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# BENCHMARKING BEAM ENVELOPE MODELS FOR THE EUROPEAN SPALLATION SOURCE

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## Abstract

TraceWin [1] is used at the European Spallation Source (ESS) as the design tool, while fast and accurate on-line models will be needed during the operations. Three models are compared: the ESS Linac Simulator (ELS) [2], TraceWin and the OpenXAL [3].

In all of the benchmarked models, dynamics of each beam-line element is, to the first order, represented by a transfer matrix. Differences in the matrices occur, since different reference frames are used and as well different assumptions about the energy of the particles are made.

General transformations of the reference frames will be presented. Using those, the comparison of transfer maps among TraceWin and OpenXAL are given. When the differences between TraceWin and OpenXAL were unclear, the benchmark versus other code, like MAD-X [4] and Dynac [5] was done. The best implementations were combined into a new on-line model implementation Java ELS (or JELS) and at last the comparison of the latter with TraceWin is given.

## INTRODUCTION

A single particle in the model is described by its state vector, i.e. position and momenta. However to decrease numerical error, the position is calculated relative to the reference particle.

The relative position of the particle may be described in laboratory frame or reference particle frame. In models we compared, the momenta are tracked as derivatives with respect to path of the reference particle. There are also different choices, how longitudinal momentum is described.

As the particle traverses different accelerator structures its state is changed. This is described by transfer matrices  $R$  and in specific cases, an additional translation.

Different solutions are used to simulate a bunch composed of many particles. Typically in fast models only statistical moments of the bunch are calculated, which are represented by covariance matrices  $\sigma$  and bunch's relative center position.

The choice of the state vector of a single particle influences how transfer and covariance matrices are written.

## TRANSFORMATIONS OF MATRICES

OpenXAL describes single particle in the reference particle frame with longitudinal coordinates expressed as  $(z, z')$ , while TraceWin describes it in the laboratory frame and

uses for longitudinal coordinates  $(z, \Delta p/p)$ , where  $\Delta p$  is difference in the longitudinal momentum  $p$  of the reference particle. Relativistic mechanics gives  $z' = \frac{dz}{ds} = \frac{1}{\gamma^2} \frac{\Delta p}{p}$ .

Transformations to account for this on transfer matrices are:

$$R_{\text{xal}} = R_{\gamma_o}^{(6)} R_{\gamma_o}^{(5)} R_{\text{tw}} R_{\gamma_i}^{(5)} R_{\gamma_i}^{(6)}$$

where  $R_{\text{xal}}$  and  $R_{\text{tw}}$  denote OpenXAL and TraceWin's transfer matrices respectively,  $\gamma_i$  and  $\gamma_o$  are input and output relativistic  $\gamma$ , and  $R_{\gamma}^{(5)}$ ,  $R_{\gamma}^{(6)}$  are diagonal matrices with following values:

$$R_{\gamma}^{(5)} = \text{diag}(1, 1, 1, 1, \gamma, 1) \quad R_{\gamma}^{(6)} = \text{diag}(1, 1, 1, 1, 1, \gamma).$$

To give a better idea what is going on, the same transformations can be written as a tensor product:

$$R_{\text{xal}} = \begin{pmatrix} 1 & & & & \gamma_i^{-1} & \gamma_i \\ & 1 & & & \gamma_i^{-1} & \gamma_i \\ & & 1 & & \gamma_i^{-1} & \gamma_i \\ & & & 1 & \gamma_i^{-1} & \gamma_i \\ \gamma_o & \gamma_o & \gamma_o & \gamma_o & \gamma_o \gamma_i^{-1} & \gamma_o \gamma_i \\ \gamma_o^{-1} & \gamma_o^{-1} & \gamma_o^{-1} & \gamma_o^{-1} & \gamma_o^{-1} \gamma_i^{-1} & \gamma_o^{-1} \gamma_i \end{pmatrix} \otimes R_{\text{tw}}$$

Similarly the transformation on beam covariance matrix is:

$$\sigma_{\text{xal}} = R_{\gamma_o}^{(6)} R_{\gamma_o}^{(5)} \sigma_{\text{tw}} R_{\gamma_i}^{(5)} R_{\gamma_i}^{(6)}$$

where  $\sigma_{\text{xal}}$  and  $\sigma_{\text{tw}}$  represent OpenXAL and TraceWin's covariance matrices, respectively.

## COMPARISON BY ELEMENT

We have first compared transfer matrices of basic accelerator elements (i.e. drift, quad, thick dipole, RF gap) based on the documentation of TraceWin [1] and OpenXAL [3], and the implementation of OpenXAL. We later backed this up by doing numerical comparison.

### Ideal Drift and Quadrupole

Comparison of drift's and quadrupole's transfer matrices showed they are the same, except for the aforementioned transformation.

For example a longitudinal part of the transfer matrix for a drift looks like:

$$R_{\text{xal}}^{zz} = \begin{bmatrix} 1 & \Delta s \\ & 1 \end{bmatrix} \quad R_{\text{tw}}^{zz} = \begin{bmatrix} 1 & \frac{\Delta s}{\gamma^2} \\ & 1 \end{bmatrix}$$

### Bending Dipole

Bending dipoles are represented by three transfer matrices: entering and exiting edge and the main section in between.

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**Edge** Edges (called faces in OpenXAL) of bending dipoles are almost equal in OpenXAL and TraceWin.

Difference is that OpenXAL does not account for  $K_2$  fringe factor, i.e.:

$$\Psi_{\text{tw}} = K_1 \frac{g}{|\rho|} \left( \frac{1 + \sin^2 B}{\cos B} \right) \left( 1 - K_1 K_2 \frac{g}{|\rho|} \tan B \right)$$

$$\Psi_{\text{xal}} = K_1 \frac{g}{|\rho|} \left( \frac{1 + \sin^2 B}{\cos B} \right)$$

which we added to JELS implementation.

**Main Section** While transversal parts of transfer matrices ( $R^{xx}$  and  $R^{yy}$ ) are the same, there were subtle difference in longitudinal part of transfer matrices  $R^{zz}$ :

- TraceWin:

$$R_{\text{tw}}^{zz} = \begin{bmatrix} 1 & -\frac{h^2(k_x \Delta s \beta^2 - \sin(k_x \Delta s))}{k_x^3} + \frac{\Delta s}{\gamma^2} \left( 1 - \frac{h^2}{k_x^2} \right) \\ & 1 \end{bmatrix}$$

- OpenXAL documentation:

$$R_{\text{xal doc}}^{zz} = \begin{bmatrix} 1 & -\frac{h^2(k_x \Delta s \beta^2 - \sin(k_x \Delta s))}{k_x^3} + \Delta s \left( 1 - \frac{h^2}{k_x^2} \right) \\ & 1 \end{bmatrix}$$

- OpenXAL implementation:

$$R_{\text{xal}}^{zz} = \begin{bmatrix} 1 & -\frac{h^2 \gamma^2 (k_x \Delta s - \sin(k_x \Delta s))}{k_x^3} + \Delta s \\ & 1 \end{bmatrix}$$

- Transformation of TraceWin to OpenXAL:

$$R^{zz} = \begin{bmatrix} 1 & -\frac{h^2 \gamma^2 (k_x \Delta s \beta^2 - \sin(k_x \Delta s))}{k_x^3} + \Delta s \left( 1 - \frac{h^2}{k_x^2} \right) \\ & 1 \end{bmatrix}$$

and differences in mixed components  $R^{zx}$ ,  $R^{xz}$ :

- TraceWin:

$$R_{\text{tw}}^{zx} = \begin{bmatrix} \frac{-h \sin(k_x \Delta s)}{k_x} & \frac{-h(1 - \cos k_x \Delta s)}{k_x^2} \\ 0 & 0 \end{bmatrix}$$

$$R_{\text{tw}}^{xz} = \begin{bmatrix} 0 & \frac{h(1 - \cos k_x \Delta s)}{k_x^2} \\ 0 & \frac{h \sin(k_x \Delta s)}{k_x} \end{bmatrix}$$

- OpenXAL documentation and implementation:

$$R_{\text{xal}}^{zx} = \begin{bmatrix} \frac{-h \sin(k_x \Delta s)}{k_x} & \frac{-h(1 - \cos k_x \Delta s)}{k_x^2} \\ 0 & 0 \end{bmatrix}$$

$$R_{\text{xal}}^{xz} = \begin{bmatrix} 0 & \frac{\gamma^2 h(1 - \cos k_x \Delta s)}{k_x^2} \\ 0 & \frac{\gamma^2 h \sin(k_x \Delta s)}{k_x} \end{bmatrix}$$

- Transformation of TraceWin to OpenXAL:

$$R^{zx} = \begin{bmatrix} \gamma \frac{-h \sin(k_x \Delta s)}{k_x} & \gamma \frac{-h(1 - \cos k_x \Delta s)}{k_x^2} \\ 0 & 0 \end{bmatrix}$$

$$R^{xz} = \begin{bmatrix} 0 & \gamma \frac{h(1 - \cos k_x \Delta s)}{k_x^2} \\ 0 & \gamma \frac{h \sin(k_x \Delta s)}{k_x} \end{bmatrix}$$

Because of all the differences, we compared the transfer matrices with MAD-X [4] implementation. We have chosen it because it has been used extensively on bending dipoles. The results showed MAD-X implementation matches TraceWin's, so we used it in JELS as well.

### RF Gap

Again transversal parts match, while longitudinal  $R^{zz}$  have differences:

- TraceWin:

$$R_{\text{tw}}^{zz} = \begin{bmatrix} 1 & 0 \\ \frac{k_z}{\beta_o \gamma_o} & \frac{\beta_i \gamma_i}{\beta_o \gamma_o} \end{bmatrix}$$

- OpenXAL documentation (here  $\bar{\gamma}$  is an average  $\gamma$ ):

$$R_{\text{xal doc}}^{zz} = \begin{bmatrix} 1 & 0 \\ \frac{k_z \bar{\gamma}^2}{\beta_o \gamma_o^3} & \frac{\beta_i \gamma_i^3}{\beta_o \gamma_o^3} \end{bmatrix}$$

- OpenXAL implementation:

$$R_{\text{xal}}^{zz} = \begin{bmatrix} 1 & 0 \\ \frac{k_z}{\beta_o \gamma_o} & \frac{\beta_i \gamma_i}{\beta_o \gamma_o} \end{bmatrix}$$

- Transformation from TraceWin to OpenXAL:

$$R^{zz} = \begin{bmatrix} \frac{\gamma_o}{\gamma_i} & 0 \\ \frac{k_z}{\gamma_i \beta_o \gamma_o^2} & \frac{\beta_i \gamma_i^2}{\beta_o \gamma_o^2} \end{bmatrix}$$

Further numerical comparison showed the biggest differences occur at low energies. In such regime Dynac [5] has been used extensively, so we numerically compared the results and they matched TraceWin's which we used in JELS.

## NUMERICAL COMPARISON

We have compared transfer and covariance matrices (using the transformation described in first section) of OpenXAL and our JELS implementations with TraceWin. Only the basic algorithm, without space-charge was used.

Each beam-line element was compared using qualitatively different parameters and using beam with different initial energies. Besides already described elements, we also tested elements composed of the basic ones, i.e. a cell of the Drift Tube Linac (DTL cell) and a multi-gap cavity (NCELLS element in TraceWin).

For comparison, second matrix norm was used to compute relative error. The following equations show how numerical error is computed:

$$R'_{\text{tw}} = R_{\gamma_o^{-1}}^{(6)} R_{\gamma_o}^{(5)} R_{\text{tw}} R_{\gamma_i^{-1}}^{(5)} R_{\gamma_i}^{(6)}$$

$$\sigma'_{\text{tw}} = R_{\gamma_o^{-1}}^{(6)} R_{\gamma_o}^{(5)} \sigma_{\text{tw}} R_{\gamma_i^{-1}}^{(5)} R_{\gamma_i}^{(6)}$$

$$\epsilon_R = \frac{\|R_{\text{xal}} - R'_{\text{tw}}\|_2}{\|R'_{\text{tw}}\|_2} \quad \epsilon_{\sigma} = \frac{\|\sigma_{\text{xal}} - \sigma'_{\text{tw}}\|_2}{\|\sigma'_{\text{tw}}\|_2} \quad \epsilon_{\gamma} = \frac{\gamma_{\text{xal}} - \gamma_{\text{tw}}}{\gamma_{\text{tw}}}$$

Comparisons show that JELS implementation differs from TraceWin only by numerical errors within  $\sim 1\text{E-}7$  as per Table 1. On the other hand comparison of OpenXAL and TraceWin had differences of up to 20%, as per Table 2, which is large for an envelope simulation.

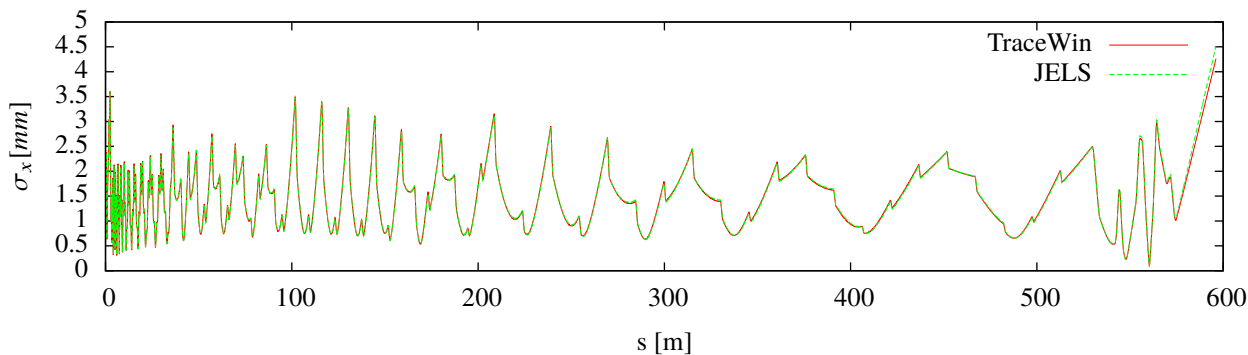


Figure 1: Comparison of JELS and TraceWin simulation on ESS beam-line starting with MEBT section with initial energy 3 MeV and without space-charge.

Table 1: Comparison of JELS and TraceWin results. Initial energy  $E_i = 2.5$  MeV was used for RF gaps, DTL cells, NCELLS and  $E_i = 3$  MeV for rest.

Element	$\epsilon_R$	$\epsilon_\sigma$	$\epsilon_\gamma$
drift	4.0E-09	4.4E-07	5.0E-11
focusing quad	9.2E-08	9.0E-08	5.0E-11
defocussing quad	9.2E-08	1.4E-07	5.0E-11
horizontal bend $N = 0$	1.9E-07	8.9E-08	5.0E-11
horizontal bend $N = 0.2$	1.7E-07	8.5E-08	5.0E-11
vertical bend $N = 0$	1.9E-07	1.3E-07	5.0E-11
vertical bend $N = 0.9$	1.9E-07	1.2E-07	5.0E-11
RF gap without TTF	2.8E-08	2.9E-07	1.5E-10
RF gap with TTF	3.8E-08	8.6E-08	4.6E-10
DTL cell, no quads, no TTF	1.9E-07	4.6E-08	4.4E-10
DTL cell, no quads, TTF	8.4E-08	3.0E-07	3.8E-10
DTL cell	8.5E-08	3.7E-08	3.8E-10
NCELLS $m = 0$	1.0E-07	2.2E-07	-1.6E-10
NCELLS $m = 1$	1.4E-07	5.7E-08	-2.8E-10
NCELLS $m = 2$	3.3E-07	1.7E-07	5.4E-11
NCELLS no TTF, $m = 0$	2.9E-08	2.8E-07	-2.8E-10
NCELLS no TTF, $m = 1$	2.9E-08	1.2E-08	2.4E-10
NCELLS no TTF, $m = 2$	7.3E-08	3.0E-08	-4.5E-10

Table 2: Comparison of OpenXAL and TraceWin results. Initial energy  $E_i = 2.5$  MeV was used for RF gaps, DTL cells, NCELLS and  $E_i = 3$  MeV for rest.

Element	$\epsilon_R$	$\epsilon_\sigma$	$\epsilon_\gamma$
drift	4.0E-09	4.4E-07	5.0E-11
focusing quad	9.2E-08	9.0E-08	5.0E-11
defocussing quad	9.2E-08	1.4E-07	5.0E-11
horizontal bend $N = 0$	1.5E-03	2.6E-03	5.0E-11
horizontal bend $N = 0.2$	1.5E-03	2.6E-03	5.0E-11
vertical bend $N = 0$	1.5E-03	2.3E-03	5.0E-11
vertical bend $N = 0.9$	1.5E-03	2.3E-03	5.0E-11
RF gap without TTF	4.3E-03	6.3E-03	1.5E-10
RF gap with TTF	1.3E-01	7.3E-02	-1.5E-05
DTL cell, no quads, no TTF	5.3E-03	2.0E-02	4.4E-10
DTL cell, no quads, TTF	1.8E-01	2.2E-01	-2.8E-05
DTL cell	6.9E-02	5.1E-02	-2.8E-05

## OVERALL COMPARISON

Last but not least overall comparison was made for the ESS accelerator structure, starting at MEBT section. Besides the comparison on Fig. 1, we have also compared simulation with slightly perturbed energy, other initial parameters (including off-centered beam). All the simulations are within 1%. Comparisons with original OpenXAL implementation is not given, since at the time RF gap phases were not calculated correctly. All the tests we have done were automated to provide quality control of the code.

## CONCLUSION

Precise numerical comparison of TraceWin and OpenXAL showed differences which may otherwise go unnoticed at specific energy for which simulation is used. The methodology, i.e. comparing software models, is not perfect. But even if ab ovo deduction of all the transfer matrices was done, possible mistakes might go unnoticed. Next step is to do precise comparison of the simulations using space charge.

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