Computational Statistical Physics

Rarefied Gas Dynamics

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https://moodle-app2.let.ethz.ch/course/view.php?id=22042

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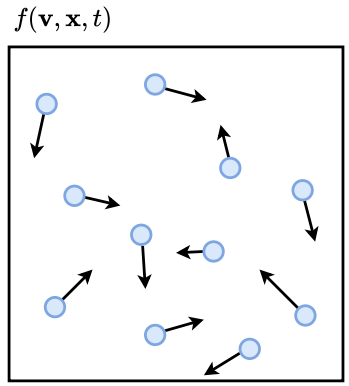
1.1 Kinetic Theory I

- Consider a particle system at rest:

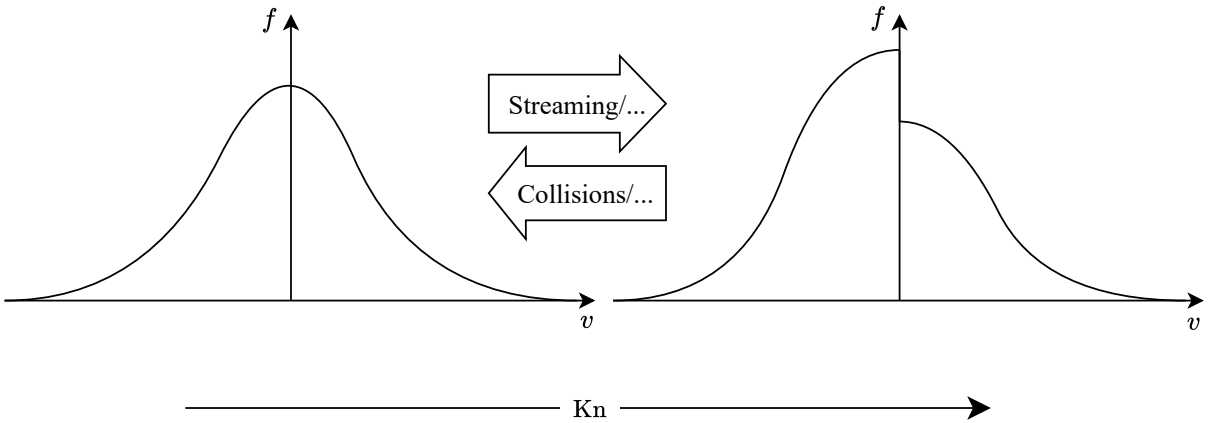


- At equilibrium, the distribution of particle velocity reach Gaussian (Maxwell-Boltzmann) distribution:

$$f^{\mathrm{eq}}(\boldsymbol{v}, \boldsymbol{x}, t) = n_0 \mathcal{N}(\boldsymbol{U}, \frac{k_b T}{m} \boldsymbol{I}) \tag{1}$$

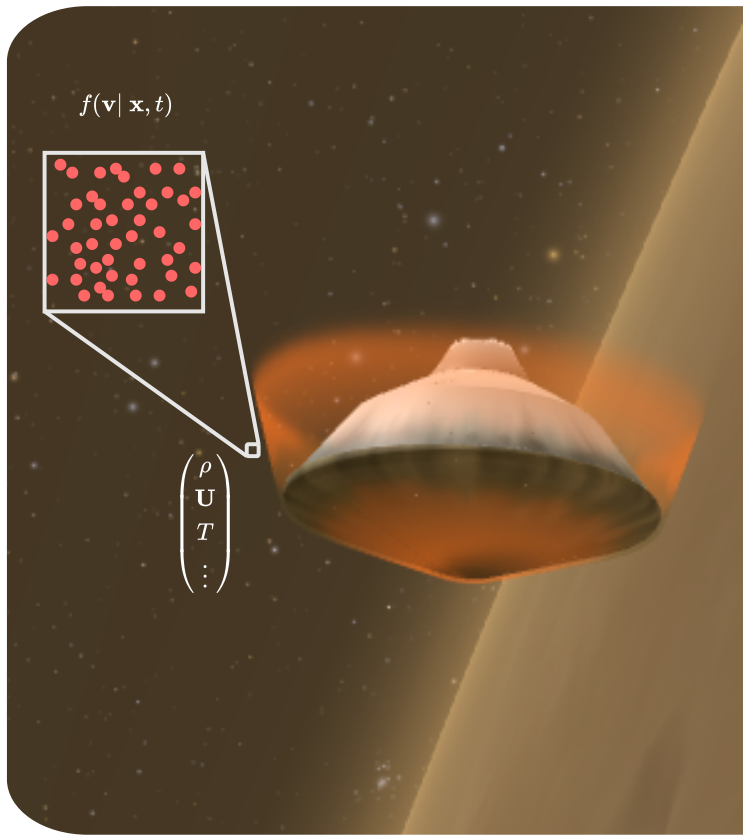
- Similarly, if we record the velocity of each particle in time, again we observe a Gaussian distribution.
- The idea is to describe a particle system statistically with a single particle distribution function, rather than N-body one.

1.1 Kinetic Theory II



$$\underbrace{\frac{\partial f}{\partial t}}_{\textit{transient}} + \underbrace{\nabla_{\boldsymbol{x}} \cdot (\boldsymbol{v} f)}_{\text{advection}} + \underbrace{\nabla_{\boldsymbol{v}} \cdot (\boldsymbol{H} f)}_{\text{long-range}} = \underbrace{S[f]}_{\text{short-range}}$$

Here, Knudsen number $\mathrm{Kn} := \lambda / L$, defined as the ratio of mean free path λ to problem length-scale L, is an indicator of rarefaction.



Ref.: nasa.gov/perseverance

1.2 Macroscopic Properties I

$$\text{Number Density:} \quad n(\boldsymbol{x}, t) = \int f(\boldsymbol{v}|\boldsymbol{x}, t) d\boldsymbol{v} \tag{2}$$

$$\text{Mass Density:} \quad \rho(\boldsymbol{x}, t) = m\ n(\boldsymbol{x}, t) \tag{3}$$

$$\text{Bulk Velocity:} \quad U_i(\boldsymbol{x}, t) = \frac{1}{n(\boldsymbol{x}, t)} \int v_i f(\boldsymbol{v}|\boldsymbol{x}, t) d\boldsymbol{v} \tag{4}$$

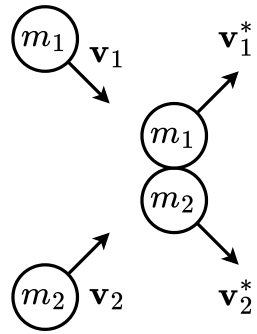
$$\text{Temperature:} \quad T = \frac{m}{3n(\boldsymbol{x}, t)k_b} \sum_{i=1}^{3} \int (v_i')^2 f(\boldsymbol{v}|\boldsymbol{x}, t) d\boldsymbol{v} \tag{5}$$

$$\text{Pressure Tensor:} \quad \pi_{ij}(\boldsymbol{x}, t) = \frac{1}{n(\boldsymbol{x}, t)} \int v_i' v_j' f(\boldsymbol{v}|\boldsymbol{x}, t) d\boldsymbol{v} \tag{6}$$

$$\text{Heat Flux:} \quad q_i(\boldsymbol{x}, t) = \frac{1}{2n(\boldsymbol{x}, t)} \int v_i' (\sum_j v_j') f(\boldsymbol{v}|\boldsymbol{x}, t) d\boldsymbol{v} \tag{7}$$

Here, $\boldsymbol{v}' := \boldsymbol{v} - \boldsymbol{U}$ is the fluctuating velocity, k_b is the Boltzmann constant, and m denotes the mass of each molecule.

1.3 Collision Rule I



- Consider momentum conservation

$$m_1 \boldsymbol{v}_1 + m_2 \boldsymbol{v}_2 = m_1 \boldsymbol{v}_1^* + m_2 \boldsymbol{v}_2^* \ . \tag{8}$$

Note: eq. (8) implies that the center of mass velocity $\boldsymbol{v}_m$ is conserved

$$\boldsymbol{v}_m = (m_1 \boldsymbol{v}_1 + m_2 \boldsymbol{v}_2)/(m_1 + m_2) \tag{9}$$

$$= (m_1 \boldsymbol{v}_1^* + m_2 \boldsymbol{v}_2^*)/(m_1 + m_2) \ . \tag{10}$$

1.3 Collision Rule II

Let us denote relative velocity by $\boldsymbol{g}$

$$\boldsymbol{g} = \boldsymbol{v}_1 - \boldsymbol{v}_2 \tag{11}$$

$$\boldsymbol{g}^* = \boldsymbol{v}_1^* - \boldsymbol{v}_2^* \tag{12}$$

and rewrite pre/post-collision velocity as

$$\boldsymbol{v}_1 = \boldsymbol{v}_m + \frac{m_2}{m_1 + m_2}\boldsymbol{g} \tag{13}$$

$$\boldsymbol{v}_2 = \boldsymbol{v}_m - \frac{m_1}{m_1 + m_2}\boldsymbol{g} \tag{14}$$

and

$$\boldsymbol{v}_1^* = \boldsymbol{v}_m + \frac{m_2}{m_1 + m_2}\boldsymbol{g}^* \tag{15}$$

$$\boldsymbol{v}_2^* = \boldsymbol{v}_m - \frac{m_1}{m_1 + m_2}\boldsymbol{g}^* \ . \tag{16}$$

1.3 Collision Rule III

- Consider the conservation of energy

$$m_1 v_1^2 + m_2 v_2^2 = m_1 v_1^{*2} + m_2 v_2^{*2} \ . \tag{17}$$

Let us reformulate cons. of energy in terms of $\boldsymbol{v}_m$ and $\boldsymbol{g}$

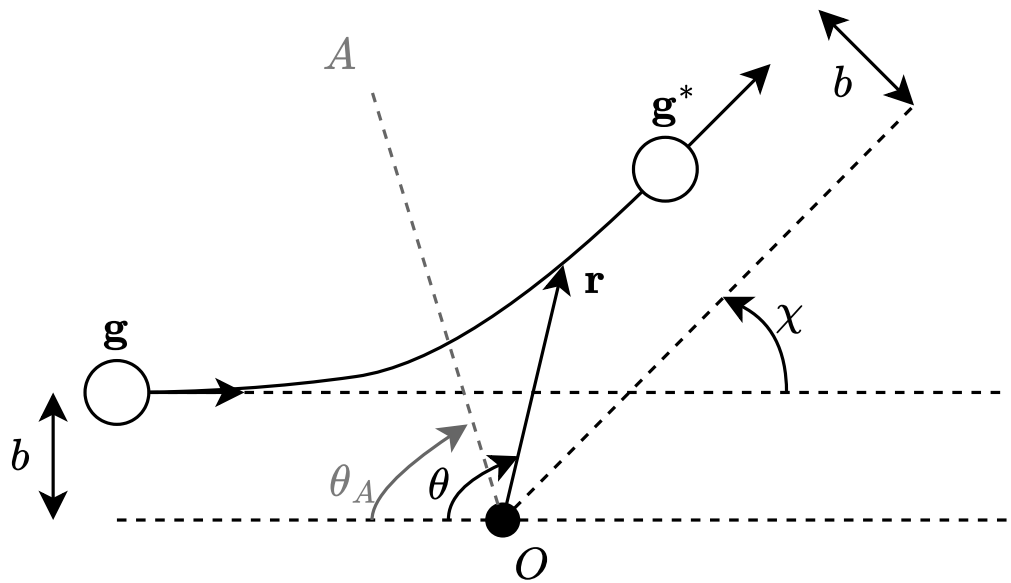
$$(m_1 + m_2) v_m^2 + m_r g^2 = (m_1 + m_2) v_m^2 + m_r g^{*2} \tag{18}$$

where $m_r = m_1 m_2 / (m_1 + m_2)$.
Note: eq. (18) implies that $g = g^*$.

1.3 Collision Rule IV

- Conservation of angular momentum enforces impact parameter b to be conserved during collision, i.e.

$$r^2\dot{\theta} = \text{const} = bg \tag{19}$$



Since both $\boldsymbol{g}$ and $\boldsymbol{v}_m$ can be computed from the pre-collision velocities, determining the post-collision velocity reduces to calculating the change in direction of relative velocity vector.

1.3 Collision Rule V

The energy within the force field is

$$\frac{1}{2}m_r(\dot{r}^2 + r^2\dot{\theta}^2) + \phi = \text{const} = \frac{1}{2}m_r g^2 \tag{20}$$

where ϕ is the intermolecular potential. Using conservation of angular momentum $r\dot{\theta} = bg$, we obtain the equation for orbit

$$\left(\frac{dr}{d\theta}\right)^2 = \frac{r^4}{b^2} - r^2 - \frac{\phi r^4}{\frac{1}{2}m_r g^2 b^2} \ . \tag{21}$$

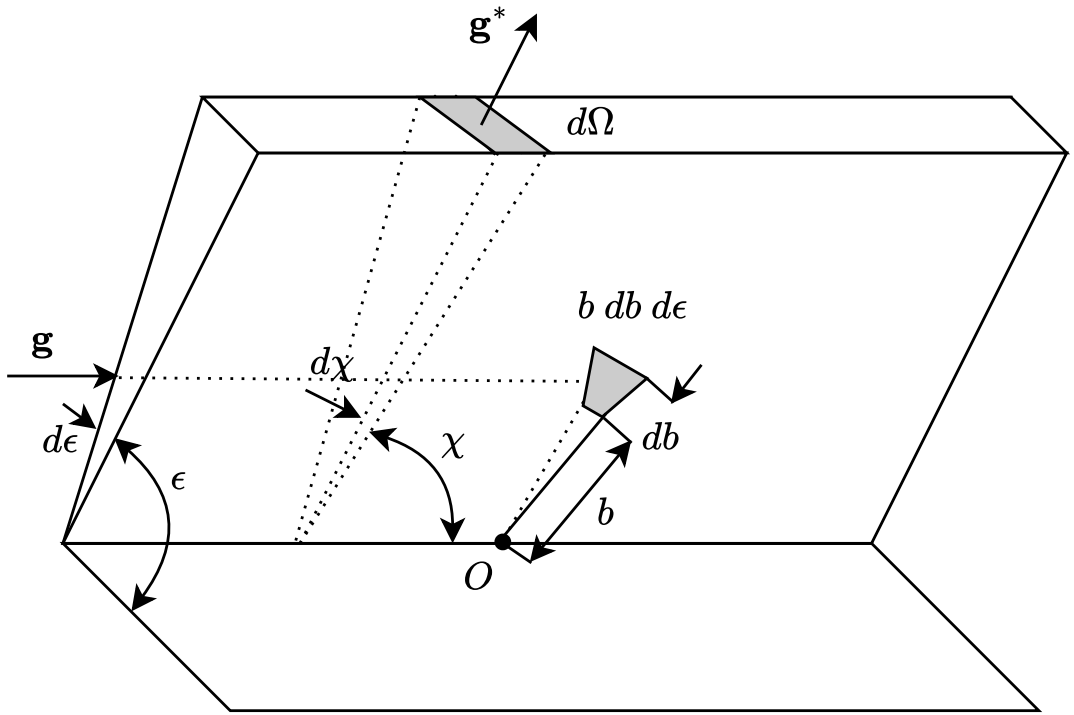
Consider $W = b/r$. The angle θ_A can be found by setting $dW/d\theta = 0$:

$$\theta_A = \int_0^{W_1} \sqrt{1 - W^2 - 2\phi/(m_r g^2)}\, dW \tag{22}$$

where W_1 is the positive root of $1 - W^2 - 2\phi/(m_r g^2) = 0$.
Deflection angle becomes $\chi = \pi - 2\theta_A$.

1.4 Boltzmann Collision Operator I

$$S[f(\boldsymbol{v}|.)] = \int_{\mathbb{R}^3} \int_0^{2\pi} \int (f(\boldsymbol{v}^*|.)f(\boldsymbol{v}_1^*|.) - f(\boldsymbol{v}|.)f(\boldsymbol{v}_1|.))gb \; dbd\epsilon d\boldsymbol{v}_1$$



Collisional cross-section $\sigma d\Omega$ relates to the impact parameters via

$$\sigma d\Omega = b \; db \; d\epsilon \tag{23}$$

1.4 Boltzmann Collision Operator II

$d\Omega$ is the unit solid angle about the vector $\boldsymbol{g}^*$ with

$$d\Omega = \sin(\chi)\ d\chi\ d\epsilon \tag{24}$$

so that

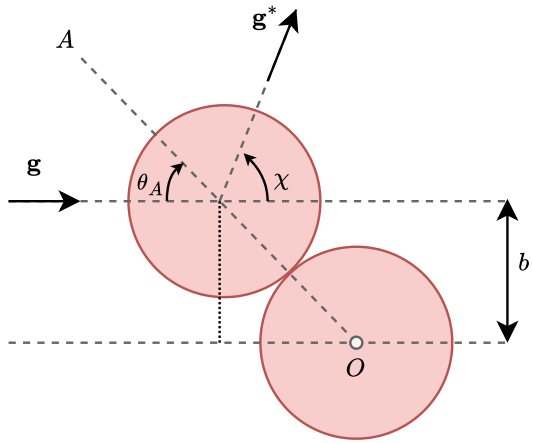
$$\sigma = \frac{b}{\sin(\chi)} \left| \frac{db}{d\chi} \right| . \tag{25}$$

Total collision cross section may be computed via substitution

$$\sigma_T = \int \sigma d\Omega = 2\pi \int_0^\pi \sigma \sin(\chi) d\chi \tag{26}$$

As we see later, this integral diverges for some molecular potentials, unless a finite **cut-off** for the impact parameter is introduced.

1.5 Hard Sphere Potential I



Denote $d_{12} := (d_1 + d_2)/2$

$$b = d_{12} \sin(\theta_A) = d_{12} \cos(\chi/2) \tag{27}$$

$$|db/d\chi| = \frac{1}{2} d_{12} \sin(\chi/2) \tag{28}$$

leading to

$$\sigma = d_{12}^2/4 \ . \tag{29}$$

1.5 Hard Sphere Potential II

Note that σ is independent of χ, hence the scattering is isotropic in the center of mass frame of reference, i.e. all directions are equally likely for $\boldsymbol{g}^*$.

Total cross section

$$\sigma_T = \int \sigma d\Omega = \pi d_{12}^2 \ . \tag{30}$$

1.6 Conservation Laws I

- It has been shown that the Boltzmann collision operator conserves mass/momentum/energy, leading to the conservation laws

$$\text{Mass Cons.:} \quad \frac{\partial}{\partial t}(\rho) + \sum_j \frac{\partial}{\partial x_j}(\rho U_j) = 0$$

$$\text{Momentum Cons.:} \quad \frac{\partial}{\partial t}(\rho U_i) + \sum_j \frac{\partial}{\partial x_j}(\rho U_i U_j + \pi_{ij}) + \rho H_i = 0$$

$$\text{Energy Cons.:} \quad \frac{\partial}{\partial t}(E) + \sum_i \frac{\partial}{\partial x_i}(E U_i + q_i + \pi_{ij} U_j) + \rho U_i H_i = 0$$

- Here, $E = \rho c_v T + \rho \boldsymbol{U} \cdot \boldsymbol{U}$ is the total energy, $c_v = 3k_b/(2m)$ is the heat capacity at constant volume.
- By perturbing f around equilibrium f^{eq}, i.e. small Kn, it is shown (Chapman-Enskog theory) that the outcome moment equations are the Euler equations for the zeroth and the Navier-Stokes-Fourier system of equations for the 1st order approximation.

1.7 H-Theorem I

- Consider spatially homogeneous system. Fractional change of f to $f + \Delta f$ is $\Delta f / f$ or $\Delta(\log f)$.
- Consider evolution of H function $H = \int f \log(f) d\boldsymbol{v}$.

$$\frac{\partial}{\partial t} \int f \log f \; d\boldsymbol{v} = \int S[f] \log f \; d\boldsymbol{v} \tag{31}$$

$$= \frac{1}{4} \int \int \int (\log f + \log f_1 - \log f^* - \log f_1^*) \left(f^* f_1^* - f f_1\right) \boldsymbol{g} \sigma d\Omega d\boldsymbol{v} d\boldsymbol{v}_1 \tag{32}$$

$$= \frac{1}{4} \int \int \int \log\left(f f_1 / f^* f_1^*\right) \left(f^* f_1^* - f f_1\right) \boldsymbol{g} \sigma d\Omega d\boldsymbol{v} d\boldsymbol{v}_1 \leq 0 \tag{33}$$

- Equality holds when $\log f$ is summational invariant

$$f^* f_1^* = f f_1, \quad \text{or equivalently} \tag{34}$$

$$\log f + \log f_1 = \log f^* + \log f_1^* \; . \tag{35}$$

It can be shown that at $\partial H / \partial t = 0$,

$$f = f^{\mathrm{eq}} \; . \tag{36}$$

1.8 Direct Simulation Monte Carlo I

Initialize $\boldsymbol{X}, \boldsymbol{V} \sim f(\boldsymbol{v}|\boldsymbol{x}, t = 0)$;
while $t < t_{final}$ **do**
  for *cell*$= 1, ..., N_{cells}$ **do**
    $N_{\mathrm{Cand}} = nN_{p/cell}\max(\sigma_T g)\Delta t$;
    for $j = 1, ..., N_{Cand}$ **do**
      Pick two particles from the cell;
      Draw $r \sim \mathcal{U}[0, 1]$;
      if $\sigma_T g / \max(\sigma_T g) > r$ **then**
        Draw $\epsilon \in [0, 2\pi]$ and χ given molecular potential ϕ;
        Collide selected particles following collision rule;
      end
    end
  end
  $\boldsymbol{X} = \boldsymbol{X} + \boldsymbol{V}\Delta t$ and apply BC;
  $t = t + \Delta t$;
end

1.8 Direct Simulation Monte Carlo II

- DSMC is considered the exact solution to the Boltzmann equation

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = \int \int \int (f(\boldsymbol{v}^*|.) f(\boldsymbol{v}_1^*|.) - f(\boldsymbol{v}|.) f(\boldsymbol{v}_1|.)) g \sigma d\Omega d\boldsymbol{v}_1 \ .$$

  For the proof, see [J. Stat. Phys. 66 (1992): 1011-1044].
- DSMC is heavily used in simulating rarefied gas dynamics and nano-scale fluid problems.
- It is the preferred numerical method for simulating non-equilibrium gas dynamics, since it is
  1. Consistent
  2. Conservative
  3. Stable
  4. Simple
- However, it faces challenges such as
  1. Statistical Noise.
  2. Complexity of $\mathcal{O}(1/\mathrm{Kn})$.

1.9 Variance Reduced DSMC I

Consider velocity moment $R(\boldsymbol{v}) \in \{1, v_i, v_i v_j ...\}$ of $f(\boldsymbol{v}|\boldsymbol{x}, t)$

$$\int Rf \; d^3\boldsymbol{v} = \int R\left(f - f^{\mathrm{eq}}\right) d^3\boldsymbol{v} + \int Rf^{\mathrm{eq}} d^3\boldsymbol{v}.$$

Defining weight as

$$w(\boldsymbol{v}|\boldsymbol{x}, t) = \frac{f^{\mathrm{eq}}(\boldsymbol{v}|\boldsymbol{x}, t)}{f(\boldsymbol{v}|\boldsymbol{x}, t)}$$

leads to

$$\int Rf \; d^3\boldsymbol{v} = \int R\left(1 - w\right) f d^3\boldsymbol{v} + \int Rf^{\mathrm{eq}} d^3\boldsymbol{v},$$

$$\langle R \rangle_{\mathrm{VR}} \approx N_{\mathrm{eff}} \sum_{i=1}^{N_p} R(\boldsymbol{V}^{(i)})(1 - W^{(i)}) + \underbrace{\int Rf^{\mathrm{eq}} d^3\boldsymbol{v}}_{\text{analytical comp.}} .$$

1.9 Variance Reduced DSMC II

$$S[f^{\mathrm{eq}}] = \frac{C}{2}\int(\delta_1^* + \delta_2^* - \frac{\delta_1}{w_2} - \frac{\delta_2}{w_1})w_1 w_2 f_1 f_2 \hat{g}\, b db d\epsilon d\boldsymbol{v}_1 d\boldsymbol{v}_2$$
$$+ \frac{C}{2}\int(-\delta_1 - \delta_2 + \frac{\delta_1}{w_2} + \frac{\delta_2}{w_1})\left(\frac{\hat{g}}{1-\hat{g}}\right) w_1 w_2 f_1 f_2 (1-\hat{g})\, b db d\epsilon d\boldsymbol{v}_1 d\boldsymbol{v}_2 \ .$$

$N_{\mathrm{Cand}} = nN_{p/cell}\max(\sigma_T \hat{g})\Delta t$;
for $j = 1, ..., N_{Cand}$ **do**
  Pick two particles from the cell;
  Draw $r \in \mathcal{U}[0,1]$;
  if $\sigma_T \hat{g}/\max(\sigma_T \hat{g}) < r$ **then**
    Collide selected particles;
    $W_1, W_2 = W_1 W_2$;
  end
  else
    $W_1 = W_1(1 - W_2\hat{g})/(1-\hat{g})$;
    $W_2 = W_2(1 - W_1\hat{g})/(1-\hat{g})$;
  end
end

Consistent

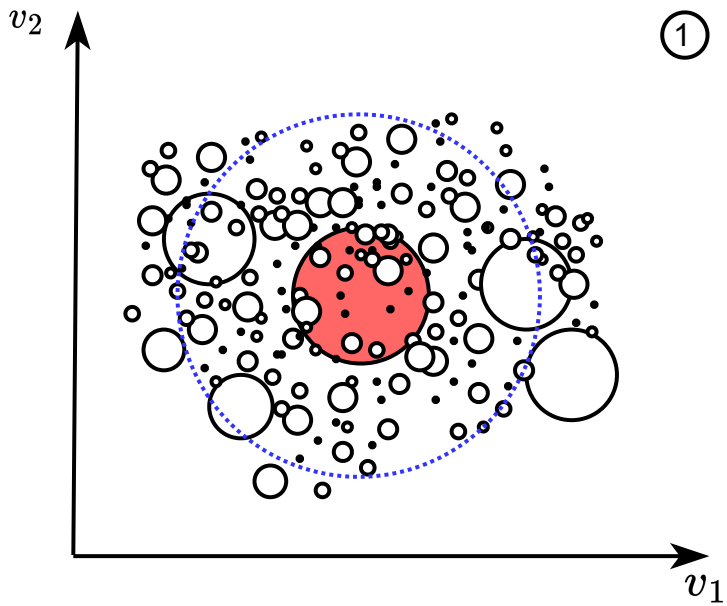
Unstable weight process

Non-conservative

Low variance without bias

1.9.1 Stabilization with kernel density estimation I

$$w^{\mathrm{KDE}}(\boldsymbol{v}|\boldsymbol{x},t) = \frac{\int \mathcal{K}(\boldsymbol{v}-\boldsymbol{v}'|h) w(\boldsymbol{v}'|\boldsymbol{x},t) f(\boldsymbol{v}'|\boldsymbol{x},t) d^3\boldsymbol{v}'}{\int \mathcal{K}(\boldsymbol{v}-\boldsymbol{v}'|h) f(\boldsymbol{v}'|\boldsymbol{x},t) d^3\boldsymbol{v}'}$$



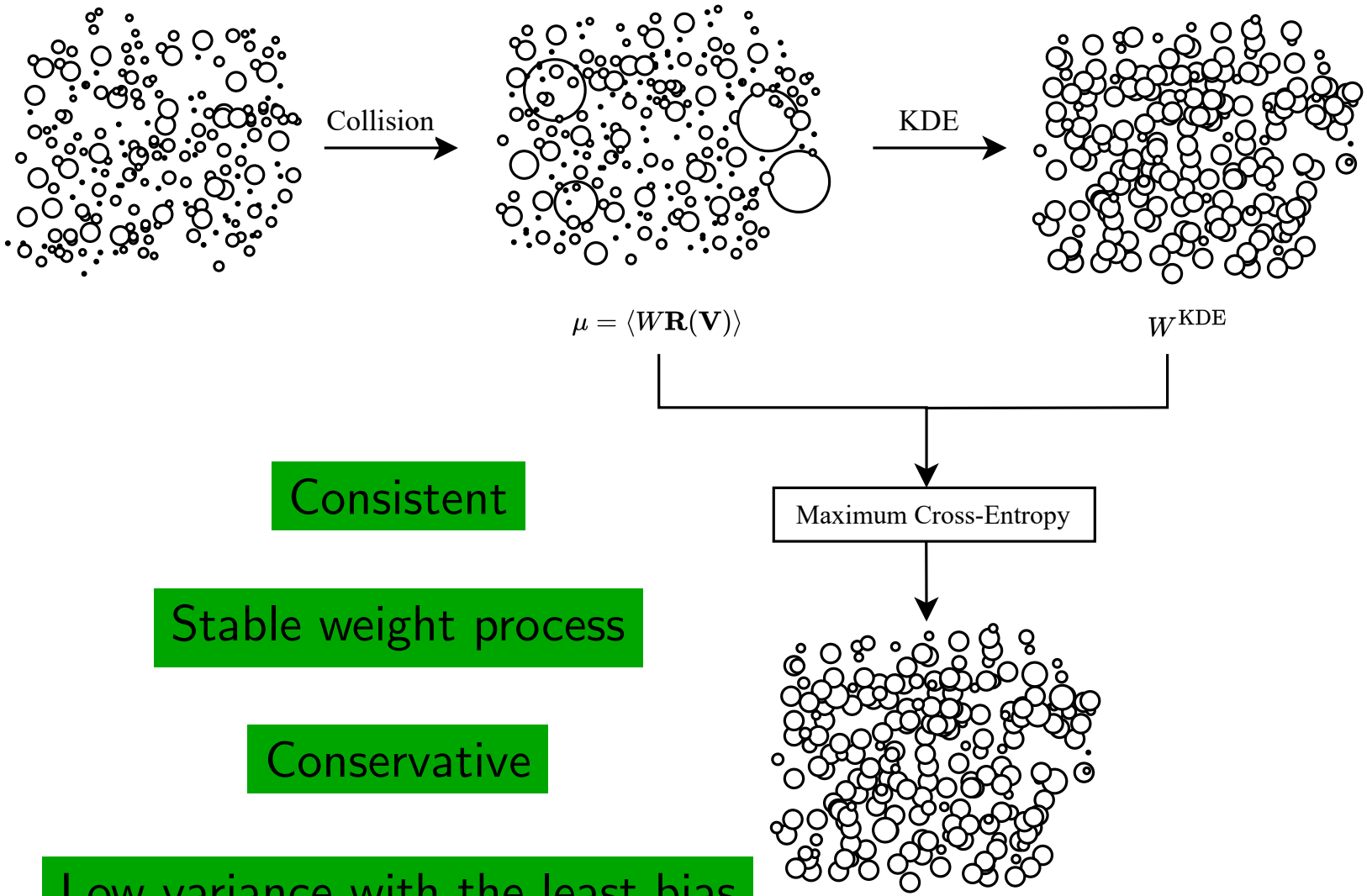
Consistent

Stable weight process

Non-conservative

Low variance with bias

1.9.2 Least Biased Variance Reduced DSMC I



Consistent

Stable weight process

Conservative

Low variance with the least bias

1.9.2 Least Biased Variance Reduced DSMC II

Given $\mathcal{F}^{\text{prior}}$ with samples $(\boldsymbol{V}, W^{\text{prior}})$ and target moments $\boldsymbol{\mu}$, let us find $\mathcal{F}$ using method of Lagrange multipliers

$$C[\mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t)] := \int \mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t) \log\left(\mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t)/\mathcal{F}^{\text{prior}}(\boldsymbol{v}|\boldsymbol{x},t)\right) d^3\boldsymbol{v} + \sum_{i=1}^{M} \lambda_i \left(\int R_i(\boldsymbol{v}) \mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t) d^3\boldsymbol{v} - \mu_i(\boldsymbol{x},t) \right).$$

The variational calculus gives us

$$\mathcal{F}(\boldsymbol{v}|\boldsymbol{x},t) = \mathcal{F}^{\text{prior}}(\boldsymbol{v}|\boldsymbol{x},t) \exp\left(\sum_{i=1}^{M} \lambda_i(\boldsymbol{x},t) R_i(\boldsymbol{v}) \right)$$

leading to weight update

$$W^{(k)} = W^{\text{prior},\,(k)} \exp\left(\sum_{i=1}^{M} \lambda_i R_i(\boldsymbol{V}^{(k)}) \right) \quad \text{for } k = 1, \ldots, N_p.$$

1.9.2 Least Biased Variance Reduced DSMC III

Lagrange multipliers can be computed using Newton-Raphson method

$$\boldsymbol{\lambda}^{(k+1)} = \boldsymbol{\lambda}^{(k)} - \boldsymbol{H}^{-1}(\boldsymbol{\lambda}^{(k)})\boldsymbol{g}(\boldsymbol{\lambda}^{(k)}),$$

where k indicates the iteration,

$$g_i = \mu_i - \int R_i \mathcal{F}^{\text{prior}} \exp\left(\sum_l \lambda_l R_l\right) d^3\boldsymbol{v} \quad \text{for } i = 1, ..., M \quad \text{and}$$

$$H_{i,j} = -\int R_i R_j \mathcal{F}^{\text{prior}} \exp\left(\sum_l \lambda_l R_l\right) d^3\boldsymbol{v} \quad \text{for } i, j = 1, ..., M \ .$$

Results: DSMC for Fourier problem

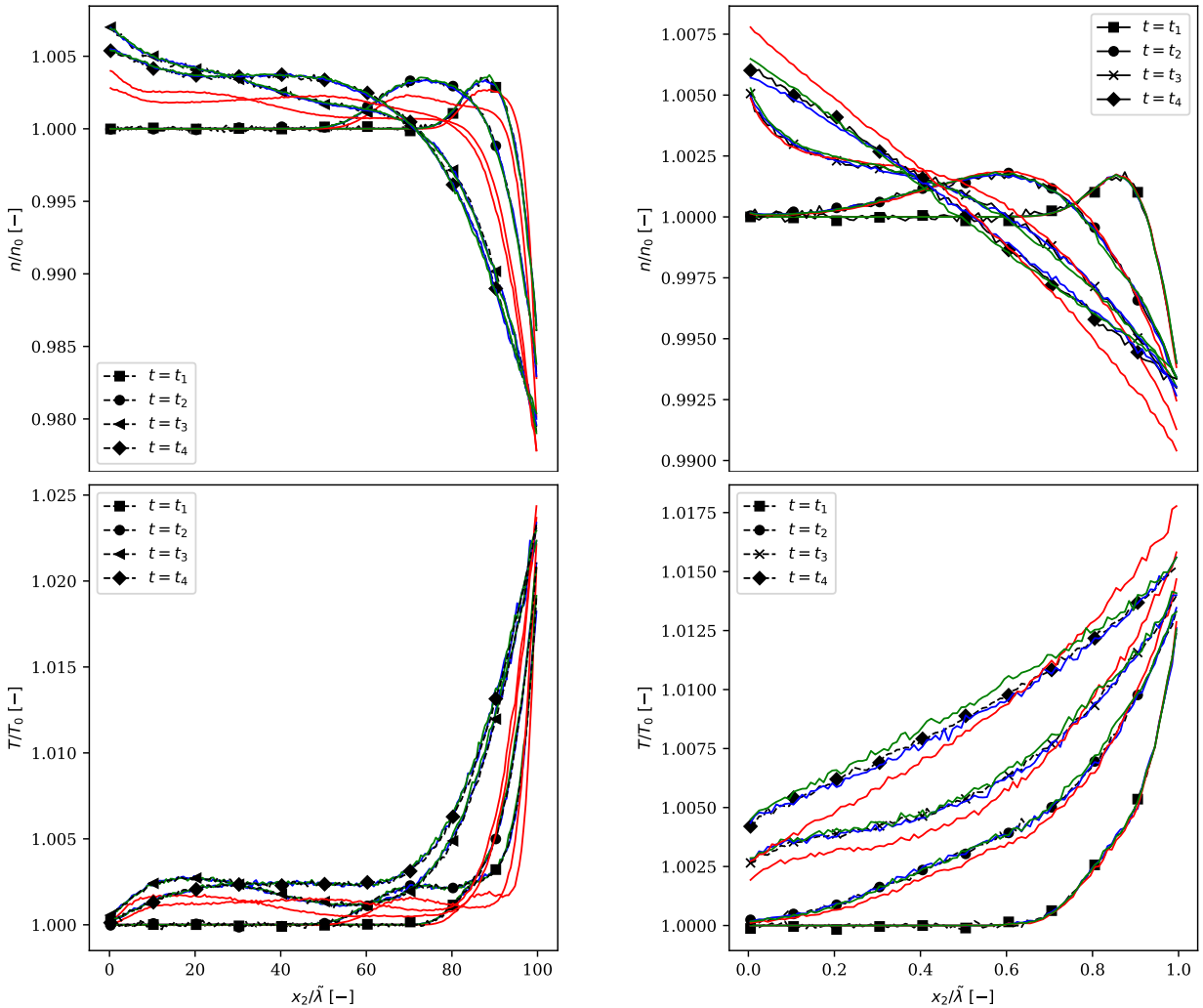
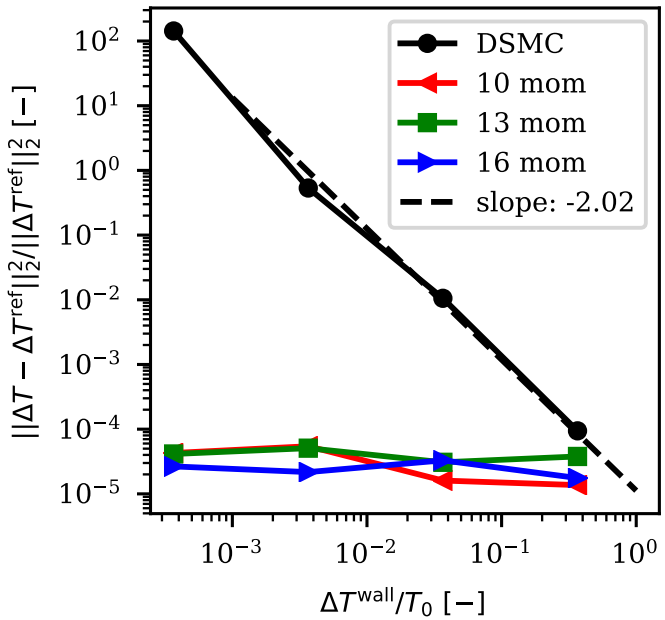
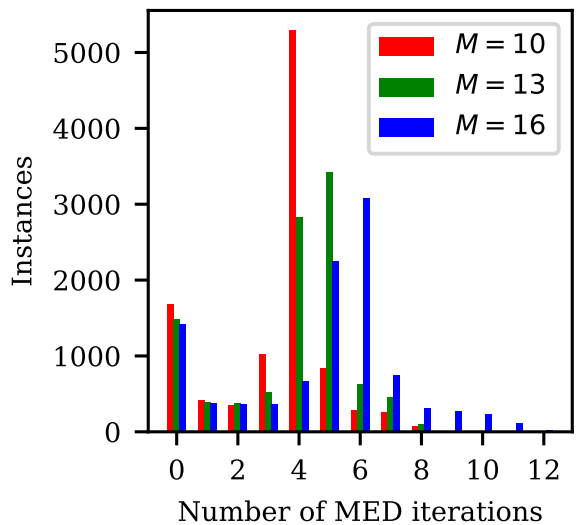
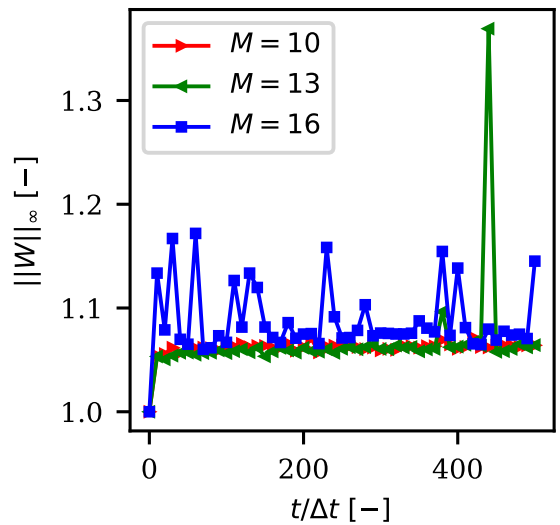


Figure: DSMC using 10^5 ensembles (black), ME-VRDSMC with $M = 10$ (red), $M = 13$ (blue) and $M = 16$ (green) using 50 ensembles. Left: $\mathrm{Kn} = 0.01$, right: $\mathrm{Kn} = 1$

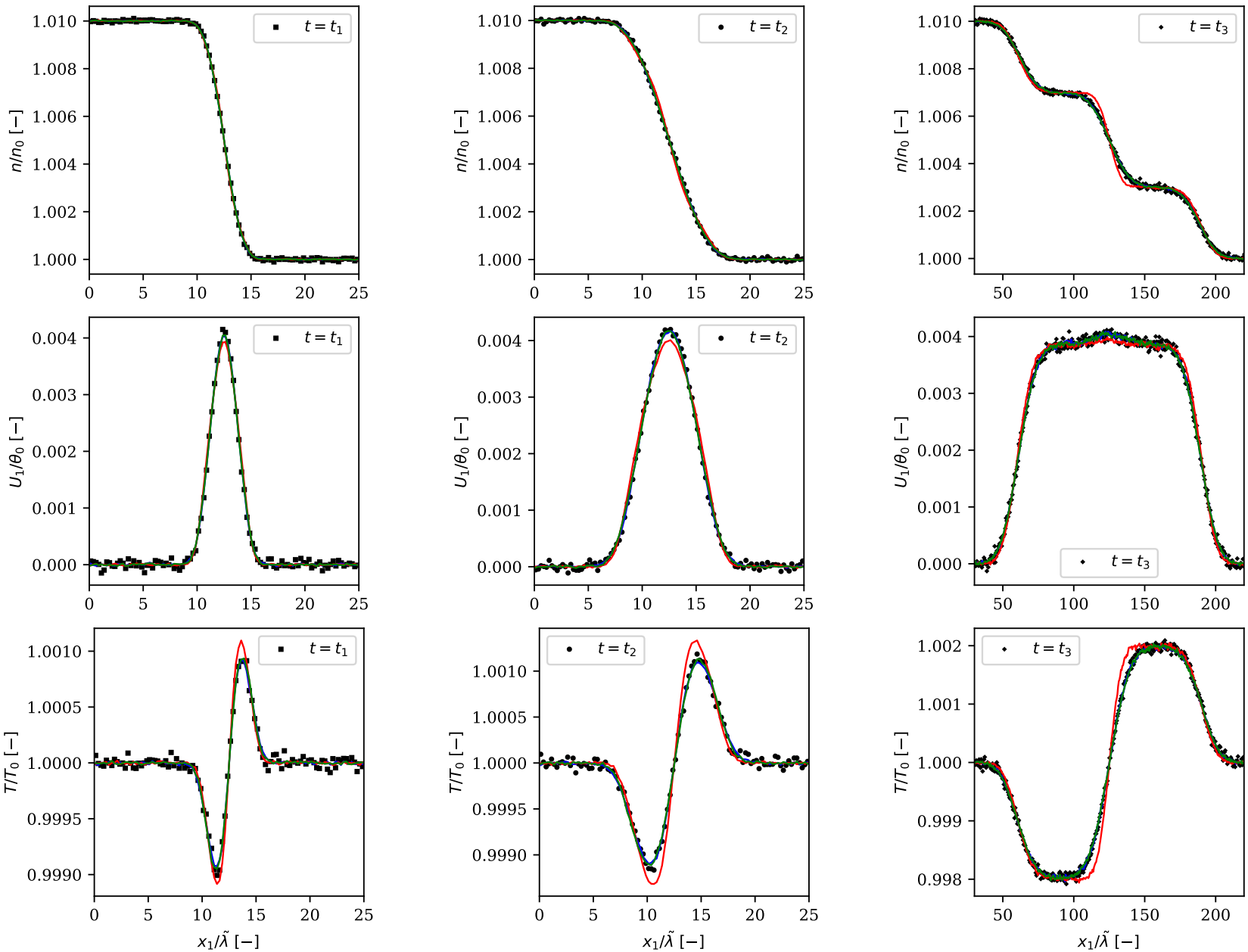
Results: DSMC for Fourier problem -cont.







Results: DSMC for shock tube test case



Results: DSMC for shock tube test case -cont.

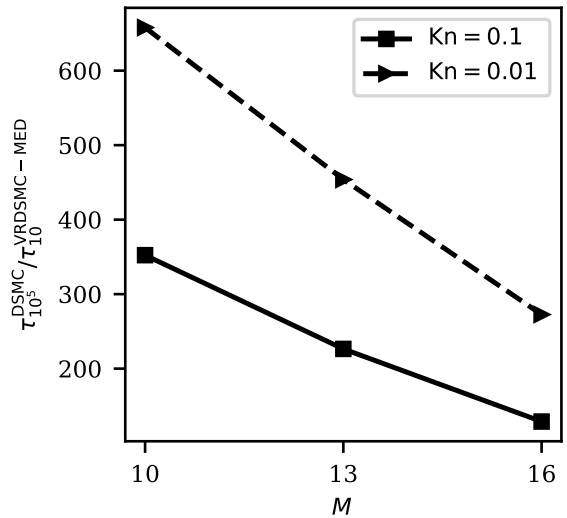


Figure: Speed-up in CPU time.

1.10 Coulomb interaction I

- For the Coulomb interaction with potential $\phi = q_1 q_2/(4\pi\epsilon_0 r)$, Rutherford found a relation between impact parameter b and the deflection angle χ

$$b = \frac{q_1 q_2}{4\pi\epsilon_0^2 m_r g^2} \cot(\chi/2) \tag{37}$$

where ϵ is the vacuum permittivity. Then,

$$\sigma = \frac{b}{\sin(\chi)} \left| \frac{db}{d\chi} \right| \tag{38}$$

$$= \left(\frac{q_1 q_2}{8\pi\epsilon_0 m_r g \sin^2(\chi/2)} \right)^2 . \tag{39}$$

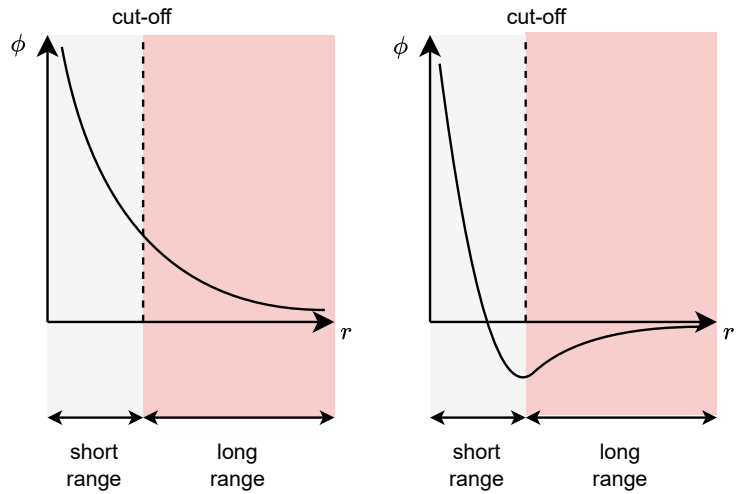
- Total cross sections

$$\sigma_T = 2\pi \int_0^\pi \sigma \sin(\chi) d\chi = 2\pi \int \left(\frac{q_1 q_2}{8\pi\epsilon_0 m_r g \sin^2(\chi/2)} \right)^2 d\chi \tag{40}$$

is divergent due to singularity of integrant at the small deflection angle, i.e. distant particles with large impact parameter b.

1.10 Coulomb interaction II

To cope with the singularity, a cut-off is needed to be introduced. This allows us to only treat short-range interactions with collision, while the long-range interaction is taken care of using the mean-field limit.



Let us deploy a cut-off r_{cut} and model the long-range interactions through the mean-field-theory in the evolution of single particle distribution function

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f - \underbrace{\nabla_{\boldsymbol{v}} \cdot \int_{r > r_{\text{cut}}} \int \nabla_{\boldsymbol{x}} \phi(\boldsymbol{x}, \boldsymbol{x}') f^{(2)}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{x}', \boldsymbol{v}') d\boldsymbol{x}' d\boldsymbol{v}'}_{I_{\text{long-range}}} = \underbrace{S(f)}_{\text{collision}} .$$

1.10 Coulomb interaction III

Using molecular chaos assumption, i.e. $f^{(2)}(\boldsymbol{x}, \boldsymbol{v}, \boldsymbol{x}', \boldsymbol{v}') = f(\boldsymbol{x}, \boldsymbol{v}) f(\boldsymbol{x}', \boldsymbol{v}')$, we obtain

$$
\begin{aligned}
I_{\text{long-range}} &= \nabla_{\boldsymbol{v}} \cdot \int_{r>r_{\text{cut}}} \int \nabla_{\boldsymbol{x}} \phi(\boldsymbol{x} - \boldsymbol{x}') \; f(\boldsymbol{x}, \boldsymbol{v}) f(\boldsymbol{x}', \boldsymbol{v}') d\boldsymbol{x}' d\boldsymbol{v}' \\
&= \nabla_{\boldsymbol{v}} f(\boldsymbol{x}, \boldsymbol{v}) \cdot \int_{r>r_{\text{cut}}} \nabla_{\boldsymbol{x}} \phi(\boldsymbol{x} - \boldsymbol{x}') \left(\int f(\boldsymbol{x}', \boldsymbol{v}') d\boldsymbol{v}' \right) d\boldsymbol{x}' \\
&= \nabla_{\boldsymbol{v}} f(\boldsymbol{x}, \boldsymbol{v}) \cdot \int_{r>r_{\text{cut}}} \nabla_{\boldsymbol{x}} \phi(\boldsymbol{x} - \boldsymbol{x}') n(\boldsymbol{x}') d\boldsymbol{x}' \\
&= \nabla_{\boldsymbol{v}} f(\boldsymbol{x}, \boldsymbol{v}) \cdot \nabla_{\boldsymbol{x}} \int_{r>r_{\text{cut}}} \phi(\boldsymbol{x} - \boldsymbol{x}') n(\boldsymbol{x}') d\boldsymbol{x}' \; . \qquad (41)
\end{aligned}
$$

1.10 Coulomb interaction IV

Substituting $\phi = qq'/4\pi r$ and taking the limit $r_{\text{cut}} \to 0$, i.e. assuming that the entire particle-particle interaction can be approximated with the mean-field limit, i.e.

$$I_{\text{long-range}} = q\nabla_{\boldsymbol{v}} f(\boldsymbol{x}, \boldsymbol{v}) \cdot \nabla_{\boldsymbol{x}} \underbrace{\int \frac{q'}{4\pi|\boldsymbol{x} - \boldsymbol{x}'|} n(\boldsymbol{x}') d\boldsymbol{x}'}_{\psi(\boldsymbol{x})} \ , \tag{42}$$

we quickly realize that the potential ψ is the fundamental solution to the Poisson equation in unbounded domains, i.e.

$$\nabla^2 \psi = -qn \ . \tag{43}$$

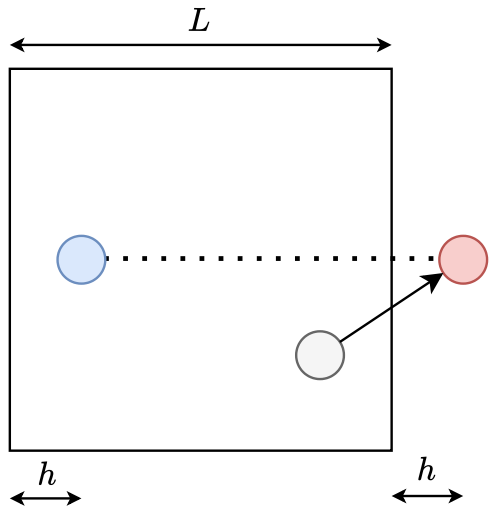
This allows us to compute the Coulomb interaction using fast Poisson solvers where short-range interactions do not need to be resolved.

However, for applications in the transition ($0.01 < \mathrm{K}n < 1$) and collisional regime ($\mathrm{K}n < 0.01$) , both long and short range interactions need to be simulated accurately.

1.10 Coulomb interaction V

This can done by combining a DSMC-based solver that resolves the Coulomb collision for the short-range interaction and use mean-field limit approximation with Poisson solver for the long-range interaction.

1.11.1 Periodic I

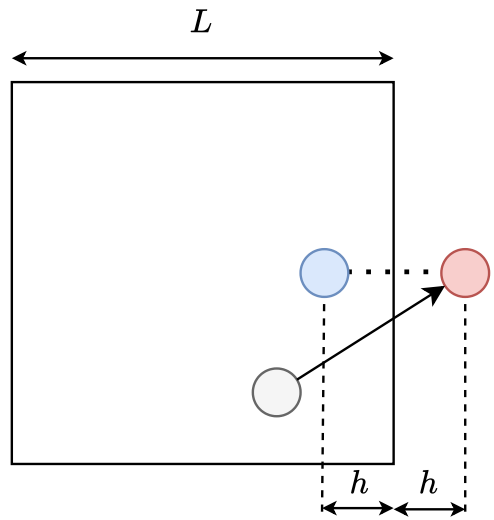


Periodic boundary condition can be simply implemented by re-entering the particles form the opposite side to the domain.

1.11.2 Specular Wall I

In case of specular wall, particles are simply reflected at the boundary. This corresponds to the BC on distribution

$$f(\boldsymbol{v}, \boldsymbol{x}, t) = f(\boldsymbol{v}, -\boldsymbol{x}, t) \ . \tag{44}$$



1.11.3 Thermal Wall I

For thermal wall, the particle velocity needs to be resampled from the wall's distribution. Often, the wall is assumed to be at equilibrium. The normal to the wall component of the new velocity should be sampled from the flux of Gaussian, i.e.

$$V_1 \sim v_1 \mathcal{N}(v_1 | 0, k_b T_{\text{wall}}/m) \tag{45}$$

$$= \pm\sqrt{2 k_b T^{\text{wall}}/m}\sqrt{-\log(\alpha)} \tag{46}$$

where $\alpha \sim \text{Uniform}([0,1])$. Then, particles need to be launched from the boundary back to the domain with the new velocity.