



J-PARC Trace3D Upgrades

Christopher K. Allen
Los Alamos National Laboratory



Trace3D “Project”

- Split the big FORTRAN file
 - Each SUBROUTINE has file
 - Project built using a Makefile (K. Furukawa)
 - Version controlled (K. Furukawa)
 - Repository `jkksv01.j-parc.jp:/jk/master/t3d_cka`
- Can reassemble back into the big FORTRAN file if desired



General Additions

- **Debugging and Data I/O**

- Added output subroutines for debugging and recording Twiss parameters along beamline

- InputDump – stores input “deck” to disk (file “InputData.txt”) to check that data is being properly input
 - TwissDump – stores Twiss parameters along beamline to disk file “TwissDump.txt”. Twiss parameters are stored during simulation since trajectory data is not kept in Trace3D memory.

- **Convenience Matrix Functions**

- Multiply, scalar multiply, commutator
 - Matrix exponent
 - Matrix logarithm (E. Forest)



General Additions (cont.)

○ **Steering Magnets**

Added steering magnets to the element library.

- Note that only the centroid tracking is affected by this element, it has no effect on the second-order moment dynamics.
- The type identifier is 19 (NT=19).
- The parameters is $\Delta x'$, $\Delta y'$



General Additions (cont.)

- Arbitrarily Oriented Beam Ellipsoids

To compute the electric self forces of the beam Trace3D performs a coordinate transform to “eigen-coordinates” of ellipsoid

- In the current version this transform fails when the beam is skewed arbitrarily off the design axis
 - That is, skewed in a direction other than one of the two transverse directions.
- This condition was fixed.



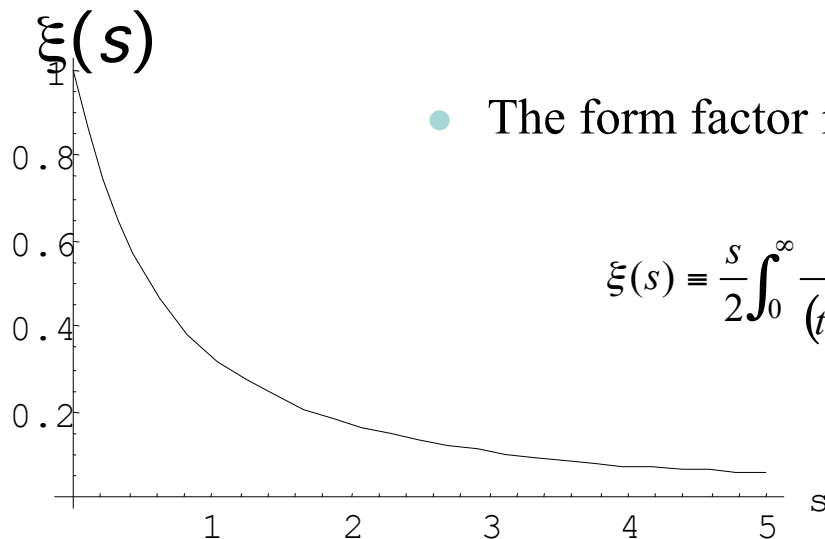
Choice of Elliptic Integral R_D or Form Factor ξ

- For the space charge calculations you may switch between the use of the form factor and direct (numerical) evaluation of the elliptic integral.
 - This feature is available using the input variable **iFlgUseRd** in the \$DATA section of the Trace3D input file
 - $iFlgUseRd = 0$: use form factor ξ (default)
 - $iFlgUseRd = 1$: use elliptic integral RD

Form Factor vs. Elliptic Integral

- Original Trace3D uses a “form factor” ξ in the self field calculations.
 - λ The function $\xi(s)$ is part of an analytic approximation to an elliptic integral R_D , which is defined

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



- The form factor is defined

$$\xi(s) \equiv \frac{s}{2} \int_0^\infty \frac{dt}{(t+1)(t+s^2)^{1/2}} = \frac{1}{1-s^2} \begin{cases} 1 - \frac{s}{\sqrt{1-s^2}} \cos^{-1} s & \text{for } s < 1 \\ 1 - \frac{s}{\sqrt{s^2-1}} \cosh^{-1} s & \text{for } s > 1 \end{cases}$$



Form Factor vs. Elliptic Integral (cont.)

The approximations for R_D in terms of the form factor are then given as

$$R_D(Z^2, Y^2, X^2) = \frac{3}{XZ} \frac{1}{X+Y} \left[1 - \xi \left(\frac{Z}{\sqrt{XY}} \right) \right] + O(\varepsilon),$$

$$R_D(Z^2, X^2, Y^2) \approx \frac{3}{YZ} \frac{1}{X+Y} \left[1 - \xi \left(\frac{Z}{\sqrt{XY}} \right) \right] + O(\varepsilon),$$

$$R_D(X^2, Y^2, Z^2) \approx \frac{3}{XYZ} \xi \left(\frac{Z}{\sqrt{XY}} \right) + O(\varepsilon^2),$$

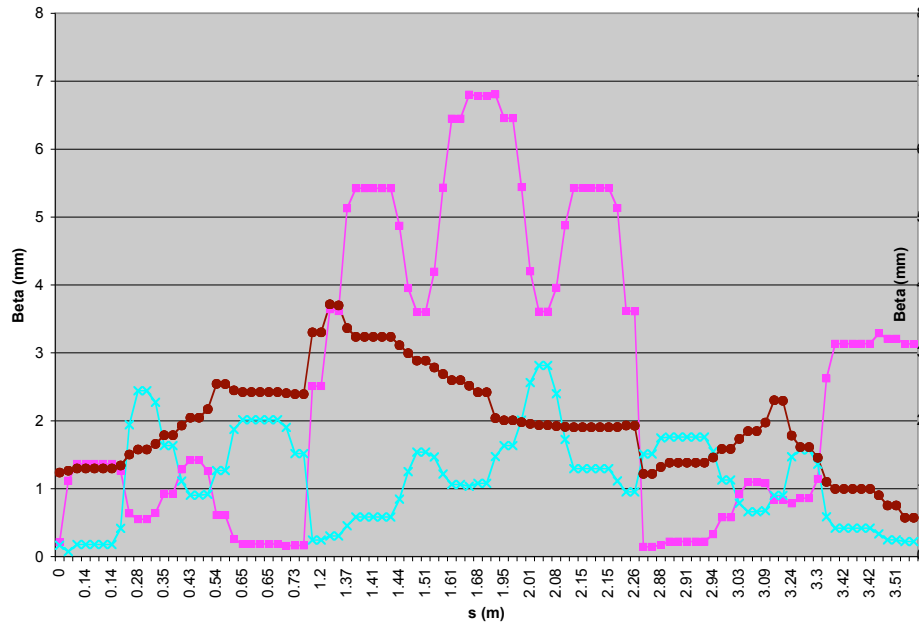
Where X , Y , and Z are the semi-axes of the beam ellipsoid and

$$\varepsilon = (X-Y)/2$$

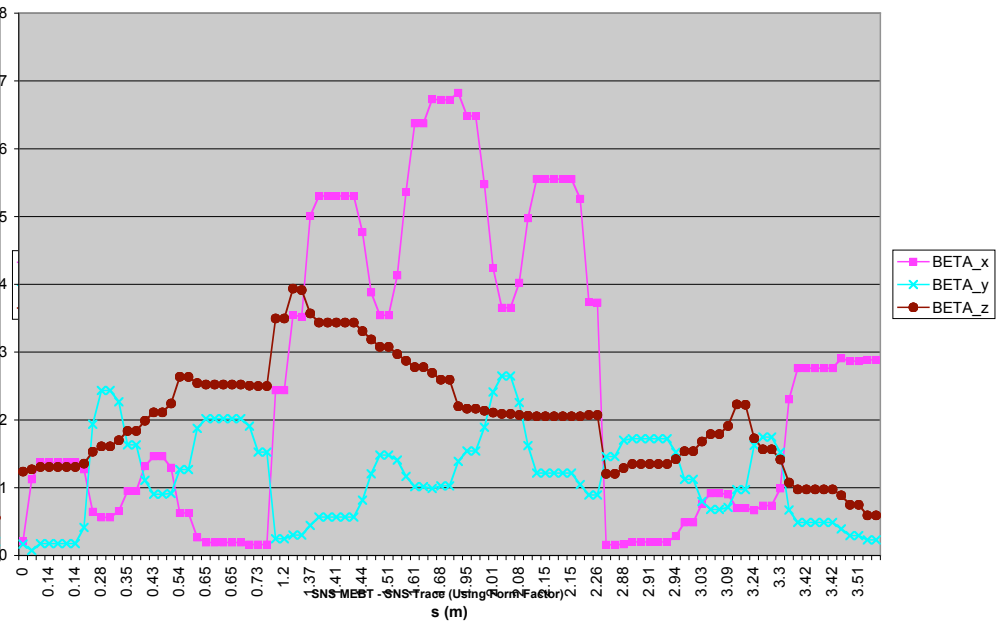
is related to the eccentricity of the transverse ellipse

Comparison of Trace3D elliptic integral and form factor simulations

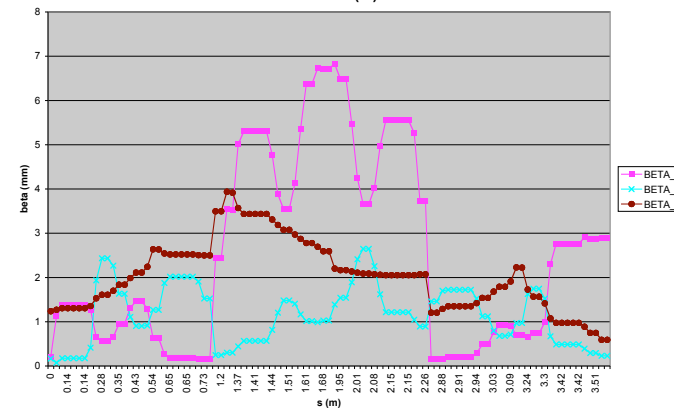
SNS MEBT - KEK Trace3D (Using Rd)



SNS MEBT - KEK Trace3D (Using Form Factor)



SNS Version of Trace3D (form fac)





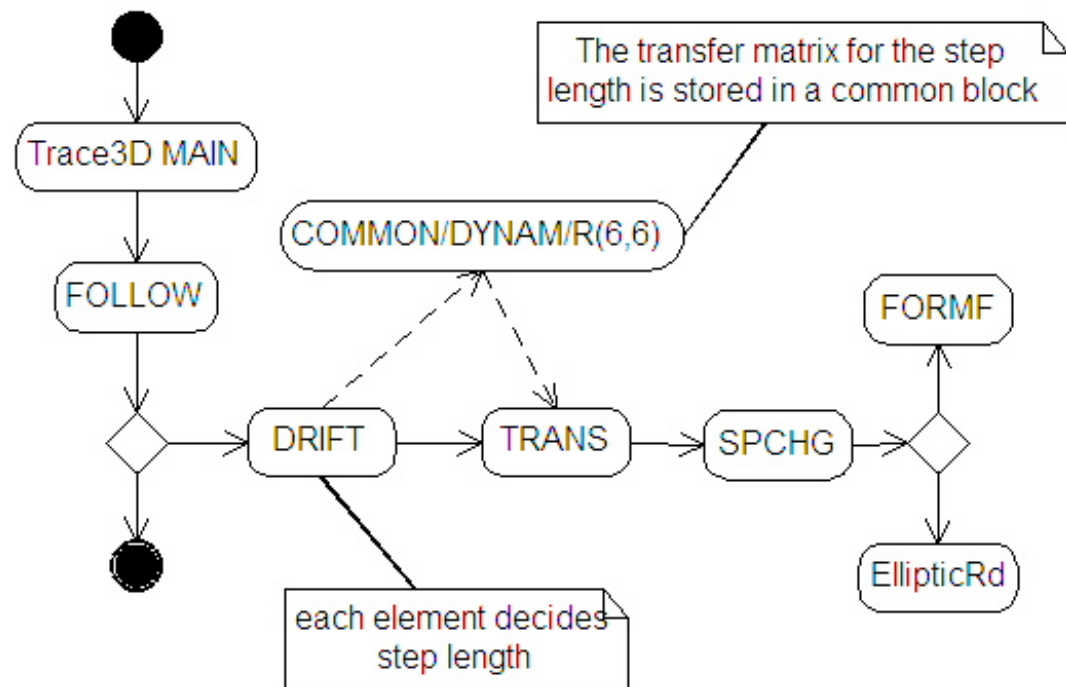
Adaptive Integration Stepping

Approach

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

Adaptive Stepping and Trace3D

- Due to Trace3D “architecture” implementing adaptive stepping **may** require a major rewrite
 - Brittle – dangerous
- Implementation possible if it can be done in SUBROUTINE TRANS
 - Compute $\log(\Phi) = \Delta s \mathbf{A}$
 - λ Compute $\exp(h\mathbf{A})$
 - λ May be too CPU intensive



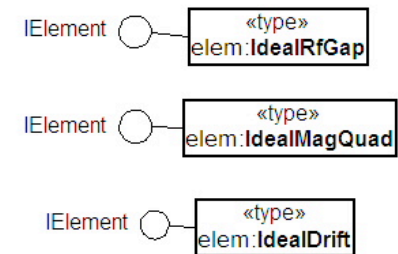
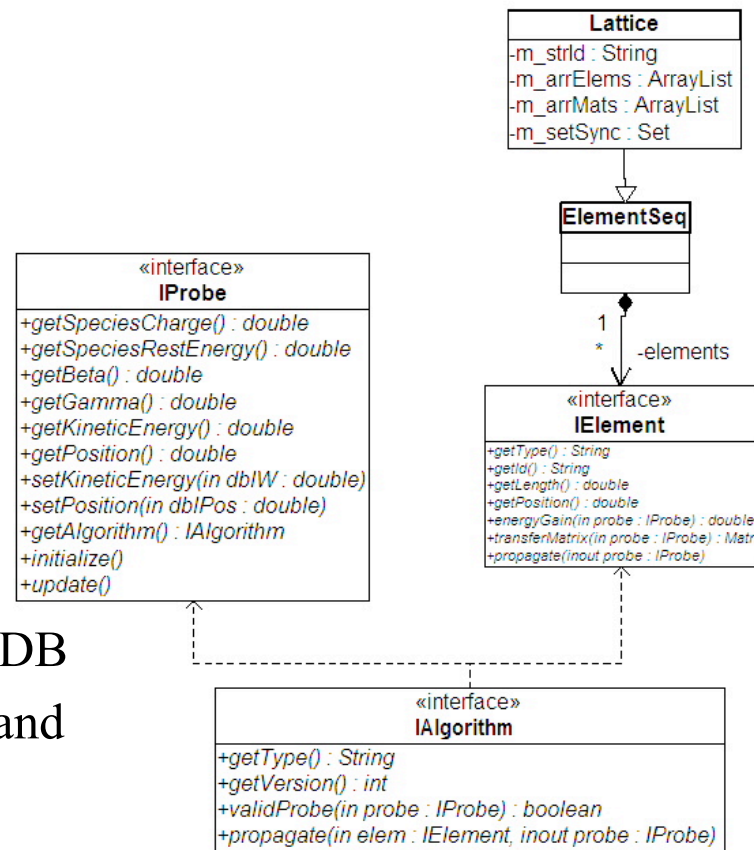
XAL Architecture

Y XAL Architecture is modern

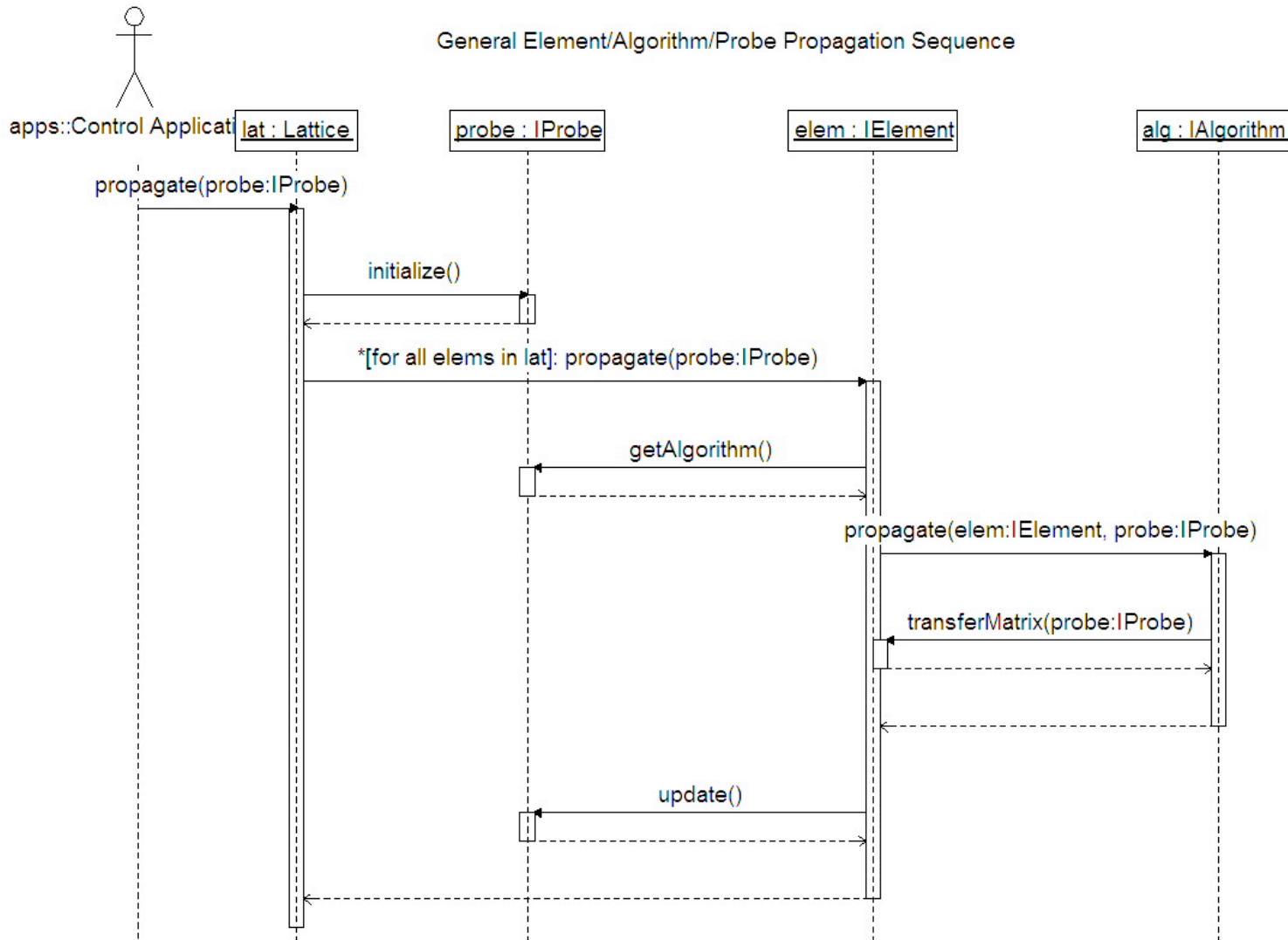
- λ Not coupled
- λ Easier to upgrade
- λ Easier to maintain

Y XAL Appl. Devel

- λ Hard part is setting up DB
- λ API is object oriented and documented (easy)
- λ New features are (relatively) easily installed



XAL Architecture – Sequence Diagram





Summary

- Adding adaptive stepping to Trace3D may not be worth the effort
 - Ability to implement it in TRANS
 - Compute matrix logarithms and exponentials
- Add space charge to SAD?
 - Unknown effort – inexperienced with SAD
- Add J-PARC features to XAL?
 - Is XAL a player?
 - Very familiar with XAL



4. Space Charge Algorithm (cont.)

Assume that \mathbf{A} and \mathbf{B} are constant

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

γ For practical reasons, we are usually *given* $\Phi_{\mathbf{A}}$ and $\Phi_{\mathbf{B}}$

- λ Beam optics provides $\Phi_{\mathbf{A}}(s)$
- λ In ellipsoid coordinates $\Phi_{\mathbf{B}}(s)$ has simple form because $\mathbf{B}^2 = \mathbf{0}$

$$\Phi_{\mathbf{B}}(s) = e^{s\mathbf{B}} = \mathbf{I} + s\mathbf{B}$$

Define $\Phi_{ave}(s) = \frac{1}{2} [\Phi_{\mathbf{A}}(s)\Phi_{\mathbf{B}}(s) + \Phi_{\mathbf{B}}(s)\Phi_{\mathbf{A}}(s)]$

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

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

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



4. Space Charge Algorithm (cont.)

- We now have a stepping procedure which is second-order accurate in step length h .
- Υ Now consider the effects of “step doubling”
 - λ Let $\tau_1(s+2h)$ denote the result of taking one step of length $2h$
 - λ Let $\tau_2(s+2h)$ denote the result of taking two steps of length h

$$\Delta(h) \equiv \tau_1(s+2h) - \tau_2(s+2h) = 6ch^3$$

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

- Υ Consider ratio of $|\Delta|$ for steps of differing lengths h_0 and h_1

$$h_1 = h_0 [|\Delta_1|/|\Delta_0|]^{1/3}$$



4. Space Charge Algorithm (cont.)

We use the formula $h_1 = h_0 [|\Delta_1|/|\Delta_0|]^{1/3}$ as the basis for adaptive step sizing

Given $|\Delta_1| = \varepsilon$, a prescribed solution residual error we can tolerate

For each iteration k

- λ Let $|\Delta_0| = |\tau_1(s_k+2h) - \tau_2(s_k+2h)|$, the residual error
- λ Let $h_0 = h_k$ be the step size at iteration k
- λ Let $h_1 = h_{k+1}$ be the step size at iteration $k+1$

$$h_{k+1} = h_k [\varepsilon / |\tau_1(s_k+2h) - \tau_2(s_k+2h)|]^{1/3}$$

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