# CALCULATION AND OPTIMIZATION OF HIGH-ENERGY BEAM TRANSFER LINES BY THE MONTE CARLO METHOD

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## Abstract

The calculation of high-energy beam lines consists of tracing of the proton beam trajectories along the transport channel from the source. The PROTON MK program code was developed to carry out such calculations using the Monte Carlo method. The beam from the accelerator is introduced in the form of a multivariate Gaussian distribution in x,x', z,z', dp/p phase space. In the case when an absorber (absorber, air section, window in the channel, etc.) is installed in the transport channel the beam parameters after the absorber are calculated using the GEANT4. The output file of this code can be used as input for the program. The program allows calculation of any beam parameters - intensity, spatial or phase density, energy distribution, etc. The program includes a block for the optimization of beam parameters presented in a functional form. Random search method with learning for search correction based on analysis of intermediate results (so-called statistical gradient method) is used for obtaining the global maximum of a function of many variables. The program has been tested in calculations of the beam transport lines for IC-80 cyclotron and for the development of the beam line for ophthalmology.

#### **INTRODUCTION**

There is a many of programs in the world for calculating the optics of high-energy beams [1, 2]. In most of them, the ion source is represented in the phase space in the form of a multidimensional ellipsoid, inside which particles and their initial parameters are uniformly distributed while there are no particles outside. Moreover, it is assumed that the beam emittance is conserved during the transport of the beam along the channel, which means that there are no beam losses in the channel. In particular, it is not possible to compute the effect of collimators on the intensity and other parameters of the beam. These assumptions greatly facilitate the mathematical formulation of the problem, but they do not quite reflect the experimental situation. In this work, a more adequate representation of the ion source is proposed.

#### **REPRESENTATION OF SOURCES**

In the experiment, the beam profile i.e. the distribution of the beam intensity over the transverse coordinates is well approximated by the Gaussian distribution, and the beam spot, i.e. intensity distribution in x, z-plane is an ellipse. This situation is typical for a multivariate Gaussian distribution, where any marginal or partial distribution along any axis is also described by a Gaussian distribution. Let's assume that the beam in the ion source can be  $\dagger$  amerkanov da@pnpi.nrcki.ru

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described by a five-dimensional normal distribution with a distribution function in space  $(x, x', z, z', \delta)$ :

$$f(\mathbf{X}, \mathbf{Z}, \mathbf{s}, \boldsymbol{\delta}) = \frac{1}{(2\pi)^{5/2} |\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2} \begin{pmatrix} X \\ Z \\ \boldsymbol{\delta} \end{pmatrix}^{T} \boldsymbol{\Sigma}^{-1} \begin{pmatrix} X \\ Z \\ \boldsymbol{\delta} \end{pmatrix}\right\}$$

where  $\Sigma$  is a 5x5 symmetric matrix, which is the covariance matrix of the adopted distribution, i.e. the mathematical expectation of the distribution and its elements are of interest, X is a vector (x, x'), Z is a vector (z, z'). The components of the matrix  $\Sigma$  have the form where  $\sigma_{k\ell} = \langle y_k \cdot y_e \rangle \, y_k$ ,  $y_e$  are the components of the random vector  $(x, x', z, z', \delta)$ .

In most cases, the movements along x and z are independent and then  $\sum_{xz}=0.$ In the case when the magnetic analysis takes place only in the x-plane  $\sum_{zp}=0.$ Based on the general properties of the multivariate normal distribution, it is possible to write the bivariate Gauss distribution in x, x' space in the form:

$$f(X) = \frac{1}{(2\pi) |\Sigma_{xx}|^{1/2}} \exp\left\{-\frac{1}{2} X^T \Sigma_{xx}^{-1} X\right\}$$

The elements of the correlation matrix  $\Sigma_{xx}$  are the mathematical expectations of the vector  $(x_i x_j')$  i.e. M  $(x_i x_j)$ , where i, j = 1, 2 and  $x_1 = x$ ,  $x_2 = x'$ . The matrix  $\Sigma_{xx}$  has the form:

$$\sum_{xx} = \begin{pmatrix} M(x^2) & M(xx') \\ M(xx') & M(x'') \end{pmatrix} = \begin{pmatrix} \sigma_x^2 & \rho \sigma_x \sigma_{x'} \\ \rho \sigma_x \sigma_{x'} & \sigma_{x'}^2 \end{pmatrix}$$

where M (x, x') =  $\rho \sigma_x \sigma_{x'}$  by definition of the correlation coefficient  $\rho$ .

Then the bivariate Gaussian distribution on the plane takes the form:

$$f(x,x') = \frac{1}{2\pi \sqrt{1-\rho^2}} \sigma_x \sigma_{x'} \exp\left\{-\frac{1}{2\left(1-\rho^2\right)}\lambda^2\right\}$$

where  $\sigma_x \sigma_{x'}$  are the standard deviations and  $\rho$  is the correlation coefficient. From the general form of the probability density of two random variables, it follows that the probability density is constant in all points of the xx plane at which

$$\lambda^2 = \left(\frac{x^2}{\sigma_x^2} - 2\rho \frac{xx'}{\sigma_x \sigma_{x'}} + \frac{x'^2}{\sigma_{x'^2}}\right)$$

where  $\lambda$  is an arbitrary value.

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The curve on the xx' plane, defined by the equations above, is the so-called ellipse of equal probabilities. In the case of a Gaussian distribution, instead of one ellipse, there is a set of concentric ellipses each of which corre-

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sponds to the fraction of the beam particles lying inside the ellipse contour. Let's denote by  $P(\lambda)$  the probability of a beam particle to fall inside an ellipse with a given value of  $\lambda$  parameter and  $F(\lambda)$  the area of this ellipse in phase space.

$$P(\lambda) = \iint_{\lambda} f(x, x') dx dx' = 1 - \exp(-\lambda^{2}),$$
  
$$F(\lambda) = \iint_{\lambda} dx dx' = \sigma_{x} \sigma_{x'} \frac{\lambda^{2}}{\sqrt{1 - \rho^{2}}},$$

If  $\delta$  is a fraction of particles outside the ellipse, then

$$P(\lambda) = 1 - \delta, \ \lambda^2 = -2\ln\delta(1 - \rho^2)$$

The area of the ellipse F ( $\lambda$ ) divided by  $\pi$  determines the emittance of the beam enclosed within the ellipse. The emittance of the beam increases with an increase in the amount of the beam contained within the ellipse. The results presented in the Table 1. demonstrate a relationship between the probability of a beam particle to fall inside an ellipse with a given value of the parameter  $\lambda$  and the beam emittance for the case of a straight ellipse i.e. when  $\rho = 0$ .

Table 1: Inside an Ellipse Probability of a Beam Particle

$\lambda^2$	δ	Ρ (λ)	F(λ)/ π
1	0.61	0.39	$\sigma_x \; \sigma_{x'}$
2	0.37	0.63	$2\sigma_x \sigma_{x'}$
3	0.22	0,74	$3\sigma_x \sigma_{x'}$
4	0.14	0.86	$4\sigma_x \sigma_{x'}$
6	0.05	0.95	$6\sigma_x \sigma_{x'}$

Gaussian distribution parameters can be determined by characteristic points of the ellipse. The ellipse of the beam and its three characteristic points  $x_1$ ,  $x_2$  and  $x_2$ ' is shown in Fig. 1.



Figure 1: Ellipse of the beam.

$$\sigma_x = \frac{x_2}{\rho \sqrt{-2 \ln \delta}}, \ \sigma_x = \frac{x_2}{\sqrt{-2 \ln \delta}}, \ \rho = \frac{x_2}{x_2^2} + x_1^2$$

The sign of  $\rho$  corresponds to the sign of  $x_2$ . If  $x_2 > 0$  then the beam diverges and  $\rho > 0$ . If  $x_2 < 0$  then  $\rho < 0$  and the beam converges. In the case of  $\rho = 0$ , the beam is described by a straight ellipse.

#### **GEANT CODE USAGE**

Another way of the generation of the particle source is used when an energy degrader, scattering foil or vacuum window is presented in the channel.

In this situation, the beam behavior in the degrader material is calculated by using the GEANT code. On the output of the program, a file containing the energy, transverse coordinates and velocities of the particles is produced. The file is used as input for further tracing of trajectories through the channel.

### THE BEAM TRANSPORT ALONG A CHANNEL

The calculation algorithm is as follows: a fivedimensional vector (x, x', z, z', dp/p) randomly generated according to Gaussian distribution determines the initial conditions for a particle at the entrance of the channel. Then the particle with the chosen initial conditions is traced along the channel. The transport channel consists of standard magnetic elements located in different positions: quadruple lenses, various types of magnets, which provide deflection of the beam in different directions. In a linear approximation, the relationship between the input and output coordinates and velocities in the transport element can be obtained using the transition matrix, which is different for each element.

The mathematical expression for the transition matrices has been formulated in many works. In this work, we used the coordinate system and transition matrices from Steffen's monograph [3]. The calculation of the trajectory of a particle along the channel is carried out step-by-step by application of transition matrices for magnetic elements. At the output of each element, the x and z coordinates are compared with the apertures. If a particle falls out of the aperture, then its transport is stopped and it is counted as a lost particle. As a result of multiple repetitions of this procedure (several thousand times), the beam parameters are evaluated at the output of each element.

### **OPTIMIZATION**

In addition to the problem of calculating the beam parameters in a channel with a given configuration, it is often necessary to obtain the optimal value of some beam parameters by varying the magnetic field in channel elements or configuration of the channel. This problem is solved in this work by using the Monte Carlo method. The different beam parameters such as intensity, energy distribution and so on are calculated using the above technique. In our case, one of the random search methods, the statistical gradient method, was used for optimization. The calculation algorithm is as follows. A sequence of random vectors is selected whose components are variable parameters with a normal distribution.

$$\vec{X}^{K} = (x_{1}^{K}, x_{2}^{K}, x_{3}^{K}, \dots, x_{n}^{K}), \quad K = 1, 2, \dots, n$$

With dispersions  $\sigma_i$  and mean value  $X_0$ . For each set of randomly selected parameters, i.e. for each vector, the

quality function  $\Phi(\vec{X}^K)$  is calculated, the maximum  $\Phi_m = \max \Phi(X)$  and the vector  $\vec{X}^M$  at which  $\Phi = \max \Phi$  are found. Then the statistical weight of each variable element is calculated.

$$g_{i} = \frac{1}{N} \sum_{K=1}^{N} (\Delta \Phi^{K} \cdot \Delta x_{i}^{K}) / \sigma_{i}^{2},$$
  
$$\Delta \Phi^{K} = \Phi^{K} - \Phi^{0}, \quad \Delta x_{i}^{K} = x_{i}^{K} - x_{i}^{0}$$

It is convenient to use normalized statistical weights

$$y_i = g_i / \sqrt{\sum_{i=1}^n g_i^2},$$

where n is the number of variables. Based on a series of trial calculations of the quality function, an attempt is made to move to a point with a larger value of maximum obtained at random search

$$x_i^r = x_i^m + \varepsilon \cdot y_i$$

where  $\varepsilon$  is a pre-selected factor. Then the function  $\Phi^r = \Phi(\vec{X}^r)$  is calculated and compared with  $\Phi_m$ . If  $\Phi_m < \Phi^r$ , then one more step is made in the direction of the gradient, but if  $\Phi_m \ge \Phi^r$ , then  $\Phi_m$  is taken equal to the original  $\Phi_0$  and a new cycle of calculations is performed. To reach a better precision it is envisaged to reduce the range of random vectors by reducing values of  $\sigma_i$  and step  $\varepsilon$ . The process is repeated until the change in  $\Phi$  or all parameters  $x_i$  becomes smaller than a predetermined value.

Constraints on the parameter ranges are easily included in the procedure that is not always possible with regular search methods. As shown in [4], in the presence of constraints on the range of parameter variation in the form:

$$\varphi_j(X) \ge 0$$
,  $j = 1 \dots m$ 

The global maximum search algorithm remains unchanged, and the quality function  $\Phi$  is assumed to be equal to zero when the coupling condition is violated.

#### **ALGORITHM REALIZATION**

Based on the described algorithm, a code with a graphical interface PROTON\_MK was developed. The program was written in C ++ and can be compiled to produce an executable file for Windows.

PROTON\_MK provides the following opportunities:

- Calculation of the high energy beam transport lines which consist of quadruple lenses, bending magnets, free space, collimators.
- Generation of the particle source the sample of N particles with the axial momentum of the channel  $p_0$  and parameters of the Gaussian distribution  $\sigma_0$ ,  $\sigma_x$ ,  $\sigma_x$ ',  $\sigma_z$ ,  $\sigma_z'$ ,  $\rho_x$ ,  $\rho_z$ ,  $\Delta p / p$ .
- Beam import after the absorber according to GEANT4 calculation.
- The output of beam parameters at any channel element.

- Variation of the operation modes of a large number of optical elements of the channel to optimize the output beam parameters.
- The calculation results are presented in the output report.

The program was tested during the development of the beams with energy of 50-900 MeV by decelerating the primary proton beam with energy of 1000 MeV in a copper absorber. Good agreement of calculation results with experimental data was achieved. Another example of the application of the program was the design of the beam for ophthalmology with a high degree of homogeneity [5] at the IC-80 accelerator. A beam with an intensity of 10 µA is extracted from the accelerator and then is focused onto a thin 300 µm tantalum scattering plate. The collimator after the foil preserves the central and uniform part of the scattered beam in such a way that a beam with a diameter of 60 mm and an intensity of 10<sup>10</sup> s<sup>-1</sup> falls into the patient's irradiation room with a 5% uniformity in intensity and a minimum divergence. The beam line for ophthalmology and the beam envelopes are shown in Fig. 2.



Figure 2: Ophthalmic beam line and beam envelopes on the level 95% of the intensity. 1 - corrector magnet, 2,3,4 – quadruple lenses triplet, 5 - tantalum scattering foil  $300\mu m$  thick, 6 - collimator, 7 – radiation shielding wall in front of the irradiation room.

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