

# Nontracking approach for the optimization of secondary beamlines

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Historically, the design and operation of secondary beamlines at CERN's North and East Areas relied on simplified particle distributions and a beamline acceptance determined solely by collimators. The formalism presented here makes as few simplifying assumptions as possible and can be used to match and design secondary beamlines without time-consuming HPC tracking studies. In this study, the formalism is applied to the development of a new neutrino beamline within the Physics Beyond Colliders framework at CERN. The code is expressed generically, providing tools for designing secondary beamlines with small relative losses.

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## I. INTRODUCTION

Within the Physics Beyond Colliders (PBC) initiative [1], which investigates physics cases complementary to the LHC physics program and that are aligned with the European Strategy for Particle Physics, the feasibility of a short baseline neutrino beamline at CERN is currently being evaluated [2–4]. Lately, the nuSCOPE collaboration has formed with the aim of performing high-precision neutrino cross-section measurements utilizing the SBN-nuSCOPE beamline. The number of required protons on target (PoT) to attain sufficient precision for an energy-dependent  $\nu_{e,\mu}$  cross-section measurement must be minimized to make it competitive with other experiments that are operated within the CERN accelerator complex. A proton beam produces  $K^+$  and  $\pi^+$  mesons in a primary target at the start of the SBN-nuSCOPE beamline. These mesons are guided by the beamline magnets into a decay tunnel—that is, a 40-m-long evacuated tube with a 2 m diameter—until a fraction of these particles decay ( $\pi^+ \rightarrow \mu^+ + \nu_\mu$  and  $K^+ \rightarrow e^+ + \nu_e + \pi^0$  are the relevant decay channels) and eventually produce a pointed neutrino beam downstream of that decay tube. In the past, the beamline design for CERN's North Area was performed manually. This approach often relied on simplifying assumptions: collimators exclusively defining the acceptance and an idealized beam distribution that is a delta function in transverse position. Such assumptions are unrealistic—a real beam exiting a production target has a finite size and angular spread, meaning the beam waist

and the optical focus do not coincide in general. Beam tuning that moves the focal point therefore partially undermines any prior acceptance optimization. An optimization process that makes neither of these assumptions is necessary for secondary beamlines, in particular for those that mainly focus on transmission and therefore lack tight collimator settings. Conventional and well-established techniques certainly do not fail to achieve a good design for such beamlines; however, there is a risk of not necessarily designing a beamline that is close to the global maximum. Another more subtle effect that makes common design techniques less applicable is the eventual decay of unstable beam particles. As will be explained in the next section, the SBN-nuSCOPE beamline is designed to primarily guide  $K^+$  and  $\pi^+$  mesons at single-digit GeV/c particle momenta. An efficient design strategy must be able to quantitatively evaluate the inevitable compromise between ideal beamline optics and the beamline length. The classic quadrupole dilemma of envisaging quadrupoles with the largest aperture and strongest field possible is now extended by ideally making magnets as short as possible to reduce the quantity of particle decays before the start of the decay tunnel.

The authors propose a straightforward yet effective formalism that can be integrated into an optimization algorithm that surpasses conventional approaches by optimizing not only beamline optics but also the beamline design itself. The computational efficiency of the developed formalism enables simultaneous optimization of various beamline parameters, such as magnet specifications, type, number of magnets, and even the production target specifications. Optimizing such a large number of quantities is particularly valuable during the design process of a beamline.

## II. THE SBN-NUSCOPE BEAMLINE STUDY

The SBN-nuSCOPE beamline will serve as an example for the design process throughout this paper. The SBN-nuSCOPE beamline merges the previously proposed

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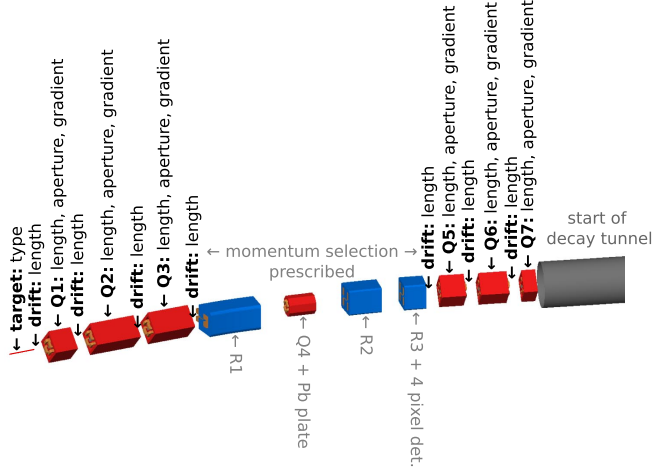


FIG. 1. The beamline elements within the SBN-nuSCOPE beamline are depicted in the GEANT4 viewer [9]. In subsequent chapters, an optimization of the beamline is conducted. All elements with adjustable parameters are highlighted in black; however, the center momentum-selection section of the beamline, comprising three dipoles (blue boxes) and the fourth quadrupole (Q4), is fixed and unchanged by the optimization process (printed in gray). The other quadrupoles (red boxes) are subject to free optimization.

monitored neutrino beamline, ENUBET [5], with the beamline concept proposed by NuTag [6]. ENUBET has designed an initial beam section to produce  $K^+$  mesons in a graphite target struck by a high-energy proton beam, similar to the beam at CERN’s SPS [7,8]. The beamline aims to select  $K^+$  and  $\pi^+$  mesons within a momentum range of  $\Delta p/p_0 \in [-10\%, 10\%]$  centered at  $p = 8.5$  GeV/c. The  $K^+$  then decay in a fully instrumented decay tunnel downstream of the magnetic structure of the beamline, enabling the detection of positrons emitted during the  $K_{e3}$  (three-body decay). The ENUBET collaboration seeks to determine the  $\nu_e$  cross section with a statistical uncertainty down to 1% on the inclusive cross section. The  $\pi^+$  decay also leads to the possibility of measuring the  $\nu_\mu$  cross section. For that, the NuTag collaboration aims at using pixel detectors to measure the beam kinematics before ( $\pi^+$ ) and after the decay process ( $\mu^+$ ) to determine the neutrino kinematics of the  $\nu_e$ . For more details, refer to [5,6]. A sketch of the beamline is depicted in Fig. 1.

An improved design for CERN’s SBN-nuSCOPE beamline has been proposed [10–13], but a full transmission optimization was pending. The approach presented here couples the linear optics calculation with precomputed particle-matter interaction histograms (computed once, before the optimization). The optimizer finds solutions that are virtually impossible to reach by hand; the improvements were validated with start-to-end BDSIM [14]/GEANT4 [9] simulations.

### III. A NONTRACKING APPROACH TO BEAMLINE OPTIMIZATION

The nontracking approach focuses on optimizing transmission efficiency, beam size at key locations, and optionally the momentum distribution at the experiment. The method presented here evaluates the beamline performance within fractions of a CPU second, enabling the full optimization of a beamline within minutes to hours on a single CPU core with the option of parallelization. The optimization routine is a multiobjective genetic algorithm (MOGA), well established in accelerator physics [15–17].

In the next sections, a method for determining both the transmission efficiency and the beam size without any tracking is presented.

#### A. Key concept: The linear acceptance

The key ingredient for a nontracking approach is the beamline acceptance: all particles whose phase space coordinates at the target fall within it are transmitted. For a short beamline with only dipoles and quadrupoles, higher-order effects are small, and the acceptance can be computed analytically by back-projecting all apertures to the target location using the first-order  $\mathbf{R}$  matrix [18] (see Appendix A; valid at zero momentum offset). For off-momentum particles, the acceptance is computed with a standard optics code (MAD-X [19] or ELEGANT [20]) at the desired  $\Delta p/p_0$ . The result is two acceptance domains,  $A_u = \{(\bar{u}_i, \bar{u}'_i) | 1 \leq i \leq N_{\text{acc}}\}$  with  $u \in \{x, y\}$  (hereafter *linear acceptance*), sampled at  $N_{\text{acc}}$  phase-space points (Appendix A). In polar coordinates, these are written  $(\bar{R}_{u,i}, \bar{\phi}_{u,i})$ .

The linear optics obtained from MAD-X with  $\Delta p \neq 0$  are not necessarily accurate because MAD-X employs a pseudo-nonlinear approach. The nominal particle with  $\Delta p/p_0 \neq 0$  no longer passes through the magnet centers due to dipole magnets in the beamline. Specifically, the magnetic field strength is adjusted to account for the trajectory offset and the rigidity offset of the particle. However, geometrical and chromatic aberrations are still present. Nevertheless, for a small enough momentum offset of  $O(3\%)$ , the calculation of the linear acceptance is sufficiently accurate to compare two solutions and determine the better-shaped acceptance. Figure 2 shows the horizontal acceptance of the SBN-nuSCOPE beamline (Fig. 1) for the nominal momentum and a respective line scan that is achieved via nonlinear tracking using PTC.

The discrepancy between linear and exact (tracked) acceptances grows with  $|\Delta p/p_0|$  (Fig. 3), but this is not a problem as long as the *hierarchy* is preserved: a solution A with a larger linear acceptance than B should also have a larger tracked acceptance. This is demonstrated numerically in Sec. IV.

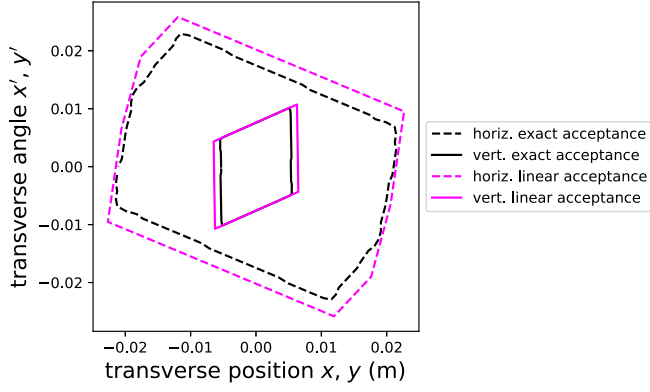


FIG. 2. The plot shows the horizontal (dashed magenta line) and vertical linear acceptance (solid magenta line) of the SBN-nuSCOPE beamline using a good "guess" for the initial optics. A line scan was performed via tracking (MAD-X's PTC [21]) to obtain the nonlinear acceptance (black solid and black dashed lines).

## B. Intensity estimate

In this section, a method to determine the transmission efficiency of a beamline is presented. The  $K^+$  transmission is taken as an example; other particle types behave analogously.

### 1. Analytic description

The acceptance plots can be used to calculate the beamline transmission. To do this, the particle distribution that emerges from the target must be known. This distribution is obtained from FLUKA [22] or GEANT4/BDSIM simulations. However, it is crucial that the distribution is determined in the perpendicular plane with respect to the beam direction at the end of the production target. This location typically corresponds to the beginning of the beamline that one aims to optimize. If applicable, the distribution should also include the production angle between the beam and the beamline. For example, BDSIM simulations of the target were conducted with a scoring plane that was horizontally rotated by  $0.5^\circ$  immediately after the production target to precisely obtain the required histogram for the optimization process. Figure 4 (both in Cartesian and polar coordinates) depicts histograms of the CNGS target. The yield of  $\pi^+$  and  $K^+$  particles is momentum-dependent, as it is illustrated in Fig. 5. The intensity is obtained by counting how many particles from the target fall within the acceptance at each momentum offset (Fig. 3 shows how the acceptance varies with  $\Delta p/p_0$ ; Fig. 4 shows the overlap at  $\Delta p/p_0 = 0$ ), weighted by the yield at that offset (Fig. 5):

$$I = \int_0^\infty dp \iint_{A_x} dR_x d\phi_x \iint_{A_y} dR_y d\phi_y \cdot \rho \cdot \epsilon(p). \quad (1)$$

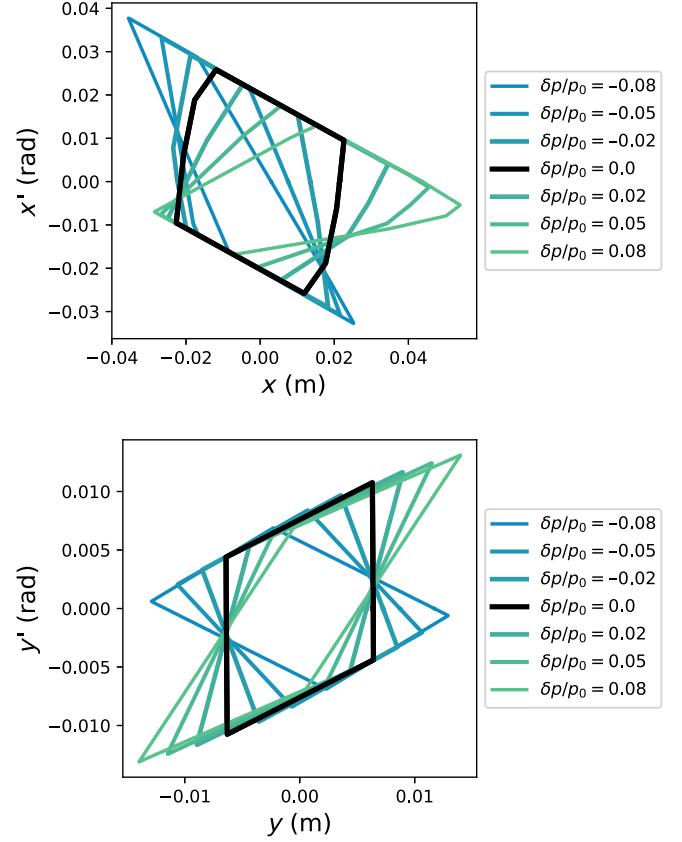


FIG. 3. Linear horizontal (top) and vertical (bottom) acceptance curves for different relative momentum offsets for the initial SBN-nuSCOPE design.

In this equation, the particle density function at the start of the beamline  $\rho$  is a function of  $p$ ,  $R_x$ ,  $\phi_x$ ,  $R_y$ , and  $\phi_y$ . The factor  $\epsilon(p)$

$$\epsilon(p) = \exp\left(-\frac{L_{\text{line}} m}{\tau_0 p}\right) \quad (2)$$

accounts for the reduction in intensity of the  $K^+$  and  $\pi^+$  mesons due to particle decay. In Eq. (2),  $\tau_0$  represents the lifetime of the respective meson of mass  $m$  at rest, while  $L_{\text{line}}$  denotes the distance between the target and the end of the guiding beamline.

### 2. Numerical solution

Discretizing Eq. (1), the density function  $\rho$  is factorized into three independent subspaces:

$$\rho(\Delta p, R_x, \phi_x, R_y, \phi_y) = N h_p(\Delta p) h_x(R_x, \phi_x) h_y(R_y, \phi_y). \quad (3)$$

The transverse distributions  $h_x$  and  $h_y$  are expressed in polar coordinates:

$$x = R_x \cos \phi_x, \quad x' = R_x \sin \phi_x, \quad (4)$$

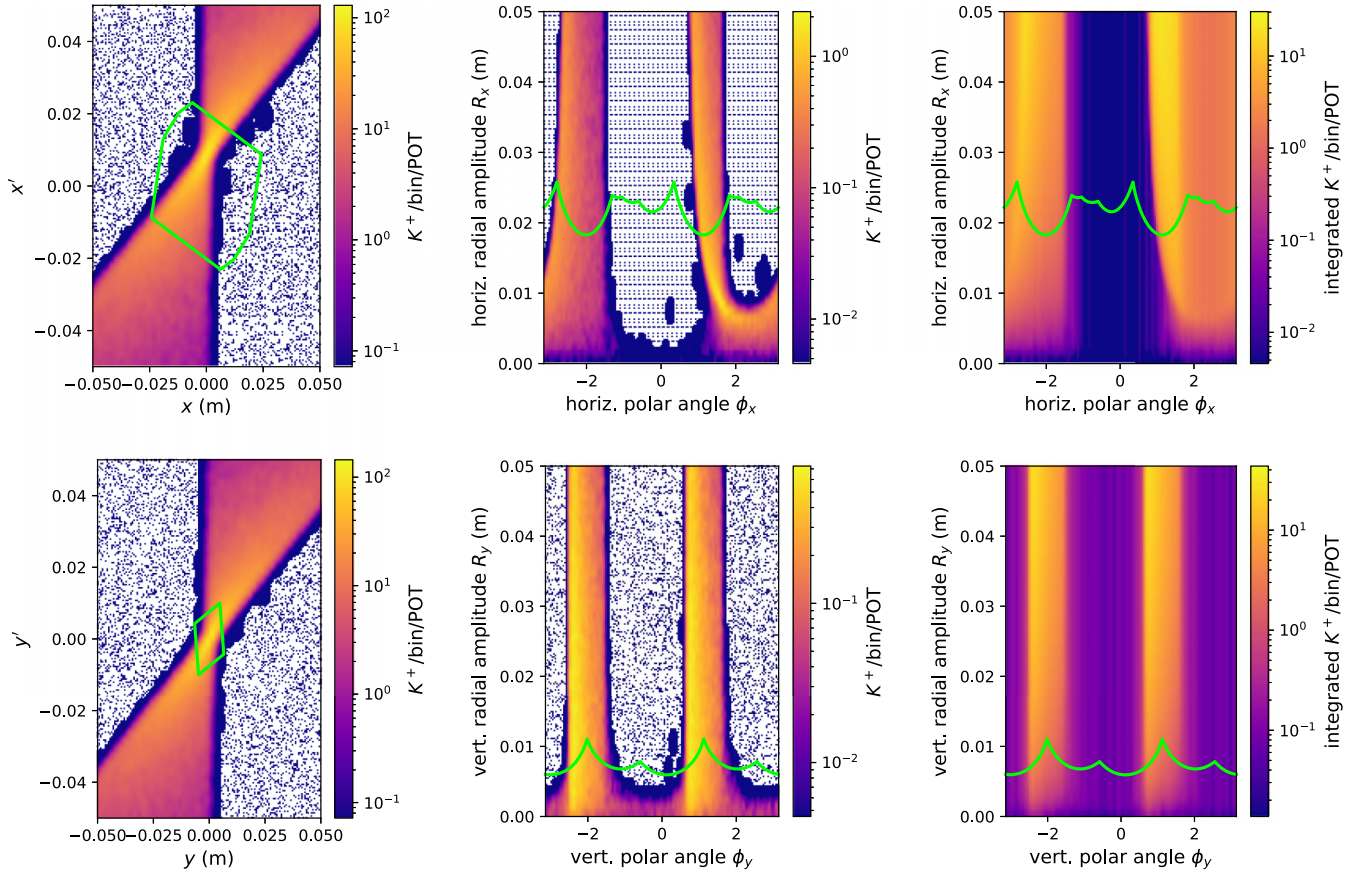


FIG. 4. Left: histograms  $h_x$  (top) and  $h_y$  (bottom) for  $K^+$  mesons at the end face of the 70-cm-long and 6-cm-wide cylindrical-shaped CNGS target. All particles within the acceptance at  $\Delta p/p_0 = 0$  (green polygons) are successfully transported to the start of the decay tunnel. The histogram for the horizontal plane includes the production angle of  $0.5^\circ$ . Center: the two plots show in the horizontal plane (top) and the vertical plane (bottom) the overlap of the acceptance (green curves) in polar coordinates. Right: the two plots show the cumulative distribution functions (CDFs)  $\tilde{h}_x$  (top) and  $\tilde{h}_y$  (bottom) in polar coordinates to simplify the intensity evaluation since the intensity can be read out directly from the histogram via a line integral along the curve of the acceptance.

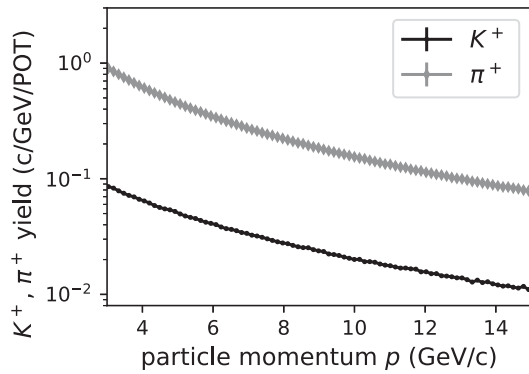


FIG. 5. Number of produced  $K^+$  (black) and  $\pi^+$  (gray) versus momentum at the end face of a graphite target (ENUBET type [5,13]) when impinged by a proton beam with a proton momentum of  $p = 400$  GeV/c.

$$y = R_y \cos \phi_y, \quad y' = R_y \sin \phi_y. \quad (5)$$

Polar coordinates are used because the acceptance curve is single-valued in  $R$  for each angle  $\phi$  (unlike Cartesian phase space), greatly simplifying the domain integration.

$h_x$  and  $h_y$  are the transverse phase-space histograms (shown in Fig. 4). The momentum distribution  $h_p(\Delta p) \approx a_0 + a_1 \Delta p$  is linearized over the relevant momentum range (Fig. 5); higher-order terms can be included if needed.  $N$  is the total number of particles in the five-dimensional phase space.

The factorization of  $\rho$  requires ignorable transverse correlations. For the cylindrically symmetric SBN-nuSCOPE target, this is expected by symmetry; it is confirmed by the  $K^+$  correlation matrix at  $p = 8.5$  GeV (CNGS target, 400 GeV/c protons):

$$\frac{\text{cov}(A, B)}{\sigma_A \sigma_B} = \begin{pmatrix} \mathbf{1} & \mathbf{0.908} & 0.001 & 0.001 & -0.001 \\ & \mathbf{1} & 0.001 & 0.002 & -0.002 \\ & & \mathbf{1} & \mathbf{0.908} & 0.003 \\ & & & \mathbf{1} & 0.004 \\ & & & & \mathbf{1} \end{pmatrix}. \quad (6)$$

In this equation, the coordinates are arranged in the order  $(x, p_x, y, p_y, p_z)$ , and  $A$  and  $B$  represent different permutations of these five quantities. The block diagonal elements (printed in bold) are significantly larger than the off-diagonal elements by at least two orders of magnitude. Therefore, the approximation of ignoring these correlations is valid in the first order; however, higher-order correlations may exist.

The momentum is sliced as  $p(r) = p_0 + r\Delta p$  for  $r \in [-N_p, N_p]$ ; polar angles and radii are discretized with steps  $\Delta\phi$  and  $\Delta R$ . The shorthand  $\epsilon(r)$ ,  $h_p(r)$ ,  $h_{x,y}(i, j)$  refers to the respective functions evaluated at  $r\Delta p$ ,  $i\Delta R$ ,  $j\Delta\phi$ . Equation (1) becomes

$$I = \sum_{r=-N_p}^{N_p} N_s(r) h_p(r) \epsilon(r\Delta p) I_x(r) I_y(r) \quad (7)$$

with

$$I_u(r) = \sum_{i=0}^{N_u(j,r)} \sum_{j=1}^{N_\phi} h_u(i, j). \quad (8)$$

The functions  $h_x$  and  $h_y$  are both depicted in Fig. 4 on the left and in the middle in Cartesian as well as polar coordinates. The quantity  $N_u(j, r) = \bar{R}_u/\Delta R$  is the index for the radius that reaches the acceptance of the  $r$ th momentum slice at the  $j$ th polar angle  $\bar{\phi}_u = j\Delta\phi$  with  $u \in \{x, y\}$ . The number of steps in terms of the polar angles  $\phi_x$  and  $\phi_y$  reads  $N_\phi = 2\pi/\Delta\phi$ . The quantity  $N_s(r)$  is the total number of particles within the  $r$ th momentum slice. This definition then forces the normalization of the three histograms

$$\sum_{r=-N_p}^{N_p} h_p(r) = \sum_{i=0}^{N_R} \sum_{j=1}^{N_\phi} h_x(i, j) = \sum_{i=0}^{N_R} \sum_{j=1}^{N_\phi} h_y(i, j) = 1. \quad (9)$$

The normalization in Eq. (9) avoids *double counting* of intensity information when determining the intensity contents in the acceptance in the  $h_p$ ,  $h_x$ , and  $h_y$  histograms.

It is important to note that the histograms  $h_x$  and  $h_y$  are not correlated with  $p$  in this formalism. This is not necessarily true for all target types and can be included in the formalism if desired by preparing the histograms  $h_x$  and  $h_y$  at the respective momenta one plans to consider.

In the following, the average histogram of the relevant momentum bite  $\Delta p/p_0 \in [-10\%; 10\%]$  is used since no relevant correlations have been observed for all the cases we studied [see, e.g., Eq. (6)]. Precomputing the CDFs

$$\tilde{h}_x(i, j) = \sum_{r=0}^i h_x(r, j) \quad \text{and} \quad \tilde{h}_y(i, j) = \sum_{r=0}^i h_y(r, j), \quad (10)$$

(shown in Fig. 4, right) reduces the 2D radial integration to a 1D line integral along the acceptance curve. This is done once before the optimization, as  $\tilde{h}_{x,y}$  are target properties. Equation (7) then simplifies to

$$I = \sum_{r=-N_p}^{N_p} I_s(r), \quad (11)$$

if one combines the different parameters to obtain the intensity of a single momentum slice

$$I_s(r) = N_s(r) h_p(r) \epsilon(r) \cdot \underbrace{\left( \sum_{j=1}^{N_\phi} \tilde{h}_x(N_x(j, r), j) \right)}_{=I_x(r)} \underbrace{\left( \sum_{n=1}^{N_\phi} \tilde{h}_y(N_y(n, r), n) \right)}_{=I_y(r)}. \quad (12)$$

Using this form of precalculating respective histograms, a five-dimensional phase-space integration is reduced to a three-dimensional integration (only three sums are required), as can be seen in Eqs. (11) and (12).

### C. Beam size along the beamline

The beam size  $\sigma_{x,y}$  at any location  $s$  can be calculated without tracking by propagating the acceptance for each momentum slice to the location of interest, as detailed below.

#### 1. Step 1: Preparation

The beam size is the standard deviation  $\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ . In polar coordinates [Eqs. (4) and (5)], this becomes

$$\sigma_x = \sqrt{\langle R_x^2 \cos^2 \phi_x \rangle - \langle R_x \cos \phi_x \rangle^2}. \quad (13)$$

The quantities  $\langle R_{x,y} \rangle(i, j)$  and  $\langle R_{x,y}^2 \rangle(i, j)$  are precomputed 2D histograms (functions of polar radius and angle) that encode the target distribution. Once the acceptance is known,  $\langle R_{x,y} \rangle$  and  $\langle R_{x,y}^2 \rangle$  are read off directly by evaluating these histograms at the acceptance coordinates  $(R_{x,y}, \phi_{x,y})$ .

The mean radius for each polar angle of the  $h_x$  and  $h_y$  histograms is determined using the following equation

$$\langle R_u \rangle(R_u, \phi_u) = \frac{1}{N_u(\phi_u)} \int_0^{R_u} R_u^* h_u(R_u^*, \phi_u) dR_u^*, \quad (14)$$

where  $u$  can be either  $x$  or  $y$ , and  $N_u(\phi_u)$  represents the total number of particles within the infinitesimal angular slice at  $\phi_u$  that extends up to the radius  $R_u$ . In discrete coordinates, this equation can be expressed as follows:

$$\langle R_u \rangle(i, j) = \frac{\Delta R_u}{\bar{h}_u(i, j)} \sum_{r=0}^i r h_u(r, j). \quad (15)$$

The next step involves calculating the mean radius squared for each polar angle of the  $h_x$  and  $h_y$  histograms, as follows:

$$\langle R_u^2 \rangle(R_u, \phi_u) = \frac{1}{N_u(\phi_u)} \int_0^{R_u} R_u^{2*} h_u(R_u^*, \phi_u) dR_u^*. \quad (16)$$

In discrete coordinates, this equation transforms to

$$\langle R_u^2 \rangle(i, j) = \frac{\Delta R_u^2}{\bar{h}(i, j)} \sum_{r=0}^i r^2 h_u(r, j). \quad (17)$$

$\langle R_u \rangle(i, j)$  and  $\langle R_u^2 \rangle(i, j)$  are 2D histograms giving the mean and mean-square radius at  $(i\Delta R, j\Delta\phi)$ ; summing them along the acceptance curve (a 1D line integral) yields the corresponding quantities for the full momentum slice.

## 2. Step 2: Beam-size calculation

We use  $u = x$  (horizontal); the vertical  $y$  is analogous. The acceptance is propagated to  $s^*$  via  $\mathbf{R}$ , giving  $A_x^* = \{(\bar{R}_{x,j}^*, \bar{\phi}_{x,j}^*) | 1 \leq j \leq N_\phi\}$ . For off-momentum slices, the orbit offset  $x_{\text{orb}}^*$  is excluded from the propagation but included directly in the mean-value calculation below. Using Eqs. (15)–(17) and the Cartesian relation  $x = R_x \cos \phi_x$ , two vectors are formed:

$$\langle x \rangle(j) = \frac{\bar{R}_{x,j}^*}{\bar{R}_{x,j}} \langle R_x \rangle(N_{R,x}(j), j) \cos \bar{\phi}_{x,j}^* + x_{\text{orb}}^*, \quad (18)$$

$$\begin{aligned} \langle x^2 \rangle(j) = & \left( \frac{\bar{R}_{x,j}^*}{\bar{R}_{x,j}} \right)^2 \langle R_x^2 \rangle(N_{R,x}(j), j) \cos^2 \bar{\phi}_{x,j}^* + x_{\text{orb}}^{*2} \\ & + 2 \frac{\bar{R}_{x,j}^*}{\bar{R}_{x,j}} \langle R_u \rangle(N_{R,x}(j), j) \cos \bar{\phi}_{x,j}^* x_{\text{orb}}^*. \end{aligned} \quad (19)$$

An index  $r$  for the momentum slice was omitted in Eqs. (18) and (19) for readability. The factor  $\bar{R}_{x,j}^*/\bar{R}_{x,j}$  linearly rescales both the acceptance and the enclosed distribution (a direct consequence of linear transport), so

mean values and rms values scale identically. Summing along the acceptance curve then yields the momentum-slice averages

$$\langle x \rangle_s = \frac{1}{I_x} \sum_{j=1}^{N_\phi} \tilde{h}_x(N_{R,x}(j), j) \cdot \langle x \rangle(j), \quad (20)$$

$$\langle x^2 \rangle_s = \frac{1}{I_y} \sum_{j=1}^{N_\phi} \tilde{h}_x(N_{R,x}(j), j) \cdot \langle x^2 \rangle(j). \quad (21)$$

Here, it is important to note that the orbit and the acceptance are momentum-dependent and different for each momentum slice. An additional index  $r$  was omitted in Eqs. (20) and (21). In consequence, if one aims to calculate the beam size of the entire beam (the set of all momentum slices), the intensity of the different momentum slices has to be used as a weight to obtain the correct beam size,

$$\sigma_x = \sqrt{\sum_{r=-N_p}^{N_p} \frac{I_s(r)}{I} \langle x^2 \rangle_s(r) - \left( \sum_{r=-N_p}^{N_p} \frac{I_s(r)}{I} \langle x \rangle_s(r) \right)^2}. \quad (22)$$

For definitions of  $I$  and  $I_s$ , see Eqs. (11) and (12). For beamlines with significant decay over their length,  $L_{\text{line}}$  in Eq. (2) can be replaced by the exact position  $s$ . The only approximation in the entire beam-size calculation is the assumption of linear transport; no assumptions are made about the underlying particle distribution.

Often, the combined beam size of both transverse planes has to be minimized (more rarely maximized). It is then convenient to minimize the combined variance

$$\Sigma_{xy}^2(s^*) = \sigma_x^2(s^*) + \sigma_y^2(s^*) \quad (23)$$

at the respective location  $s^*$  since this expression displays a well-behaved convex nature. This procedure corresponds to a minimization of the beam envelope in both transverse planes—a so-called *double waist*.

## D. Beam divergence

The beam divergence  $\sigma_{x'}$  is calculated analogously to the beam size, with the substitution  $x' = R_x \sin \phi_x$  (instead of  $x = R_x \cos \phi_x$ ). This amounts to replacing the cosine in Eqs. (18) and (19) with the sine and introducing the orbit angle  $x_{\text{orb}}'^*$  at  $s^*$ :

$$\langle x' \rangle(j) = \frac{\bar{R}_{x,j}^*}{\bar{R}_{x,j}} \langle R_x \rangle(N_{R,x}(j), j) \sin \bar{\phi}_{x,j}^* + x_{\text{orb}}'^*, \quad (24)$$

$$\begin{aligned} \langle x'^2 \rangle(j) = & \left( \frac{\bar{R}_{x,j}^*}{\bar{R}_{x,j}} \right)^2 \langle R_x^2 \rangle(N_{R,x}(j), j) \sin^2 \bar{\phi}_{x,j}^* + x_{\text{orb}}'^{*2} \\ & + 2 \frac{\bar{R}_{x,j}^*}{\bar{R}_{x,j}} \langle R_u \rangle(N_{R,x}(j), j) \sin \bar{\phi}_{x,j}^* x_{\text{orb}}'^{*} \end{aligned} \quad (25)$$

Equations (20)–(22) then apply with the substitutions above, giving  $\sigma_{x'}$  and the combined divergence

$$\Sigma_{x'y'}^2(s^*) = \sigma_{x'}^2(s^*) + \sigma_{y'}^2(s^*). \quad (26)$$

### E. Momentum spread at the end of the beamline

An additional parameter that can be optimized is the momentum spread of the transmitted beam. In this work, the following definition is used for defining the relative momentum spread

$$\frac{\sigma_p}{p_0} = \sqrt{\frac{1}{I} \sum_{r=-N_p}^{N_p} \left( \frac{r \Delta p}{p_0} \right)^2 I_s(r)} \quad (27)$$

with  $r$  being the index of the respective momentum slice and  $r \Delta p$  being the absolute momentum offset with respect to the nominal momentum  $p_0$ . This equation implies that a shift of the mean momentum increases the momentum spread since the mean momentum is not taken into consideration.

### F. MOGA optimization, its free parameters, and the objectives

The optimizer is free to modify essentially any beamline parameter within designer set constraints, including magnet specifications, number of magnets, and collimator gaps. Multiobjective optimization is used to avoid constructing a potentially flawed scalar cost function and to reveal trade-offs between competing objectives. Among the algorithms tested, NSGA-III [23], SMS-EMOA [24], and AGE-MOEA [25] from the PyMoo library [26] were selected. MOGA is well established in accelerator lattice optimization [15–17].

Initially, the authors focused on optimizing relatively simple beamline parameters, such as magnet strengths and drift space lengths. However, these changes might not fully optimize the beamline. For instance, altering a magnet's type (length, aperture, and maximum gradient) could yield benefits for the overall beamline design that are not immediately apparent. Additionally, selecting the target is not a straightforward task. The particle flux alone does not necessarily indicate the optimal target type. By allowing the optimization process to freely choose targets, it can determine the most suitable target that, when combined with a fully optimized line (specific to that target), results in the best overall transmission. The authors

have identified the following generic beamline parameters that the optimization process should have access to: (i) Production target: The optimizer selects the best target from a precomputed list of phase-space histograms (see Fig. 4), since particle-matter simulations are not run inline. (ii) Drift spaces: Freely varied above a lower limit set by instrumentation and vacuum hardware. (iii) Quadrupole type (aperture, peak gradient, and current): The aperture sets the pole-tip distance; the maximum gradient follows from a  $g \propto 1/R$  scaling. The optimizer freely chooses any gradient up to this maximum (i.e., implicitly the current) and the magnet length, subject to constraints within the span of existing magnet designs. (iv) Collimator gap width: Allows optimization of the momentum selection (not used in the optimization presented here). (v) Dipole edges: Entrance and exit edge angles can be optimized for large deflections (not used here).

Optimizing the quadrupole type by hand is impractical: the interplay between aperture, length, gradient, inter-magnet distances, and particle decay probabilities is too complex to balance intuitively. For example, a longer quadrupole may improve acceptance but simultaneously increase decay losses—a trade-off the optimizer handles naturally.

The authors consider the following generic optimization objectives as easily obtainable within the optimization process: (i) beam size  $\sigma_{x,y}$ —see Eq. (22), (ii) beam divergence  $\sigma_{x',y'}$ —see Eq. (22) with substitutions, (iii) transmission efficiency  $I$ —see Eq. (11), and (iv) momentum spread  $\sigma_p/p_0$ —see Eq. (27).

Other optimization objectives can surely be considered.

## IV. THE OPTIMIZATION OF THE SBN-NUSCOPE SHORT-BASELINE NEUTRINO BEAMLINE

The SBN-nuSCOPE beamline is a short, horn-free line driven by a slowly extracted high-energy proton beam that impinges on a graphite target. The resulting charged hadrons are guided by quadrupoles to a momentum-selection section comprising three dipoles and a central quadrupole acting as a field lens, which nullifies the first-order dispersion  $D_x$  at the section exit. A thin Pb plate in the momentum-selection section serves as a positron degrader: positrons lose energy in the plate and are therefore more strongly deflected in the second bending magnet, reducing the positron flux in the NuTag pixel detectors to a compatible level. The mechanism is depicted in Fig. 6. While the Pb plate is not considered in the optimization process, it plays a vital role in modifying the energy of on-momentum positrons ( $p \approx 8.5$  GeV/c) that have escaped the target and reached the longitudinal position of the Pb plate. The third dipole is surrounded by two upstream and two downstream pixel detectors [30,31] to achieve a precise momentum measurement on a particle-by-particle basis,

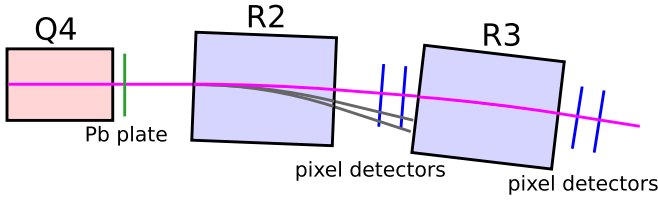


FIG. 6. Sketch of the second half of the momentum-selection section of the SBN-nuSCOPE beamline (beam travels left to right). An on-momentum  $K^+$  or  $\pi^+$  particle (magenta line) is barely influenced by the Pb plate (thickness of two radiation lengths) and remains centered within the pixel detectors (blue lines) at the third bending magnet (R3) in the beamline. The momentum of positrons (gray lines), however, is strongly influenced by the Pb plate, and the positrons, therefore, are more strongly deflected in the R2 bending magnet. The positrons eventually pass through the pixel detectors at a transverse offset (reduced particle rate in the pixel detectors' center).

similar to the approach employed in the K12 line for the NA62 experiment [32]. The final triplet of the beamline performs the necessary focusing to achieve a parallel beam that remains small within the 40-m-long decay tunnel.

### A. Free parameters

The beamline elements, modeled in BDSIM [14], are shown in Fig. 1. The momentum selection covers  $\Delta p/p_0 \in [-10\%, 10\%]$ . Seven drift spaces are free (lower bound 0.65 m; 0.7 m before Q1 for shielding), and the six quadrupoles outside the momentum-selection section contribute 18 free parameters (length, aperture, and gradient each). The target type is the 27th free parameter. The bending magnets and the dispersion-canceling quadrupole in the momentum-selection section are fixed.

The optimization of the quadrupoles demands special attention due to the quadrupole aperture's limitation on the maximum field gradient. To accommodate realistic magnetic element choices, the quadrupoles have varying lengths ranging from 0.6 to 2.1 m, while the aperture can extend from 4 to 10.5 cm. From the aperture, the maximum gradient can be estimated using a modified  $1/r$  scaling based on data points from existing North Area and East Area magnets [33].

The optimizer selects one target from a list of 19 graphite targets with varying lengths, widths, and densities. The list is presented in Table I. It was quickly discovered that a collapsed version of the CNGS target (a continuous graphite rod without multiple gaps between graphite pieces, unlike the original CNGS target) yields the best performance. Consequently, we have expanded the list to encompass various target variants, enabling a comprehensive exploration of the parameter space. The initial target types were inspired by existing experiments or proposals for accelerator neutrino experiments.

TABLE I. The list of considered production targets. The  $K^+$  and  $\pi^+$  yield is a linear fit in order to include the dependence on the particle momentum in the  $p = 8.5$  GeV range. Fourteen (14) collapsed CNGS target types have been analyzed with different lengths, radii, and densities.

| Name                       | Geometry      | Length<br>$L$ (m) | Radius<br>$r$ (mm) | Density<br>$\rho$ (g/cm <sup>2</sup> ) |
|----------------------------|---------------|-------------------|--------------------|----------------------------------------|
| ENUBET [5,13]              | Cylinder      | 0.70              | 30                 | 2.3                                    |
| ENUBET thin                | Cylinder      | 0.70              | 10                 | 2.3                                    |
| NuMI [27]                  | Cylinder      | 0.94              | 3.7                | 1.7                                    |
| T2K [28]                   | Cylinder      | 0.91              | 13                 | 1.7                                    |
| CNGS [29]                  | Multicylinder | 1.30              | 2, 3               | 1.8                                    |
| CNGS collapsed $\times 14$ | Cylinder      | 0.7–1.4           | 2.50–3.25          | 1.7–2.2                                |

### B. Optimization objectives

Three objectives are minimized/maximized: (i)  $K^+$  transmission [Eq. (12)] to the decay tunnel entrance (end of Q7);  $\pi^+$  intensity is nearly perfectly correlated with  $K^+$  and is therefore not treated as an independent objective. (ii) Combined beam-size variance  $\Sigma_{xy}^2$  [Eq. (23)] at the end of the decay tunnel, to keep the beam contained. (iii)  $\Sigma_{xy}^2$  at the Pb plate, where multiple scattering must be minimized (a double waist is desired).

### C. Optimization convergence

The SMS-EMOA algorithm is used with the updated ENUBET beamline [13] as a starting point. A population of 200 solutions is evolved; the *offspring* are generated by combining pairs of solutions, and an offspring replaces a population member if it increases the *hypervolume*—the objective-space volume enclosed by the *Pareto front*—keeping the population size fixed.

#### 1. Initial optimization with low precision

The rough scan uses 200 polar-angle sample points per plane, seven momentum slices, and an offspring size of 20. Constraints are applied on minimum transmission ( $1.7 \times 10^{-3}$   $K^+$ /PoT), primary beam trajectory, and maximum beam-size variance ( $\Sigma_{xy}^2 < 500$  cm<sup>2</sup>) at the tunnel end. Figure 7 shows the hypervolume [34] evolution: growth slows after  $\sim 200$  generations.

#### 2. Maintaining hierarchy

The MOGA relies on nondominant sorting and does not require the exact acceptance or particle count—it only needs to correctly rank solutions relative to one another. It therefore suffices to show that a solution A outperforming solution B in the linear approximation also outperforms B under exact tracking (hierarchy preservation). We verify this using the 200 solutions after 500 generations, comparing the linear and tracking-based acceptance areas  $A_x$ ,  $A_y$ ,

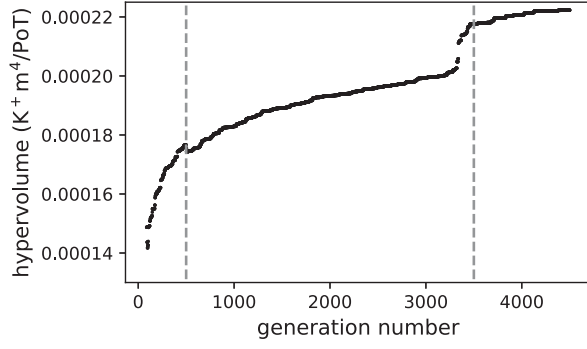


FIG. 7. The evolution of the hypervolume during the optimization process. The initial scan is conducted up to generation 500 (first gray line). The minimum transmission is increased after generation 500, and the calculation is resumed with improved numerical precision. At generation 3500, the sampling rate is increased once more (second gray line).

and their product  $A_x A_y$  via the linear correlation coefficient  $r$  (Fig. 9). As shown in Table II, the correlation coefficient of  $A_x A_y$  exceeds  $r > 0.98$  for all three momentum offsets. The low  $r$  for the vertical acceptance alone reflects the fact that the vertical aperture in the momentum-selection section is identical across solutions, keeping  $A_y$  nearly constant. Summing the three  $A_x A_y$  slices gives  $r = 0.9986$ , confirming that the hierarchy is robustly preserved. No broken hierarchy has been observed in any application of this method; nonetheless, performing this check is recommended when applying the approach to a new beamline.

### 3. Follow-up optimization with increased precision

Starting from the 200 solutions after 500 generations, the precision is increased to 11 momentum slices and 600 polar angles (up to generation 3500) and then to 1000 polar

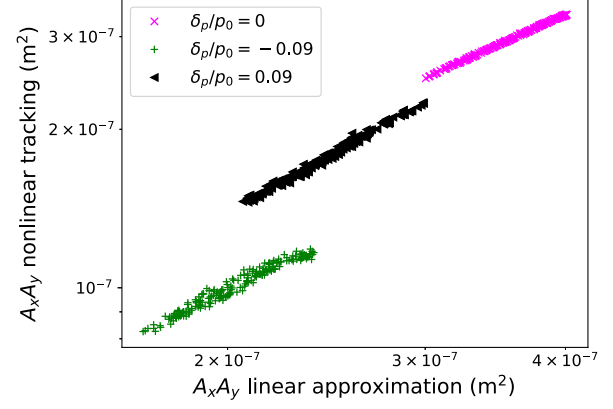


FIG. 9. The figure illustrates the values of the area enclosed by the transverse beamline acceptance, which is the product of  $A_x$  and  $A_y$ . In the case of a uniform density distribution in phase space originating from the target, this value is directly proportional to the intensity. The analysis presents the 200 diverse beamline designs that emerged after 500 generations of MOGA optimization. The linear approximation of the acceptance is plotted on the abscissa, while the PTC tracking result for the acceptance is displayed on the ordinate. Different markers represent various momentum slices at  $\Delta p/p_0 = 0$ ,  $\Delta p/p_0 = -0.09$ , and  $\Delta p/p_0 = 0.09$ . The corresponding linear correlation coefficients are presented in Table II.

angles (up to generation 4500, second gray line in Fig. 7). The hypervolume stagnates between generations 4000 and 4500, at which point the optimization is terminated.

## D. Comparison of optimized design with initial guess

### 1. Transmission improvements

The optimized solution is selected from three-dimensional Pareto front as shown in Fig. 8. In the selection process, increased weight is put on the beamline transmission and beam size in the decay tunnel (visible in the

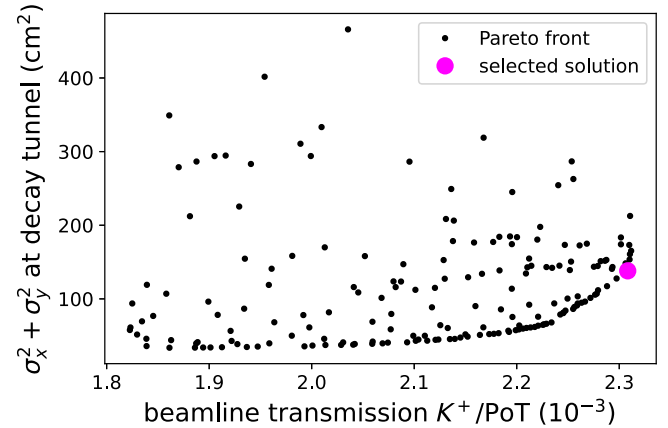
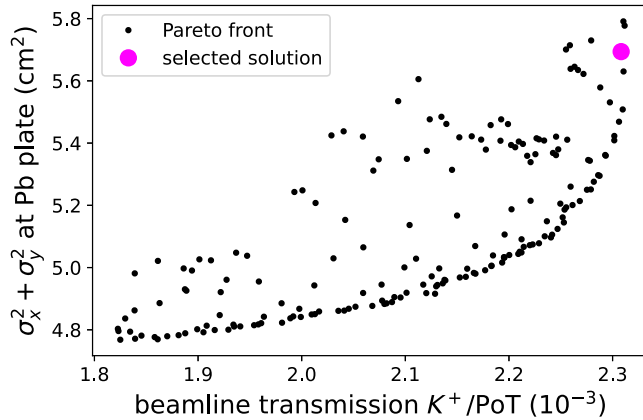


FIG. 8. The figure shows two projections of the three-dimensional Pareto front after 1200 generations. The left plot shows the beam size at the Pb plate versus the beamline transmission, while the right plot displays the beam size in the decay tunnel versus the beamline transmission. The solution that is selected for the evaluation of the performance with a start-to-end BDSIM simulation is marked with a magenta dot.

TABLE II. The linear correlation coefficients that indicate the correlation between the enclosed area calculated using the linear approximation and that of the exact tracking calculation (as depicted in Fig. 9) ultimately serve as an indicator of whether the hierarchy between the linear approximation and tracking is maintained. The correlation coefficient is close to 1 for all three momentum slices.

| Quantity                          | Momentum slice |        |        |
|-----------------------------------|----------------|--------|--------|
| Momentum offset $\Delta p/p_0$    | 0              | -0.09  | 0.09   |
| $r$ horizontal ( $A_x$ )          | 0.9996         | 0.9930 | 0.9959 |
| $r$ vertical ( $A_y$ )            | 0.1473         | 0.0674 | 0.0039 |
| $r$ full transverse ( $A_x A_y$ ) | 0.9995         | 0.9800 | 0.9954 |

right plot in Fig. 8). The initial beamline design did not anticipate the use of a Pb plate to remove positrons from the beam. Therefore, the comparison is conducted without the Pb plate, as if silicon pixel detectors were not inserted into the beamline. The top section of Table III presents the beamline transmission of  $K^+$  and  $\pi^+$  within the  $\Delta p/p_0 \in [-10\%, 10\%]$  range in the linear approximation, while the bottom section shows the corresponding results from equivalent BDSIM simulations. The BDSIM values are derived from the beamline spectra depicted in Fig. 10.

It is evident from Table III that significant improvements are achieved in both the linear model (used by the optimizer) and within BDSIM for the newly optimized beamline. The linear model clearly overestimates the meson yield, predicting a kaon yield of  $9.96 \times 10^{-4}$   $K^+$ /PoT while BDSIM only indicates a  $6.19 \times 10^{-4}$   $K^+$ /PoT yield. This discrepancy arises from a linear acceptance that exceeds that obtained through tracking. However, the relative change improvement in the transmission compared to the initial design can be predicted more accurately: in the linear model, the relative improvement for the  $K^+$  ( $\pi^+$ ) yield is predicted to be at +132% (+100%). BDSIM simulation yields a +124% (+93%) relative improvement that closely matches the prediction from the linear model.

The increase in yield can be easily explained by the change in production target and the sophisticated shaping of the transverse beamline acceptance. The solution

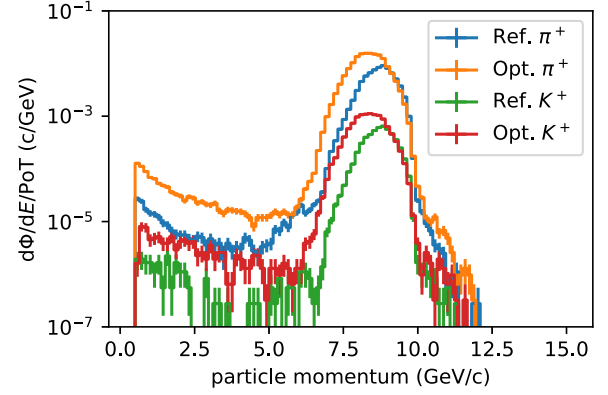


FIG. 10. The  $K^+$  and  $\pi^+$  flux of the reference beamline (Ref.) and the optimized beamline (Opt.) as a function of the particle momentum as produced by a start-to-end BDSIM simulation. The number of transmitted particles in the  $\Delta p/p_0 \in [-10\%, 10\%]$  range around  $p = 8.5$  GeV/c are given in Table III. A  $p = 500$  MeV/c momentum cut is applied within the simulation.

chosen from the Pareto front utilizes a collapsed CNGS target with a length of  $L = 1.30$  m, a radius of  $r = 3.0$  mm, and a density of  $\rho = 2.26$  g/cm<sup>3</sup>.

The optimized beamline's acceptance is well matched to the target distribution shown in Fig. 11. Notably, the substantial  $y$ - $y'$  correction of the vertical acceptance leads to a much higher acceptance of particles by the line compared to the plots depicted in Fig. 4.

## 2. Beamline optics changes

The optimization process of the beamline has changed the layout of the beamline significantly, as can be seen in the schematic comparison features in Fig. 12. The beamline length decreased by roughly 4 m, a feature that reduces the number of  $K^+$  decays. The decreased beamline length is obtained by using much shorter quadrupoles in the final triplet and for the first quadrupole in the beamline. The final quadrupole triplet that recovers the beam coming out of the achromat and is weak and does not aim for some sort of focus ( $R_{12} = R_{34} = 0$ ) anywhere near the decay tunnel as can be seen in Fig. 13. Instead, the optimizer

TABLE III. Comparison of the optimization objectives (transmission and beam size) between the previous design (reference) and the optimized beamline design (optimized). The results from the proposed linear approach are given in the top part of the table, while the values of a full BDSIM simulation are given in the bottom part. While absolute performance cannot be precisely quantified by the linear model, it can predict a relative transmission improvement with an 8% precision in this specific case. The BDSIM simulation results are extracted from the spectra shown in Fig. 10. The beam size at the Pb plate, as well as the end of the decay tunnel, is also listed.

| Design    | Framework | $K^+$ /PoT( $10^{-4}$ ) | $\pi^+$ /PoT( $10^{-3}$ ) | $\Sigma_{xy}$ Pb plate (cm) | $\Sigma_{xy}$ decay tunnel (cm) |
|-----------|-----------|-------------------------|---------------------------|-----------------------------|---------------------------------|
| Reference | Linear    | 9.96                    | 15.42                     | 2.3                         | 16.3                            |
| Optimized | Linear    | 23.08 (+132%)           | 30.89 (+100%)             | 2.4 (+2%)                   | 11.8 (-28%)                     |
| Reference | BDSIM     | 6.19                    | 10.74                     | 2.0                         | 13.2                            |
| Optimized | BDSIM     | 13.87 (+124%)           | 20.68 (+93%)              | 2.2 (+9%)                   | 10.0 (-24%)                     |

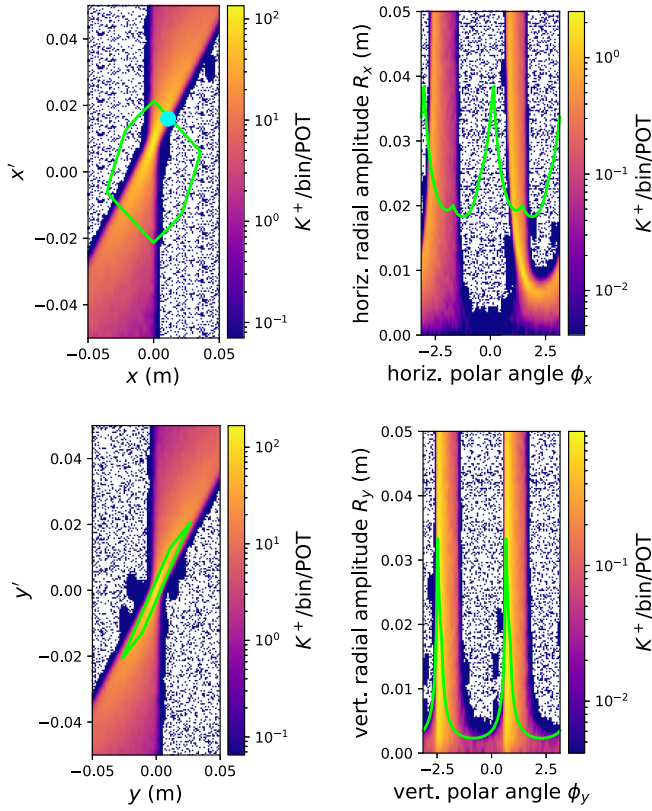


FIG. 11. Top left: the overlap of the horizontal acceptance (green polygon) after the optimization process with the histogram coming out of the optimized target. The production angle of  $0.5^\circ$  causes a  $x'$  shift of the distribution, so that one edge of the acceptance (cyan marker) gets close to the beam core. Top right: the same plot as in the top left plot in polar coordinates. Bottom left: the overlap of the vertical acceptance with the histogram of the optimized target. The acceptance polygon follows the  $y$ - $y'$  correlation of the target histogram. Bottom right: the bottom left plot is shown here in polar coordinates. The optimized acceptance (two large peaks) overlaps very efficiently with the histogram.

maximizes the beam size toward the start of the decay tunnel as is shown in Fig. 14 (right) to minimize the phase advance within in the decay tunnel. This leads to a beam that stays as small as possible throughout the decay tunnel. This is particularly evident in the vertical plane (see Fig. 14, bottom right). Initially, the optics were designed to generate a parallel beam in the decay tunnel by nullifying the  $R_{22}$  and  $R_{44}$  matrix elements. The  $R_{12}$  and  $R_{34}$  terms then remain constant throughout the decay tunnel, as illustrated in Fig. 13. The rationale behind this design was to preserve the beam size of a particle distribution originating from the production target, which is predominantly spread out in transverse momentum rather than transverse position (ignoring the target's length). However, this approach of solely focusing on minimizing the contribution of transverse momentum to the beam size in the decay tunnel inadvertently allows the contribution

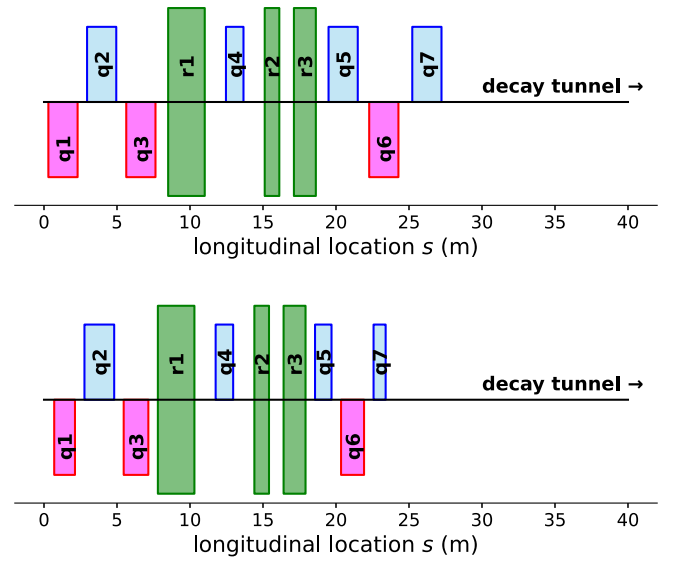


FIG. 12. Top: a schematic view of the initial guess for the magnet arrangement. The magenta-colored boxes represent focusing quadrupoles, while the blue-colored boxes indicate defocusing quadrupoles. The bending magnets are colored in green. Bottom: after the optimization process, it is evident that the quadrupole magnets, particularly those in the final triplet, have become shorter. The optimized line is now only about 23 m long, compared to the initial length of  $\sim 27$  m.

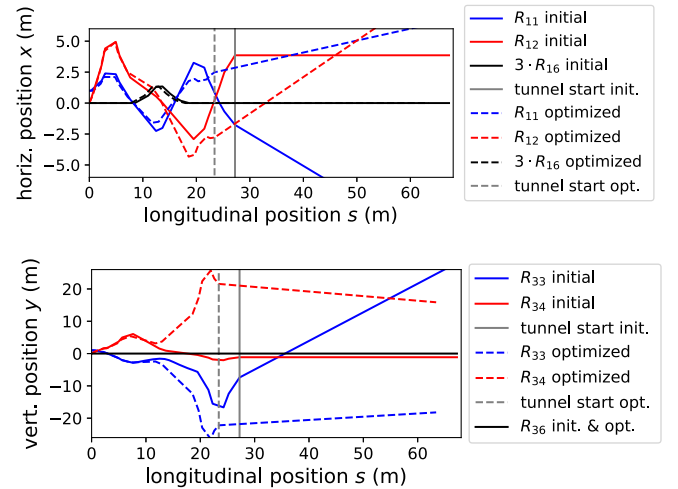


FIG. 13. Top: comparison of the horizontal transport matrix elements between the initial guess and the optimized design. The optimized design features a decay tunnel that starts  $\sim 4$  m earlier than in the initial design. Bottom: the analogous plot for the vertical plane.

of transverse position to increase uncontrollably. This is evident in Fig. 14 (left).

An important feature that can be observed in Fig. 14 is the deviation of the tracked beam size from that estimated by the analytic approach. This disagreement is caused by the production angle of  $\Delta x' = 0.5^\circ$  as evident from Fig. 11

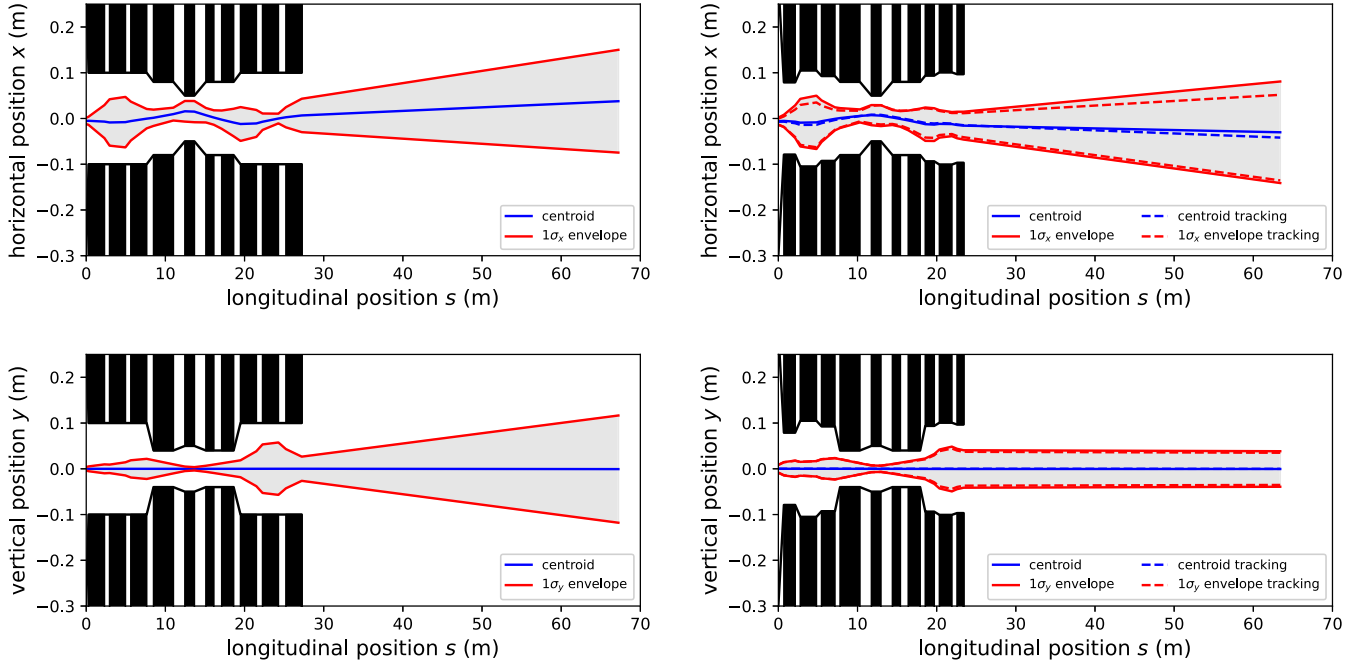


FIG. 14. Beam-size prediction by the linear model. Top left: the horizontal centroid (blue) and its corresponding  $1\sigma$  envelope (red) within  $\Delta p/p_0 \in [-10\%; 10\%]$  of the initial beamline. The black lines and areas denote the aperture. Bottom left: the analogous plot for the vertical plane for the initial beamline design. Top right: the horizontal beam size for the optimized beamline. The decay tunnel begins at  $s \approx 23$  m instead of  $s \approx 27$  m. The values obtained from a corresponding BDSIM tracking simulation are indicated by the colored dashed lines. The horizontal production angle amplifies geometric aberrations, resulting in an overestimate of the beam size in the positive  $x$  direction in the linear model. Bottom right: the analogous plot for the vertical plane of the optimized beamline. A better agreement between tracking (dashed lines) and the predicted behavior (solid lines) is achieved in the vertical plane due to the absence of the production angle.

(cyan indicator in the top left plot). The edge of the horizontal acceptance intersects with a high-density region of the histogram, leading to a loss of acceptance due to geometric aberration. Consequently, the beam fraction not captured by the acceptance in reality results in a (mostly) one-sided deviation of the tracked and calculated beam size in Fig. 14. Furthermore, Fig. 2 shows that at the equivalent location in  $x$ - $x'$  space, the acceptance obtained from tracking is slightly smaller than that obtained from the linear calculation.

The beam size at the Pb plate (at the end of the decay tunnel) is predicted to be  $\Sigma_{xy} = 2.4$  cm ( $\Sigma_{xy} = 11.8$  cm) in the linear model after optimization, as shown in Table III. This represents a relative change of 2% (–28%) compared to the original design. The BDSIM simulation yields beam sizes at these two locations that are 8%–19% smaller than those calculated by the linear model. The relative change in beam size between the original beamline and the optimized beamline in the BDSIM simulation closely matches the relative changes predicted by the linear model; for instance, a +9% increase at the Pb plate and a –24% decrease at the end of the decay tunnel. The absolute differences in beam size are once again attributed to the one-sided (in terms of acceptance in  $x$ - $x'$  space)

enhancement of geometric aberrations caused by the horizontal production angle, as previously explained.

The combination of employing a linear model with an MOGA algorithm proves highly effective in this scenario. The MOGA algorithm facilitates relative comparisons, while the linear framework presented throughout this paper accurately predicts the relative difference between beamline designs. Tracking is undoubtedly essential for obtaining the most precise beamline prediction; however, it is not necessarily crucial in an optimization process that is solely based on optics.

## V. WORKING EXAMPLE

An example for the optimization of the H4-VLE beamline that guides the beam to one of the ProtoDUNE detectors in CERN’s North Area is provided at [35].

## VI. CONCLUSION

The formalism presented in this paper led to a significant improvement in the transmission of the SBN-nuSCOPE beamline, as confirmed by a comprehensive start-to-end BDSIM simulation. The transmission was enhanced by a substantial 93% for  $\pi^+$  and 124% for

$K^+$  transmission. It is worth noting that a well-informed initial guess significantly accelerated the convergence of the algorithm. The algorithm's performance is robust enough for practical applications. The authors successfully implemented the algorithm during a short beamline optimization session of the H4-VLE beamline. The transmission could be improved without a substantial time investment, achieving a  $4.3 \pm 3.1(\text{stat.})\%$  improvement under the assumption of a perfect beamline setup, which was clearly not realistic. The framework presented in this paper provides a powerful tool to determine all necessary information based on two readily obtainable pieces of data: particle production at the target level and the linear optics of the beamline. With these two simple inputs, the typical challenges encountered during beamline design and optimization are overcome. Simplifying assumptions regarding particle production are no longer necessary, while the computationally intensive approach of optimizing the beamline by tracking is effectively avoided. At the same time, if the target and acceptance stage of the beamline is determined by a high-dimensional parameter space (e.g., target in combination with a magnetic horn), then the evaluation of such a system can be decoupled from the downstream beamline design to avoid a computationally expensive optimization process.

## ACKNOWLEDGMENTS

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## DATA AVAILABILITY

The data are available from the authors upon reasonable request. A working example of the presented framework is provided at [35].

## APPENDIX: ANALYTIC CALCULATION OF THE LINEAR ACCEPTANCE

### 1. Linear method

An aperture can be represented by a vector equation at some location  $s$  along the beamline with the respective aperture  $\pm a_x$  on either side in phase space, as (horizontal plane taken as an example)

$$\begin{pmatrix} x \\ x' \end{pmatrix} = \begin{pmatrix} \pm a_x \\ 0 \end{pmatrix} + t \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (\text{A1})$$

$$\mathbf{w} = \mathbf{k} + t \cdot \mathbf{v} \quad (\text{A2})$$

with Eq. (A2) as an alias for Eq. (A1). The aperture  $a_x$  represents just an infinite vertical line in the  $x$ - $x'$  phase space (or  $y$ - $y'$  phase space) with  $t \in \mathbb{R}$ . The acceptance is

defined as the smallest area around the nominal particle's trajectory enclosed by the  $\mathbf{w}(t)$  functions that are all projected to the target position (typically, for secondary lines at  $s = 0$ ). The acceptance can be obtained from the  $\mathbf{R}$  matrices calculated by, e.g., the TWISS command in MAD-X, in combination with the linear expressions of all apertures as shown in Eq. (A2).

The  $\mathbf{R}$  matrix reads

$$\mathbf{R}_{x,y} = \begin{pmatrix} R_{11,33} & R_{12,34} \\ R_{21,43} & R_{22,44} \end{pmatrix}. \quad (\text{A3})$$

For each beamline element at any position  $s$ , the inverse matrix

$$\mathbf{R}_{x,y}^{-1} = \begin{pmatrix} R_{22,44} & -R_{12,34} \\ -R_{21,43} & R_{11,33} \end{pmatrix} \quad (\text{A4})$$

is applied to  $\mathbf{w}(t)$  at this particular position

$$\mathbf{R}^{-1}\mathbf{w}(t) = (\mathbf{R}^{-1}\mathbf{k}) + t \cdot (\mathbf{R}^{-1}\mathbf{v}). \quad (\text{A5})$$

Equation (A5) has the form of an aperture again [see Eq. (A2)]; however, it is propagated backward to the start of the beamline, which is the target's location. This process of propagating the aperture backward has to be repeated for all apertures. Examples of the projected apertures can be viewed in Fig. 3.

A convenient way to get the final acceptance shape at the initial ( $s = 0$ ) position now is to generate *lines*  $\mathbf{p}(r, \phi)$  from the origin in polar coordinates

$$\mathbf{p}(r, \phi) = r \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix} \quad (\text{A6})$$

with  $r \in \mathbb{R}^+$  and  $\phi \in [0, 2\pi[$ . The intersection of these lines with the back-projected apertures is obtained by setting Eq. (A5) equal to Eq. (A6) for any one of the calculated  $\mathbf{R}^{-1}\mathbf{w}(t)$  vectors

$$\underbrace{r \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix}}_{\mathbf{a}=(a_0, a_1)^T} = \underbrace{(\mathbf{R}^{-1}\mathbf{k})}_{\mathbf{k}'=(k'_0, k'_1)^T} + t \underbrace{(\mathbf{R}^{-1}\mathbf{v})}_{\mathbf{v}'=(v'_0, v'_1)^T}. \quad (\text{A7})$$

One can express Eq. (A7) as two equations of the same form

$$ra_0 = k'_0 + tv'_0, \quad (\text{A8})$$

$$ra_1 = k'_1 + tv'_1. \quad (\text{A9})$$

An expression for the free parameter  $t$  is easily obtained from the two equations

$$r = \frac{k_0 v_1 - k_1 v_0}{a_0 v_1 - a_1 v_0}. \quad (\text{A10})$$

It needs to be noted that the  $\mathbf{p}$  vector [defined in Eq. (A6)] can become (for certain  $s$  positions) (anti)parallel to the aperture vector  $\mathbf{v}' = \mathbf{R}^{-1}\mathbf{v}$  that gives the direction the aperture is extending in (so there is no intersection). The scalar  $r$  is the actual distance in phase space between the origin of the coordinate system and the projected aperture divided by the intersection with that aperture. This is due to the fact that  $|\mathbf{p}(r, \phi)| = |r|$ . For a single angle  $\phi$ , one obtains a number of different  $r$  values since the vector  $\mathbf{p}(r, \phi)$  that originates from the coordinate origin will intersect not only with a single but also with many of the projected apertures. The  $r$  corresponding to the actual acceptance is the smallest  $r$  that is larger than 0 since  $r \in \mathbb{R}^+$ .

The calculated acceptance is a list of  $(\phi_i, r_i)$  with  $i$  being the number of steps the polar angle  $\phi$  is sampled with. This list can be projected in either the (Cartesian)  $x$ - $x'$  or  $y$ - $y'$  planes via  $\mathbf{p}_i(r_i, \phi_i) = r_i(\cos \phi_i, \sin \phi_i)$ . A linear approximation between these points will yield a polygon in the  $x$ - $x'$  or  $y$ - $y'$  phase space. Since the vectors  $\mathbf{w}(r)$  are linear in phase space (before and after the back projection) and the interpolation is also linear, there is no interpolation error. The only possible source of interpolation error lies in the corners of the polygon: in corners, the acceptance changes direction, and a small triangle will not be considered in the interpolated acceptance (a vanishing underestimation if the increment in terms of polar angle is sufficiently small). An interpolation error only occurs at a very small number of corners. Otherwise, the calculation is analytic and exact within the first-order matrix approximation and can be extended to off-momentum particles.

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