Efficient Monte Carlo description of multi-phase and multi-scale fluid flows in kinetic theory

Mohsen Sadr

PhD candidate, Applied and Computational Mathematics, RWTH Aachen, Germany

Advisors: Dr. Hossein Gorji (EPFL)
       Prof. Manuel Torrilhon (RWTH Aachen)

June 25, 2020
Kinetic description of multi-phase fluid flows
Dilute vs. dense gases

Dilute

Point particle:

**Boltzmann** collision operator
Dilute .vs. dense gases

**Dilute**

Point particle: **Boltzmann** collision operator

**Dense**

Particles with Sutherland potential: **Enskog** collision operator
+ **attraction** (long-range)
Ideal gas (Boltzmann equation)

Assuming molecular chaos and point particles, Boltzmann derived an evolution equation for single-particle molecular velocity distribution of monatomic gas, i.e.

\[
\frac{\partial F}{\partial t} + \frac{\partial (Fv_i)}{\partial x_i} = S^{Boltz}(F), \tag{1.1}
\]

where

\[
S^{Boltz}(F) = \frac{1}{m} \int \int \int \left[ F(v^*,x)F(v_1^*,x) - F(v,x)F(v_1,x) \right] g\hat{b}d\hat{b}d\hat{\epsilon}d^3v_1. \tag{1.2}
\]

- $\hat{b} \in [0, \infty)$ and $\hat{\epsilon} \in [0, 2\pi)$ are impact parameters.
- Specifics of $g\hat{b}d\hat{b}$ are determined by the molecular potential.
- $(.)^*$ indicates post-collision state.
Kinetic equation for dense gases (Enskog eq.)

Enskog extended Boltzmann equation to dense regime

$$\frac{\partial F}{\partial t} + \frac{\partial (Fv_i)}{\partial x_i} = S_{\text{Ensk}},$$

by including diameter of hard sphere particles in the collision operator

$$S_{\text{Ensk}}(F) = \frac{1}{m} \int \int \int \left[ Y(x + \frac{1}{2} \sigma \hat{k})F(v^*, x)F(v_1^*, x + \sigma \hat{k}) 
\right.
\left. - Y(x - \frac{1}{2} \sigma \hat{k})F(v, x)F(v_1, x - \sigma \hat{k}) \right] gH(g \cdot \hat{k})bd\hat{d}d\hat{e}d^3v_1.$$

- $\sigma$: effective diameter of particles.
- $Y$: pair correlation function.
- $H(.)$: Heaviside step function.
Kinetic equation for dense gases (Enskog eq.)

Enskog extended Boltzmann equation to dense regime

\[
\frac{\partial F}{\partial t} + \frac{\partial (Fv_i)}{\partial x_i} = S^{\text{Ensk}},
\]

(1.3)

by including diameter of hard sphere particles in the collision operator

\[
S^{\text{Ensk}}(F) = \frac{1}{m} \int \int \int \int \left[ Y(x + \frac{1}{2} \sigma \hat{k})F(v^*, x)F(v^*_1, x + \sigma \hat{k}) - Y(x - \frac{1}{2} \sigma \hat{k})F(v, x)F(v_1, x - \sigma \hat{k}) \right] g\mathcal{H}(g \cdot \hat{k})\hat{b}d\hat{b}d\hat{\epsilon}d^3v_1.
\]

- \(\sigma\): effective diameter of particles.
- \(Y\): pair correlation function.
- \(\mathcal{H}(.)\): Heaviside step function.

For hard-sphere \(g\hat{b}d\hat{b}d\hat{\epsilon} = (g \cdot \hat{k})dA_{\partial B(x, \sigma)}\),
\[
\hat{b} = \sigma \cos(\chi/2) \text{ and } \chi \in [0, \pi).
\]
Including long-range interactions (Enskog-Vlasov eq.)

Conservative attractive forces are included in the kinetic equation

\[
\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F} v_i)}{\partial x_i} - H_i \frac{\partial \mathcal{F}}{\partial v_i} = S^{\text{Ensk}}(\mathcal{F})
\]

where

\[
H_i(x, t) = \frac{1}{m} \frac{\partial \eta(x, t)}{\partial x_i}, \quad \text{and} \quad (1.4)
\]

\[
\eta(x, t) = \int_{r > \sigma} \phi(r) n(y, t) d^3y, \quad (1.5)
\]

with Sutherland molecular potential for particles at distance \(r := |y - x|\)

\[
\phi(r) = \begin{cases} 
+\infty & r < \sigma, \\
-\epsilon \left(\frac{\sigma}{r}\right)^6 & r \geq \sigma.
\end{cases} \quad (1.6)
\]
Computational complexity of Enskog-Vlasov eq.

- Curse of high dimensionality (similar to Boltzmann eq.).
- Non-local collision operator.
- Numerical cost of $O(N_{\text{cells}} N_{\text{quad}})$ in evaluation of Vlasov integral.

Using direct Monte Carlo methods that resolve high-dim. lead to
- $O(N_p n \sqrt{T})$ collisions, once collision scale is resolved.
- outside cell collisions which prevents cell-based parallelization.
- cost of long-range interaction remains $O(N_{\text{cells}} N_{\text{quad}} + N_p)$.

Here, cost analysis of Monte Carlo method does not include the statistical errors.
Computational complexity of Enskog-Vlasov eq.

- Curse of high dimensionality (similar to Boltzmann eq.).
- Non-local collision operator.
- Numerical cost of $O(N_{\text{cells}} N_{\text{quad}})$ in evaluation of Vlasov integral.

Using direct Monte Carlo methods that resolve high-dim. lead to
- $O(N_p n \sqrt{T})$ collisions, once collision scale is resolved.
- outside cell collisions which prevents cell-based parallelization.
- cost of long-range interaction remains $O(N_{\text{cells}} N_{\text{quad}} + N_p)$.

Objective

Devising a Fokker-Planck-Poisson model as an approximation to Enskog-Vlasov eq. to cope with above mentioned challenges.

Here, cost analysis of Monte Carlo method does not include the statistical errors.
A Fokker-Planck model for short-range interactions
Let us assume that the underlying jump process of collision operator can be approximated with a continuous one

\[
\begin{align*}
\begin{cases}
    dV_i &= A_i dt + D dW_{t,i} & \text{and} \\
    dX_i &= V_i dt,
\end{cases}
\end{align*}
\]

where \( dW_{t,i} := W_i(t + dt) - W_i(t) \) and \( dW_{t,i} \sim \mathcal{N}(0, dt) \).

Using Itô’s lemma, a Fokker-Planck equation can be derived

\[
\frac{\partial F}{\partial t} + \frac{\partial (F v_i)}{\partial x_i} = -\frac{\partial (F A_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 F)}{\partial v_i \partial v_i}.
\]

see Jenny, Torrilhon & Heinz (2010) [1].
Let us assume that the underlying jump process of collision operator can be approximated with a continuous one

\[
\begin{aligned}
    dV_i &= A_i dt + D dW_{t,i} \quad \text{and} \\
    dX_i &= V_i dt,
\end{aligned}
\]

where \(dW_{t,i} := W_i(t + dt) - W_i(t)\) and \(dW_{t,i} \sim \mathcal{N}(0, dt)\).

Using Itô’s lemma, a Fokker-Planck equation can be derived

\[
\frac{\partial F}{\partial t} + \frac{\partial (F v_i)}{\partial x_i} = - \frac{\partial (F A_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 F)}{\partial v_i \partial v_i}.
\] (1.8)

**Task**

Model drift \(A\) and diffusion \(D\) such that FP model follows collision operator up to a desired degree of moments.

---

see Jenny, Torrilhon & Heinz (2010) [1].
Velocity moments $\psi = [1, v_i, \frac{1}{2} v_j v_j]$ of Fokker-Planck equation

$$\frac{\partial F}{\partial t} + \frac{\partial (F v_i)}{\partial x_i} = -\frac{\partial (FA_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 F)}{\partial v_i \partial v_i}$$

immediately provides us conservation laws

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_j)}{\partial x_j} = 0,$$  \hspace{1cm} (1.9)

$$\frac{\partial (\rho U_i)}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho U_i U_j + \int v'_i v'_j F d^3 v \right) = 0 \quad \text{and} \quad (1.10)$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \left( EU_j + \frac{1}{2} \int v'_j v'_k v'_k F d^3 v + U_k \int v'_j v'_k F d^3 v \right) = 0,$$  \hspace{1cm} (1.11)

as far as $\int \psi_l \left[ -\frac{\partial (FA_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 F)}{\partial v_i \partial v_i} \right] d^3 v = 0$. 

Mohsen Sadr
MathCCES, RWTH Aachen University
June 25, 2020
Velocity moments $\psi = [1, v_i, \frac{1}{2} v_j v_j]$ of Fokker-Planck equation

$$\frac{\partial F}{\partial t} + \frac{\partial (F v_i)}{\partial x_i} = - \frac{\partial (FA_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 F)}{\partial v_i \partial v_i}$$

immediately provides us conservation laws

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_j)}{\partial x_j} = 0,$$  \hspace{1cm} (1.9)

$$\frac{\partial (\rho U_i)}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho U_i U_j + \int v'_i v'_j F d^3 v \right) = 0 \quad \text{and}$$  \hspace{1cm} (1.10)

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} \left( EU_j + \frac{1}{2} \int v'_i v'_k v'_k F d^3 v + U_k \int v'_j v'_k F d^3 v \right) = 0,$$  \hspace{1cm} (1.11)

as far as $\int \psi_l \left[ -\frac{\partial (FA_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 F)}{\partial v_i \partial v_i} \right] d^3 v = 0.$

Q?

How pressure tensor and heat flux relax because of collision?
Step 1: fixing relaxation rates

First, let us fix the rate at which non-advective fluxes relax. Hence, we should make sure that drifts and diffusion in

\[ S_{FP} = -\frac{\partial (FA_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 \mathcal{F})}{\partial v_i \partial v_i} \quad (1.12) \]

guarantee that

\[ \int_{\mathbb{R}^3} v'_i v'_j S_{FP} (\mathcal{F}) d^3 v = \int_{\mathbb{R}^3} v'_i v'_j S_{Ensk} (\mathcal{F}) d^3 v \quad \text{and} \quad (1.13) \]
\[ \int_{\mathbb{R}^3} v'_i v'_j v'_j S_{FP} (\mathcal{F}) d^3 v = \int_{\mathbb{R}^3} v'_i v'_j v'_j S_{Ensk} (\mathcal{F}) d^3 v. \quad (1.14) \]

If spatial dependency of \( S_{Ensk} \) is ignored, i.e. considering decomposition

\[ S_{Ensk} = Y S^{Boltz} + S_\phi \quad (1.15) \]

where \( S_\phi \) includes all spatial dependencies, explicit expressions for the right hand side can be obtained.
One can fix the relaxation rates of $S^{FP}$ with the ones from $S^{Ensk}$ in homogeneous setting, i.e. considering $S_\phi = 0$,

$$
\int_{\mathbb{R}^3} \left( A_i v'_j + A_j v'_i - \frac{2}{3} A_k v'_k \delta_{ij} + \frac{2}{3} \delta_{ij} D^2 \right) \mathcal{F} d^3 v = -Y \frac{p^{\text{kin}}}{\mu^{\text{kin}}} \pi^{\text{kin}}_{ij}, \quad (1.16)
$$

$$
\int_{\mathbb{R}^3} (A_i v'_j v'_j + 2 A_j v'_j v'_i) \mathcal{F} d^3 v = -Y \frac{2}{3} \frac{p^{\text{kin}}}{\mu^{\text{kin}}} q^{\text{kin}}_i. \quad (1.17)
$$

Next, we bring in spatial dependency of operator by modeling collisional transport of Enskog operator.

---

Here, $v' = v - \int v \mathcal{F} d^3 v / \rho$ is the fluctuating velocity, $p^{\text{kin}}$ kinetic equilibrium pressure, $q^{\text{kin}}$ kinetic heat flux, $\pi^{\text{kin}}$ kinetic stress tensor and $\mu^{\text{kin}}$ is the kinetic viscosity coefficient.
Step 2: fixing collisional transport

Hard spheres admit transfer of $\psi = [v_i, \frac{1}{2} v_j v_j]^T$ during collision, i.e.,

$$\int \psi_l S_{\text{Ensk}}(F) d^3 v \neq 0 \quad \text{for } l = 1, \ldots, \text{dim}(\psi).$$

(1.18)

In fact, it can be shown that

$$\int \psi_l S_{\text{Ensk}}(F) d^3 v = \frac{\sigma^3 Y}{2m} \frac{\partial \psi^\phi_{lk}}{\partial x_k} \bigg|_{h=\sigma/2}$$

where

(1.19)

$$\psi^\phi_{lk}(x, h) = \int \int \int (\psi^* - \psi_l) F(x + h \hat{k}) F_1(x - h \hat{k}) \hat{k}_k (g \cdot \hat{k}) \mathcal{H}(g \cdot \hat{k}) d^2 \hat{k} d^3 v_1 d^3 v.$$

Using first order Taylor expansion around $x$, considering $\partial_x F \sim \partial_x F_{\text{Max}}$, the flux can be estimated in terms of moments.

The flux nature of collisional transfer motivates introducing spatial drift.
Consider the FP model

\[ S_{DFP} = -\frac{\partial (FA_i)}{\partial v_i} + \frac{1}{2} \frac{\partial^2 (D^2 F)}{\partial v_i \partial v_i} - \frac{\partial (F \hat{A}_i)}{\partial x_i} \]  \hspace{1cm} (1.20)

where spatial drift \( \hat{A} \) can provide us with the collisional transfer, i.e.,

\[ \int_{\mathbb{R}^3} \hat{A}_i F d^3 v = 0, \]  \hspace{1cm} (1.21)

\[ \int_{\mathbb{R}^3} \hat{A}_i v_j F d^3 v = nbY(p^{\text{kin}} \delta_{ij} + 2/5 \pi^{\text{kin}}_{ij}) - w\left(\frac{\partial U_k}{\partial x_k} \delta_{ij} + \frac{5}{6} \frac{\partial U_{\langle i}}{\partial x_j}\right), \]  \hspace{1cm} (1.22)

\[ \frac{1}{2} \int_{\mathbb{R}^3} \hat{A}_i v_j v_j F d^3 v = \frac{3}{5} nbYq_i^{\text{kin}} - c_v w \frac{\partial T}{\partial x_i}. \]  \hspace{1cm} (1.23)

Now, all it remains is devising an ansatz for \( A, \hat{A} \) and \( D \), substituting them in the closures Eqs. (1.16)-(1.17) as well as Eqs (1.21)-(1.23), and finding the free parameters of the ansatz.
Consider the ansatz

\[ A_i = c_{ij} v_j' + \gamma_i \left( v_j' v_j' - \frac{3 k_b T}{m} \right) + \Lambda \left( \frac{v_i' v_j' v_j' - 2 q_{i \text{kin}}}{\rho} \right), \quad (1.24) \]

\[ D = \sqrt{\frac{k_b T}{\tau m}} \quad (1.25) \]

and

\[ \hat{A}_i = \hat{c}_{ij} v_j' + \hat{\gamma}_i \left( v_j' v_j' - \frac{3 k_b T}{m} \right) + \hat{\Lambda} \left( \frac{v_i' v_j' v_j' - 2 q_{i \text{kin}}}{\rho} \right). \quad (1.26) \]

The cubic terms make sure of stability of SDEs with their coeff. set to

\[ \Lambda = -\left| \frac{\text{det}(u_{ij})}{(u^{(2)})^4} \right| \quad \text{and} \quad \hat{\Lambda} = -\epsilon \frac{nb Y}{k_b T / m}. \quad (1.27) \]

Here \( \epsilon = 10^{-3} \), \( \text{det}(\cdot) \) indicates the determinant and

\[ u_{i_1...i_n}^{(k)} := \frac{1}{\rho} \int_{\mathbb{R}^3} |v'\rangle^k v_{i_1}' v_{i_2}' ... v_{i_n}' \mathcal{F} d^3 v ; \quad i_k \in \{1, 2, 3\}. \quad (1.28) \]
Computing coeff. of $A$ and $\hat{A}$

Substituting the Ansatz back in closure equations, we obtain

\[
    c_{ik} u_{kj}^{(0)} + c_{jk} u_{ki}^{(0)} + \gamma_i u_j^{(2)} + \gamma_j u_i^{(2)} = -2\Lambda u_{ij}^{(2)} \quad \text{and} \quad \tag{1.29}
\]

\[
    c_{ij} u_j^{(2)} + 2 c_{jk} u_{ijk}^{(0)} + \gamma_i (u^{(4)} - (u^{(2)})^2) + 2 \gamma_j (u_{ij}^{(2)} - u^{(2)} u_{ij}) \\
    = -\Lambda (3 u_i^{(4)} - u_i^{(2)} u^{(2)} - 2 u_j^{(2)} u_{ij}^{(0)}) + \frac{5}{6} \frac{Y_{p}^{\text{kin}}}{\mu^{\text{kin}}} q_i^{\text{kin}}, \tag{1.30}
\]

which fixes relaxation rates and equivalently for $\hat{A}$ (coll. transfer) we get

\[
    \hat{c}_{jk} \pi_{ik}^{\text{kin}} + \hat{c}_{ji} p^{\text{kin}} + 2 \hat{\gamma}_j q_i^{\text{kin}} = -\rho \hat{\Lambda} u_{ij}^{(2)} \\
    + nb Y (p^{\text{kin}} \delta_{ij} + 2/5 \pi_{ij}^{\text{kin}}) - w \left( \frac{\partial U_k}{\partial x_k} \delta_{ij} + \frac{5}{6} \frac{\partial U_{\langle i}}{\partial x_j} \right) \quad \text{and} \quad \tag{1.31}
\]

\[
    \hat{c}_{ij} q_j^{\text{kin}} + \frac{1}{2} \rho \hat{\gamma}_i (u^{(4)} - (u^{(2)})^2) = \frac{3}{5} nb Y q_i^{\text{kin}} - wc_v \frac{\partial T}{\partial x_i} - \frac{1}{2} \rho \hat{\Lambda} (u_i^{(4)} - u_i^{(2)} u^{(2)}) \tag{1.32}
\]
A screened-Poisson model for long-range interactions
Conservative attractive forces are included in the kinetic equation

\[
\frac{\partial F}{\partial t} + \frac{\partial (Fv_i)}{\partial x_i} - H_i \frac{\partial F}{\partial v_i} = S_{\text{Ensk}}(F)
\]

where

\[
H_i(x, t) = \frac{1}{m} \frac{\partial \eta(x, t)}{\partial x_i}, \quad \text{and} \quad (2.1)
\]

\[
\eta(x, t) = \int_{r>\sigma} \phi(r) n(y, t) d^3y, \quad (2.2)
\]

with Sutherland molecular potential for particles at distance \( r := |y - x| \)

\[
\phi(r) = \begin{cases} 
+\infty & r < \sigma, \\
-\epsilon \left(\frac{\sigma}{r}\right)^6 & r \geq \sigma.
\end{cases} \quad (2.3)
\]
A screened-Poisson model for long-range interactions

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

$$(a, \lambda) = \arg\min_{r \in (\sigma, \infty)} \left( \| \partial_r \phi(r) - \partial_r \tilde{\phi}(r) \|_2^2 \right).$$

Then, rewrite

$$\eta(x, t) \approx a \int_{r > \sigma} G(r)n(y, t) d^3y$$

$$= a \int_{r > 0} G(r)n(y, t) d^3y - a \int_{r < \sigma} G(r)n(y, t) d^3y,$$

where

$$\left( \Delta - \lambda^2 \right) \tilde{n}(x, t) = n(x, t); \quad (\forall x \in \mathbb{R}^3).$$
Screened-Poisson model for long-range interactions

- For simulations in a bounded domain of $\Omega$, Poisson solver can be used to solve

$$
(\Delta - \lambda^2) \tilde{\eta}(x, t) = n(x, t) \quad (\forall x \in \Omega) \quad \text{and} \quad (2.8)
$$
$$
\tilde{\eta}(y, t) = g(y, t) \quad (\forall y \in \partial \Omega), \quad (2.9)
$$

where $g$ is the Dirichlet boundary condition computed directly.

- The second integral can be approximated via

$$
\hat{\eta}_{r<\sigma}(x, t) = \int_{r<\sigma} G(|x - y|)n(y, t)d^3y
$$
$$
= \int_{|y|<\sigma} G(|y|)n(x - y, t)d^3y. \quad (2.10)
$$

Assuming regularity for $n$

$$
\hat{\eta}_{r<\sigma}(x, t) \approx n(x, t) \int_{|y|<\sigma} G(|y|)d^3y + \frac{1}{2} \frac{\partial^2 n(x, t)}{\partial x_j \partial x_j} \int_{|y|<\sigma} G(|y|)y_jy_j d^3y. \quad \text{analytical expr.}
$$
A Monte Carlo solution algorithm for Fokker-Planck-Poisson model
Solution algorithm for Fokker-Planck-Poisson model

Initialize samples of $X$ and $V$;

while $t < t_{\text{final}}$ do

    Estimate moments in each cell using samples;
    Solve SP eq. and estimate attractive forces $H_i = \partial \eta / \partial x_i$ at $X$;
    Compute $A$, $\hat{A}$ and $D$ in each cell;
    Solve $dV = Adt + DdW_t$ numerically for short-range interactions;
    Incorporate attractive forces by $V \leftarrow V + H \Delta t$;
    $X \leftarrow X + (V + \hat{A}) \Delta t$;
    Apply boundary conditions;
    Increment $t$;

end
Solution algorithm for Fokker-Planck-Poisson model

Initialize samples of $X$ and $V$;

\begin{verbatim}
while $t < t_{\text{final}}$ do
    Estimate moments in each cell using samples;
    Solve SP eq. and estimate attractive forces $H_i = \partial \eta / \partial x_i$ at $X$;
    Compute $A$, $\hat{A}$ and $D$ in each cell;
    Solve $dV = Adt + DdW_t$ numerically for short-range interactions;
    Incorporate attractive forces by $V \leftarrow V + H\Delta t$;
    $X \leftarrow X + (V + \hat{A})\Delta t$;
    Apply boundary conditions;
    Increment $t$;
end
\end{verbatim}

\textbf{cost of short-range interaction} $\sim \mathcal{O}(N_p)$

\textbf{cost of long-range interaction} $\sim \mathcal{O}(N_c \log(N_c) + N_p)$
**Figure:** Initial density and temperature are picked from stable region of phase diagram. Particles leaving the domain are reinitialized inside the liquid to obtain a constant mass flux in the system. Furthermore, the liquid is thermostated to maintain a desired temperature.
Evaporation of liquid Argon to vacuum

Mohsen Sadr
MathCCES, RWTH Aachen University
June 25, 2020
Inverted Temperature Gradient (1D): setup

Figure: Initial density and temperature are picked from stable region of phase diagram. Here, walls are fully diffusive and liquid phase is thermostated to maintain a desired temperature.
Inverted Temperature Gradient (1D)

\[ n\sigma^3 \] vs. \( x_2/\sigma \)

\[ T \text{ [K]} \] vs. \( x_2/\sigma \)

\[ U_2/\sqrt{(k_bT_c)/m} \] vs. \( x_2/\sigma \)

\[ \frac{q_{\text{kin}}}{\rho_e(k_bT_c/m)^{3/2}} \] vs. \( x_2/\sigma \)

Mohsen Sadr
MathCCES, RWTH Aachen University
June 25, 2020 22 / 29
Inverted Temperature Gradient (1D)

3.5 × 10^6 particles, 140 spatial cells, ×3.1 speed-up, \( \frac{||E[n_{DFP-SP}] - E[n_{EV}]||_2}{||E[n_{EV}]||_2} \approx 0.053 \)

Mohsen Sadr
MathCCES, RWTH Aachen University
June 25, 2020 22 / 29
Figure: Initial density and temperature of each phase is chosen within stable region of the phase diagram for Argon. Here, specular walls are deployed and no thermostat is used.
Argon droplet in equilibrium (2D)
Argon droplet in equilibrium (2D)

DFP-SP  Enskog-Vlasov

DFP-SP  Enskog-Vlasov

Mohsen Sadr  MathCCES, RWTH Aachen University  June 25, 2020  24 / 29
Argon droplet in equilibrium (2D)

DFP-SP  
Enskog-Vlasov

$\rho$ [\(\sigma\)]

$T$ [K]

$t = 0.187$ [ps]

Mohsen Sadr  
MathCCES, RWTH Aachen University  
June 25, 2020
Argon droplet in equilibrium (2D)

DFP-SP
Enskog-Vlasov

$\rho \sigma$ [-]

$t = 0.560 \text{ [ps]}$

DFP-SP
Enskog-Vlasov

$x/\sigma$ [-]

$T \text{ [K]}$

$n \sigma^3$ [-]

DFP-SP
Enskog-Vlasov

$t = 0.560 \text{ [ps]}$
Argon droplet in equilibrium (2D)

DFP-SP vs. Enskog-Vlasov

$\text{DFP-SP}$ $\text{Enskog-Vlasov}$

$\begin{array}{c}
t = 1.866 \text{[ps]} \\
T [K]
\end{array}$

$\begin{array}{c}
x_0/\sigma [-] \\
\rho [\text{a}^3]
\end{array}$

$t = 1.866 \text{[ps]}$
Argon droplet in equilibrium (2D)

$2 \times 10^6$ particles, $40 \times 40$ spatial grid, $\times 9.5$ speed-up, $\frac{\|E[n_{DFP-SP}] - E[n_{EV}]\|_2}{\|E[n_{EV}]\|_2} \approx 0.031$
Collaboration with Marcel Pfeiffer, University of Stuttgart
finalized during lockdown due to Coronavirus
Figure: Initial density and temperature are picked from an unstable region of phase diagram for Argon (enclosed by the green curve). Specular walls are considered here and no thermostat is used.
Spinodal decomposition (droplet formation)

Above-figures show the evolution of density for the spinodal decomposition of Argon. The results are obtained in collaboration with Marcel Pfeffer at the University of Stuttgart using their in-house code called PICLas.
Spinodal decomposition (droplet formation)

\[ T_0 = 120 \text{ [K]}, \ n_0 = 5 \times 10^{27} \text{ [m}^{-3}], \ N_p = 1.5 \times 10^8 \ & 250 \times 250 \text{ cells} \]

Above-figures show the evolution of density for the spinodal decomposition of Argon. The results are obtained in collaboration with Marcel Pfeiffer at the University of Stuttgart using their in-house code called PICLas.

4 days execution time using 40 cores
Spinodal decomposition (bubble formation)

Above-figures show the evolution of density for the spinodal decomposition of Argon. The results are obtained in collaboration with Marcel Pfieffer at the University of Stuttgart using their in-house code called PICLas.
Spinodal decomposition (bubble formation)

\[ T_0 = 120 \text{ [K]}, \ n_0 = 8 \times 10^{27} \text{ [m}^{-3}\text{]}, \ N_p = 1.5 \times 10^8 \ & 250 \times 250 \text{ cells} \]

Above-figures show the evolution of density for the spinodal decomposition of Argon. The results are obtained in collaboration with Marcel Pfieffer at the University of Stuttgart using their in-house code called PICLas.

4 days execution time using 40 cores
Published works:


Papers in review:


**Thanks for your attention**
Collision cross section, maxwell mol, Y factor

FP for ideal gas

FP for dense gas
  - How numerics of DFP is obtained?

Vlasov mean field limit, Screened-Poisson
  - FMM
  - Attractive pressure

Analysis of phase transition, phase diagram, scales

Incompressible limit of dense fluids

Multi-Scale Fluid Flows

SDEs
  - Conv rate, def.
  - Wagner-Platen expansion
  - Ito’s lemma
  - Deriving FP from SDE
  - Existence and uniqueness of SDEs
  - Regularity of FP

MLMC

Central limit and Girsanov theorems
Impact parameters (Bird [2])

In general, $\epsilon \in [0, 2\pi)$, $\chi \in [0, \pi)$ and $b \in [0, \infty)$. The colliding pair lies in the volume $(gdt)(bdbd\epsilon)$. 

Fig. 2.3 Illustration of the impact parameters.
For molecular potential of $\phi(r) = \frac{\kappa}{r^{\eta-1}}$, the collision cross section is

$$g \hat{b} d \hat{b} d \hat{\epsilon} = W_0 (\kappa/mg^2)^{2/\eta-1} dW_0 d\hat{\epsilon} \quad (3.1)$$

$$W_0 = \hat{b}(mg/\kappa)^{1/(\eta-1)} \quad (3.2)$$

Note that $\int g \hat{b} d \hat{b} d \hat{\epsilon}$ diverges for any choice of $\eta$. However, introducing cut-off for $W_0$

$$\int_0^{2\pi} \int_0^{W_{0,max}} W_0 (\kappa/mg^2)^{2/\eta-1} dW_0 d\hat{\epsilon} = \pi W_{0,max}^2 (\kappa/mg^2)^{2/\eta-1} \quad (3.3)$$

Now if $\eta = 5$, i.e., $\phi = \kappa/r^4$, the dependency of collision operator on $g$ disappears and moments of Boltzmann can be computed analytically, see Bird [2].
Hard-sphere collision (Bird [2])

\[ b = \sigma \sin(\theta_A) = \sigma \cos(\chi/2). \]

\[ bdbdB \epsilon = \frac{\sigma^2}{4} \sin(\chi) d\chi d\epsilon. \]
The factor $Y$ (which comes form virial expansion)

$$Y := \frac{Z - 1}{nb}$$ (3.4)

for hard-sphere can be calculated exactly as done by Ree-Hoover [3]

$$Y = 1 + 0.625nb + 0.2869(nb)^2 + 0.115(nb)^3 + \ldots$$ (3.5)

or approximated by a closed expression as suggested by Carnahan-Starling [4]

$$Y^{CS} = \frac{1 - nb/8}{(1 - nb/4)^3}.$$ (3.6)
Review of Fokker-Planck model for ideal gases
In order to provide consistent relaxation rates, Cubic FP was designed by Gorji et al. (2011) [5]

\[ A_i = c_{ij}v_j' + \gamma_i \left( v_j'v_j' - \frac{3kT}{m} \right) + \Lambda \left( v_i'v_i'v_j' - \frac{2q_i}{\rho} \right), \quad (4.1) \]

\[ D_{ij} = \sqrt{\frac{2kT}{\tau m}} \delta_{ij} \quad \text{and} \quad \tau = 2\mu^\text{kin}/p, \quad (4.2) \]

where coefficients of higher order terms \( c \) and \( \gamma \) are set satisfying homogeneous relaxation rates\(^1\),

\[ \frac{\partial \pi_{ij}}{\partial t} \bigg|_{\text{col.}} = -\frac{p}{\mu} \pi_{ij} \quad \text{and} \]

\[ \frac{\partial q_i}{\partial t} \bigg|_{\text{col.}} = -\frac{2p}{3\mu} q_i. \quad (4.5) \]

---

\(^1\) see Truesdell and Muncaster (1980) [6].
Conditions on any $S_{\text{coll}}$ describing monatomic dilute gas:

- $S_{\text{coll}}$ must conserve mass, momentum an energy i.e. for any $\psi_{\text{cons}} \in \{1, v_i, v_j v_j\}$

\[
\int_{\mathbb{R}^3} \psi_{\text{cons}} S_{\text{coll}}(\mathcal{F}) d^3v = 0 \quad \text{for any } \mathcal{F}.
\] (4.6)

- Considering a homogeneous setting, the equilibrium is a Maxwellian distribution

\[
S(\mathcal{F}) = 0 \rightarrow \mathcal{F} = \mathcal{F}_M.
\] (4.7)

- In order to obtain identical transport properties

\[
\int_{\mathbb{R}^3} \psi S_{\text{model}}(\mathcal{F}) d^3v = \int_{\mathbb{R}^3} \psi S_{\text{coll}}(\mathcal{F}) d^3v,
\] (4.8)

where $\psi = \{v_i v_j, v_i v_j v_k, ..., v_{i_1} ... v_{i_M}\}$.

- Relaxation rates of the shear stress and the heat fluxes must be

\[
\left. \frac{\partial \pi_{ij}}{\partial t} \right|_{\text{col.}} = -P \frac{\pi_{ij}}{\mu} \quad \text{and}
\]

\[
\left. \frac{\partial q_i}{\partial t} \right|_{\text{col.}} = -\frac{2}{3} P \frac{q_i}{\mu}.
\] (4.9)
A Fokker-Planck model for dense gases
Let us simplify Enskog operator using the decomposition

\[ S^{\text{Ensk}} = Y(x)S^{\text{Boltz}} + S_{B}(x, \sigma) \]  \hspace{1cm} (5.1)

where \( S_{B}(x, \sigma) \) includes all derivative of \( F \) and \( Y \) in \( x \).

Relaxation rates of shear stress and heat fluxes then become

\[ \frac{\partial \pi_{ij}^{\text{kin}}}{\partial t} \bigg|_{\text{col.}} = -Y \frac{p}{\mu^{\text{kin}}} \pi_{ij}^{\text{kin}} \]  \hspace{1cm} (5.2)

and

\[ \frac{\partial q_{i}^{\text{kin}}}{\partial t} \bigg|_{\text{col.}} = -Y \frac{2}{3} \frac{p}{\mu^{\text{kin}}} q_{i}^{\text{kin}} , \]  \hspace{1cm} (5.3)

Drift and diffusion coefficients of cubic model of \( \mathcal{A} \) must satisfy this relaxation rates for dense gases.

Spatial dependence of Enskog operator needs to be modeled.
Conservation equations of Enskog equation

Taking velocity moments $\psi \in \{1, v_j, v_jv_j/2\}$ of $S^{\text{Ensk}}$

$$J = \int_{\mathbb{R}^3} \psi S^{\text{Ensk}} d^3 v. \quad (5.4)$$

Deploying Taylor expansion near $x$ for $F$ and $Y$

$$J = J_0 + J_1 + J_2 + \ldots \quad (5.5)$$

where for $Y = Y(x)$, $F = F(v^*, x)$ and $F_1 = F(v_1^*, x)$

$$J_0 = 0, \quad (5.6)$$

$$J_1 = -\frac{\partial}{\partial x_i} \left[ \frac{\sigma^2}{2} \int \int \int \int (\psi^* - \psi) YF_1 k_i g \hat{b} d \hat{b} d \hat{e} d^3 v_1 d^3 v \right], \quad (5.7)$$

$$J_2 = -\frac{\partial}{\partial x_i} \left[ \frac{\sigma^2}{4} \int \int \int \int (\psi^* - \psi) YF_1 \frac{\partial}{\partial x_j} \left( \ln \frac{F}{F_1} \right) k_i k_j g \hat{b} d \hat{b} d \hat{e} d^3 v_1 d^3 v \right]. \quad (5.8)$$
Conservation equations of Enskog equation

- Taking velocity moment \( \psi \in \{1, v_j, v_jv_j/2\} \) of expanded Enskog equation leads to

\[
\int_{\mathbb{R}^3} \psi \left( \frac{\partial F}{\partial t} + v_i \frac{\partial F}{\partial x_i} \right) d^3v = -\frac{\partial \Psi^\phi_i}{\partial x_i}.
\]  

(5.9)

By keeping only first derivatives in Taylor expansion, one can show

\[
\Psi^\phi_i = \frac{Y \sigma^2}{2} \int \int \int \int \int (\psi^* - \psi) F F_1 k_i g \hat{b} d \hat{b} d \hat{c} d^3 v_1 d^3 v
\]
\[
+ \frac{Y \sigma^2}{4} \int \int \int \int \int (\psi^* - \psi) k_i k_j F F_1 \frac{\partial}{\partial x_j} \ln \left( \frac{F}{F_1} \right) g \hat{b} d \hat{b} d \hat{c} d^3 v_1 d^3 v.
\]

(5.10)

- Unlike Boltzmann, moments of Enskog operator does not vanish! This contribution is called \textbf{Collisional Transfer}. 

Mohsen Sadr  
MathCCES, RWTH Aachen University  
June 25, 2020
\( \Psi_i^\phi \) is approximated by\(^2\)
- Ignoring Higher order terms.
- \( \partial_x \ln(\mathcal{F}/\mathcal{F}_1) \approx \partial_x \ln(\mathcal{F}^0/\mathcal{F}_1^0) \), where \( \mathcal{F}^0 \) is the Maxwellian VDF.

**Mass Conservation:**

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j) = 0. \]  
(5.11)

**Momentum Conservation:**

\[ \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} \left( \rho U_i U_j + \pi_{ij}^{\text{kin+col}} + p^{\text{kin+col}} \delta_{ij} \right) = 0. \]  
(5.12)

**Energy Conservation:**

\[ \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_i} \left( EU_i + q_i^{\text{kin+col}} + p^{\text{kin+col}} \delta_{ik} U_k + \pi_{ik}^{\text{kin+col}} U_k \right) = 0, \]

where \( E = \rho c_v T + \frac{1}{2} \rho U_k U_k \) and \( c_v = 3 k_b/(2m) \).

---

\(^2\) see Chapman and Cowling (1953) [7]
Therefore, kinetic and collisional pressure tensor and heat fluxes can be derived

\[ p^{\text{kin+col}} = nk_b T (1 + nb Y) - w \frac{\partial U_k}{\partial x_k}, \]  
(5.13)

\[ \pi^{\text{kin+col}}_{ij} = (1 + 2 nb Y / 5) \pi_{ij} - \left( \frac{5w}{6} \right) \frac{\partial U_{\langle i}}{\partial x_{j}^{\rangle}}, \]  
(5.14)

and

\[ q^{\text{kin+col}}_i = (1 + 3 nb Y / 5) q_i - c_v w \frac{\partial T}{\partial x_i}, \]  
(5.15)

with \( w = (nb)^2 Y \sqrt{mk_b T} / (\pi^{3/2} \sigma^2) \) being bulk effect.

We used these expressions to correct pressure tensor and heat fluxes in FP of dense gases.
Cubic FP: conservation equations

- **Mass conservation:**
  \[
  \frac{\partial \rho}{\partial t} + \frac{\partial (\rho U_i)}{\partial x_i} = 0. \tag{5.16}
  \]

- **Momentum conservation:**
  \[
  \frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_i U_j) + \frac{\partial}{\partial x_j} (\pi_{ij}^{\text{kin}} + p^{\text{kin}} \delta_{ij}) \\
  + \frac{\partial}{\partial x_j} \int_{\mathbb{R}^3} \hat{A}_i v_j \mathcal{F} \, d^3 v = 0. \tag{5.17}
  \]

- **Energy conservation:**
  \[
  \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_i} \left( E U_i + q_i^{\text{kin}} + p^{\text{kin}} \delta_{ik} U_k + \pi_{ik}^{\text{kin}} U_k \right) \\
  + \frac{1}{2} \frac{\partial}{\partial x_i} \int_{\mathbb{R}^3} \hat{A}_i v_k v_k \mathcal{F} \, d^3 v = 0. \tag{5.18}
  \]
Monte Carlo solution of DFP

\[
\begin{align*}
V_i^{(n+1)} &= \langle V_i \rangle^{(n)} + \alpha_c \tilde{V}_i^{(n)} \\
X_i^{(n+1)} &= X_i^{(n)} + V_i^{(n+1)} \Delta t + \delta \tilde{X}_i^{(n)}
\end{align*}
\]

(5.19a)  
(5.19b)

where

\[
\tilde{V}_i^{(n)} = V_i'^{(n)} e^{-\Delta t Y^{(n)}/\tau^{(n)}} + c_{ij}^{(n)} V_j'^{(n)} + \gamma_i^{(n)} (V_j'^{(n)} V_j'^{(n)} - 3 k_B T^{(n)}/m) \\
+ \Lambda (V_i'^{(n)} V_j'^{(n)} V_j'^{(n)} - 2 q_i^{(n)}/\rho^{(n)}) + \sqrt{\frac{k T^{(n)} Y^{(n)}}{\tau^{(n)} m}} \left(1 - e^{\frac{-2 \Delta t Y^{(n)}}{\tau^{(n)}}}\right) \xi_i
\]

and

\[
\delta \tilde{X}_i^{(n)} = \left(\hat{c}_{ij}^{(n)} V_j'^{(n)} + \hat{\gamma}_i^{(n)} (V_j'^{(n)} V_j'^{(n)} - 3 k_B T^{(n)}/m) + \hat{\Lambda} (V_i'^{(n)} V_j'^{(n)} V_j'^{(n)} - 2 q_i^{(n)}/\rho^{(n)}) \right) \Delta t.
\]
The scaling factor $\alpha^{(c)}$ in cell $(c)$ guarantees conservation of kinetic energy in moments during a time step, i.e.,

$$\alpha^{(c)} = \frac{\langle V_j^{'(n)} V_j^{'(n)} \rangle^{(c)}}{\langle \tilde{V}_j^{(n)} \tilde{V}_j^{(n)} \rangle^{(c)}}. \quad (5.20)$$

Moments of velocity polynomials $\phi(v)$ is estimated through particles, i.e.,

$$\int_{\mathbb{R}^3} \phi \mathcal{F} d^3 v \approx \langle \Phi \rangle^{(c)}, \quad \text{where}$$

$$\langle \Phi \rangle^{(c)} := \sum_{m=1}^{N_p^{(c)}} \frac{w_m \Phi_m}{N_p^{(c)}}. \quad (5.22)$$
Closing $A$ & $D$

Plugging the ansatz for $A$ and $D$ in the equality of relaxation rates

$$\int_{\mathbb{R}^3} v'_i v'_j S_{FP}(\mathcal{F}) d^3 v \approx \int_{\mathbb{R}^3} v'_i v'_j S_{Ensk}(\mathcal{F}) d^3 v \quad \text{and} \quad (5.23)$$

$$\int_{\mathbb{R}^3} v'_i v'_j v'_j S_{FP}(\mathcal{F}) d^3 v \approx \int_{\mathbb{R}^3} v'_i v'_j v'_j S_{Ensk}(\mathcal{F}) d^3 v \quad (5.24)$$

leads to a system of equations for coefficients $c$ and $\gamma$, i.e.,

$$c_{ik} u^{(0)}_{kj} + c_{jk} u^{(0)}_{ki} + \gamma_i u^{(2)}_j + \gamma_j u^{(2)}_i = -2\Lambda u^{(2)}_{ij} \quad \text{and} \quad (5.25)$$

$$c_{ij} u^{(2)}_j + 2c_{jk} u^{(0)}_{ijk} + \gamma_i (u^{(4)} - (u^{(2)})^2) + 2\gamma_j (u^{(2)}_i - u^{(2)} u_{ij})$$

$$= -\Lambda (3u^{(4)}_i - u^{(2)}_i u^{(2)} - 2u^{(2)}_j u^{(0)}_{ij}) + \frac{5}{6} \frac{Y_p}{\mu_{\text{kin}}} q_i, \quad (5.26)$$

where $i, j, k = 1, 2, 3$. For convenience, note the abbreviation

$$u^{(l)}_{i_1...i_n} = \frac{1}{\rho} \int_{\mathbb{R}^3} |v'|^l v'_{i_1} v'_{i_2}...v'_{i_n} \mathcal{F} d^3 v. \quad (5.27)$$
Plugging in the ansatz for $\hat{A}$ in the approximation

$$\frac{\partial}{\partial x_k} \int_{\mathbb{R}^3} \hat{A}_k \psi_l \mathcal{F} d^3\mathbf{v} \approx \int_{\mathbb{R}^3} \psi_l S_{\text{Ensk}}^{\mathcal{F}}(\mathcal{F}) d^3\mathbf{v} \quad \text{for } l = 1, \ldots, \text{dim}(\psi), \quad (5.28)$$

gives us a system of equations for coefficients $\hat{c}$ and $\hat{\gamma}$, i.e.,

$$\hat{c}_{jk} \pi_{ik} + \hat{c}_{ji} p + 2\hat{\gamma}_{j} q_i = -\rho \hat{\Lambda} u_{ij}^{(2)}$$

$$+ nb Y (\rho \delta_{ij} + 2/5 \pi_{ij}) - w \left( \frac{\partial U_k}{\partial x_k} \delta_{ij} + \frac{5}{6} \frac{\partial U_i}{\partial x_j} \right) \quad \text{and} \quad (5.29)$$

$$\hat{c}_{ij} q_j + \frac{1}{2} \rho \hat{\gamma}_i (u^{(4)} - (u^{(2)})^2) = \frac{3}{5} nb Y q_i - \hat{w} c_v \frac{\partial T}{\partial x_i} - \frac{1}{2} \rho \hat{\Lambda} (u_i^{(4)} - u_i^{(2)} u^{(2)}). \quad (5.30)$$
Hence, for 3D velocity and 3D position problems, in each cell a $9 \times 9$ and a $12 \times 12$ linear system of equations need to be solved, i.e.,

$$
A_v \begin{pmatrix} c_{1,1} \\ \vdots \\ c_{3,3} \\ \gamma_1 \\ \vdots \\ \gamma_3 \end{pmatrix} = b_v \quad \text{and} \quad A_x \begin{pmatrix} \hat{c}_{11} \\ \vdots \\ \hat{c}_{3,3} \\ \hat{\gamma}_1 \\ \vdots \\ \hat{\gamma}_3 \end{pmatrix} = b_x,
$$

where the matrices $A_v$ and $A_x$ and right hand sides $b_v$ and $b_x$ are read from Eqs.(1.29)-(5.26) and Eqs.(5.29)-(5.30), respectively.
Temperature contours and heat fluxes of the lid-driven cavity flow at $Kn = 0.1$, $nb = 0.1$ and $U_w = 300$ m/s.
How is the numerical scheme for DFP obtained?
For simplicity consider $V = V'$, i.e., $U = 0$, and 1D setting:

$$dV = \left( cV + \gamma(V^2 - k_b T/m) + \Lambda(V^3 - 2q/\rho) \right) dt + \sqrt{\frac{2k_b T}{m\tau}} dW_t$$

$$dX = V dt + \left( \hat{c}V + \hat{\gamma}(V^2 - k_b T/m) + \hat{\Lambda}(V^3 - 2q/\rho) \right) dt$$

We know the analytical solution of the linear FP for $V$, i.e.,

$$dV = -\frac{1}{\tau} V dt + \sqrt{\frac{2k_b T}{m\tau}} dW$$

$$\implies V(t_0 + \Delta t) = V(t_0) e^{-\Delta t/\tau} + \sqrt{\frac{k_b T}{m}} (1 - e^{-2\Delta t/\tau}) \xi$$

We add the higher order terms

$$V(t_0 + \Delta t) = V(t_0) e^{-\Delta t/\tau} + \sqrt{\frac{k_b T}{m}} (1 - e^{-2\Delta t/\tau}) \xi + e^{-\Delta t/\tau} \int_0^{\Delta t} e^{\Delta t/\tau} (A + \frac{1}{\tau} V) dt$$
We use Euler for the remaining terms, leading to a scheme with at least $\gamma = 1$ strong and $\beta = 1$ weak convergence rate in velocity, i.e.,

$$
\int_0^{\Delta t} e^{t/\tau} A(V(t), t) dt = A(V(t_0), t_0)\tau(e^{\Delta t/\tau} - 1)
$$

We used backward Euler in the position update

$$
X(t_0 + \Delta t) = X(t_0) + \int_{t_0}^{t_0+\Delta t} \left( V(t) + \hat{A}(V(t), t) \right) dt
\approx X(t_0) + \left( V(t_0 + \Delta t) + \hat{A}(V(t + t_0), t_0) \right) \Delta t
$$

which has $\gamma = 1$ strong (since the terms with Wiener process don’t show up) and $\beta = 1$ weak convergence rate in position.
Screened-Poisson equation for long-range interactions
Attractive forces

Let us include the attractive forces from $\phi(r)$, where $r := |x - x'|$, through mean field theory in evolution of single particle distribution function

$$\frac{\partial F}{\partial t} + \frac{\partial (Fv_j)}{\partial x_j} - \frac{1}{m} \frac{\partial}{\partial v_i} \int_{r > \sigma} \int \frac{\partial \phi}{\partial x_i} F^{(2)}(x, v, x', v') \, dx' \, dv' = S_{\text{Ensk}}^{\text{repulsion}}(F).$$

(6.1)

Considering molecular chaos, i.e. $F^{(2)}(x, v, x', v') = F(x, v)F(x', v')$

$$I_{\text{attr}} = \frac{\partial}{\partial v_i} \int_{r > \sigma} \int \frac{\partial \phi}{\partial x_i} F(x, v)F(x', v') \, dx' \, dv'$$

$$= \frac{\partial F(x, v)}{\partial v_i} \int_{r > \sigma} \frac{\partial \phi}{\partial x_i} \left( \int F(x', v') \, dv' \right) \, dx'$$

$$= \frac{\partial F(x, v)}{\partial v_i} \int_{r > \sigma} \frac{\partial \phi}{\partial x_i} n(x') \, dx'$$

$$= \frac{\partial F(x, v)}{\partial v_i} \frac{\partial}{\partial x_i} \int_{r > \sigma} \phi(r) n(x') \, dx' \, .$$

(6.2)
Idea: Relating Vlasov integral

$$U(x) = \int_{r > \sigma} \phi(r) n(x') d^3x'$$  \hspace{1cm} (6.3)

to a Poisson-type PDE.

- Approximate $\phi$ 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 \frac{e^{-\lambda r}}{4\pi r}$$

$$= a \underbrace{G(r)}_{\tilde{\phi}(r)}$$  \hspace{1cm} (6.4)

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

$$(\nabla^2 - \lambda^2) u(x) = -n(x), \quad \forall x \in \mathbb{R}^3.$$  \hspace{1cm} (6.5)
Rewrite the Vlasov integral as:

\[
U(x) = \int_{r>0} \phi(r)n(x')d^3x' - \int_{r<\sigma} \phi(r)n(x')d^3x'.
\]  

(6.6)

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

\[
(\nabla^2 - \lambda^2) u(x) = -n(x), \quad \forall x \in \mathbb{R}^3.
\]  

(6.7)

**Challenge:** we cannot solve the PDE numerically in \( \mathbb{R}^3 \).
Bounded domains

For a bounded domain $\Omega \subset \mathbb{R}^3$, solution of a screened-Poisson problem

\[
\begin{aligned}
\begin{cases}
(\nabla^2 - \lambda^2)u &= -n \quad \text{in } \Omega \quad \text{and} \\
\quad u &= g \quad \text{on } \partial \Omega
\end{cases}
\end{aligned}
\tag{6.8}
\]

is given by

\[
u(x) = \int_{\Omega} G(y - x)n(y)d^3y \\
+ \int_{\partial\Omega} \left(G(y - x)\frac{\partial u(y)}{\partial \nu} - u(y)\frac{\partial G(y - x)}{\partial \nu}\right)dS(y)
\tag{6.9}
\]

where $G(y - x)$ denotes fundamental solution of unbounded screened-Poisson PDE.

**Challenges:**

- The integral is $\int_{\Omega}(.)d^3y$ instead of our target $U := \int_{\mathbb{R}^3}(.)d^3y$.
- How to set $g$?
- How can we avoid $\int_{\partial\Omega}(.)dS$, $\forall x \in \Omega$?
Bounded domains, cont.

What we want is the solution of unbounded screened-Poisson

\[
(\nabla^2 - \lambda^2)u(x, t) = n(x, t) \quad (\forall x \in \mathbb{R}^3),
\]

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

\[
(\nabla^2 - \lambda^2)\psi(x, t) = n(x, t) \quad (\forall x \in \Omega) \quad \text{and} \quad \psi(y, t) = g(y, t) \quad (\forall y \in \partial\Omega). \tag{6.11}
\]

Uniqueness of screened-Poisson equation with Dirichlet BC implies

\[
\psi(x, t) = u(x, t) \quad (\forall x \in \Omega) \tag{6.13}
\]

provided

\[
g(y, t) = u(y, t) \quad (\forall y \in \partial\Omega). \tag{6.14}
\]

Note \(u(y, t)\) on \(\partial\Omega\) can be calculated directly.
Instead of density, expand potential $e^{\lambda|y-x|/(4\pi|y-x|)}$ around $x$ in

$$
\tilde{\eta}_{r>\sigma}(x, t) = \int_{r:=|y-x|>\sigma} \frac{e^{-\lambda|y-x|}}{4\pi|y-x|} n(y) d^3y.
$$

(6.15)

Alternatively, one can split the kernel using multipole expansion. Then, for any point $x = (\rho, \theta, \phi) \in \mathbb{R}^3$ from an origin that $\rho > a$ we have

$$
\tilde{\eta}_{r>\sigma}(x, t) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} M^i_j k_i(\lambda \rho) Y^j_i(\theta, \phi)
$$

(6.16)

The error in keeping only $p$ terms is

$$
\left| \tilde{\eta}_{r>\sigma}(x, t) - \sum_{i=0}^{p} \sum_{j=-i}^{i} M^i_j k_i(\lambda \rho) Y^j_i(\theta, \phi) \right| = O \left( (a/\rho)^p \right).
$$

(6.17)

FMM for $e^{-\lambda r}/(4\pi r)$ has been done before by Greengard [8].
\[ \tilde{\eta}_{r>\sigma}(\mathbf{x}, t) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} M_{ij}^i k_i(\lambda \rho) Y_i^j(\theta, \phi) \]

Here:

\[ M_{ij}^i = \frac{2\lambda}{\pi} \sum_{l=1}^{N} n_l i_i(\lambda \rho_l) Y_{i}^{-j}(\theta_l, \phi_l) \] (6.18)

\( Y_i^j(\theta, \phi) \) is the spherical harmonics of degree \( i \) and order \( j \), \( i_i(\rho) \) is the modified spherical Bessel, and \( k_i(\rho) \) is the spherical Henkel functions where \( k_0(\lambda \rho) = \frac{\pi}{2} \frac{e^{-\lambda \rho}}{\lambda \rho} \).
How can one get attractive pressure?
Obtaining attractive pressure

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho U_i) = 0, \]  
\[ (6.19) \]

\[ \frac{\partial (\rho U_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_i U_j + p_{ij}^{\text{kin+col}}) - \rho H_i = 0 \]
\[ (6.20) \]

where \( H_i(x) = \frac{\partial \Phi(\rho(x))}{\partial x_i}. \) e.g. in 1D:

\[ \Phi(x) = \int_{|x-x'|>\sigma} G(x-x')\rho(x')dx' \]
\[ (6.21) \]

\[ = \int_{|x'|>\sigma} G(x')\rho(x-x')dx' \]
\[ (6.22) \]

\[ = \int_{|x'|>\sigma} G(x')[\rho(x) + \frac{\partial \rho(x)}{\partial x}(x-x') + ...]dx' \]
\[ (6.23) \]

\[ = \rho(x) \int_{|x'|>\sigma} G(x')dx' + \frac{\partial \rho(x)}{\partial x} \int_{|x'|>\sigma} G(x')(x-x')dx' + ... \]
\[ (6.24) \]
Obtaining attractive pressure -cont

\[ \Phi(x) \approx \rho(x)L^{(0)} + \sum_{i=1}^{\infty} \frac{\partial^i \rho(x)}{\partial x^i} L^{(i)} \]  

(6.25)

Then, \( \rho \partial \Phi / \partial x \) becomes

\[ \rho(x) \frac{\partial \Phi(x)}{\partial x} = \rho(x) \frac{\partial \rho(x)}{\partial x} L^{(0)} + ... \]  

(6.26)

\[ = \frac{1}{2} \frac{\partial \rho^2(x)}{\partial x} L^{(0)} + ... \]  

(6.27)

\[ = \frac{\partial}{\partial x} \left( \frac{1}{2} \rho^2(x) L^{(0)} + ... \right) \]  

(6.28)

Similar trick can be done for other terms which leads to Korteweg tensor (not unique [9]).
Scale analysis of phase transition

Observation:

\[ \frac{\Delta \rho}{\Delta x} \bigg|_{\text{interface}} \text{ increases as } T \text{ decreases.} \]  \hspace{1cm} (6.29)

Does it make sense?

\[ T_{\text{Left}} < T_{\text{Right}} < T_{\text{Critical}} \]
Figure: Indicated points are the states that are taken as initial conditions from stable region of phase diagram. Unstable region is the region where pressure increases as density reduces, i.e., area enclosed with the green curve.
Scale analysis of phase transition

Observation:
\[
\left. \frac{\Delta \rho}{\Delta x} \right|_{\text{interface}} \text{ increases as } T \text{ decreases.} \tag{7.1}
\]

Does it make sense?

With some approx., Van der Waals surface tension \( \gamma \) can be related to 2nd moment of potential via \( \Delta \rho/\Delta x \)

\[
\left. \frac{\Delta \rho}{\Delta x} \right|_{\text{interface}} \approx \gamma / \int r^2 \phi(r) d^3 r \tag{7.2}
\]

Where \( \gamma \) increases monotonically as \( T \) decreases, i.e., \( \gamma \sim -\log(T/T_C) \)

INCOMPRESSIBLE LIMIT OF DENSE FLUIDS
Applying operator

\[ \mathcal{L}[u] := (\Delta - \chi^2)u \]  

(8.1)
on

\[ \Phi(x) = a \int_{r>0} \tilde{\phi}(r)n(x')d^3x' - a \int_{r<\sigma} \tilde{\phi}(r)n(x')d^3x' \]

(8.2)
leads to

\[ \Phi = \Phi_{r>0} - \Phi_{r<\sigma} \]  

(8.3)

\[ \implies m\mathcal{L}[\Phi] = -\rho/a - m\mathcal{L}[\Phi_{r<\sigma}] . \]  

(8.4)

Let \( \rho \to \infty \) as \( \epsilon \to 0 \), i.e. \( \rho = \bar{\rho}/\epsilon \) where \( \bar{\rho} < \infty \). Let \( \hat{\rho} := -am\mathcal{L}[\Phi_{r<\sigma}] \), then

\[ \begin{cases} 
\frac{\partial F}{\partial t} + \frac{\partial (Fv_i)}{\partial x_i} - \frac{\partial \Phi}{\partial x_i} \frac{\partial F}{\partial v_i} = S(F) \quad \text{and} \\
ma \epsilon \mathcal{L}[\Phi] = \hat{\rho} - \bar{\rho} . 
\end{cases} \]  

(8.5)
Incompressible limit of dense liquids

Conservation of mass:

\[
\frac{\partial \rho}{\partial t} + U_i \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial U_i}{\partial x_i} = 0. \tag{8.6}
\]

Note that

\[
\frac{\partial \rho}{\partial t} = -ma\epsilon L[\Phi_t] \quad \text{and} \quad \frac{\partial \rho}{\partial x_i} = -ma\epsilon L[\Phi_{x_i}] \tag{8.7, 8.8}
\]

Then

\[-ma\epsilon L[\Phi_t] - U_i ma\epsilon L[\Phi_{x_i}] + \rho \frac{\partial U_i}{\partial x_i} = 0.\]

Letting \(\epsilon \to 0\)

\[
\frac{\partial U_i}{\partial x_i} = 0. \tag{8.9}
\]
Part II: Multi-scale fluid flows far from equilibrium
Samples of $X$ and $V$ with measure $\mathcal{F}$ s.t.

\[
\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial (\mathcal{F}v_j)}{\partial x_j} = \mathcal{S}^{\text{Boltz.}}(\mathcal{F}).
\]

We shall find a unique $\mathcal{F}$, which has the least bias.

This leads to finding $\mathcal{F}$ that minimizes the entropy $\int \mathcal{F} \ln(\mathcal{F}) dv$ in bounded domains $\Omega$ with constraints on moments, i.e.,

\[
C_N^\lambda[\mathcal{F}] := \int_{\Omega} \mathcal{F} \ln(\mathcal{F}) dv + \lambda_j \left( \int_{\Omega} \mathcal{F} \phi_j dv - p_j \right).
\]

Here, $p$ and $\phi$ are the vectors of moments and velocity polynomials.
Maximum entropy distribution (MED)

The normalized extremum of $C^\lambda_N[.]$ is called MED, i.e.,

$$\mathcal{F}^\lambda_N(v) = Z_\lambda^{-1} \exp \left( - \sum_{j=1}^N \lambda_j \phi_j \right).$$

(9.2)

Newton’s method of line-search for the dual problem

$$\lambda(p) = \arg\min_{\lambda^* \in \mathbb{R}^N} \left\{ Z_{\lambda^*} - \sum_{j} \lambda_j^* p_j \right\}$$

(9.3)

with iteration scheme

$$\sum_{j=1}^N H_{ij}(\lambda^n) \Delta \lambda^n_j = g_i(\lambda^n) \quad \text{and} \quad \lambda_i^{n+1} = \lambda_i^n + \beta^n \Delta \lambda^n_i,$$

(9.4)

(9.5)

can become costly.

$H$ and $g$ are Hessian and gradient of $C^\lambda_N[.]$ and $\beta$ is damping factor.
Maximum entropy distribution (MED)

The normalized extremum of $C_N^\lambda[.]$ is called MED, i.e.,

$$F_N^\lambda(v) = Z_\lambda^{-1} \exp \left( - \sum_{j=1}^{N} \lambda_j \phi_j \right). \tag{9.2}$$

Newton’s method of line-search for the dual problem

$$\lambda(p) = \arg \min_{\lambda^* \in \mathbb{R}^N} \left\{ Z_{\lambda^*} - \sum_j \lambda^*_j p_j \right\} \tag{9.3}$$

with iteration scheme

$$\sum_{j=1}^{N} H_{ij}(\lambda^n) \Delta \lambda_j^n = g_i(\lambda^n) \text{ and } \lambda_i^{n+1} = \lambda_i^n + \beta^n \Delta \lambda_i^n, \tag{9.4}$$

and (9.5)

Cost depends on initial guess & condition number of $H(\lambda^n)$.

$H$ and $g$ are Hessian and gradient of $C_N^\lambda[.]$ and $\beta$ is damping factor.
Existence and uniqueness of MED in $\mathbb{R}$ [11]

**Theorem (Existence)**

If the MED for $N - 1$ moments, i.e. $\mu_0, ..., \mu_{N-1}$, is associated with $\lambda_0, ..., \lambda_{N-1}$, then MED exists for $N$ moments only if

$$\mu_N \leq \int_0^\infty x^N e^{-\sum_{i=0}^{N-1} \lambda_i x^i} \, dx. \quad (9.6)$$

**Theorem (Uniqueness)**

If a MED exists for a given moment vector, then it is unique.

Both proofs benefit from the fact that

$$\sum_i d\mu_i d\lambda_i < 0, \quad (9.7)$$

where $d\mu_i = - \int_0^\infty x^i \left( \sum_j d\lambda_j x^j \right) e^{-\sum_j \lambda_j x^j} \, dx. \quad (9.8)$
Gaussian process regression
for maximum entropy distribution
Here we approximate the unique map $\Psi_i : p \to \lambda_i, \ i = 1, \ldots, N$ by Gaussian process

$$\tilde{\Psi}_i \sim \mathcal{GP}(0, K_i) \quad (9.9)$$

given a positive semi-definite kernel function $K(p, p')$. Hyperparameters are found by maximizing log-likelihood on data set $D$,

$$\ln \left[ \tilde{f} \left( \tilde{\Psi}_i(p) \mid p \in D \right) \right] \quad (9.10)$$

Predicting $\lambda^*_i$ for the input $p^*$ follows

$$\left( \tilde{\Psi}_i(p^*) \mid \tilde{\Psi}_i(p) = \Psi_i(p) \right) \sim \mathcal{N}(\bar{m}_i, \bar{\Sigma}_i), \quad (9.11)$$

where

$$\bar{m}_i = K_{\Theta_i}(p^*, p')K_{\Theta_i}(p, p')^{-1}\Psi_i(p) \quad (9.12)$$

and

$$\bar{\Sigma}_i = K_{\Theta_i}(p^*, p^*) - K_{\Theta_i}(p^*, p)K_{\Theta_i}(p, p')^{-1}K_{\Theta_i}(p^*, p). \quad (9.13)$$

see Sadr, Torrilhon, and Gorji (2019) [12].
Here we approximate the unique map $\Psi_i : p \rightarrow \lambda_i, \ i = 1, ..., N$ by Gaussian process

$$\tilde{\Psi}_i \sim \mathcal{GP}(0, \mathcal{K}_i)$$ (9.9)

given a positive semi-definite kernel function $\mathcal{K}(p, p')$. Hyperparamaters are found by maximizing log-likelihood on data set $D$,

$$\ln \left[ \tilde{f} \left( \tilde{\Psi}_i(p) \mid p \in D \right) \right]$$ (9.10)

Predicting $\lambda_i^*$ for the input $p^*$ follows

$$\left( \tilde{\Psi}_i(p^*) \mid \tilde{\Psi}_i(p) = \Psi_i(p) \right) \sim \mathcal{N}(\bar{m}_i, \bar{\Sigma}_i),$$ (9.11)

where

$$\bar{m}_i = \mathcal{K}(p^*, p') \mathcal{K}(p, p')^{-1} \Psi_i(p)$$ (9.12)

and

$$\bar{\Sigma}_i = \mathcal{K}(p^*, p^*) - \mathcal{K}(p^*, p) \mathcal{K}(p, p')^{-1} \mathcal{K}(p, p^*).$$ (9.13)

See Sadr, Torrilhon, and Gorji (2019) [12].
Results: recovering bi-modal distribution

\[ f(x) \]

(a) \( f^\text{bi} \)

(b) \( f^\lambda_4 \)

(c) \( f^\lambda_6 \)

\( f^\lambda_8 \)

Test Case: 10^{-6}, 10^{-4}, 10^{-2}, 10^0, 10^2, 10^4, 10^6

\[ \| \lambda^\text{est} - \lambda^\text{ex} \|_2 / \| \lambda^\text{ex} \|_2 \]

\[ N = 4, 6, 8 \]

Test Case: 10^{-7}, 10^{-5}, 10^{-3}, 10^{-1}, 10^0, 10^1

\[ \| \text{Var}(\lambda^\text{est}) \|_2 / \| \lambda^\text{est} \|_2 \]

\[ N = 4, 6, 8 \]

\[ \tau^\text{pred} \text{ GPR} / \tau^\text{direct} \]

\[ N = 4, 6, 8 \]

Mohsen Sadr  
MathCCES, RWTH Aachen University  
June 25, 2020  
46 / 69
Coupling SPH with DSMC

Initialization with SPH particles in every cell;

while $t < t_{\text{final}}$ do
  - Evolve particles;
  - Apply boundary conditions;
  for $cell = 1, \ldots, N_{\text{cells}}$ do
    - Estimate $f_3^\lambda$ from moments using GPR;
    if $\mathcal{I}(f^{\text{eq}} | f_3^\lambda) > \epsilon$ and $cell_{\text{flag}} == \text{SPH}$ then
      - Replace SPH particles with samples of $f_3^\lambda$;
    end
    if $\mathcal{I}(f^{\text{eq}} | f_3^\lambda) < \epsilon$ and $cell_{\text{flag}} == \text{DSMC}$ then
      - Remove DSMC particles;
      - Generate SPH particles with values based on the moments;
    end
  end
  - Increment $t$;
end

$\mathcal{I}(f^{\text{eq}} | f_3^\lambda) := \int_{\Omega} f^{\text{eq}} \left[ \nabla \ln \left( \frac{f^{\text{eq}}}{f_3^\lambda} \right) \right]^2 dv$

SPH: Smoothed Particle Hydrodynamics
DSMC: Direct Simulation Monte Carlo
Results: Sod’s shock tube

Figure: Sod’s shock tube with initial value of $\rho_0 = 10^{-4}$ [kg.m$^{-3}$] at $t = 2.01 \times 10^{-4}$ [s]. Here GPR as the MED estimator is used for the hybrid solution algorithm.
Figure: Sod’s shock tube with initial value of $\rho_0 = 10^{-4}$ [kg.m$^{-3}$] at $t = 2.01 \times 10^{-4}$ [s]. Here $GPR$ as the MED estimator is used for the hybrid solution algorithm.
Convergence rate of numerical schemes for SDEs

- **Strong convergence with order** \( \gamma \)

\[
\mathbb{E}[|X_T - X_T^\Delta|] \leq C \Delta^\gamma
\]

(10.1)

- **Weak convergence with order** \( \beta \)

\[
\left| \mathbb{E}[g(X_T)] - \mathbb{E}[g(X_T^\Delta)] \right| \leq C_g \Delta^\beta
\]

(10.2)

\( \Delta \): denotes step size

\( X_T^\Delta \): discrete-time approximation of solution \( X_T \) at time \( T \).

\( g : \mathbb{R}^d \to \mathbb{R} \) and \( g \in \tilde{C}_P(\mathbb{R}^d, \mathbb{R}) \), which is the set of all polynomials.
Wagner-Platen expansion

Consider process $X = \{X_t, t \in [t_0, T]\}$ satisfying

$$X_t = X_{t_0} + \int_{t_0}^{t} a(X_s)ds + \int_{t_0}^{t} b(X_s)dW_s. \quad (10.3)$$

For any $f : \mathbb{R} \to \mathbb{R}$, $f \in C^2$, note Itô’s formula

$$f(X_t) = f(X_0) + \int_{t_0}^{t} \left( a(X_s) \frac{\partial}{\partial x} + \frac{1}{2} b^2(X_s) \frac{\partial^2}{\partial x^2} \right) f(X_s)ds + \int_{t_0}^{t} b(X_s) \frac{\partial}{\partial x} f(X_s)ds. \quad (10.4)$$

Considering $f = a$ and $f = b$, it can be shown that

$$X_t = X_{t_0} + a(X_0) \int_{t_0}^{t} ds + b(X_0) \int_{t_0}^{t} dW_s + R_2, \quad (10.5)$$
Wagner-Platen expansion -cont

\[
R_2 = \int_{t_0}^{t} \int_{t_0}^{s} \left( L^0 a(X_z) dz ds + L^1 a(X_z) dW_z ds \right) + \int_{t_0}^{t} \int_{t_0}^{s} \left( L^0 b(X_z) dz dW_s + L^1 b(X_z) dW_z dW_s \right).
\] (10.6)

- Using Hölder inequality, one can show that Euler-Maruyama has strong convergence rate of \( \gamma = 1/2 \).
- If diffusion is additive, i.e., \( b(X_t, t) = b(t) \), then \( \gamma = 1 \).
- One can obtain higher order schemes by keeping higher order terms. Also, Stratonovich equation instead of Itô is typically used.
- See [13] for derivation of other higher order schemes such as Milstein among others.
For some $\beta \in \{1, 2, \ldots\}$ and autonomous SDE for $X$ let $X^\Delta$ be a weak Taylor scheme of order $\beta$. Suppose that $a$ (drift) and $b$ (diffusion) are Lipschitz continuous with components $a^k, b^{k,j} \in C_2^{\beta+1}(\mathbb{R}^d, \mathbb{R})$ for all $k \in \{1, 2, \ldots, d\}$ and $j \in \{0, 1, \ldots, m\}$, and that the $f_\alpha$ satisfy a linear growth bound

$$|f_\alpha(t, x)| \leq K(1 + |x|)$$

(10.7) for all $\alpha \in \Gamma_\beta$, $x \in \mathbb{R}^d$ and $t \in [0, T]$, where $K < \infty$. Then for each $g \in C_2^{\beta+1}(\mathbb{R}^d, \mathbb{R})$ there exists a constant $C_g$, which does not depend on $\Delta$, such that

$$\left| \mathbb{E}[g(X_T)] - \mathbb{E}[g(X^\Delta_T)] \right| \leq C_g \Delta^\beta$$

(10.8) that is $X^\Delta$ converges with weak order $\beta$ to $X$ at time $T$ as $\Delta \to 0$.

- One can show that Euler-Maruyama has weak convergence of $\beta = 1$. 
\[ f_\alpha(t, x) = L^{j_1} \ldots L^{j_{l-1}} b^{j_l} \] 

for all \( (t, x) \in [0, T] \times \mathbb{R}^d \), all multi-indices 
\( \alpha = (j_1, \ldots, j_l) \in \mathcal{M}_m, \ m \in \{1, 2, \ldots\} \)
\[ dX_t = a(X_t)dt + b(X_t)dW_t \]  

(10.10)

Taylor expansion of a smooth function \( f(X_t) \) up to second order

\[ df[X_t] = f'[X_t]dx + \frac{1}{2}f''[X_t]dx^2. \]

Substitute \( dX_t \) for \( dx \):

\[ df[X_t] = f'[X_t](adt + bdW_t) + \frac{1}{2}f''[X_t](a^2dt^2 + b^2dW_t^2 + 2adtdW_t) \]

Quadratic variance, i.e. \( dW_t^2 = dt \) and ignoring higher order terms:

\[ df[X_t] = \left( af'[X_t] + \frac{b^2}{2}f''[X_t] \right) dt + bf'[X_t]dW_t \]  

(10.11)
Deriving Fokker-Planck equation using Ito’s lemma

Take average of Ito’s formula for the Ito process

\[
\langle df[X_t] \rangle = \langle (af'[X_t] + \frac{b^2}{2} f''[X_t])dt \rangle + \langle bf'[X_t]dW_t \rangle
\]

\[
= \langle (af'[X_t] + \frac{b^2}{2} f''[X_t])dt \rangle + \langle bf'[X_t] \rangle \langle dW_t \rangle = 0
\]

Note that \( \langle f[X_t] \rangle = \int f[x]p(x, t|x_0, t_0)dx \). Hence

\[
\int f[x] \partial_t p dx = \int (af' + \frac{b^2}{2} f'')p dx
\] (10.12)

Applying integration by parts on rhs, assuming \( p \in L^2 \), one gets

\[
\int f[x] \partial_t p dx = \int f[x] \left( (ap)' + \left( \frac{b^2}{2} p \right)'' \right) dx
\] (10.13)

Since \( f[.] \) is arbitrary \( \Rightarrow \partial_t p = (ap)' + \left( \frac{b^2}{2} p \right)'' \).
Existence of solution to SDEs

**Theorem (3.8, Khasminskii [14])**

\[ X(t) = X(t_0) + \int_{t_0}^{t} a(X(s))ds + \sum_i \int_{t_0}^{t} b_i(X(s))dW_i(s) \]

where \( a \) and \( b \) are \( \theta \)-periodic, i.e. joint-distr of \( a(t_1 + h), \ldots a(t_n + h) \) is indep of \( h \), and satisfy

\[ |a(s, x) - a(s, y)| + \sum_i |b_i(s, x) - b_i(s, y)| \leq B|x - y| \quad (10.14) \]

and

\[ |a(s, x)| + \sum_i |b_i(s, x)| \leq B(1 + |x|) \quad (10.15) \]

in every cylinder \( I \times U \). Also, suppose there exists a function \( V(t, x) \in C^2 \)

\( \theta \)-periodic in \( t \), and satisfies

\[ \sup_{|x| > R} LV(t, x) \to -\infty \text{ as } R \to \infty, \quad (10.16) \]

\[ \inf_{|x| > R} V(t, x) \to \infty \text{ as } R \to \infty. \quad (10.17) \]

Then, SDE has a solution which is a \( \theta \)-periodic Markov process.
Existence of solution to SDEs

E.g.: \( dX = -(X + X^2 + X^3) \, dt + \underbrace{a}_{\text{a}} \, dt + \underbrace{b}_{\text{b}} \, dW \). Consider \( V(x) = x^2 \).

\[
L(.) := \frac{\partial}{\partial t}(.) + a(t, x) \frac{\partial}{\partial x}(.) + \frac{b^2(t, x)}{2} \frac{\partial^2}{x^2}(.)
\] (10.18)

\[
L(V(x)) = -(x + x^2 + x^3)(2x) + 1
\] (10.19)

\[
= -2x^4 - 2x^3 - 2x^2 + 1
\] (10.20)

As \( R \to \infty, \, |x| \to \infty \),

\[
\sup_{|x| > R} LV(x) \to -\infty \checkmark
\] (10.21)

\[
\inf_{|x| > R} V(x) \to \infty \checkmark
\] (10.22)

Hence, solution exists.
Uniqueness of SDE

Uniqueness means that one should show solution of

\[ Lf = 0 \quad \text{(10.23)} \]

\[ L = \frac{\partial}{\partial s} + a(s, x) \frac{\partial}{\partial x} + \frac{1}{2} b(s, x)^2 \frac{\partial^2}{\partial x^2} \quad \text{(10.24)} \]

is unique.

Lemma (3.3, Khasminskii [14])

*If the conditions for existence hold, assuming \( f(s, x) \) is a bounded and continuous function on \( (t_0, T) \times U \), the solution is unique*

\[ f(s, x) = \mathbb{E}^{s,x}[f(\tau_U(T), X(\tau_U(T)))] \quad \text{(10.25)} \]

*where \( \tau_U \) is the time the corresponding process \( X(t) \) reaches the boundaries of \( U \).*
Regularity of FP

We know from Pinsker’s inequality for probability distributions $F, G$

$$\sup(|F - G|_1) \leq \sqrt{\frac{1}{2} D_{KL}(F||G)}.$$ (10.26)

similar thing can be written for pdf.

In case of FP, the cross entropy $H(f, g) = \int f \log(f/g)dv$, where $g$ is Maxwell,

$$\frac{\partial H}{\partial t} = C(A, D)$$ (10.27)

- Not for any drift and diffusion, $C(A, D) \leq 0$.
- Next, one should consider Entropic-Fokker-Planck more where

$$\int \log(f/g)S^{FP}(f)dv = \int \log(f/g)S^{coll}(f)dv.$$ (10.28)
All kinds of conv.: seq. of rand. var. $X_n$ to $X$

- **Point-wise** convergence or sure convergence:
  \[ X_n(\omega) \to X(\omega), \forall \omega \in \Omega. \]  
  \[ (10.29) \]

- **Almost sure** convergence or convergence with probability 1:
  \[ P(\{\omega | X_n(\omega) \to X(\omega)\}) = 1. \]  
  \[ (10.30) \]

- **Convergence in probability**:
  \[ \lim_{n \to \infty} P(|X_n - X| > \epsilon) = 0, \forall \epsilon > 0. \]  
  \[ (10.31) \]

- **Convergence in rth mean**:
  \[ \lim_{n \to \infty} \mathbb{E}[|X_n - X|^r] = 0. \]  
  \[ (10.32) \]

- **Convergence in dist. or weak conv.** ($\xrightarrow{D}$):
  \[ \lim_{n \to \infty} F_{X_n}(x) = F_X(x), \forall x \in \mathbb{R}. \]  
  \[ (10.33) \]
Given \( N \) samples \( \omega \) of the random variable \( V \), law of large numbers gives

\[
\mathbb{E}[V] \approx \frac{\sum_{n=1}^{N} V(\omega^{(n)})}{N} \quad \text{&} \quad \text{Var}[\mathbb{E}^\Delta[V]] = \frac{N \text{Var}[V]}{N^2} = \frac{\text{Var}[V]}{N} \sim \frac{T}{N}.
\]

(11.1)

Consider levels of accuracy/cost for \( \mathbb{E}[.] \) based on MC simulations.

\[
\mathbb{E}[V_L] = \mathbb{E}[V_0] + \sum_{l=0}^{L} \mathbb{E}[V_l - V_{l-1}]
\]

(11.2)

\[
\mathbb{E}^\Delta[V_L] = \frac{1}{N_0} \sum_{n=1}^{N_0} V_0^{(0,n)} + \sum_{l=1}^{L} \left\{ \frac{1}{N_l} \sum_{n=1}^{N_l} \left( V_l^{(n,l)} - V_{l-1}^{(n,l)} \right) \right\}
\]

(11.3)

\(^3\text{see Giles (2015) [15].}\)
Multi-Level Monte Carlo

Task: find \( N_l \) that minimizes \( \text{Var}[\mathbb{E}^A[V_L]] \) with constraint on cost.

\( C_0 \) & \( s_0 \) := cost and variance of one sample of \( V_0 \).

\( C_l \) & \( s_l \) := cost and variance of one sample of \( V_l - V_{l-1} \).

\[
L := \sum_{l=0}^{L} \left( N_l^{-1} s_l + \mu^2 N_l C_l \right) \tag{11.4}
\]

Extremum is at \( N_l = \mu \sqrt{s_l / C_l} \). For overall variance of \( \epsilon^2 \):

\[
\mu = \epsilon^{-2} \sum_{l=0}^{L} \sqrt{s_l C_l} \tag{11.5}
\]

\[
\text{and } C_{\text{total}} = \epsilon^{-2} \left( \sum_{l=0}^{L} \sqrt{s_l C_l} \right)^2 \tag{11.6}
\]

Levels could be cell size or/and time step size?
How many particles per level? Do we need to generate new particles during simulation?
Central Limit Theorem

**Theorem**

Let \( \{X_i\} \) be a sequence of i.i.d random variables with mean \( \mathbb{E}[X] \) and non-zero variance \( \sigma_X^2 < \infty \). Let \( Z_n = \frac{S_n - n\mathbb{E}[X]}{\sigma_X \sqrt{n}} \). Then, we have

\[
Z_n \xrightarrow{D} \mathcal{N}(0, 1), \quad \text{i.e.} \quad \lim_{n \to \infty} F_{Z_n} = \int_{\infty}^{0} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx.
\]

Proof uses characteristic function of \( Z_n \), i.e. \( \phi_X(x) = \mathbb{E}[e^{itX}] \), leading

\[
\phi_{Z_n} = \phi \sum \frac{1}{n} Y_i(t) = (\phi_{Y_1}(t/\sqrt{n}))^n \quad (12.1)
\]

where \( Y_i = (X_i - \mathbb{E}[X]) / \sigma_X \). Then, \( \phi_{Y_1} \) is expanded using Taylor and only up-to second order term is kept. What remains is characteristic func of normal distribution.
Theorem

Let $u \in L^2[0, T]$ be a deterministic function. Then the process

$$X_t = \int_0^t u(s) \, ds + W_t, \quad 0 \leq t \leq T$$

(12.2)

is a Brownian motion with respect to the probability measure $Q$ given by

$$dQ = e^{\int_0^T u(s) \, dW_s - \frac{1}{2} \int_0^T u(s)^2 \, ds} \, dP.$$  

(12.3)
A solution algorithm for the fluid dynamic equations based on a stochastic model for molecular motion.  

*Molecular gas dynamics and the direct simulation of gas flows*.  

Fifth and sixth virial coefficients for hard spheres and hard disks.  

Equation of state for nonattracting rigid spheres.  
Fokker–Planck model for computational studies of monatomic rarefied gas flows. 

Fundamentals of Maxwel’s Kinetic Theory of a Simple Monatomic Gas: Treated as a Branch of Rational Mechanics, volume 83. 

The mathematical theory of non-uniform gases: an account of the kinetic theory of viscosity, thermal conduction and diffusion in gases. 
[8] Leslie F Greengard and Jingfang Huang.  
A new version of the fast multipole method for screened coulomb interactions in three dimensions.  

Non-local korteweg stresses from kinetic theory point of view.  

The surface properties of a Van der Waals fluid.  
On the existence of a class of maximum-entropy probability density functions (corresp.).

Gaussian process regression for maximum entropy distribution.

*Numerical solution of stochastic differential equations with jumps in finance*, volume 64.

Multilevel monte carlo methods. 