# SIMULATING APERTURES IN THE UNIFORM EQUIVALENT EQUIVALENT BEAM MODEL 

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## Abstract

The uniform equivalent beam model is useful for simulating particle beam envelopes. Beam root-meansquare (rms) sizes, divergences, and emittances of an equivalent uniform beam approximate well the rms properties of more realistic beam distributions, even in the presence of space charge. Envelope simulation codes for high current beams using the model, such as TRACE 3-D, are central to particle optics design. However, the modeling of apertures has required multi-particle simulation codes. Multi-particle codes do not typically have the fitting and optimization capabilities common to envelope codes, so the evaluation of aperture effects is often a secondary study that may result in further design iteration. To incorporate aperture effects into the optics design at the start, a method has been developed for simulating apertures in the context of a uniform equivalent beam. The method is described and its TRACE 3-D implementation is outlined. Comparisons with multiparticle simulations are used to validate the method and examine regions of applicability.

## INTRODUCTION

The uniform equivalent beam ("UEB") model [1] provides a useful approximation for simulating particle beam envelopes in transfer lines and accelerator structures. Beam dynamics design often begins with the use of an envelope simulation that utilizes the UEB such as TRACE 3-D [2]. To help incorporate apertures into the initial optics design, a method has been developed for simulating apertures within the context of the UEB model. This paper outlines the method and its implementation in TRACE 3-D. Comparisons with multi-particle simulation codes, with and without space charge, are used to validate the method and examine potential regions of applicability.

It is convenient to examine three cases of a beam passing through an aperture, as illustrated in Fig. 1.


Figure 1: Three cases of beams intercepting an aperture. The apertures are drawn red while the beams are in blue.

Figure 1 shows an elliptical aperture (red) with a vertical (y) to horizontal (x) aspect ratio of 2 . Three beam cases are illustrated by blue ellipses. Case (a) corresponds to the situation where the beam cross section (i.e. y-x plane) is entirely within the aperture. Case (c) is the situation where the beam covers the aperture, so that the beam cross section is effectively replaced by the aperture cross section. Case (b) illustrates the situation where a part of the beam passes through the aperture ellipse, but a portion of the beam is intercepted and lost.

In the context of the equivalent uniform beam, the spatial particle density is described by an uniformly filled ellipsoid of three dimensions (3-D) for bunched beams, or of two dimensions (2-D) for continuous beams. The Kapchinsky-Vladimirsky [3], or KV, beam is a useful model for continuous beams. The approach to modeling apertures is to determine suitable equivalent uniform beams that approximate the beams which survive after encountering the aperture.

## APERTURE METHOD

## Transmission Factor $T_{f}$

The normalized two-dimensional distribution function, $f(\mathrm{x}, \mathrm{y})$, for a beam uniformly distributed within an ellipse, can be represented in terms of the Heaviside step function $\Theta$ by:

$$
\begin{align*}
& f(\mathrm{x}, \mathrm{y})=\Theta\left[\mathrm{A}-\mathrm{B}\left(\mathrm{x} / \mathrm{x}_{\mathrm{b}}\right)\left(\mathrm{y} / \mathrm{y}_{\mathrm{b}}\right)-\left(\mathrm{x} / \mathrm{x}_{\mathrm{b}}\right)^{2}-\left(\mathrm{y} / \mathrm{y}_{\mathrm{b}}\right)^{2}\right], \\
& \text { where } \\
& \text { and }  \tag{2}\\
& \mathrm{A}=\left(1-\mathrm{r}_{\mathrm{xy}}^{2}\right), \\
& \mathrm{B}=2 \mathrm{r}_{\mathrm{xy}} \tag{3}
\end{align*}
$$

The beam ellipse parameters $\mathrm{x}_{\mathrm{b}}$ and $\mathrm{y}_{\mathrm{b}}$ are the maximum extents of the ellipse in the horizontal and vertical directions, respectively, and are given by the square roots of the beam sigma matrix elements $\sigma_{11}$ and $\sigma_{33}$, respectively. Note that these are not the semi-axes parameters for the ellipse ${ }^{1}$. The parameter $r_{x y}$ is the $x-y$ correlation of the beam: $r_{\mathrm{xy}}=\mathrm{r}_{13}=\sigma_{13} /\left(\mathrm{x}_{\mathrm{b}} \mathrm{y}_{\mathrm{b}}\right)$.

The aperture transmission function, $T(x, y)$, can similarly be represented by the Heaviside function as:

$$
\begin{equation*}
T(\mathrm{x}, \mathrm{y})=\Theta\left[1-\left(\mathrm{x} / \mathrm{x}_{\mathrm{a}}\right)^{2}-\left(\mathrm{y} / \mathrm{y}_{\mathrm{a}}\right)^{2}\right] \tag{4}
\end{equation*}
$$

${ }^{1}$ If the semi-axes parameters of the beam ellipse are $a$ and $b$, then $\mathrm{r}_{\mathrm{xy}}$ is related to the rotation angle, $\theta$, by:

$$
\mathrm{r}_{\mathrm{xy}}=-\alpha_{\mathrm{xy}} /\left(1+\alpha_{\mathrm{xy}}{ }^{2}\right)^{1 / 2}
$$

where $\quad \alpha_{x y}=-\left(b^{2}-a^{2}\right) \sin (2 \theta) /(2 a b)$
The beam ellipse parameters $\mathrm{x}_{\mathrm{b}}$ and $\mathrm{y}_{\mathrm{b}}$ are given by:

$$
\begin{gathered}
\mathrm{x}_{\mathrm{b}}=2^{1 / 2} a b /\left[\left(b^{2}+a^{2}\right)+\left(b^{2}-a^{2}\right) \cos (2 \theta)\right]^{1 / 2}, \\
\mathrm{y}_{\mathrm{b}}=2^{1 / 2} a b /\left[\left(b^{2}+a^{2}\right)-\left(b^{2}-a^{2}\right) \cos (2 \theta)\right]^{1 / 2}
\end{gathered}
$$

where $x_{a}$ and $y_{a}$ are the aperture ellipse semi-axes in the horizontal and vertical directions respectively. Letting $g(\mathrm{x}, \mathrm{y})$ denote the beam distribution after the aperture, then

$$
\begin{equation*}
g(\mathrm{x}, \mathrm{y})=T(\mathrm{x}, \mathrm{y}) f(\mathrm{x}, \mathrm{y}) \tag{5}
\end{equation*}
$$

Case (a) simply gives $g(\mathrm{x}, \mathrm{y})=f(\mathrm{x}, \mathrm{y})$, while case (c) results in $g(\mathrm{x}, \mathrm{y})=T(\mathrm{x}, \mathrm{y})$. For case (b) $g(\mathrm{x}, \mathrm{y})$ is again a Heaviside step function, but the argument is a more complicated function of four segments from the inner most boundaries of the beam and aperture ellipses.

In case (b) the beam and aperture ellipses intersect at four points. The coordinates $\left(\mathrm{x}_{\mathrm{i}}, \mathrm{y}_{\mathrm{i}}\right)$ for the intersection points are found by equating the arguments of (1) and (4). The result can be written as a quadratic equation for the square of one of the intersection coordinates. Selecting to solve for $y^{2}$ yields:

$$
\begin{equation*}
a y^{4}+b y^{2}+c=0, \tag{6}
\end{equation*}
$$

where:

There are four solutions to equation (6) for the intersection coordinate $y_{i}$, each with a corresponding $x_{i}$ coordinate. The coordinate pairs ( $\mathrm{x}_{\mathrm{i}}, \mathrm{y}_{\mathrm{i}}$ ) for the intersection points in this work are labeled with i increasing from 1 to 4 in a counterclockwise sense from the first quadrant, with $\mathrm{x}_{1}$ corresponding to the largest positive value. Thus pairs $\left(\mathrm{x}_{1}, \mathrm{y}_{1}\right)$ and $\left(\mathrm{x}_{4}, \mathrm{y}_{4}\right)$ are located in the upper half plane $\left(\mathrm{y}_{\mathrm{i}}>0\right)$ while $\left(\mathrm{x}_{2}, \mathrm{y}_{2}\right)$ and $\left(\mathrm{x}_{3}, \mathrm{y}_{3}\right)$ are located in the lower half plane ( $\mathrm{y}_{\mathrm{i}}<0$ ).

Each segment defining the interior of the beam capture region in Fig. 1(b) is part of an ellipse. The beam transmission fraction, $T_{\mathrm{f}}$, given by the integral over $g(\mathrm{x}, \mathrm{y})$ of equation (5) divided by the beam area, can be computed analytically, with the results expressed in terms of arcsin and algebraic functions of the four intersection coordinates $x_{i}$. Only the contribution for $y>0$ need be computed as the contribution for $\mathrm{y}<0$ will be the same.

For the example in Fig. 1(b), where $\mathrm{x}_{\mathrm{b}}>\mathrm{x}_{\mathrm{a}}, T_{\mathrm{f}}$ is:

$$
\begin{align*}
T_{\mathrm{f}} & =\left(\pi \mathrm{F}_{\mathrm{xy}}\right)^{-1}\left\{\left[(\pi / 2)+\arcsin \left(\mathrm{R}_{\mathrm{a} 4}\right)+\mathrm{R}_{\mathrm{a} 4} \mathrm{~F}_{\mathrm{a} 4}\right]\right. \\
& +\mathrm{F}_{\mathrm{xy}}\left[\arcsin \left(\mathrm{R}_{\mathrm{b} 1}\right)+\mathrm{R}_{\mathrm{b} 1} \mathrm{~F}_{\mathrm{b} 1}-\arcsin \left(\mathrm{R}_{\mathrm{b} 4}\right)+\mathrm{R}_{\mathrm{b} 4} \mathrm{~F}_{\mathrm{b} 4}\right] \\
& \left.+\mathrm{r}_{\mathrm{xy}}\left[\mathrm{R}_{\mathrm{b} 1}{ }^{2}-\mathrm{R}_{\mathrm{b} 4}{ }^{2}\right]+\left[(\pi / 2)-\arcsin \left(\mathrm{R}_{\mathrm{a} 1}\right)-\mathrm{R}_{\mathrm{a} 1} \mathrm{~F}_{\mathrm{a} 1}\right]\right\}, \tag{10}
\end{align*}
$$

where:

$$
\mathrm{R}_{\mathrm{a} 1}=\mathrm{x}_{1} / \mathrm{x}_{\mathrm{a}}, \mathrm{R}_{\mathrm{a} 4}=\mathrm{x}_{4} / \mathrm{x}_{\mathrm{a}}, \mathrm{R}_{\mathrm{b} 1}=\mathrm{x}_{1} / \mathrm{x}_{\mathrm{b}}, \quad \mathrm{R}_{\mathrm{b} 4}=\mathrm{x}_{4} / \mathrm{x}_{\mathrm{b}},
$$

$$
\mathrm{F}_{\mathrm{a} 1}=\left(1-\mathrm{R}_{\mathrm{a} 1}^{2}\right)^{1 / 2}, \mathrm{~F}_{\mathrm{a} 4}=\left(1-\mathrm{R}_{\mathrm{a} 4}^{2}\right)^{1 / 2},
$$

$$
\begin{equation*}
\mathrm{F}_{\mathrm{b} 1}=\left(1-\mathrm{R}_{\mathrm{b} 1}^{2}\right)^{1 / 2}, \mathrm{~F}_{\mathrm{b} 4}=\left(1-\mathrm{R}_{\mathrm{b} 4}^{2}\right)^{1 / 2}, \tag{11}
\end{equation*}
$$

and

$$
\begin{equation*}
\mathrm{F}_{\mathrm{xy}}=\left(1-\mathrm{r}_{\mathrm{xy}}{ }^{2}\right)^{1 / 2} \tag{12}
\end{equation*}
$$

The first and last terms in square brackets in equation (10) correspond to the left-most and right-most region between $\left(-\mathrm{x}_{\mathrm{a}}, \mathrm{x}_{4}\right)$ and $\left(\mathrm{x}_{1}, \mathrm{x}_{\mathrm{a}}\right)$, respectively. The two

$$
\begin{align*}
& \mathrm{a}=\left[\left(\mathrm{x}_{\mathrm{b}}{ }^{2} \mathrm{y}_{\mathrm{a}}{ }^{2}-\mathrm{x}_{\mathrm{a}}{ }^{2} \mathrm{y}_{\mathrm{b}}{ }^{2}\right)^{2}+4 \mathrm{r}_{\mathrm{xy}}{ }^{2}\left(\mathrm{x}_{\mathrm{b}} \mathrm{y}_{\mathrm{a}} \mathrm{x}_{\mathrm{a}} \mathrm{y}_{\mathrm{b}}\right)^{2}\right] /\left(\mathrm{y}_{\mathrm{a}}{ }^{4} \mathrm{x}_{\mathrm{b}}{ }^{4} \mathrm{y}_{\mathrm{b}}{ }^{4}\right),  \tag{7}\\
& \mathrm{b}=2\left\{\left(\mathrm{x}_{\mathrm{b}}{ }^{2} \mathrm{y}_{\mathrm{a}}{ }^{2}-\mathrm{x}_{\mathrm{a}}{ }^{2} \mathrm{y}_{\mathrm{b}}{ }^{2}\right)\left(\mathrm{x}_{\mathrm{a}}{ }^{2} \mathrm{y}_{\mathrm{b}}{ }^{2}-\mathrm{x}_{\mathrm{b}}{ }^{2} \mathrm{y}_{\mathrm{b}}{ }^{2}\right)+\right. \\
& \left.\mathrm{r}_{\mathrm{xy}}{ }^{2}\left[\left(\mathrm{x}_{\mathrm{b}}{ }^{2} \mathrm{y}_{\mathrm{a}}{ }^{2}-\mathrm{x}_{\mathrm{a}}{ }^{2} \mathrm{y}_{\mathrm{b}}{ }^{2}\right) \mathrm{x}_{\mathrm{b}}{ }^{2} \mathrm{y}_{\mathrm{b}}{ }^{2} .-2 \mathrm{x}_{\mathrm{b}}{ }^{2} \mathrm{y}_{\mathrm{a}}{ }^{2} \mathrm{x}_{\mathrm{a}}{ }^{2} \mathrm{y}_{\mathrm{b}}{ }^{2}\right]\right\} /\left(\mathrm{y}_{\mathrm{a}}{ }^{2} \mathrm{x}_{\mathrm{b}}{ }^{4} \mathrm{y}_{\mathrm{b}}{ }^{4}\right),  \tag{8}\\
& \text { and } \quad c=\left[\left(\mathrm{x}_{\mathrm{a}}{ }^{2}-\mathrm{x}_{\mathrm{b}}{ }^{2}\right)+\mathrm{r}_{\mathrm{xy}}{ }^{2} \mathrm{x}_{\mathrm{b}}{ }^{2}\right]^{2} /\left(\mathrm{y}_{\mathrm{b}}{ }^{4}\right) \text {. } \tag{9}
\end{align*}
$$

middle terms in the square brackets of equation (10) correspond to the region of $\left(\mathrm{x}_{4}, \mathrm{x}_{1}\right)$. For the situation with $\mathrm{x}_{\mathrm{b}}<\mathrm{x}_{\mathrm{a}}, T_{\mathrm{f}}$ can also be expressed analytically but is not shown due to space limits.

The transmission factor is used to compute the beam current after the aperture, $I_{\text {after }}=T_{\mathrm{f}} I_{\text {before, }}$, where $I_{\text {before }}$ is the beam current incident on the aperture.

## Beam Ellipsoid ( $\sigma$-matrix) Parameters

The beam ellipsoid parameters following the aperture are determined by the second moments, including correlated moments, of the distribution function $g(\mathrm{x}, \mathrm{y})$. For case (a) the beam parameters are simply those of the initial beam. For case (b) the beam spatial parameters are determined by the aperture parameters. For case (c) the second moments can be computed following the same procedure as used to compute the transmission factor, with the integrals involved appropriately weighted with the $x^{2}, x y$, or $y^{2}$, as well as $x$ or $y$ for the phase space correlation elements. That procedure gives well-defined second moments, but may not represent the best UEB beam. A simpler procedure for case (c) has been used where the values for each second moment are determined by the smaller of the values for the initial beam or the aperture itself. For example, the values after the aperture of the $\sigma$-matrix parameters in the x -x' phase space are:

$$
\begin{gather*}
\sigma_{11}=\mathrm{F}_{\mathrm{x}}^{2} \mathrm{x}_{\mathrm{b}}^{2}  \tag{13}\\
\sigma_{12}=\mathrm{F}_{\mathrm{x}} \mathrm{r}_{12} \mathrm{x}_{\mathrm{x}} \mathrm{x}_{\mathrm{b}}^{\prime},  \tag{14}\\
\sigma_{22}=\mathrm{x}_{\mathrm{b}}^{\prime 2}, \tag{15}
\end{gather*}
$$

where $\mathrm{x}_{\mathrm{b}}^{\prime}$ and $\mathrm{r}_{12}$ are beam divergence and x - x ' correlation parameters before the aperture, and the scale factor $F_{x}$ is:

$$
\begin{align*}
& \mathrm{F}_{\mathrm{x}}=1 \quad \text { if } \quad \mathrm{x}_{\mathrm{b}}<\mathrm{x}_{\mathrm{a}}, \quad \text { and } \\
& \mathrm{F}_{\mathrm{x}}=\mathrm{x}_{\mathrm{a}} / \mathrm{x}_{\mathrm{b}} \text { if } \mathrm{x}_{\mathrm{b}}>\mathrm{x}_{\mathrm{a}} . \tag{16}
\end{align*}
$$

## Model Comparison with Numerical Simulations

The aperture method described has been added to the TRACE 3-D code available as a Module to the PBO Lab software [4]. MARYLIE [5] has been used for multiiparticle simulations of apertures. MARYLIE has a good KV beam distributions algorithm and is also available as a PBO Lab Module [6], making comparisons easy.

Table 1 summarizes selected $T_{\mathrm{f}}$ results using the TRACE 3-D aperture method and compares them to MARYLIE calculations. The examples are for a 2 MeV proton beam (mass 938.28 MeV ) and an aperture with $x_{a}=1 \mathrm{~mm}$ and $y_{a}=3 \mathrm{~mm}$. The initial beam is parameterized in terms of starting values of the semi-axes for the beam cross section, $a$ and $b$, together with a roll angle, $\theta$. The values of $a$ and $b$ used are 3 mm and 2 mm , respectively, and the roll angle $\theta$ is varied to cover a variety of the conditions for case (b) of Fig. 1. The results
show that the analytic results for $T_{\mathrm{f}}$ have been correctly programmed in the TRACE 3-D Module software. The differences between the MARYLIE simulations and the analytic (TRACE 3-D) model are around $1 \%$ (for 10,000 particles), and of the same order as the differences between $+\theta$ and $-\theta$ MARYLIE simulations.

Table 1. Selected transmission factor $\left(T_{\mathrm{f}}\right)$ results for the PBO Lab TRACE 3-D Module aperture model (T3D) with comparisons to MARYLIE 10,000 particle simulations (MARY). The Diff column shows the percent difference of the $T_{\mathrm{f}}$ (MARY) results from the $T_{\mathrm{f}}$ (T3D) model, while the last column shows the percent difference observed with MARYLIE for $\pm \theta$ values.

| $\theta$ (deg) | $T_{\mathrm{f}}$ (T3D) | $T_{\mathrm{f}}$ (MARY) | Diff (\%) | Diff(MARY) |
| :---: | :---: | :---: | :---: | :---: |
| 0 | 0.3870352 | 0.3842 | -0.73 | - |
| 10 | 0.3895167 | 0.3856 | -1.01 | -0.39 |
| 20 | 0.3969442 | 0.3923 | -1.17 | -1.11 |
| 40 | 0.4259730 | 0.4207 | -1.24 | -2.09 |
| 60 | 0.4678598 | 0.4649 | -0.63 | -1.94 |
| 80 | 0.4978750 | 0.5036 | 1.15 | 0.04 |
| 90 | 0.5000000 | 0.5043 | 0.86 | 0.00 |



Figure 2: Transmission factors $\left(T_{\mathrm{f}}\right)$ for the Example B beamline from PARMILA-2 when (A) the quadrupoles are fit ignoring apertures (red) and (B) using the aperture method (blue), as a function of current. The black curve shows the $T_{\mathrm{f}}$ aperture method estimate from TRACE 3-D.

A typical transfer line problem was used to explore the utility of using TRACE 3-D with the aperture method. The Example B transfer line problem from the TRACE 3D documentation [2] is representative and has been studied in detail previously. The Example B - Modified version [7] uses 4 quadrupoles to transport a beam, with given initial Twiss parameters, to a match point downstream, where the quadrupole strengths are varied to
achieve different Twiss parameters at the match point. One cm (radius) apertures were added at the middle of each of the 4 "matching" quadrupoles, as well as at the match point, which is in the middle of a 5th quadrupole. TRACE 3-D was used to find the 4 required quadrupole strengths either (A) ignoring the apertures, or (B) including apertures. The "matched" quadruple strengths were determined for currents $I$ between 0 and 150 mA .

Once the matched quadruples are set by TRACE 3-D, the PARMILA-2 program $[8,9]$ was used for multiparticle simulations ( 10,000 particles) with space charge through the transfer lines for (A) and (B). Fig. 2 summarizes the total transmission factor $\left(T_{\mathrm{f}}\right)$ results. The data displayed in Fig. 2 show that if the aperture method is included, when using TRACE 3-D to find the matched quadrupole strengths, that PARMILA-2 predicts higher transmission through the line (B), than if the strengths were fit ignoring the apertures (A). The TRACE 3-D calculations with the aperture method appear to give a reasonable estimate of the PARMILA-2 transmission, even though that beam is not a UEB distribution.

## SUMMARY

A method for modeling apertures within the context of the uniform equivalent beam (UEB) model has been derived. The method was added to the PBO Lab TRACE 3-D Module. Comparisons to multi-particle simulations are used to validate the method, and to indicate that the method may have utility in beamline design.

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