

## Abstract

The capability for three-dimensional RMS envelope simulation, including space charge, has been implemented in the SAD (for Strategic Accelerator Design) [5] accelerator modeling environment used at KEK. The dynamics within the model are similar to that used by Trace3D [3] and TRANSPORT [2]. Specifically, the matrix of all second-order beam moments is propagated using a linear beam optics model for the beamline. However, the current simulation employs an adaptive space-charge algorithm. It maintains the integration step size as large as possible while enforcing a given error tolerance. We concentrate on the adaptive nature of the RMS simulation, since this is the novel feature.

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## Background - Linear Beam Optics Model

- Phase coordinates  $\mathbf{z}(s)$  at axial position  $s$  is a point in phase space.

$$\mathbf{z} = (x, x', y, y', z, \delta) \in \mathbb{R}^6$$

- Correlation matrix is defined  $\boldsymbol{\tau} = \langle \mathbf{z}\mathbf{z}^T \rangle$

$$\boldsymbol{\tau} = \begin{pmatrix} \langle x^2 \rangle & \langle xx' \rangle & \langle xy \rangle & \langle xy' \rangle & \langle xz \rangle & \langle x\delta \rangle \\ \langle xx' \rangle & \langle x'^2 \rangle & \langle x'y \rangle & \langle x'y' \rangle & \langle x'z \rangle & \langle x'\delta \rangle \\ \langle xy \rangle & \langle x'y \rangle & \langle y^2 \rangle & \langle yy' \rangle & \langle yz \rangle & \langle y\delta \rangle \\ \langle xy' \rangle & \langle x'y' \rangle & \langle yy' \rangle & \langle y'^2 \rangle & \langle y'z \rangle & \langle y'\delta \rangle \\ \langle xz \rangle & \langle x'z \rangle & \langle yz \rangle & \langle y'z \rangle & \langle z^2 \rangle & \langle z\delta \rangle \\ \langle x\delta \rangle & \langle x'\delta \rangle & \langle y\delta \rangle & \langle y'\delta \rangle & \langle z\delta \rangle & \langle \delta^2 \rangle \end{pmatrix}$$

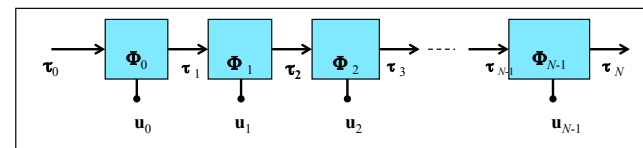
- Entrance of each stage is at  $s = s_n$  so that

$$\boldsymbol{\tau}_n = \boldsymbol{\tau}(s_n)$$

- Beamline element  $n$  is represented by matrix  $\Phi_{n,sc}$  including space charge

- Propagation equations for  $\{\boldsymbol{\tau}_n\}$  are

$$\boldsymbol{\tau}_{n+1} = \Phi_{n,sc} \boldsymbol{\tau}_n \Phi_{n,sc}^T$$



- Transfer matrix  $\Phi_{n,sc}(h)$  for element  $n$  through length  $h$  can be written

$$\Phi_{n,sc}(h) = \Phi_{sc}(h/2) \Phi_n(h) \Phi_{sc}(h/2) + O(h^3)$$

- $\Phi_n(h)$  is the transfer matrix for element  $n$  w/out space charge
- $\Phi_{sc}(h)$  is the transfer matrix for space alone

- Letting  $\Phi(h) = \Phi_{sc}(h/2) \Phi_n(h) \Phi_{sc}(h/2)$ , define

$$S_h(\boldsymbol{\tau}) = \Phi(h) \boldsymbol{\tau} \Phi(h)^T$$

- Then if  $\boldsymbol{\tau}(s+h)$  is exact solution

$$S_h(\boldsymbol{\tau}) = \boldsymbol{\tau}(s+h) + h^3 \mathbf{C}$$

$$\mathbf{C} = \boldsymbol{\tau}'''(s_0) \text{ some } s_0 \in [s, s+h]$$

## Adaptive Stepping

- Error residual of  $\boldsymbol{\tau}(s+h)$  for step size  $h$  is given by

$$\epsilon(h) = h^3 \|\mathbf{C}\|$$

- Objective is to find largest  $h_i$  such that  $\epsilon(h_i) \leq \bar{\epsilon}$  where  $\bar{\epsilon}$  is a given error tolerance.

- Use *step doubling*

$$\begin{aligned} \boldsymbol{\tau}^1(s+2h) &= S_{2h}(\boldsymbol{\tau}) = \boldsymbol{\tau}(s+2h) + (2h)^3 \mathbf{C} \\ \boldsymbol{\tau}^2(s+2h) &= S_h(S_h(\boldsymbol{\tau})) = \boldsymbol{\tau}(s+2h) + 2(h^3 \mathbf{C}) \end{aligned}$$

- Let  $\Delta(h) = \boldsymbol{\tau}^1(s+2h) - \boldsymbol{\tau}^2(s+2h)$  so that for any matrix norm  $\|\cdot\|$

$$\epsilon(h) = (1/6) \|\Delta(h)\|$$

- Assume we are given a step size  $h_i$  and wish the next step  $h_{i+1}$  to maintain the error  $\bar{\epsilon}$ , that is,

$$\epsilon(h_{i+1}) = \bar{\epsilon}$$

from  $\epsilon(h_{i+1})/\epsilon(h_i) = [h_i/h_{i+1}]^3$ , we have

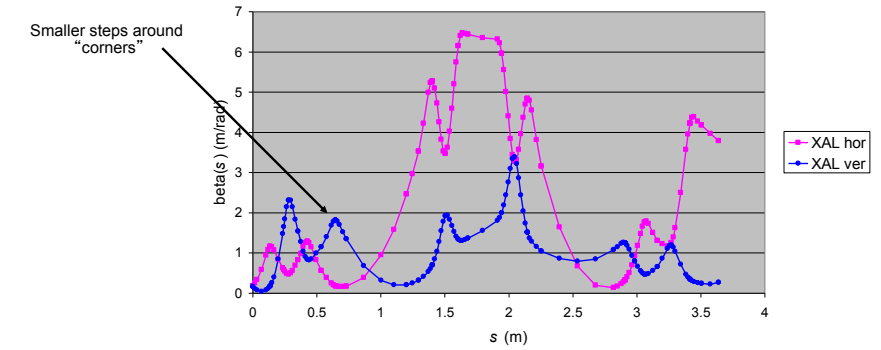
$$h_{i+1} = h_i \left[ \frac{6\bar{\epsilon}}{\|\boldsymbol{\tau}^1(s+2h) - \boldsymbol{\tau}^2(s+2h)\|} \right]^{1/3}$$

## Summary

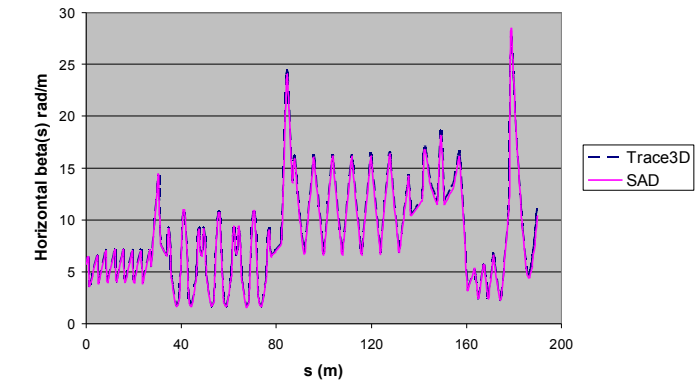
The adaptive integration algorithm is based upon discrete transfer equations for the correlation matrix and an adaptive step sizing formula which maintains a predetermined error tolerance. At each iteration, the algorithm keeps the step size as large as possible while maintaining this error tolerance, however it does require some computational overhead. We must compute three applications of  $S_h$  for a single iteration. Yet each iterate actually propagates  $\boldsymbol{\tau}$  a distance  $2h$  and, consequently, must be compared to two applications of  $S_h$ . Thus, the adaptive procedure requires a computational overhead of at least 150% that of a non-adaptive algorithm.

Although a fixed-step approach may then seem faster, what we lose is the guarantee of a given solution accuracy. Moreover, we also lose the guarantee of self-consistency in the space-charge calculations. In adaptive stepping, in most cases, we expect a significant computational advantage by taking potentially much larger steps. Considering the overall advantages contrasted with the small amount of additional code development, the adaptive stepping process appears as a clear benefit in RMS envelope simulation.

## Simulation Results

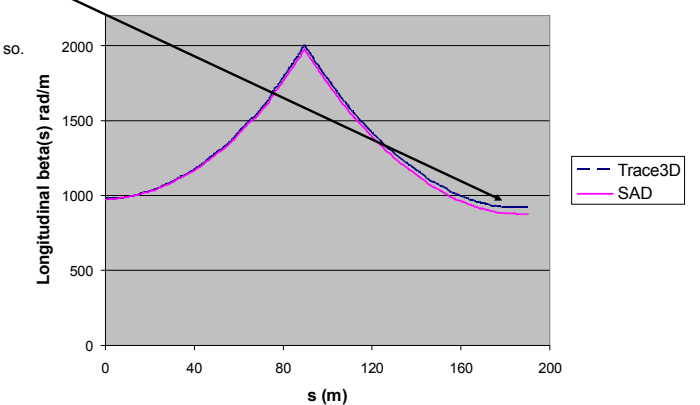


XAL simulation of SNS MEBT (Demonstrates adaptive stepping)



simulation results for SAD versus Trace3D horizontal beta

Small discrepancy in longitudinal case. More space charge effect for Trace3D.  
SAD is symplectic  
Trace3 equations of motion  
- but still uncertain why this is so.



simulation results for SAD versus Trace3D longitudinal beta

SAD vs Trace3D simulations are of J-PARC transport line between 181 MeV linear accelerator and 3 GeV synchrotron. Beam is H<sup>+</sup> at 30 mA.

In all simulations we have chosen  $\bar{\epsilon} = 10^{-5}$ ,  $\delta_n = 0.05$ , initial step size  $h_0 = 3$  cm, and used the  $l_1$  matrix norm. Trace3D uses a constant step size of  $h = 1$  cm.