Monte-Carlo particle methods for non-equilibrium multiphase flows

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I. Introduction

Probabilistic description of dense fluids with Sutherland potential

$$\phi(r) = \begin{cases} +\infty & r < \sigma \\ \phi_0\left(\frac{\sigma}{r}\right)^6 & r \geq \sigma \end{cases}$$

far from equilibrium can be described by Enskog-Vlasov Eq. [1]

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial(\mathcal{F}v_i)}{\partial x_i} - \frac{\xi_i}{m}\frac{\partial \mathcal{F}}{\partial v_i} = S^{\text{Ensk}}(\mathcal{F})$$

where collisions are incorporated with Enskog operator

$$S^{\text{Ensk}}(\mathcal{F}) = \frac{1}{m}\iiint \Big[Y(\boldsymbol{x} + \frac{1}{2}\sigma\hat{\boldsymbol{k}})\mathcal{F}(\boldsymbol{v}^*, \boldsymbol{x})\mathcal{F}(\boldsymbol{v}_1^*, \boldsymbol{x} + \sigma\hat{\boldsymbol{k}}) - Y(\boldsymbol{x} - \frac{1}{2}\sigma\hat{\boldsymbol{k}})\mathcal{F}(\boldsymbol{v}, \boldsymbol{x})\mathcal{F}(\boldsymbol{v}_1, \boldsymbol{x} - \sigma\hat{\boldsymbol{k}}) \Big] \mathcal{H}(\boldsymbol{g}\cdot\hat{\boldsymbol{k}}) g\hat{b}d\hat{b}d\hat{\epsilon}d^3\boldsymbol{v}_1$$

and long-range forces are included via $\xi_i = \partial_{x_i} U$ where

$$U(\boldsymbol{x}, t) = \int_{r>\sigma} \phi(r) n(\boldsymbol{y}, t) d^3\boldsymbol{y} \ .$$

Challenges:
1. **Resolving collision operator is costly.**
2. **Long tail Vlasov integral restricts computation of attractive forces.**

II. Modelling long range interactions

IDEA: i. Modeling attractive part of $\phi(r)$ with Green function of an elliptic PDE.
ii. Solve the PDE globally instead.

MODEL: approximate $\phi(r)$ by $\tilde{\phi}(r) = aG(r)$ with

$$G(r) = \frac{e^{-\lambda r}}{4\pi r}$$

where a and λ are obtained from

$$(a, \lambda) = \underset{r\in(\sigma,\infty)}{\text{argmin}}(||\partial_r\phi(r) - \partial_r\tilde{\phi}(r)||_2) \ .$$

Rewrite the potential $U(\boldsymbol{x}, t)$ as

$$U(\boldsymbol{x}, t) \approx \underbrace{a\int_{r>0} G(r)n(\boldsymbol{y}, t)d^3\boldsymbol{y}}_{u(\boldsymbol{x},t)} - \underbrace{a\int_{r<\sigma} G(r)n(\boldsymbol{y}, t)d^3\boldsymbol{y}}_{\tilde{U}_{r<\sigma}} \ .$$

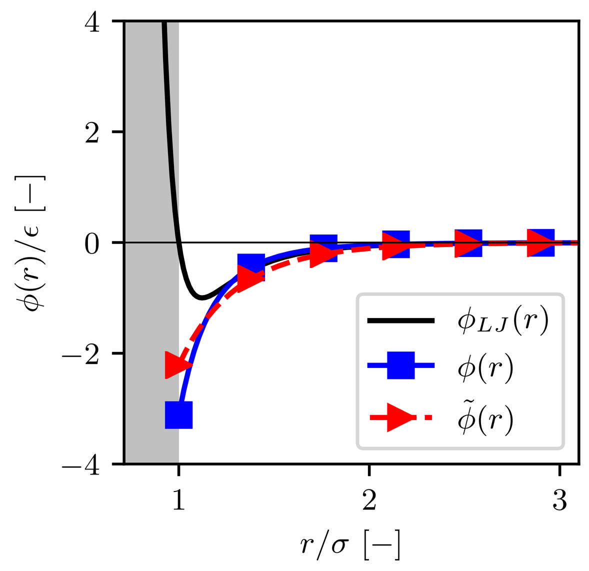

Figure 1: Lennrad-Jones molecular potential $\phi_{LJ}(r)$ along with Sutherland $\phi(r)$ and the Coulomb-type potential $\tilde{\phi}(r)$ for Argon with $\epsilon = 119.8k_b$ and $\sigma = 3.405 \times 10^{-10}$m.

The first term $u(\boldsymbol{x}, t)$ is the fundamental solution to Screened-Poisson (SP) Eq.

$$\left(\Delta - \lambda^2\right) u(\boldsymbol{x}, t) = n(\boldsymbol{x}, t); \quad (\forall \boldsymbol{x} \in \mathbb{R}^3)$$

and $\tilde{U}_{r<\sigma}$ can be approximated assuming regularity on density for $r \in (0, \sigma)$ [4].

The long range potential can be computed using efficient Poisson solvers.

IV.c Inverted Temperature Gradient

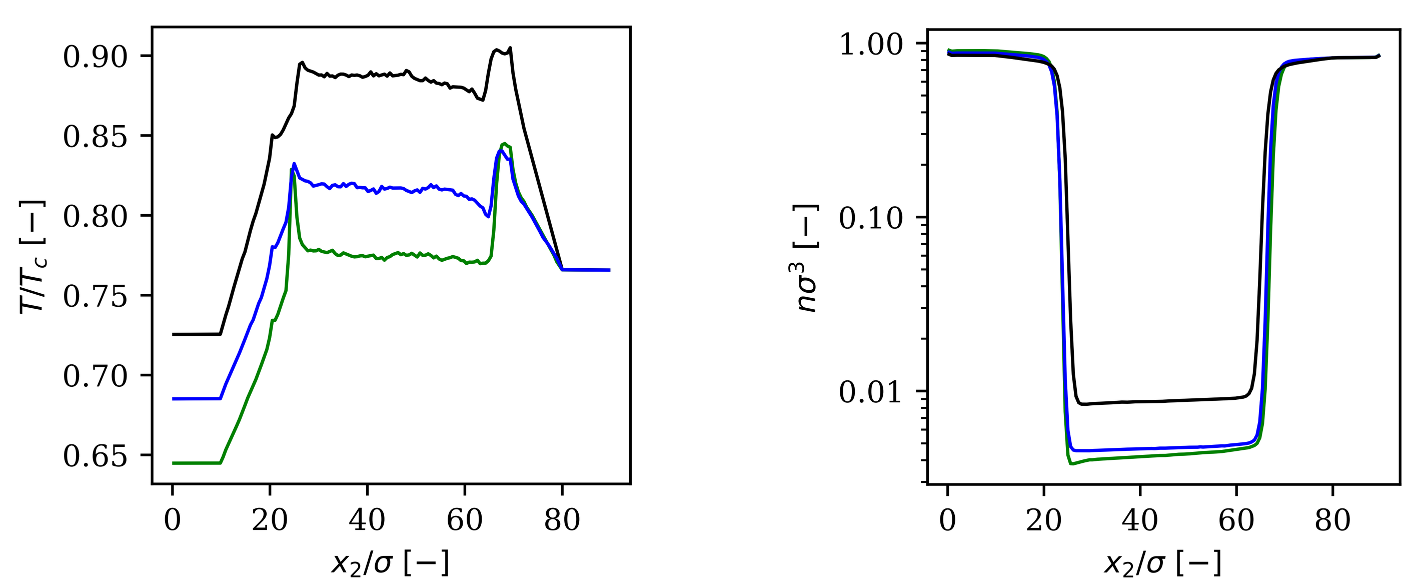

Figure 2: Normalized profiles of temperature and number density of two droplets and the vapour between obtained via DFP-SP model where $T_{\text{hot}} = 95$ K while $T_{\text{cold}} = 80$, 85 and 90 K.

III. Fokker-Planck model for dense gases

IDEA: i. Approximate jump process with a continuous one.
$\xrightarrow{\text{needed}}$ **relaxation rates**
ii. Include dense effects with spatial drift.
$\xrightarrow{\text{needed}}$ ***collisional transfer***

i. **Relaxation rates** of Enskog operator are

$$\frac{\partial \pi_{ij}}{\partial t}|_{\text{coll}} = -Y\frac{p}{\mu^{\text{kin}}}\pi_{ij} \quad \& \quad \frac{\partial q_i}{\partial t}|_{\text{coll}} = -Y\frac{2}{3}\frac{p}{\mu^{\text{kin}}}q_i \ .$$

ii. ***Collisional transfer*** $\boldsymbol{\Psi}^\phi$ appearing in the velocity moments of Enskog equation

$$\int \psi\left(\frac{\partial \mathcal{F}}{\partial t} + v_i\frac{\partial \mathcal{F}}{\partial x_i}\right)d^3\boldsymbol{v} = -\frac{\partial \Psi_i^\phi}{\partial x_i}$$

has explicit form up to second order term.

MODEL: a Fokker-Planck model for Dense gases (DFP) can be designed [3]

$$S^{\text{DFP}}(\mathcal{F}) = \underbrace{-\frac{\partial(\mathcal{F}A_i)}{\partial v_i} + \frac{1}{2}\frac{\partial^2(D^2\mathcal{F})}{\partial v_j\partial v_j}}_{\text{ensures consistent relaxation rates}} - \underbrace{\frac{\partial(\mathcal{F}\hat{A}_i)}{\partial x_i}}_{\text{spatial drift}}$$

to approximate Enskog operator with a spatial drift $\hat{\boldsymbol{A}}$ which is closed by

$$\frac{\partial}{\partial x_i}\int \hat{A}_i\psi\mathcal{F}d^3\boldsymbol{v} = \frac{\partial \Psi_i^\phi}{\partial x_i} \ .$$

Efficient particle methods for the equivalent SDEs can be used.

Once $\boldsymbol{A}$, $\hat{\boldsymbol{A}}$ and D are sampled, the random variables for velocity $\boldsymbol{V}$ and position $\boldsymbol{X}$ are evolved via Itō process

$$\begin{cases} d\boldsymbol{V} = \boldsymbol{A}dt + Dd\boldsymbol{W}_t \ , \\ d\boldsymbol{X} = \hat{\boldsymbol{A}}dt + \boldsymbol{V}dt \ . \end{cases}$$

IV. Results

IV.a Lid-Driven Cavity

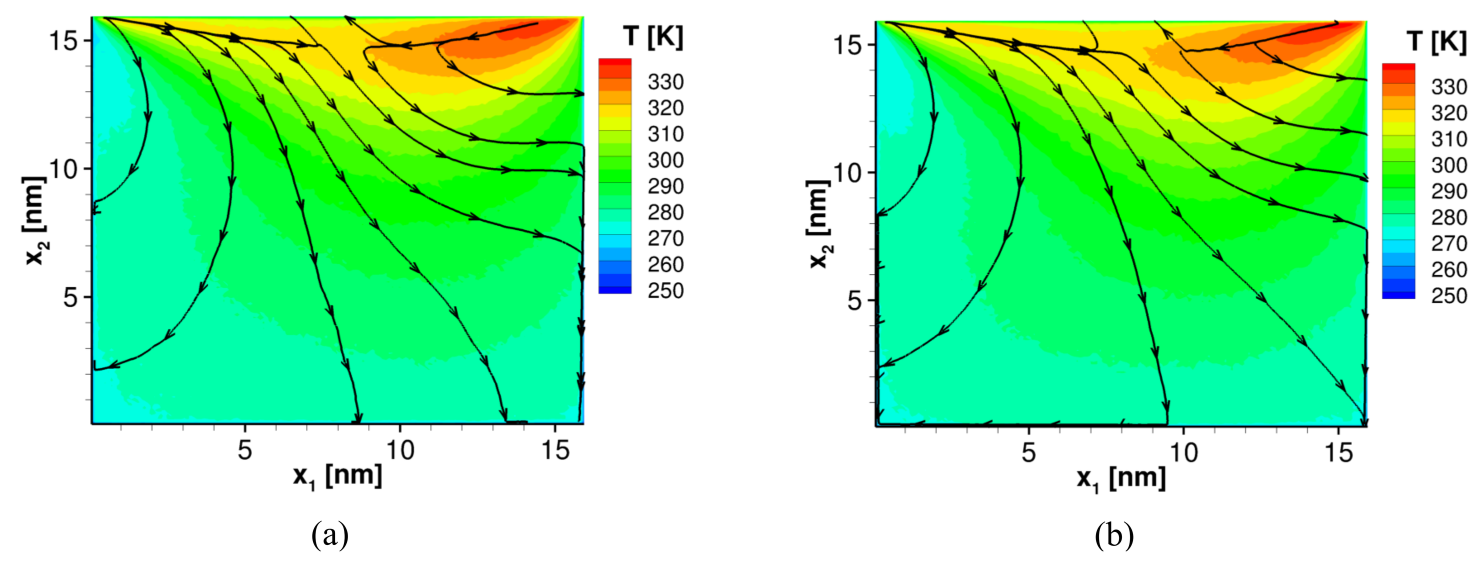

Figure 3: Temperature contours along with heat fluxes of a **lid-driven cavity** flow with wall velocity of 300 m/s at Kn = 0.1 using (a) DFP model and (b) Enskog Simulation Monte Carlo (ESMC) method [2].

IV.b Evaporation

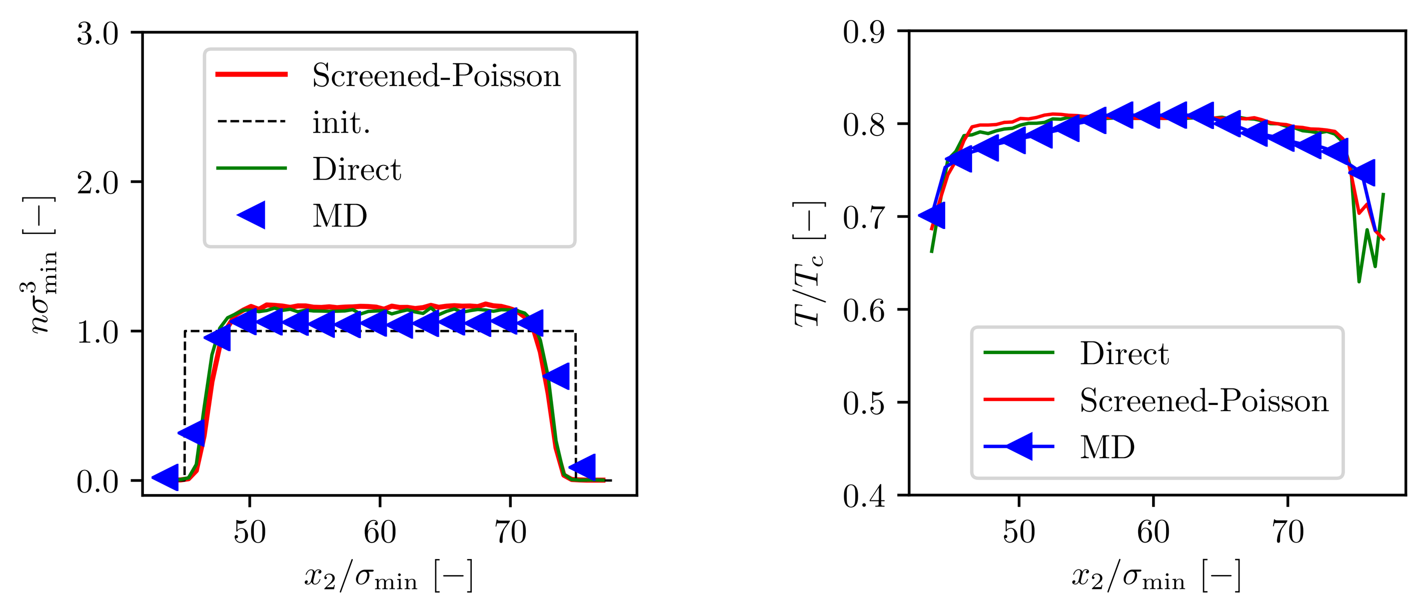

Figure 4: Normalized density and temperature profiles for the **evaporation** of liquid argon to vacuum at $T_{\text{initial}} = 0.8\ T_c$. Here, ESMC [2] is used to solve the collision operator while the the Vlasov integral is computed using the direct method and screened-Poisson model [4], respectively. Furthermore, good agreement with Molecular Dynamics (MD) result is observed. Note that $T_c = 124.1367$ K and $\sigma_{\min} = 2^{1/6}\sigma$.

References

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