Bunched-Beam RMS Envelope Simulation with Space Charge

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Abstract

We discuss an algorithm for treating the first-order effects of space charge in bunched beam RMS envelope simulation. The envelope simulation is assumed to be of the type employed by TRACE3D or TRANSPORT. Specifically, transfer matrices are used to propagate the Courant-Snyder parameters along the beamline. Thus, to include space charge effects we must determine a transfer matrix representing the dynamics caused by the self electric fields. Because the space charge matrices depend upon the Courant-Snyder parameters, and the Courant-Snyder parameters in turn depend upon the space charge matrices, we are also faced with some self-consistency issues. We present an adaptive technique for applying the space charge matrices that maintains a specified level of accuracy.

Outline

1. Overview
   1. Motivation
   2. Basic Approach
2. Beam Dynamics Model
3. Self Field Representation
4. Space Charge Algorithm
5. Summary

1. Overview

Motivation

To develop a *fast* simulation engine for intense charged-particle beams systems that is first-order accurate.

Such an engine is useful for

- Initial machine design
- A (fast) online model for Model Reference Control (MRC) applications during machine operation

1. Overview (cont.)

Approach – Extension of Linear Beam Optics

- In a straightforward manner, the linear beam optics model for single particle dynamics can be extended to the dynamics for the second moments of the beam.
- For intense beams, space charge effects are significant and must be included. For a beam optics model, this means a matrix $\mathbf{\Phi}_{sc}$ that accounts for space charge (linear force!).
- For ellipsoidally symmetric beams, we can produce such a $\mathbf{\Phi}_{sc}$ that is almost independent of the actual beam profile.
- Since the second moments depend upon $\mathbf{\Phi}_{sc}$ and $\mathbf{\Phi}_{sc}$ depends upon the second moments, we have self-consistency issues. We employ an adaptive propagation algorithm that maintains certain level of consistency.

2. Beam Dynamics Model

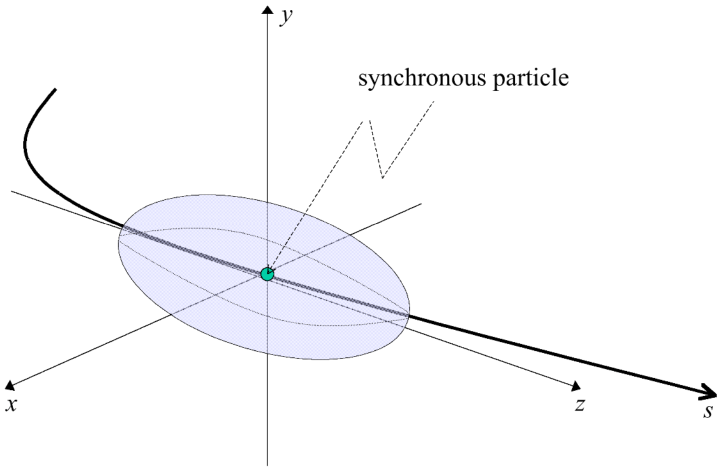
Overview

- Introduce *homogeneous* phase space coordinates $\mathbf{z}$
- Linear beam optics - transfer matrices $\mathbf{z}(s_1) = \mathbf{\Phi}(s_1,s_0)\ \mathbf{z}(s_0)$
- Moment operator $\langle\cdot\rangle$
- Moment matrix $\boldsymbol{\tau} = \langle\mathbf{z}\mathbf{z}^T\rangle$
- Propagation of moment matrix $\boldsymbol{\tau}(s)$

2. Beam Dynamics Model

Phase Space

- Let s be the *path length parameter* along the design trajectory
- Let $\mathbf{z}(s)$ denote a particle's phase space coordinate in beam frame at axial position s.
- We parameterize phase space by *homogeneous coordinates* in $P^6 \times \{1\}$



$$\mathbf{z} \equiv (x,x',y,y',z,z',1)^T \in P^6 \times \{1\}$$

Homogenous coordinates are used because
- Translation, rotation, scaling - all be performed by matrix multiplication
- Allows coupling between 1^{st} and 2^{nd} order moments in RMS simulation

2. Beam Dynamic Model (cont.)

Linear Beam Optics Review

Assume that the particle phase $\mathbf{z}(s)$ can be propagated according to

$$\mathbf{z}(s) = \mathbf{\Phi}_{\mathbf{A}}(s;s_0)\mathbf{z}_0$$

where

- $\mathbf{z}_0$ is the initial particle phase at $s = s_0$
- $\mathbf{\Phi}_{\mathbf{A}}(s;s_0)$ is the *transfer matrix* for the beamline

Notes:

- $\mathbf{\Phi}_{\mathbf{A}}'(s;s_0) = \mathbf{A}(s)\mathbf{\Phi}_{\mathbf{A}}(s;s_0)$ where $\mathbf{A}(s)$ is matrix of *applied* forces
- If $\mathbf{A}$ is constant, then $\mathbf{\Phi}_{\mathbf{A}}(s;s_0) = e^{(s-s_0)\mathbf{A}}$
- Semigroup property $\mathbf{\Phi}_{\mathbf{A}}(s_2;s_0) = \mathbf{\Phi}_{\mathbf{A}}(s_2;s_1)\,\mathbf{\Phi}_{\mathbf{A}}(s_1;s_0)$
- $\mathbf{\Phi}_{\mathbf{A}}(s;s_0)$ is symplectic, i.e., $\mathbf{\Phi}_{\mathbf{A}}(s;s_0) \in Sp(6) \subset \mathrm{P}^{7\_7}$

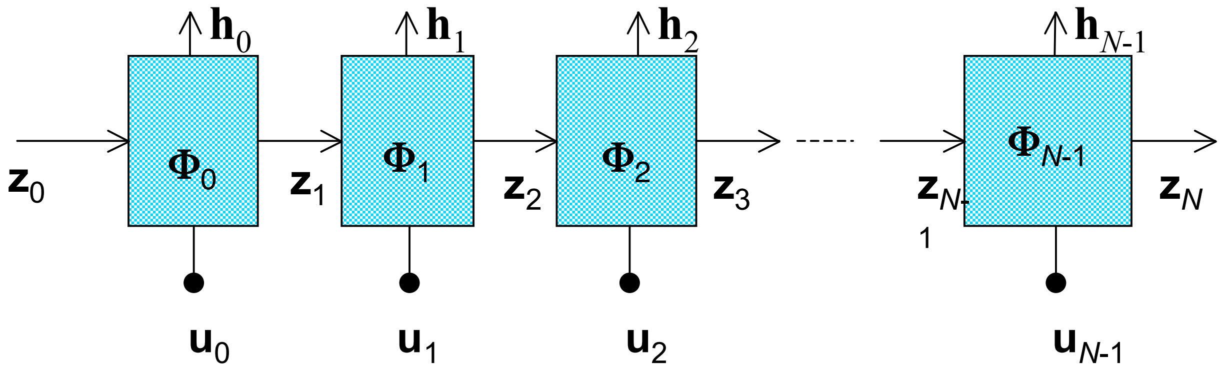
2. Beam Dynamics Model (cont.)

TRACE3D, TRANSPORT Type Beam Simulation

Divide beamline into N *stages,* one element per stage

- Entrance position of stage n defined as $s \equiv s_n$
- Define $\mathbf{z}_n = \mathbf{z}(s_n)$
- The action of stage n is represented by a *transfer matrix* $\mathbf{\Phi}_n(\mathbf{u}_n) = \mathbf{\Phi}_\mathbf{A}(s_{n+1},s_n)$ where $\mathbf{u}_n$ is the *control vector* for the element (magnet strengths, etc.)

Then $\quad \mathbf{z}_{n+1} = \mathbf{\Phi}_n(\mathbf{u}_n)\mathbf{z}_n$



2. Beam Dynamics Model (cont.)

Example – Ideal Steering Dipole

An ideal steering dipole magnet can be model with a transfer matrix $\mathbf{\Phi}_{SM}$ of the form

$$\mathbf{\Phi}_{SM}(\mathbf{u}) \equiv \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & \Delta x' \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & \Delta y' \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

where $\mathbf{u} \equiv (\Delta x', \Delta y')$ are the dipole strengths

2. Beam Dynamics Model (cont.)

The RMS Moments

- Let the beam be described by the distribution function $f : P^6 \times \{1\} \rightarrow P$

- Define the moment operator $\langle \cdot \rangle$ as $\langle g \rangle \equiv \int g(\mathbf{z}) f(\mathbf{z}) d^6\mathbf{z}$

- Now define the following:
  - $\boldsymbol{\mu} \equiv \langle \mathbf{z} \rangle \in P^6 \times \{1\}$ is the mean value vector (beam *centroid*)
  - $\boldsymbol{\tau} \equiv \langle \mathbf{z}\,\mathbf{z}^T \rangle \in P^{7\times 7}$ is the *moment matrix*

$$
\hat{\mathbf{o}} \equiv \left\langle \mathbf{z}\mathbf{z}^T \right\rangle = \begin{pmatrix}
\langle x^2 \rangle & \langle xx' \rangle & \langle xy \rangle & \langle xy' \rangle & \langle xz \rangle & \langle xz' \rangle & \langle x \rangle \\
\langle xx' \rangle & \langle x'^2 \rangle & \langle x'y \rangle & \langle x'y' \rangle & \langle x'z \rangle & \langle x'z' \rangle & \langle x' \rangle \\
\langle xy \rangle & \langle x'y \rangle & \langle y^2 \rangle & \langle yy' \rangle & \langle yz \rangle & \langle yz' \rangle & \langle y \rangle \\
\langle xy' \rangle & \langle x'y' \rangle & \langle yy' \rangle & \langle y'^2 \rangle & \langle y'z \rangle & \langle y'z' \rangle & \langle y' \rangle \\
\langle xz \rangle & \langle x'z \rangle & \langle yz \rangle & \langle y'z \rangle & \langle z^2 \rangle & \langle zz' \rangle & \langle z \rangle \\
\langle xz' \rangle & \langle x'z' \rangle & \langle yz' \rangle & \langle y'z' \rangle & \langle zz' \rangle & \langle z'z' \rangle & \langle z' \rangle \\
\langle x \rangle & \langle x' \rangle & \langle y \rangle & \langle y' \rangle & \langle z \rangle & \langle zz' \rangle & 1
\end{pmatrix}
$$

2. Beam Dynamics Model (cont.)

RMS Envelope Transport Equations

The dynamics of $\boldsymbol{\tau}$ are given by

$$\boldsymbol{\tau}(s) = \langle \mathbf{z}(s)\, \mathbf{z}^T(s) \rangle = \langle (\boldsymbol{\Phi}_\mathbf{A}(s)\mathbf{z}_0)\, (\boldsymbol{\Phi}_\mathbf{A}(s)\mathbf{z}_0)^T \rangle = \boldsymbol{\Phi}_\mathbf{A}(s)\langle \mathbf{z}_0\, \mathbf{z}_0^T \rangle \boldsymbol{\Phi}_\mathbf{A}^T(s)$$

$$= \boldsymbol{\Phi}_\mathbf{A}(s;s_0)\boldsymbol{\tau}_0\boldsymbol{\Phi}_\mathbf{A}^T(s;s_0)$$

NOTES:

- The moment matrices $\boldsymbol{\tau}(s)$ carry the 2nd order statistics, or "RMS envelopes"
- Transfer matrices $\boldsymbol{\Phi}_\mathbf{A}(s;s_0)$ propagate the moment matrices $\boldsymbol{\tau}$ (as well as $\mathbf{z}$)
- Transfer equations for $\boldsymbol{\tau}$ allow coupling between 1st and 2nd order moments

Space Charge:

- To include space charge we must represent it with a transfer matrix $\boldsymbol{\Phi}_\mathbf{B}$

Require a linear representation of the self electric fields

3. Self Field Representation

Approach

- Use weighted, least-squares expansion the electric self fields
  - The weight is the distribution function f itself

    (Expansion is then more accurate in dense regions)
  - Self force is then represented as $\mathbf{F}_{sc}[\mathbf{z};s] = \mathbf{B}(s)\mathbf{z}$
  - $\mathbf{B}$ requires determination of field moments $\langle xE_x\rangle$, $\langle yE_y\rangle$, $\langle zE_z\rangle$

- Assume an ellipsoidally symmetric beam in phase space
  - Can compute these moments in terms of $\boldsymbol{\tau}$
  - $\langle xE_x\rangle$, $\langle yE_y\rangle$, $\langle zE_z\rangle$ values only weakly coupled to distribution f

3. Self Field Representation (cont.)

Field Expansions

To accommodate a space charge transfer matrix $\mathbf{\Phi_B}$, each electric self-field component E_x, E_y, E_z must have a representation of the form

$$E_x = a_0 + a_1 x + a_2 y + a_3 z \qquad \text{(e.g., for } x \text{ plane)}$$

- Multiplying the above equation by the functions $\{1,x,y,z\}$ then taking moments

$$\begin{pmatrix} \langle 1\rangle & \langle x\rangle & \langle y\rangle & \langle z\rangle \\ \langle x\rangle & \langle x^2\rangle & \langle xy\rangle & \langle xz\rangle \\ \langle y\rangle & \langle xy\rangle & \langle y^2\rangle & \langle yz\rangle \\ \langle z\rangle & \langle xz\rangle & \langle yz\rangle & \langle z^2\rangle \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} \langle E_x\rangle \\ \langle xE_x\rangle \\ \langle yE_x\rangle \\ \langle zE_x\rangle \end{pmatrix}$$

which we can solve for the a_i in terms of the $\langle xE_x\rangle$, $\langle yE_y\rangle$, $\langle zE_z\rangle$

This is the *weighted, least-squares, linear approximation* for the self fields

3. Self Field Representation (cont.)

- The self force component $\mathbf{F}_{sc}[\mathbf{z}]$ of the dynamics is then given by

$$\mathbf{F}_{sc}(\mathbf{z}) = \mathbf{B}[\hat{\mathbf{o}}(s)]\mathbf{z}(s) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_x^x & 0 & a_y^x & 0 & a_z^x & 0 & a_0^x \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_x^y & 0 & a_y^y & 0 & a_z^y & 0 & a_0^y \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_x^z & 0 & a_y^z & 0 & a_z^z & 0 & a_0^z \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ x' \\ y \\ y' \\ z \\ z' \\ 1 \end{pmatrix}$$

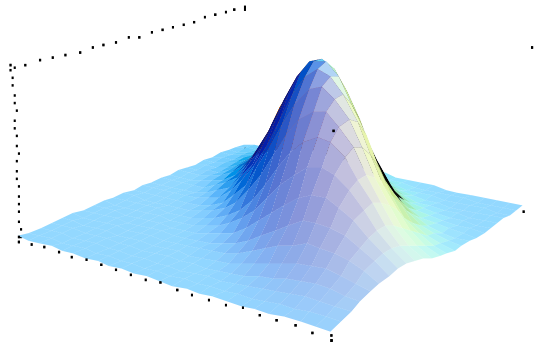
where the $a^i_j = a^i_j(\boldsymbol{\tau})$ are the expansion coefficients

- The space charge transfer matrix $\boldsymbol{\Phi}_{\mathbf{B}}(s)$ is now defined by the equation

$$\boldsymbol{\Phi}_{\mathbf{B}}'(s) = \mathbf{B}(s)\,\boldsymbol{\Phi}_{\mathbf{B}}(s)$$

3. Self Field Representation (cont.)

- Assume that the distribution f has (hyper) ellipsoidal symmetry. Then f has the form



$$f(z) = f[(\mathbf{z}-\boldsymbol{\mu})^T \boldsymbol{\sigma}^{-1}(\mathbf{z}-\boldsymbol{\mu})]$$

where

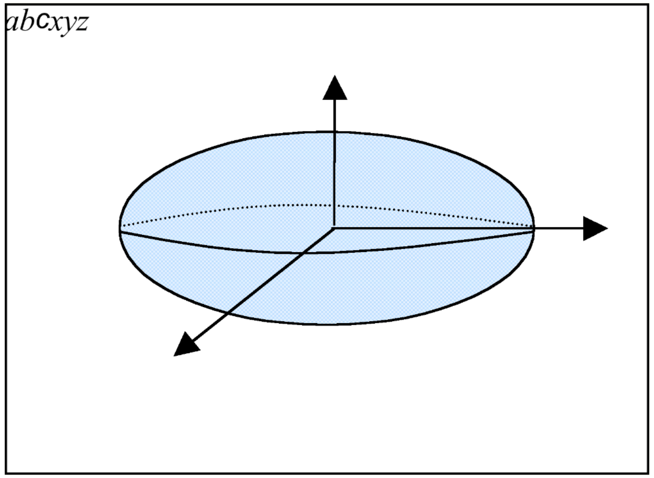
  - $\boldsymbol{\mu} \equiv \langle \mathbf{z} \rangle$ is the mean-value vector (centroid location)
  - $\boldsymbol{\sigma} \equiv \langle \boldsymbol{\tau} \rangle - \boldsymbol{\mu}\,\boldsymbol{\mu}^T$ is the *covariance matrix*

- There exists rigid motion $\mathbf{M} = \mathbf{R}^T\mathbf{T}$ that aligns the ellipsoid to coordinate axes
  - $\mathbf{T} \in P^3 \subset P^7$ is the translation by $(\langle x \rangle, \langle y \rangle, \langle z \rangle)$
  - $\mathbf{R} \in SO(3) \subset SO(7)$ is the rotation which diagonalizes the matrix

$$\begin{pmatrix} \langle x^2 \rangle - \langle x \rangle^2 & \langle xy \rangle - \langle x \rangle\langle y \rangle & \langle xz \rangle - \langle x \rangle\langle z \rangle \\ \langle xy \rangle - \langle x \rangle\langle y \rangle & \langle y^2 \rangle - \langle y \rangle^2 & \langle yz \rangle - \langle y \rangle\langle z \rangle \\ \langle xz \rangle - \langle x \rangle\langle z \rangle & \langle yz \rangle - \langle y \rangle\langle z \rangle & \langle z^2 \rangle - \langle z \rangle^2 \end{pmatrix}$$

3. Self Field Representation (cont.)

In the ellipsoid coordinates $(a,b,c) = \phi(x,y,z)$, all the cross moments are zero and the only non-zero field moments are the following



$$\langle aE_a \rangle = \Gamma(f)\frac{q\pi}{6\varepsilon_0}\frac{a^2b^2c^2}{N}a^2 R_D(c^2,b^2,a^2),$$

$$\langle bE_b \rangle = \Gamma(f)\frac{q\pi}{6\varepsilon_0}\frac{a^2b^2c^2}{N}b^2 R_D(a^2,c^2,b^2),$$

$$\langle cE_c \rangle = \Gamma(f)\frac{q\pi}{6\varepsilon_0}\frac{a^2b^2c^2}{N}c^2 R_D(a^2,b^2,c^2),$$

$$G(r) \equiv \int_r^\infty f(s)\,ds,$$

$$\Gamma(f) \equiv \int_0^\infty G^2(r^2)\,dr,$$

where $\Gamma(f)$ is almost constant (F. Sacherer) and R_D is the elliptic integral

$$R_D(x,y,z) \equiv \frac{3}{2}\int_0^\infty \frac{dt}{(t+x)^{1/2}(t+y)^{1/2}(t+z)^{3/2}}$$

In these coordinates field approximations have simply form $\quad E_a \approx \dfrac{\langle aE_a \rangle}{\langle a^2 \rangle}a$

3. Self Field Representation (cont.)

Summary

- Aligned ellipsoid to coordinate axes with rigid motion $\mathbf{M}(\boldsymbol{\tau})$
- Expanded the self fields as $E_i = [\langle x_i E_i \rangle / \langle x_i^2 \rangle]\, x_i$
- Solved for the self moments $\langle x_i E_i \rangle$ in terms of matrix $\boldsymbol{\tau}$
- For small changes in s self force matrix $\mathbf{B}$ is constant
  - Then space charge matrix is $\boldsymbol{\Phi}_{\mathbf{B}}(s) = \mathbf{M}^{-1} e^{s\mathbf{B}} \mathbf{M}$

4. Space Charge Algorithm

Approach

- Form a transfer matrix $\mathbf{\Phi}(s;s_0)$ that includes space effects to second order (2^{nd} order accurate)
- Choose error tolerance ε in the solution (~ 10^{-5} to 10^{-7})
- Use $\mathbf{\Phi}(s;s_0)$ to propagate $\boldsymbol{\tau}$ in steps h whose length is determined adaptively to maintain ε

4. Space Charge Algorithm (cont.)

Assume that **A** and **B** are constant

- Then full transfer matrix $\boldsymbol{\Phi}(s;s_0) = e^{(s-s_0)(\mathbf{A}+\mathbf{B})}$

- For practical reasons, we are usually *given* $\boldsymbol{\Phi}_{\mathbf{A}}$ and $\boldsymbol{\Phi}_{\mathbf{B}}$
  - Beam optics provides $\boldsymbol{\Phi}_{\mathbf{A}}(s)$
  - In ellipsoid coordinates $\boldsymbol{\Phi}_{\mathbf{B}}(s)$ has simply form because $\mathbf{B}^2 = \mathbf{0}$

$$\boldsymbol{\Phi}_{\mathbf{B}}(s) = e^{s\mathbf{B}} = \mathbf{I} + s\mathbf{B}$$

Define $\boldsymbol{\Phi}_{ave}(s) = \_[\ \boldsymbol{\Phi}_{\mathbf{A}}(s)\boldsymbol{\Phi}_{\mathbf{B}}(s) + \boldsymbol{\Phi}_{\mathbf{B}}(s)\boldsymbol{\Phi}_{\mathbf{A}}(s)\ ]$

- By Taylor expanding $\boldsymbol{\Phi}(s) = e^{s(\mathbf{A}+\mathbf{B})}$ we find

$$\boldsymbol{\Phi}(s) = \boldsymbol{\Phi}_{ave}(s) + O(s^3)$$

That is, $\boldsymbol{\Phi}_{ave}(s)$ is a second-order accurate approximation of $\boldsymbol{\Phi}(s)$

4. Space Charge Algorithm (cont.)

- We now have a stepping procedure which is second-order accurate in step length h.

- Now consider the effects of "step doubling"
  - Let $\boldsymbol{\tau}_1(s+2h)$ denote the result of taking one step of length $2h$
  - Let $\boldsymbol{\tau}_2(s+2h)$ denote the result of taking twos steps of length h

$$\boldsymbol{\Delta}(h) \equiv \boldsymbol{\tau}_1(s+2h) - \boldsymbol{\tau}_2(s+2h) = 6\mathbf{c}h^3$$

where the constant $\mathbf{c} = d\boldsymbol{\tau}(s')/ds$ for some $s' \in [s, s+2h]$

- Consider ratio of $|\boldsymbol{\Delta}|$ for steps of differing lengths h_0 and h_1

$$h_1 = h_0 \, [|\boldsymbol{\Delta}_1| / |\boldsymbol{\Delta}_0|]^{1/3}$$

4. Space Charge Algorithm (cont.)

We use the formula $h_1 = h_0\ [|\mathbf{\Delta}_1| / |\mathbf{\Delta}_0|]^{1/3}$ as the basis for adaptive step sizing

Given $|\mathbf{\Delta}_1| = \varepsilon$, a prescribed solution residual error we can tolerate

For each iteration k

- Let $|\mathbf{\Delta}_0| = |\ \boldsymbol{\tau}_1(s_k+2h) - \boldsymbol{\tau}_2(s_k+2h)\ |$, the residual error
- Let $h_0 = h_k$ be the step size at iteration k
- Let $h_1 = h_{k+1}$ be the step size at iteration k+1

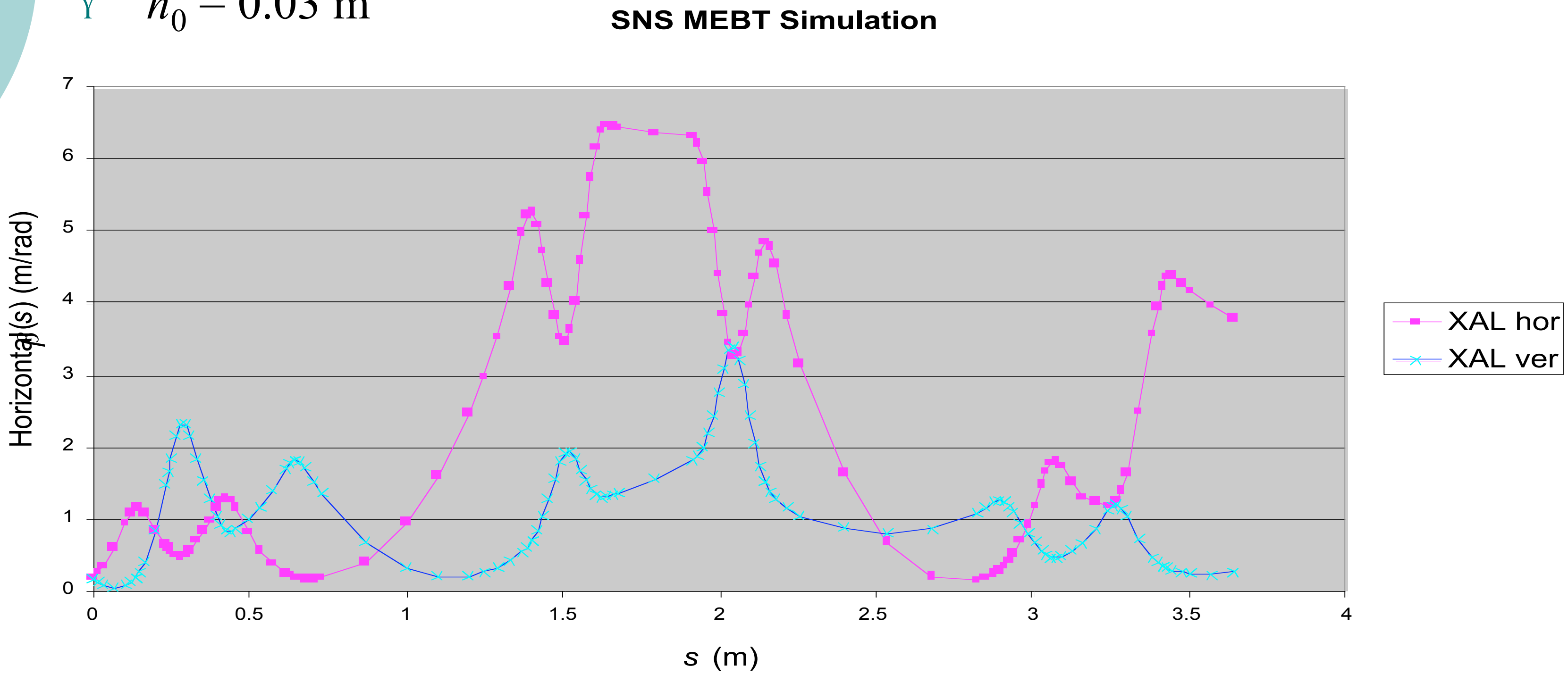
$$h_{k+1} = h_k\ [\varepsilon / |\ \boldsymbol{\tau}_1(s_k+2h) - \boldsymbol{\tau}_2(s_k+2h)\ |]^{1/3}$$

where if $h_{k+1} < h_k$, we must re-compute the k^{th} step using the new steps size h_{k+1} to maintain the same solution accuracy

4. Space Charge Algorithm (cont.)

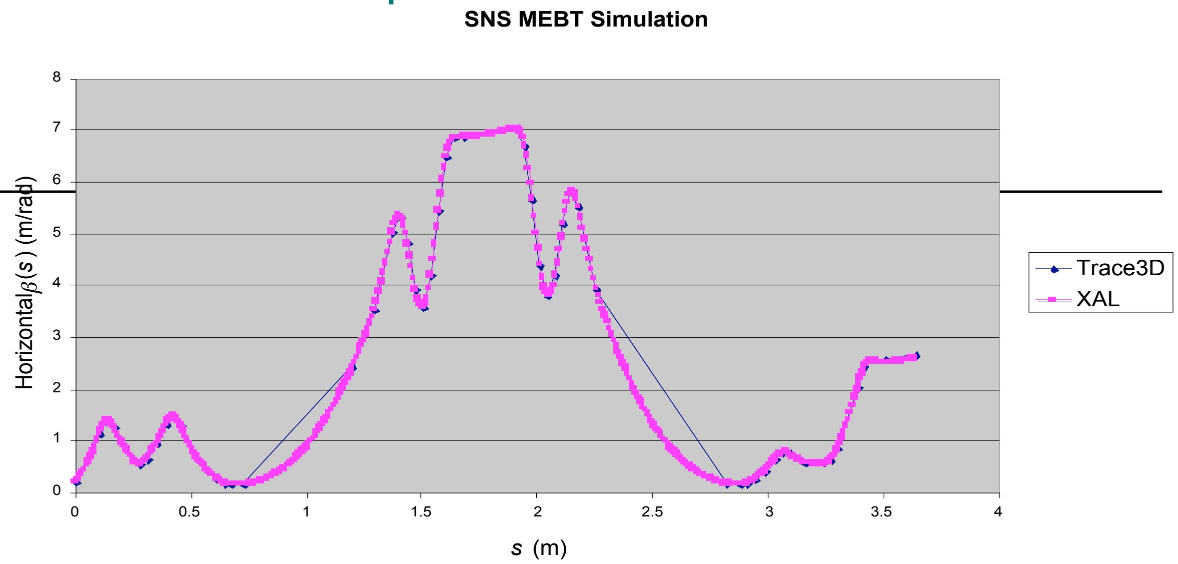
Example – Simulation of SNS MEBT

- $\varepsilon = 10^{-5}$
- $h_0 = 0.03$ m

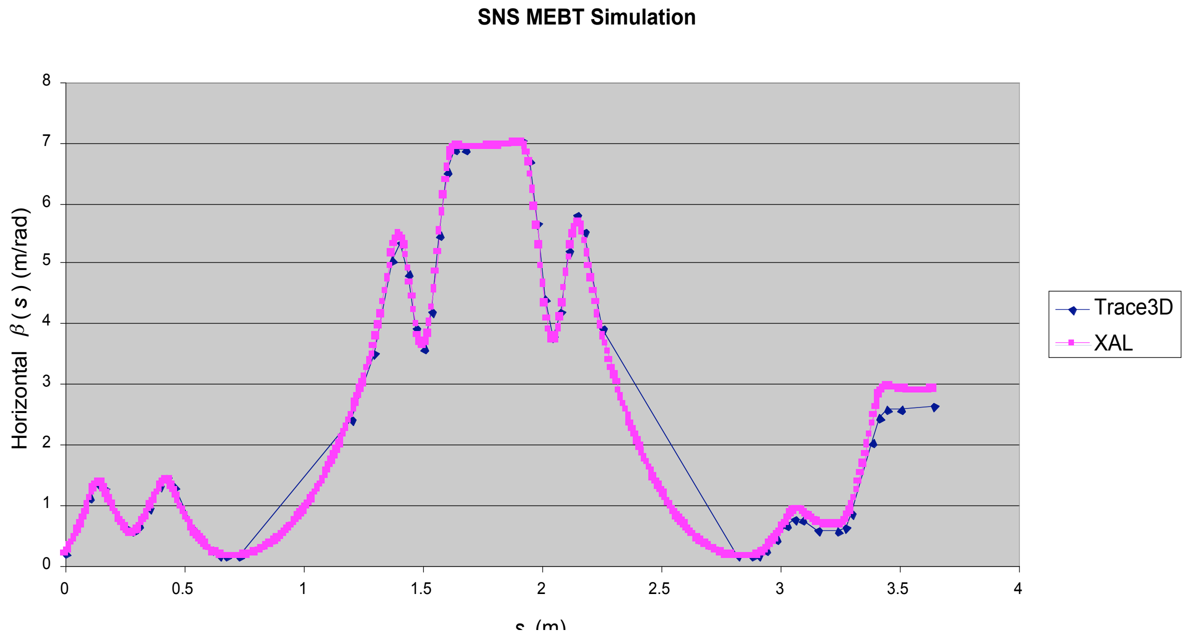


Trace3D Verification of XAL Envelope Simulation

- Implementing Trace3D R_D approximation



- Numerically evaluating R_D (*a la* Carlson)



5. Summary

- We can include the effects of space charge in a linear beam optics model for RMS envelopes
  - The dynamics are accurate to first order
  - The simulation is fast

- Key points (from experience)
  - To maintain self-consistent solution we should employ an adaptive stepping algorithm
  - A second-order accurate stepping methods seems best
  - Use accurate numerical evaluation of the elliptic integrals
  - Use accurate method for determining rigid motion $\mathbf{M}$