# A SPACE CHARGE ALGORITHM FOR ELLIPSOIDAL BUNCHES WITH ARBITRARY BEAM SIZE AND PARTICLE DISTRIBUTION 

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## Abstract

We propose an universal and precise method of electric field calculation in the case of an ellipsoidal bunch. The distribution function is fitted by the polynom of a certain degree and further calculations are made for this polynomial expansion. In the case of axisymmetric bunches the analytic solution is derived. Tests illustrate the high accuracy of this method.

## INTRODUCTION

The problem of space charge calculation is not new. The problem of analytical or semi-analytical space charge calculation has been considered for linac applications with the goal of combining accuracy with efficiency [1][2]. We are presenting an algorithm, which is applied to linac code benchmarking (HIPPI-project), where high accuracy is required. The same algorithm can be applied to the space charge problem in the FAIR project [3], where particle losses must be calculated during a long term storage involving more than $10^{5}$ turns. For either appication it is important to avoid or estimate the artificial noise of electric field from Poisson solvers. For this reason, an analytic model of the space charge is considered. We restrict ourselves to bunches with ellipsoidal symmetry, where the charge distribution is given by $\rho(x, y, z)=Q n(x, y, z)$ with $Q$ the total charge in the bunch. The normalized 3D particle distribution $n(x, y, z)$ is defined as

$$
\begin{gather*}
n(x, y, z)=\frac{\hat{n}(T)}{4 \pi a b c}  \tag{1}\\
T=x^{2} / a^{2}+y^{2} / b^{2}+z^{2} / c^{2}
\end{gather*}
$$

where $a, b, c$ are the bunch axis and $T$ is the isodensity parameter. The function $\hat{n}(t)$ characterizes the distribution and satisfies the condition

$$
\int_{0}^{1} \hat{n}\left(t^{2}\right) t^{2} d t=1
$$

In Ref. [4] is derived the following general formula for the electric field created by 3D ellipsoidal bunch

$$
\begin{equation*}
E_{x}=\frac{Q}{2} x \int_{0}^{\infty} \frac{\hat{n}(\hat{T})}{\left(a^{2}+t\right)^{3 / 2}\left(b^{2}+t\right)^{1 / 2}\left(c^{2}+t\right)^{1 / 2}} d t \tag{2}
\end{equation*}
$$

with

$$
\hat{T}=\frac{x^{2}}{\left(a^{2}+t\right)}+\frac{y^{2}}{\left(b^{2}+t\right)}+\frac{z^{2}}{\left(c^{2}+t\right)}
$$

Similar expressions hold for $E_{y}, E_{z}$.

## SOLUTION FOR AXISYMMETRIC ELLIPSOIDAL BUNCH

In this section we study the electric field of an axisymmetric bunch with axis $a=b, a \ll c$. The isodensity parameter reads $T=r^{2} / a^{2}+z^{2} / c^{2}$, where $r^{2}=x^{2}+y^{2}$. We restrict ourselves to bunches with distribution function $\hat{n}$, which is a polynom of degree $N$

$$
\begin{equation*}
\hat{n}(t)=\sum_{l=0}^{N} c_{l} t^{l} \tag{3}
\end{equation*}
$$

Since we consider bunches with an edge, the distribution function $\hat{n}(t)$ has to be zero on the edge, which is identified by the condition $t=1$, i.e. $\hat{n}(1)=0$, and zero outside $(t>1)$. The general solution in this case can be found substituting Eq. 3 in Eq. 2

$$
\begin{gather*}
\frac{E_{x}}{x}=\frac{E_{y}}{y}=\frac{Q}{2} \sum_{l=0}^{N} c_{l} \sum_{i+j=l} \frac{l!}{i!j!} r^{2 i} z^{2 j} I_{i+1, j}(\tau)  \tag{4}\\
\frac{E_{z}}{z}=\frac{Q}{2} \sum_{l=0}^{N} c_{l} \sum_{i+j=l} \frac{l!}{i!j!} r^{2 i} z^{2 j} I_{i, j+1}(\tau) \tag{5}
\end{gather*}
$$

where

$$
\begin{equation*}
I_{i, j}(\tau)=\int_{\tau}^{\infty} \frac{1}{\left(a^{2}+t\right)^{1+i}\left(c^{2}+t\right)^{1 / 2+j}} d t \tag{6}
\end{equation*}
$$

The lower integration limit $\tau$ depends on the particle position: $\tau=0$ if the particle is inside the bunch, $\tau=B / 2+$ $\left(B^{2} / 4+C\right)^{1 / 2}$ if the particle is outside. The quantities $B$ and $C$ are $B=r^{2}+z^{2}-a^{2}-c^{2}, C=r^{2} c^{2}+z^{2} a^{2}-a^{2} c^{2}$. It follows then that the integral Eq. 6 has to be computed for each particle which is outside the beam edge. The analytic expressions of $I_{i, j}(\tau)$ have already been found in [5], but the complexity of such formulas makes their use difficult for large value of $i, j$. An alternative way of calculating $I_{i, j}(\tau)$ is found by using hypergeometric functions [6] as follows

$$
I_{i, j}(\tau)=\frac{{ }_{2} F_{1}(1+i, 0.5+i+j, 1.5+i+j, \phi)}{(0.5+i+j)\left(\tau+c^{2}\right)^{0.5+i+j}}
$$

where

$$
\begin{gathered}
{ }_{2} F_{1}(l, m, n, k)=1+\frac{l m}{1!n} k+\frac{l(l+1) m(m+1)}{2!n(n+1)} k^{2}+\ldots \\
\phi=\left(c^{2}-a^{2}\right) /\left(c^{2}+\tau\right)
\end{gathered}
$$

This expression allows to calculate analytically through Eqs. 4-6 the electric field for ellipsoidal axisymmetric bunches described by an arbitrary polynom $\hat{n}(t)$.

## GENERAL SOLUTION FOR 3D ELLIPSOIDAL BUNCH

In the previous section we saw that for axisymmetric bunches with a polynomial distribution the electric field can be written as a series. We then consider a polynomial approximation $\hat{n}_{p}(t)$ of an arbitrary particle distribution $\hat{n}(t)$, which needs not be of a polynomial nature (a Gaussian for instance). We also observed in the previous section that particles inside the bunch edge have the same integral $I_{i, j}=I_{i, j}(0)$. We propose then to take $\hat{n}_{p}(t)$ such that its edge is far enough to describe all the space where a particle may be found. In this way the particle is always inside the bunch and the integrals $I_{i, j}$ must be computed only once. For a Gaussian there is no beam edge and characteristic beam sizes are described in terms of rms quantities. Then we use the same description for the "interpolating" bunch defined by the polynomial function

$$
\hat{n}_{p}(t)=\sum_{l=0}^{N} c_{l} t^{l}
$$

defined now on $\left[0, T_{\max }\right]$. Here $T_{\max }$ is the bunch edge and it has to be large enough to contain all possible particle positions. An upper bound for $T_{\max }$ is typically hundred. The isodensity parameter $T=x^{2} / a^{2}+y^{2} / b^{2}+z^{2} / c^{2}$ uses the $r m s$ sizes $a, b, c$ which are now arbitrary. Then Kellog's formulas can be transformed to the following

$$
\begin{align*}
& E_{x}=\frac{Q}{2} x \sum_{l=0}^{N} c_{l} \sum_{i+j+k=l} \frac{l!}{i!j!k!} x^{2 i} y^{2 j} z^{2 k} I_{i+1, j, k}, \\
& E_{y}=\frac{Q}{2} y \sum_{l=0}^{N} c_{l} \sum_{i+j+k=l} \frac{l!}{i!j!k!} x^{2 i} y^{2 j} z^{2 k} I_{i, j+1, k}, \\
& E_{x}=\frac{Q}{2} z \sum_{l=0}^{N} c_{l} \sum_{i+j+k=l} \frac{l!}{i!j!k!} x^{2 i} y^{2 j} z^{2 k} I_{i, j, k+1}, \tag{7}
\end{align*}
$$

where

$$
I_{i, j, k}=\int_{0}^{\infty} \frac{1}{\left(a^{2}+t\right)^{1 / 2+i}\left(b^{2}+t\right)^{1 / 2+j}\left(c^{2}+t\right)^{1 / 2+k}} d t
$$

The computation of $I_{i, j, k}$ can be done numerically by variable replacement $t=\xi /(1-\xi)$. In order to precisely calculate $I_{i, j, k}$ the new interval of integration $[0,1]$ is divided into the following subintervals $\left[0,10^{-10}\right],\left[10^{-10}, 10^{-5}\right],\left[10^{-5}, 10^{-3}\right],\left[10^{-3}, 1\right]$, and we apply Gaussian Quadrature for 96 points to each subinterval. The relative error of calculation is less than $10^{-5}$.

## FITTING OF THE DISTRIBUTION FUNCTION

A critical issue to be considered is how to fit the "real" distribution function $\hat{n}(t)$ with the interpolating polynom $\hat{n}_{p}(t)$ on the interval [ $\left.0, T_{\max }\right]$. Our goal is to find the fitting polynom $\hat{n}_{p}(t)$ of the lower order $N$ which can be considered as being of sufficient accuracy. To minimize the error $\left|\hat{n}_{p}(t)-\hat{n}(t)\right|$ on the interval $\left[0, T_{\max }\right]$ we use Chebyshev nodes [7],

$$
t_{k}=T_{\max }\left\{\frac{1}{2}+\frac{1}{2} \cos \left[\frac{(2 k+1) \pi}{2 N+2}\right]\right\}
$$

which define the polynom with the smallest absolute error on the whole interval in the class of polynoms of order $N$. Here $k=0, . ., N$. Requiring that on these nodes the approximating polynom $\hat{n}_{p}(t)$ is equal to the "real" distribution function $\hat{n}(t)$, i.e. $\hat{n}\left(t_{k}\right)=\hat{n}_{p}\left(t_{k}\right)$ we find the following system of equations

$$
\left\{\begin{array}{l}
c_{0}+c_{1} t_{0}+\ldots+c_{N} t_{0}^{N}=\hat{n}\left(t_{0}\right) \\
c_{0}+c_{1} t_{1}+\ldots+c_{N} t_{1}^{N}=\hat{n}\left(t_{1}\right) \\
\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \\
c_{0}+c_{1} t_{N}+\ldots+c_{N} t_{N}^{N}=\hat{n}\left(t_{N}\right)
\end{array}\right.
$$

This system has a Waan-der-Mond determinant

$$
W\left(t_{0}, \ldots, t_{N}\right)=\prod_{i>j}\left(t_{i}-t_{j}\right)
$$

which is always different from zero because Chebyshev nodes have the property $t_{i} \neq t_{j} \forall i, j$. Therefore the system has always a unique solution $c_{0}, \ldots, c_{N}$. Our purpose is to obtain the required small error from the fitting and at the same time to minimize the number of nodes (that means the polynom degree) in order to increase the speed and the accuracy of the electric field calculations. We studied a Gaussian distribution function $\hat{n}(t)=\exp (-t / 2)$ and investigated the dependence of the number of nodes required for having a relative error less than $1 \%$ and $10 \%$ as function of the interval $\left[0, T_{\max }\right]$, where $T_{\max } \leq 30$. One can see


Figure 1: Number of nodes to be used in the interval $\left[0, T_{\max }\right], T_{\max } \leq 30$ in order to have a maximum relative error of polynomial interpolation in $\left[0, T_{\max }\right]$ less than $1 \%$, and $10 \%$ for a Gaussian distribution function.
from Fig. 1 that for a Gaussian distribution function on this interval the number of nodes for having an error less than $1 \%$ or $10 \%$ can be extrapolated as

$$
N_{\text {nodes }}=0.55 T_{\max }+\lambda
$$

where $\lambda=0.9$ for having $10 \%$ and $\lambda=2$ for having $1 \%$. This law is specific for a Gaussian distribution function,
and whether it can be used for other distribution functions remains a subject of further studies. In Fig. 1 the interval is restricted to $T_{\max }<30$, because for $t>30$ the relative error of $\hat{n}_{p}(t)$ with respect to $\hat{n}(t)$ becomes very large as the values of the real function $\hat{n}(t)=\exp (-t / 2)$ and the fitting polynom $\hat{n}_{p}(t)$ tend to be very close to zero. Therefore in this case we do not study the relative but the absolute error. Fig. 2 shows the dependence of maximum absolute error $\left|\hat{n}_{p}(t)-\hat{n}(t)\right|$ in the interval $[0,100]$ versus the number of interpolating nodes (for Gaussian distribution function). The optimal number of nodes for the fitting


Figure 2: Maximum absolute error on the interval $\left[0, T_{\max }\right], T_{\max }=100$ as function of the number of nodes.
of Gaussian distribution on the interval $[0,100]$ is found to be in the range between 20 and 30 .

## STATIC BENCHMARKS

As a first test we compare the electric field computed for an axisymmetric bunch with the fully analytic expressions obtained in [5] for distribution functions up to the 3rd order. We found a perfect agreement. A much stronger test has been made by using Gausses law. Given the electric field computed with Eqs. 7 and applying Gausses law $\vec{\nabla} \cdot \vec{E}(\vec{x})=4 \pi \rho^{\prime}(\vec{x})$ we can re-derive the local charge density. Here $\vec{x}=(x, y, z)$ are the particle coordinates in the bunch frame. In this procedure we make use of analytic formulas for $\vec{\nabla} \cdot \vec{E}(\vec{x})$ obtained from Eqs. 7 as well as a numerical derivative of the electric field, which is however computed with high accuracy: the derivative $\partial_{x} E_{x}(\vec{x})=\left[E_{x}(\vec{x}+\Delta x)-E_{x}(\vec{x})\right] / \Delta x$ is calculated with $\Delta x=10^{-6}$. From $\vec{x}$ we find the corresponding isodensity parameter $T$ and by using the local reconstructed charge density $\rho^{\prime}(\vec{x})$ in Eq. 1 we determine the value of $\hat{n}^{\prime}$, which is the "reconstructed" distribution function $\hat{n}^{\prime}(t)$. By considering sufficiently many test points $\vec{x}$ uniformly distributed into the full allowed space defined by $T_{\text {max }}=100$ we can reconstruct completely $t \rightarrow \hat{n}^{\prime}(t)$. For test points belonging to the same shell the value of
$\hat{n}^{\prime}(t)$ must be unchanged and eventually $\hat{n}^{\prime}(t)$ should be equal to the original distribution function $\hat{n}(t)$. We perform this comparison by plotting $\left|\hat{n}(t)-\hat{n^{\prime}}(t)\right|$ in the interval $\left[0, T_{\max }\right]$. In Fig. 3 we show this comparison for the Gaussian distribution function $\hat{n}(t)=\exp (-t / 2)$. This test has been made for a bunch with different axis as $a=0.001 \mathrm{~m}$, $b=0.01 \mathrm{~m}$, and $c=1 \mathrm{~m}$. As we can see, to each value of


Figure 3: Reconstruction error $\left|\hat{n}(t)-\hat{n^{\prime}}(t)\right|$ for the Gaussian distribution on the interval $\left[0, T_{\max }\right]$.
the isodensity parameter corresponds a band of values containing all points in this shell. Note that most of the points lie on a central peak located at zero and the average error band width is much less then $10^{-6}$.

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