Grid dependent noise and entropy growth in anisotropic 3d particle-in-cell simulation of high intensity beams

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The numerical noise inherent to particle-in-cell (PIC) simulation of 3d anisotropic high intensity bunched beams in periodic focusing is compared with the analytical model by Struckmeier [*Part. Accel.* 45, 229 (1994)]. The latter assumes that 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. The PIC simulations are carried out with the TRACEWIN code widely used for high intensity beam simulation. The resulting noise can lead to growth of the six-dimensional rms emittance. The logarithm of the latter is shown to qualify as rms-based entropy. We confirm the dependence of this growth on the bunch temperature anisotropy as predicted by Struckmeier. However, we also find a grid and focusing dependent component of noise not predicted by Struckmeier. Although commonalities exist with well-established models for collision effects in PIC-simulation of extended plasmas, a distinctive feature is the presence of a periodic focusing potential, wherein the beam one-component plasma extends only over relatively few Debye lengths. Our findings are applied in particular to noise in high current linac beam simulation, where they help for optimization of the balance between the number of simulation particles and the grid resolution.

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I. INTRODUCTION

In modeling of high intensity beams by particle-in-cell (PIC) computer simulation it is of importance to understand whether any observed emittance growth or beam loss is caused by real physical processes, or by nonphysical processes like numerical discretization and grid effects from the Poisson solver, which can be also seen as pseudo-collisions with the grid charge distribution. Our emphasis is on the numerical noise generated by the discreteness of the spatial grid used for the Poisson solver, collision effects between simulation super-particles and the presence of a periodic focusing potential.

It is commonly accepted that real physical processes leading to amplitude and emittance growth can be: initial mismatch, mismatch at structure transitions, errors, external or internal resonances as well as the fact that with space charge strictly periodic stationary distribution functions are not explicitly known in 3d (as discussed in Ref. [1]). In storage rings intra-beam scattering is often observed as another kind of real physical process, which can lead to emittance growth under certain circumstances. Numerical noise, on the other hand, can have a similar heating effect on the beam as real intra-beam scattering; it can be also

significantly different, if grid heating effects play a role. It is one of the challenges of high intensity beam simulation to be able to distinguish between physical and numerical growth effects. Toward this end an in-depth understanding and parametrization of numerical noise is crucial.

Collision or noise effects can, in principle, be associated with entropy growth. The concept of entropy in accelerator beams was first discussed in general terms by Lawson *et al.* [2]. Later on the Fokker-Planck equation—see Ref. [3] for a detailed discussion of its applicability to intra-beam scattering—was employed to analyze mismatch and turbulent heating of a sheet beam by Bohn [4]. A significant step ahead in this direction has been the noise and entropy growth model by Struckmeier [5–7], which provides a useful theoretical framework based on second order moments of the Vlasov-Fokker-Planck equation. It assumes that collisional behavior and temperature anisotropy can drive 6d rms emittance growth, which is used to define a rms entropy growth.

Compared with high intensity beams, the subject of collisions and noise has in the past received much wider and systematic attention in the area of plasma PIC simulation, and much can be learnt from the associated literature (see, for example, Refs. [8,9]). In contrast with the usually extended plasmas, the beams considered here are a one-component “beam-plasma” confined by a periodically varying external potential (lenses, rf gaps), which is thus time-dependent in a frame moving with the bunch. Furthermore, even for high-intensity beams, the spatial

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extent is at best over a few Debye shielding lengths. These differences require modifications of the well-established results obtained for extended plasmas.

For our study we use the TRACEWIN code [10] as a widely used candidate of PIC-code developed primarily for linear accelerators. It employs the PICNIC space charge routine with an rz as well as an xyz option. We claim that the established dependencies on grid resolution, number of particles, anisotropy or intensities are generic to many 3d PIC-scheme. Nonetheless every code has specific issues of smoothing and interpolation some of which—specific to the TRACEWIN algorithm—are discussed in the appendix. We note that an earlier reference to rms entropy growth by “spurious collisions” in a linac environment—using the PICNIC space charge routine within the PARMILA code—was given in Ref. [11]. In any case, detailed comparison with results from other codes is desirable and should be pursued in future work.

Here we mention that collisional behavior in 2d beams is essentially different from that in 3d due to the very different range of the Coulomb force. A steadily increasing rms emittance for increasing mesh resolution was already evidenced by simulation results in a paper by Haber and Rudd [12], who studied 2d beams very close to the space charge limit. In a forthcoming companion paper to the present study by Boine-Frankenheime *et al.* [13] the collision and noise effects in 2d isotropic beams with space charge and their connection with entropy and noise, also on the basis of Struckmeier’s equations, has been given detailed consideration.

II. RMS APPROACH TO ENTROPY GROWTH

In analytical descriptions of high intensity beams it is generally assumed that the flow of particles in 6d phase space can be described by a Hamiltonian with—in general—time-dependent external forces and a time-dependent self-consistent space charge potential. Liouville’s theorem applies, which implies that the volume of a phase space element occupied by particles remains invariant in time. In such a system there is no entropy growth, if infinite phase space resolution is assumed and the Boltzmann entropy as logarithm of probabilities in 6d or μ space is evaluated accordingly.

The same applies to a Hamiltonian flow in the 6N-dimensional phase space (Γ space), which includes systems with Coulomb collisions. Growth of the Gibbs entropy (logarithm of probabilities in Γ space) requires introduction of a “coarse-grained” phase space—as opposed to the “fine-grained” infinite resolution phase space—which breaks the Hamiltonian nature of the flow. There is a certain analogy between coarse-graining in Γ space and the PIC-code technique of distributing particles on a 3d grid to solve Poisson’s equation. The latter also breaks the Hamiltonian nature of the flow in 6d phase space and is a source of entropy growth. Under certain circumstances

the interaction with this grid can be also looked at as “collisions” with the grid charge distribution.

The idea of a probability based approach to entropy by using the logarithm of the rms emittance was introduced by Lawson *et al.* [2]. For a time-independent Kapchinskij-Vladimirskij distribution in 4d phase space they thus obtained

$$S = k \ln \epsilon, \quad (1)$$

where k is the Boltzmann constant.

An important step toward dynamically evolving distributions has been the approach by Struckmeier [6,7]. He demonstrated that the rms—second order moments—approach originally introduced by Sacherer [14] to derive envelope equations, and later generalized to include the field energy in 6d (see Ref. [15]), 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

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

where $s = \beta c t$ measures the distance and $k_f \equiv \beta_f / \beta c \gamma$, with β_f the dynamical friction coefficient, which is proportional to the Coulomb logarithm. The r_{nm} are rms based “temperature ratios” or ratios of intrinsic spreads of velocities given here in non-relativistic approximation:

$$r_{xy}(s) \equiv \frac{T_y(s)}{T_x(s)}, \quad r_{xz}(s) \equiv \frac{T_z(s)}{T_x(s)}, \quad r_{yz}(s) \equiv \frac{T_z(s)}{T_y(s)}, \quad (3)$$

For upright ellipses we simply have the familiar rms expressions

$$\frac{T_y(s)}{T_x(s)} \equiv \frac{\epsilon_y^2 / \langle y^2 \rangle}{\epsilon_x^2 / \langle x^2 \rangle} = \frac{\epsilon_y k_y}{\epsilon_x k_x} \quad (4)$$

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 the strict sense. In the above 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, which is only valid for not too large deviation from thermal equilibrium.

It is important to note that Eq. (2) suggests a separation of a “friction term” (given by k_f) and a “temperature anisotropy term” I_A defined by the bracket on the right-hand side (r.h.s.) of Eq. (2). For the present study we shall

not be concerned further about a more rigorous justification of k_f , which is left to future work. Instead, we adopt a phenomenological approach with the goal to demonstrate that this separation is a practical ansatz. The details of the numerical scheme and of the Coulomb logarithm are assumed to enter into the coefficient k_f , which is separated from the “driving” anisotropy term. Note that—as one may expect for infinite plasmas—no growth of the rms emittance is predicted from Eq. (2), if all temperatures are identical everywhere and the r.h.s. vanishes. This issue will be examined and discussed further below.

As the r.h.s. of Eq. (2) is either zero or positive, $\ln \epsilon_x \epsilon_y \epsilon_z$ cannot decrease. Noting that the probability of decoupled events is the product of individual probabilities and that entropy should be an “extensive” (i.e., additive) quantity, it is justified to relate this logarithm to the entropy in an rms sense analogous to the static KV-case in Ref. [2]:

$$\frac{1}{k} \frac{dS}{ds} = \frac{d}{ds} \ln \epsilon_x(s) \epsilon_y(s) \epsilon_z(s) = \frac{k_f}{3} I_A \geq 0. \quad (5)$$

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 also cause growth of individual rms emittances, but at the same time a decrease of ϵ_{6d} . An example of this is given in Sec. III A, where the steep initial evolution (in < 20 m) is due to a nonlinear mechanism, here a 4th order space charge driven emittance coupling. In this case correlation terms in the six-dimensional matrix appear, and a different—more refined—approach to entropy would be needed. This is indicated in simulations by initial oscillatory increase and decrease of ϵ_{6d} , which is not consistent with an entropy definition and at the same time an indicator for the breakdown of the rms entropy concept during such a phase.

III. 3D BUNCHES IN PERIODIC SOLENOID WITH r_z POISSON SOLVER

In the TRACEWIN code particles are advanced in x , y , and z with thin lens kicks and optionally with field maps. The 3d advancement of particles in these field models is not symplectic, but sufficiently accurate for linac applications. Focusing and accelerating fields are calculated at grid points—a grid moving with the bunch—and applied by interpolation with neighboring grid points.

In all examples of this section we assume a bunched beam in a periodic lattice with thin solenoid lenses and thin rf gaps at the same location to ensure absence of temperature anisotropy at every position. Due to the rotational symmetry the r_z 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 number of axial cells from $-Z_{\max}$ to $Z_{\max}$. For these maximum grid extent

FIG. 1. Envelope of spherical bunch in standard periodic solenoid lattice with bars indicating positions of combined solenoid and rf kicks (5 periodic cells).

values we have assumed the values 3σ (in Secs. III and IV) as well as 3.5σ (in Sec. V, where a comparison is made), with σ the rms size in each direction. Beyond the grid limits PICNIC determines fields analytically assuming a Gaussian density distribution of the same rms sizes. TRACEWIN foresees two options to determine fields: nearest grid point, “weight = 0,” used in Secs. III and IV; or linear interpolation, “weight = 1,” used and compared with “weight = 0” in the Appendix.

Typical matched periodic envelopes over 5 cells—assuming a length of 1 m per cell—for a spherical (breathing) bunch with equal emittances in x, y, z and $k_{0x,y,z} = 60^\circ$ are shown in Fig. 1. Note that we have set the energy of the protons arbitrarily to 10 MeV—what matters is the space charge tune depression, which is defined further below. In all cases—unless mentioned otherwise—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 functions we employ the TRACEWIN standard options “6d-ellipsoid” (randomly generated in the six-dimensional phase space ellipsoid with parabolic density profiles), “Gaussian” (Parmila type 36), or “Gaussian in 6d ellipse.”

A. Distinction of different noise regimes

As mentioned above the validity of the rms entropy concept is limited to incoherent noise effects typical for matched “equilibrium” beams, whereas intense beams often reveal highly dynamical, coherent behavior. It is useful to compare here our spatially confined bunched beams with regimes related to extended plasma PIC simulation [9]: plasma waves have their counterpart in resonant (coherent) interactions in the beams; enhanced

collision effects due to super-particles carrying much higher charge than real particles, which are common to both; finally upper bounds to grid cell lengths—typically $\Delta x < \lambda_{\text{Debye}}$ —to avoid grid aliasing and related grid heating [16], in comparison with the need to sufficiently resolve the spatial and self-field profiles of spatially confined beams, which may also lead to grid heating.

Thus, a distinction between essentially three regimes is recognized in Fig. 2, where the noise effect is enhanced for

FIG. 2. Rms emittances (top); ϵ_{6d} (center, with dashed lines indicating transitions between different regimes); and stability chart (bottom; color scale indicating theoretical rates of emittance change) for $\epsilon_z/\epsilon_{xy} = 3$ including tune footprint over 1000 periodic cells (m).

easier demonstration by choosing a particle number as low as 1000. An initial anisotropy with $\epsilon_{x,y}/\epsilon_z = 0.35$ is assumed for a zero current phase advance $k_{0,x,y,z} = 60^\circ$. This results in space charge depressed tunes of $k_{x,y,z} = 32/32/38^\circ$, which lead to a $\lambda_{\text{Debye}} \approx \sigma/3$. The number n_c of grid cells (in r, z) is chosen as 16, thus $\Delta z/\lambda_{\text{Debye}} \approx 1$ and $\Delta x/\lambda_{\text{Debye}} \approx 0.5$. The starting distribution function is the “6d-ellipsoid” option. Results of the emittance evolution are shown in Fig. 2. Three regimes of emittance behavior are identified: (i) Coherent resonance regime: It is noted that in less than 20 cells a partial exchange occurs between transverse and longitudinal emittances. This is caused by the coherent space charge driven fourth order resonance with a stop-band around $k_z/k_{x,y} = 1$ as shown in the stability chart of Fig. 2 for the initial emittance values (details see Ref. [17]). The tune foot print (evolving from larger to smaller values of $k_z/k_{x,y}$ due to the self-consistently changing emittances) indicates the rapid initial changes of the tune ratio over the first few cells. During this resonant phase there is a steep increase of ϵ_{6d} , followed by pronounced oscillations. Therefore, ϵ_{6d} cannot be interpreted as entropy—which should be increasing only—and thus not used as a measure for noise. In this case the underlying dynamics is driven by the nonlinear space charge force—hence beyond the second order frame of the above rms-based description. Consequently, a suitable noise or entropy quantity would have to be more refined and beyond second order momenta. Note that the approach to equipartition in this regime is only partial, which is a typical self-stabilizing mechanism. (ii) Anisotropy dominated collisional regime: The remaining anisotropy slowly vanishes in the subsequent anisotropy dominated regime. Here collisional noise and anisotropy gradually lead to equal emittances and tunes at about 500 m, where $k_{x,y,z} \approx 36^\circ$. Hence the beam becomes fully equipartitioned; once this point is reached the vanishing r.h.s. of Eq. (2) predicts that no further emittance or entropy growth should occur. (iii) Grid noise regime: We find, however, that there is a continuing growth of ϵ_{6d} beyond the point of equipartition, which is unexpected in the frame of Eq. (2). We assume this growth is dominated by grid heating and presumably enhanced by a violation of the assumption of a locally isotropic collision type diffusion process in our periodic focusing system—the underlying assumption in the derivation of Eq. (2). It can be assumed that this violation is also influenced by the fact that the periodic modulation of focusing introduces a “coherent” streaming against the grid, which is not slow compared with “collision times.” This subject is also discussed in Ref. [13]. We conclude that it is appropriate to introduce a predominately grid-related noise term I_{GN} in Eq. (5), which is independent of the temperature anisotropy term:

$$\frac{d}{ds} \ln \epsilon_x(s) \epsilon_y(s) \epsilon_z(s) = \frac{k_f^*}{3} (I_A + I_{\text{GN}}). \quad (6)$$

Note that we have 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} .

Derivation of such a modified equation from first principles is beyond the scope of this paper. Instead, we take this phenomenological approach and present further support of it in the following sections.

B. Scaling with intensity

We first study the relative increase in ϵ_{6d} over 1000 cells for a strictly spherical bunch with Gaussian distribution function, $\epsilon_{x,y}/\epsilon_z = 1$, $k_{0x,y,z} = 60^\circ$ and $k_{x,y,z} \approx 33^\circ$. An example for $N = 4000$ is shown in Fig. (3) for an rz Poisson solver setting with $n_c = 16$ grid cells within 3σ . Note that Fig. 3 indicates strong initial variations of ϵ_{6d} , which damp within the first 25 m. This is caused by a lack of matching of the initial Gaussian profile—only rms matching was applied. As a result, the nonlinear space charge field energy specific to this profile is transformed into a change of rms emittances (for details see Ref. [15]). Beyond 25 m ϵ_{6d} evolves linearly in time, which gives the collision and grid induced rms entropy growth; the superimposed relatively large jitter is due to the low number of particles in this case.

The explicit dependence of this noise on space charge is shown in Fig. 4, where the linac current is varied. Here, as in all following graphs, we show the growth of ϵ_{6d} relative to its initial value, i.e., $\Delta\epsilon_{6d}/\epsilon_{6d}$. 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 ϵ_{6d} bends downward due to a strongly growing emittance, hence only the initial gradient of ϵ_{6d} was used and extrapolated to the same value of 1000 cells. We thus obtain from Eq. (6):

$$\frac{1}{k} \Delta S = \frac{\Delta\epsilon_{6d}}{\epsilon_{6d}} = \Delta s \frac{k_f^*}{3} (I_A + I_{GN}). \quad (7)$$

FIG. 3. Example of evolution of ϵ_{6d} for $N = 4000$.

FIG. 4. Relative growth of ϵ_{6d} for varying linac current I (mA), $N = 4000$ and fully isotropic bunch.

On the current scale of Fig. 4, the example of Fig. 3 with a space charge depressed tune of $k_{x,y,z} \approx 33^\circ$ is equivalent to $I = 5$ mA. The effect of space charge results in a steeper than linear, but not quite quadratic dependence on the current. This is reflected by the second order polynomial fitting shown on graph. Note that for $I = 0$ one would expect vanishing grid noise; the small offset in the fitting curve is due to the effect of nonlinear coupling terms in the rf gap model. They are beyond our second order rms entropy model, as demonstrated by this example.

C. Scaling with N and grid in rz

While the emittance exchange in the coherent regime of Fig. 2 changes only slightly for a larger number N of macro particles, the rates in the collisional and grid noise dominated regimes decrease with increasing N . Noting that the charge per simulation particle is $\propto 1/N$ we expect a corresponding decrease of the noise level for large N . Such a scaling is also supported by a recent study by Kesting *et al.*, who find that the noise level generated by fluctuations of the electric field should be inversely proportional to the number of simulation particles as long as electric field fluctuations are uncorrelated [18].

A more complete picture is shown in Fig. 5, where the relative growth of ϵ_{6d} —proportional to the rms entropy—is

FIG. 5. Relative growth of ϵ_{6d} for N from 1000 to 128.000 macro particles indicating transition to *grid resolution limited* regions.

plotted against $1/N$ (note the double-logarithmic scale, with the dashed line indicating a fictitious linear fit through the origin). For the 16×16 grid a linear dependence of $\Delta\epsilon/\epsilon$ is noted in the range from 1000 up to $\approx 20,000$ particles:

$$\Delta\epsilon_{6d}/\epsilon_{6d} \propto N^{-1} \quad (8)$$

For higher N we find, however, that $\Delta\epsilon/\epsilon$ levels off. We also show cases with grid resolution of only 12×12 and find that the departure from a linear law occurs even with less particles, and even more for 8×8 grids. The data indicate that for sufficiently large N we enter into a *grid resolution limited region* with grid heating, where further increasing of N has only little effect on the reduction of growth of ϵ_{6d} , unless the grid resolution is increased. This transition region is characterized by a typical average number of particles per cell. For a (toroidal) cell in $\Delta r \Delta z$ it is given as $N/(n_c^2 * 3.14/4)$, and we find that the transition occurs typically for 80–100 particles per toroidal cell (equivalent to about 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, if the grid resolution is not increased. This connection should be considered if one wishes to optimize the efficiency of a simulation with regard to cpu-time.

In Fig. 6 we show the rms emittance and entropy growth as function of the number of grid cells n_c , which is chosen as equal in r and z . As observed above, a resolution above 16 cells has no further benefit for only 16,000 particles, and some kind of saturation is reached. The 128,000 particles case, instead, shows progressive benefit for increasing n_c , and saturation has not yet been reached for n_c as high as 22. We remind here that n_c counts the number of cells from axis to 3σ or—as later in Sec. V— 3.5σ ; this is equivalent to much larger numbers of grid cells in other PIC codes, where the grid extends to the actual beam pipe many σ 's

FIG. 6. Relative growth of ϵ_{6d} for $N = 16,000/128,000$ and increasing number of grid cells in r, z indicating transition from a *grid resolution limited region* to a *collision dominated region*.

away. On the other hand, a n_c as low as 8 shows only a factor 2 reduction of ϵ_{6d} by increasing N from 16,000 to 128,000 due to the lack of grid resolution and grid heating. We mention that in beam dynamics studies for 3d ellipsoidal bunches of protons or ions—in linacs usually close to spherical— n_c is usually chosen around 10 for cpu time reasons. For the equilibrium beam studied here this choice is sufficiently well supported by Fig. 6. On the other hand there is no evidence in proton or ion linac applications of sharp density transitions or fine structures that would require much higher resolution. A sharp equilibrium beam edge, for example, would be expected for very strong tune depression approaching zero (“cold beam limit,” see Ref. [19]), which is impractical for rf linacs.

It is worth noting that the rise of $\Delta\epsilon_{6d}/\epsilon_{6d}$ for small n_c —in the grid resolution limited region—can be related quantitatively to the lack of spatial resolution of the beam profile, hence the space charge potential. $n_c = 6$, for example, involves only two radial grid and one axial grid cell over 1σ of the beam profile, which is obviously too coarse. For comparison with the plasma grid heating criterion by Langdon [16] this amounts to $\Delta x/\lambda_{\text{Debye}} \approx 3/2$ and $\Delta z/\lambda_{\text{Debye}} \approx 3$. Under such parameters (unphysical) aliasing with grid harmonics and related heating are possible consequences in extended plasma simulation. We assume, however, that for our “beam plasma” confined in a potential well it is more suitable to explain the grid heating by the lack of spatial resolution of the equilibrium beam profile.

In practice, the noise level or cpu time arguments may not be the only ones for selecting the number of simulation particles N . A reliable statistical level to ensure small fractional beam loss at the level of 10^{-4} to 10^{-6} can be reached only with an adequately large N .

IV. TEMPERATURE ANISOTROPY DRIVEN COLLISIONAL NOISE

For a comparison of simulations with the analytical model of Eq. (2) it is important to work in a region, where collisional noise dominates rather than noise by grid heating. In a grid heating dominated (small n_c) regime there is no reason to assume that temperature anisotropy relaxes toward equal temperatures or equipartition. We have tested this with the example of Fig. 2 and found that the collisional merging of longitudinal and transverse emittance was absent and both had a tendency to grow.

Justification of the separation of k^* and a “kinetic” term $I_A + I_{\text{GN}}$ needs careful examination. It is not *a priori* clear that I_{GN} is fully independent of, for example, space charge, if we notice that the collision distance relative to the focusing period is not independent of space charge. In order to gain some insight we study in the following the entropy growth as function of the transverse:longitudinal temperature ratio for $N = 4000$ and a relatively high resolution grid with $n_c = 16$.

FIG. 7. Relative growth of ϵ_{6d} for $k_{0xyz} = 60^\circ$ and varying (initial) temperature anisotropy.

A. Anisotropy effects with equal external focusing

In the first example we assume $k_{0xyz} = 60^\circ$ with the “6d-ellipsoid” initial distribution. The linac current is chosen again such that $k_{xyz} = 33^\circ$ for equal emittances. Different initial 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. 7 is determined via Eq. (4) using actual emittances and space charge dependent tunes k from TRACEWIN. In Fig. 7 we show $\Delta\epsilon_{6d}/\epsilon_{6d}$ determined from the initial gradient of the 6d emittance from TRACEWIN data (determined over the first 100 or few hundred cells, but as before normalized to the growth over the nominal length of 1000 cells): 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. (3) are all equal to unity. In order to check the applicability of the analytical I_A in Eq. (2) we need to fit k_f and a suitable value for I_{GN} to the numerical data using Eq. (7). The thus resulting “theoretical” curve in Fig. 7 shows good agreement with the simulation data.

B. Anisotropy effects with weaker longitudinal focusing strength

We also test this comparison for split tunes $k_{0xyz} = 60^\circ/60^\circ/47^\circ$ —this time using a Gaussian input distribution—and find again reasonably good agreement

FIG. 8. $\Delta\epsilon_{6d}/\epsilon_{6d}$ for $k_{0xyz} = 60/60/47^\circ$ and varying (initial) temperature anisotropy.

as shown in Fig. 8. The isotropic offset is slightly higher than in the example of Fig. 7, $\Delta\epsilon_{6d}/\epsilon_{6d} \approx 0.04$, which might be connected with the stronger tune depression in the weaker focusing direction (z).

V. 3D BUNCHES WITH xyz POISSON SOLVER

The findings obtained for rz symmetry also have an equivalent in the use of the xyz Poisson solver option. The $n_{cx,y,z}$ are understood here as half number of cells between the maximum grid extent values. We also consider variation of the number of space charge “steps of calculation”—keeping the Tracewin input number of “lattice calculations per m” fixed at 20/m. A Gaussian distribution function with equal rms emittances and phase advances, hence no average anisotropy, is used throughout.

A. xyz versus rz Poisson solver

We first consider the identical periodic solenoidal case used in Figs. 1, 5, 6 and replace the rz Poisson solver by the xyz option. This is shown in Fig. 9 employing (as before) 14 space charge steps per lattice cell. We find, however, that for 16.000 particles $\Delta\epsilon/\epsilon$ saturates around 0.08—more than 5 times than for the rz solver. For 128.000 particles, instead, the xyz -solver results are roughly only a factor of 2 larger than the corresponding values for the rz solver.

For $N = 16.000$ we note that increasing the number of space charge kicks from seven to eleven per cell leads to only half the growth of ϵ_{6d} for values of $n_c \approx 10$. Less frequent space charge kicks are “harder,” and it is understandable that they enhance entropy growth. This difference, however, is less pronounced for larger N .

The distinction between “collision and statistics limited” and “grid resolution limited” is even more visible than for the rz Poisson solver: (i) *Grid resolution limited*: For small n_c there is only weak benefit by increasing N from 16.000 to 128.000 due to insufficient grid resolution. As discussed above for Fig. 6, small n_c cannot resolve the beam profile.

FIG. 9. Relative growth of ϵ_{6d} for $N = 16.000/128.000$, as function of number of grid cells in x, y, z for periodic solenoid lattice of Fig. 1.

(ii) *Collision and statistics limited*: Increasing n_c above 6 enhances again the emittance growth for the case $N = 16.000$; in this case the average number of particles per grid cell falls under 10 and particle statistics on the grid becomes insufficient, besides the dominance of collision effects. Raising N to 128.000 has visible benefit due to the reduced collision effect, and no saturation is seen, although the noise reduction above $n_c \approx 8 \dots 10$ is only minor.

B. Focusing-drift-defocusing-drift (FODO) lattice

Getting closer to real applications we adopt in this section a periodic FODO lattice, including rf gaps, and set the cell length again as 1 m as shown in Fig. 10. The lattice is “equivalent” to that of Fig. 1 in the sense that the same phase advances per m are used, together with identical emittances in x, y, z . This results in approximately the same space charge depressed tunes.

The alternating focusing causes a strong modulation and local imbalance of “temperatures,” which is described in Ref. [6] as source of entropy growth. We expect that this mechanism amplifies respectively adds to the already mentioned “non-Markov” effects found for the periodic solenoid. Results are shown in Fig. 11 as function of n_c and for different N . We note that the number of space charge steps per lattice cell has been chosen here as 15 (10/m in TRACEWIN); comparison with the lower value 11 (3/m in TRACEWIN) gives only a minor difference of a few % in the growth of ϵ_{6d} , hence the chosen number of space charge steps per lattice cell is considered safe. For this and the following examples we have selected in TRACEWIN the options “linear interpolation” (on the grid) and 3.5σ for the transition mesh-analytical for the space charge potential (see Appendix for some details).

Note that $n_c = 7$ implies only two grid points per 1σ of the Gaussian profile. This can explain the steeply rising noise for less resolution, with only small differences

FIG. 10. Basic cell of equivalent FODO lattice with rf gaps.

FIG. 11. Relative growth of ϵ_{6d} in FODO for $N = 16.000/32.000/128.000$, as function of the number of grid cells in x, y, z .

between numbers of particles. All three cases show that an *optimum value* of n_c exists, where the noise is minimum. It is the higher the larger N . As before, large N is efficient only if the grid resolution is sufficiently large.

The increase of $\Delta\epsilon_{6d}/\epsilon_{6d}$ above the optimum n_c is most pronounced for the case $N = 16.000$, where an estimate shows that the number of simulation particles per grid cell is only as low as approximately 1 for $n_c = 16$, which explains the strong rise of the noise. For $N = 128.000$ the gentle increase of the noise when rising above $n_c = 10$ might be indicative of an increase of the Coulomb logarithm with higher resolution of the colliding charges. This is apparently different from the rz Poisson solver case in Fig. 9, where this region is not yet reached. It is worth noting here that in the 2d simulations of Ref. [13] the collisional growth of ϵ_{6d} is significantly more pronounced for high grid resolution—apparently due to the different range of the Coulomb force in 2d.

Comparing with Fig. 9 for the periodic solenoid, we find a generally enhanced noise level, which we ascribe to the FODO alternating gradient lattice. The results of Fig. 11 also differ from the result reported in Ref. [11], where low and high particle number (transverse) emittance growth values are 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.

C. DTL lattice

In TRACEWIN—when applied to linac design or error studies—it is customary to employ the compressed and faster option of drift tube Linac (DTL) cells. It simplifies space charge calculation to one single step of calculation per DTL cell, or optionally to three steps (marked by 1/cell and 3/cell).

We apply this method to the FODO lattice shown in Fig. 10 and obtain the results of Fig. 12. They indicate that the frequently used 1/cell option implies a not insignificant additional noise level. It thus appears preferable to choose the option 3/cell, which is equivalent—in our example—to

FIG. 12. Drift tube Linac cell option for FODO: Relative growth of ϵ_{6d} for $N = 16,000/128,000$, as function of number of grid cells in x, y, z in same lattice structure as Fig. 11.

about 36 space charge calculations per effective betatron period.

VI. CONCLUSION AND OUTLOOK

We have explored space charge and grid induced noise in 3d PIC simulation with the TRACEWIN code, and compared results with the analytical rms entropy growth equation by Struckmeier based on a purely collisional approach. Our findings support that the 6d rms emittance—defined as product of the three 2d rms emittances—can be taken as suitable measure for equilibrium beam entropy growth driven by grid *and* collision induced noise. This suggests to use it as relevant “quality measure” for optimizing computer simulation of high intensity beams. In particular, we find that an optimum combination of N and grid resolution exists: further increasing of the grid resolution is useful only, if N is increased as well. Likewise, a larger number of simulation particles has limited benefit unless there is sufficient grid resolution. The usefulness of a simulation optimization based on matched equilibrium properties in highly dynamical situations—deviations due to mismatch or resonances—is not obvious and requires careful examination in future studies.

We also find that our 3d PIC simulations are in a mixed grid effect and collision physics controlled regime. This differs from the assumption of only local collisions acting in the work by Struckmeier, where anisotropy is needed to drive entropy growth. Instead, we obtain entropy growth even in fully isotropic cases with no temperature differences.

Further theoretical work would be useful to explore in more detail the transition between the “grid effect dominated regime” and a “collision dominated regime,” where the (Markov type) particle-particle collisions are resolved. The latter can be assumed to be increasingly relevant at much higher grid resolution than employed here. Transient effects due to the rapidly changing focusing need to be taken into account, furthermore the presence of “coherent flow” in periodic focusing—as opposed to incoherent temperature-like

motion typical for steady state plasmas—needs to enter in a suitable way into more detailed analytical studies.

Filters [20] can reduce the noise at high frequencies, but can also smooth out important small-scale effects in beams. High-order interpolation [21] reduces the noise, but increases the computing times. Therefore one often prefers to use a larger number of macro-particles instead of higher-order interpolation schemes. Both measures, filters and higher order interpolation, should only weakly affect the scaling of the artificial emittance growth with current and macro-particle number. However, a detailed study of the possible advantage of filters and higher-order interpolation schemes is left to future work. Energy conserving PIC schemes (see, e.g., Ref. [22]) can avoid or delay the onset of grid heating. This comes at the cost of by far more complex evolution algorithms. In beams the emittance growth due to artificial collision is more important. Here the emittance growth is caused by the nonconservation of the entropy and not by the nonconservation of energy. Therefore, we would expect the results to be similar in the case of energy conserving schemes. However, detailed comparisons of momentum and energy conserving PIC schemes for beams are also beyond the scope of this study.

Further work is also required to extend this analysis to very nonspherical 3d bunches with substantially different oscillation frequencies—like slow synchrotron motion—in order to explore the role of PIC simulation noise for circular accelerators in a similar framework.

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APPENDIX: TRACEWIN SPECIFIC ISSUES

Our comparison between PIC noise and analytical models is based on a specific code—here the TRACEWIN

FIG. 13. Dependence of relative emittance growth on grid interpolation (“weight = 0/1” corresponding to no/linear interpolation) and mesh boundary (at 3/3.5 rms) as function of N (in units of 1000).

code. We must assume that some code specific issues exist which enter into the quantitative analysis.

We assume the most important candidates for this are the TRACEWIN-specific features of grid interpolation and of the definition of the mesh boundary, where the grid is continued by an analytical model for the potential. One may expect that these mechanisms somewhat modify the strength of noise. To this end we study the influence of the relevant parameters in the case $n_c = 8$ of Fig. 11. Results are shown in Fig. 13. For low particle numbers it is beneficial to employ the linear interpolation scheme as compared with no interpolation at all. This is understandable as fewer particles per cell cause larger statistical variations, which can be smoothed by interpolation.

The choice of the mesh boundary at 3.5σ rather than 3σ also reduces slightly the noise. Not surprisingly, it is also reduced by the choice of linear interpolation.

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