Overview of Particle Beam Optics Utilized in the Matrix, Envelope, and Tracking Codes: TRACE 3-D, Beamline Simulator (TRANSPORT & TURTLE)

George H. Gillespie

G. H. Gillespie Associates, Inc.
P. O. Box 2961
Del Mar, California 92014, U.S.A.

Presented at

King Abdulaziz City for Science and Technology (KACST)
Riyadh, Saudi Arabia
October 2014

Presentation Outline - Part I

Overview of Particle Beam Optics Utilized in the Matrix, Envelope, and Tracking Codes: TRACE 3-D, Beamline Simulator (TRANSPORT & TURTLE)

Part II ⇒ **Use the PBO Lab TRACE 3-D Module to work some examples**

4. Introduction to TRACE 3-D

- **TRACE 3-D**
  - **Primarily a First-Order Code with a Space Charge Model**
  - **Evolved from an Earlier Two-Dimensional Code (TRACE)**
  - **Similar to an Early (LBNL) TRANSPORT Spin-Off**
  - **Includes several radiofrequency (RF) components**
- **Solves (Numerically "Integrates") the Envelope Equations**
  - **Beam is an Ellipsoid in Three Dimensions - "Bunched"**
  - **Differential Matrix Model of Optical Components**
  - **Beam Envelopes Advanced in Steps, Using R-Matrices for Elements of Short Length, Δs**
  - **Space Charge Impulse Applied at Each Step**
  - **Can Include Models for Fringe Fields, Higher-Orders, Non-Linearities - But Only Computes Their Effect on the Second Moments of the Beam Distribution (σ Matrix)**
- **Principle Uses Are for Ion and (Low-Energy) Electron Beams**
  - **Especially for Radiofrequency Acceleration, Space Charge**
- **PBO-Lab Version Can Also Model ElectroStatic (ES) Elements**
  - **Einzel Lenses, ES Quadrupoles, ES Columns, ES Deflectors**
  - **Useful with DC Acceleration, with or without Space Charge**

4. Introduction to TRACE 3-D (continued)

- **Initial Beam Usually Specified with 3-D Twiss (CS) Parameters**
  - **May Also Specify the Initial σ Matrix Directly**

{ Recall: If Particle Coordinates Transform as $[q_{i\,b}] = \Sigma_j R_{ij}\, q_{ja} \equiv R[q_{i\,a}]$
It Can Be Shown that the Sigma Matrix $[\sigma_{ij\,b}]$ Transforms as:

$$[\sigma_{ij\,b}] = \Sigma_k R_{ik}\, \Sigma_m R_{mj}\, [\sigma_{km\,a}] \equiv R[\sigma_{ij\,a}]R^T$$

where R^T is the Transpose of R. }

- **6×6 σ Matrix Advanced, from Location j to j+1, through an Increment, $\Delta s = s_{j+1} - s_j$, Along the Reference Trajectory:**

$$\sigma(j+1) = R(\Delta s)\, \sigma(j)\, R(\Delta s)^T$$

- $R(\Delta s)$ **is the First-Order Transfer Matrix for Optical Element of Length Δs**
- **At Each Increment, a Space Charge Impulse is Applied Using a Thin Lens R Matrix Based Upon 3-D Ellipsoid**
- **Since $R(\Delta s)$ is Computed At Each Increment j, Non-Constant (& Non-Linear) Fields Can be Modeled by Using $R(j, \Delta s)$**

4. Introduction to TRACE 3-D (continued)

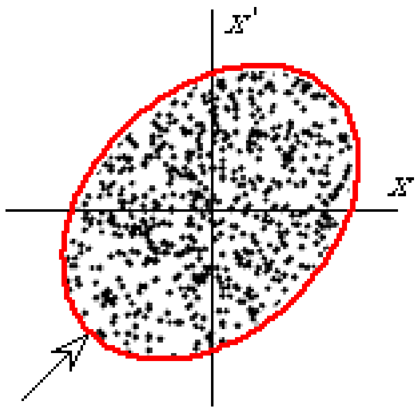
- **Sixteen Built-in Optical Elements in Standard Version**
  - **Six are Common (e.g. TRANSPORT) Elements:**
    Drift, Quad, Solenoid, Bend, Edge, Rotate
  - **Three are "Compound" Magnet Elements:**
    Anti-Symmetric Doublet, Symmetric Triplet,
    and Permanent Magnet Quad (PMQ) with Fringe Fields
  - **Four are Radiofrequency Elements:**
    RF Gap, RFQ Cell, RF Cavity, Coupled Cavity Tank
  - **Thin Lens**
  - **Alias (Identical) - Takes on the Identity of a Specified Element**
  - **Special = Free Electron Laser (FEL) Wiggler**

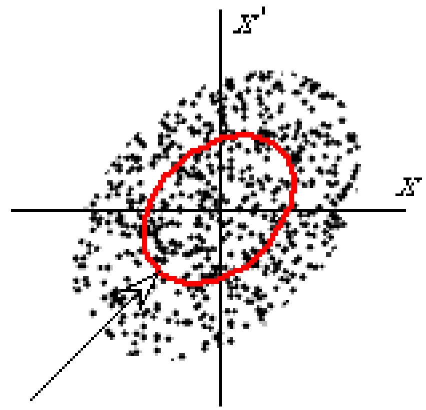
- **PBO Lab TRACE 3-D Has Additional Optical Elements Available**
  - **2 Traveling Wave RF Accelerator Elements for Electron Linacs**
  - **Electrostatic (ES) Elements**
    3 Einzel Lenses, 3 Prisms (Deflectors), 2 DC Columns, 2 ES Quads
  - **TRANSPORT / MAD S-Bend and R-Bend Supported**

- **PBO Lab TRACE 3-D Supports Overlapping Fields for Einzel Lenses and DC Columns**

4. Introduction to TRACE 3-D (continued)

- **TRACE 3-D Uses an "Equivalent Uniform Beam" Model of A Beam**
- **Emittance Values are for the Laboratory Emittance, 5 × RMS**





TRACE 3-D Boundary Emittance **RMS Emittance**

Boundary "bnd" Emittance ≡ bnd Emittance = 5 × RMS Emittance

(• **For Continuous (DC) Beams Can Assume Laboratory Emittance, 4 × RMS**)

- **Boundary, RMS, or *Other* Emittance ⇒ 1st Order Same, if no Space Charge**
- **Equivalent Uniform Beam Model, With Boundary Emittance:**
  ⇒ **Useful for Computing Space Charge Effects**

4. Introduction to TRACE 3-D (continued)

Space Charge Model in TRACE 3-D

- **The Charge Density of a Uniformly Filled 3-D Ellipsoid is**

$$\rho(x,y,z) = \rho_o \,\Theta\, [1 - (x/x_m)^2 - (y/y_m)^2 - (z/z_m)^2]$$

Where Θ is the Heaviside Step Function and

$$\rho_o = \frac{3Q}{4\pi\, x_m y_m z_m}$$

With Q Equal to the Total Charge in the Ellipsoid

- **The Three Semi-Axes of the Ellipsoid Are Computed from**

$$x_m = (\sigma_{11})^{1/2} \qquad y_m = (\sigma_{33})^{1/2} \qquad z_m = (\sigma_{55})^{1/2}$$

$\Rightarrow$ **Important to get σ_{55} correct, even for continuous (unbunched) beams**

- **A Particle Will See an Electric Field Due to This Charge Density**
  - **Inside the Ellipsoid, the Field is Linear in x, y, z**
  - **The Coefficients of the Linear Field Depend Upon x_m, y_m, z_m**
  - **TRACE 3-D Model Has No "Particles" Outside the Ellipsoid**

4. Introduction to TRACE 3-D (continued)

Space Charge Model in TRACE 3-D (con't)

- **Particles Experience an Electric Field Due to** $\rho(x,y,z)$
  Inside the Ellipsoid, this Field in the Beam Frame is Given by:

$$E_x = \frac{\rho_o}{\varepsilon_o} \left[\frac{(y_m)}{(x_m+y_m)} \right] (1 - f)\, x$$

$$E_y = \frac{\rho_o}{\varepsilon_o} \left[\frac{(x_m)}{(x_m+y_m)} \right] (1 - f)\, y$$

$$E_z = \frac{\rho_o}{\varepsilon_o} f\, z$$

- $f = f(p)$ **is the Ellipsoidal *Form Factor* Which Depends Upon the Semi-Axes of the Ellipsoid (**x_m, y_m, z_m**) Through the Ratio** p**:**

$$p = \left[z_m/(x_m y_m)^{1/2} \right]$$

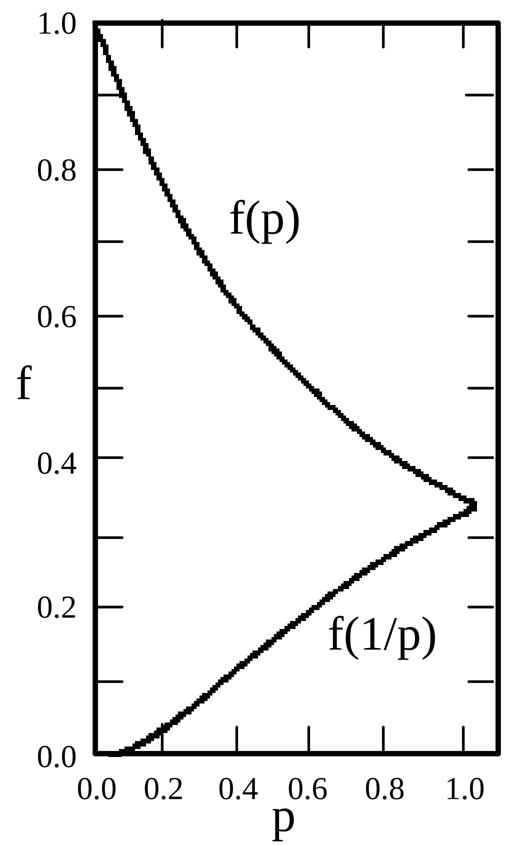
4. Introduction to TRACE 3-D (continued)

Space Charge Model in TRACE 3-D (con't) Ellipsoidal Form Factor

- **For** $0 \le p \le \infty$**, the Ellipsoidal Form Factor is** $0 \le f(p) \le 1$
- **When** $p \cong 1$ **(near spherical bunch) then** $f(p) \cong 1/(3p)$

$$f(p) = \begin{cases} \dfrac{1}{1-p^2} - \dfrac{p}{\left(1-p^2\right)^{3/2}} \cos^{-1}(p) \quad , \quad \text{for } p < 1 \; ; \\ \dfrac{p \ln \cdot \left[p + \sqrt{p^2 - 1}\right]}{\left(p^2 - 1\right)^{3/2}} - \dfrac{1}{p^2 - 1} \quad , \quad \text{for } p > 1 \quad . \end{cases}$$

$$f(1) = \frac{1}{3}$$



4. Introduction to TRACE 3-D (continued)

Space Charge Model in TRACE 3-D (con't)

- **For One Beam Bunch Passing a Point in the Beamline Every RF Cycle, the Total Charge is Related to the Beam Current** I**:**

$$Q = I/f = (\lambda/c)I$$

- **For Relativistic Beams with Kinectic Energy** $W = (\gamma-1)mc^2$**:**

$$(E_{x,y})_{\text{lab frame}} = (E_{x,y})_{\text{beam frame}} / \gamma$$
$$(z_m)_{\text{lab frame}} = (z_m)_{\text{beam frame}} / \gamma$$

- **Effective** R **Matrix is Equivalent to a 3-D Diverging Thin Lens**

$$R_{21} = -1/f_x = qe\,(\partial E_x/\partial x)\,\Delta s\,/\,(\gamma\,\beta^2\,mc^2)$$

$$R_{43} = -1/f_y = qe\,(\partial E_y/\partial y)\,\Delta s\,/\,(\gamma\,\beta^2\,mc^2)$$

$$R_{65} = -1/f_z = qe\,(\partial E_z/\partial z)\,\Delta s\,/\,(\gamma\,\beta^2\,mc^2)$$

- **A Few Computational Details (Automated in TRACE 3-D)**
  - **Ellipsoid May Be Tilted** $\Rightarrow$ **Must Transform Coordinates**
  - **Calculation Accuracy** $\Rightarrow$ **Elements at** $\Delta s/2$**, Some Adjust** Δs

4. Introduction to TRACE 3-D (continued)

Continuous Beam Space Charge

- **It Can Be Shown That the TRACE 3-D Equivalent Uniform Beam Model for 3-D Space Charge Can Approximate the KV (Equivalent Uniform Beam) 2-D Space Charge Model By Making the Beam Bunch Sufficiently Long**

- **Use a "Long" Bunch" in TRACE 3-D**

  Bunch Length r_z Greater than the Beamline Length L

- **Pick the RF Wavelength λ Long Compared to the Beamline Length L**

- **Set the TRACE 3-D Bunched Beam Current I_b To:**

$$I_b = (4/3)(r_z / \beta\lambda)\ I_{dc}\ .$$

  Where I_{dc} Is the Continuous (DC) Beam Current

  Suggestion: Select r_z and λ so $(4/3)(r_z / \beta\lambda) = 1$

- **Bunch Length r_z Remains Unchanged & Transverse Space Charge is KV**

- **Results are Independent of Precise Values of r_z and λ - Provides Tests**

  ⇒This Method is Largely Automated in the PBO Lab TRACE 3-D Module

4. Introduction to TRACE 3-D (continued)

TRACE 3-D Fitting ("Matching") Capabilities

- **“Matching” is TRACE 3-D Equivalent to TRANSPORT “Fitting”**

- **Fourteen (14) Matching Options in TRACE 3-D**
  - **Four (4) Find Twiss (C-S) Parameters for Matched Beams**
  - **One Varies Initial Beam Parameters to Produce Specified Twiss Parameters at the Output**
  - **Six (6) Vary (Match) Beamline Parameters to Produce Specified Twiss Parameters at the Output**
  - **Three (3) Vary Beamline Parameters to Produce**
    Specified R Matrix Elements (for Overall Beamline)
    Specified σ Matrix (Modified) Elements (at Output)
    Specified Phase Advances μ_x, μ_y, μ_z (at Output)

- **Number of Beamline Element Vary ("Match") Parameters Limited to 6**

(Number of Vary Parameters Can Be Increased with Optimization Module)

4. Introduction to TRACE 3-D (continued)

TRACE 3-D Fitting ("Matching") Capabilities

Some Useful R-Matrix Fitting Constraints

- **For point-to-point optics in the horizontal (x) direction:** $R_{12} = 0$
- **For parallel-to-parallel optics in the horizontal (x) direction:** $R_{21} = 0$
- **For parallel-to-point optics in the horizontal (x) direction:** $R_{11} = 0$
- **For point-to-parallel optics in the horizontal (x) direction:** $R_{22} = 0$
- **Similar conditions for the vertical (y) direction involving** R_{yy} **submatrix**
- **For achromatic optics in the horizontal (x) direction:** $R_{16} = R_{26} = 0$

Useful Beam (σ) Matrix Constraints

- **For a beam waist in the horizontal (x) direction:** $\alpha_x = 0$ **or** $r_{12} = 0$
- **For beam size in the horizontal (x) direction:** $[\sigma_{11}]^{1/2} = X_{size}$

TRACE 3-D Capabilities

Other Useful Commands

- **Trace of** R-Matrix **for stability in a periodic system:** $(1/2)\ |Tr[R]| \le 1$

⇒ **PBO Lab TRACE 3-D Command "Calculate Phase Advance" Finds Matched Beam Phase Space Parameters *if* a Matched Beam Exists (i.e. if** $(1/2)\ |Tr[R]| \le 1$**)**

- **Longitudinal phase space parameters of output beam:**

⇒ **PBO Lab TRACE 3-D Command "Calculate Phase and Energy" Gives Synchronous Phase, Beam Energy, Phase Spread, Bunch Length, Energy Spread, Momentum Spread, Longitudinal Emittance, at the Output (Exit End of Beamline)**

- **Transfer matrix for beamline:**

⇒ **PBO Lab TRACE 3-D Command "Show R Matrix" Gives** R-Matrix

- **Beam parameters at the output:**

⇒ **PBO Lab TRACE 3-D Command "Show Modified Sigma" Gives Reduced** σ-Matrix

- **PBO Lab has other useful capabilities that supplement these**

4. Introduction to TRACE 3-D (continued)

TRACE 3-D Mismatch Factor

- **Useful to Have One Number (Figure of Merit) to Compare Two Ellipses**
- **One Measure of Comparison is the Mismatch Factor (MMF)**
  - **Two Ellipses (a and b) with Different Twiss Parameters in x Plane**
  - **Mismatch Factor Between Ellipses a and b Defined as**

$$MMF_x = \left[(1/2)(R_x + [(R_x^2 - 4)]^{1/2})\right]^{1/2} - 1$$

where $R_x = \beta_a \gamma_b + \gamma_a \beta_b - 2\, \alpha_a \alpha_b$

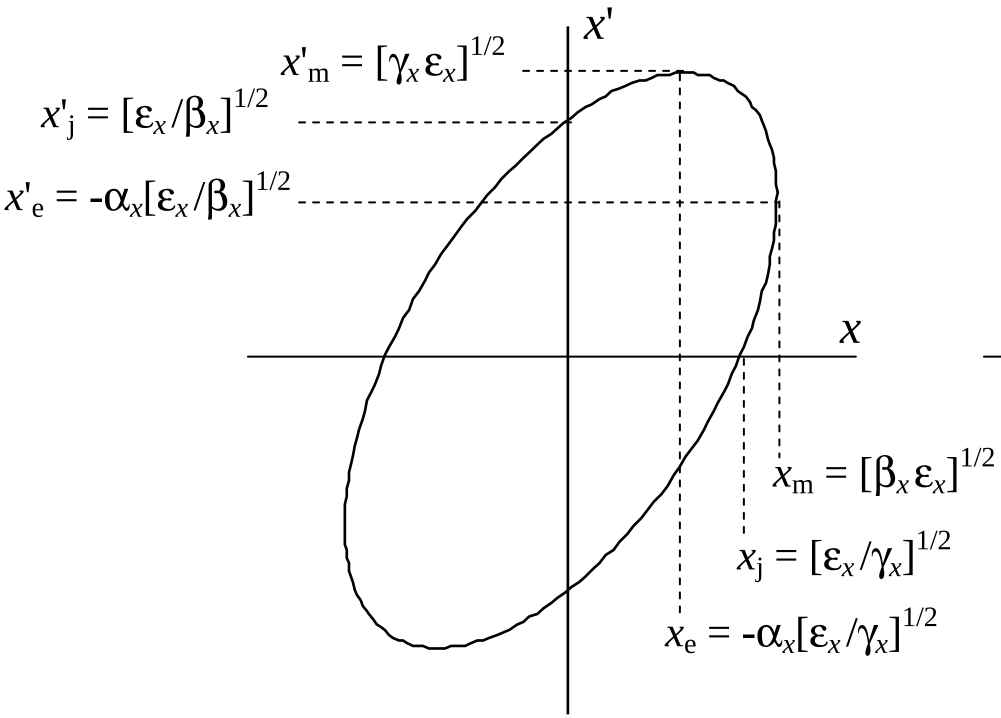
  - **If Ellipses Are Identical (a=b):** $R_x = 2(\beta_a\gamma_a - \alpha_a^2) = 2$ & $MMF_x = 0$
  - **Different Ellipses** $MMF_x > 0$

- **Most TRACE 3-D Fitting Minimizes Mismatch Factors** MMF_x, MMF_y, MMF_z
- **Mismatch Factor (MMF) defined by Twiss Parameters.**
- **This MMF Definition is Independent of the Beam Emittances.**

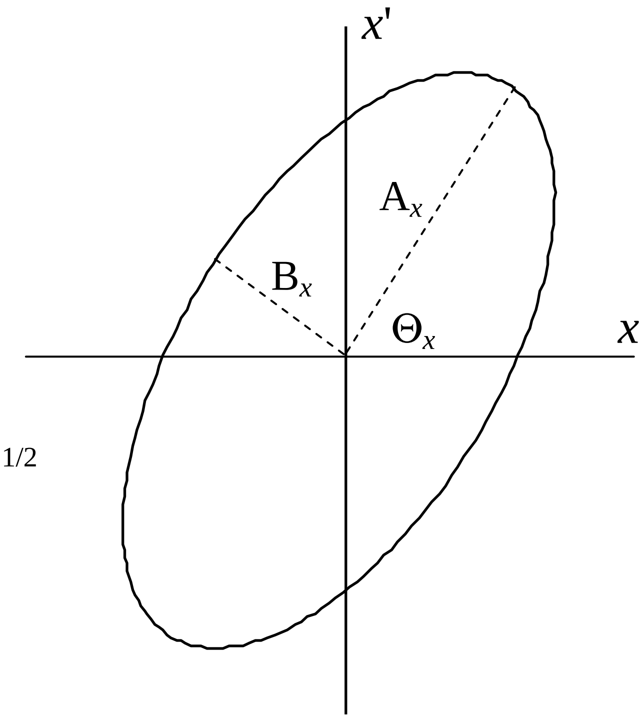
⇒ **What is the geometrical / physical interpretation of the MMF?**

Mismatch Factor - Ellipse Parameterization

Twiss Representation



Geometric Parameterization



$$\gamma_x / \varepsilon_x = (\cos\Theta_x / A_x)^2 + (\sin\Theta_x / B_x)^2$$

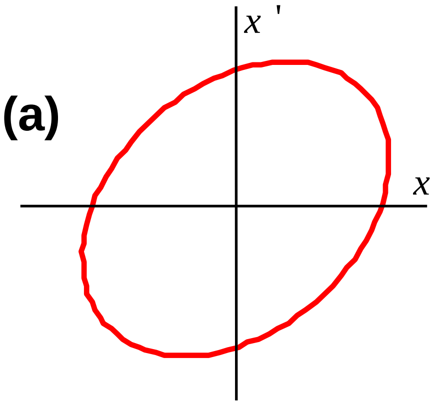
$$\beta_x / \varepsilon_x = (\sin\Theta_x / A_x)^2 + (\cos\Theta_x / B_x)^2$$

$$\alpha_x / \varepsilon_x = \cos\Theta_x \sin\Theta_x \; [(1 / B_x)^2 - (1 / A_x)^2]$$

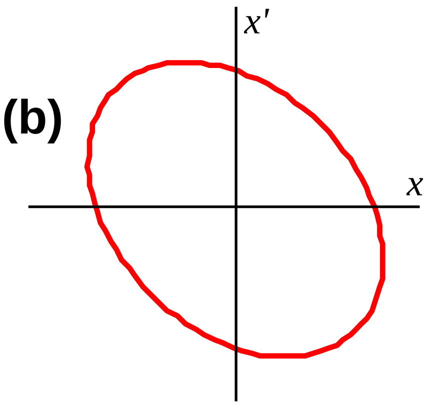
Mismatch Factor - Ellipse Transformations

Starting Ellipses

Ellipse (a)

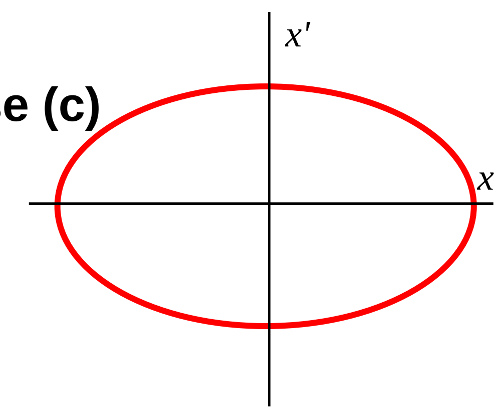


Ellipse (b)

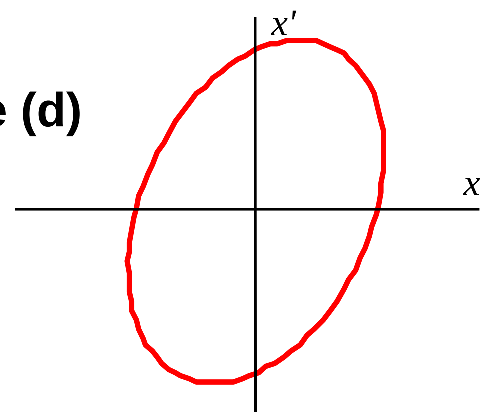


Rotate Ellipses Through an Angle (e.g. Θ_a) To Make Ellipse (a) Upright

Ellipse (c)



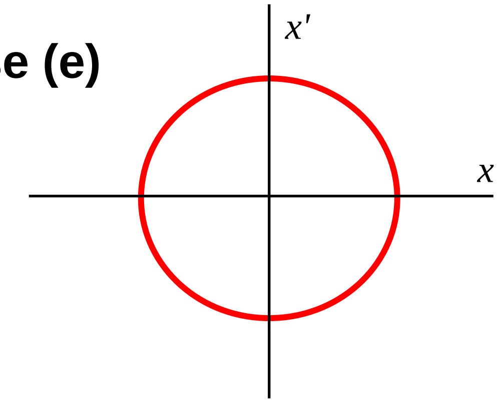
Ellipse (d)



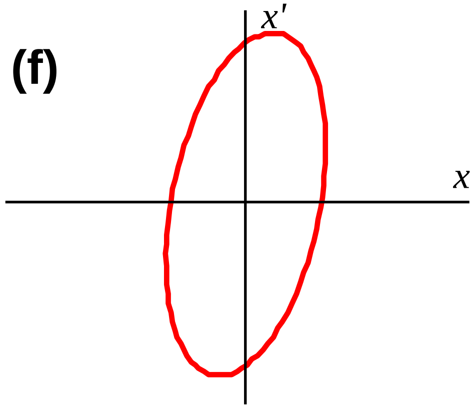
Mismatch Factor - Ellipse Transformations

Scale Coordinates So That Upright Ellipse (c) Becomes a Circle

Ellipse (e)



Ellipse (f)



Semi-Axes of Ellipse (e) are Equal (Circle):

$$r = (\text{Area}/\pi)^{1/2}$$

Define for Ellipse (f):

$$r_e = \text{Larger of Semi-axes } (a,b)$$

Then Mismatch Factor Can Be Expressed As:

$$\text{MMF} = (r_e \,/\, r) \text{ -1} \geq 0$$

4. Introduction to TRACE 3-D (continued)

Some Other TRACE 3-D Features

- **TRACE 3-D Can Run Beam in Reverse (Backward) Direction**
  - **- PBO-Lab Put "Initial" Beam at End of Beamline, "Final" Beam at Start**
  - $\Rightarrow$ **Use with Caution if Space Charge is Important!**

- **Supports Misalignment of Elements (computes beam centroid)**

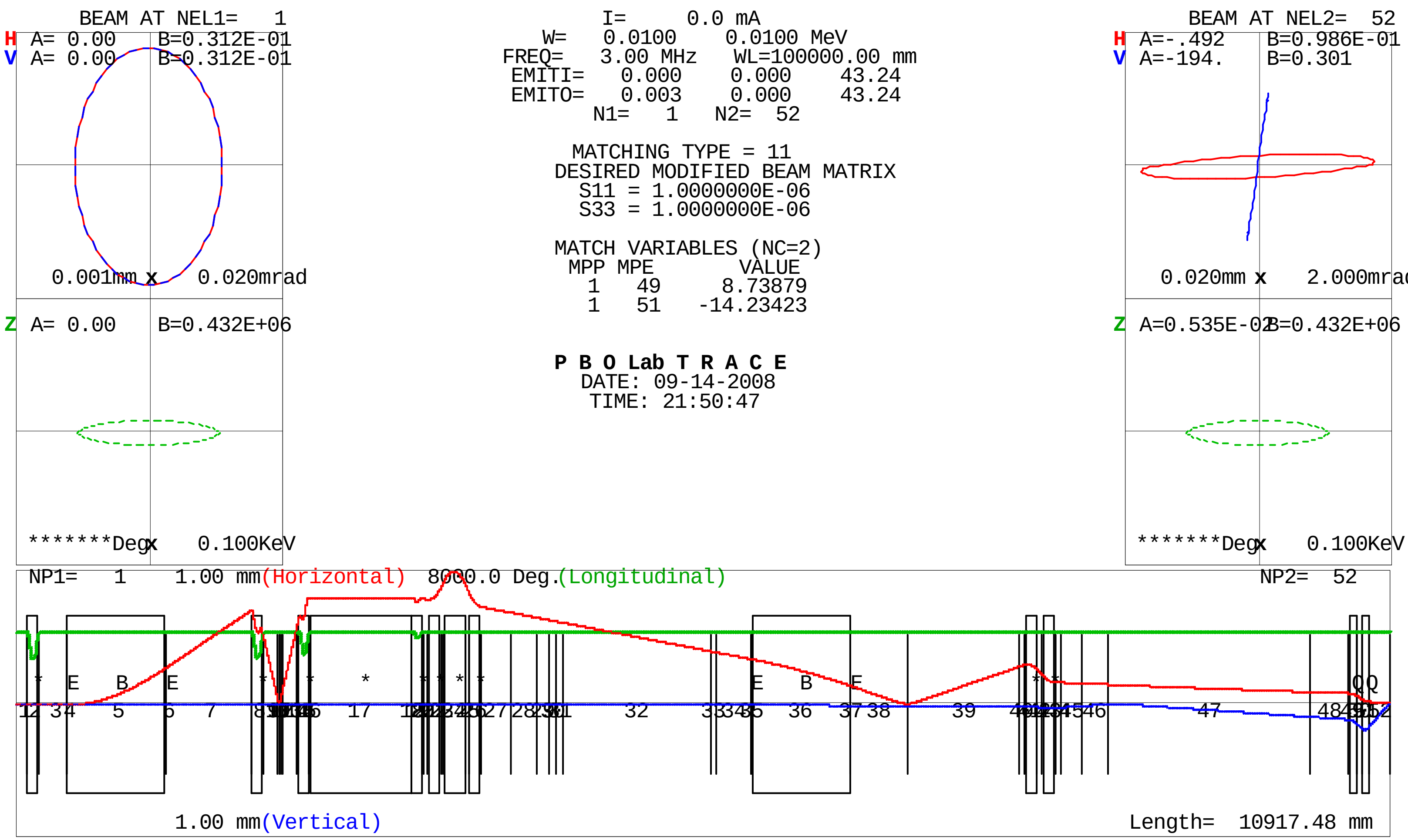
- **Can Couple Elements Parameters to Match Parameters**
  - **- k=+1 Coupling: Couple Parameter = Match Parameter**
  - **- k=-1 Coupling: Couple Parameter = - Match Parameter,**
    EXCEPT for Drift Lengths: Sum of 2 Drifts = Constant

- **PBO Lab version of TRACE 3-D**
  - **- Electrostatic (ES) Elements that can be used by TRACE 3-D**
  - **- Can Import TRACE 3-D Input Files from other TRACE 3-D versions***
  - **- Can Write TRACE 3-D Input Files for other TRACE 3-D versions***
    ***Assuming versions have some degree of compatibility!**

- **Display Options Limited: Profiles and Phase Space Plots**
  - **- Can Overlay ("Trace on Background") Profiles for Comparison**

4. Introduction to TRACE 3-D (continued)

Primary Graphical Output: "Graph Beam Line"



5. Introduction to Beamline Simulator

- **Developed by Morgan & Kurt Dehnel (D-PACE)**
- **Standalone Program - *Not* a PBO Lab Module**
- **Six Magnetic Optical Elements**
  - **Five are Common (e.g. TRANSPORT) Elements:**
    Drift, Quad, Solenoid, Bend (S-Bend, normal entry), Rotate
  - **Thin Lens**
- **Can Also Enter a "Non-Standard" Element via R-matrix Element**
- **Supports Misalignment of Elements via "Perturbation" Element**
- **Can Compute Beam Envelopes Through Beamline**
- **Can Track Individual Particles ("rays") Through Beamline: 1 to 10,000**
  $\Rightarrow$ **"Performance Code" Rather Than a "Design Code"**
- **Single Parameter Fitting**
- **Provides a Unique Simulated Real-time Tuning Capability**
- **Good Suite of Graphics & Plot Tools**
- **Good and Very Detailed Manual: "Using Beamline Simulator"**

5. Introduction to Beamline Simulator (continued)

- **Uses a 5×5** R-Matrix **rather than 6×6** R-Matrix
  - **Recall that for Magnetic Optics the Momentum (& Energy) Conserved**

$$\Rightarrow \quad d\delta/ds = 0$$

  - **So** $R_{66} \equiv 1$ **and** $R_{6i} \equiv 0$ **for all** $i < 6$**. In addition** $R_{i5} \equiv 0$ **for all** $i < 5$

    Ignore the path-length (bunch length) variable l **then**

    $\Rightarrow$ **No need for full 6×6** R-Matrix **(magnetic systems)**

  - **5-D coordinates same as 5 of the "Standard" 6-D coordinates:**

Beamline Simulator:	$(q_i)=(x,x',y,y', \delta)$
TRACE 3-D, TRANSPORT:	$(q_i)=(x,x',y,y', l,\delta)$

- **Several "pure magnetic" codes use this "simplified" 5×5** R-Matrix
- **Cannot readily model acceleration / deceleration:**
  - **No ElectroStatic (ES) Elements**
  - **No RadioFrequency (RF) Elements**
  - **Does not model bunched beams**

5. Introduction to Beamline Simulator (continued)

- **Beam uses a 5×5** σ-Matrix **rather than 6×6** σ-Matrix

- **Initial Beam Input is "almost" Standard:**
  - **Semi-Axis Parameters**
  - σ **Matrix Directly**

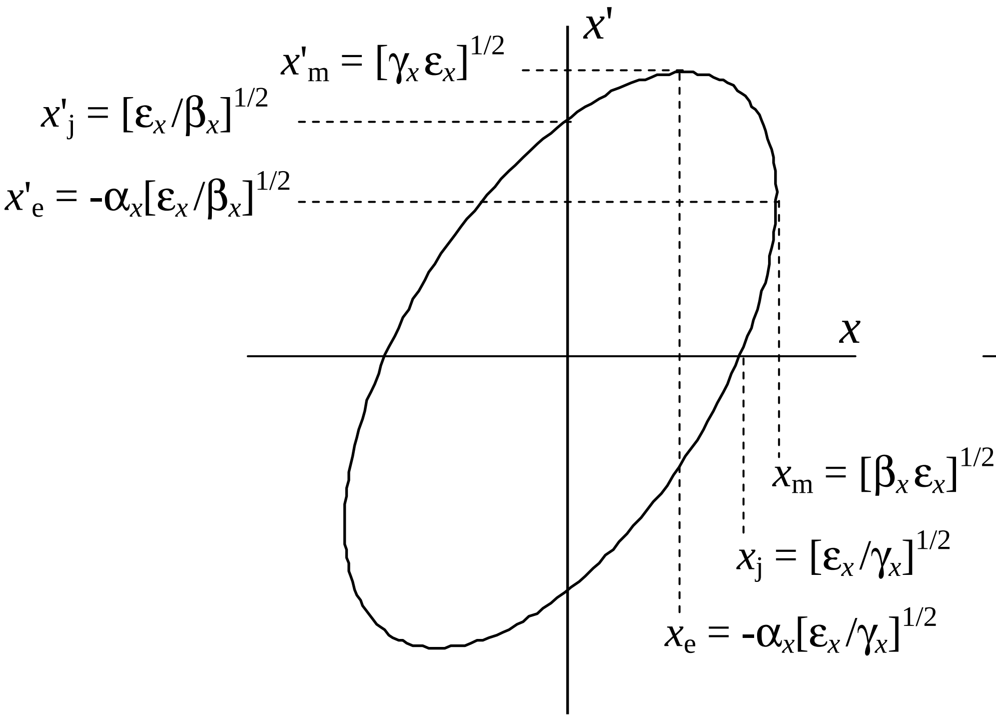
- **Semi-Axis Beam Parameters are a Little "Non-Standard"**
  - **Beam Size and Beam Divergence are Standard**
  - **Reduced** σ **Matrix (i.e. Correlation Parameters** r_{ij}**) Not Used**

  $\Rightarrow$ **Possible to Input Off-Diagonal** σ_{ij} **Such That** $r_{ij} > 1$.

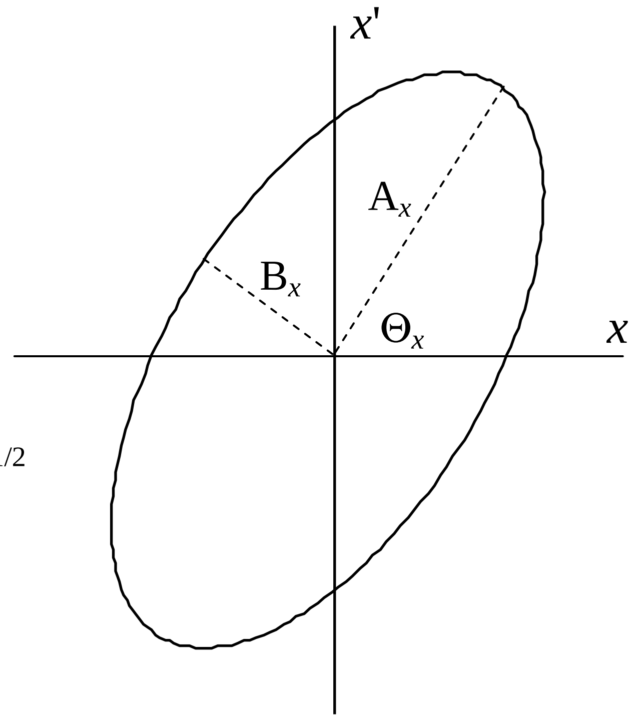
- **No Direct Twiss Parameter Representation, But Other Capability:**
  - **Initial Phase-Space Can Defined by "Virtual" Drifts & Thin-Lenses**
  - **The "Geometry Representation" Angle** Θ **is Calculated & Displayed**
    Use these "Angles" with Caution

5. Introduction to Beamline Simulator (continued)

Twiss Representation



Geometric Parameterization



$$\gamma_x /\varepsilon_x = (\cos\Theta_x / A_x)^2 + (\sin\Theta_x / B_x)^2$$

$$\beta_x /\varepsilon_x = (\sin\Theta_x / A_x)^2 + (\cos\Theta_x / B_x)^2$$

$$\alpha_x /\varepsilon_x = \cos\Theta_x \sin\Theta_x \ [(1 / B_x)^2 - (1 / A_x)^2]$$

5. Introduction to Beamline Simulator (continued)

After a Little Algebra it Can Be Shown for the Geometric Representation that:

$$\tan(2\Theta_x) = 2\,\alpha_x / (\beta_x - \gamma_x) \quad \text{(but units!?!)}$$

Let's Try an Example:

$$x_m = 1.00 \text{ mm}, \qquad x'_m = 10.0 \text{ mrad} = 0.010 \text{ rad}$$

$$\sigma_{11} = 1.00 \text{ mm}^2 \qquad \sigma_{22} = 0.0001 \text{ rad}^2 \quad \sigma_{12} = 0.005 \text{ mm-rad}$$

$$\varepsilon_x = 8.660254 \;\; \pi\text{-mm-mrad}, \quad r_{12} = 0.5$$

$$\alpha_x = -\, r_{12}/(1 - r_{12}^{\,2})^{1/2} = -\, 0.577350 \text{ radians}$$

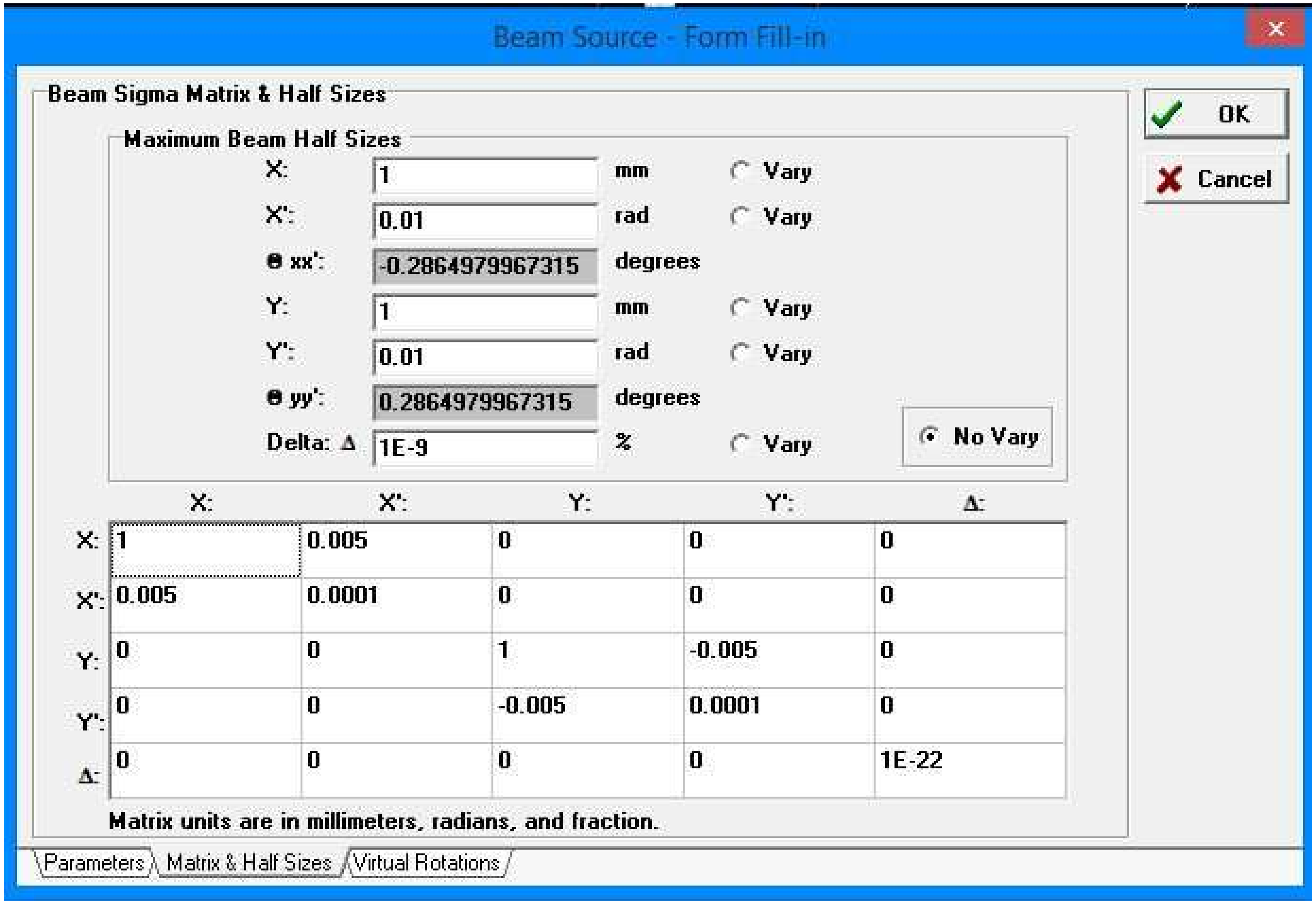
$$\beta_x = 0.115470 \text{ mm/mrad} \qquad \gamma_x = (1 - \alpha_x^{\,2}) \,/\, \beta_x = 5.773508 \;\; \text{mrad/mm}$$

Or in Different Units:

$$\beta_x = 115.470 \quad \text{mm/rad} \qquad \gamma_x = 0.005773508 \;\; \text{rad/mm}$$

* **Results in** Blue **on this page are from** PBO Lab **for this example.**

5. Introduction to Beamline Simulator (continued)



	X:	X':	Y:	Y':	Δ:
X:	1	0.005	0	0	0
X':	0.005	0.0001	0	0	0
Y:	0	0	1	-0.005	0
Y':	0	0	-0.005	0.0001	0
Δ:	0	0	0	0	1E-22

5. Introduction to Beamline Simulator (continued)

Units Choice 1 (PBO Lab Defaults for Twiss Parameters):

$$\beta_x = 0.115470 \text{ mm/mrad} \qquad \gamma_x = (1- \alpha_x^{\,2}) / \beta_x = 5.773508 \text{ mrad/mm}$$

$$\tan(2\Theta_x) = 2\,\alpha_x / (\beta_x - \gamma_x) = 1.1547 / 5.658038 = 0.204081 \text{ (units!?!)}$$

$$(2\Theta_x) = 11.535° \quad \text{or} \quad \Theta_x = 5.7675°$$

Units Choice 2 (Beamline Simulator):

$$\beta_x = 115.470 \text{ mm/rad} \qquad \gamma_x = 0.005773508 \text{ rad/mm}$$

$$\tan(2\Theta_x) = 2\,\alpha_x / (\beta_x - \gamma_x) = 1.1547 / 115.464 = 0.0100005 \text{ (units!?!)}$$

$$(2\Theta_x) = 0.57297° \text{ or } \Theta_x = 0.28648°$$

Beamline Simulator gives for this example $\Theta_{xx'} = - 0.286497996...°$

6. Summary of Part I

- **Overview of Coordinate Systems and Basic Matrix Descriptions**
- **Relationship Between Semi-Axes and Twiss Beam Description**
- **Overview of Drift, Quad, and Bend Equations of Motion & Matrix Solutions**
- **Guide to Fitting Constraints (Point-to-Point, etc.)**
- **Summary of Primary TRACE 3-D Capabilities**
- **Brief Introduction to Beamline Simulator**

Part II $\Rightarrow$ **Use the PBO Lab TRACE 3-D Module to work some examples**