Monte Carlo method with negative particles

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The long range Coulomb collisions in plasma can be modeled by Landau-Fokker-Planck (LFP) equation

$$\frac{\partial f}{\partial t} = Q_{LFP}(f,f),$$

with binary collision term

$$Q_{LFP}(f,f) = \frac{1}{4} \frac{\partial}{\partial v_i} \int_{\mathbb{R}^3} u^{-3}(u^2 \delta_{ij} - u_i u_j) \left( \frac{\partial}{\partial v_j} - \frac{\partial}{\partial w_j} \right) f(w)f(v) \, dw.$$  

Problem in DSMC

- As $f \to m$, most computation is spent on the collision between particles sampled from $m$.
- $Q_{LFP}(m,m) = 0$. The major part of collisions has no net effect.

Highly inefficient!
Hybrid methods with “negative” particles

Apply splitting

\[ f(v) = m(v) + f_d(v), \]

- Equilibrium \( m(v) \): evolved according to a fluid equation – cheap
  - In spatial homogeneous case, \( m(v) \) can be constant.
- Deviation \( f_d(v) \): represented by particles – expensive

To minimize the deviation part, we allow \( f_d(v) < 0 \). Write

\[ f(v) = m(v) + f_p(v) - f_n(v), \]

with \( f_p(v) \geq 0, f_n(v) \geq 0 \).

We introduce “negative particles” to represent \( f_n \).

- \( f_p \) and \( f_n \) are represented by P and N particles.
Negative particle methods for rarefied gas

(Hadjiconstantinou 05)

One negative particle means the number of particle is $-1$.

- An $N$ particle cancels a $P$ particle with the same velocity
  \[ w_+ + w_- = 0 \text{ particle.} \]

- A $P$-$N$ collision cancels a regular $P$-$P$ collision
  \[
  \begin{align*}
  \text{P-P: } & \quad v_+, w_+ \rightarrow v_+', w_+', \\
  \text{P-N: } & \quad v_+, w_- \rightarrow 2v_+, v_-, w_-.
  \end{align*}
  \]

This can be derived from the Boltzmann equation.
Particle number increases!

In rarefied gas (charge free),
- short range collision $\Rightarrow$ # collisions in one time step = $O(\Delta t)$
- The particle number grows in the physical scale

$$\left. (N_p + N_n) \right|_{t+\Delta t} = (1 + c\Delta t) \left. (N_p + N_n) \right|_t.$$ 

In Coulomb gas (charged),
- long range collision $\Rightarrow$ # collisions in one time step = $N$
- The particle number grows in the numerical scale in Coulomb collisions!

$$\left. (N_p + N_n) \right|_{t+\Delta t} = \left(1 + \frac{N_m + 2N_n}{N_m + N_p - N_n} \right) \left. (N_p + N_n) \right|_t.$$
A new negative particle method for general binary collisions
The Boltzmann equation \( \partial_t f = Q(f,f) \) is reformulated

\[
\partial_t f = Q(f,f) = Q(f,f_p) - Q(f,f_n) + Q(f,m) = Q(f,f_p) - Q(f,f_n) + Q(f_p - f_n, m) + Q(m,m),
\]

and split:

\[
\begin{align*}
\partial_t m &= Q(m,m) = 0, \\
\partial_t f_p &= Q(f,f_p) + (Q(f_p - f_n, m))_+, \\
\partial_t f_n &= Q(f,f_n) + (Q(f_p - f_n, m))_.
\end{align*}
\]
Key idea # 1: Combine collisions

The Boltzmann equation $\partial_t f = Q(f,f)$ is reformulated

$$\partial_t f = Q(f,f) = Q(f,f_p) - Q(f,f_n) + Q(f,m)$$

$$= Q(f,f_p) - Q(f,f_n) + Q(f_p - f_n, m) + Q(m,m),$$

and split:

$\partial_t m = Q(m,m) = 0,$

$\partial_t f_p = Q(f,f_p) + (Q(f_p - f_n, m))_+, $

$\partial_t f_n = Q(f,f_n) + (Q(f_p - f_n, m))_-.$

P - P   P - N   M - M  
N - P   N - N   N - M  
M - P   M - N   P - M
Key idea # 1: Combine collisions

Apply a forward Euler method in time. A Monte Carlo method:

\[
f_p(t + \Delta t) = f_p + \Delta t Q(f, f_p) + \Delta t (Q(f_p - f_n, m))_+.
\]

regular collisions between \( f \) and \( f_p \),
\( N_p \) not change

source term,
\( N_p \) increases by
\( O(\Delta t (N_p + N_n)) \)

The particle number grows in the physical scale for any binary collisions

\[
(N_p + N_n)_{t+\Delta t} = (1 + c\Delta t) (N_p + N_n)_t.
\]
Step 1, collisions between $f$ and $f_p$

\[ f_p(t + \Delta t) = f_p + \Delta t Q(f, f_p) + \Delta t (Q(f_p - f_n, m))_. \]

Sample a particle from $f$ and collide with a P particle. How?

- $f = m + f_p - f_n$.  
- Need to recover the distributions $f_p$ and $f_n$ from P and N particles $\Rightarrow$ computationally expensive and inaccurate.
Key idea # 2: Approximate $f$ by F particles

We introduce F particles

- give a solution to the original equation $\partial_t f = Q(f, f)$.
  - Initially sampled from $f(v, t = 0)$ directly. Then perform regular DSMC method.
- To sample a particle from $f$, just randomly pick one sample from F particles.

One only needs

$(\text{F particles}) \geq N_p + N_n$.

Hence

- F particles give a coarse approximation of $f$.
- P and N particles are finer approximation of $f - m$. 
The new method

A new Monte Carlo method with negative particles

\[
\begin{align*}
\partial_t m &= 0, \\
\partial_t f_p &= Q(f, f_p) + (Q(f_p - f_n, m))_+, \\
\partial_t f_n &= Q(f, f_n) + (Q(f_p - f_n, m))_.
\end{align*}
\]
A new Monte Carlo method with negative particles

\[
\begin{align*}
\partial_t \tilde{f} &= Q(\tilde{f}, \tilde{f}), \\
\partial_t m &= 0, \\
\partial_t f_p &= Q(\tilde{f}, f_p) + (Q(f_p - f_n, m))_+, \\
\partial_t f_n &= Q(\tilde{f}, f_n) + (Q(f_p - f_n, m))_-. 
\end{align*}
\]

- $\tilde{f}$: coarse solution. Simulated by F particles.
- $f = m + f_p - f_n$: finer solution, the desired result. Simulated by P and N particles.
To summarize

- Combine collisions to reduce the total number of collisions.
- Use F particles to perform the combined collisions.
An extra step: Particle Resampling

Global interpolation

\[ f_P - f_n \]

Resample
Particle resampling is accurate but expensive. But it is only needed whenever $N_{\tilde{f}} \geq (N_p + N_n)$ is violated.

After resampling, only need to keep a subset of the F particles.
Figure: The snaps of time evolution of marginal distribution \( \int f(v_x, v_y, v_z) \, dv_y \, dv_z \) in Bump-on-Tail problem.
Figure: The snaps of time evolution of the components $m, f_p$ and $f_n$ in Bump-on-Tail problem.
Convergence test

Figure: The convergence rate for fine solution $f$ and coarse solution $\tilde{f}$ at different times. Test on Rosenbluth’s problem.
Efficiency test

Figure: The efficiency test on Rosenbluth’s problem.
Future work

- Multi-component plasma.
- Evolve Maxwellian part $m$ to further improve the efficiency.
- General non-linear operators.
- Spatial inhomogeneous. **Design a hybrid method which uses very few particles in the fluid regime.**