

HIGH CURRENT BEAM SIMULATION USING TEMPLATES*

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Abstract

Charged particle beam dynamics including space charge and image forces were simulated with a newly developed code. The formalism for this new code is based on the template potential technique and can be employed for computational approaches ranging from envelope equations to particle-in-cell (PIC) models in either two- (2D) or three-dimensional (3D) geometries. While the method is not completely self-consistent, it is appropriate for a large class of beam distributions and boundary constraints. The speed of calculations is high and memory demands are moderate in comparison with conventional PIC codes.

1 INTRODUCTION

A template formalism was previously described in [1-3] that supports beam dynamics simulation under relatively general conditions and is considerably faster than general PIC codes. This hybrid method employs particles as do PIC codes, but also uses macro objects called templates to speed up calculations. In this paper, we develop new features of the theory of templates and consider its applications to beam simulation.

A standard 3D PIC code algorithm at each step of beam simulation may be schematically represented as:

$$\left\{ \begin{array}{l} \mathbf{x}_k \\ \mathbf{x}'_k \end{array} \right\}_{old} \rightarrow [\rho_{beam}] \rightarrow \left[\begin{array}{l} u_{beam} \\ \mathbf{E}_{beam} \end{array} \right] \rightarrow \left[\begin{array}{l} \text{Trajectories} \\ \text{Integrator} \end{array} \right] \rightarrow \left\{ \begin{array}{l} \mathbf{x}_k \\ \mathbf{x}'_k \end{array} \right\}_{new} \quad (1)$$

where \mathbf{x}_k , \mathbf{x}'_k are the phase coordinates of a k -th particle, ρ_{beam} , u_{beam} , \mathbf{E}_{beam} are beam space charge density, potential, and field on a 3D spatial grid. Trajectory integration taking into account both space charge and external fields, advances the particles. Note that (1) may require 2-3 iterations for each integration step if the motion equations integrator scheme is implicit [3].

Through the use of the template formalism, it is possible to obtain the space charge potential and field without explicit computation of the grid density ρ_{beam} while still operating in a manner similar to general PIC methods [4]. Schematically this method operates as:

$$\left\{ \begin{array}{l} \mathbf{x}_k \\ \mathbf{x}'_k \end{array} \right\}_{old} \rightarrow \left[\begin{array}{l} \text{Template } u_{beam} \\ \text{Method } \mathbf{E}_{beam} \end{array} \right] \rightarrow \left[\begin{array}{l} \text{Trajectories} \\ \text{Integrator} \end{array} \right] \rightarrow \left\{ \begin{array}{l} \mathbf{x}_k \\ \mathbf{x}'_k \end{array} \right\}_{new} \quad (2)$$

Unlike scheme (1), the Template Method substitutes the grid density block, establishing a faster feedback mechanism between particles and space charge fields. The scheme (2) allows fewer particles and sparser grids ultimately resulting in lesser computational times.

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2 TEMPLATE CONCEPT

2.1 Principle of Superposition

Templates are infinitesimally thin charged discs (or slices) and template potentials $u_{imp}(\mathbf{x})$, $\mathbf{x}=(x,y,z) \in \mathfrak{R}$, are particular solutions of the 3D Poisson equation for each individual slice in a presence of boundaries $\partial\mathfrak{R}$. If the beam is represented as a sequence of slices, then from the principle of superposition, a total beam potential will satisfy Poisson equation:

$$\begin{cases} \Delta u_{imp}(\mathbf{x}) = -4\pi\rho_{imp}(\mathbf{x}) \\ u_{imp}(\mathbf{x})|_{\partial\mathfrak{R}} = \bar{U}_{imp}(\mathbf{x}) \end{cases} \rightarrow \begin{cases} \Delta u_{beam}(\mathbf{x}) = -4\pi\rho_{beam}(\mathbf{x}) \\ u_{beam}(\mathbf{x})|_{\partial\mathfrak{R}} = \bar{U}_{beam}(\mathbf{x}) \end{cases} \quad (3)$$

where $\bar{U}_{imp} = \bar{U}_{beam} = 0$ for an ideal conducting boundary (electrostatic case).

This is the essence of the template concept idea. To make the method computationally efficient, we calculate and tabulate individual potentials $u_{imp}(\mathbf{x})$ for slices with different sizes and aspect ratios. During the beam dynamics simulation, the data is extracted from that table and properly scaled and interpolated [1] resulting in a fast reconstruction of the total bunch potential.

2.2 Single Template Potential Generation and Total Beam Potential Reconstruction

A potential for each individual slice may be found by the moment method, as a sum of a free space and image charge potentials (see for details [1,4]). However, other algorithms may be also appropriate such as the successive over-relaxation algorithm (SOR-3D).

The total beam potential is a superposition of template potentials described by the shape functions $S_{x,y}(z)$ with sizes corresponding to the actual beam geometry. The total potential expressed as a superposition (convolution) is:

$$u_{beam}(x, y, z) = \int u_{imp}(x, y, z - \tilde{z}, S_{x,y}(\tilde{z})) d\tilde{z} \quad (4)$$

with $u_{imp}(\mathbf{x})$ and $u_{beam}(\mathbf{x})$ satisfying (3).

In Fig. 1, the shape functions are shown corresponding to a 3D beam without axial symmetry, carrying a total space charge potential of 10^{-11} C, and propagating along a conducting cylindrical pipe of 4 cm in diameter.

Given in Fig. 2 are the template potentials, distributed according to the shape functions $S_{x,y}(z)$ and the total beam potential calculated as a convolution (4).

The shape functions $S_{x,y}(z)$ change as the beam evolves. However, the reconstruction of the beam total potential via the integral (4) always employs the table of pre-calculated template potentials. The number of templates

required to compute properly the potentials depends on the $S_{x,y}(z)$ behavior as discussed below.

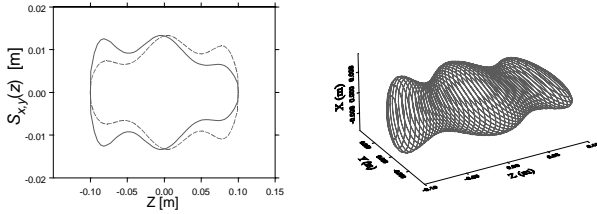


Figure 1: Shape functions (left) and a corresponding general 3D beam represented as a “sliced” bunch (right).

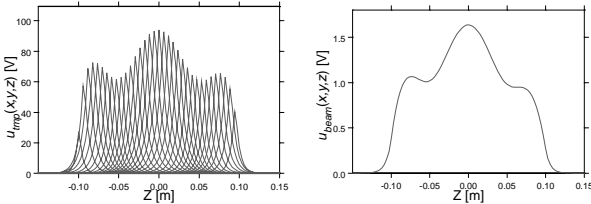


Figure 2: Template potentials $u_{imp}(x,y,z)$ (left) and the total beam potential $u_{beam}(x,y,z)$ (right) for: $x=y=0$ for the beam from Fig. 1 (right), plotted as a function of “ z ”.

2.3 Generalization for Equivalent Beams

For the case of constant charge density, the implementation of the template potential technique is straightforward. For beams with non-uniform charge densities, the concept of equivalent beams [5,3] is used. A large family of 2D charge densities may be expressed using the representation:

$$\sigma(x,y,p) = \sigma_m(p) \left(1 - x^2/x_m^2(p) - y^2/y_m^2(p) \right)^p \quad (5)$$

where x_m, y_m are the beam’s envelopes and $\sigma(x,y,p)$ is the 2D charge density with $\sigma_m(p) = \sigma(0,0,p)$.

An analysis was done for 3D beams having the same rms size (“equivalent beams”) of 2D slices with charge densities depending on “ p ” (5). The total potential is calculated by the integral (4) including a form-factor proportional to the linear beam density and the shape functions (beam envelopes) that now depend on “ p ” and the space charge computations based on the Template Technique are organized as: Particles $\rightarrow \langle x^2 \rangle^{1/2}(p), \langle y^2 \rangle^{1/2}(p) \rightarrow S_{x,y}(z,p) \rightarrow$ Convolution integral (4) $\rightarrow u(x,y,z), E_{x,y,z}$ (see for details [4]).

2.4 Library of Templates, Parameterization

The stored $u_{imp}(\mathbf{x})$ data array is used to evaluate potentials (4) for all possible beam configurations via interpolation and scaling. To provide a large range of possible templates without significant memory requirements, $u_{imp}(\mathbf{x})$ is analytically parameterized as a function of one variable “ z ”:

$$u_{imp}(\mathbf{x}) = \exp(P_n(\mathbf{x})) \text{ with } P_n(\mathbf{x}) = \sum a_n(x,y) \cdot z^n \quad (6)$$

for $z < 0$ and $u_{imp}(x,y,z) = u_{imp}(x,y,-z)$ (even functions).

The coefficients a_i are obtained by a least squares minimization of the array $u_{imp}(\mathbf{x})$ as function of “ z ” for fixed (x,y) . The 2nd order polynomial $P_2(x,y,z) = a_2(x,y) \cdot z^2 + a_1(x,y) \cdot z + a_0(x,y)$ was found to give nearly an ideal approximation of the original template potential in (6). Thus, instead of storing functions of “ z ”, we store only 3 coefficients $a_{0,1,2}$ for each potential.

For axially-symmetric beams, 100 pre-calculated templates with different radii (10 \times) and different off-axis positions (10 \times) are used. For cases with less symmetry, e.g. for an elliptical beam, the number of template potentials increases to 3000 to include different azimuthal positions (3 \times) and aspect ratios (10 \times). Thus, the total array of coefficients a_i , will consist of 9000 numbers [4].

The parameterization (6) is also very convenient for fast and accurate space charge field representation without the necessity of numerical differentiation and interpolation. The longitudinal space charge field is:

$$E_{z,imp}(\mathbf{x}) = -(2a_2z + a_1) \exp(P_2(\mathbf{x})) \quad \text{for } z < 0 \quad (6')$$

with $E_{z,imp}(x,y,z) = -E_{z,imp}(x,y,-z)$ (odd functions).

In Fig. 3, the longitudinal template fields (6’) are plotted and the total beam field computed as a convolution of these individual template fields. The same coefficients a_i , derived for $u_{imp}(\mathbf{x})$ are used for longitudinal field generation. No additional stored data is required.

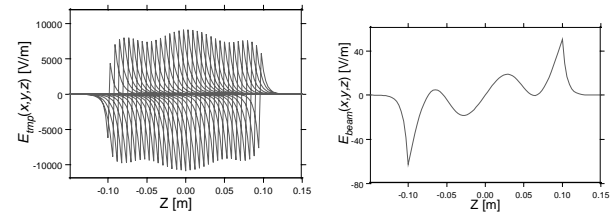


Figure 3: Template fields $E_{z,imp} = -\partial u_{imp}/\partial z$ (left) and beam longitudinal field $E_{z,beam} = -\partial u_{beam}/\partial z$ (right) for $x=y=0$, plotted as functions of “ z ”, for the bunch from Fig. 1.

In a similar manner, a parameterization may be carried out for transverse fields $E_{x,y}$ although all field components can be derived from the potential data.

The template potentials may be interpreted as the macro Green’s functions [6] and the template table has an analogy with a library of special functions. That data ($\approx 10^4$ numbers), calculated prior beam simulation, provides with interpolation and scaling the information necessary for the evolving beam field evaluation during the dynamics modeling. As discussed below, in some cases the table should include template information for a few different values of “ p ” of equation (5). Even so, the memory demands remain quite modest.

2.5 Other Applications

The template method can also be used to extend the rms envelope equations both for 2D and 3D models. In [3] we demonstrated a 2D code, based on the extended rms envelope equations, including image charge effects. The same approach may be fulfilled for the 3D case [4].

3 BEAM DYNAMICS SIMULATION

A PIC code (2) was developed with the trajectories integrator [3] and the sub-3D Poisson Solver [2], approaching conventional PIC formalism in generality.

As an example, we considered an ellipsoidal-like electron beam with semi-axes 0.35cm×0.67cm×1cm, propagating along a metal pipe 4 cm in diameter through a FODO focusing lattice (Fig. 4). The beam was assumed to have a uniform distribution with initial rms emittances $\epsilon_{x,y} = 5 \cdot 10^{-5} \pi$ m-rad, $\Delta p/p = 0$ (i.e. $\epsilon_z = 0$), an energy of 10 keV and a current of 5 mA. The number of particles used for simulation was $5 \cdot 10^4$ and the number of templates, used to reconstruct the beam potential, was taken 50.

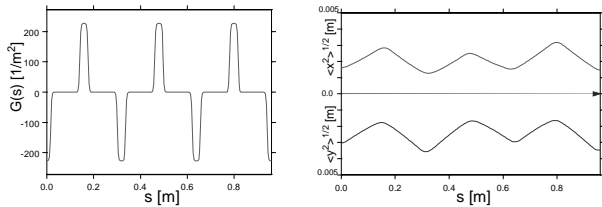


Figure 4: Left: FODO structure. Right: beam rms envelopes within three periods.

Beam envelopes through 3 periods ($s = 3 \times 0.32$ m), initial and final (x,y) distributions are plotted in Figs. 4,5. The phase distributions are given in Fig. 6 and beam passage through the last lens is shown in Fig.7.

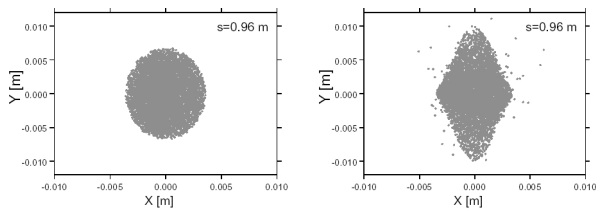


Figure 5: (x,y) particles distribution for $s=0$ and $s=0.96$ m.

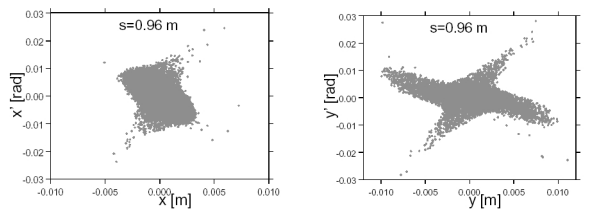


Figure 6: (x,x') and (y,y') phase distributions at $s=0.96$ m.

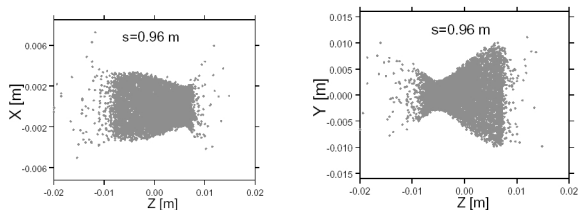


Figure 7: Beam passing the last defocusing lens, shown as particles in (z,x) and (z,y) planes at $s=0.96$ m.

4 DISCUSSION AND CONCLUSION

Field calculations in (2) use the shape functions $S_{x,y}(z)$, that together with template potentials $u_{tmp}(\mathbf{x})$ represent macro objects. Though such a substitution may omit certain micro-level effects and the PIC (2) is not completely self-consistent, the shape-functions respond adequately to beam evolutions and accommodate rather general particle distributions (See e.g., Fig. 1). A flexibility of the formalism can be further upgraded [4], using the extended template library for different parameters “ p ” in (5).

The code (2) requires many fewer particles than would otherwise be used in (1) for density calculations. The calculational speed of (2) is derived from the smaller number ($\approx 10^4$) of macro-particles necessary to adequately reproduce the rms envelopes and $S_{x,y}(z)$. There is a one to two orders of magnitude decrease in computational times in comparison with (1). Therefore, it would be possible to use optimization in conjunction with the template-based PIC codes.

There is a large gap between envelope models and general PIC codes both in terms of computational intensity (speed, memory) and beam model detail. The template-based codes fill this gap. In addition, a more general extension of the template potentials theory may be used for cases of $\bar{U}_{tmp}, \bar{U}_{beam} \neq 0$ in (3) to make wakefield effect calculations.

5 REFERENCES

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