

HERSC: A NEW 3 DIMENSIONAL SPACE CHARGE ROUTINE FOR HIGH INTENSITY BUNCHED BEAMS

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Abstract

The Coulomb forces between particles in a bunch yield to the 3D electrostatic Dirichlet-Neumann problem within boundary conditions often hard to define. The present routine derives from the typical procedure adopted in mathematical physics; the problem is transposed from some point to point correspondence onto a functional space spanned by a finite sequence of 3D Hermite functions, where the analytical set of beam self-field equations is found without any sort of restriction or basic hypothesis.

1 INTRODUCTION

A new generation of high intensity, high energy accelerators is under consideration, typically requiring particle loss levels below 1W/m. Therefore simulation methods in space charge computations are being improved for more detailed studies of exact beam evolution under any circumstance. The objective of the present work is a routine allowing accurate 3D space charge computations without any sort of restriction or basic hypothesis.

2 THE DENSITY OF THE BUNCH

The distributions of bunches, even of complicated distinct non-symmetrical shapes, can be represented within a compact region by bounded, continuous and positive functions [1]. Hermite functions $\hat{h}_n(u)$, requiring no strict limit provided that they are properly scaled, are appropriate to represent such distributions. These Hermite functions are shown after normalization in Fig.1.

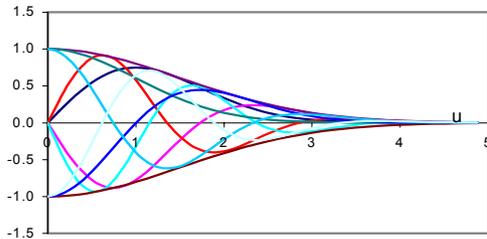


Figure 1: Even and odd normalized Hermite functions $\hat{h}_n(u)$ for n varying from 0 to 7 are represented with the envelopes. One notices that these functions decrease rapidly to zero and can be considered null when $u \geq 4$.

The Hermite functions are extended in 3 dimensions from the relation:

$$\delta_{lmn}(x, y, z) = \hat{h}_l(x)\hat{h}_m(y)\hat{h}_n(z) \quad (1)$$

Endowed with an adequate metric, a finite sequence of these δ_{lmn} constitutes a complete 3D orthogonal basis. The metric is defined from:

$$\left\{ \begin{aligned} \langle f, g \rangle &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, z)g(x, y, z)d\varpi \\ \|f\| &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y, z)f(x, y, z)d\varpi \end{aligned} \right. \quad (2)$$

where $d\varpi = e^{-(x^2+y^2+z^2)/2} dx dy dz$

The orthogonality relationship is

$$\|\delta_{lmn}\| = (2\pi)^{3/2} l!m!n! \quad (3)$$

and the inner product is null.

$\rho(x, y, z)$ being the distribution of the bunch, one considers the following limited Hermite series expansion:

$$S(\rho) = \sum_{l=0}^l \sum_{m=0}^m \sum_{n=0}^n A_{lmn} \delta_{lmn} \quad (4)$$

$$\text{with : } A_{lmn} = \frac{\langle \rho, \delta_{lmn} \rangle}{\|\delta_{lmn}\|} \quad (5)$$

One proves that $S(\rho)$ respects the conditions required by the ‘Mini-Max’ theorem of Chebitcheff. Then, $S(\rho)$ oscillates regularly around ρ in each Cartesian direction such that two successive oscillations are identical but with alternate sign [2]. The beam self-fields being computed from the integration of $S(\rho)$ instead of the one of ρ , with regard to $d\varpi$, the compensation between two successive identical oscillations of opposite sign minimizes the difference between this integration and the one of the distribution ρ . By increasing the values l, m, n in Eq.4, the magnitude of the oscillations falls off to zero and an estimate of the error in the integration with regard to l, m, n is possible [2]. The problem is then to find the lower upper limits l, m and n providing these regular oscillations. The distributions of clouds of particles having identical analytical characteristics, one proves [2] that these lower upper limits are always similar. Among all the terms occurring in the Hermite series expansions from these upper limits, just a few tens of the more significant terms are sufficient to provide the regularity of the oscillations; the other terms can be removed. These few significant terms are selected from a parameter which must be defined. The method to find this parameter at once as well as the lower upper limits consists of using typical analytical functions having identical characteristics to the distributions and from which the beam self-fields can be

predicted and compared to the ones obtained from the potential equation (Eq.7). As soon as the regularity of the oscillations exists, the beam self-field errors become negligible[2].

3 COMPUTATION OF THE HERMITE COEFFICIENTS A_{lmn}

$H_l(x_i)$ being the Hermite polynomial, one shows that:

$$A_{lmn} = \frac{1}{\|\delta_{lmn}\|} \sum_{i=1}^N H_l(x_i) H_m(y_i) H_n(z_i) \quad (6)$$

Here (x_i, y_i, z_i) are the coordinates of the particles. The accuracy of these coefficients depends more on the closeness of the points in the bunch than on the importance of the statistics (see Fig.4) [2].

4 THE BEAM SELF-FIELDS

Through the substitution of ρ by the series expansion $S(\rho)$ in the potential equation, one can write:

$$\nabla U^* = -q / \varepsilon_0 \sum_{l=0}^l \sum_{m=0}^{m^*} \sum_{n=0}^{n^*} A_{lmn} \hat{h}_l(x) \hat{h}_m(y) \hat{h}_n(z) \quad (7)$$

One considers separately each term in Eq.7:

$$\nabla U_{lmn} = -A_{lmn} \hat{h}_l(x) \hat{h}_m(y) \hat{h}_n(z) \quad (8)$$

from which one obtains in the x-direction:

$$E_{lmn} = (-i)^{l+m+n+1} \frac{q}{\varepsilon_0} A_{lmn} (2\pi)^{-3/2} \times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\hat{x}^{l+1} \hat{y}^m \hat{z}^n}{\hat{x}^2 + \hat{y}^2 + \hat{z}^2} e^{-(\hat{x}^2 + \hat{y}^2 + \hat{z}^2)/2} e^{i(\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z})} d\hat{x} d\hat{y} d\hat{z} \quad (9)$$

The integral, computed analytically, yields the set of beam self-field equations of the Dirichlet-Neumann problem within an arbitrary bunch [2]. Examples of beam self-fields are shown in Fig.2.

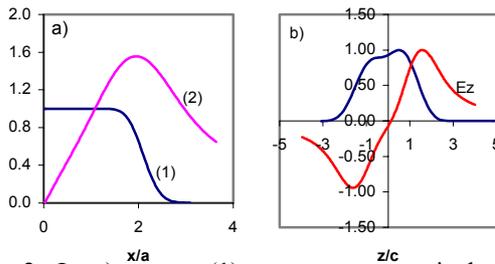


Figure 2: In a), curve (1) represents a typical density function from which the field can be obtained at once. Curve (2) is the field E_x for this density function computed from Eq.7 with the 70 most significant $A_{lmn} \delta_{lmn}$ terms. A perfect agreement exists with the field predicted. In b), for a bunch of 40000 macro-particles at the end of the SNS/ORNL DTL, one represents the longitudinal distribution and the corresponding field E_z computed from the 50 most significant terms in Eq.7. Both have been normalized with regard to the longitudinal direction. These terms being sufficient to provide regular oscillations of the Hermite series

expansion around the density, by increasing to 250 the number of significant terms, the accuracy is not improved. It is a consequence of the ‘Mini-Max’ theorem of Chebitcheff: As soon as the regularity of the oscillations is obtained, the field errors become negligible.

5 COMPARISON WITH OTHER SPACE CHARGE METHODS

With Particle In Cell (PIC) methods, the space is mapped with a mesh constituted by rectangles, such as SCHEFF [3], or cubes, such as PICNIC [4]. The fields at the nodes of a box are computed in assuming this box uniformly charged with regard to the number of particles confined in the box. The fields acting on the particles inside the box are computed from the nodes of this box. The fields in such a box, often subject to statistical noise and being ‘unaware’ of the other boxes not adjacent to this box cannot be mathematical solutions of the electrostatic Dirichlet-Neumann problem. Another approach is the routine SCHERM [5] where the bunch is considered to be consisting of several ellipsoids in the longitudinal direction, whereas in the transverse directions it keeps only one ellipsoid (note that this contrasts with the complex shape of the transverse density). Fig.3 and Fig.4 depict comparisons of results obtained with the above-mentioned types of space charge routines.

In Fig.3, for a given setting of the 81 cavities of the SNS super-conducting linac (SCL), the evolution of the quantity $R = \sqrt{E_x^2 + E_y^2}$ (where E_x and E_y are the horizontal and the vertical emittance) has been plotted as computed with the Fortran code DYNAC [6] using HERSC, SCHERM, and SCHEFF.

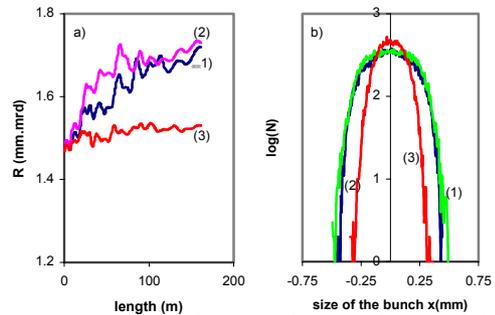


Figure 3: a), For a given setting of the SNS SCL, the evolution of the quantity R has been computed results from HERSC (1), SCHERM (2), and SCHEFF (3). In b), one shows the logarithm of the number of particles in the bunch as a projection along the x-axis at the end of the SCL for HERSC (1), SCHERM (2), SCHEFF (3) from SCHEFF.

The differences in Fig 3 a) can be explained as follows: The rotational symmetry around the longitudinal direction not always being respected, with SCHEFF the assumption of this rotational symmetry eliminates coupling effects between x and y and tends to reduce the evolution of the transverse emittances. With SCHERM the hypothesis of

the transverse density equivalent to a simple shape could affect the coupling effects between x and y . The differences in Fig 3 b) is mainly due to the few % from the 40000 particles forming a halo around the core of the bunch.

One is mainly concerned by the validity of the solution of the Dirichlet-Neumann problem in the *physics sense*, therefore differences between the simulated and real beam should be studied carefully (e.g. dependence of the simulation results on the number of particles, on the type of input distribution etc). Fig 4 a) shows that for HERSC the maximum beam extent does not vary with the number of macro-particles used. In Fig 4 b) one notices that results from the simulation discussed in Fig 4 a) yields more than double the number of particles beyond 3 RMS in HERSC than in some other space charge routines. Note that these other methods cannot be solutions to the Dirichlet-Neumann problem.

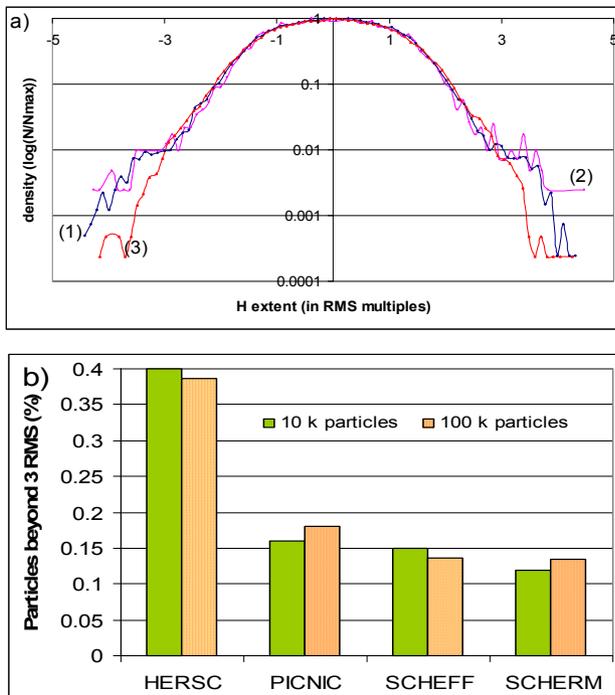


Figure 4: In a), one shows the logarithm of the number of particles (normalized) in the bunch at the SNS DTL output as projected along the x axis for HERSC with 100k particles (1), for PICNIC with 100k particles (3) and curve (2) is like (1), but with 10k particles. In b), one compares the particles beyond 3 RMS computed with HERSC and three other space charge methods. Results are shown for 10k and 100k particles at the SNS DTL output.

6 COMPUTING TIME WITH HERSC

Typically computing time is proportional to the number of particles. In HERSC one has a mesh constituted by cuboids automatically overlapping most of the cloud of particles. Contrary to other space charge methods that employ a mesh, in HERSC the values at the nodes of the mesh are computed by taking into account the statistics in

its integrity, and are independent of the number of particles lying in each box. The fields acting on the points in the boxes are obtained through a very accurate and adequate interpolation. The few remaining points are computed like the nodes. The computer time becomes roughly proportional to the number of nodes in the mesh; of the order of 500 nodes are generally sufficient for accurate interpolations [2]. With these improvements the routine is relatively fast (see Fig.5).

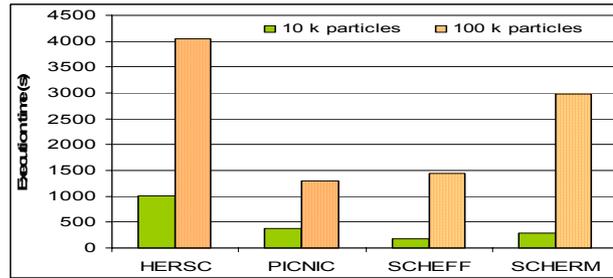


Figure 5: Execution time for 10k and 100k particles through SNS MEBT-DTL (on a 750 MHz, 250 MB laptop). As shown in Fig.4, with HERSC only 10k particles are sufficient for the accuracy. Other routines typically need 100k particles for similar accuracy.

7 CONCLUSIONS

HERSC is an accurate and relatively fast space charge routine. It has been integrated into the Fortran code DYNAC and could be a good tool for understanding the mechanism of generation of halo phenomena and for studies of the evolution of beam halo, particularly when misalignments exist in the machine. The analytical set of beam self-field equations, constituting the solution of the 3D Dirichlet-Neumann problem within an arbitrary bunch, is obtained without any sort of restriction or basic hypothesis. The approach can also be applied in several other branches in mathematical physics where the field is reduced to the potential equation as, for instance, in the gravitational problem.

8 REFERENCES

- [1] S.S. WILKS, "Mathematical Statistics", John Wiley & Sons, Inc New York, London, 1962.
- [2] "An analytical solution of the 3D electrostatic Dirichlet-Neumann problem applied to high intensity bunched beams", by the authors, in preparation.
- [3] F.Gay, Los Alamos Group AT-1 Memorandum AT-1:85-90, March 6,1985
- [4] N. Pitchoff et al, "Simulation results with an alternate 3D space charge routine, PICNIC", Proc. Linear Acc. Conf. Chicago, 1998, pp.141-143.
- [5] P. Lapostolle et al, "A modified space-charge routine for high intensity bunched beams", NIM, A 379 (1996), pp. 21-40.
- [6] "DYNAC: A multi-particle code in beam dynamics computations in complex accelerating elements", presented at this conference by the authors.