SELF FIELD OF SHEET BUNCH: A SEARCH FOR IMPROVED METHODS

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ABSTRACT

We consider a sheet bunch represented by a random sample of $\mathcal{N}$ simulation particles moving in a 4D phase space. The mean field (='self field') of the bunch is computed from Maxwell's equations in the lab frame with a smoothed charge/current density. The particles are tracked in the beam frame, thus requiring a transformation of densities from lab to beam frame. We seek improvements in speed and practicality in two directions: (a) choice of integration variables and quadrature rules for the field calculation; and (b) finding smooth densities from scattered data. For item (a) we compare our singularity-free formula with the retarded time as integration variable, which we currently use, with a formula based on Frenet-Serret coordinates. The latter suggests good approximations in different regions of the retardation distance which could save both time and storage. For item (b) we discuss Fourier vs. kernel density estimation and mention quasi vs. pseudo-random sampling.

INTRODUCTION

In this paper we discuss current and future approaches to numerically integrating the Vlasov-Maxwell system for a sheet bunch. More information on our current work can be found in [1]-[3]. We first present the mathematical problem in the lab frame. We write the field as an integral of the time history of the source. Then the initial value problem (IVP) for the Vlasov equation defines the $u = ct$ evolution of the phase space density, f_L. The coefficients of the Vlasov equation depend on the Maxwell self field and thus contain integrals over the time history of f_L.

It is both physically and computationally advantageous to determine the so-called beam frame phase space density, f_B. We define the beam frame phase space variables in terms of the lab frame. The independent variable in the lab frame (LF) is u and the independent variable in the beam frame (BF) is arc length s along a suitably defined reference orbit. The lab to beam phase space variable transformation gives the relation between f_B and f_L and f_B satisfies a BF Vlasov equation. Our goal is an efficient computation of the s-evolution of f_B given its value f_{B0} at say $s = 0$. However, this problem is not well posed; solutions are not unique. The root of this is a causality issue; at s, certain coefficients of the BF Vlasov equation need information about f_B outside the interval $[0, s]$. This problem, which is pertinent to the BF and absent in the LF, is easily resolved to what we believe is a good approximation.

We want to numerically integrate the 4D BF Vlasov equation and we do this in terms of a random sample of $\mathcal{N}$ points which simulate the 4D phase space density. We work in a high performance computing (HPC) environment. Even so, we do not have a fast enough algorithm to take $\mathcal{N}$ large enough to obtain an accurate estimate of the 4D density. Furthermore, there are probably more efficient ways to obtain the 4D density, e.g., the method of local characteristics. However, the self field calculation only needs the BF spatial density, ρ_B, and a 2D current density type function, which we denote by τ_B. We believe our sample of 4D points is large enough to accurately estimate these 2D quantities and this makes a simulation approach feasible. We randomly generate an initial sample of BF phase space points from f_{B0}, and move this sample according to the BF equations of motion. Having resolved the causality issue, the self field can be computed at arc length s from the history of $g_B = (\rho_B, \tau_B)$. The calculation of g_B requires a density estimation procedure from our scattered data which we discuss. To move the points from s to $s + \delta s$ we freeze the self field at s and move the points according to the equations of motion. Important to our approach is the discovery of an s-independent grid on which to represent the spatial density and a parallel implementation of our algorithm.

STATEMENT OF PROBLEM FOR SHEET BUNCH IN LAB FRAME

We consider particle motion in the $Y = 0$ plane in a right handed coordinate system, (Z, X, Y), under an external magnetic field $\mathbf{B}_{ext}(Z, X, Y) = B_{ext}(Z)\mathbf{e}_Y$. The equations of motion without self field are

$$\dot{\mathbf{R}} = \frac{\mathbf{P}}{m\gamma(\mathbf{P})c}, \ \dot{\mathbf{P}} = qB_{ext}(Z)\frac{1}{m\gamma(\mathbf{P})c}\begin{pmatrix} P_X \\ -P_Z \end{pmatrix}, \quad (1)$$

where $\mathbf{R} = (Z, X)^T$, $\mathbf{P} = (P_Z, P_X)^T$, $\dot{} = d/du$, m is the electron rest mass, q is the electron charge and γ is the Lorentz factor. The associated 4D phase space density, $f_L(\mathbf{R}, \mathbf{P}; u)$, evolves according to the Liouville equation $\partial_u f_L + \dot{\mathbf{R}} \cdot \partial_{\mathbf{R}} f_L + \dot{\mathbf{P}} \cdot \partial_{\mathbf{P}} f_L = 0$, where f_L is normalized so that its integral over a phase space region represents the fraction of the beam in that region. All densities in this paper are normalized in this way.

We are interested in the evolution of f_L when coupled to the self field and we begin with the coupled Vlasov-Maxwell initial boundary problem in 3D with a shielding boundary condition and initial data at $u = u_i$ where u_i will be specified further below. In general, the self field will push the particles out of the $Y = 0$ plane unless the bunch is a 'sheet bunch' and the self

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field is 'symmetric'. We call the bunch a 'sheet bunch at u' if its phase space density f has, at time u, the form $f(Z,X,Y,P_Z,P_X,P_Y;u) = \delta(Y)\delta(P_Y)f_L(\mathbf{R},\mathbf{P};u)$. Denoting the components of the self field by $E_Z, E_X, E_Y, B_Z, B_X, B_Y$ we call the self field "symmetric at u" if $E_Z(\mathbf{R},Y;u), E_X(\mathbf{R},Y;u), B_Y(\mathbf{R},Y;u)$ are even in Y and if $E_Y(\mathbf{R},Y;u), B_Z(\mathbf{R},Y;u), B_X(\mathbf{R},Y;u)$ are odd in Y. The point here is that if the initial bunch is a sheet bunch and if the initial self field is symmetric then, thanks to the reflection symmetry of Maxwell's equations with respect to the $Y = 0$ plane, the bunch is a sheet bunch for all $u \geq u_i$ and the self field is symmetric for all $u \geq u_i$. We assume that these initial conditions on f and the self field are fulfilled whence, for all $u \geq u_i$, $E_Y(\mathbf{R},0;u) = B_Z(\mathbf{R},0;u) = B_X(\mathbf{R},0;u) = 0$. Thus no particle is pushed out of the $Y = 0$ plane.

We now focus on the self field components $\mathcal{F}_L(\mathbf{R};u) = (E_Z(\mathbf{R},0;u), E_X(\mathbf{R},0;u), B_Y(\mathbf{R},0;u)) \equiv (E_Z(\mathbf{R};u), E_X(\mathbf{R};u), B_Y(\mathbf{R};u))$ which together with $B_{ext}(Z)$ are responsible for the in plane forces. The solution of the initial boundary problem for $\mathcal{F}_L$, with $\mathcal{F}_L(\mathbf{R};u) = \partial_u\mathcal{F}_L(\mathbf{R};u) = 0$ at $u = u_i$ and the shielding boundary condition $\mathcal{F}_L = 0$ for $Y = \pm h/2$, is

$$\mathcal{F}_L(\mathbf{R};u) = -\frac{1}{4\pi}\sum_{k=-\infty}^{\infty}(-1)^k \times$$

$$\int_{\mathbb{R}^2} d\mathbf{R}' \frac{\mathbf{S}(\mathbf{R}';u-\left[|\mathbf{R}'-\mathbf{R}|^2+(kh)^2\right]^{1/2})}{\left[|\mathbf{R}'-\mathbf{R}|^2+(kh)^2\right]^{1/2}}. \quad (2)$$

The source is

$$\mathbf{S}(\mathbf{R};u) = Z_0 Q H(u-u_i)\begin{pmatrix} c\partial_Z\rho_L + \partial_u J_{L,Z} \\ c\partial_X\rho_L + \partial_u J_{L,X} \\ \partial_X J_{L,Z} - \partial_Z J_{L,X}\end{pmatrix}, \quad (3)$$

where H is the indicator function on $[0,\infty)$ and $\mathbf{J}_L = (J_{L,Z}, J_{L,X})^T$. This solution is obtained by writing the Maxwell equations in the wave equation form and using the retarded Green function and the method of images. If the initial condition is not zero a homogeneous solution must be added. Without the boundary condition only the $k = 0$ term remains.

The Vlasov IVP for the LF phase space density is

$$\partial_u f_L + \dot{\mathbf{R}}\cdot\partial_{\mathbf{R}} f_L + \dot{\mathbf{P}}\cdot\partial_{\mathbf{P}} f_L = 0,$$
$$f_L(\mathbf{R},\mathbf{P};u_i) = f_{L0}(\mathbf{R},\mathbf{P}), \quad (4)$$

where

$$\dot{\mathbf{R}} = \frac{\mathbf{P}}{m\gamma(P)c}, \quad (5)$$

$$\dot{\mathbf{P}} = \frac{q}{c}\left(\begin{pmatrix} E_Z(\mathbf{R};u) \\ E_X(\mathbf{R};u)\end{pmatrix} + \frac{[B_{ext}(Z)+B_Y(\mathbf{R};u)]}{m\gamma(\mathbf{P})}\begin{pmatrix} P_X \\ -P_Z\end{pmatrix}\right).$$

The Vlasov equation and the self field are coupled by the 2D charge and current densities, $Q\rho_L$ and $Q\mathbf{J}_L$, where

$$\rho_L(\mathbf{R};u) = \int_{\mathbb{R}^2} d\mathbf{P} f_L(\mathbf{R},\mathbf{P};u), \quad (6)$$

$$\mathbf{J}_L(\mathbf{R};u) = \int_{\mathbb{R}^2} d\mathbf{P}(\mathbf{P}/m\gamma(\mathbf{P}))f_L(\mathbf{R},\mathbf{P};u). \quad (7)$$

We believe the IVP (4) is well posed, that is, there exists a unique solution depending continuously on the initial data. Furthermore, given $f_L(\cdot;u), \mathcal{F}_L(\cdot;u)$ and a small positive δu the solution at $u+\delta u$ can be determined approximately by freezing the field at u and moving forward along characteristics defined by the Vlasov equation in (4). Note that $\mathcal{F}_L(\mathbf{R},u)$, requires knowing $\rho_L(\cdot;v)$ and $\mathbf{J}_L(\cdot;v)$ for $u_i \leq v \leq u$.

In this paper we focus on the numerical solution of the IVP (4). It is computationally intensive even in a HPC environment and so a fast algorithm is utmost on our mind. Actually, for several reasons, the Vlasov equation is integrated in the beam frame and this will be discussed in the next section. Several approximations will be involved. Ultimately the approximations must be judged by how accurately they give an approximation to $f_L(\cdot;u)$ as defined by (4).

The physical problem we have in mind is a single pass four magnet chicane, and this determines $B_{ext}(Y)$ (e.g., see [1]). We take u_i to be the time at which the head of the bunch reaches the chicane. To have a well defined "head", as well as for other reasons, we consider a bunch of compact spatial support, and we assume this in the following (see [2]). In the regime we have studied we believe the self field at $u = u_i$ is negligible and so (2) is appropriate. In applications such as this, it is important to determine the evolution of the so-called BF phase space density, f_B, with the arc length s along a reference orbit as the independent variable, and with f_B given at $s = 0$, which we take to be the entrance to the chicane. This frame is also convenient as the phase space variables are small and so linearizations are possible. We now turn our attention to the beam frame.

BEAM FRAME FOR SHEET BUNCH

The beam frame is defined in terms of the reference orbit $\mathbf{R}_r(s) = (Z_r(s), X_r(s))^T$ in the $Y = 0$ plane, which in turn is defined by the Lorentz equations without the self field given in (1). Here s is the arc length along the orbit and $\mathbf{R}_r(0) = 0$ is the entry point of the reference orbit into the chicane. The unit tangent vector, $\mathbf{t}$, to the reference orbit is just $\mathbf{t}(s) = \mathbf{R}_r'(s)$ and we define the unit normal vector, $\mathbf{n}$, by $\mathbf{n}(s) = (-X_r'(s), Z_r'(s))^T$ so that $\mathbf{n}$ is a $\pi/2$ counterclockwise rotation from $\mathbf{t}$. It follows from (1) that $\mathbf{t}'(s) = -qB_{ext}(Z_r(s))\mathbf{n}(s)/P_r$ where $P_r = m\gamma_r\beta_r c$ is the momentum of the reference particle. This determines the curvature κ up to a sign and we choose $\kappa(s) = qB_{ext}(Z_r(s))/P_r$. Thus $\mathbf{t}'(s) = -\kappa(s)\mathbf{n}(s)$ and $\mathbf{n}'(s) = \kappa(s)\mathbf{t}(s)$.

The BF Frenet-Serret coordinates are $\xi = (s,x)$, where x is the perpendicular distance along $\mathbf{n}$. Let $\mathbf{T} : U := \mathbb{R}\times(-x_M, x_M) \to \mathbf{T}(U) \subset \mathbb{R}^2$, where $\mathbf{T}(\xi) = \mathbf{R}_r(s) + x\mathbf{n}(s)$ and $x_M > 0$ is chosen sufficiently small so that $\mathbf{T}$ is a bijection. This leads to the phase space variable transformation $(\mathbf{R},\mathbf{P}) \leftrightarrow (s,x,p_s,p_x)$ defined by

$$\mathbf{R} = \mathbf{T}(\xi), \quad \mathbf{P} = \mathbf{P}(s,p_s,p_x), \quad (8)$$

where $\mathbf{P}(s,p_s,p_x) := P_r(p_s\mathbf{t}(s) + p_x\mathbf{n}(s))$. Our lab to beam transformation has two more transformations so that we have $(\mathbf{R},\mathbf{P};u) \to (s,x,p_s,p_x;u) \to (u,x,p_s,p_x;s) \to (z,x,p_z,p_x;s)$. We have included the independent variables and in the second transformation the variables s and u are interchanged making s the new independent variable. In the final transformation $z := s - \beta_r u$ replaces u as a dependent variable and $p_z := (\gamma - \gamma_r)/\gamma_r$ replaces p_s. Note that the variables $\mathbf{r} := (z,x)^T$ and $\mathbf{p} := (p_z,p_x)^T$ are small near the reference orbit which corresponds to $\mathbf{r} = \mathbf{p} = 0$.

The main objects in this paper are the phase space densities. The exact relation between the LF phase space density, f_L, and the BF phase space density, f_B, is

$$f_B(\mathbf{r},\mathbf{p};s) = \frac{P_r^2}{\beta_r^2} f_L\{\mathbf{T}(\xi), P_r[p_s(\mathbf{p})\mathbf{t}(s) + p_x\mathbf{n}(s)]; (s-z)/\beta_r\}, \quad (9)$$

where

$$p_s(\mathbf{p})^2 = (\frac{1}{\beta_r})^2(1+p_z)^2 - p_x^2 - \frac{1}{\gamma_r^2\beta_r^2}. \quad (10)$$

Recall that we consider $f_L(\cdot;u)$ to be well defined by (4) for $u \geq u_i$ and note that $f_B(\cdot;s)$ requires $f_L(\cdot;u)$ for a range of u values. This density transformation is unusual in that there is an interchange of u and s in their roles as independent and dependent variables and this requires that in the dynamics s must be an increasing function of u. There are subtleties in the derivation of the transformation (9) and details will be given in [2].

Introducing the inverse of (8), we write

$$f_L(\mathbf{R},\mathbf{P};u) = \frac{\beta_r^2}{P_r^2} f_B\{s(\mathbf{R}) - \beta_r u, x(\mathbf{R}), p_z(\mathbf{P},s(\mathbf{R})), \mathbf{P}\cdot\mathbf{n}(s(\mathbf{R}))/P_r; s(\mathbf{R})\}, \quad (11)$$

where $(s(\mathbf{R}),x(\mathbf{R})) = \mathbf{T}^{-1}(\mathbf{R})$ for $\mathbf{R} \in \mathbf{T}(U)$, $p_s(\mathbf{p}) = \mathbf{P}\cdot\mathbf{t}(s)/P_r$ can be solved for $p_z(\mathbf{P},s)$ using (10) and $p_x = \mathbf{P}\cdot\mathbf{n}(s(\mathbf{R}))/P_r$. Because $\mathbf{R} = \mathbf{T}(\xi)$ in (8) is only locally invertible we require the coordinate densities $\rho_L(\mathbf{R};u)$ and $\rho_B(\mathbf{r};s)$ to have compact support.

To define the BF Vlasov equation we need the BF equations of motion. Using (5) and (8) we obtain

$$\begin{aligned}
z' &= 1 - \frac{\mathcal{K}(\xi)(1+p_z)}{p_s(\mathbf{p})}, \qquad x' = \frac{\mathcal{K}(\xi)p_x}{p_s(\mathbf{p})},\\
p_z' &= \frac{q\mathcal{K}(\xi)}{m\gamma_r c^2}\Big(\mathbf{E}_\parallel(\mathbf{T}(\xi);\frac{s-z}{\beta_r})\cdot\mathbf{t}(s)\\
&\quad + \frac{p_x}{p_s(\mathbf{p})}\mathbf{E}_\parallel(\mathbf{T}(\xi);\frac{s-z}{\beta_r})\cdot\mathbf{n}(s)\Big)\\
p_x' &= \frac{1}{P_r}\Big(P_r p_s(\mathbf{p})\kappa(s) - q\mathcal{K}(\xi)B_{ext}(Z_r(s) - xX_r'(s))\Big)\\
&\quad + \frac{q(1+p_z)}{P_r p_s(\mathbf{p})\beta_r c}\mathcal{K}(\xi)\mathbf{E}_\parallel(\mathbf{T}(\xi);\frac{s-z}{\beta_r})\cdot\mathbf{n}(s)\\
&\quad - \frac{q}{P_r}\mathcal{K}(\xi)B_Y(\mathbf{T}(\xi);\frac{s-z}{\beta_r}). \qquad (12)
\end{aligned}$$

Here $' = d/ds$, $\mathbf{E}_{||} := (E_Z,E_X)^T$ and $\mathcal{K}(\xi) := 1+\kappa(s)x$.

The BF phase space density f_B, given in (9), satisfies the Vlasov equation

$$\partial_s f_B + \mathbf{r}'\cdot\nabla_{\mathbf{r}} f_B + \mathbf{p}'\cdot\nabla_{\mathbf{p}} f_B = 0, \quad (13)$$

where the coefficients are given by (12). This can be verified by simply plugging (9) into (13) and using (4). It is also consistent with the BF equations of motion themselves, as it must be, since the Vlasov equation for (12) is (13). In this context it is worth mentioning that the vector field in (12) is divergence free (see [2]).

Since there exists a unique f_L defined by the IVP (4), Eq. (9) gives us a unique f_B which we want to compute. However, we want to compute it based on the $s = 0$ IVP for (13), where

$$f_B(\mathbf{r},\mathbf{p};0) =: f_{B0}(\mathbf{r},\mathbf{p}), \quad (14)$$

by using an algorithm which marches forward in s. The initial condition can be determined from (9) given f_{L0} and the solution of (4) for a small forward time interval starting at u_i. However, in our applications, e.g. [1], we have been given f_{B0}, not f_{L0}.

Clearly, (13) is a nonlinear partial differential integral equation where the $\mathbf{p}'$ coefficient depends on the self field $\mathcal{F}_L(\mathbf{R}(s,x),(s-z)/\beta_r)$ and thus on f_B through f_L. However, there is a causality issue. The quantity $\mathcal{F}_L(\mathbf{R}(s,x),(s-z)/\beta_r)$ requires knowledge of $f_B(\cdot;\tau)$, not only for $\tau \in [0,s]$, but also for some τ outside this interval. Nevertheless, since the main contribution to $\mathbf{p}'$ comes from $[0,s]$, we obtain a feasible s-stepping algorithm for f_B given the initial condition (14). In the next section we discuss what we do when knowledge of $f_B(\cdot;\tau)$ is needed for $\tau \notin [0,s]$.

The basic computational issue is to solve the IVP (13-14) in such a way that to good approximation (9) is satisfied, with f_L defined by (4). This requires determining f_{L0} from f_{B0}, which we discuss in [2].

Before leaving this section we note that in our computations we use the approximate BF equations of motion,

$$\begin{aligned}
z' &= -\kappa(s)x, \qquad & p_z' &= F_{z1}(z,x;s) + p_z F_{z2}(z,x;s),\\
x' &= p_x, & p_x' &= \kappa(s)p_z + F_x(z,x;s), \qquad (15)
\end{aligned}$$

where

$$\begin{aligned}
F_{z1} &= \frac{q}{P_r c}\mathbf{E}_\parallel(\mathbf{R}(\xi);\frac{s-z}{\beta_r})\cdot\mathbf{t}(s),\\
F_{z2} &= \frac{q}{P_r c}\mathbf{E}_\parallel(\mathbf{R}(\xi);\frac{s-z}{\beta_r})\cdot\mathbf{n}(s), \qquad (16)\\
F_x &= \frac{q}{P_r c}[\mathbf{E}_\parallel(\mathbf{R}(\xi);\frac{s-z}{\beta_r})\cdot\mathbf{n}(s) - cB_Y(\mathbf{R}(\xi);\frac{s-z}{\beta_r})].
\end{aligned}$$

These equations were obtained from the exact BF equations (12) by linearizing the terms without the self field and by approximating the coefficients of the self field terms (see [2]). Without the self field, the general solution of (15) can be written in terms of the dispersion function, $D(s)$, and the

momentum compaction function, $R_{56}(s)$. We have found that it is numerically more efficient to integrate (15) in the interaction picture based on this zero self field solution (see [1]).

SELF FIELD FROM BF PHASE SPACE DENSITY AND CAUSALITY DISCUSSION

An $s-$stepping algorithm to evolve an approximation to $f_B(\cdot;s)$ according to (13-14) needs to compute

$$\mathcal{F}_L(\mathbf{T}(\xi);(s-z)/\beta_r) = \quad (17)$$
$$-\int_{\mathbb{R}^2} d\mathbf{R}' \frac{\mathbf{S}[\mathbf{R}';(s-z)/\beta_r - |\mathbf{R}'-\mathbf{T}(\xi)|]}{4\pi|\mathbf{R}'-\mathbf{T}(\xi)|},$$

approximately, where $\mathcal{F}_L(\mathbf{R};u)$ was defined in (2). Here we ignore the shielding, as it adds little computational complexity. To compute (17) we need $\rho_L(\mathbf{R}';v(\mathbf{R}'))$ and $\mathbf{J}_L(\mathbf{R}';v(\mathbf{R}'))$ in terms of f_B as $\mathbf{R}'$ varies over the support of $\rho_L(\mathbf{R}';v(\mathbf{R}')$, where $v(\mathbf{R}') = (s-z)/\beta_r - |\acute{\mathbf{R}}-\mathbf{T}(\xi)|$. Using (11) we obtain

$$\rho_L(\mathbf{R};u) = \quad (18)$$
$$\beta_r^2 \int d\mathbf{p} f_B\{s(\mathbf{R})-\beta_r u, x(\mathbf{R}), \mathbf{p}; s(\mathbf{R})\}|\partial_{p_z} p_s(\mathbf{p})|,$$

and a similar formula for $\mathbf{J}_L(\mathbf{R};u)$. Thus given $f_B(\cdot;\tau)$ over a suitable τ domain, (17) can be computed. Furthermore, using the fact that f_B is nonnegative and continuous, it follows that the support of $\rho_L(\mathbf{R};u)$ is the same as the support of $\rho_B\{s(\mathbf{R})-\beta_r u, x(\mathbf{R}); s(\mathbf{R})\}$.

There are two issues here. First, it would be inefficient to integrate (17) over all of $\mathbb{R}^2$. Thus it is important to determine a good superset for the region where the integrand is nonzero. However, this $\mathbf{R}'$ region appears to be difficult to determine efficiently. In the next section we explore two sets of integration variables better suited to the integration in (17). Second, we must deal with the issue that (17) requires knowledge of $f_B(\cdot;\tau)$ for $\tau \notin [0,s]$. to good approximation becomes

We begin by considering $s=0$. We assume that the support of the initial $z-$density, $\int dx dp_z dp_x f_{B0}$, is $[-a,a]$. For $s=0$ we have $z=-\beta_r u$, so the arrival time at $s=0$ of the particle with $z-$coordinate ξ is $u=-\xi/\beta_r$. Thus the head of the bunch corresponds to $z=a$ and the tail to $z=-a$. Recall that we defined u_i to be the time at which the head of the bunch enters the chicane, thus $u_i=-a/\beta_r$. To evaluate (17) we need $f_L(\mathbf{R}',\mathbf{P};-z/\beta_r-|\mathbf{R}'-\mathbf{T}[(0,x)]|)$ and so we need $f_L(\mathbf{R}',\mathbf{P};v)$ for $v\in[u_i=-a/\beta_r, a/\beta_r]$. This will be discussed in [2].

We claim that at s we need partial information on $f_B(\cdot;\tau)$ for some $\tau > s$, i.e., there is a causality issue. To demonstrate this we choose $\mathbf{r}=0$ and $\mathbf{R}'=\mathbf{R}_r(s)+\Delta\mathbf{t}(s)$ in the integrand of (17), where Δ is positive and small relative to the bunch size. Thus the integrand requires the value of $\rho_L(\mathbf{R}_r(s)+\Delta\mathbf{t}(s);s/\beta_r-\Delta)$ and by (18) $f_B\{s(\mathbf{R}_r(s)+\Delta\mathbf{t}(s))-s+\beta_r\Delta, x(\mathbf{R}_r(s)+\Delta\mathbf{t}(s)),\mathbf{p};s(\mathbf{R}_r(s)+\Delta\mathbf{t}(s)\}$ is needed. Now applying Taylor's theorem $s(\mathbf{R}_r(s)+\Delta\mathbf{t}(s))=s+\Delta+O(\Delta^2)$ and $x(\mathbf{R}_r(s)+\Delta\mathbf{t}(s))=O(\Delta^2)$ and we obtain $f_B\{(1+\beta_r)\Delta+O(\Delta^2),O(\Delta^2),\mathbf{p};s+\Delta\}$. Thus we need partial information on $f_B(\cdot;s+\Delta)$ and this completes the claim.

A geometrical argument may be more insightful. Take $\mathbf{r}=0$, then the LF observation point is at $(\mathbf{R}_r(s),s/\beta_r)$. The 'backward lightcone' of this event is $C_L=\{(\mathbf{R}',u'): |\mathbf{R}'-\mathbf{R}_r(s)|=s/\beta_r-u',\mathbf{R}'\in\mathbf{T}(U)\}$ with BF image $C_B=\{(z',x',s'): |\mathbf{R}_r(s')+x'\mathbf{n}(s')-\mathbf{R}_r(s)|=(z'-s'+s)/\beta_r,\xi'\in U)\}$. Solving $|\mathbf{R}_r(s')+x'\mathbf{n}(s')-\mathbf{R}_r(s)|=(z'-s'+s)/\beta_r$ for small $\Delta:=s'-s$ gives $z'=\Delta+\beta_r\sqrt{\Delta^2+x'^2}$. Thus there are small positive Δ with (z',x') in the beam, i.e., C_B contains points in the beam $s'>s$. In the drift, this argument even works without the small Δ assumption.

We suspect that whenever causality is violated, within the support of f_B, it is only violated in a small τ interval for $\tau>s$. However, in our applications $f_B(\cdot;s)$ is slowly varying, that is, $f_B(\cdot;s+\Delta)\approx f_B(\cdot;s)$ for $|\Delta|$ less than the $z-$size of the beam. Thus we believe that to good approximation (17) can be determined from $f_B(\cdot;\tau)$ for $\tau\le s$, if we take $f_B(\cdot;\tau)=f_B(\cdot;s)$ when $\tau>s$, and this resolves the causality issue. Recall that the IVP (4) defines $f_L(\mathbf{R},\mathbf{P};u)$ for $u\ge u_i$, given $f_{L0}(\mathbf{R},\mathbf{P})$. So the true test of any approximation is, does the $f_B(\mathbf{r},\mathbf{p};s)$ we calculate approximately satisfy (9)? We believe our approximations do, but have no proof.

For each s, the computation of $\mathcal{F}_L$ in (17) must be done for a large number of $\mathbf{r}$ values, thus both arguments of $\mathcal{F}_L$ vary. However, since $f_B(\cdot;s)$ is slowly varying we believe that $\mathcal{F}_L(\mathbf{T}[(s,x)],(s-z)/\beta_r)$ is also slowly varying in s, for fixed $\mathbf{r}$. Replacing s by $s+z$ and expanding gives $\mathcal{F}_L(\mathbf{R}_r(s)+x\mathbf{n}(s),(s-z)/\beta_r)\approx\mathcal{F}_L(\mathbf{R}_r(s)+M(s)\mathbf{r},s/\beta_r)$, where $M(s)=[\mathbf{t}(s),\mathbf{n}(s)]$. Thus to move points, the second argument is independent of z, and this increases the efficiency. This is what we do in the code. There is still a causality issue but it can be resolved as above.

OUTLINE OF CALCULATION OF THE BEAM FRAME SPATIAL DENSITY

Our ultimate goal is to compute the evolution of $f_B(\cdot;s)$ for $s>0$ given f_{0B}, i.e., the solution of the IVP (13-14), but this is beyond our current capability as mentioned in the Introduction. However the computation of the evolution of the associated spatial density $\rho_B(\cdot;s)$ is possible. From (10) $\partial_{p_z}p_s(\mathbf{p})$ is $1/\beta_r^2$ to good approximation, thus by (11) we can take $\rho_L(\mathbf{R};u)=\rho_B\{s(\mathbf{R})-\beta_r u, x(\mathbf{R});s(\mathbf{R}))$. Also, to good approximation, $\mathbf{J}_L$ can be determined from ρ_B and τ_B where $\tau_B(\mathbf{r},s)=\beta_r\int_{\mathbb{R}^2}p_x f_B(\mathbf{r},\mathbf{p};s)d\mathbf{p}$ (see [1]-[3]). Thus, from the history of $g_B:=(\rho_B,\tau_B)$, the self field (17) can be computed. Our current goal is a fast method to calculate $g_B(\cdot;s)$, for $s>0$ given f_{B0}, consistent with the IVP (13-14).

We begin by generating an initial, $s=0$, set of phase space points from f_{B0} using a random number genera-

tor. We currently use pseudo random points and are in the process of investigating quasi random points, which are known to have a significant advantage in numerical integration. From the scattered data we calculate $g_B(\cdot;0)$ using a density estimation procedure. We follow the phase space points using (15) in the interaction picture. At s we have the scattered set of phase space points and the history of $g_B(\mathbf{r};\tau)$ for $-2a \le \tau < s$ on a 3D grid in $(\mathbf{r},\tau)$. To go from $s \to s+\delta s$ we first calculate $g_B(\cdot;s)$ from scattered data using well known density estimation procedures from Statistics. Then from the knowledge of $g_B(\cdot;\tau)$ for $-2a \le \tau \le s$ we calculate the self field from (17) and use this and (15) to move the points from $s \to s+\delta s$. The bulk of the calculations are done in parallel.

The main issues for a fast algorithm are the field calculation, the density estimation and the parallel implementation. The latter is elementary, the first two are discussed in the next two sections.

FIELD CALCULATION

The bunch is small and moving. Thus, for each s, it is important to have a good estimate of the location and spatial extent of the bunch. This allows for an s-independent grid on which to represent $g_B(\mathbf{r};s)$. We first discuss a model we currently use in our bunch compressor studies, which gives a compact, s-independent grid. Then we discuss two sets of integration variables for the integration in (17).

Compact Support Model of Bunch

The location and spatial extent of the bunch depends on the initial phase space density. The one we use in our microbunching studies, [1], is

$$f_{B0}(\mathbf{r},\mathbf{p}) = (1+\varepsilon(z))\mu(z)\rho_c(p_z - hz)\rho_t(x,p_x), \quad (19)$$

where $\varepsilon(z) = A\cos(k_0 z)$, μ is a flat top with support $[-a,a]$, ρ_c is $N(0,\sigma_u)$ and ρ_t is $N(0,\mathrm{diag}(\sigma_{x_0},\sigma_{p_{x_0}}))$, where σ_u and $\sigma_{p_{x_0}}$ are small. Taking $\sigma_u = 0$ and $\sigma_{p_{x_0}} = 0$, the initial conditions for (15) have the form $z = \tilde{z}$, $p_z = h\tilde{z}$, $x = \tilde{x}$, and $p_x = 0$ and without the self field the solution is

$$z = (1+hR_{56}(s))\tilde{z} - D'(s)\tilde{x}, \quad x = hD(s)\tilde{z} + \tilde{x}. \quad (20)$$

Here h is the chirp parameter and $D(s)$ and $R_{56}(s)$ were introduced in the context of (15). Using $(\tilde{z},\tilde{x})$ as coordinates we find that the support of $g_B(\cdot;s)$ is essentially independent of s.

To obtain our compact support model we scale the tilde variables and our final transformation is $\mathbf{r} = A(s)\tilde{\mathbf{r}} = A(s)\Sigma\hat{\mathbf{r}} =: B(s)\hat{\mathbf{r}}$. Here Σ is a diagonal matrix chosen so that the support of the beam is just inside the circle $\hat{\mathbf{r}}^T\hat{\mathbf{r}} = 1$. Thus the support of $g_B(\mathbf{r};s)$ is given by

$$\mathbf{r}^T E(s)\mathbf{r} \le 1, \quad E(s) = B(s)^{-T}B(s)^{-1}, \quad (21)$$

that is, it is the interior of an ellipse. Using (21) to determine the $\mathbf{R}'$ region of integration seems complicated. We now introduce two sets of integration variables which simplify the determination of the support and the task of integration.

Polar Coordinates

We transform to polar coordinates (χ,θ) in (2) and then take the temporal argument v in place of the radial coordinate χ. That is, we make the transformation $\mathbf{R}' \to (\theta,v)$ via $\mathbf{R}' = \mathbf{R} + \chi\mathbf{e}(\theta), \mathbf{e}(\theta) = (\cos\theta,\sin\theta)^T, v = u - \sqrt{\chi^2+(kh)^2}$.

This removes the integrable singularity giving the field simply as an integral over the source,

$$\mathcal{F}_L(\mathbf{R},u) = -\frac{1}{4\pi}\int_{u_i}^{u} dv \int_{-\pi}^{\pi} d\theta\ \mathbf{S}[\mathbf{R}+(u-v)\mathbf{e}(\theta),v], \quad (22)$$

where we have ignored shielding. Using the slowly varying assumption, as discussed at the end of Section 4, we obtain

$$\mathcal{F}(,(s-z)/\beta_r) \approx \mathcal{F}(\mathbf{R}_r(s)+M(s)\mathbf{r}, s/\beta_r)$$
$$= -\frac{1}{4\pi}\int_{u_i}^{s/\beta_r} dv \int_{-\pi}^{\pi} d\theta \mathbf{S}[\tilde{\mathbf{R}}(\theta,v;\mathbf{r},s),v], \quad (23)$$

where $\tilde{\mathbf{R}}(\theta,v;\mathbf{r},s) = \mathbf{R}_r(s) + M(s)\mathbf{r} + (s/\beta_r - v)\mathbf{e}(\theta)$. This is what we must calculate, at arc length s, as $\mathbf{r}$ varies over the bunch. Note that for $\mathbf{r} = 0$ the approximation is exact. Also taking $\mathbf{r} = 0$, $v = s/\beta_r - \Delta$ and $\mathbf{e}(\theta) = \mathbf{t}(s)$, we see the same causality issue as before and resolve it in the same way.

Except for v close to s/β_r the θ support in (23) is tiny and it is important for a fast algorithm to compute this accurately. Using the slowly varying approximation and (18), it can be shown that the support of $\mathbf{S}(\tilde{\mathbf{R}},v)$ is, to good approximation, the same as $\rho_B(M^T(\beta_r v)(\tilde{\mathbf{R}} - \mathbf{R}_r(\beta_r v)),\beta_r v)$. The support of the latter is given by (21) with $\mathbf{r}$ replaced by $M^T(\beta_r v)(\tilde{\mathbf{R}} - \mathbf{R}_r(\beta_r v))$ and s replaced by $\beta_r v$. This gives a quartic in $\exp(i\theta)$ and solving this gives reasonable θ limits. This is discussed in some detail in [1] and [3].

Currently the θ integration is done with the superconvergent trapezoidal rule. The remaining $v-$integrand varies with v, $\mathbf{R}$ and u in ways we have not yet quantified and so we use an adaptive integrator based on the Gauss-Kronrod algorithm. We are investigating two improvements. The adaptive integrator is slow and we are studying the v dependence of the integrand after the θ integration with the hope of using a non-adaptive algorithm. Solving the quartic to determine the θ support may not be the best approach. The ellipse in (21) is quite elongated and we are investigating replacing it by a parallelogram which should simplify the calculation.

The computational effort for the calculation of one component of the self field is $O(N_z N_x N_v N_\theta)$, where N_z and N_x are the number of grid points in $\hat{z}$ and $\hat{x}$ respectively, N_v is the number of evaluations for the v integra-

tion, and N_θ is the number of evaluations for the θ integration. Typical values for our simulations in [1] are $N_z = 1000$, $N_x = 128$, $N_v = N_\theta = 1000$, therefore $O(N_z N_x N_v N_\theta) = O(10^{12})$.

Beam Frame Coordinates

The transformation $\mathbf{R}' \to \xi'$ via $\mathbf{R}' = \mathbf{T}(\xi')$ in (2) gives

$$\mathcal{F}_L(\mathbf{T}(\xi); (s-z)/\beta_r) = -\frac{1}{4\pi}\int_{\mathbb{R}^2} d\xi' \frac{\mathcal{K}(\xi')}{|\mathbf{T}(\xi') - \mathbf{T}(\xi)|} \times \mathbf{S}[\mathbf{T}(\xi'); \frac{s-z}{\beta_r} - |\mathbf{T}(\xi') - \mathbf{T}(\xi)|]. \quad (24)$$

The nonsingular part of the integrand for $\mathbf{E}_{||}$ is given by

$$\begin{aligned} &\mathcal{K}(\xi')\mathbf{S}_{||}[\mathbf{T}(\xi'); \frac{s-z}{\beta_r} - |\mathbf{T}(\xi') - \mathbf{T}(\xi)|]/QZ_0c \\ &= [(\frac{1}{\gamma_r^2} - \beta_r^2 x'\kappa(s'))D_1\rho_B() + D_3\rho_B()]\mathbf{t}(s') \\ &+ \quad \mathcal{K}(\xi')[D_2\rho_B() + D_1\tau_B()]\mathbf{n}(s'), \end{aligned} \quad (25)$$

where $() = (z', x'; s')$, $z' = s' - s + z - \beta_r|\mathbf{T}(\xi') - \mathbf{T}(\xi)|$ and $\mathbf{S}_{||}$ is defined in the obvious way. Thus the support of the integrand is the support of $g_B(z', x'; s')$. For each s', the x' region of integration can now be determined from (21) by solving $\mathbf{r}(\xi')^T E(s')\mathbf{r}(\xi') = 1$ where $\mathbf{r}(\xi')^T = (s' - s + z - \beta_r|\mathbf{T}(\xi') - \mathbf{T}(\xi)|, x')$. This is a quartic equation in x', which is not so surprising as x' is analogous to θ in the previous subsection. We can now write (24) as an iterated integral as in (23).

We are in the process of comparing this with the polar coordinate approach. The integrand is given naturally in terms of g_B which is nice. For example, one sees the factor, $D_3\rho_B$, which gives rise to the compression and is not there for a rigid bunch. Also, studies by Warnock suggest (i) this is a natural framework for the study of 1D collective force approximations, (ii) it could lead to a good approximation for s' near s, which includes the singularity, and (iii) a multipole expansion for s' a few bunch lengths from s is possible and may save time and storage. We are pursuing these ideas.

DENSITY ESTIMATION

Density estimation is a significant and active area of Statistics, see for example [4] and [5]. We compare the computational effort of three methods for the same level of accuracy.

One approach to density estimation is based on orthogonal series and we have studied the Fourier series case in some detail following [4]. Here ρ_L and $\mathbf{J}_L$ are obtained at every s step by computing the Fourier coefficients of the truncated Fourier series via Monte Carlo integration of the random sample of phase space points. Details are given in [1] and [3]. The computational effort is $O(\mathcal{N} J_z J_x) + O(N_z N_x J_z J_x)$, where $\mathcal{N}$ is the number of simulated points, and J_z and J_x are the number of Fourier coefficients in $\hat{z}$ and $\hat{x}$ respectively. Typical values in our microbunching simulations are $\mathcal{N} = 5\times10^8$, $J_z = 150$ and $J_x = 50$. Therefore the computational effort is $O(10^{12})$ and is of the same order as the computational effort for the polar coordinate field calculation discussed previously.

A second approach employs cloud in cell charge deposition where at every s step the random sample is placed on our fixed grid (See Section3.5 of [5] and [6]). Here ρ_L and $\mathbf{J}_L$ are obtained by computing the Fourier coefficients of the truncated Fourier series by a simple quadrature. The computational effort in this case is $O(\mathcal{N})+O(N_z N_x J_z J_x)$. We have found that using $\mathcal{N}, J_z, J_x$ as above, $N_z = 1000$ and $N_x = 128$, gives the same approximation as the Monte Carlo approach of the previous paragraph. This computational effort of $O(10^9)$ is much smaller than for the orthogonal series method and negligible with respect to the computational effort for the polar coordinate field calculation. This is the present method implemented in our code.

A third approach applies kernel density estimator techniques to the random sample. This approach is still in the testing phase where we are investigating standard kernels like bivariate Gaussians or bivariate Epanechnikov kernels (all with a uniform bandwith, h). The computational effort for the bivariate Epanechnikov kernel is $O(\mathcal{N}\tilde{N}_z\tilde{N}_x)$, where $\mathcal{N}$ is as before but now $\tilde{N}_z\tilde{N}_x$ is the number of grid points inside the square which encloses the circle of radius h centered at the scattered particle position $\hat{z}, \hat{x}$. For $\mathcal{N} = 5\times10^8, N_z = 1000, N_x = 128$ we approximately get $\tilde{N}_z = 24, \tilde{N}_x = 3$, $O(\mathcal{N}\tilde{N}_z\tilde{N}_x) = O(10^{10})$. Thus this method is comparable in speed to the second method and is worthy of further investigation.

So far, for all three approaches, the initial random sample is generated from pseudo-random numbers but quasi-random numbers will be tested soon.

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