# 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 $\lambda$ are obtained from

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

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

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

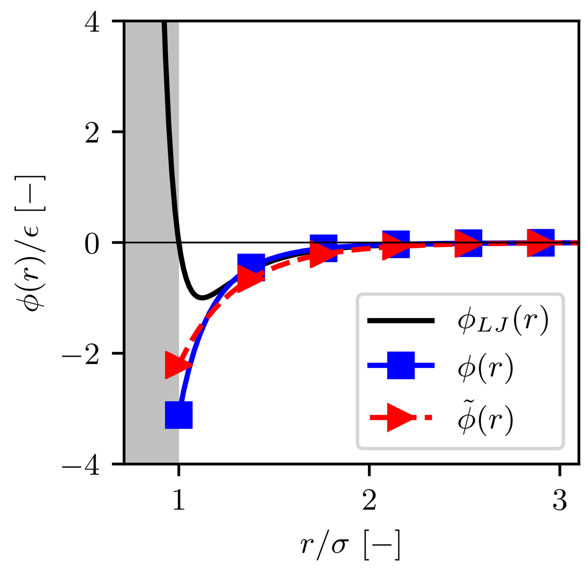

Figure 1: Lennrad-Jones molecular potential $\phi_{LJ}(r)$ along with Sutherland $\phi(r)$ and the Coulomb-type potential $\tilde{\phi}(r)$ for Argon with $\epsilon=119.8k_b$ and $\sigma=3.405\times10^{-10}\text{m}$.

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

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

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

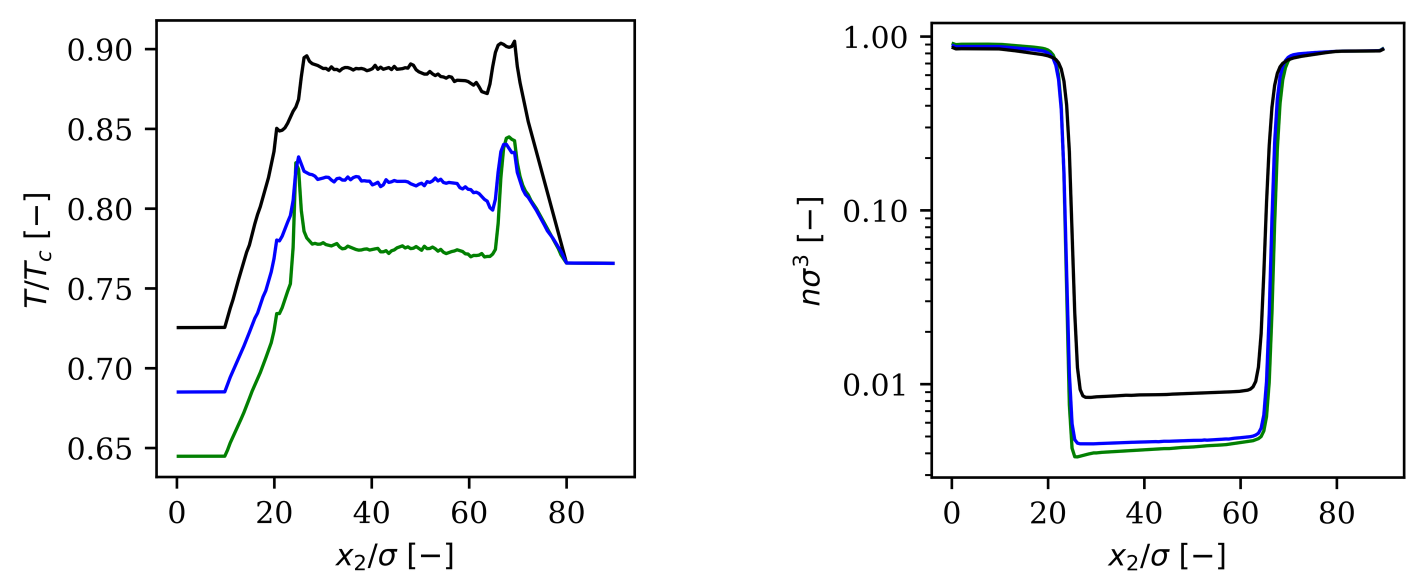

Figure 2: Normalized profiles of temperature and number density of two droplets and the vapour between obtained via DFP-SP model where $T_{\text{hot}}=95$ K while $T_{\text{cold}}=80,\ 85$ and $90$ K.

## 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

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

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

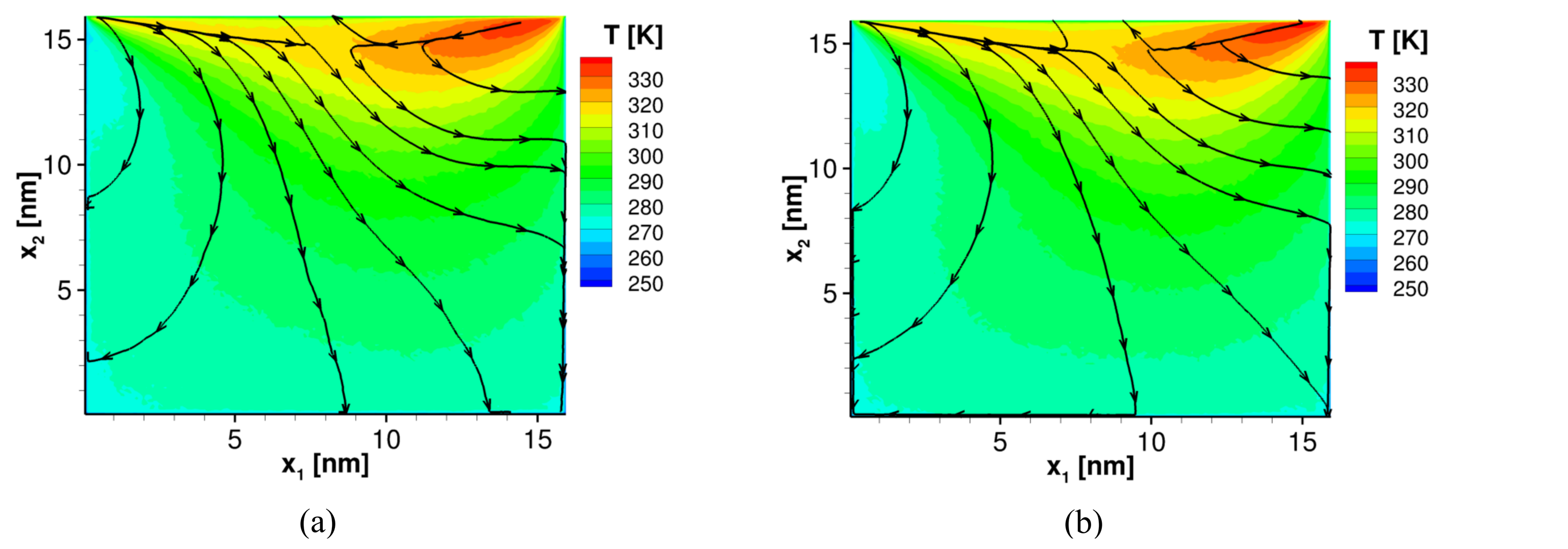

Figure 3: Temperature contours along with heat fluxes of a **lid-driven cavity** flow with wall velocity of 300 m/s at $\text{Kn}=0.1$ using (a) DFP model and (b) Enskog Simulation Monte Carlo (ESMC) method [2].

IV.b Evaporation

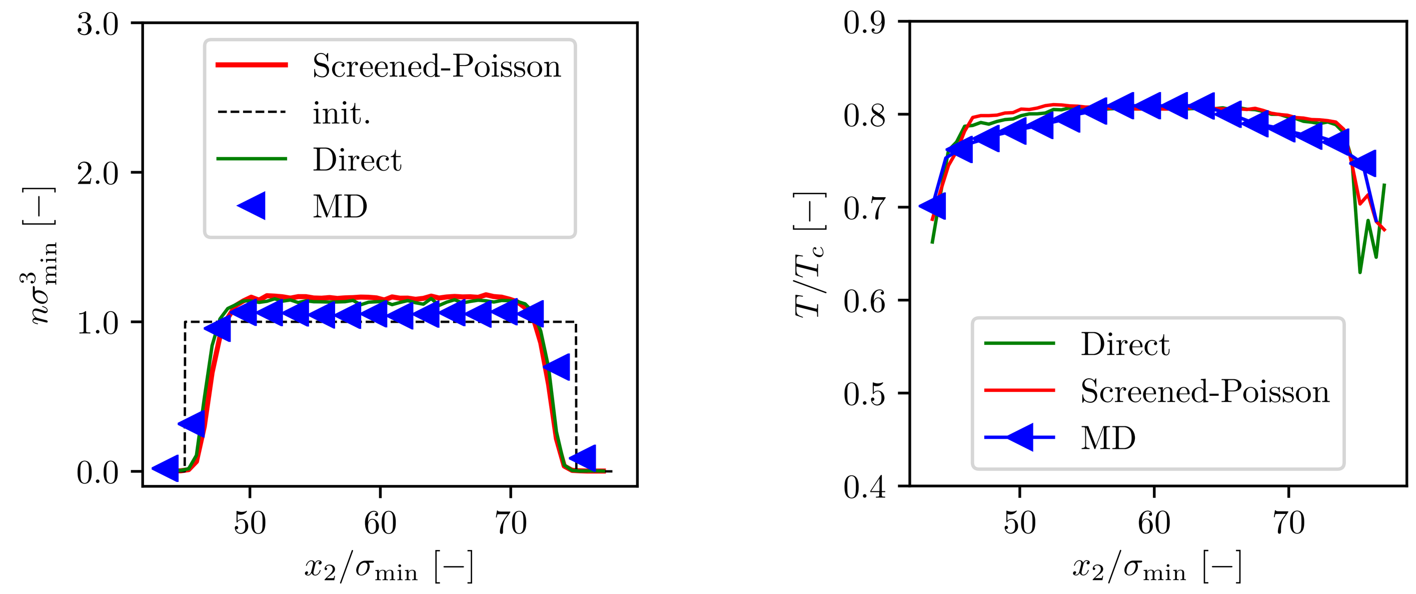

Figure 4: Normalized density and temperature profiles for the **evaporation** of liquid argon to vacuum at $T_{\text{initial}}=0.8\ T_c$. Here, ESMC [2] is used to solve the collision operator while the the Vlasov integral is computed using the direct method and screened-Poisson model [4], respectively.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

## References

[1] A Frezzotti, L Gibelli, & LS Lorenzani, Phys. Fluids , Vol. 17, (2005).
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