

# FAST ENVELOPE TRACKING FOR SPACE CHARGE DOMINATED INJECTORS\*

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## Abstract

High brightness injectors are increasingly pushing against space charge effects. Usually, particle tracking codes such as ASTRA, GPT, or PARMELA are used to model these systems however these can be slow to use for detailed optimization. It becomes increasingly challenging in future projects such as LCLS-II where space charge effects are still significant after BC1 and BC2 at 250 and 1600 MeV respectively. This talk will describe an envelope tracking approach that compares well against the particle tracking codes and could facilitate much faster optimization.

## INTRODUCTION

Commonly, particle tracking simulation codes are used to design and then commission and finally have operators tune accelerators. Only a few particles would be needed if they act individually, but if space charge fields are significant, this rises to  $10^5$  to  $10^6$  or even more. A known, simpler technique is to track rms sizes and correlations (second moments), since then space charge can be included at little cost.

In this note, we expand this technique to more complex cases, beyond the usual integrable ones such as drifts, solenoids, quadrupoles and dipoles. In particular, we apply it to time-varying fields such as in linear accelerators.

## SACHERER ENVELOPE THEORY REVIEW

Instead of multiparticle simulations, we look at the “envelope”, i.e. treat the beam statistically. [1]

If there is a distribution of particles, one would like to calculate the final distribution from the initial. The behaviour of the beam centroid

$$\langle \mathbf{X} \rangle = \sum_{i=1}^N \mathbf{X} / N \quad (1)$$

(where  $N$  is the number of particles, and  $\mathbf{X}$  is the column vector  $(x, P_x, y, P_y, z, P_z)^T$  as in eqn. 6) is determined by the same transfer matrix  $\mathbf{M}$  as for an individual particle. This is the equation of ‘first moments’. At the next level, one would like to calculate the evolution of the beam widths, or, ‘second moments’ given by

$$\sigma \equiv \frac{1}{N} \sum_{i=1}^N \mathbf{X} \mathbf{X}^T \quad (2)$$

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For example,  $\sigma_{11} = \langle x^2 \rangle$ ,  $\sigma_{12} = \langle x P_x \rangle$ ,  $\sigma_{13} = \langle xy \rangle$ , ... For a distribution of particles so dense that we do not see graininess on any scale of our diagnostics, the sums go over into integrals.

Here,  $s$  is the independent variable, so coordinates 5 and 6 are resp. time and energy:  $z = \beta_0 c \Delta t$ ,  $P_z = (\beta_0 c)^{-1} \Delta E$ . (This is further explained below.)

By direct substitution into the definition of  $\sigma$ , we find

$$\sigma_f = \mathbf{M} \sigma_i \mathbf{M}^T \quad (3)$$

As well, we can define an *infinitesimal transfer matrix*  $\mathbf{F}$  where  $\mathbf{X}' = \mathbf{F} \mathbf{X}$  and the transfer matrix of an infinitesimal length  $ds$  is  $\mathbf{M} = \mathbf{I} + \mathbf{F} ds$ , we find directly

$$\sigma' = \mathbf{F} \sigma + \sigma \mathbf{F}^T. \quad (4)$$

This is the **envelope equation**. For the full 6D case, it represents 21 equations. (Because  $\sigma$  is symmetric.)

## Infinitesimal Transfer Matrix

The general Hamiltonian can be Taylor-expanded by orders in the 6 dependent variables<sup>1</sup>,

$$H(\mathbf{x}; s) = \sum_i \frac{\partial H}{\partial x_i} \Big|_0 x_i + \frac{1}{2} \sum_{i,j} \frac{\partial^2 H}{\partial x_i \partial x_j} \Big|_0 x_i x_j + \dots \quad (5)$$

The subscript 0 means that the derivatives are evaluated on the reference trajectory  $\forall i$ ,  $x_i = 0$ . Terms of first order are eliminated by transforming to a coordinate system measured with respect to the reference trajectory. The remaining terms are second order and higher, and for linear motion, we simply truncate at the second order.

Then the Hamiltonian looks like  $H = Ax^2 + BxP_x + Cxy + \dots + UP_z^2$ : there are 21 independent terms.  $A = \frac{1}{2} \frac{\partial^2 H}{\partial x^2}$ , and so on; all derivatives are evaluated on the reference trajectory, and may be a function of the independent variable. We know the equations of motion from the Hamiltonian to be:  $x' = \partial H / \partial P_x$ ,  $P'_x = -\partial H / \partial x$ , etc., where primes denote derivatives w.r.t. the independent variable. Therefore the equations of motion:

$$\begin{pmatrix} x' \\ P'_x \\ y' \\ P'_y \\ z' \\ P'_z \end{pmatrix} = \begin{pmatrix} \frac{\partial^2 H}{\partial P_x \partial x} & \frac{\partial^2 H}{\partial P_x^2} & \cdots & \frac{\partial^2 H}{\partial P_x \partial P_z} \\ -\frac{\partial^2 H}{\partial x^2} & -\frac{\partial^2 H}{\partial x \partial P_x} & \cdots & -\frac{\partial^2 H}{\partial x \partial P_z} \\ \frac{\partial^2 H}{\partial P_y \partial x} & \frac{\partial^2 H}{\partial P_y \partial P_x} & \cdots & \frac{\partial^2 H}{\partial P_y \partial P_z} \\ -\frac{\partial^2 H}{\partial y \partial x} & -\frac{\partial^2 H}{\partial y \partial P_x} & \cdots & -\frac{\partial^2 H}{\partial y \partial P_z} \\ \frac{\partial^2 H}{\partial P_z \partial x} & \frac{\partial^2 H}{\partial P_z \partial P_x} & \cdots & \frac{\partial^2 H}{\partial P_z^2} \\ -\frac{\partial^2 H}{\partial z \partial x} & -\frac{\partial^2 H}{\partial z \partial P_x} & \cdots & -\frac{\partial^2 H}{\partial z \partial P_z} \end{pmatrix} \begin{pmatrix} x \\ P_x \\ y \\ P_y \\ z \\ P_z \end{pmatrix} \quad (6)$$

<sup>1</sup> In this shorthand,  $x_1 = x$ ,  $x_2 = P_x$ ,  $x_3 = y$ , ...

or,

$$\mathbf{X}' = \mathbf{F}\mathbf{X},$$

where  $\mathbf{F}$  is called the ‘infinitesimal transfer matrix’. Of the 36 elements of  $\mathbf{F}$  there are only 21 independent ones. This equation is easily integrated if  $\mathbf{F}$ =constant.

### Example: Quadrupole

A particular case is where the beamline consists only of elements that keep all 3 degrees of freedom independent of each other, and there is only a focusing force  $K(s)$  that varies with  $s$ . In other words, the Hamiltonian is eqn. 7,

$$H = \frac{p_x^2}{2} + K(s) \frac{x^2}{2} + \frac{p_y^2}{2} - K(s) \frac{y^2}{2} + \frac{p_z^2}{2\gamma^2}, \quad (7)$$

so

$$\mathbf{F} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -K & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & K & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\gamma^2} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (8)$$

When  $K$  is a constant, equation set 6 is easily solved, and these solutions are built into matrix codes such as TRANSPORT. But if not constant, eqns. 6 must be integrated numerically.

### Space Charge Part of $\mathbf{F}$

The beam is in bunches rather than continuous, so we need the electric field of an ellipsoidal distribution of charge. It turns out, surprisingly [1], that the RMS linear part of the space charge self-field depends mainly on the RMS size of the distribution and only very weakly on its exact form. To within a few percent, the RMS linear part of space charge is the same as that for a uniformly populated ellipsoid. The space charge infinitesimal transfer matrix is

$$\mathbf{F}_{sc} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ K_{xsc} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & K_{ysc} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & K_{zsc} & 0 \end{pmatrix} \quad (9)$$

where

$$K_{xsc} = \frac{Q}{4\pi\epsilon_0(mc^2/e)\beta^2\gamma^3} \frac{1}{a^3} g\left(\frac{b^2}{a^2}, \frac{c^2}{a^2}\right) \quad (10)$$

$$K_{ysc} = \frac{Q}{4\pi\epsilon_0(mc^2/e)\beta^2\gamma^3} \frac{1}{b^3} g\left(\frac{c^2}{b^2}, \frac{a^2}{b^2}\right) \quad (11)$$

$$K_{zsc} = \frac{Q}{4\pi\epsilon_0(mc^2/e)\beta^2\gamma^3} \frac{1}{c^3} g\left(\frac{a^2}{c^2}, \frac{b^2}{c^2}\right) \quad (12)$$

where  $Q$  is the bunch charge, the ellipsoid semi-axes in the  $x, y, z$  directions are  $a, b, c$ , and the function  $g$  is

$$g(u, v) = \frac{3}{2} \int_0^\infty (1+s)^{-3/2} (u+s)^{-1/2} (v+s)^{-1/2} ds \quad (13)$$

This is from the family of Carlson elliptic integrals [2].

**Arbitrary bunch distributions, orientations:** For arbitrary distributions of the type  $f(x, y, z) = f\left(\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2}\right)$ , replace  $a, b, c$  with the RMS values according to the values they have for the uniform case, namely,  $a^2 = 5\sigma_{11}$ ,  $b^2 = 5\sigma_{33}$ . Because of relativity,  $c^2$  is a special case:  $c^2 = 5\gamma^2\sigma_{55}$  [3].

Though the optics of individual particles is still linear, the envelope equations are highly nonlinear, and with space charge they now depend recursively upon these elliptic functions of beam size. For arbitrary orientations of the ellipsoid, one must apply a rotation matrix to  $F$ , thus making also  $F_{23}, F_{25}, F_{41}, F_{45}, F_{61}, F_{63}$  also non-zero. Elaborated for the case with space charge, DC (unbunched), uncoupled, the equations can be reduced to the (better-known) Kapchinsky-Vladimirsky eqns. [4] For further reading, again refer to [1], but also [5].

## TRANSOPTR

If all elements are integrable then the transfer matrices  $\mathbf{M}$  are known, and they are simply multiplied together to find the matrix of the whole beamline or synchrotron, and the final beam is found from the initial as in eqn. 3. This is the traditional approach, e.g. TRANSPORT, TRACE3D. To incorporate space charge, elements were subdivided and appropriate thin defocus lenses inserted. In TRACE3D, there are space charge impulses applied in the approximation of long bunches.

These techniques are approximate and non-adaptive: Why not use the equations of motion directly? There are only 21 of them. In TRANSOPTR, eqn. 4 is solved with a Runge-Kutta integrator. This allows not only space charge, but any general case with no closed-form solution to equations of motion, e.g. varying axial fields, linacs, short-soft-edge quads, etc.

The original version was written by Mark deJong, Ed Highway at Chalk River, Canada, [5] and applied to: beam-lines, achromatic fitting, space charge. Since that time, it has been expanded to include complex transport problems such as einzel lenses, axial electric fields for accelerator columns and soft-landing, soft solenoids, cyclotron inflectors, synchrotron closed orbit fitting finding  $\beta$ -functions with space charge, and now also linacs [6]. As well, its optimization routines have expanded to include simplex method and simulated annealing.

## APPLICATION TO LINEAR ACCELERATOR

Firstly, it is important for devices, such as linacs, where the energy deviation (coordinate 6) changes according to the particle's phase (coordinate 5), that we use properly canonical definitions of those coordinates. And here we are bothered by a persistent error originating from the earliest days of the field of accelerator physics. SLAC-75 [7] mentions “At any position in the system...”. This means that path length  $s$  rather than time  $t$  is the independent variable. Then goes on:

“...particle represented by a vector”:

$$(x, \theta, y, \phi, l, \delta)$$

(where  $l$  is trajectory length and  $\delta \equiv \Delta P/P$ ). This is wrong: The canonical pair are  $(t - t_0, E - E_0)$  or  $(\Delta t, \Delta E)$ , **not**  $(l, \Delta P/P)$ . The reason it works usually is by applying a trick: If we scale by  $\beta_0 c$ , we can make them match, since  $\beta_0 c \Delta t = z$ , and in magnetic elements,  $\Delta E/(\beta_0 c) = \Delta P$ , but this is **only** true of magnetic elements, and leads the analysis astray when there are electric fields. We use this same trick because then coordinate 6 only deviates from the usual  $\Delta P/P$  in regions where electric potential  $\Phi \neq 0$ . Further, the coordinate 5 is not “path length difference” as stated by Brown, but the time difference with respect to the reference particle, scaled by the reference particle’s speed.

### Hamiltonian

With the distance along the reference trajectory  $s$  as the independent variable, the Hamiltonian is

$$H(x, P_x, y, P_y, t, E; s) = -qA_s \quad (14)$$

$$-\sqrt{\left(\frac{E - q\Phi}{c}\right)^2 - m^2 c^2 - (P_x - qA_x)^2 - (P_y - qA_y)^2}$$

**Potentials:** The case of RF axially-symmetric electric field can be handled entirely with no electric potential ( $\Phi = 0$ ), and time-varying vector potential. This has been presented a number of times in the past e.g. E.E. Chambers [8] who uses an analytic electric field, but we are interested in the following more experimentally-useful case: The electric field along the axis  $\mathcal{E}(s)$  has been measured and is therefore known, and the geometry is exactly axially symmetric.

Rob Ryne [9] has treated this case; the vector potential  $\vec{A}(x, y, s, t)$  is

$$A_x = \frac{\mathcal{E}'(s)}{2} \frac{\sin(\omega t + \theta)}{\omega} x \quad (15)$$

$$A_y = \frac{\mathcal{E}'(s)}{2} \frac{\sin(\omega t + \theta)}{\omega} y$$

$$A_s = \left( -\mathcal{E}(s) + \frac{x^2 + y^2}{4} \left[ \mathcal{E}''(s) + \frac{\omega^2}{c^2} \mathcal{E}(s) \right] \right) \frac{\sin(\omega t + \theta)}{\omega}$$

This is Coulomb/Lorenz gauge, satisfies Maxwell equations to second order in transverse coordinates, gives correct on-axis  $\vec{\mathcal{E}} = -\partial \vec{A}/\partial t = \mathcal{E} \cos(\omega t + \theta)$ .

But we needn’t use this gauge. There’s a simpler much vector potential where the lowest order transverse components vanish, leaving only the  $s$  component, and it also gets rid of the second derivative of  $\mathcal{E}$ .

I propose the following function

$$\Psi(x, y, s, t) = -\frac{\mathcal{E}' \sin(\omega t + \theta)}{2} \frac{x^2 + y^2}{\omega} \quad (16)$$

Add the gradient of this function to the previous vector potential (15). We find  $A_x = A_y = 0$  and

$$A_s = -\mathcal{E}(s) \left( 1 - \frac{\omega^2}{c^2} \frac{x^2 + y^2}{4} \right) \frac{\sin(\omega t + \theta)}{\omega} \quad (17)$$

This is considerably simpler, but now there is a scalar potential:

$$\Phi = -\frac{\partial \Psi}{\partial t} = \mathcal{E}' \cos(\omega t + \theta) \frac{x^2 + y^2}{4} \quad (18)$$

**Find reference trajectory:** A complication is that *a priori*, we do not know the reference particle’s energy and time coordinates. We need these in order to expand about them. (See eqn. 5.) They can be found from the equations of motion for  $x = y = P_x = P_y = 0$ :

$$\frac{dE}{ds} = \frac{\partial H}{\partial t} = q\mathcal{E} \cos(\omega t + \theta) \quad (19)$$

$$\frac{dt}{ds} = -\frac{\partial H}{\partial E} = \frac{E}{P} = \frac{1}{\beta_0 c}$$

These two equations are added to the 21 mentioned previously, so 23 simultaneous equations must now be integrated together.

(From here on, I drop the 0 subscript:  $\beta$  and  $\gamma$  are implicitly assumed to be the relativistic parameters of the reference particle.)

These give the functions  $E_0(s)$  and  $t_0(s)$  about which  $t$  and  $E$  are expanded:  $E = E_0 + \Delta E$ ,  $t = t_0 + \Delta t$ . So we transform the canonical variables  $t$  and  $-E$  to  $(\Delta t, -\Delta E)$ , using as generating function

$$G = -\left( t - \int \frac{ds}{\beta(s)c} \right) (\Delta E + E_0) \quad (20)$$

(Check:  $\frac{\partial G}{\partial t} = -E$ ,  $\frac{\partial G}{\partial(-\Delta E)} = \Delta t$ .) The Hamiltonian gets the added terms

$$\frac{\partial G}{\partial s} = \frac{\Delta E + E_0(s)}{\beta(s)c} - \Delta t E'_0(s).$$

Finally, we wish to transform from  $(\Delta t, -\Delta E)$  to  $(z, P_z) = (-\beta c \Delta t, \Delta E/(\beta c))$ . (The reason for the sign change is as follows: an early arrival implies  $\Delta t < 0$ , but this means the particle is **ahead** so  $z > 0$ .) The generating function is

$$G = -\beta c \Delta t P_z \quad (21)$$

(Check:  $\frac{\partial G}{\partial \Delta t} = -\Delta E$ ,  $\frac{\partial G}{\partial(P_z)} = z$ .) The term to be added to the Hamiltonian is

$$\frac{\partial G}{\partial s} = \frac{\beta'}{\beta} z P_z = \frac{\gamma'}{\beta^2 \gamma^3} z P_z = \frac{q\mathcal{E}C}{\beta c P \gamma^2} z P_z,$$

where  $C \equiv \cos(\omega t_0 + \theta)$ .

Now, expanding the Hamiltonian, we get the result:

$$H_z = \frac{P_x^2}{2P} + \frac{P_y^2}{2P} + \frac{q}{2\beta c} \left( \mathcal{E}'C - \mathcal{E}S \frac{\omega\beta}{c} \right) \frac{r^2}{2} +$$

$$\frac{P_z^2}{2\gamma^2 P} + \frac{q\mathcal{E}C}{\beta c} \frac{z P_z}{\gamma^2 P} - \frac{q\mathcal{E}\omega S}{\beta^2 c^2} \frac{z^2}{2} \quad (22)$$

( $C \equiv \cos(\omega t_0(s) + \theta)$ ,  $S \equiv \sin(\omega t_0(s) + \theta)$ )

We can recognize individual terms. (1) The factor in parentheses represents usual the focal power of an RF gap, e.g. a buncher. (2) Taking the limit as  $\omega \rightarrow 0$  reproduces precisely the Hamiltonian of the DC accelerator [3]. Note that in that case,  $\mathcal{E}' = -\phi''$ .

### Infinitesimal Transfer Matrix $F$

Now that the Hamiltonian for linear motion (eqn. 22) has been obtained, it is a simple matter to find the infinitesimal transfer matrix  $F$ . Writing the equations of motion ( $x' = \partial H / \partial P_x$ ,  $P'_x = -\partial H / \partial x$ , etc.), the following  $F$ -matrix is found for the axially symmetric linear accelerator:

$$F = \begin{pmatrix} 0 & \frac{1}{P} & 0 & 0 & 0 & 0 \\ \mathcal{A}(s) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{P} & 0 & 0 \\ 0 & 0 & \mathcal{A}(s) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{B'}{\beta} & \frac{1}{\gamma^2 P} \\ 0 & 0 & 0 & 0 & \mathcal{B}(s) & -\frac{B'}{\beta} \end{pmatrix}. \quad (23)$$

where we have defined:

$$\mathcal{A}(s) = \frac{-q}{2\beta c} \left( \mathcal{E}' C - \mathcal{E} S \frac{\omega \beta}{c} \right), \quad \mathcal{B}(s) = \frac{q \mathcal{E} \omega S}{\beta^2 c^2}. \quad (24)$$

This matrix has been coded as subroutine SCLINAC into TRANSPTR. Along with additional the two additional eqns. 19, this sets up to calculate through any axially symmetric linac or buncher. Function  $\mathcal{E}(s)$  is input as a set of points (usually 10 per cell is sufficient), which are then spline interpolated.

### Example Calculations



Figure 1: TRIUMF linac EINJ.

The TRIUMF injector electron linac, EINJ, takes bunches at 300 keV to ~ 10 MeV if properly phased and the peak gradient is 20 MV/m. Fig. 2 shows the input  $\mathcal{E}(s)$ . Three example calculations are shown, Figs. 3,4,5.

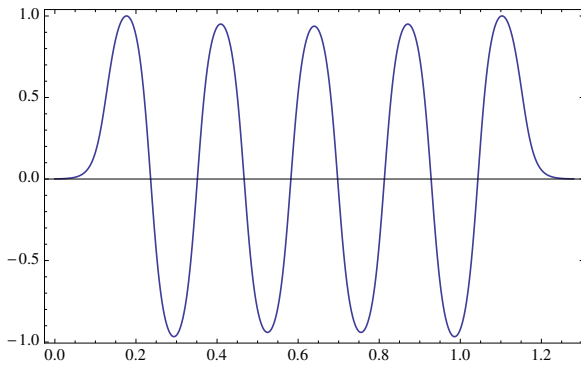


Figure 2: Electric field on axis  $\mathcal{E}(s)$  for EINJ.

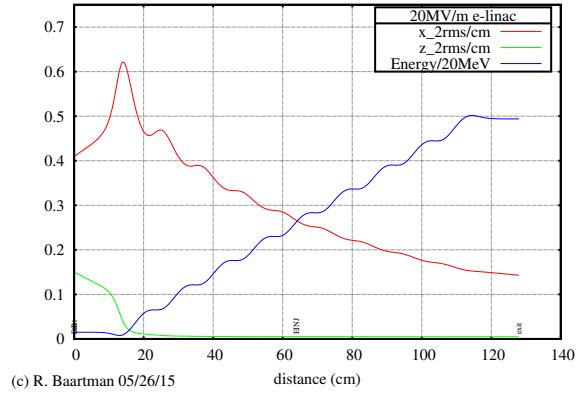


Figure 3: This is an example for phase  $\theta = 0$  at the start of the calculation. Red is the 2rms transverse size, and green is the 2rms longitudinal (bunch length). The input bunch parameters are somewhat arbitrary, roughly the condition for a minimum beam size at exit. This particular case has zero bunch charge.

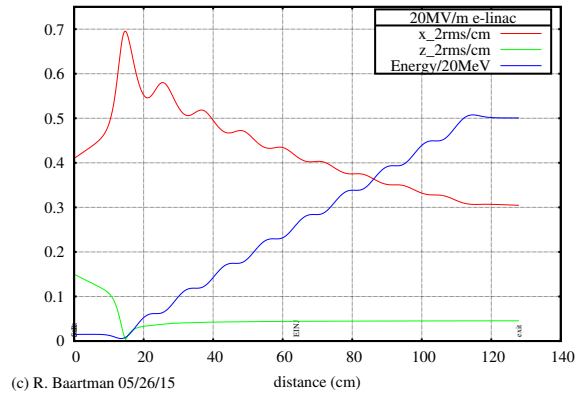


Figure 4: In this second example, TRANSPTR is instructed to fit the 65 matrix element to zero. This makes energy insensitive to input phase, thus finding the peak energy gain phase. This phase turns out to be  $\theta = -15.46^\circ$ .

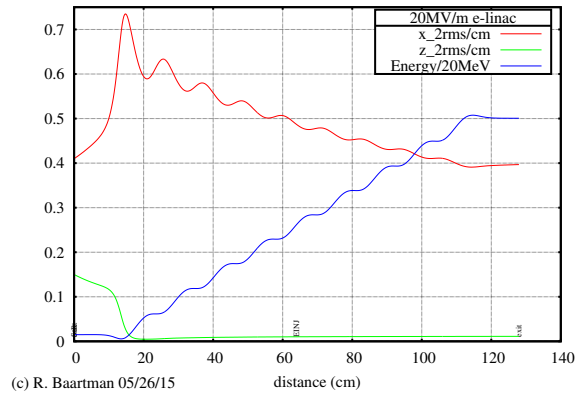


Figure 5: In the third example, bunch charge has been raised to 30 pC.



## Compute Efficiency

Each calculation above takes roughly 400 Runge-Kutta steps for 2400 calls to the SCLINAC routine. This gives 5-figure accuracy to the transfer matrix and the  $\sigma$ -matrix, and is easily enough for describing reality considering that the on-axis field is only known to 2 or 3 significant figures. The extra precision is useful, however for fitting matrix or beam matching, which is done with a downhill simplex method, or simulated annealing for cases of more than 3 fitting parameters.

On my unremarkable, circa 2006 Intel single core desktop, each run through the linac takes about 17 milliseconds with zero bunch charge and 25 milliseconds with space charge. The difference is due to the Carlson elliptic integrals needed for the space charge case.

On a typical optics matching case, one varies 2 solenoids, the buncher amplitude, and the linac phase, to minimize the bunch size and energy spread at the linac output. A calculation with such a fit requires typically a half million total calls to SC (the space charge routine for no-linac case) and SCLINAC, and so takes about 5 seconds CPU time. The result is shown below. Each calculation starts from the cathode (it would have been more efficient to store the beam parameter set at the buncher entrance and start it from there, but the savings are only a few %). The DC acceleration to 300 keV from the cathode is described in reference [3]. The Buncher itself, located at  $s = 85$  cm, is calculated as just another linac, phased to give no energy gain.

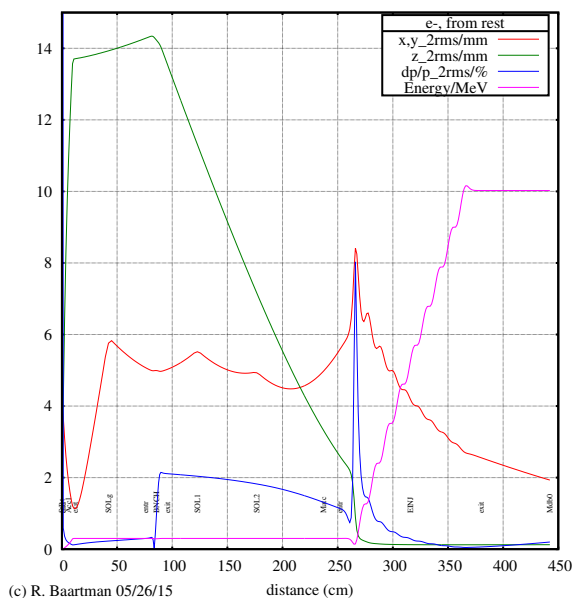


Figure 6: Typical injector optimization calculation. The bunch charge is 15 pC.

Figure 6 is a matching optimization calculation as typically performed through a Graphical User Interface (GUI) by an operator. For details on the GUI, see Jung [10]. Such a calculation takes a few seconds if initial settings are not

near optimum because then simulated annealing is used. However, for small changes to parameters such as cavity gradient, re-match calculation takes only a split second. A further use of the GUI is that any input parameter can be explored. These are set up as sliders and the turnaround time for an individual calculation is so rapid (25 ms) that the envelopes are seen to change continuously as the slider is moved.

## CONCLUSIONS

Envelope calculations (TRANSOPTR) are the most efficient method when optics is linear, with space charge. Typically these are 4 or 5 orders of magnitude faster than multiparticle space charge simulations.

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