

# ARTIFICIAL COLLISIONS, ENTROPY AND EMITTANCE GROWTH IN COMPUTER SIMULATIONS OF INTENSE BEAMS

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## Abstract

Artificial collisions during particle tracking with self-consistent space charge lead to diffusion-like, numerical effects. The artificial collisions generate a stochastic noise spectrum. As a consequence the entropy and the emittance can grow along periodic focusing structures. The growth rates depend on the number of simulation macro-particles and on the space charge tune shifts. For long-term tracking studies the numerical diffusion can lead to incorrect beam loss predictions. In our study we present analytical prediction for the numerical friction and diffusion in 2D simulations. For simple focusing structures we derive a relation between the friction coefficient and the entropy growth. The scaling of the friction coefficient with the macro-particle number and the space charge tune shift is obtained from 2D simulations and compared to the analytic predictions.

## INTRODUCTION

The prediction of beam loss and emittance growth in intense beams relies on particle tracking codes with space charge solvers. The Particle-In-Cell (PIC) scheme is employed in order to obtain the space charge force self-consistently at every time step. Because of the finite amount of simulation macro-particles the PIC scheme also adds noise to the dynamics of the computer beam. The noise in PIC codes can be related to artificial collisions in the computer beam, similar to Schottky noise and intra-beam scattering in real beams. In a number of studies the artificial noise in computer beams has been used to predict the Schottky noise in real beams (see e.g. [1]). The artificial collisions cause an undesired emittance growth in computer beams [2, 3]. Especially for long-term tracking studies or for very intense beams the effects of artificial collisions and noise should be well controlled. This is usually achieved by an increase of the macro-particle number in combination with higher order interpolation or smoothing of the beam density on the grid. In order to estimate the required number of macro-particles for given machine and beam parameters this study aims to provide scaling laws for the emittance growth induced by artificial collisions.

## ENTROPY AND EMITTANCE GROWTH IN COMPUTER BEAMS

The theory of artificial collisions and stochastic noise is well developed for Particle-In-Cell plasma simulations [4]. There it is shown that the effect of the fluctuations generated from the finite amount of macro-particles can be cast into the form of collision operators. The artificial collisions between macro-particles cause a thermal relaxation, with different

rates in 1D, 2D and 3D PIC codes [5]. Also the effect of different interpolation schemes has been studied [6]. For particle beams expressions for the entropy and emittance increase due to artificial collisions were derived in Refs. [2,3] and compared to 2D PIC simulations. Following Ref. [2] the diffusion term is approximated through the Einstein relation as a constant

$$D \approx \nu \frac{k_B T_{eff}}{m} \quad (1)$$

where  $\nu$  is the collision frequency. However, instead of the local temperature  $T = (T_x + T_y)/2$  at position  $s$  we define an effective beam temperature in a periodic focusing channel as

$$T_{eff} = \alpha \langle T \rangle + (1 - \alpha) T \quad (2)$$

where  $\langle \dots \rangle$  represents the average over one focusing cell. Our effective temperature is a weighted average of the local and the cell averaged temperature with the positive weighting factor  $\alpha \leq 1$ . The motivation for this effective temperature is that the relevant collision times ( $\approx \nu^{-1}$ ) for small angle scattering events between macro-particles can be assumed to be of the order of or longer than the focusing cell length (or the typical modulations of the betatron functions). Therefore an averaged expression for the temperatures should be used and not the local one. Only in the special case of a FODO cell with phase advances  $\mu_x = \mu_y$  the sum of the local transverse temperatures  $T_x + T_y$  remains constant and the effective temperature is  $T_{eff} = (T_x + T_y)/2 = \langle T_x + T_y \rangle / 2$ . In two dimensions the entropy growth resulting from Equation 1 is (see Ref. [2], Eq. 12)

$$\frac{dS}{dt} = k_B \nu \left( \frac{T_{eff}}{T_x} + \frac{T_{eff}}{T_y} - 2 \right) \quad (3)$$

or

$$\frac{dS}{dt} = k_B \nu \left[ \alpha \left( \langle T \rangle \frac{T_x + T_y}{T_x T_y} - 2 \right) + \frac{1 - \alpha}{2} \frac{(T_x - T_y)^2}{T_x T_y} \right] \quad (4)$$

The corresponding emittance growth is

$$\frac{1}{\varepsilon} \frac{d\varepsilon}{dt} = \frac{1}{k_B} \frac{dS}{dt}, \quad \varepsilon = \varepsilon_x \varepsilon_y \quad (5)$$

The emittance growth per cell is

$$\frac{\Delta\varepsilon}{\varepsilon_0} \approx \beta_0 c L \nu (A + G) \quad (6)$$

where  $L$  is the cell length and the anisotropy factor is defined as

$$A = \frac{1 - \alpha}{2} \left\langle \frac{(T_x - T_y)^2}{T_x T_y} \right\rangle \quad (7)$$

and the ripple factor

$$G = \alpha \left( \langle T \rangle \left\langle \frac{T_x + T_y}{T_x T_y} \right\rangle - 2 \right) \quad (8)$$

For weak space charge we can use  $\sigma_x^2 \approx \hat{\beta} \varepsilon_x$  and the averaging can be performed using the  $\hat{\beta}$ -functions.

## COLLISION FREQUENCY IN COMPUTER BEAMS

In order to estimate the emittance growth Equation 6 we need an approximate expression for the collision frequency  $\nu$  in a computer beam. Because in synchrotrons the bunches are usually long relative to the pipe diameter PIC codes for beams employ 2D or 2.5D space charge models. In 2.5D space charge models the bunch is sliced along the longitudinal direction. For each slice a 2D space charge solver is employed. In both cases, 2D and 2.5D, the particle motion is 3D, but the transverse space charge forces are calculated on a 2D grid. Therefore the macro-particles are effectively charged rods extending in the longitudinal direction. The collisions between the rods takes place in the 2D transverse plane. In 2D the force between a test particle and a beam particle (or rod) is

$$F_p(\vec{r}) = \frac{Qq'}{2\pi\epsilon_0 r} \quad (9)$$

where  $q'$  is the line charge of the beam particle and  $Q$  is charge of the test particle. For the above force the deflection angle  $\theta$  depends only on the relative velocity  $u$  and only weakly on the impact parameter  $b$ .

$$\theta(b) = \frac{Qq'}{\pi\epsilon_0 m u^2} \arccos \frac{b}{\lambda_D} \quad (10)$$

The upper cutoff parameter is chosen at the Debye length  $\lambda_D$ . For  $b > \lambda_D$  we assume that the force between particles is shielded off. The concept of the Debye length in particle beams is discussed in Ref. [7]. The velocity for a  $90^\circ$  deflection can be obtained from

$$v_\perp^2 = \frac{Qq'}{2\pi\epsilon_0 m} \quad (11)$$

For a given distribution  $f$  and density  $n$  of beam particles the friction force on the test particle is

$$F(\vec{v}) = m\nu\vec{v} = m \int d^2v db u f(\vec{v}) \Delta\vec{v} \quad (12)$$

where the velocity change is

$$\Delta\vec{v} = -u \sin^2(\theta/2) \approx -\frac{u}{4} \theta^2 \quad (13)$$

From the friction force the collision frequency can be obtained as

$$\nu \approx \left( \frac{v_\perp}{v} \right)^4 n v \lambda_D \quad (14)$$

The above formalism applies to real and to computer beams in 2D. For computer beams there are three main differences. First, the charge of the test macro-particle  $Q$  is much higher than the charge of the real beam ions  $q$ . If  $M$  is the number of macro-particles and  $N$  the number of real beam ions, then  $Q = qN/M$ . Second, in beam simulations the collisions take place between the test macro-particle (charge  $Q$ ) and the  $M$  beam macro-particles (charge  $q$ ). Therefore the macro-particle density seen by the test macro-particle is lower than the real beam density by  $\frac{M}{N}n$ . Third, the macro-particle charge profile is distributed over a grid cell. We will assume an effective size of the macro-particle  $\Delta = \Delta_x = \Delta_y$ , which is of the order of the grid spacing. Therefore a lower cutoff at  $b \approx \Delta$  has to be applied. In a 2D computer beam the relative velocity for  $90^\circ$  deflection increases according to

$$v_\perp^2 = \frac{N}{M} v_\perp^2 \quad (15)$$

compared to a 2D 'real' beam. Therefore more particles are affected by large angle collisions. The scaling law for the collision frequency in a 2D computer beam is then

$$\nu \approx \frac{N}{M} \nu \propto \frac{N^{3/2}}{M} \left( 1 - \frac{\Delta}{\lambda_D} \right) \quad (16)$$

## SIMULATION RESULTS

As an example case we study the artificial emittance growth in a simple FODO channel. The phase advance in both directions is set to  $\mu_0 = 60^\circ$ . The initial beam distribution is first matched with 2D space charge using the rms envelope equations. Afterwards the distribution is tracked for about 1000 cells with the code PATRIC [1]. The results obtained for the FODO channel are compared to a symmetric FODO channel (FODOxx). In the FODOxx cell the focusing gradients are symmetric and so are the resulting envelopes and local temperatures ( $T_x = T_y$ ). Any artificial emittance case in a FODOxx cell will be entirely due to the ripple of the lattice functions ( $G > 0$ ,  $A = 0$ ). The final emittance growth for the FODO and FODOxx channels and fixed macro-particle number  $M = 5000$  as a function of the space charge induced phase advance shift  $\Delta\mu \propto N$  is shown in Figure 1. Very similar results have been obtained with the code py-ORBIT [8]. The results are compared to  $N^{3/2}$  and  $N^2$  scaling laws. One can see that the emittance growth varies very strongly for weak and moderately strong space charge ( $|\Delta\mu| \lesssim 20^\circ$ ). This can be explained in part by the combination of structure resonances (indicated in Figure 1) and low frequency fluctuations of the space charge force. For strong space charge the emittance growth can be roughly described by  $N^{3/2}$  and  $N^2$  scaling laws. In this regime the emittance growth is about a factor of two larger for the FODO compared to the FODOxx channel. This difference is in agreement with the evaluation of Equation 6 with  $\alpha = 0.5$  for the effective temperature.  $\alpha = 1$  would result in a similar emittance growth for the FODO and FODOxx lines. For  $\alpha = 0$  the predicted emittance growth for the FODOxx line would be zero. As a next step we fix the

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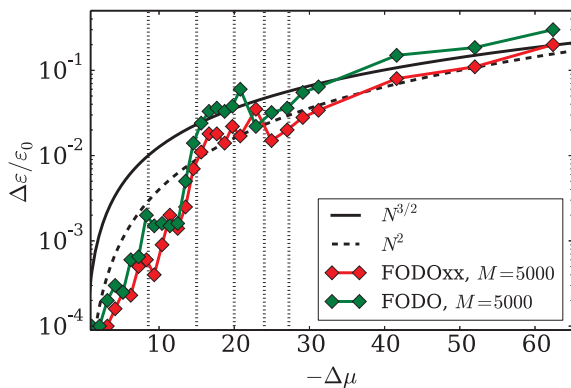


Figure 1: Emittance growth as a function of the beam intensity for  $M = 5000$  in PATRIC.

beam particle number  $N$  and obtain the emittance growth as a function of the macro-particle number  $M$ , as shown in Figure 2. The emittance growth decrease with increas-

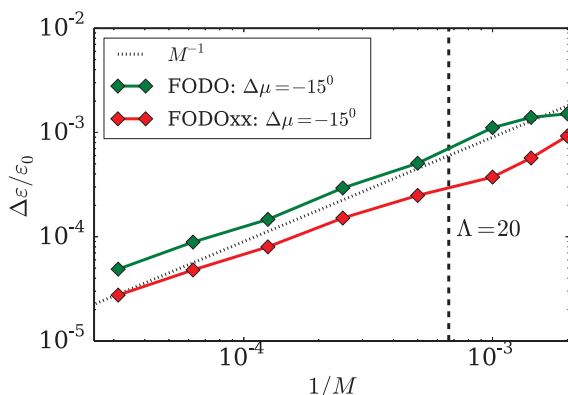


Figure 2: Emittance growth as a function of the inverse macro-particle number  $1/M$  for  $\mu = -15^\circ$ .

ing  $M$ . The decrease follows approximately a  $1/M$  scaling law. Again we observe a factor of 2 difference between the FODO and the FODOxx channels. For very low macro-particle numbers ( $\lesssim 2000$ ) there are deviations from this scaling law because large angle collisions start to play an important role (coupling parameter  $\Lambda = v_{rms}/v_\perp$ ). At last, we study the effect of the grid spacing  $\Delta x = \Delta y$ . Figure 3 depicts the change of the emittance growth with changing grid spacing (normalized by  $\lambda_D$ ). The emittance growth reduces on a coarser grid, because the collisions are smoothed out. For the FODO channel the emittance decrease follows approximately Equation 6. For  $\Delta x \gtrsim 3\lambda_D$  we find that the emittance growth increases again.

## CONCLUSION

The entropy and emittance growth caused by numerical effects in particle tracking codes with 2D self-consistent

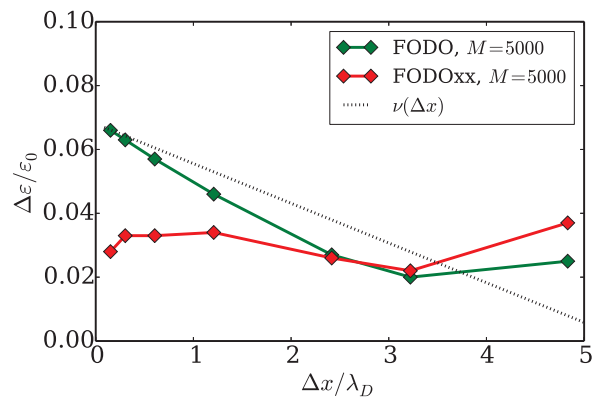


Figure 3: Emittance growth as a function of the grid spacing for  $M = 5000$  and  $\Delta\mu = -30^\circ$ .

space charge solvers has been studied. The obtained emittance growth in FODO channels can in part be attributed to artificial collisions between macro-particles, as demonstrated by comparison with an analytic scaling law. In our analytic model we introduced an effective, non-local temperature in order to account for the observed emittance growth in isotropic beams. For weak space charge the emittance growth is dominated by a low frequency noise spectrum in combination with structure resonances. For strong space charge the noise spectrum extends to higher frequencies and artificial collisions dominate. In 3D space charge codes for linacs a different scaling law for the artificial collisions applies. However, in such codes the emittance growth is often dominated by the coarse 3D grids [9].

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