NEW APPROACH TO SPACE CHARGE CALCULATION IN ENSEMBLE MODEL*

M. Krassilnikov†, T. Weiland#, FB18-TEMF, Technische Universität Darmstadt, Germany

Abstract

Based on the Ensemble Model, V-Code has been developed for fast beam dynamics simulations. The Single-Ensemble Model (SEM) considers a beam as an Ensemble, incorporating internal particles motion in phase space. A SEM code, including space charge model, has been successfully tested and applied to the TTF (TESLA Test Facility, DESY). It demonstrates good agreement in beam trajectory and beam sizes. However, for the emittance simulations the Multi-Ensemble Model (MEM) is needed. Whereas the external fields can be implemented by generalization of the SEM, the space charge force implementation needs more efforts. A new approach for space charge treatment, available for the MEM has been developed. The method is based on the Multi-Centered Gaussian Expansion (MCGE) of the Ensemble distribution function and yields significant advantage in simulation time in comparison with direct methods.

1 INTRODUCTION

The Ensemble Model [1] is derived from Vlasov equation and includes besides a centroid motion also internal particles motion. The beam is represented by a set of sub-beams or Ensembles. The Single Ensemble Model (SEM) treats a beam as one Ensemble and the space charge forces are calculated with a help of analytical approximation [2]. Forces acting on particles are taken in linear approximation, what corresponds to invariance of the Ensemble emittance. For simulations of nonlinear effects the beam has to contain several Ensembles, i.e. Multi-Ensemble Model (MEM) has to be developed. Whereas nonlinear external fields can be implied automatically, the space charge force needs additional consideration. Several approaches for the space charge field calculations in MEM (direct integration, Poisson solver, distribution function expansion) are discussed. The algorithm based on the Multi-Centered Gaussian Expansion (MCGE) demonstrates better properties being applied to the MEM.

2 THE ENSEMBLE MODEL

Time development of Ensemble parameters is described by 6 differential equations for the averaged center in phase space

$$\frac{d\langle\vec{p}\rangle}{d(ct)}=\vec{\mathbf{F}}\left(\langle\vec{r}\rangle,\langle\vec{p}\rangle\right);\quad \frac{d\langle\vec{r}\rangle}{d(ct)}=\hat{\mathbf{W}}\langle\vec{p}\rangle \qquad (1)$$

and by 21 equations for the second order moments of the Ensemble distribution function

$$\frac{d\hat{\mathbf{M}}_{pp}}{d(ct)}=\hat{\mathbf{F}}^{X}\hat{\mathbf{M}}_{xp}+\hat{\mathbf{F}}^{P}\hat{\mathbf{M}}_{pp}+\left(\hat{\mathbf{F}}^{X}\hat{\mathbf{M}}_{xp}+\hat{\mathbf{F}}^{P}\hat{\mathbf{M}}_{pp}\right)^{T},$$

$$\frac{d\hat{\mathbf{M}}_{xp}}{d(ct)}=\hat{\mathbf{V}}\hat{\mathbf{M}}_{pp}+\hat{\mathbf{M}}_{xx}\left(\hat{\mathbf{F}}^{X}\right)^{T}+\hat{\mathbf{M}}_{xp}\left(\hat{\mathbf{F}}^{P}\right)^{T}, \qquad (2)$$

$$\frac{d\hat{\mathbf{M}}_{xx}}{d(ct)}=\hat{\mathbf{M}}_{xp}\hat{\mathbf{V}}+\hat{\mathbf{V}}\hat{\mathbf{M}}_{xp}{}^{T},$$

where

$$\langle\xi\rangle=\int\xi\psi\,d\vec{r}\,d\vec{p},$$
$$M_{\xi\nu}=\langle\Delta\xi\Delta\nu\rangle=\int(\xi-\langle\xi\rangle)(\nu-\langle\nu\rangle)\psi\,d\vec{r}\,d\vec{p} \qquad (3)$$

Here $\xi,\nu=x,y,z,p_x,p_y,p_z$ and $\psi=\psi(t,\vec{r},\vec{p})$ is an Ensemble distribution function. Auxiliary matrices

$$\left[V_{ij};W_{ij}\right]=\frac{1}{\gamma_m}\left(\delta_{ij}-\left[\langle p_i\rangle\langle p_j\rangle;\hat{\mathbf{M}}_{p_ip_j}\right]\Big/\gamma_m^2\right)$$

use mean energy $\gamma_m=\sqrt{1+\sum_{n=x}^{z}\left\{\langle p_n\rangle^2+M_{p_np_n}\right\}}$. Vector $\vec{\mathbf{F}}\left(\langle\vec{r}\rangle,\langle\vec{p}\rangle\right)=\vec{F}\left(\langle\vec{r}\rangle,\langle\vec{p}\rangle\right)\Big/mc^2$ is normalized Lorentz force acting on the Ensemble center. Matrices $\hat{\mathbf{F}}^{X},\hat{\mathbf{F}}^{P}$ are derivatives of the Lorentz force

$$\hat{\mathbf{F}}^{X}_{ij}=\frac{1}{mc^2}\frac{\partial\vec{F}_i}{\partial r_j}\bigg|_{\langle\vec{r}\rangle,\langle\vec{p}\rangle},\quad \hat{\mathbf{F}}^{P}_{ij}=\frac{1}{mc^2}\frac{\partial\vec{F}_i}{\partial p_j}\bigg|_{\langle\vec{r}\rangle,\langle\vec{p}\rangle} \qquad (4)$$

2.1 Space Charge Model for Single Ensemble

A space charge algorithm for the SEM assumes an Ensemble to be a homogeneously charged ellipsoid. Space charge field gradient at the ellipsoid center can be calculated by integration over the thin charged shell. Action of charges in this shell is not compensated and they forms the Lorentz force in the Ensemble center vicinity [2]:

$$\vec{F}=\hat{G}\left(2\gamma\sigma_z\Big/\left(\sigma_x+\sigma_y\right)\right)\cdot eQ\gamma^{-2}V_G^{-1}\left(\vec{r}-\langle\vec{r}\rangle\right), \qquad (5)$$

where Q is Ensemble charge, V_G is geometrical volume of the Ensemble:

$$V_G^2=\det\hat{\mathbf{M}}^{G};\quad \hat{\mathbf{M}}^{G}_{ij}=\left\{\hat{\mathbf{M}}_{ij}\right\}_{i,j=x,y,z}. \qquad (6)$$

*Work supported in part by DESY, Hamburg.
†kras@remf.de, #weiland@temf.de

To take into account relativistic effect factor $\hat{G}$ has been introduced:

$$\left\{\hat{G}(u)\right\}_{ij} : \left(1-\exp(u)\right)\cdot\left(\delta_{ij}+\delta_{iz}\cdot\left(\gamma/u-1\right)\right). \quad (7)$$

The Single Ensemble space charge model, being a semi-analytical one, does not require long computational times, the V-Code [3], based on it, is very fast and has demonstrated high applicability to a several beam dynamics applications. In particular, it was shown [3], that sizes and momentum spreads of the beam in photoinjectors, simulated with conventional PIC-code and with SEM version of V-Code are in very good agreement. However, for many important problems, i.e. for the beam emittance simulations, "one-ensemble-beam" is not enough. Extension of the Single Ensemble space charge model to a "multi-ensemble beam" is impossible because of the model assumptions: the small offset from the driving Ensemble center has no place in general case, field discontinuity at the boundary of homogeneously charged ellipsoid demands additional complications.

2.2 Space Charge Model for Multi-Ensemble Beam

Driving Ensemble field with derivatives has to be continuous and needs to be calculated only at centers of other Ensembles. A smooth Ensemble charge distribution function provides the field continuity. The Gaussian distribution is the most probable candidate for it:

$$\psi(\vec{r},\vec{p}) = \frac{\exp\left(-\Delta\vec{\xi}^{T}\cdot\hat{\mathbf{M}}^{-1}\cdot\Delta\vec{\xi}/2\right)}{(2\pi)^3\det\hat{\mathbf{M}}}, \quad (8)$$

where $\Delta\vec{\xi}=\vec{\xi}-\left\langle\vec{\xi}\right\rangle$, $\vec{\xi}=\{\vec{r},\vec{p}\}$ and $\hat{\mathbf{M}}$ is 6×6 matrix of the second order moments (3).

To find a fields generated by Ensemble with charge distribution (8) several methods are available.

1. Direct Integration implies straightforward calculations from the retarded potential approach [4].This approach includes many physical effects (such as a synchrotron radiation), but multidimensional integration makes it very slow and the singularity complicates its implementation.

2. Using Poisson Solver with Lorentz transformations assumes no momentum spreads are taken into account. After coordinates transformation (which corresponds to the matrix $\hat{\mathbf{M}}$ diagonalization) and integration (8) in pulse space, we have for charge distribution function:

$$\psi(\tilde{x},\tilde{\sigma}_x,\tilde{y},\tilde{\sigma}_y,\tilde{z},\tilde{\sigma}_z) = \prod_{i=x}^{z}\psi_G(\Delta\tilde{\xi}_i,\tilde{\sigma}_{\xi_i}), \quad (9)$$

where $\psi_G(u_i,\sigma)=\exp\left(-u^2/2\sigma^2\right)\Big/\sqrt{2\pi\sigma^2}$ is one dimensional Gaussian distribution. In the Ensemble rest system the Poisson equation has to be solved:

$$\tilde{\Delta}\varphi = -4\pi Q\cdot\psi(\tilde{x},\tilde{\sigma}_x,\tilde{y},\tilde{\sigma}_y,\tilde{z},\tilde{\sigma}_z). \quad (10)$$

In general case the z axis does not coincide with direction of vector $\left\langle\vec{\beta}\right\rangle=\left\langle\vec{p}\right\rangle\Big/\sqrt{1+\left\langle\vec{p}\right\rangle\cdot\left\langle\vec{p}\right\rangle}$, so the coordinates transformation can be performed as

$$\tilde{\vec{r}} = \hat{\mathbf{T}}\cdot\left(\vec{r}-\left\langle\vec{r}\right\rangle\right), \quad (11)$$

where $\hat{\mathbf{T}}$ is transformation matrix:

$$\hat{\mathbf{T}}=\hat{\mathbf{\Phi}}_M\cdot\hat{\mathbf{\Gamma}}\cdot\hat{\mathbf{\Phi}}_\beta;\quad \hat{\mathbf{\Phi}}_\beta\cdot\left\langle\vec{\beta}\right\rangle=\left\{0,0,\left|\left\langle\vec{\beta}\right\rangle\right|\right\}^T;$$
$$\hat{\mathbf{\Gamma}}_{ij}=\delta_{ij}\cdot[1-\left\langle\vec{\beta}\right\rangle\cdot\left\langle\vec{\beta}\right\rangle\delta_{iz}]^{-1/2};\quad i,j=x,y,z \quad (12)$$

Matrix $\hat{\mathbf{\Phi}}_M$ has to be found from the diagonalization of the matrix $\hat{\mathbf{M}}^G$:

$$\left[\hat{\mathbf{\Phi}}_M^T\cdot\hat{\mathbf{M}}^G\cdot\hat{\mathbf{\Phi}}_M\right]_{ij}=\tilde{\sigma}_i^2\delta_{ij} \quad (13)$$

The equation (10) with boundary conditions (exact or asymptotic), can be solved using grid based methods, which give solution at all points of discretization, what significantly exceeds needs of the Ensemble Model. Moreover most of these methods are valid for any arbitrary right part of the Poisson equation, so the regularity of the Gaussian distribution is not used.

3. Multi-Centered Gaussian Expansion (MCGE) is based on the expansion of the Ensemble charge density in distributed basis functions with known solutions of the field equation. For symmetrical basis functions

$$\psi_{nml}=\psi_G(x-x_n,\sigma_0)\psi_G(y-y_m,\sigma_0)\psi_G(z-z_l,\sigma_0) \quad (14)$$

electric field can be calculated analytically:

$$\vec{E}_{nml}(x,y,z)=\frac{q_{nml}}{\sigma_0^2}\cdot S\left(\left|\vec{r}_{nml}\right|\Big/\sqrt{2}\sigma_0\right)\cdot\frac{\vec{r}_{nml}}{\left|\vec{r}_{nml}\right|}, \quad (15)$$

where $S(x)=x^{-2}\cdot\left\{\mathrm{erf}(x)-2/\sqrt{\pi}\cdot x\cdot\exp\left(-x^2\right)\right\}$ and $\vec{r}_{nml}=\{x-x_n,y-y_m,z-z_l\}$ is a radius-vector from the basis function ψ_{nml} center to the observation point, q_{nml} is a weight part of the Ensemble charge.

Distribution function (9) is approximated by a series

$$\psi\approx\tilde{\psi}=\sum_{n,m,l}w_{nml}\cdot\psi_{nml} \quad (16)$$

where $w_{nml}=Q/q_{nml}$. Unfortunately the basis (14) is not orthogonal, but factorization of the weights $w_{nml}=w_n^x\cdot w_m^y\cdot w_l^z$ reduces three dimensional weights problem to three independent one dimensional ($\xi=x,y,z$):

$$\sum_j w_j^\xi\cdot\exp\left(-\frac{(\xi-\xi_j)^2}{2\sigma_0^2}\right)\approx\frac{\sigma_0}{\sigma_\xi}\cdot\exp\left(-\frac{\xi^2}{2\sigma_\xi^2}\right) \quad (17)$$

Standard procedure yields a system of linear equations for weights w_j^ξ, the matrix elements can be calculated analytically.

The main approximation parameters are: 1) α is normalized distance between two basis functions

($\xi_j = \alpha j \sigma_0$); 2) $K_\xi = \alpha \sigma_0 N_\xi / \sigma_\xi$ is asymptotic parameter, determined by N_ξ - a number of terms in sum (16) for truncation; 3) σ_0 is rms basis function size. By choosing $\sigma_0 = \min \sigma_\xi = \sigma_\nu$ we obtain $N_\nu = 0$ and $w_0^\nu = 1$. Centers of the basis functions are located at the plane $\xi_\nu = 0$. If all three dimensions of the Ensemble are significantly different triangular truncation [5] in 2D sums can be used to reduce computation time. Using MCGE a space charge field at the point of interest (x, y, z) can be calculated by summing up of (15):

$$\vec{E}(x,y,z) = \sum_{nml} \vec{E}_{nml}(x,y,z), \qquad (18)$$

moreover a sum with index equal ν is degenerated, so it can be simply omitted. Other advantage of the MCGE is the capability of analytical expressions (in terms of corresponding sums) for derivatives of the space charge field, what is necessary for matrices (4) computation.

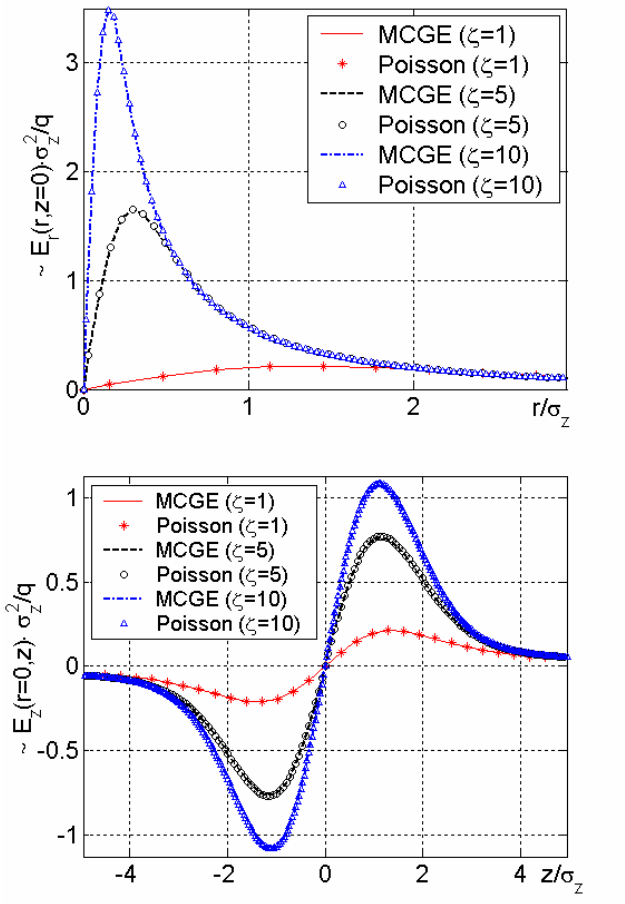

Figure 1. Electric field of round Gaussian Ensemble, calculated using MCGE in comparison with conventional Poisson solver.

Electric field of a round ($\sigma_x = \sigma_y = \sigma_\perp$) Gaussian distribution calculated with conventional Poisson solver (solid lines) and using MCGE (markers) is shown in Fig.1 for different $\zeta = \sigma_z / \sigma_\perp$ values. The results are in very good agreement, 100×100 mesh has been used for Poisson solver, whereas the MCGE for the fields calculation treats $N_z(\zeta) = 1 \div 30$ terms in sum (18) (for the round beam two sums in (18) are degenerated). Field gradients $(\partial E_r / \partial r ; \partial E_z / \partial z)$ at the driving Ensemble center are calculated using Single Ensemble space charge model (5) and MCGE and shown in Fig.2.

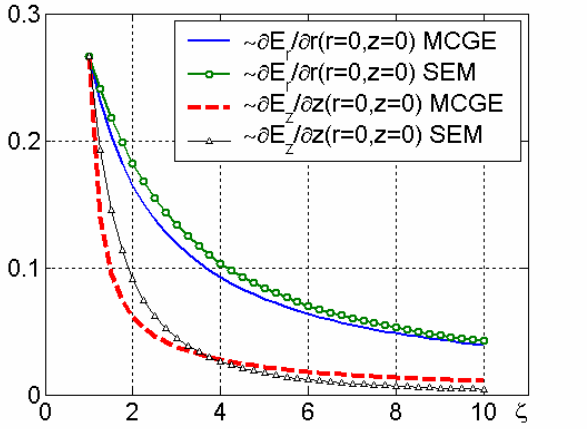

Figure 2. Electric field gradient of round Gaussian Ensemble, calculated using MCGE in comparison with SEM analytical approximation (5).

3 CONCLUSIONS

A new approach to space charge calculation in Ensemble Model has been developed. Based on the Multi Centered Gaussian Expansion of Ensemble distribution function it has advantages in comparison with direct methods and conventional Poisson solvers as well. The field gradient at the Ensemble center calculated using MCGE is in good agreement with analytical approximation of Single Ensemble Model.. The results of space charge field simulations by MCGE agree with obtained by conventional Poisson solver, whereas the calculation with MCGE takes less time.

4 REFERENCES

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