

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

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

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

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

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 $U(\mathbf{x}, t)$ as

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

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

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

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.

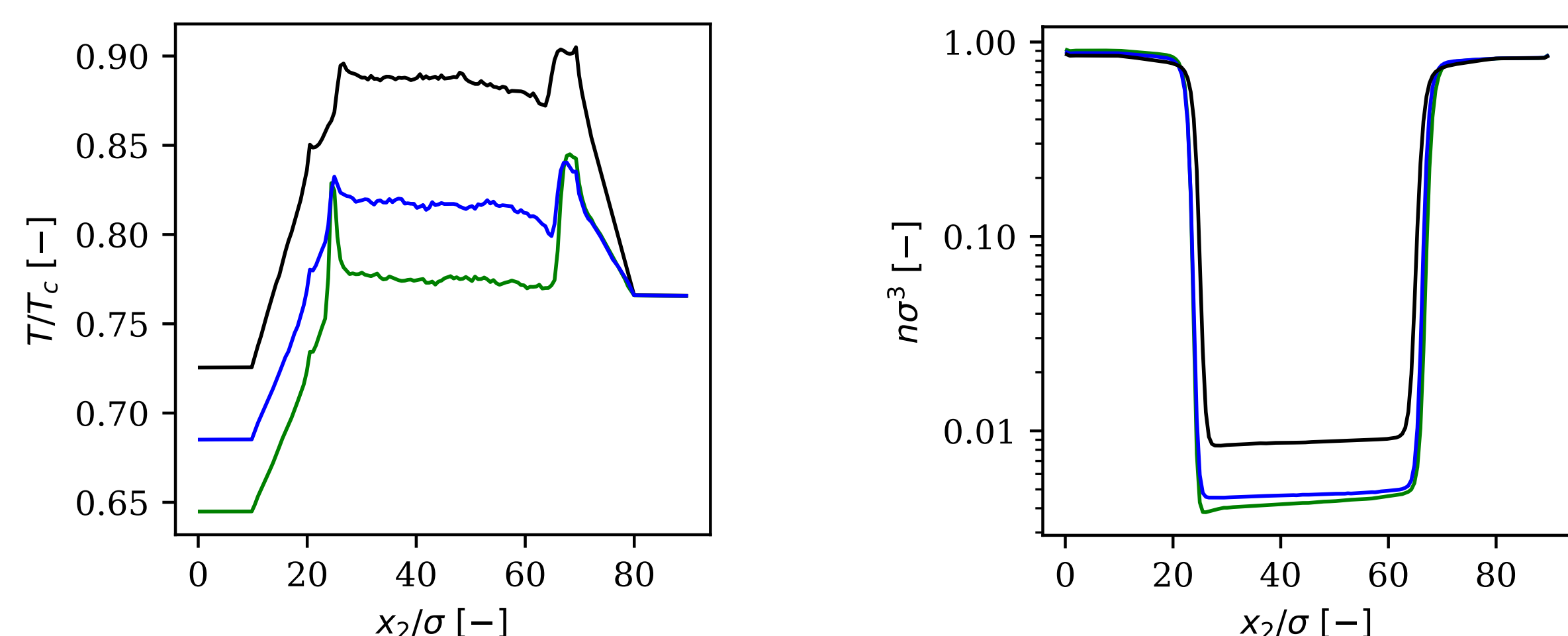


Figure 2: Normalized profiles of temperature and number density of two droplets and the vapour between obtained via DFP-SP model where $T_{\text{hot}} = 95$ K while $T_{\text{cold}} = 80, 85$ and 90 K.

III. Fokker-Planck model for dense gases

- IDEA:
 - i. Approximate jump process with a continuous one.
 needed \rightarrow **relaxation rates**
 - ii. Include dense effects with spatial drift.
 needed \rightarrow **collisional transfer**

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

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

ii. **Collisional transfer** Ψ^ϕ appearing in the velocity moments of Enskog equation

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

has explicit form up to second order term.

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

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

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

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

Efficient particle methods for the equivalent SDEs can be used.

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

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

IV. Results

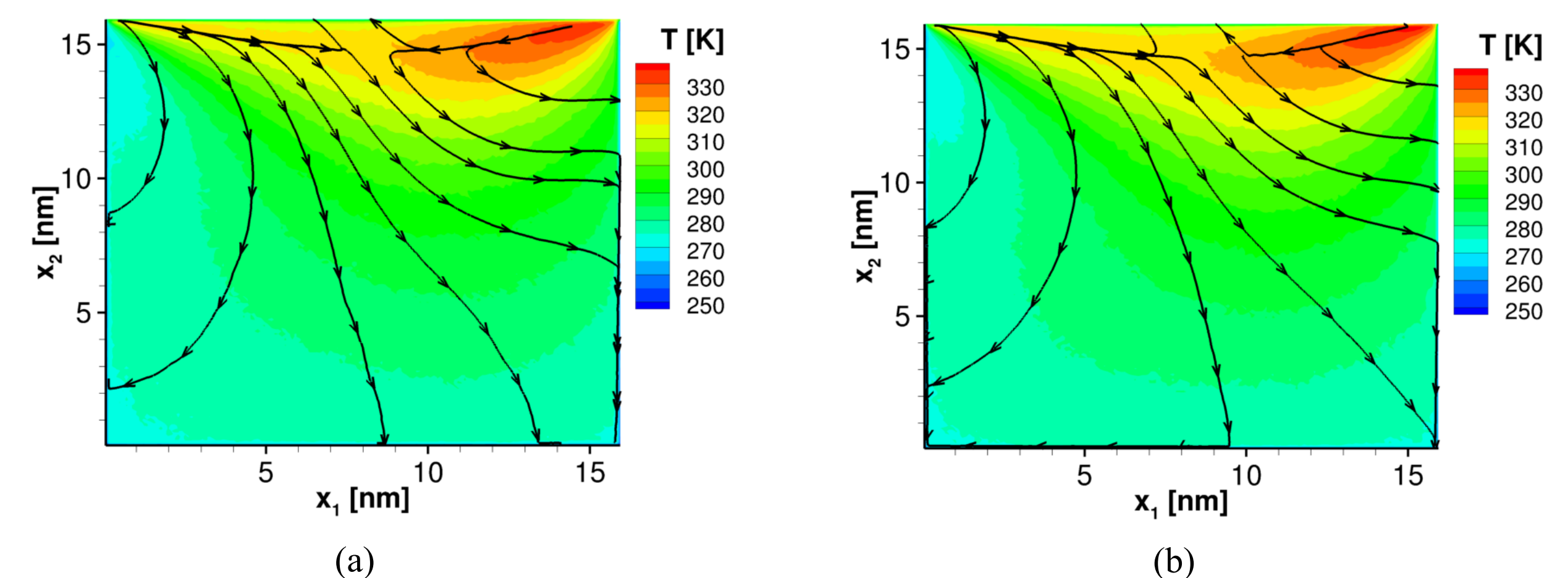


Figure 3: Temperature contours along with heat fluxes of a **lid-driven cavity** flow with wall velocity of 300 m/s at $Kn = 0.1$ using (a) DFP model and (b) Enskog Simulation Monte Carlo (ESMC) method [2].

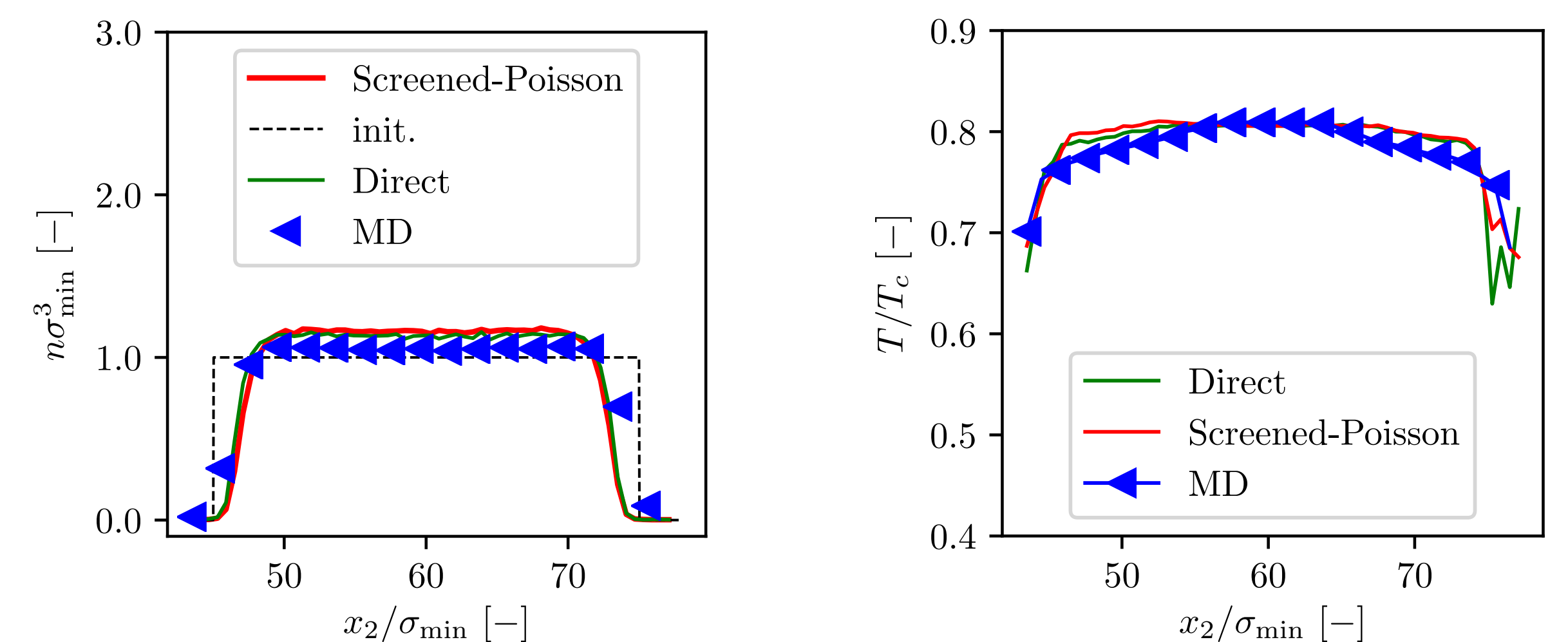


Figure 4: Normalized density and temperature profiles for the **evaporation** of liquid argon to vacuum at $T_{\text{initial}} = 0.8 T_c$. Here, ESMC [2] is used to solve the collision operator while the the Vlasov integral is computed using the direct method and screened-Poisson model [4], respectively. 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

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- [2] JM Montanero & A Santos, Phys. Rev. E Vol. 54 (1996).
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