

STOCHASTIC NOISE EFFECTS IN HIGH CURRENT PIC SIMULATION

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Abstract

The numerical noise inherent to particle-in-cell simulation of 3D high intensity bunched beams is studied with the TRACEWIN code and compared with the analytical model by Struckmeier [1]. The latter assumes the six-dimensional rms emittance or rms entropy growth can be related to Markov type stochastic processes due to temperature anisotropy and the artificial "collisions" caused by using macro-particles and calculating the space charge effect. Our entropy growth confirms the dependency on bunch temperature anisotropy as predicted by Struckmeier. However, we also find noise generation by the non-Liouvillian effect of the Poisson solver grid, which exists in periodic focusing systems even when local temperature anisotropy is absent - contrary to predictions by Struckmeier's model.

INTRODUCTION

In modelling of high intensity beams by particle-in-cell (PIC) computer simulation it is of importance to understand the numerical noise generated by the discreteness of the spatial Poisson solver grid and the finite number of particles. We focus on beam parameters typical for high intensity linear accelerators, but our findings can also be extended to circular accelerators with very different ratio of transverse to longitudinal parameters.

Numerical noise can have a similar effect on the beam as real collisions or intra-beam scattering. It is one of the challenges of high intensity beam simulation to be able to distinguish between physical and numerical growth effects. Towards this end an in-depth understanding and parametrisation of numerical noise is crucial. Such collision or noise effects can, in principle, be associated with entropy growth [2, 3]. The rms entropy model by Struckmeier [4, 5] assumes that collisional behaviour and temperature anisotropy are driving a 6d rms emittance growth, which leads to the rms entropy growth. An observation of such an emittance growth in a linac beam context using the PICNIC space charge routine within the PARMILA code was presented in Ref. [6].

RMS APPROACH TO ENTROPY GROWTH

Lawson et al. [2] first discussed a probability based approach to entropy by using the logarithm of the rms emittance. For a time-independent Kapchinskij-Vladimirskij distribution in 4d phase space they thus obtained the relation $S = k \ln \epsilon$, where k is the Boltzmann constant. An important step ahead for dynamically evolving distributions has been the approach by Struckmeier [4, 5] who demonstrated that the rms envelope equations can be extended to

the full Vlasov-Fokker-Planck equation. The thus obtained equation applies to the product of the three rms emittances, which can be understood as a six-dimensional rms emittance, $\epsilon_{6d} \equiv \epsilon_x \epsilon_y \epsilon_z$, hence

$$\frac{1}{k} \frac{dS}{ds} = \frac{d}{ds} \ln \epsilon_x(s) \epsilon_y(s) \epsilon_z(s) = \frac{k_f}{3} I_A = \frac{k_f}{3} \left(\frac{(1-r_{xy})^2}{r_{xy}} + \frac{(1-r_{xz})^2}{r_{xz}} + \frac{(1-r_{yz})^2}{r_{yz}} \right) \geq 0 \quad (1)$$

where $s = \beta ct$ measures the distance and $k_f \equiv \beta_f / \beta c \gamma$ with β_f the dynamical friction coefficient. The r_{nm} are rms based "temperature ratios" or ratios of intrinsic spreads of velocities given here in non-relativistic approximation:

$$r_{xy}(s) \equiv \frac{T_y(s)}{T_x(s)}, r_{xz}(s) \equiv \frac{T_z(s)}{T_x(s)}, r_{yz}(s) \equiv \frac{T_z(s)}{T_y(s)}, \quad (2)$$

For upright ellipses we simply have the familiar rms expressions

$$\frac{T_y(s)}{T_x(s)} \equiv \frac{\epsilon_y^2 / \langle y^2 \rangle}{\epsilon_x^2 / \langle x^2 \rangle} = \frac{\epsilon_y k_y}{\epsilon_x k_x} \quad (3)$$

and similar for the remaining ratios. Some caution is necessary when using a concept like "temperature". Strictly speaking, it cannot be defined properly for our beams, which are not in an equilibrium state. In this model the concept of locally near-isotropic temperatures is formally adopted as basis for the validity of the Einstein relation connecting isotropic diffusion and friction coefficients.

Eq. 1 suggests a separation of a "friction term" (given by k_f) and a "temperature anisotropy term" I_A defined by the bracket on the r.h.s. of Eq. 1. Details of the numerical scheme and of the Coulomb logarithm are assumed to enter into k_f , which is separated from the "driving" anisotropy term. No growth of the rms emittance is predicted from Eq. 1, if all temperatures are identical everywhere and the r.h.s. vanishes.

In the remainder of this work growth of ϵ_{6d} is thus used as a synonym to entropy growth. It is, however, necessary to apply some caution here. An entropy definition based on rms quantities cannot be applied to collective or resonant processes beyond second order, which may cause growth of individual rms emittances, but at the same time a decrease of ϵ_{6d} and thus the rms entropy is not excluded.

3D BUNCHES IN PERIODIC SOLENOID WITH r_z POISSON SOLVER

The TRACEWIN code [7] is employed here with a bunched beam and a periodic lattice with thin solenoid lenses and thin rf gaps at the same location. Due to

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the rotational symmetry the rz Poisson solver option of TRACEWIN/PICNIC is sufficient. It is characterized by the number n_{cr} of radial cells from the origin to R_{max} ; and n_{cz} as radial cells from $-Z_{max}$ to Z_{max} . For these maximum grid extent values we have assumed throughout the values 3σ , where σ is the rms size in each direction. Beyond it PICNIC determines fields analytically assuming a Gaussian density distribution of the same rms sizes. We assume a length of 1 m per cell and a spherical bunch with equal emittances in x, y, z and $k_{0x,y,z} = 60^\circ$. We set the option "steps of calculation" to 20/10 in TRACEWIN, which implies 20 lattice calculations and 10 space charge steps per meter of drift space, in addition to one lattice calculation and one space charge step per solenoid. Due to a rounding up algorithm this amounts to 14 space charge steps per lattice cell, which is found as sufficient. As starting distribution we employ either the TRACEWIN standard option "6d-ellipsoid" (randomly generated in the six-dimensional phase space ellipsoid with parabolic density profiles) or the option "Gaussian" (Parmila type 36).

Here we study the relative increase in ϵ_{6d} over 1000 cells for a strictly spherical bunch with Gaussian initial distribution function, $\epsilon_{x,y}/\epsilon_z = 1$, $k_{0x,y,z} = 60^\circ$ and $k_{x,y,z} \approx 33^\circ$. The dependence on N is shown in Fig. 1, where the relative growth $\Delta S/k = \Delta\epsilon_{6d}/\epsilon_{6d}$ is plotted against $1/N$ as measure of the charge per macro particle (note the double-logarithmic scale, with the dashed line is indicating an hypothetical strictly linear extrapolation through the origin). Throughout this study $\Delta\epsilon_{6d}$ is normalized to 1000 lattice cells, which makes use of a practically linear evolution of ϵ_{6d} in s ; except for relatively small values of N , where the initial gradient of ϵ_{6d} was determined and extrapolated to the same value of 1000 cells.

In spite of the absence of anisotropy, hence $I_A = 0$, all cases show a finite growth of ϵ_{6d} , which is unexpected in the frame of Eq. 1. We assume this growth is caused by a violation of the assumption of a locally isotropic collision type diffusion process - the underlying assumption in the derivation of Eq. 1 - in our periodic focussing system. It must be assumed that this violation is actually a combined effect of: (1) Coulomb interaction taken via charges on a relatively coarse grid rather than direct particle-particle interaction; (2) a periodic modulation of focusing introducing a "coherent" streaming against the grid, which is not slow compared with "collision times". This subject is discussed in further detail in Ref. [8].

We therefore introduce a purely grid-related noise term I_{GN} in Eq. 1, which is independent of the temperature anisotropy term:

$$\frac{d}{ds} \ln \epsilon_x(s)\epsilon_y(s)\epsilon_z(s) = \frac{k_f^*}{3} (I_A + I_{GN}). \quad (4)$$

We have also introduced a k_f^* to take into account that these grid related effects might also have an effect on k_f , besides the offset term I_{GN} .

For the 16x16 grid a linear dependence of $\Delta\epsilon/\epsilon$ is noted in the range from 1000 up to ≈ 20.000 particles:

$$\Delta\epsilon_{6d}/\epsilon_{6d} \propto N^{-1} \quad (5)$$

For higher N we find that $\Delta\epsilon/\epsilon$ bends off, however. We also show cases with grid resolution of only 12x12 and find that the departure from a linear law occurs even with less particles, and even more for 8x8 grids. The data indicate that for sufficiently large N we enter into a *grid resolution limited region*, where further increasing of N doesn't help much to reduce growth of ϵ_{6d} , unless the grid resolution is increased as well. This transition region is characterized by

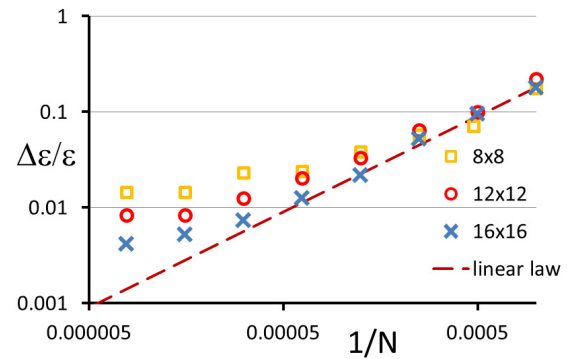


Figure 1: Relative growth of ϵ_{6d} for N from 1000 to 128.000 macro particles indicating transition to *grid resolution limited regions*.

a typical average number of particles per cell. With the average number of particles per (toroidal) cell in $\Delta r \Delta z$ given as $N/(n_c^2 * 3.14/4)$ we find that the transition occurs typically for 80-100 particles in a toroidal cell (for example for 16.000 particles for $n_c = 16$). This suggests that for significantly less particles statistical fluctuations of charges on the grid become large, hence more particles will help to reduce the noise effect. Using significantly more particles, instead, has no further benefit unless the grid resolution is increased as well.

TEMPERATURE ANISOTROPY DRIVEN NOISE

Justification of the separation of k^* with the assumption of a "kinetic" term $I_A + I_{GN}$ needs careful examination. We assume $k_{0xyz} = 60^\circ$, $N=4000$, a 16x16 grid with the "6d-ellipsoid" initial distribution. The linac current is chosen again such that $k_{xyz} = 33^\circ$ for equal emittances. Different emittances in transverse and longitudinal directions are realized in such a way that the product $\epsilon_x \epsilon_y \epsilon_z$ remains invariant. The initial temperature anisotropy on the abscissa of Fig. 2 is determined via Eq. 3 using actual emittances and space charge dependent tunes k from TRACEWIN, while $\Delta\epsilon_{6d}/\epsilon_{6d}$ is extracted from the gradients of ϵ_{6d} taken over the first 100 or few hundred cells.

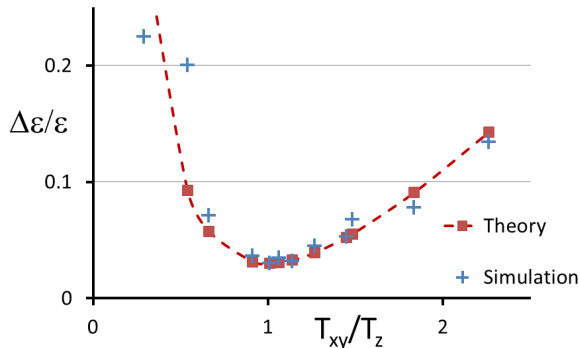


Figure 2: Relative growth of ϵ_{6d} for $k_{0xyz} = 60^\circ$ and varying (initial) temperature anisotropy.

The simulation results confirm the existence of a minimum emittance growth of $\Delta\epsilon_{6d}/\epsilon_{6d} \approx 0.03$ at the point, where the temperature ratios r in Eq. 2 are all equal to unity. In order to check the applicability of the analytical I_A in Eq. 1 we need to fit k_f^* and I_{GN} to the numerical data using Eq. 4. The thus resulting "theoretical" curve in Fig. 2 shows good agreement with the simulation data. We have also tested this comparison for split k_{0xy} and k_{0z} to $60^\circ/60^\circ/47^\circ$ and find reasonably good agreement as well.

3D BUNCHES WITH xyz POISSON SOLVER IN FODO LATTICE

We adopt an "equivalent" periodic FODO lattice with rf gaps and cell length again 1 m. The same phase advance per m is chosen as in the previous examples as well as identical emittances, which results in approximately the same space charge depressed tunes. The alternating focusing causes a stronger modulation and local imbalance of "temperatures", which is described in Ref. [4] as source of entropy growth. We expect that this mechanism amplifies or adds to the already mentioned "non-Markov" effects found for the periodic solenoid. This is shown in Fig. 3 as function of n_c and for different N as well as space charge steps. Note that the difference by decreasing the number of space charge steps per cell from 15 (10/m in TRACEWIN) to 11 (3/m in TRACEWIN) is minor. Both cases, low and high particle numbers, show that an optimum n_c exists, which is the higher the larger N . As before, large N is efficient only if the grid resolution is sufficiently large.

Comparing with the periodic solenoid we find an enhanced noise level. The results of Fig. 3 also differ from the result reported in Ref. [6], where low and high particle number (transverse) emittance growth is nearly identical around $n_c = 8$. For this grid resolution we find that 16.000 particles lead to practically four times the growth in ϵ_{6d} than 128.000 particles. Theoretically, following the result of Fig. 1 and Eq. 5, the difference could be even as large as a factor eight.

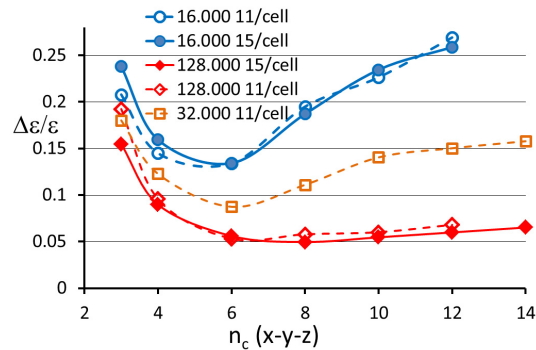


Figure 3: Relative growth of ϵ_{6d} in FODO for different N as function of number of grid cells in x, y, z and different numbers of space charge steps.

The needed high resolution may turn out impractical - in particular jointly with large N .

CONCLUSION AND OUTLOOK

Our simulations are in a grid effect dominated regime, which differs from the assumption of a collisional regime assumed in the work by Struckmeier. Thus, we obtain entropy growth even in fully isotropic cases with no temperature differences. Further work is needed to explore in more detail the transition between two distinct regimes: the "grid effect dominated regime" - claimed here - where particles interact in a non-Liouvillian way with the charge distribution on a grid; and a "particle collision regime", where (Markov type) particle-particle collisions are resolved. The latter can be assumed to be increasingly relevant at much higher grid resolution than employed here.

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