# Conservation of invariants in binary collisions in fluctuating fields

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## Introduction

Charged particles in a plasma interact with each other through the long-range Coulomb collisions and, in a particle-in-cell simulation, these interactions can be modelled with the so-called binary collision (BC) methods. The two widely-used schemes are presented in Refs. [1, 2]. If equal particle weights are used, both these methods preserve kinetic momentum and energy in local homogeneous simulations, which explains the popularity of these two schemes. The convergence properties of the methods are well established in terms of time step and particle number [3, 4] but the testing has been done excluding electromagnetic (EM) fields. In global simulations, including configuration-space effects, the conservation properties generally depend on time step, number of test particles, particle sampling method, interpolation schemes and implementation of EM fields as well. The account of these effects is less established. If EM fluctuations are included in the simulation model, they contribute to both the conserved toroidal angular momentum and the energy (see, e.g., [5]). Consequently, the BC models should be considered in conjunction with the invariants of the collisionless dynamics. In this work, we discuss the conserved quantities in a drift-kinetic EM model, and how the accuracy of the conservation properties could potentially be improved while still using the standard BC model.

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## Binary collisions model

In performing particle-in-cell simulations and using the widely used BC models [1, 2], collisional effects are naturally implemented so that they only change those parts of momentum and energy that directly depend on the particle distribution function. For example, in the 6D Vlasov-Maxwell model, the fields $E$ and $B$ are kept fixed during the collisional step. Correspondingly, the global functionals

$$P_F = \sum_s \int m_s v F_s dv dx \tag{1}$$

$$E_F = \sum_s \int \frac{1}{2} m_s |v|^2 F_s dv dx, \tag{2}$$

should remain constant during the collisional step. Here, $m_s$ and $F_s$ are the mass and distribution function of species $s$, and $x$ and $v$ are the location of particle in configuration and velocity space, respectively.

In a BC algorithm with equal particle weights, implementing this strategy amounts to requesting that the kinetic energy and momentum are conserved in a pair-wise collision between the particles $p_1$ and $p_2$. Effectively, one requires that the following conditions are met

$$m_{p_1} v_{p_1}(t_n) + m_{p_2} v_{p_2}(t_n) = m_{p_1} v_{p_1}(t_{n+1}) + m_{p_2} v_{p_2}(t_{n+1}), \tag{3}$$

$$m_{p_1} |v_{p_1}(t_n)|^2 + m_{p_2} |v_{p_2}(t_n)|^2 = m_{p_1} |v_{p_1}(t_{n+1})|^2 + m_{p_2} |v_{p_2}(t_{n+1})|^2, \tag{4}$$

where $t_{n+1} = t_n + \Delta t$ and $\Delta t$ is the time step.

If EM fluctuations are included in the simulations, they affect the quantities that are conserved by the collisionless dynamics. Considering then also the collisional dynamics, the BC model should retain the invariants of the colllision-free model. For fusion plasmas, an EM drift-kinetic model that results as the $k_\perp \rho \ll 1$ limiting case of the EM gyrokinetic model [6] is of particular interest. The analysis of the conserved quantities for such a model can be found, e.g., in [5].

For this case, the "kinetic-momentum"- and the "kinetic energy"-like functionals, that the binary-collision algorithm should leave invariant for fixed values of the fields $E_1$ and $B_1$, are given by

$$P_F = \sum_s \int F_s \left( e_s A_0 + m_s u b_0 - \frac{\partial K_s}{\partial E_1} \times B_1 \right) \cdot e_\varphi du d\mu dx, \tag{5}$$

$$E_F = \sum_s \int \left( K_s - \frac{\partial K_s}{\partial E_1} \cdot E_1 \right) F_s du d\mu dx, \tag{6}$$

where the summation over $s$ again refers to particle species. Here, $B_0 = \nabla \times A_0$ is the background magnetic field, with $b_0 = B_0/|B_0|$ the corresponding unit vector. The dynamical fields in the system are the distributional densities $F_s$, which include the phase-space Jacobian, and the electric and magnetic field perturbations $E_1$ and $B_1$. The single drift-center kinetic energy function in the model ([5]) is given by

$$K = \frac{1}{2} m u^2 + \mu |B_0| \left( 1 + \frac{b_0 \cdot B_1}{|B_0|} + \frac{|B_{1\perp}|^2}{2|B_0|^2} \right) - \frac{m}{2|B_0|^2} |E_{1\perp} + u b_0 \times B_1|^2. \tag{7}$$

From the global functionals, we identify the individual particle contributions, namely

$$P(x,u) = \left( e A_0 + m u b_0 - \frac{\partial K}{\partial E_1} \times B_1 \right) \cdot e_\varphi, \tag{8}$$

$$E(x,u,\mu) = K - \frac{\partial K}{\partial E_1} \cdot E_1. \tag{9}$$

Regardless of what exactly a conservative BC algorithm does, it should satisfy the pair-wise conservation of toroidal angular momentum and total energy

$$P_{1,n} + P_{2,n} = P_{1,n+1} + P_{2,n+1}, \tag{10}$$

$$E_{1,n} + E_{2,n} = E_{1,n+1} + E_{2,n+1}, \tag{11}$$

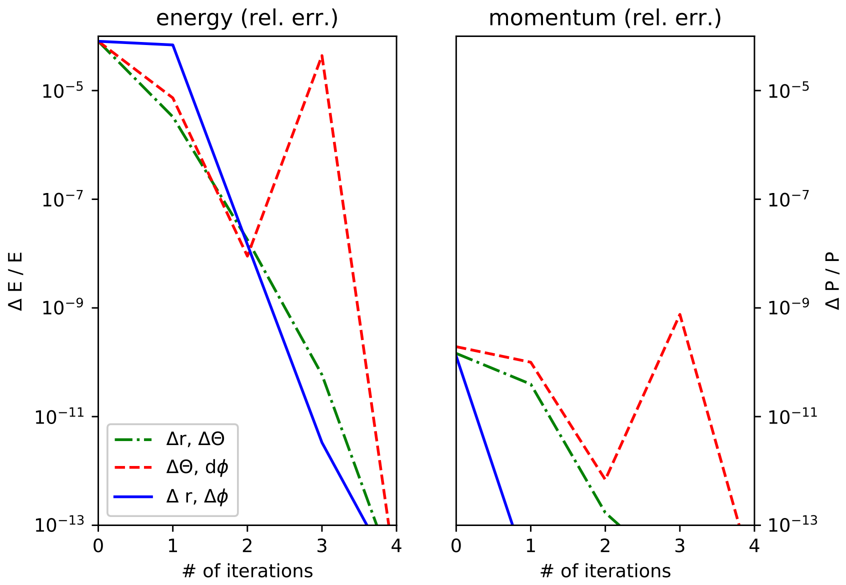


Figure 1: *Relative change of E and P just after BCs (index "0" in xlabel) and after iterative corrections.*

with the notation $P_{1,n} \equiv P(x_{1,t_n}, u_{1,t_n})$ etc. and $(x_{t_n}, u_{t_n}, \mu_{t_n})$ and $(x_{t_{n+1}}, u_{t_{n+1}}, \mu_{t_{n+1}})$ referring to the particle coordinates before and after the collisional time step $\Delta t$.

The standard BC algorithms, however, are not designed to preserve these particular invariants in the presence of the perturbations $E_1$ and $B_1$, resulting in deviations $\Delta P$ and $\Delta E$ such that

$$P_{1,n} + P_{2,n} = P_{1,n+1} + P_{2,n+1} + \Delta P, \tag{12}$$

$$E_{1,n} + E_{2,n} = E_{1,n+1} + E_{2,n+1} + \Delta E. \tag{13}$$

Since the field fluctuations by definition are supposed to be small, the new values for velocities from a standard BC step nevertheless are expected to approximately retain the invariants, and significant errors to accumulate only over time. Consequently, a small perturbation, e.g., a shift in the location or velocity of particle one, $x_1$, at every time step, could potentially be used to make the deviations $\Delta E$ and $\Delta P$ to vanish.

**Potential corrections to conserving P and E**

Using $(x_1, x_2, x_3)$ for the configuration space coordinates of particle 1 after the standard BC step has been taken and the errors $\Delta P$ and $\Delta E$ are known, we could adjust, say, two of the coordinates according to

$$\begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix} = \begin{bmatrix} dP/dx_1 & dP/dx_2 \\ dE/dx_1 & dE/dx_2 \end{bmatrix}^{-1} \begin{bmatrix} \Delta P \\ \Delta E \end{bmatrix} \tag{14}$$

to reduce the error. Further, this corrective step can be iterated to suppress the error significantly. In 3D case, there is freedom to choose any two out of the three available components for tuning the quantities $P$ and $E$. In toroidal coordinates, the relative errors in momentum appear to be quite small. The correction terms depend much on the numerical parameters and mainly on radial coordinate, $P \approx P(r)$. Other corrections are very small.

In Fig. 1, the correction method is tested with a simple test case for sinusoidal $|B_1|/|B_0| = \mathscr{O}(10^{-3})$ fluctuations. Repeated binary collisions of two particles are carried out and, after each BC, $P$ and $E$ are corrected using Eq. (14). The standard deviation of the error compared to $P$ ($E$) before the BC is shown. It can be seen that correction in $P$ is small, $\mathscr{O}(10^{-10})$, while relative error in $E$ is order of $10^{-4}$. Tuning with $\Delta r$ together with poloidal ($\Delta\theta$) or toroidal ($\Delta\phi$) correction shows the best performance confirming that in practise the radial coordinate $r$ tunes $P \approx P(r)$ after which the fine tuning of E is done with either $\theta$ or $\phi$.

If a scheme, such as the one described above, is adopted to enforce the conservation properties, one can expect at least some level of artificial transport which in [7] was estimated to be

$$D = \frac{(\Delta r)^2}{\Delta t} \sim \left(\frac{B_0}{B_{0,p}}\right)^2 \left(\frac{B_1}{B_0}\right)^4 \rho_0^2 \nu. \tag{15}$$

i.e. even if the magnetic fluctuations were comparable to the poloidal magnetic field, the term $(B_0/B_{0,p})^2(B_1/B_0)^4$ would remain considerably less than one. Consequently, we expect that the transport from the corrective algorithm would remain at most at the level of classical diffusion and likely be significantly less than that.

## Conclusions

In this work, we suggested one possibility to modify the existing BC algorithms to regain the conservation of the quantities important in transport simulations when EM fluctuations are present. We expect such minor modifications to be also practical enough for implementations.

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