Structure-preserving marker-particle discretizations of Coulomb collisions for particle-in-cell codes

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PIC codes commonly use the following representation for the distribuion function

$$f_h(\boldsymbol{z},t)d\boldsymbol{z} = \sum_p w_p \delta(\boldsymbol{x}-\boldsymbol{x}_p(t))\delta(\boldsymbol{v}-\boldsymbol{v}_p(t))d\boldsymbol{z}. \tag{1}$$

Here, and throughout, the notation $\boldsymbol{z}=(\boldsymbol{x},\boldsymbol{v})$ rerefs to phase-space coordinates. For convenience, we also group the variables together into spatial positions $\boldsymbol{X}=\{\boldsymbol{x}_p\}_p$, velocities $\boldsymbol{V}=\{\boldsymbol{v}_p\}_p$, and marker weights $W=\{w_p\}_p$. Ideally, an implementation of Coulomb collisions in a PIC code should preserve the discrete versions of the kinetic momentum and energy, namely

$$\boldsymbol{P}(\boldsymbol{X},\boldsymbol{V};W) = \sum_p w_p m \boldsymbol{v}_p, \tag{2}$$

$$K(\boldsymbol{X},\boldsymbol{V};W) = \sum_p w_p \frac{m}{2}|\boldsymbol{v}_p|^2. \tag{3}$$

Additionally, the collisions should dissipate entropy.

Evaluating the standard entropy expression with respect to the distribution (1), however, is not generally possible, and an approximation of some level must be introduced. Carrillo et al. [1] introduced the idea of using a regularized entropy, where the distribution is smoothed out with a radial basis function ψ_ε and the entropy replaced by an expression such as

$$S_\varepsilon[\boldsymbol{X},\boldsymbol{V};W] = -\int \sum_p w_p \psi_\varepsilon(\boldsymbol{z}-\boldsymbol{z}_p)\ln\left(\sum_{p'} w_{p'}\psi_\varepsilon(\boldsymbol{z}-\boldsymbol{z}_{p'})\right)d\boldsymbol{z}. \tag{4}$$

This realization enabled a construction of a deterministic marker-particle integrator for Coulomb collisions. While the integrator presented in [1] preserves the kinetic momentum, it does not preserve the kinetic energy.

To fix the missing energy conservation, I have proposed in [2] the following collisional single-species particle-update scheme which can be generalized to multiple species

$$\frac{\boldsymbol{v}_p^{n+1}-\boldsymbol{v}_p^n}{\Delta t} = \frac{\nu}{m}\sum_{\bar{p}} w_{\bar{p}} \mathbf{1}(p,\bar{p})\mathbb{Q}(\boldsymbol{v}_p^{n+1/2}-\boldsymbol{v}_{\bar{p}}^{n+1/2})\cdot\boldsymbol{\Gamma}(S_\varepsilon^n,p,\bar{p}). \tag{5}$$

Here $\nu = 2\pi e^2 \ln\Lambda$ is the collisional coefficient, the midpoint velocity is defined according to $\boldsymbol{v}_p^{n+1/2} = (\boldsymbol{v}_p^{n+1}+\boldsymbol{v}_p^n)/2$, and the notation $A^n = A(\boldsymbol{X},\boldsymbol{V}^n;W)$ refers to the function A being

evaluated with respect to $\boldsymbol{v}_p^n$. The indicator function $\mathbf{1}(p,\bar{p})$ is either one or zero depending on whether the coordinates $\boldsymbol{x}$ of particles p and $\bar{p}$ are within the same spatial collision cell or not. The matrix $\mathbb{Q}(\boldsymbol{\xi})$ is the expression familiar from the Landau collision operator, a scaled projection onto a plane perpendicular to $\boldsymbol{\xi}$

$$\mathbb{Q}(\boldsymbol{\xi}) = \frac{1}{|\boldsymbol{\xi}|}\left(\mathbb{I} - \frac{\boldsymbol{\xi}\boldsymbol{\xi}}{|\boldsymbol{\xi}|^2}\right), \tag{6}$$

with $\mathbb{I}$ the identity matrix in three dimensions. The vector $\boldsymbol{\Gamma}(A,p,\bar{p})$ is defined as

$$\boldsymbol{\Gamma}(A,p,\bar{p}) = \frac{1}{mw_p}\frac{\partial A}{\partial \boldsymbol{v}_p} - \frac{1}{mw_{\bar{p}}}\frac{\partial A}{\partial \boldsymbol{v}_{\bar{p}}}. \tag{7}$$

For a detailed description of the derivation of this scheme, the reader should consult [2].

This new scheme will conserve the kinetic energy for

$$\begin{aligned}
\frac{K^{n+1}-K^n}{\Delta t} &= \sum_p w_p m \boldsymbol{v}_p^{n+1/2} \cdot \frac{\boldsymbol{v}_p^{n+1}-\boldsymbol{v}_p^n}{\Delta t} \\
&= \nu \sum_{p,\bar{p}} w_p w_{\bar{p}} \mathbf{1}(p,\bar{p}) \boldsymbol{v}_p^{n+1/2} \cdot \mathbb{Q}(\boldsymbol{v}_p^{n+1/2} - \boldsymbol{v}_{\bar{p}}^{n+1/2}) \cdot \boldsymbol{\Gamma}(S_\varepsilon^n, p, \bar{p}) \\
&= \frac{\nu}{2} \sum_{p,\bar{p}} w_p w_{\bar{p}} \mathbf{1}(p,\bar{p}) (\boldsymbol{v}_p^{n+1/2} - \boldsymbol{v}_{\bar{p}}^{n+1/2}) \cdot \mathbb{Q}(\boldsymbol{v}_p^{n+1/2} - \boldsymbol{v}_{\bar{p}}^{n+1/2}) \cdot \boldsymbol{\Gamma}(S_\varepsilon^n, p, \bar{p}) \\
&= 0,
\end{aligned} \tag{8}$$

owing the the projection property of the matrix $\mathbb{Q}$ and the antisymmetry of the vector $\boldsymbol{\Gamma}$. The scheme also preserves the discrete-time kinetic momentum for

$$\begin{aligned}
\frac{\boldsymbol{P}^{n+1}-\boldsymbol{P}^n}{\Delta t} &= \sum_p w_p m \frac{\boldsymbol{v}_p^{n+1}-\boldsymbol{v}_p^n}{\Delta t} \\
&= \nu \sum_{p,\bar{p}} w_p w_{\bar{p}} \mathbf{1}(p,\bar{p}) \mathbb{I} \cdot \mathbb{Q}(\boldsymbol{v}_p^{n+1/2} - \boldsymbol{v}_{\bar{p}}^{n+1/2}) \cdot \boldsymbol{\Gamma}(S_\varepsilon^n, p, \bar{p}) \\
&= \frac{\nu}{2} \sum_{p,\bar{p}} w_p w_{\bar{p}} \mathbf{1}(p,\bar{p}) (\mathbb{I} - \mathbb{I}) \cdot \mathbb{Q}(\boldsymbol{v}_p^{n+1/2} - \boldsymbol{v}_{\bar{p}}^{n+1/2}) \cdot \boldsymbol{\Gamma}(S_\varepsilon^n, p, \bar{p}) \\
&= 0.
\end{aligned} \tag{9}$$

The simple integrator does not guarantee a strict algebraic dissipation of entropy. This can be obtained, though, with a so-called discrete gradient integrator. Similarly, with the help of discrete gradients, an energy and density conserving and entropy dissipating marker-particle discretization of the electrostatic gyrokinetic Landau collision operator is possible. Due to space contraints, these are not discussed in the current exposition. Instead, the reader is directed to [2] for details.

To back up the claims regarding the momentum and energy conservation, an example simulating the collisional relaxation of a double-Maxwellian distribution function in a reduced 2-D

setting is provided. Essentially, the demonstration will be a replication of the example 3 described in Sec. 4.3 of Ref. [1] but with a different algorithm.

The physical parameters, m, ν, as well as the integral of the distribution over the dimensionless velocity space, are set to one. The initial state for the distribution is chosen as

$$f(\boldsymbol{v},t=0)=\frac{1}{4\pi}\left[\exp\left(-\frac{(\boldsymbol{v}-\boldsymbol{u}_1)^2}{2}\right)+\exp\left(-\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{2}\right)\right], \tag{10}$$

where the peaks of the Maxwellians are $\boldsymbol{u}_1=(-2,1)$ and $\boldsymbol{u}_2=(0,-1)$. The energy and momentum of this distribution are $E=2.5$ and $\boldsymbol{P}=(-1,0)$ respectively. The radial basis function ψ_ε is chosen to be the Gaussian

$$\psi_\varepsilon(\boldsymbol{v})=\frac{1}{2\pi\varepsilon}\exp\left(-\frac{|\boldsymbol{v}|^2}{2\varepsilon}\right), \tag{11}$$

with $\varepsilon=0.64h^{1.98}$, the parameter $h=2L/\sqrt{N}$, $L=10$, and the total particle number $N=60^2=3600$. The particles are initialized in a regular grid in the domain $[-L,L]\times[-L,L]$ and the weights adjusted to match the initial distribution. The discrete entropy functional is computed with a 2-D Gauss-Hermite quadrature, localizing a 6-by-6 mesh of quadrature points to the velocity position of each particle.

In this demonstration, I will push the particles with the scheme (5) using a time step of $\Delta t=1/16$. The resulting nonlinear system is solved using fixed-point iteration with the tolerance for the iteration set to 1E-15. The program for the demonstration has been written in `Python`, parallelized with `CUDA` via use of the `Numba` package, and the simulations have been performed on a single `NVIDIA` Quaddro K2200 GPU card. The source code for the implementation is available upon request from the author. The collisional evolution of the distribution function according to the chosen implicit particle push is illustrated in Fig. 1 by evaluating $\psi_\varepsilon * f_h$ on a regular mesh in the domain $[-L,L]\times[-L,L]$. The panels indicate the time steps #(1,10,30,60,120,200) from left to right and top down. The corresponding values for the kinetic momentum and energy are recorded in Table 1 demonstrating the conservation laws.

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References

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[2] Eero Hirvijoki. Structure-preserving marker-particle discretizations of Coulomb collisions for particle-in-cell codes. *Plasma Physics and Controlled Fusion*, 63(4):044003, April 2021. doi: 10.1088/1361-6587/abe884.

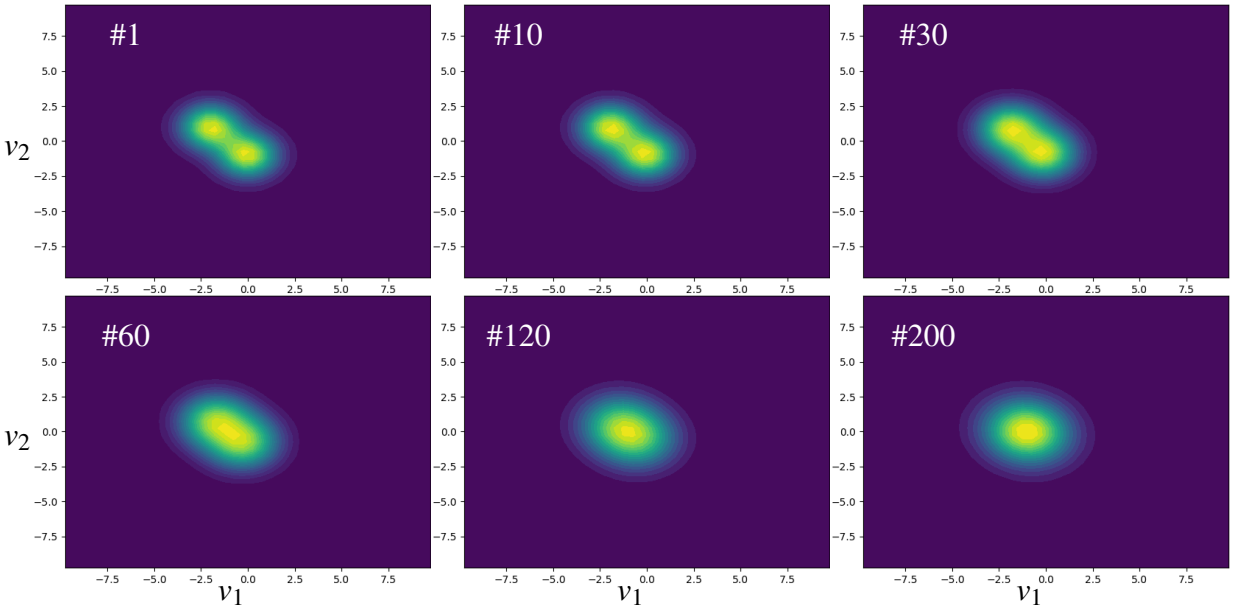

Figure 1: Collisional relaxation of a double Maxwellian (10). The panels describe snapshots of the steps #$(1, 10, 30, 60, 120, 200)$ from left to right and top down. The axes in the panels refer to the velocity coordinates (v_1, v_2) in the domain $[-L, L] \times [-L, L]$ and the color indicates the level sets of the distribution function from zero (deep blue) to the instantaneous maximum values (bright yellow) for optimal visual contrast.

Step #	P_1	P_2	E
1	-0.9999999999999982	-1.8617208789871285E-16	2.499999999999991
10	-0.9999999999999984	-4.263625043299246E-16	2.4999999999999907
30	-0.9999999999999981	-1.4125799054770516E-16	2.500000000000011
60	-0.9999999999999984	-1.2262462096082616E-15	2.5000000000000293
120	-0.9999999999999974	4.1795993749316196E-17	2.500000000000039
200	-0.9999999999999982	-4.68985202235761E-16	2.500000000000042

Table 1: Conservation of momentum and energy during the collisional relaxation of a double Maxwellian. The step numbers correspond to the panels in Fig.1.