SELF-CONSISTENT PIC SIMULATIONS OF BEAM-CAVITY INTERACTIONS USING RICIAN SUB-BEAMS

L.Serafini, M.Zanin, A.Peretti and C.Pagani
University of Milano and INFN
Via Celoria 16, 20133 Milano, Italy.

Abstract

Particle In Cell codes, typically used in the simulations of beam dynamics in presence of strong interactions between the beam and its self-field (space charge and/or wake-field), deal with the problem of assigning the beam charge and current distributions at the mesh nodes on the basis of particle positions and velocities. In this paper a new assignment algorithm is presented, suitable for axi-symmetric beams, based on Rician distributed macro-particles: this method has been successfully implemented[1] in the PIC self-consistent code ITACA, extensively used for the design and study of RF electron guns.

The relevance of such a new algorithm on the calculation of beam emittances and other beam parameters is discussed: it is shown that the minimization of unphysical fluctuations in the e.m. field propagation allows a noise-free evolution of the beam-field interaction process reaching a greater accuracy in the beam dynamic simulation.

Introduction

The subject of assignment algorithms in PIC simulations and its relevance for the control of the unphysical charge fluctuations within the cells, has been extensively discussed in the literature[2]. These studies have shown that the gaussian assignment algorithm is in this respect far superior to other commonly used techniques. In the following section we discuss a particular version of this algorithm suitable for the simulation of axi-symmetric beams. Indeed, cylindrical charge and current distributions can be described by an ensemble of 2D macro-particles distributed within a 4D (r,p_r,z,p_z) phase space, saving a lot in computation time with respect to a 6D (x,p_x,y,p_y,z,p_z) phase space description, which needs larger numbers of 3D macro-particles to guarantee the same particle density in the phase space. Here the term macro-particle is used to define a representative (sample) point in a nD phase space, that is associated to a charge and current distribution in the corresponding (n/2)D real space.

The development of an axi-symmetric assignment algorithm should start from usual basic requirements[2]:

a) the charge assigned to a mesh node M from a macro-particle Q should scale like the charge of the macro-particle and should decrease as the distance between M and Q

b) the charge assigned to a mesh node M from an infinitely large ensemble of uniformly distributed macro-particles should be independent on the position of M

c) the charge and current density distributions ρ and J must satisfy the continuity equation

Condition c) is implicitly satisfied by most 3D algorithms, while it must be explicitly checked in the axi-symmetric case. Indeed, a simple extension of the gaussian algorithm to the cylindrical coordinate system can be shown to violate such a condition. Let us take the following expression for the charge density distribution:

$$\rho^G(r,z) = \rho_o^G(r_p)\, e^{-\left[(z-z_p)^2/2\sigma_z^2 + (r-r_p)^2/2\sigma_r^2\right]} \qquad (1)$$

where (r_p,z_p) are the particle coordinates on the mesh and the normalization coefficient $\rho_o^G(r_p)$, given by:

$$\rho_o^G(r_p) = \frac{Q}{(2\pi)^{3/2}\sigma_z\sigma_r^2}\left[e^{-(r_p^2/2\sigma_r^2)} + \frac{r_p}{\sigma_r}\sqrt{2\pi}\,\mathrm{erf}\left(\frac{r_p}{\sigma_r}\right)\right]^{-1}$$

(erf(x) is the error function) is needed to assure $Q = \int_{V_\infty}\rho^G dv$.

It can be seen at a glance that the radial derivative of the charge density distribution $\partial\rho^G/\partial r$ calculated on axis (r=0) is different from zero for $r_p>0$, in contrast with the requirement of axi-symmetry. Moreover, the continuity equation $\nabla \bullet \mathbf{J} + \partial\rho^G/\partial t = 0$ is violated at r=0, as shown elsewhere[3], when the 2D macro-particle Q moves radially off-axis.

The Rician assignment algorithm

To overcome this problem we developed an *ad hoc* distribution: we look at a single 2D macro-particle (hereafter referred as 2Dmp), positioned at a point (z_p,r_p) on the mesh, as given by the superposition of several 3D gaussian micro-distributions whose centroids are spread over the circle C of radius r_p, laying in the plane (x,y) and centred on the z symmetry axis at $z=z_p$. If the centroids are uniformly distributed with linear density λ on the circle, the 2Dmp distribution will be given by:

$$\rho(r,z) = 2\pi\, r_p\, \lambda \int_0^{2\pi}\tilde{\rho}\, d\theta \qquad (2)$$

where $\tilde{\rho}$ are 3D gaussian functions $(G(a,b,c)\equiv e^{-(a^2+b^2+c^2)/2})$ of argument $((x-x_p)/\sigma_r,(y-y_p)/\sigma_r,(z-z_p)/\sigma_z)$, under the condition $x_p^2 + y_p^2 = r_p^2$ (the gaussian widths σ_x and σ_y of the micro-distributions are taken equal to a common value σ_r in order to preserve the cylindrical symmetry). Rearranging terms under the integral in (2), it can be found[3]:

$$\rho(r,z) = 4\pi\, r_p\, \lambda\, e^{-(z-z_p)^2/2\sigma_z^2}\int_0^{\pi} e^{-(r^2+r_p^2)/2\sigma_r^2}\, e^{r r_p\cos\theta/\sigma_r^2} d\theta$$

Since the linear density λ must scale like $1/r_p$ in order to keep the 2Dmp charge Q invariant under change of its radial position r_p, the expression for the 2Dmp distribution $\rho(r,z)$ becomes:

$$\rho(r,z) = \frac{Q}{(2\pi)^{3/2}\sigma_r^2\sigma_z}\, e^{-\left[(z-z_p)^2/2\sigma_z^2 + (r-r_p)^2/2\sigma_r^2\right]} e^{-x} I_0(x) \quad ; \quad x \equiv \frac{r\, r_p}{\sigma_r^2} \qquad (3)$$

where $I_0(x)$ is the 0-th order modified Bessel function of the first kind.

The radial part of such 2Dmp charge density distribution is actually a modified Rician distribution, well known in the context of the statistical optics for the laser speckle studies[4].

It is plotted in Fig.1 the quantity $\rho_o(\alpha,\beta)\equiv\rho(r,z=z_p)$ as function of the normalized radial position $\alpha\equiv r/\sigma_r$ of the computation mesh node, for different values of the radial 2Dmp position $\beta\equiv r_p/\sigma_r$. It can be clearly seen that $\rho_o(\alpha,\beta)$ is actually a gaussian function of α, i.e. $e^{-\alpha^2/2}$, at $\beta=0$, while it is close to a gaussian function of α with an enlarged width, i.e. $e^{-\alpha^2/2x}$ $x>1$, for small β's and, after assuming a strongly perturbed shape for intermediate β's, it resembles again a gaussian of $\alpha-\beta$, i.e $\frac{e^{-(\alpha-\beta)^2/2}}{\sqrt{2\pi\beta}}$, for large β's .

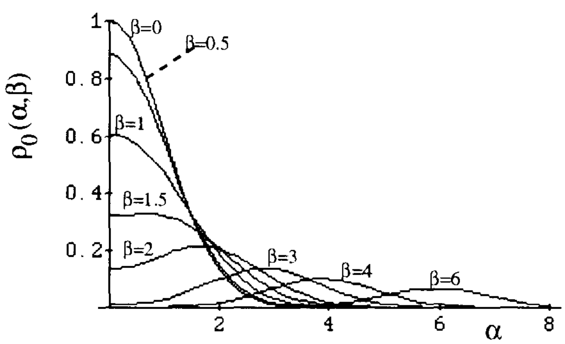

Fig.1 - Rician distribution form factors (arb. units) for the radial part of the 2D macro-particle charge density ρ as functions of the normalized mesh node radius α, at different normalized radial positions β of the 2D macro-particle.

This is easily verified recalling the asymptotic behaviour of $I_0(x) \sim e^x/\sqrt{2\pi x}$ when $x \gg 1$. The normalization condition $Q = \int_0^{2\pi} d\theta \int_0^{\infty} r dr \int_{-\infty}^{\infty} \rho(r,z)dz$ can be either proved using the result[5] $\int_0^{\infty} e^{-ax} I_0(b\sqrt{x})dx = \frac{e^{b^2/4a}}{a}$. Therefore, each 2Dmp comes out to be represented by a charge density cloud which assumes different shapes depending upon the 2Dmp radial position r_p. When the 2Dmp sits on-axis ($r_p=0$) the charge cloud is distributed actually like an axi-symmetric 3D gaussian with centroid located at ($x_p=0,y_p=0,z_p$) and widths σ_r and σ_z, such that the equi-density surfaces are ellipsoids defined by the equation $x^2/\sigma_r^2 + y^2/\sigma_r^2 + z^2/\sigma_z^2 = \text{const}$. When the 2Dmp is shifted slightly off-axis (i.e. $r_p<\sigma_r$) the density distribution remains qualitatively of the same kind, but the peak charge density at the centroid is decreased as long as the effective radial width σ_r is enlarged. For larger r_p the charge cloud resembles the behaviour of a smoke ring, with an increasing hollow-like behaviour: eventually, the cloud reaches a thoroidal-like distribution when the particle is well far off-axis ($r_p \gg \sigma_r$). At that time the charge density distribution approaches asymptotically a thoroidal gaussian function of the type:

$$\rho(r,z) \sim \frac{Q}{(2\pi)^2\sigma_z\sigma_r r_p} e^{-[(z-z_p)^2/2\sigma_z^2+(r-r_p)^2/2\sigma_r^2]}$$

The construction of the current density distribution associated to a 2Dmp whose charge density is specified by eq. (3) can be developed as in the following: assuming that the 2Dmp can move freely on the mesh in the (r,z) plane, with a velocity specified by $\mathbf{v} = v_r\mathbf{e}_r + v_z\mathbf{k}$, the corresponding propagation of its associated charge density distribution can be thought to be generated by the centroid motion of all the 3D micro-distributions $\tilde{\rho}$, moving all with the same v_r and v_z components. This guarantees that the linear density λ of the centroids distributed on the circle C (of radius r_p) remains uniform all over the circle, varying like $1/r_p$ as the circle C is expanding (or collapsing) in radius. In this way the cylindrical symmetry can be preserved and, as shown later on, the continuity equation can be either satisfied all over the space.

To find out the actual expression for $J(r,z) = J_r(r,z)\mathbf{e}_r + J_z(r,z)\mathbf{k}$, first we observe that the axial component J_z has the same behaviour vs r and z of the charge density, hence is simply given by $J_z(r,z) = v_z\rho(r,z)$; the radial component J_r must be instead calculated by[3]

$$J_r(r,z) = 2\pi\, r_p\, \lambda v_r \int_0^{2\pi} \tilde{\rho}\cos\theta d\theta \qquad (4)$$

which, upon integration, gives

$$J_r(r,z) = v_r\, \rho(r,z)\, \frac{I_1(x)}{I_0(x)} \quad ; \quad x \equiv \frac{r\, r_p}{\sigma_r^2} \qquad (5)$$

where $I_1(x)$ is the 1st order modified Bessel function of first kind. The radial behaviour of J_r calculated at the 2Dmp z-position (i.e. $J_r(r,z=z_p)$) is plotted in Fig.2 as a function of α for different values of the normalized 2Dmp radial position β.

Again for large β (i.e. $r_p \gg \sigma_r$) we get a gaussian profile for J_r, peaked at r_p at an amplitude scaling like $1/r_p$, as typical of the current density distribution of a thoroidal gaussian charge density distribution which is propagating radially outward: this is actually due to the result $I_1(x)/I_0(x) \sim 1$ for $x \gg 1$. The behaviour at low β is more complex: it is worth

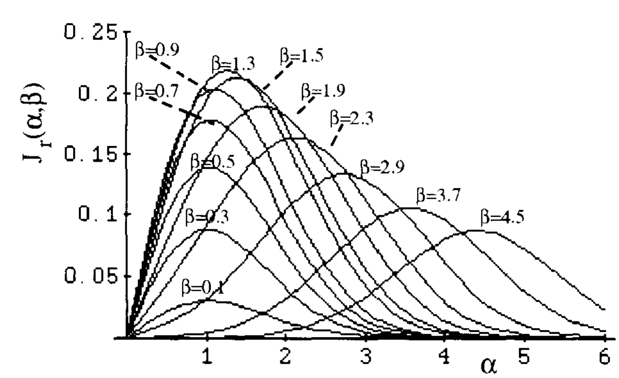

Fig.2 - Rician distribution form factors (arb. units) for the 2D macro-particle radial current density J_r, as functions of the normalized mesh node radius α, for different values of the normalized 2D macro-particle radial position β.

noting that J_r close to the axis (low α) scales like β, since the condition of axi-symmetry ask for a vanishing transverse component of the current on axis.

In case the 2Dmp has an azimuthal velocity component $v_\theta = \omega_p r_p e_\theta$, the azimuthal component J_θ of the current density distribution is clearly given by $J_\theta(r,z) = \omega_p\, r\, \rho(r,z)$: this is of interest for the simulation of cylindrical beams injected into the magnetostatic field of a solenoid.

The modified Rician charge and current distributions (3) and (5) have a number of useful properties when applied to an axi-symmetric assignment algorithm:

I) - despite the infinite range of the distribution, due to its fast decrease only the mesh nodes contained inside the ellipse E of equation $(z-z_p)^2/(4\sigma_z)^2 + (r-r_p)^2/(4\sigma_r)^2 = 1$, centred on the 2Dmp position (r_p,z_p), are assigned a charge and current density value according to (3) and (5). The total charge contained inside the ellipse E, i.e. $Q_E \equiv \int_E \rho dv$, can be analytically calculated only at $r_p=0$, where it is found $Q_E=Q(2\mathrm{erf}(4)-1-8e^{-8}/\sqrt{2\pi})$, and at $r_p \gg \sigma_r$, where $Q_E=Q(1-e^{-8})$. It has been numerically checked that Q_E is less than Q by a quantity not larger than $10^{-3}Q$ all over the range of r_p.

II) - By applying a standard method[2], we evaluated the unphysical charge fluctuations produced by the assignment algorithm: uniformly distributing a large ensemble of 2Dmp's on the nodes of a regular mesh of step d_p and moving such a 2Dmp mesh over a regular calculation mesh of step d_c, it is possible to compute (numerically) the normalized deviation D, defined as the the difference between the maximum and minimum value of the charge density over the calc. mesh, i.e. $D\equiv(\rho^{max}-\rho^{min})/\rho^{max}$. An ideal assignment algorithm (obeying the condition b) mentioned above) should get D=0 at all values of the parameter r, defined as the ratio between the two mesh steps, $r\equiv d_c/d_p$ (D gives actually a measure of the unphysical fluctuation amplitude). We found that the Rician assignment algorithm assures D<1% when r>0.55 , meaning that at least 0.3 particle per cell are needed to keep the unphysical fluctuations below 1% (note that the number of particle per cell scales like r^2). Such a performance is a little better than the gaussian assignment algorithm, which needs[2] more than 0.64 particle per cell to keep D<1% . The required particles per cell can be further decreased as long as larger Rician widths σ_r and σ_z are used (previous data have been achieved setting $\sigma_r=\sigma_z=d_c$): in practice we found that the best compromise between high resolution (i.e. smaller Rician widths) and low unphysical fluctuations (larger Rician widths) is achieved setting $\sigma_r=\sigma_z=1.25d_c$.

III) - It can be analytically proved[3] that the distributions (3) and (5) satisfy the continuity equation, that, for an axi-symmetric beam, reads : $\frac{1}{r}\frac{\partial}{\partial r}(rJ_r) + \frac{\partial J_z}{\partial z} + \frac{\partial \rho}{\partial t} = 0$. The proof follows from $\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial r_p}\frac{dr_p}{dt} + \frac{\partial \rho}{\partial z_p}\frac{dz_p}{dt} = \frac{\partial \rho}{\partial r_p}v_r + \frac{\partial \rho}{\partial z_p}v_z$ and by the equations $\frac{dI_0(x)}{dx} = I_1(x)$, $\frac{dI_1(x)}{dx} = I_0(x)-I_1(x)/x$. The relevance of such a property of the Rician distribution (matching the required condition c) previously mentioned) comes out clearly when a wave-equation integration is applied to describe the field propagation in presence of coupling to the beam current[1]: in this case, the capability of the assignment algorithm to satisfy the continuity equation allows to respect Gauss theorem (i.e. gauge invariance) during the integration even if not explicitly imposed.

PIC simulations with Rician sub-beams

The PIC code ITACA has been equipped with the Rician assignment algorithm and tested in the context of RF laser-driven guns[6]. In Fig.3 the current density distributions J_r (dashed lines) and J_z (solid lines), associated to a 1 nC electron bunch, are plotted as function of z at different radii, when the bunch is still being accelerated inside the RF cavity of the gun (note the negative sign of J_r, since the beam is focussing at that location). It is worth noting that the bunch current density distribution retain the gaussian profile both in radius and in time (or z, since the bunch is travelling at v~c along z) of the laser pulse illuminating the cathode: no appreciable fluctuations can be observed. As a consequence, the noise produced in the phase space distributions is kept quite low, giving very regular dependence[7] of the beam parameters (emittances, spreads,..) versus the bunch charge and accelerating field.

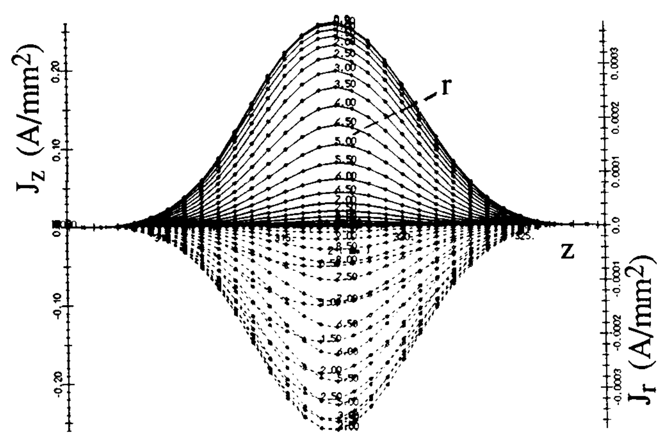

Fig.3 - Current density distributions J_r (dashed lines)and J_z (solid line) of a 1 nC electron bunch accelerated in a RF gun, as produced by the Rician assignment algorithm (see text for details).

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