Modelling and implementation of the “6D” beam-beam interaction

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Keywords: beam-beam, 6D, synchro beam mapping

Abstract

These slides illustrate the numerical modelling of a beam-beam interaction using the “Synchro Beam Mapping” approach. The employed description of the strong beam allows correctly accounting for the hour-glass effect as well as for linear coupling at the interaction point. The implementation of the method within the SixTrack code is reviewed and tested.
Modelling and implementation of the “6D” beam-beam interaction

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Outline

• Introduction

• “6D” beam beam treatment
  o Handling the crossing angles: “the boost”
  o Transverse “generalized kicks”
  o Description of the strong beam (Σ-matrix)
  o Handling linear coupling
  o Longitudinal kick

• Implementation

• Testing:
  o “Boost” and “Anti-boost”
  o Transverse kicks
  o Other derivatives of the electric potential
  o Σ-matrix propagation with linear coupling
  o Σ-matrix transformation to un-coupled frame
  o Constant charge slicing
  o Complete multi-slice interaction

• Handling the denominators
Goal: review of the 6D beam-beam lens implemented in SixTrack

Tried to answer two main questions:

• What is the code supposed to do?
  → Mathematical derivation behind the implemented numerical model

• Is the code doing what it is supposed to do?
  → Verify the implementation of the above numerical model
The code simulates a \textbf{beam-beam interaction} using the \textit{“Synchro Beam Mapping”} technique in the presence of:

- \textbf{Crossing angle} ($\phi$)
- \textbf{Arbitrary crossing plane} ($\alpha$)
- Optics at the IP described by a \textbf{general 4D correlation matrix} ($\Sigma$-matrix)

\rightarrow \text{hour glass effect, elliptic beams, alphas, and linear coupling at the IP}

are included in the modeling

This makes the \textbf{mathematical derivation quite heavy}

Implementation in Sixtrack in \textbf{largely based on}:

- [1] \textit{A symplectic beam-beam interaction with energy change}, by K. Hirata, H. W. Moshammer, F. Ruggiero, 1992
- [2] \textit{Don't be afraid of beam-beam interactions with a large crossing angle}, by K. Hirata, 1993

... but \textbf{important parts} (e.g. inverse boost, “optics de-coupling” including longitudinal derivatives) are \textbf{not reported in the papers nor anywhere else}, to our best knowledge...
• Invested some time in **understanding and re-constructing the mathematical treatment** trying to use as little as possible the source code as a reference

→ **Independent reconstruction** of the equations to verify the implementation in Sixtrack and to be used as a basis for a modern implementation (GPU compatible, for example)

→ **Parts not available in literature** (mainly inverse Lorentz boost, and a large fraction of the coupling treatment) **had to be re-derived**

• Prepared a **document** including the full set of equation to enable a possible re-implementation (and avoid that somebody has to redo the same exercise in ten years :-)

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**CERN-ACC-NOTE-XXX**
2017-12-01
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**6D beam-beam interaction step-by-step**
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Keywords: beam-beam, 6D, synchro beam mapping

**Summary**
This document describes in detail the numerical method used in different simulation codes for the simulation of beam-beam interactions using the "Synchro Beam Mapping" approach to correctly model the coupling introduced by beam-beam between the longitudinal and the transverse plane. The goal is to provide in a compact, complete and self-consistent manner the set of equations needed for the implementation in a numerical code. The effect of a "crossing angle" in an arbitrary "crossing plane" with respect to the assigned reference frame is taken into account with a suitable coordinate transformation. The employed description of the strong beam allows correctly accounting for the hour-glass effect as well as for linear coupling ad the interaction point.
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• Handling the denominators
The goal

- We want to simulate a **beam-beam interaction** taking into account the **finite longitudinal size of the two beams**

- We are in the framework on the **weak-strong treatment**: we have a particle (of the weak-beam) that we are tracking. It interacts with a strong beam that is “rigid”, i.e. unaffected by the weak beam
Hypotheses that need to be satisfied

We will use the “synchro-beam mapping” approach introduced by Hirata, Moshammer and Ruggiero [1]. To do so, the following **conditions need to be satisfied**:

- We work in **ultra-relativistic** approximation $v = c$ for both beams.
- The **strong beam is travelling backwards** $s_{\text{strong}}(t) = \sigma_{\text{strong}} + ct$.
- $P_x = P_y = 0$ for the strong beam:
  - The transverse electric field can be calculated solving a 2D Poisson problem.
- The **angles of the test particle are small** so that we can assume that it travels at the speed of light along $s$: $s(t) = \sigma - ct$.

- In the presence of a **crossing angle** a reference frame satisfying all the conditions above cannot be found by simple rotation in the lab frame, but this can be obtained by applying also a **Lorentz boost in the crossing plane** as shown by Hirata in [2].
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A dance of reference systems

Assuming that the beams are colliding (no separation):
- We assume that we are in the reference system of the weak beam
- The Interaction Point (IP) is at $s=0$
- The crossing plane is defined by our $s$-axis and by the strong beam
- We call $\alpha$ the angle between the crossing plane and the $x$-$s$ plane
- We call $\phi$ the half crossing angle

In the presence of an offset between the beams (separation), the orientation of the reference system is defined by the weak beam closed orbit and the system is centered at the IP location as defined for the strong beam → the strong beam passes always through the origin of the reference frame.
We look at the problem in the crossing plane.

We introduce move to the “barycentric” reference system in which the weak and the strong beam are at $+\phi$ and $-\phi$ respectively.
• In the crossing plane the interaction looks like this...
• To apply the Hirata, Moshammer, Ruggiero treatment we practically need to suppress the angle for the two beams (impossible by simple rotation)
In the crossing plane the interaction looks like this...

To apply the Hirata, Moshammer, Ruggiero treatment we practically need to suppress the angle for the two beams (impossible by simple rotation)

This can be achieved by using a boosted frame that is moving w.r.t. the lab
In the **boosted frame** the interaction looks like this.
This transformation is applied for positions:

\[
\begin{pmatrix}
\sigma^* \\
x^* \\
s^* \\
y^*
\end{pmatrix} = A^{-1} R_{CP}^{-1} L_{\text{boost}} R_{CA} R_{CP} A
\begin{pmatrix}
\sigma \\
x \\
s \\
y
\end{pmatrix}
\]

- \(A\) is the matrix transforming the accelerator coordinates (Courant-Snyder) to Cartesian coordinates:

\[
\begin{pmatrix}
ct \\
X \\
Z \\
Y
\end{pmatrix} = A
\begin{pmatrix}
\sigma \\
x \\
s \\
y
\end{pmatrix}
= \begin{pmatrix}
-1 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\sigma \\
x \\
s \\
y
\end{pmatrix}
\]

- \(R_{CP}\) is the rotation matrix bringing the crossing plane in the X-Z plane:

\[
R_{CA} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \phi & \sin \phi & 0 \\
0 & -\sin \phi & \cos \phi & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

- \(R_{CP}\) is the rotation matrix moving to the barycentric frame:

\[
R_{CP} = \begin{pmatrix}
1 & 0 & 1 & 0 \\
0 & \cos \alpha & 0 & \sin \alpha \\
0 & 0 & 1 & 0 \\
0 & -\sin \alpha & 0 & \cos \alpha
\end{pmatrix}
\]

- \(L_{\text{boost}}\) is the Lorentz boost in the direction of the rotated X-axis:

\[
L_{\text{boost}} = \begin{pmatrix}
1/ \cos \phi & -\tan \phi & 0 & 0 \\
-\tan \phi & 1/ \cos \phi & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]
This transformation is applied for momenta:

\[
\begin{pmatrix}
\delta^* \\
p_x^* \\
h^* \\
p_y^*
\end{pmatrix}
= B^{-1} R_{CP}^{-1} L_{\text{boost}} R_{CA} R_{CP} B
\begin{pmatrix}
\delta \\
p_x \\
h \\
p_y
\end{pmatrix}
\]

- **B** is the matrix transforming the accelerator coordinates (Courant-Snyder) to Cartesian coordinates:

\[
\begin{pmatrix}
E/c - p_0 \\
P_x \\
P_z - p_0 \\
P_y
\end{pmatrix}
= p_0
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\delta \\
p_x \\
h \\
p_y
\end{pmatrix}
\]

- **\( R_{CP} \)** is the rotation matrix bringing the crossing plane in the X-Z plane:

\[
R_{CA} =
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \phi & \sin \phi & 0 \\
0 & -\sin \phi & \cos \phi & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

\[
R_{CP} =
\begin{pmatrix}
1 & 0 & 1 & 0 \\
0 & \cos \alpha & 0 & \sin \alpha \\
0 & 0 & 1 & 0 \\
0 & -\sin \alpha & 0 & \cos \alpha
\end{pmatrix}
\]

- **\( L_{\text{boost}} \)** is the Lorentz boost in the direction of the rotated X-axis:

\[
L_{\text{boost}} =
\begin{pmatrix}
1/ \cos \phi & -\tan \phi & 0 & 0 \\
-\tan \phi & 1/ \cos \phi & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]
Not all particles with \( s=0 \) are fixed points of the transformation:

\[ \Rightarrow \text{A drift back to } s=0 \text{ needs to be performed as we are tracking w.r.t. } s \text{ and not w.r.t. time} \]

We compute the angles:

\[
\begin{align*}
p_z^* &= \sqrt{(1 + \delta^*)^2 - p_x^*^2 - p_y^*^2} \\

h_x^* &= \frac{\partial h^*}{\partial p_x^*} = \frac{p_x^*}{p_z^*} \\

h_y^* &= \frac{\partial h^*}{\partial p_y^*} = \frac{p_y^*}{p_z^*} \\

h_\sigma^* &= \frac{\partial h^*}{\partial \delta} = 1 - \frac{\delta^* + 1}{p_z^*}
\end{align*}
\]

We drift the particles to \( s=0 \):

\[
\begin{align*}
x^*(s^* = 0) &= x^*(s) - h_x^*s \\
y^*(s^* = 0) &= y^*(s) - h_y^*s \\
\delta^*(s^* = 0) &= \delta^*(s) - h_\delta^*s
\end{align*}
\]

The entire procedure needs to be reverted after the interaction, see note.
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• Handling the denominators
The synchro-beam method: transverse “generalized kicks”

The strong beam is cut in several slices having different transverse offset.
A particle with $z=0$ and a slice having $z=0$ collide at the IP.
The synchro-beam method: transverse “generalized kicks”

A particle and a slice with generic \( z \) coordinates will collide at a different \( s \) coordinate, Collision Point - CP, given by:

\[
S = \frac{\sigma^* - \sigma_{sl}^*}{2}
\]

(in sixtrack jargon \( z \) is called \( \sigma \))

... but within the tracking code, the beam-beam interaction acts as a thin element installed at the IP (i.e. the \( s \) where the synchronous particles of the two beams meet). This means that:

- Particles are tracked to the IP
- The BB interaction is applied
- Tracking restarts from the IP
- The description of the strong beam is provided at the IP
The synchro-beam method: transverse “generalized kicks”

We proceed as follows:

1. **We drift** the slice and the weak particle from the IP to the CP

\[ \bar{x}^* = x^* + p_x^* S - x_{sl}^* \]  
\[ \bar{y}^* = y^* + p_y^* S - y_{sl}^* \]

w.r.t. the slice centroid

(a particle having an angle will probe the strong-beam electric field at a different transverse coordinates)

2. **We apply the kick** at the CP:

\[ p_{x,new}^* = p_x^* + F_x^* \]
\[ p_{y,new}^* = p_y^* + F_y^* \]

3. **We drift** the particles back from the CP to the IP using the new angles:

\[ x_{new}^* = x^* - SF_x^* \]
\[ y_{new}^* = y^* - SF_y^* \]
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• **Handling the denominators**
The shape of the strong beam is described by **4D correlation matrix (Σ-matrix)**

The **phase space distribution** can be written as:

$$f(\eta) = f_0 e^{-\eta^T \Sigma^{-1} \eta} \quad \text{with} \quad \eta = \begin{pmatrix} x \\ p_x \\ y \\ p_y \end{pmatrix}$$

Points having same phase space density lie on hyper-elliptic manifolds defined by the equation:

$$\eta^T \Sigma^{-1} \eta = \text{const.}$$

Σ contains all the information about the beam shape and divergence (including linear coupling) and can be transported from the IP to the CP (assuming that we are in a drift):

\[
\begin{align*}
\Sigma_{11}^* &= \Sigma_{11}^0 + 2\Sigma_{12}^0 \Sigma + \Sigma_{22}^0 \Sigma^2 \\
\Sigma_{33}^* &= \Sigma_{33}^0 + 2\Sigma_{34}^0 \Sigma + \Sigma_{44}^0 \Sigma^2 \\
\Sigma_{13}^* &= \Sigma_{13}^0 + \left(\Sigma_{14}^0 + \Sigma_{23}^0\right) \Sigma + \Sigma_{24}^0 \Sigma^2 \\
\Sigma_{12}^* &= \Sigma_{12}^0 + \Sigma_{22}^0 \Sigma \\
\Sigma_{14}^* &= \Sigma_{14}^0 + \Sigma_{24}^0 \Sigma \\
\Sigma_{22}^* &= \Sigma_{22}^0 \\
\Sigma_{23}^* &= \Sigma_{23}^0 + \Sigma_{24}^0 \Sigma \\
\Sigma_{24}^* &= \Sigma_{24}^0 \\
\Sigma_{34}^* &= \Sigma_{34}^0 + \Sigma_{44}^0 \Sigma \\
\Sigma_{44}^* &= \Sigma_{44}^0
\end{align*}
\]

Convention:
1 → x, 2 → pₓ, 3 → y, 4 → pᵧ
In general, **linear coupling** of the strong beam can be present:

- The **coupling angle** and the **beam sizes** in the decoupled frame can be obtained by **diagonalization** of the $\Sigma$-matrix

- Coupling angle depends on the $s$-coordinate
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→ The **coupling angle** and the **beam sizes** in the decoupled frame can be obtained by **diagonalization** of the $\Sigma$-matrix

→ Coupling angle depends on the $s$-coordinate

Worked on simplifying the notation in this part:

\[
R (S) = \Sigma_{11}^* - \Sigma_{33}^* \\
W (S) = \Sigma_{11}^* + \Sigma_{33}^* \\
T (S) = R^2 + 4\Sigma_{13}^*^2
\]

Semi-axes in the decoupled frame:

\[
\hat{\Sigma}_{11}^* = \frac{1}{2} \left( W + \text{sgn}(R) \sqrt{T} \right) \\
\hat{\Sigma}_{33}^* = \frac{1}{2} \left( W - \text{sgn}(R) \sqrt{T} \right)
\]
In general, **linear coupling** of the strong beam can be present:

→ The **coupling angle** and the **beam sizes** in the decoupled frame can be obtained by **diagonalization** of the $\Sigma$-matrix

→ Coupling angle depends on the $s$-coordinate

\[ R \left( S \right) = \Sigma_{11}^* - \Sigma_{33}^* \]
\[ W \left( S \right) = \Sigma_{11}^* + \Sigma_{33}^* \]
\[ T \left( S \right) = R^2 + 4 \Sigma_{13}^* \]

\[ \cos \theta = \frac{R}{\sqrt{T}} \]
\[ \cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}} \]
\[ \sin \theta = \text{sgn}(R) \text{sgn}(\Sigma_{13}^*) \sqrt{\frac{1}{2} \left( 1 - \cos 2\theta \right)} \]
Linear coupling of the strong beam

Once the coupling angle and the beam sizes in the decoupled plain are known, we proceed as follows:

1. We calculate the particle coordinates in the **decoupled frame** at the CP:
   \[ \hat{x}^* = x^* \cos \theta + y^* \sin \theta \]
   \[ \hat{y}^* = -x^* \sin \theta + y^* \cos \theta \]

2. We calculate the **kick** from the slide in the decoupled reference frame:
   \[ \hat{f}_x^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{x}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}, \hat{\Sigma}_{33} \right) \]
   \[ \hat{f}_y^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{y}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}, \hat{\Sigma}_{33} \right) \]
   where \( \hat{U}^* \) is the electric potential
   \[
   K_{sl} = \frac{N_{sl} q_{sl} q_0}{P_0 c}
   \]

For Gaussian (uncoupled) beams, closed forms exist to evaluate these quantities.

**For a bi-Gaussian beam (elliptic) [2]:**

\[
\hat{f}_x^* = -\frac{\partial \hat{U}^*}{\partial \hat{x}^*} = \frac{1}{2\epsilon_0 \sqrt{2\pi} (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})} \text{Im} \left[ \frac{\hat{x}^* + i\hat{y}^*}{\sqrt{2 (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})}} - \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}} \right) \right]
\]

\[
\hat{f}_y^* = -\frac{\partial \hat{U}^*}{\partial \hat{x}^*} = \frac{1}{2\epsilon_0 \sqrt{2\pi} (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})} \text{Re} \left[ \frac{\hat{x}^* + i\hat{y}^*}{\sqrt{2 (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})}} - \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}} \right) \right]
\]

**Bassetti-Erskine**

\[
\left[ \frac{\hat{x}^* \sqrt{\hat{\Sigma}_{33} + i\hat{y}^* \sqrt{\hat{\Sigma}_{11}}} \sqrt{\hat{\Sigma}_{11} - \hat{\Sigma}_{33}}}{\sqrt{2 (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})}} \right] \left[ \frac{\hat{x}^* \sqrt{\hat{\Sigma}_{33} + i\hat{y}^* \sqrt{\hat{\Sigma}_{11}}} \sqrt{\hat{\Sigma}_{11} - \hat{\Sigma}_{33}}}{\sqrt{2 (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})}} \right]
\]

\[
\left[ \frac{\hat{x}^* \sqrt{\hat{\Sigma}_{33} + i\hat{y}^* \sqrt{\hat{\Sigma}_{11}}} \sqrt{\hat{\Sigma}_{11} - \hat{\Sigma}_{33}}}{\sqrt{2 (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})}} \right] \left[ \frac{\hat{x}^* \sqrt{\hat{\Sigma}_{33} + i\hat{y}^* \sqrt{\hat{\Sigma}_{11}}} \sqrt{\hat{\Sigma}_{11} - \hat{\Sigma}_{33}}}{\sqrt{2 (\hat{\Sigma}_{11} - \hat{\Sigma}_{33})}} \right]
\]
Once the coupling angle and the beam sizes in the decoupled plain are known, we proceed as follows:

1. We calculate the particle coordinates in the **decoupled frame** at the CP:
   \[
   \hat{x}^* = \bar{x}^* \cos \theta + \bar{y}^* \sin \theta \\
   \hat{y}^* = -\bar{x}^* \sin \theta + \bar{y}^* \cos \theta 
   \]

2. We calculate the **kick** from the slide in the decoupled reference frame:
   \[
   \hat{F}_x^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{x}^*} (\hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^*) \\
   \hat{F}_y^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{y}^*} (\hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^*) 
   \]
   where
   \[
   \hat{U}^* \text{ is the electric potential} \\
   K_{sl} = \frac{N_{sl} q_{sl} q_0}{P_0 c}
   \]
   For Gaussian (uncoupled) beams, closed forms exist to evaluate these quantities.

3. We **rotate the kicks** to decoupled reference frame
   \[
   F_x^* = \hat{F}_x^* \cos \theta - \hat{F}_y^* \sin \theta \\
   F_y^* = \hat{F}_x^* \sin \theta + \hat{F}_y^* \cos \theta
   \]

4. We **apply the kicks** to the transverse momenta and **drift back** to the IP (as explained before)
   \[
   p_{x, \text{new}}^* = p_x^* + F_x^* \\
   p_{y, \text{new}}^* = p_y^* + F_y^* \\
   x_{\text{new}}^* = x^* - SF_x^* \\
   y_{\text{new}}^* = y^* - SF_y^*
   \]
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• Handling the denominators
The longitudinal kick has **two components**:

\[ p_{z,\text{new}} = p_z^* + F_z^* + \frac{1}{2} \left[ F_x^* \left( p_x^* + \frac{1}{2} F_x^* \right) + F_y^* \left( p_y^* + \frac{1}{2} F_y^* \right) \right] \]

The trajectory is, in general, not perpendicular to the transverse fields of the strong beam (see Hirata [1] for detailed explanation) → this introduces this term in the longitudinal kick.
The longitudinal kick has two components:

\[ p_{z, new}^* = p_z^* + F_z^* + \frac{1}{2} F_x^* \left( p_x^* + \frac{1}{2} F_x^* \right) + F_y^* \left( p_y^* + \frac{1}{2} F_y^* \right) \]

Another component of the longitudinal kick arises from the fact that the transverse shape of the strong beam is changing along \( z \) (hour-glass effect, "rotating" coupling angle)

- The electric potential depends on \( z \)
- The gradient of the electric potential (i.e. the electric field) has a \( z \) component
- There is a \( z \)-kick, i.e. again a change in the particle energy

We need to evaluate the derivative w.r.t. \( z \) (or \( \sigma \), or small-\( s \)) of the electric potential

As we have written down most of the involved quantities as a function of the coordinate of the CP (capital-S) we just notice that:

\[ S = \frac{\sigma^* - \sigma_{sl}^*}{2} \]

\[ \frac{\partial}{\partial z} = \frac{1}{2} \frac{\partial}{\partial S} \]

\[ F_z^* = \frac{1}{2} \frac{\partial}{\partial S} \left[ \hat{U}^* \left( \hat{x}^* (\theta(S)), \hat{y}^* (\theta(S)), \hat{\Sigma}_{11}^*(S), \hat{\Sigma}_{33}^*(S) \right) \right] \]

(in sixtrack jargon

\( z \) is called \( \sigma \)
Energy change: grad-phi effect

\[ F^*_z = \frac{1}{2} \frac{\partial}{\partial S} \left[ \hat{U}^* \left( \hat{x}^* (\theta(S)), \hat{y}^* (\theta(S)), \hat{\Sigma}_{11}^*(S), \hat{\Sigma}_{33}^*(S) \right) \right] \]

Derivative rule for nested functions:

\[ F^*_z = \frac{1}{2} \left( \hat{F}^*_x \frac{\partial}{\partial S} \left[ \hat{x}^* (\theta(S)) \right] + \hat{F}^*_y \frac{\partial}{\partial S} \left[ \hat{y}^* (\theta(S)) \right] + \hat{G}^*_x \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^*(S) \right] + \hat{G}^*_y \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^*(S) \right] \right) \]

We need to evaluate these eight terms...

\[ \hat{F}^*_x = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{x}} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \quad \hat{G}^*_x = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{11}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \]

\[ \hat{F}^*_y = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{y}} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \quad \hat{G}^*_y = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{33}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{33}^*, \hat{\Sigma}_{33}^* \right) \]
Energy change: grad-phi effect

\[ F_z^* = \frac{1}{2} \left( \hat{F}_x^* \frac{\partial}{\partial S} \left[ \hat{x}^* (\theta(S)) \right] + \hat{F}_y^* \frac{\partial}{\partial S} \left[ \hat{y}^* (\theta(S)) \right] + \hat{G}_x^* \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^* (S) \right] + \hat{G}_y^* \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^* (S) \right] \right) \]

\[ \hat{F}_x^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{x}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \quad \hat{G}_x^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{11}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \]

\[ \hat{F}_y^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{y}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \quad \hat{G}_y^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{33}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \]

For these four terms a closed forms exist for transverse Gaussian beams

For a bi-Gaussian beam (elliptic) [2]:

\[ \hat{f}_x^* = -\frac{\partial \hat{U}^*}{\partial \hat{x}^*} = \frac{1}{2\epsilon_0 \sqrt{2\pi} (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)} \text{Im} \left[ w \left( \frac{\hat{x}^* + i\hat{y}^*}{\sqrt{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)}} \right) - \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) \right] \]

\[ \hat{f}_y^* = -\frac{\partial \hat{U}^*}{\partial \hat{y}^*} = \frac{1}{2\epsilon_0 \sqrt{2\pi} (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)} \text{Re} \left[ w \left( \frac{\hat{x}^* + i\hat{y}^*}{\sqrt{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)}} \right) - \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) \right] \]

\[ \hat{g}_x^* = -\frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{11}^*} = -\frac{1}{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)} \left\{ \hat{x}^* \hat{E}_x^* + \hat{y}^* \hat{E}_y^* + \frac{1}{2\pi\epsilon_0} \left[ \frac{\hat{\Sigma}_{33}^*}{\hat{\Sigma}_{11}^*} \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) - 1 \right] \right\} \]

\[ \hat{g}_y^* = -\frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{33}^*} = \frac{1}{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)} \left\{ \hat{x}^* \hat{E}_x^* + \hat{y}^* \hat{E}_y^* + \frac{1}{2\pi\epsilon_0} \left[ \frac{\hat{\Sigma}_{11}^*}{\hat{\Sigma}_{33}^*} \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) - 1 \right] \right\} \]

where \( w \) is the Faddeeva function.

Bassetti-Erskine
For these four terms a closed forms exist for transverse Gaussian beams.
Energy change: grad-phi effect

\[ F_z^* = \frac{1}{2} \left( \hat{F}_x^* \frac{\partial}{\partial S} \left[ \hat{x}^* (\theta(S)) \right] + \hat{F}_y^* \frac{\partial}{\partial S} \left[ \hat{y}^* (\theta(S)) \right] + \hat{C}_x^* \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^* (S) \right] + \hat{C}_y^* \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^* (S) \right] \right) \]

\[ \hat{x}^* = \bar{x}^* \cos \theta + \bar{y}^* \sin \theta \]
\[ \hat{y}^* = -\bar{x}^* \sin \theta + \bar{y}^* \cos \theta \]

\[ \frac{\partial}{\partial S} \left[ \hat{x}^* (\theta(S)) \right] = \bar{x}^* \frac{\partial}{\partial S} [\cos \theta] + \bar{y}^* \frac{\partial}{\partial S} [\sin \theta] \]
\[ \frac{\partial}{\partial S} \left[ \hat{y}^* (\theta(S)) \right] = -\bar{x}^* \frac{\partial}{\partial S} [\sin \theta] + \bar{y}^* \frac{\partial}{\partial S} [\cos \theta] \]

With some goniometric trick:
\[ \frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta \]
\[ \frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta \]

Before we had written:
\[ \cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}} \]
\[ \frac{\partial}{\partial S} [\cos 2\theta] = \text{sgn}(R) \left( \frac{\partial R}{\partial S} \frac{1}{\sqrt{T}} - \frac{R}{2 (\sqrt{T})^3} \frac{\partial T}{\partial S} \right) \]

with
\[ R(S) = \Sigma_{11}^* - \Sigma_{33}^* \]
\[ W(S) = \Sigma_{11}^* + \Sigma_{33}^* \]
\[ T(S) = R^2 + 4\Sigma_{13}^*^2 \]

We just need to evaluate
\[ \frac{\partial}{\partial S} \cos 2\theta \]

where we need to evaluate the derivatives of R, T and W...
Energy change: grad-phi effect

\[ F_z^* = \frac{1}{2} \left( \hat{F}_x^* \frac{\partial}{\partial S} \left[ \hat{x}^* (\theta(S)) \right] + \hat{F}_y^* \frac{\partial}{\partial S} \left[ \hat{y}^* (\theta(S)) \right] + \hat{G}_x^* \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^* (S) \right] + \hat{G}_y^* \frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^* (S) \right] \right) \]

Derivatives of R, T and W

\[
\begin{align*}
R (S) &= \Sigma_{11}^* - \Sigma_{33}^* \\
W (S) &= \Sigma_{11}^* + \Sigma_{33}^* \\
T (S) &= R^2 + 4\Sigma_{13}^* \Sigma_{13}^* \\
\Sigma_{11}^* &= \Sigma_{11}^* + 2\Sigma_{12}^* S + \Sigma_{22}^* S^2 \\
\Sigma_{33}^* &= \Sigma_{33}^* + 2\Sigma_{34}^* S + \Sigma_{44}^* S^2 \\
\Sigma_{13}^* &= \Sigma_{13}^* + \left( \Sigma_{14}^* + \Sigma_{23}^* \right) S + \Sigma_{24}^* S^2
\end{align*}
\]

\[
\begin{align*}
\frac{\partial R}{\partial S} &= 2 \left( \Sigma_{12}^* - \Sigma_{34}^* \right) + 2S \left( \Sigma_{22}^* - \Sigma_{44}^* \right) \\
\frac{\partial W}{\partial S} &= 2 \left( \Sigma_{12}^* + \Sigma_{34}^* \right) + 2S \left( \Sigma_{22}^* + \Sigma_{44}^* \right) \\
\frac{\partial \Sigma_{13}^*}{\partial S} &= \Sigma_{14}^* + \Sigma_{23}^* + 2\Sigma_{24}^* S \\
\frac{\partial T}{\partial S} &= 2R \frac{\partial R}{\partial S} + 8\Sigma_{13}^* \frac{\partial \Sigma_{13}^*}{\partial S}
\end{align*}
\]

Before we had written:

\[
\cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}}
\]

\[
\frac{\partial}{\partial S} [\cos 2\theta] = \text{sgn}(R) \left( \frac{\partial R}{\partial S} \frac{1}{\sqrt{T}} - \frac{R}{2 \left( \sqrt{T} \right)^3} \frac{\partial T}{\partial S} \right)
\]

With some trigonometric trick, we just need to evaluate \( \Sigma_{11}^*, \Sigma_{33}^* \) and \( \Sigma_{13}^* \)

where we need to evaluate the derivatives of R, T and W...
Energy change: grad-phi effect

\[ F_z^* = \frac{1}{2} \left( \hat{F}_x^* \frac{\partial}{\partial S} [\hat{x}^*(\theta(S))] + \hat{F}_y^* \frac{\partial}{\partial S} [\hat{y}^*(\theta(S))] + \hat{G}_x^* \frac{\partial}{\partial S} [\hat{\Sigma}_{11}^*(S)] + \hat{G}_y^* \frac{\partial}{\partial S} [\hat{\Sigma}_{33}^*(S)] \right) \]

\[ \hat{\Sigma}_{11}^* = \frac{1}{2} \left( W + \text{sgn}(R) \sqrt{T} \right) \]
\[ \hat{\Sigma}_{33}^* = \frac{1}{2} \left( W - \text{sgn}(R) \sqrt{T} \right) \]

\[ \frac{\partial}{\partial S} [\hat{\Sigma}_{11}^*] = \frac{1}{2} \left( \frac{\partial W}{\partial S} + \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right) \]
\[ \frac{\partial}{\partial S} [\hat{\Sigma}_{33}^*] = \frac{1}{2} \left( \frac{\partial W}{\partial S} - \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right) \]

Again what we need to know are the derivatives of R, T and W, which were already shown in the previous slides.

**Derivatives of R, T and W**

\[ R(S) = \Sigma_{11}^* - \Sigma_{33}^* \]
\[ W(S) = \Sigma_{11}^* + \Sigma_{33}^* \]
\[ T(S) = R^2 + 4\Sigma_{13}^*^2 \]

\[ \Sigma_{11}^* = \Sigma_{11}^0 + 2\Sigma_{12}^0 S + \Sigma_{22}^0 S^2 \]
\[ \Sigma_{33}^* = \Sigma_{33}^0 + 2\Sigma_{34}^0 S + \Sigma_{44}^0 S^2 \]
\[ \Sigma_{13}^* = \Sigma_{13}^0 + \left( \Sigma_{14}^0 + \Sigma_{23}^0 \right) S + \Sigma_{24}^0 S^2 \]

\[ \frac{\partial R}{\partial S} = 2 \left( \Sigma_{12}^0 - \Sigma_{34}^0 \right) + 2S \left( \Sigma_{22}^0 - \Sigma_{44}^0 \right) \]
\[ \frac{\partial W}{\partial S} = 2 \left( \Sigma_{12}^0 + \Sigma_{34}^0 \right) + 2S \left( \Sigma_{22}^0 + \Sigma_{44}^0 \right) \]
\[ \frac{\partial \Sigma_{13}^*}{\partial S} = \Sigma_{14}^0 + \Sigma_{23}^0 + 2\Sigma_{24}^0 S \]
\[ \frac{\partial T}{\partial S} = 2R \frac{\partial R}{\partial S} + 8\Sigma_{13}^* \frac{\partial \Sigma_{13}^*}{\partial S} \]
Handling the denominators

We have all the pieces, but on the way we introduced some denominators which can become zero! → we will deal with it later...

\[ R(S) = \Sigma_{11}^* - \Sigma_{33}^* \]
\[ W(S) = \Sigma_{11}^* + \Sigma_{33}^* \]
\[ T(S) = R^2 + 4\Sigma_{13}^* \]

\[ \cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}} \]
\[ \hat{\Sigma}_{11}^* = \frac{1}{2} \left( W + \text{sgn}(R) \sqrt{T} \right) \]
\[ \hat{\Sigma}_{33}^* = \frac{1}{2} \left( W - \text{sgn}(R) \sqrt{T} \right) \]

\[ \frac{\partial}{\partial S} [\hat{\Sigma}_{11}^*] = \frac{1}{2} \left( \frac{\partial W}{\partial S} + \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right) \]
\[ \frac{\partial}{\partial S} [\hat{\Sigma}_{33}^*] = \frac{1}{2} \left( \frac{\partial W}{\partial S} - \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right) \]

\[ \frac{\partial}{\partial S} [\cos 2\theta] = \text{sgn}(R) \left( \frac{\partial R}{\partial S} \frac{1}{\sqrt{T}} - \frac{R}{2} \frac{1}{(\sqrt{T})^3} \frac{\partial T}{\partial S} \right) \]

\[ \cos \theta = \sqrt{\frac{1}{2} (1 + \cos 2\theta)} \]
\[ \sin \theta = \text{sgn}(R)\text{sgn}(\Sigma_{13}^*) \sqrt{\frac{1}{2} (1 - \cos 2\theta)} \]

\[ \frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta \]
\[ \frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta \]
• Introduction
• “6D” beam beam treatment
  o Handling the crossing angles: “the boost”
  o Transverse “generalized kicks”
  o Description of the strong beam (Σ-matrix)
  o Handling linear coupling
  o Longitudinal kick
• Implementation
• Testing:
  o “Boost” and “Anti-boost”
  o Transverse kicks
  o Other derivatives of the electric potential
  o Σ-matrix propagation with linear coupling
  o Σ-matrix transformation to un-coupled frame
  o Constant charge slicing
  o Complete multi-slice interaction
• Handling the denominators
Initialization stage:

- Prepare **coefficients** for Lorentz boost
- **Slice** strong bunch
  - Compute slice charges and centroid coordinates
- **Boost strong beam** slices
  - Boost centroid coordinates
  - Boost $\Sigma$-matrix
- Store all information in a **data block**

Tracking routine:

- **Boost** coordinates of the **weak beam particle**
- Compute $S$ coordinate of the **collision point** (CP)
- **Transport strong beam** optics from the IP to the CP:
  - Transport sigma matrix to the CP
  - Compute coupling angle and beam sizes in the decoupled plane
  - Compute auxiliary quantities for the calculation of the longitudinal kick
- Compute **transverse kicks**
  - Transform coordinates of the weak beam particles to the un-coupled frame
  - Compute transverse forces in the un-coupled frame
  - Transform transverse kicks to the coupled frame
  - Apply transverse kicks in the coupled frame (change $p_x$, $p_y$)
  - Transport transverse kick from the CP to the IP and change particle positions $(x,y)$ accordingly
- Compute and apply the **longitudinal kick**
- **Anti-boost** coordinates of the weak beam particles
SixTrack implementation

Very hard to read and to debug, it can be kept alive... but definitely not ideal

...
• Started from previous work done by J. Barranco
  • Identified and described the interface of the main functional blocks
  • Built tables with the descriptions of the cumbersome notation used in the code

• Moved to the understanding and testing of the source code...
It quickly became evident that the only viable way of checking the SixTrack code was to build an independent implementation to compare against. Done keeping in mind:

- **Readability, modularity**, possibility to **interface with other codes** (PyHEADTAIL, SixTrackLib)
- **Compatibility with GPU**

```c
// Boost coordinates of the weak beam
BB6D_boost(&bb6data->parboost), &x_star, &px_star, &y_star, &py_star,
&6sigma_star, &delta_star);

// Syncrhon beam
for (i_slice=0; i_slice<N_slices; i_slice++)
{
    double sigma_slice_star = sigma_slices_star[i_slice];
    double x_slice_star = x_slices_star[i_slice];
    double y_slice_star = y_slices_star[i_slice];

    // Compute derivatives of the transformation
    double dS_x_bar_hat_star = x_bar_star*dS_costheta + y_bar_star*dS_sinhetha;
    double dS_y_bar_hat_star = -x_bar_star*dS_sinhetha + y_bar_star*dS_costheta;

    // Get transverse fields
    double Ex = Ey, Gx, Gy;
    get_Ex_Ey_Gx_Gy_gauss(x_bar_hat_star, y_bar_hat_star,
        sqrt(Sig_11_hat_star), sqrt(Sig_33_hat_star), bb6data->min_sigma_diff,
        &Ex, &Ey, &Gx, &Gy);

    // Compute kicks
    double Fx_hat_star = Ksl*Ex;
    double Fy_hat_star = Ksl*Ey;
    double Gx_hat_star = Ksl*Gx;
    double Gy_hat_star = Ksl*Gy;

    // Move kicks to coupled reference frame
    double Fx_star = Fx_hat_star*costheta - Fy_hat_star*sintetha;
    double Fy_star = Fx_hat_star*sintetha + Fy_hat_star*costheta;

    // Compute longitudinal kick
    double Fz_star = 0.5*(Fx_hat_star*dS_x_bar_hat_star + Fy_hat_star*dS_y_bar_hat_star +
        Gx_hat_star*dS_11_hat_star + Gy_hat_star*dS_33_hat_star);

    // Apply the kicks (Hirata's synchro-beam)
    delta_star = delta_star + Fz_star*0.5*(Fx_star*(px_star*0.5*Fy_star)+
        Fy_star*(py_star*0.5*Fy_star));

    x_star = x_bar_star + px_star + Fx_star;
    px_star = px_star + Fx_star;
    y_star = y_bar_star + py_star + Fy_star;
    py_star = py_star + Fy_star;

    // Compute derivatives of the transformation
    double dS_x_bar_hat_star = x_bar_star*dS_costheta + y_bar_star*dS_sinhetha;
    double dS_y_bar_hat_star = -x_bar_star*dS_sinhetha + y_bar_star*dS_costheta;

// Inverse boost on the coordinates of the weak beam
BB6D_inv_boost(&bb6data->parboost), &x_star, &px_star, &y_star, &py_star,
&6sigma_star, &delta_star);
```
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  o Constant charge slicing
  o Complete multi-slice interaction
• Handling the denominators
• Very difficult to identify problems by using the full tracking simulations
  o Need to test the single routine “on the bench”

• Procedure being performed for each functional block
  o Built a C/python implementation from the equations in the document
  o Extracted the corresponding sixtrack source code and compiled as of a stand-alone python module (f2py)
  o “Stress test” performed on the two: consistency checks, comparison against each other
<table>
<thead>
<tr>
<th>Module</th>
<th>Tests performed</th>
<th>Outcome</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boost/anti-boost</td>
<td>• Comparison Sixtrack vs C/python routine&lt;br&gt;• Checked that the two cancel each other</td>
<td>• Bug identified and <strong>corrected</strong></td>
</tr>
<tr>
<td>Beam-beam forces (with potential derivatives w.r.t. sigmas)</td>
<td>• Comparison sixtrack vs C/python routine&lt;br&gt;• Force compared against Finite Difference Poisson solver (PyPIC)&lt;br&gt;• Other derivatives compared against numerical integration/derivation</td>
<td>• <strong>All checks passed</strong></td>
</tr>
<tr>
<td>Beam shape propagation and coupling treatment</td>
<td>• Comparison Sixtrack vs C/python routine&lt;br&gt;• Comparison against MAD for a coupled beam line&lt;br&gt;• Crosscheck with numerical derivation</td>
<td>• Bug identified and <strong>corrected</strong>&lt;br&gt;<strong>Vanishing denominators</strong> not treated correctly → <strong>correct treatment developed and implemented</strong> in the library, <strong>to be ported in SixTrack</strong></td>
</tr>
<tr>
<td>Slicing</td>
<td>• Check against independent implementation</td>
<td>• Passed but precision is quite poor (1e-3)</td>
</tr>
<tr>
<td>Computation of the kicks</td>
<td>• Check against independent implementation</td>
<td>• <strong>All checks passed</strong></td>
</tr>
</tbody>
</table>
Outline

• Introduction

• “6D” beam beam treatment
  o Handling the crossing angles: “the boost”
  o Transverse “generalized kicks”
  o Description of the strong beam ($\Sigma$-matrix)
  o Handling linear coupling
  o Longitudinal kick

• Implementation

• Testing:
  o “Boost” and “Anti-boost”
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  o Other derivatives of the electric potential
  o $\Sigma$-matrix propagation with linear coupling
  o $\Sigma$-matrix transformation to un-coupled frame
  o Constant charge slicing
  o Complete multi-slice interaction

• Handling the denominators
• Boost and anti-boost should cancel each other exactly
• “Bench-test” cases: large crossing angle, test particle very off momentum and large $px$, $py$
• Test passed for the library
• Problem identified in the Sixtrack implementation

## Error after boost + anti-boost

<table>
<thead>
<tr>
<th>Python test routine</th>
<th>SixTrack routine</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$</td>
<td>4.3e-19</td>
</tr>
<tr>
<td>$px$</td>
<td>0.0</td>
</tr>
<tr>
<td>$y$</td>
<td>4.3e-19</td>
</tr>
<tr>
<td>$py$</td>
<td>3.e3-17</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\delta$</td>
<td>1e-16</td>
</tr>
<tr>
<td>$x$</td>
<td>6.5e-19</td>
</tr>
<tr>
<td>$px$</td>
<td>0.065</td>
</tr>
<tr>
<td>$y$</td>
<td>4.3e-19</td>
</tr>
<tr>
<td>$py$</td>
<td>3.e3-17</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>0.0</td>
</tr>
<tr>
<td>$\delta$</td>
<td>2.0e-17</td>
</tr>
</tbody>
</table>
Discrepancy found between in the anti-boost between derived equations and SixTrack source code:

\[ p_x = p_x^* \cos \phi + h \cos \alpha \tan \phi \]  \hspace{1cm} (95)
\[ p_y = p_y^* \cos \phi + h \sin \alpha \tan \phi \]  \hspace{1cm} (96)

\[
\text{TRACK}(2) = (\text{TRACK}(2) + \text{CALPHA} \cdot \text{SPHI} \cdot H1) \cdot \text{CPHI} \\
\text{TRACK}(4) = (\text{TRACK}(4) + \text{SALPHA} \cdot \text{SPHI} \cdot H1) \cdot \text{CPHI}
\]

The lines should be:

\[
\text{TRACK}(2) = (\text{TRACK}(2) \cdot \text{CPHI} + \text{CALPHA} \cdot \text{TPHI} \cdot H1) \\
\text{TRACK}(4) = (\text{TRACK}(4) \cdot \text{CPHI} + \text{SALPHA} \cdot \text{TPHI} \cdot H1)
\]

• Digging a bit we found out that the issue was already present in Hirata’s code from 1996, on which the Sixtrack implementation is based
Correction implemented in SixTrack

<table>
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</tr>
<tr>
<td>px</td>
</tr>
<tr>
<td>y</td>
</tr>
<tr>
<td>py</td>
</tr>
<tr>
<td>sigma</td>
</tr>
<tr>
<td>delta</td>
</tr>
</tbody>
</table>
Problem confirmed by Riccardo simulating a beam-beam interaction with **zero** intensity in the strong beam.

### Original implementation

<table>
<thead>
<tr>
<th>Coordinates before interaction</th>
<th>Coordinates after interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="dump.jp.dat" alt="Image" /></td>
<td><img src="dump_bb.dat" alt="Image" /></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ID</th>
<th>turn</th>
<th>[s]</th>
<th>x[m]</th>
<th>y[m]</th>
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### Corrected implementation

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Boost /anti-boost
• Impact on **realistic simulation study** assessed by Dario

• Tune scans comparison with 2017 ATS optics show no dramatic change, but slightly worse DA

---

**Old version**

ATS Optics; $\beta^* = 40$ cm; $Q' = 15$; $I_{MO} = 500$ A; $\varepsilon = 2.5$ $\mu$m; $I = 1.25 \times 10^{11}$ e; $X = 150$ $\mu$rad; Min DA.

**Corrected version**

ATS Optics; $\beta^* = 40$ cm; $Q' = 15$; $I_{MO} = 500$ A; $\varepsilon = 2.5$ $\mu$m; $I = 1.25 \times 10^{11}$ e; $X = 150$ $\mu$rad; Min DA.
• Introduction
• “6D” beam beam treatment
  o Handling the crossing angles: “the boost”
  o Transverse “generalized kicks”
  o Description of the strong beam (Σ-matrix)
  o Handling linear coupling
  o Longitudinal kick
• Implementation
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  o Σ-matrix propagation with linear coupling
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  o Constant charge slicing
  o Complete multi-slice interaction
• Handling the denominators
Transverse kicks for a Gaussian beam

Transverse field for a Gaussian beam (Bassetti-Erskine)

\[ \hat{F}_x^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{x}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \]

\[ \hat{F}_y^* = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{y}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \]

\[ \hat{f}_x = -\frac{\partial \hat{U}^*}{\partial \hat{x}^*} = \frac{1}{2e_0 \sqrt{2\pi}} \frac{\text{Im}}{\sqrt{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)}} \left[ w \left( \frac{\hat{x}^* + i\hat{y}^*}{\sqrt{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)}} \right) - \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) \right] \]

\[ \hat{f}_y = -\frac{\partial \hat{U}^*}{\partial \hat{y}^*} = \frac{1}{2e_0 \sqrt{2\pi}} \frac{\text{Re}}{\sqrt{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)}} \left[ w \left( \frac{\hat{x}^* + i\hat{y}^*}{\sqrt{2 (\hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^*)}} \right) - \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) \right] \]

Library tested against Poisson solver of PyECLoud

(test repeated for tall, fat and round beams)
SixTrack tested against library
(test repeated for tall, fat and round beams)
- Introduction
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- Handling the denominators
Other derivatives of the electric potential

\[ \hat{G}_x = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{11}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{11}^*, \hat{\Sigma}_{33}^* \right) \]

\[ \hat{G}_y = -K_{sl} \frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{33}^*} \left( \hat{x}^*, \hat{y}^*, \hat{\Sigma}_{33}^*, \hat{\Sigma}_{33}^* \right) \]

\[ \hat{g}_x = -\frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{11}^*} = -\frac{1}{2 \left( \hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^* \right)} \left\{ \hat{x}^* \hat{E}_x^* + \hat{y}^* \hat{E}_y^* + \frac{1}{2 \pi \epsilon_0} \left[ \frac{\hat{\Sigma}_{33}^*}{\hat{\Sigma}_{11}^*} \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) - 1 \right] \right\} \]

\[ \hat{g}_y = -\frac{\partial \hat{U}^*}{\partial \hat{\Sigma}_{33}^*} = \frac{1}{2 \left( \hat{\Sigma}_{11}^* - \hat{\Sigma}_{33}^* \right)} \left\{ \hat{x}^* \hat{E}_x^* + \hat{y}^* \hat{E}_y^* + \frac{1}{2 \pi \epsilon_0} \left[ \frac{\hat{\Sigma}_{11}^*}{\hat{\Sigma}_{33}^*} \exp \left( -\frac{(\hat{x}^*)^2}{2\hat{\Sigma}_{11}^*} - \frac{(\hat{y}^*)^2}{2\hat{\Sigma}_{33}^*} \right) - 1 \right] \right\} \]

Library tested against numerical derivative

(test repeated for tall, fat and round beams)
Other derivatives of the electric potential

\[
\hat{G}_x = -K_{sl} \frac{\partial \hat{U}^*}{\partial \Sigma_{11}^*} \left( \hat{x}^*, \hat{y}^*, \Sigma_{11}^*, \Sigma_{33}^* \right)
\]
\[
\hat{g}_x = -\frac{\partial \hat{U}^*}{\partial \Sigma_{11}^*} = -\frac{1}{2 \left( \Sigma_{11}^* - \Sigma_{33}^* \right)} \left\{ \hat{x}^* \hat{E}_x^* + \hat{y}^* \hat{E}_y^* + \frac{1}{2 \pi \epsilon_0} \left[ \sqrt{\frac{\Sigma_{33}^*}{\Sigma_{11}^*}} \exp \left( -\frac{\hat{x}^*}{2 \Sigma_{11}^*} - \frac{\hat{y}^*}{2 \Sigma_{33}^*} \right) - 1 \right] \right\}
\]
\[
\hat{G}_y = -K_{sl} \frac{\partial \hat{U}^*}{\partial \Sigma_{33}^*} \left( \hat{x}^*, \hat{y}^*, \Sigma_{33}^*, \Sigma_{33}^* \right)
\]
\[
\hat{g}_y = -\frac{\partial \hat{U}^*}{\partial \Sigma_{33}^*} = \frac{1}{2 \left( \Sigma_{11}^* - \Sigma_{33}^* \right)} \left\{ \hat{x}^* \hat{E}_x^* + \hat{y}^* \hat{E}_y^* + \frac{1}{2 \pi \epsilon_0} \left[ \sqrt{\frac{\Sigma_{11}^*}{\Sigma_{33}^*}} \exp \left( -\frac{\hat{x}^*}{2 \Sigma_{11}^*} - \frac{\hat{y}^*}{2 \Sigma_{33}^*} \right) - 1 \right] \right\}
\]

SixTrack tested against library

(test repeated for tall, fat and round beams)
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  o Handling the crossing angles: “the boost”
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  o Longitudinal kick

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• **Handling the denominators**
Library tested against MAD-X:
- Built a simple line with a strong skew quadrupole
- Entering with a de-coupled beam
- Saves $\Sigma$-matrix at regularly spaced markers for comparison against library
Library tested against MAD-X:
- Built a simple line with a strong skew quadrupole
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• **Implementation**

• **Testing:**
  o “Boost” and “Anti-boost”
  o Transverse kicks
  o Other derivatives of the electric potential
  o \( \Sigma \)-matrix propagation with linear coupling
  o \( \Sigma \)-matrix transformation to un-coupled frame
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  o Complete multi-slice interaction

• **Handling the denominators**
Library tested against numerical diagonalization of the $\Sigma$-matrix.
Library tested against numerical diagonalization of the $\Sigma$-matrix
**Σ-matrix transformation to un-coupled frame**

**SixTrack tested against library: test failed!**
Sign error in the computation of the coupling angle

Original source code:

```plaintext
if(abs(sinth).gt.pieni) then
    sinh=(-1d0*sfac)*sqrt(sinth)
else
    sinh=zero
endif
```
**Σ-matrix transformation to un-coupled frame**

**SixTrack tested against library:** test failed!
Sign error in the computation of the coupling angle

Corrected source code:

```plaintext
if(abs(sinth).gt.pieni) then
  sinth=(sfac)*sqrt(sinth)
else
  sinth=zero
endif
```
\[ \Sigma \text{-matrix transformation to un-coupled frame} \]

Input sigma matrix:

\[
\begin{align*}
\text{Original} & : \\
\text{Corrected} & : \\
\end{align*}
\]

\[
\begin{align*}
\text{Sig}_{11} & : 2.1046670129999999e-05, \\
\text{Sig}_{12} & : 2.7725426699999999e-07, \\
\text{Sig}_{13} & : 5.9207071659999999e-06, \\
\text{Sig}_{14} & : 1.2224001670000001e-07, \\
\text{Sig}_{22} & : 3.6622825020000002e-09, \\
\text{Sig}_{23} & : 7.4141363399999994e-08, \\
\text{Sig}_{24} & : 1.495491124e-09, \\
\text{Sig}_{33} & : 3.165637487e-06, \\
\text{Sig}_{34} & : 7.9058234540000002e-08, \\
\text{Sig}_{44} & : 2.040387648e-09,
\end{align*}
\]

Checked by Kyrre using full SixTrack simulations (numerical divergence of the computed kicks)

More info at: https://github.com/SixTrack/SixTrack/issues/267#issuecomment-307333656
After bug correction derivatives were also found to be ok
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  • Handling the denominators
Library: slicing could be easily re-implemented using python inverse error function
**Sixtrack**: implementation is correct but not very accurate
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      o Complete multi-slice interaction
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Sixtrack (corrected) vs library: agreement to the 6th digit!

Compare kicks against sixtrack:

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• Introduction
• “6D” beam beam treatment
  o Handling the crossing angles: “the boost”
  o Transverse “generalized kicks”
  o Description of the strong beam (Σ-matrix)
  o Handling linear coupling
  o Longitudinal kick
• Implementation
• Testing:
  o “Boost” and “Anti-boost”
  o Transverse kicks
  o Other derivatives of the electric potential
  o Σ-matrix propagation with linear coupling
  o Σ-matrix transformation to un-coupled frame
  o Constant charge slicing
  o Complete multi-slice interaction
• Handling the denominators
Handling the denominators: case \#0

**Case T>0, \( |\Sigma_{13}^*|>0 \)**

We use the expression that we have derived before:

\[
R(S) = \Sigma_{11}^* - \Sigma_{33}^* \\
W(S) = \Sigma_{11}^* + \Sigma_{33}^* \\
T(S) = R^2 + 4\Sigma_{13}^*^2 \\
\cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}} \\
\hat{\Sigma}_{11}^* = \frac{1}{2} \left( W + \text{sgn}(R)\sqrt{T} \right) \\
\hat{\Sigma}_{33}^* = \frac{1}{2} \left( W - \text{sgn}(R)\sqrt{T} \right)
\]

\[
\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^* \right] = \frac{1}{2} \left( \frac{\partial W}{\partial S} + \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right) \\
\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^* \right] = \frac{1}{2} \left( \frac{\partial W}{\partial S} - \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right) \\
\frac{\partial}{\partial S} \left[ \cos 2\theta \right] = \text{sgn}(R) \left( \frac{\partial R}{\partial S} \frac{1}{\sqrt{T}} - \frac{R}{2 \left( \sqrt{T} \right)^3} \frac{\partial T}{\partial S} \right)
\]

\[
\cos \theta = \sqrt{\frac{1}{2} \left( 1 + \cos 2\theta \right)} \\
\sin \theta = \text{sgn}(R)\text{sgn}(\Sigma_{13}^*) \sqrt{\frac{1}{2} \left( 1 - \cos 2\theta \right)}
\]

\[
\frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta \\
\frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta
\]
Handling the denominators: case #0

Case $T>0$, $|\Sigma^*_13|>0$

Tests:

Mode: check_singularities At $s=4.0$:
$\text{SIG13}=1.0$ $T=8.0$, $a=2.0\times10^{-1}$, $b=-3.0\times10^{-2}$, $c=4.0\times10^{-1}$, $d=1.0\times10^{-1}$

Expression with denominator (apparently singular)

Expression with correction
Handling the denominators: case #0

Case $T > 0, |\Sigma^*_13| > 0$

Tests against Sixtrack:

Mode: vs_sixtrack At $s = 4.0$

$\text{SIG}13 = 1.0, T = 8.0, a = 2.0e-01, b = -3.0e-02, c = 4.0e-01, d = 1.0e-01$
Handling the denominators: case #1

Case $T>0, |\Sigma_{13}^*|=0$:

The highlighted formulas break and alternative expressions need to be found:

\[
R(S) = \Sigma_{11}^* - \Sigma_{33}^*
\]
\[
W(S) = \Sigma_{11}^* + \Sigma_{33}^*
\]
\[
T(S) = R^2 + 4\Sigma_{13}^*^2
\]
\[
\cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}}
\]
\[
\hat{\Sigma}_{11}^* = \frac{1}{2} \left( W + \text{sgn}(R) \sqrt{T} \right)
\]
\[
\hat{\Sigma}_{33}^* = \frac{1}{2} \left( W - \text{sgn}(R) \sqrt{T} \right)
\]
\[
\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^* \right] = \frac{1}{2} \left( \frac{\partial W}{\partial S} + \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right)
\]
\[
\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^* \right] = \frac{1}{2} \left( \frac{\partial W}{\partial S} - \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right)
\]
\[
\frac{\partial}{\partial S} \left[ \cos 2\theta \right] = \text{sgn}(R) \left( \frac{\partial R}{\partial S} \frac{1}{\sqrt{T}} - \frac{R}{2 \left( \sqrt{T} \right)^3} \frac{\partial T}{\partial S} \right)
\]
\[
\cos \theta = \sqrt{\frac{1}{2} (1 + \cos 2\theta)}
\]
\[
\sin \theta = \text{sgn}(R) \text{sgn}(\Sigma_{13}^*) \sqrt{\frac{1}{2} (1 - \cos 2\theta)}
\]
\[
\frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta
\]
\[
\frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta
\]
**Case T>0, \(|\Sigma_{13}^*|=0\):**

\[
\cos 2\theta = \text{sgn}(\Sigma_{11}^* - \Sigma_{33}^*) \frac{\Sigma_{11}^* - \Sigma_{33}^*}{\sqrt{\left(\Sigma_{11}^* - \Sigma_{33}^*\right)^2 + 4\Sigma_{13}^*}} \\
\sin \theta = 0
\]

\[
\frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta \\
\frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta
\]
Handling the denominators: case #1

Case $T>0, \left| \Sigma_{13}^* \right|=0$:

Around the singular point we can write:

$$\Sigma_{13}^* = c\Delta S + d\Delta S^2$$

with

$$a = \Sigma_{12}^* - \Sigma_{34}^*$$
$$b = \Sigma_{22}^* - \Sigma_{44}^*$$
$$c = \Sigma_{14}^* + \Sigma_{23}^*$$
$$d = \Sigma_{24}^*$$

$$\cos 2\theta = \frac{|R|}{\sqrt{R^2 + 4\Sigma_{13}^*}} \approx \frac{1}{\sqrt{1 + 4\frac{\Sigma_{13}^*}{R^2}}} \approx 1 - 2\frac{\Sigma_{13}^*}{R^2}$$

$$\sin \theta = \text{sgn}(R) \text{sgn}(\Sigma_{13}^*) \frac{|\Sigma_{13}^*|}{|R|} = \frac{\Sigma_{13}^*}{R}$$

$$\frac{\partial}{\partial S} \sin \theta = \frac{1}{R^2} \left[ (c + 2d\Delta S) R - \frac{\partial R}{\partial S} \left( c\Delta S + d\Delta S^2 \right) \right]$$

At the singular point

$$\frac{\partial}{\partial S} \sin \theta = \frac{c}{R}$$

Which is always regular once we assume $T>0$ and therefore $R^2>0$
Case $T>0$, $|\Sigma_{13}^*|=0$:

Tests:

Mode: check_singularities At $s=4.0$:
SIG13=0.0 $T=4.0$, $a=-5.0e-01$, $b=0.0$, $c=-3.0e-01$, $d=1.0e-01$
Handling the denominators: case #1

Case $T>0, |\Sigma^*_13|=0$:  

Tests against Sixtrack:

Mode: vs_sixtrack At $s=4.0$:
SIG13=0.0 $T=4.0, a=-5.0e-01, b=0.0, c=-3.0e-01, d=1.0e-01$
Handling the denominators: case #2

Case $T=0, |c|>0$

The highlighted formulas break and alternative expressions need to be found:

\[
R(S) = \Sigma_{11}^* - \Sigma_{33}^*
\]
\[
W(S) = \Sigma_{11}^* + \Sigma_{33}^*
\]
\[
T(S) = R^2 + 4\Sigma_{13}^*^2
\]
\[
\cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}}
\]
\[
\dot{\Sigma}_{11}^* = \frac{1}{2} \left( W + \text{sgn}(R) \sqrt{T} \right)
\]
\[
\dot{\Sigma}_{33}^* = \frac{1}{2} \left( W - \text{sgn}(R) \sqrt{T} \right)
\]

\[
\frac{\partial}{\partial S} \left[ \dot{\Sigma}_{11}^* \right] = \frac{1}{2} \left( \frac{\partial W}{\partial S} + \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right)
\]
\[
\frac{\partial}{\partial S} \left[ \dot{\Sigma}_{33}^* \right] = \frac{1}{2} \left( \frac{\partial W}{\partial S} - \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right)
\]

\[
\frac{\partial}{\partial S} \left[ \cos 2\theta \right] = \text{sgn}(R) \left( \frac{\partial R}{\partial S} \frac{1}{\sqrt{T}} - \frac{R}{2} \left( \frac{1}{\sqrt{T}} \right)^3 \frac{\partial T}{\partial S} \right)
\]

\[
\cos \theta = \sqrt{\frac{1}{2} (1 + \cos 2\theta)}
\]
\[
\sin \theta = \text{sgn}(R) \text{sgn}(\Sigma_{13}^*) \sqrt{\frac{1}{2} (1 - \cos 2\theta)}
\]

\[
\frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta
\]
\[
\frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta
\]
Handling the denominators: case #2

\[ \textbf{Case T=0, } |c|>0 \]

Around the singular point we can write:

\[ a = \Sigma_{12}^* - \Sigma_{34}^* \]
\[ b = \Sigma_{22}^* - \Sigma_{44}^* \]
\[ c = \Sigma_{14}^* + \Sigma_{23}^* \]
\[ d = \Sigma_{24}^* \]

\[ R = 2a\Delta S + b\Delta S^2 \]

\[ T = \Delta S^2 \left[ (2a + b\Delta S)^2 + 4 (c + d\Delta S)^2 \right] \]

\[ \cos 2\theta = \frac{|2a + b\Delta S|}{\sqrt{(2a + b\Delta S)^2 + 4 (c + d\Delta S)^2}} \]

\[ \frac{\partial}{\partial \Delta S} \left[ \cos 2\theta \right] = \text{sgn}(2a + b\Delta S) \left[ \frac{b}{\sqrt{(2a + b\Delta S)^2 + 4 (c + d\Delta S)^2}} - \frac{(2a + b\Delta S)(2ab + b^2\Delta s + 4cd + 4d^2\Delta S)}{\left(\sqrt{(2a + b\Delta S)^2 + 4 (c + d\Delta S)^2}\right)^3} \right] \]

\[ \Delta S = 0 \]

\[ \frac{\partial}{\partial \Delta S} \left[ \cos 2\theta \right] = \text{sgn}(2a) \left[ \frac{b}{2\sqrt{a^2 + c^2}} - \frac{a(ab + 2cd)}{2 \left(\sqrt{a^2 + c^2}\right)^3} \right] \]
Handling the denominators: case #2

Case $T=0$, $|c|>0$

$$a = \Sigma_{12}^* - \Sigma_{34}^*$$
$$b = \Sigma_{22}^* - \Sigma_{44}^*$$
$$c = \Sigma_{14}^* + \Sigma_{23}^*$$
$$d = \Sigma_{24}^*$$

$$R = 2a\Delta S + b\Delta S^2$$
$$T = \Delta S^2 \left[ (2a + b\Delta S)^2 + 4(c + d\Delta S)^2 \right]$$

$$\hat{\Sigma}_{11}^* = \frac{W}{2} + \frac{1}{2} \text{sgn} \left( 2a\Delta S + b\Delta S^2 \right) |\Delta S| \sqrt{(2a + b\Delta S)^2 + 4(c + d\Delta S)^2}$$
$$\hat{\Sigma}_{33}^* = \frac{W}{2} - \frac{1}{2} \text{sgn} \left( 2a\Delta S + b\Delta S^2 \right) |\Delta S| \sqrt{(2a + b\Delta S)^2 + 4(c + d\Delta S)^2}$$

$$\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^* \right] = \frac{1}{2} \frac{\partial W}{\partial S} + \frac{1}{2} \text{sgn} \left( 2a\Delta S + b\Delta S^2 \right) \text{sgn}(\Delta S) \left[ \sqrt{(2a + b\Delta S)^2 + 4(c + d\Delta S)^2} + \frac{\Delta S (2ab + b^2\Delta S + 4cd + 4d^2\Delta S)}{\sqrt{(2a + b\Delta S)^2 + 4(c + d\Delta S)^2}} \right]$$
$$\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^* \right] = \frac{1}{2} \frac{\partial W}{\partial S} - \frac{1}{2} \text{sgn} \left( 2a\Delta S + b\Delta S^2 \right) \text{sgn}(\Delta S) \left[ \sqrt{(2a + b\Delta S)^2 + 4(c + d\Delta S)^2} + \frac{\Delta S (2ab + b^2\Delta S + 4cd + 4d^2\Delta S)}{\sqrt{(2a + b\Delta S)^2 + 4(c + d\Delta S)^2}} \right]$$

$$\Delta S = 0$$

$$\hat{\Sigma}_{11}^* = \frac{W}{2}$$
$$\hat{\Sigma}_{33}^* = \frac{W}{2}$$

$$\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{11}^* \right] = \frac{1}{2} \frac{\partial W}{\partial S} + \text{sgn}(2a) \sqrt{a^2 + c^2}$$
$$\frac{\partial}{\partial S} \left[ \hat{\Sigma}_{33}^* \right] = \frac{1}{2} \frac{\partial W}{\partial S} - \text{sgn}(2a) \sqrt{a^2 + c^2}$$
Handling the denominators: case #2

Case $T=0, |c|>0$

Tests:

Mode: check_singularities At $s=4.0$:
$SIG_{13}=0.0$, $T=0.0$, $a=4.0e-01$, $b=0.0$, $c=1.2$, $d=1.0e-01$

Expression with denominator (apparently singular)
Expression with correction
Handling the denominators: case #2

Case \( T=0, \ |c|>0 \)

Tests against Sixtrack:

Mode: vs_sixtrack At \( s=4.0 \):
SIG13=0.0, \( T=0.0, a=4.0e-01, b=0.0, c=1.2, d=1.0e-01 \)
Handling the denominators: case #3

Case $T=0$, $c=0$, $|a|>0$

The highlighted formulas break and alternative expressions need to be found:

\[ R(S) = \Sigma_{11}^* - \Sigma_{33}^* \]
\[ W(S) = \Sigma_{11}^* + \Sigma_{33}^* \]
\[ T(S) = R^2 + 4\Sigma_{13}^* \]
\[ \cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}} \]
\[ \hat{\Sigma}_{11}^* = \frac{1}{2} \left( W + \text{sgn}(R)\sqrt{T} \right) \]
\[ \hat{\Sigma}_{33}^* = \frac{1}{2} \left( W - \text{sgn}(R)\sqrt{T} \right) \]

\[
\frac{\partial}{\partial S} [\hat{\Sigma}_{11}^*] = \frac{1}{2} \left( \frac{\partial W}{\partial S} + \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right)
\]
\[
\frac{\partial}{\partial S} [\hat{\Sigma}_{33}^*] = \frac{1}{2} \left( \frac{\partial W}{\partial S} - \text{sgn}(R) \frac{1}{2\sqrt{T}} \frac{\partial T}{\partial S} \right)
\]

\[
\frac{\partial}{\partial S} [\cos 2\theta] = \text{sgn}(R) \left( \frac{\partial R}{\partial S} \frac{1}{\sqrt{T}} - \frac{R}{2(\sqrt{T})^3} \frac{\partial T}{\partial S} \right)
\]

\[ \cos \theta = \sqrt{\frac{1}{2} (1 + \cos 2\theta)} \]
\[ \sin \theta = \text{sgn}(R)\text{sgn}(\Sigma_{13}^*) \sqrt{\frac{1}{2} (1 - \cos 2\theta)} \]

\[ \frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta \]
\[ \frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta \]
Handling the denominators: case #3

**Case T=0, c=0, \(|a|>0\)**

\[
a = \Sigma_{12}^* - \Sigma_{34}^*
\]
\[
b = \Sigma_{22}^* - \Sigma_{44}^*
\]
\[
c = \Sigma_{14}^* + \Sigma_{23}^*
\]
\[
d = \Sigma_{24}^*
\]

\[
R = 2a\Delta S + b\Delta S^2
\]
\[
T = \Delta S^2 \left[ (2a + b\Delta S)^2 + 4 (c + d\Delta S)^2 \right]
\]

We proceed as before:

\[
\cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}}
\]

\[
\cos \theta = \sqrt{\frac{1}{2} (1 + \cos 2\theta)}
\]

\[
\sin \theta = \text{sgn}(R) \text{sgn}(\Sigma_{13}^*) \sqrt{\frac{1}{2} (1 - \cos 2\theta)}
\]

\[
\frac{\partial}{\partial S} \cos \theta = \frac{1}{4 \cos \theta} \frac{\partial}{\partial S} \cos 2\theta
\]

\[
\frac{\partial}{\partial S} \sin \theta = -\frac{1}{4 \sin \theta} \frac{\partial}{\partial S} \cos 2\theta
\]

Same as before but this denominator becomes zero
Handling the denominators: case #3

Case \( T=0, c=0, |a|>0 \)

\[
\begin{align*}
    a &= \Sigma^*_{12} - \Sigma^*_{34} \\
    b &= \Sigma^*_{22} - \Sigma^*_{44} \\
    c &= \Sigma^*_{14} + \Sigma^*_{23} \\
    d &= \Sigma^*_{24}
\end{align*}
\]

\[
R = 2a\Delta S + b\Delta S^2
\]

\[
T = \Delta S^2 \left[ (2a + b\Delta S)^2 + 4 (c + d\Delta S)^2 \right]
\]

We need to expand to higher order:

\[
\cos 2\theta = \frac{1}{\sqrt{1 + \frac{4d^2\Delta S^2}{(2a+b\Delta S)^2}}} \approx 1 - \frac{2d^2\Delta S^2}{(2a+b\Delta S)^2}
\]

\[
\sin \theta = \text{sgn}(R)\text{sgn}(\Sigma^*_{13}) \sqrt{\frac{1}{2} (1 - \cos 2\theta)}
\]

\[
\sin \theta = \frac{d\Delta S}{2a} \left| 1 - \frac{b\Delta S}{2a} \right|
\]

\[
\frac{\partial}{\partial S} \sin \theta = \frac{d}{2a}
\]
Handling the denominators: case #3

Case $T=0$, $c=0$, $|a|>0$

Tests:

Mode: check_singularities At $s=4.0$:
$SIG_{13}=0.0$, $T=0.0$, $a=-6.5e-01$, $b=-5.0e-02$, $c=0.0$, $d=-1.0e-01$

![Graphs showing function behavior](image)

Expression with denominator (apparently singular)
Expression with correction
Library (with correction)

Tests against Sixtrack:

Mode: vs_sixtrack At s=4.0:
SIG13=0.0 T=0.0, a=-6.5e-01, b=-5.0e-02, c=0.0, d=-1.0e-01

Case $T=0$, $c=0$, $|a|>0$
Handling the denominators: case #4

Case $T=0$, $c=0$, $a=0$

\[
\begin{align*}
    a &= \Sigma_{12}^* - \Sigma_{34}^* \\
    b &= \Sigma_{22}^* - \Sigma_{44}^* \\
    c &= \Sigma_{14}^* + \Sigma_{23}^* \\
    d &= \Sigma_{24}^*
\end{align*}
\]

\[
\begin{align*}
    R &= b \Delta S^2 \\
    \Sigma_{13}^* &= d \Delta S^2 \\
    T(S) &= R^2 + 4\Sigma_{13}^*^2
\end{align*}
\]

\[
\cos 2\theta = \text{sgn}(R) \frac{R}{\sqrt{T}} \quad \cos 2\theta = \frac{|b|}{\sqrt{b^2 + 4d^2}} \quad \text{which is a constant...}
\]
Handling the denominators: case #4

Case $T=0$, $c=0$, $a=0$

Tests:

Mode: check_singularity At $s=4.0$:
$SIG13=0.0$ $T=0.0$, $a=0.0$, $b=-5.0e-02$, $c=0.0$, $d=1.0e-01$

Expression with denominator (apparently singular)

Expression with correction
Handling the denominators: case #4

Case T=0, c=0, a=0

Tests against Sixtrack:

Mode: vs_sixtrack At s=4.0:
SIG13=0.0 T=0.0, a=0.0, b=-5.0e-02, c=0.0, d=1.0e-01

Graphs showing data analysis for different variables against s in meters.
Summary

- Complete **mathematical derivation** needed for implementation available in the prepared note (CERN-ACC-NOTE-2018-0023)
- Implemented in a **Python/C library** for usage in other simulation codes (SixtrackLib, PyHEADTAIL) and compatible with **GPU**
  - “**Stress tests**” performed on the different functional blocks of the library → **Passed**
- **Source code** including all tests available on github
- **SixTrack implementation tested** against library. Outcome:
  - **Uncoupled case:**
    - Bug identified in “inverse boost” → **corrected** (now in the production version)
    - Other tests passed
  - **Coupled case:**
    - Suffering from a **serious bug** (wrong sign) → **corrected** (now in the production version)
    - Apparently singular cases (denominators) not correctly handled → **strategy to be defined** (requires serious re-structuring, should we just replace everything with the library code?)
- **Next steps:**
  - Tests on GPU
  - Performance profiling and, if needed, optimization
  - Real life usage (fancy GPUs in Bologna should be coming soon😊)