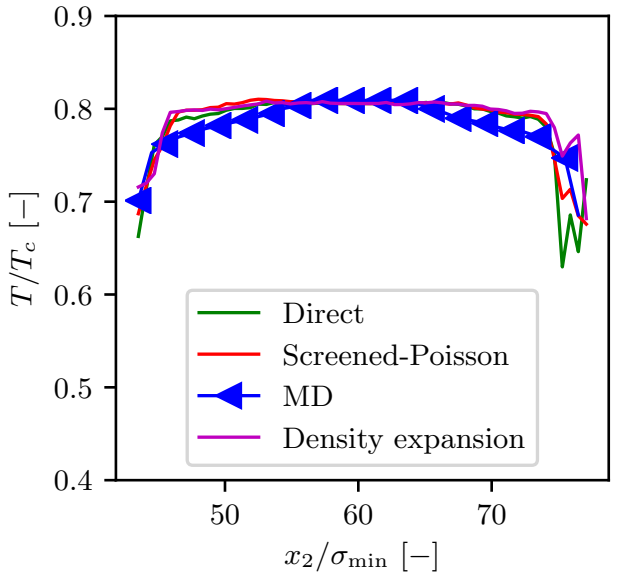
provided

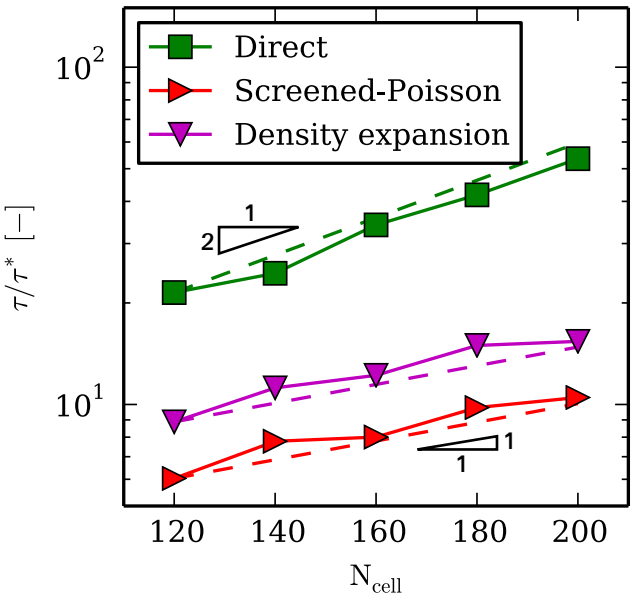
$$g(\boldsymbol{y}, t) = u(\boldsymbol{y}, t) \qquad (\forall \boldsymbol{y} \in \partial\Omega). \tag{1.26}$$

Note $u(\boldsymbol{y}, t)$ on $\partial\Omega$ can be calculated directly.

Evaporation







Evaporation/Condensation rate (DFP-SP)

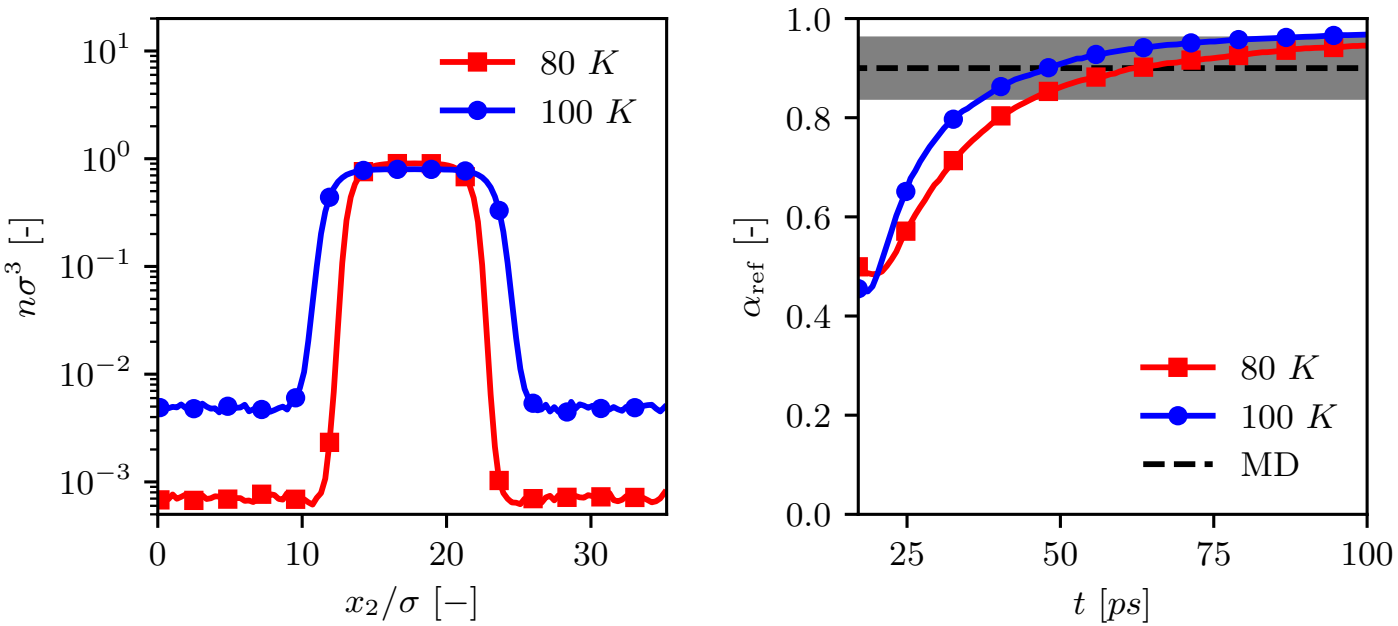


Figure 4: Normalized number density and reflective evaporation/condensation rate profiles for droplets of Argon in a box with periodic boundary condition bathed with 80 and 100 K thermostats compared with MD simulation[5].

[5] for the MD simulation, please see Yasuoka *el al.* (1994). [10]

Inverted Temperature Gradients using DFP-SP

Inverted Temperature Gradients using DFP-SP

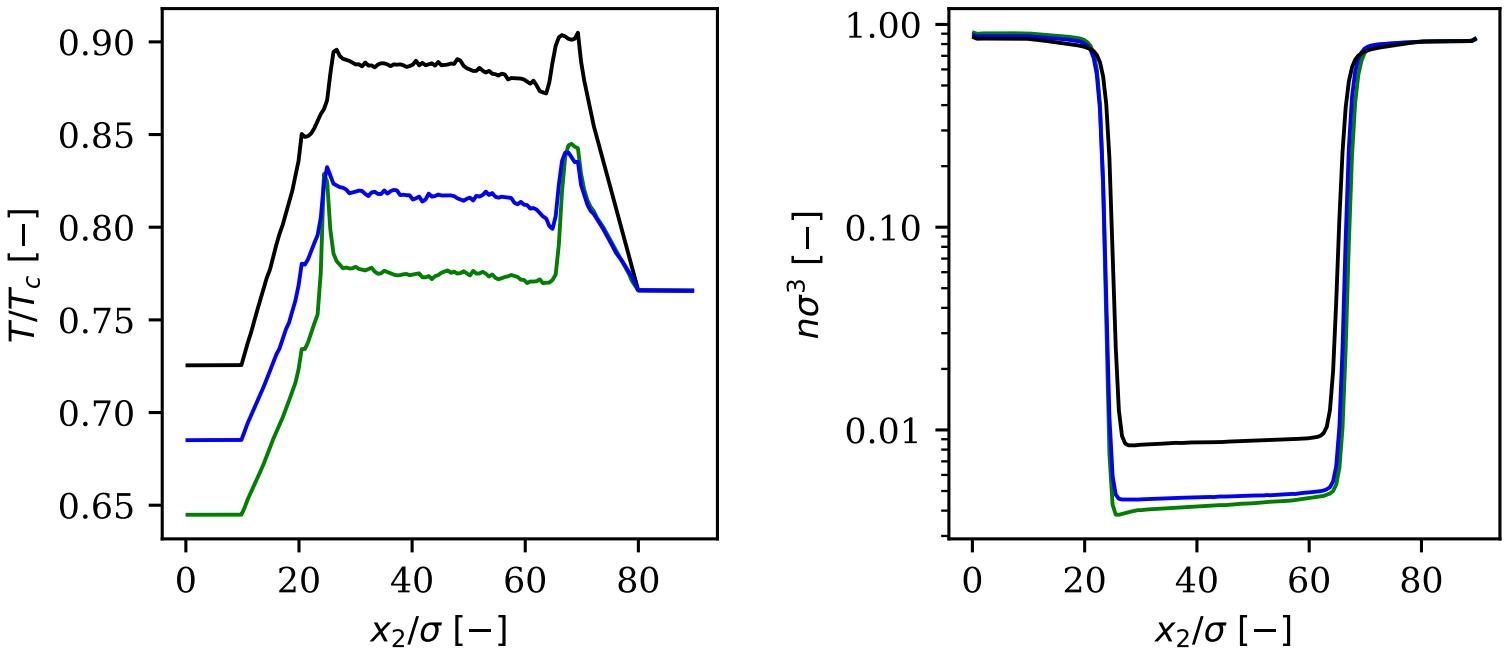


Figure 5: Normalized profiles of temperature and number density of two droplets and the vapour between obtained via DFP-SP model where $T_{\text{hot}} = 95\ \text{K}$ while $T_{\text{cold}} = 80,\ 85$ and $90\ \text{K}$.

Conclusion

- Via collision and Vlasov integral, non-equilibrium phase transition process can be described by Enskog-Vlasov equation.
- Furthermore, efficient solution algorithm can be achieved by modeling collisions through continuous stochastic process[6] and Vlasov integral by screened-Poisson equation[7] (DFP-SP).
- Several test cases showed a good agreement with benchmark at lower computational cost.
- Below critical point, the phenomenon of *inverted temperature gradient* using DFP-SP was studied here.

[6] see M Sadr & MH Gorji, Phys. Fluids, Vol. 29, (2017).

[7] see M Sadr & MH Gorji, J. Comput. Phys., Vol. 378, (2019).

Thanks for your attention.

Any questions?

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For Further Reading III

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N. F. Carnahan and K. E. Starling, "Equation of state for nonattracting rigid spheres," *The Journal of Chemical Physics*, vol. 51, no. 2, pp. 635–636, 1969.

From statistical mechanics, the virial expansion of pressure can be obtained by

$$Z := \frac{p}{nkT} = 1 + B_2 n + B_3 n^2 + B_4 n^2 ..., \tag{3.1}$$

$$B_N = \frac{1-N}{N!} \lim_{V \to 0} V^{-1} \int ... \int d\boldsymbol{r}_1 ... d\boldsymbol{r}_N V_N, \tag{3.2}$$

$$V_N = \sum \prod_{i<j}^{N} f_{ij} \tag{3.3}$$

$$\text{and} \quad f_{ij} = exp(-\phi_{ij}/kT) - 1, \tag{3.4}$$

where ϕ_{ij} is molecular potential between particles i and j.

The factor Y (which comes form virial expansion)

$$Y := \frac{Z-1}{nb} \tag{3.5}$$

for hard-sphere can be calculated exactly as done by Ree-Hoover [**?**]

$$Y = 1 + 0.625nb + 0.2869(nb)^2 + 0.115(nb)^3 + ... \tag{3.6}$$

or approximated by a closed expression as suggested by Carnahan-Starling [11]

$$Y^{CS} = \frac{1 - nb/8}{(1 - nb/4)^3}. \tag{3.7}$$