PHYSCON 2009, Catania, Italy, September, 1–September, 4 2009

MULTI-OBJECTIVE OPTIMIZATION FOR BEAM LINES

Andrey Chernyshev
Applied Mathematics and Control Processes
Saint-Petersburg State University
Russia
andr.chernyshev@gmail.com

Abstract
In the present paper some problems of global optimization for focusing beam lines are discussed. The main features of this concept are described, and there are cited solutions for a variant of micro- and nanoprobe systems. For this purpose some analytical and numerical methods and tools are realized and discussed some results of numerical experiments.

Key words
Beam line, Modeling, Optimization, Computing, Nanoprobe

1 Introduction

Today, big place in science and technology is occupied with focusing systems that form a beam on the target with size less than a micrometer (up to nanometers) and named micro- and nanoprobes. Their specifics is that their construction stage always includes a stage of theoretical research of possible choice of such systems. The thing is, that the calibration process of finished systems (the adjustment) doesn't lead to significant system improvements and therefore the need to upgrade the systems by adding new elements arises, thus increasing the installation price. The traditional process of designing and tuning of focusing systems such as micro- and nanoprobes in order to produce certain desired properties is not straightforward. So the process of searching for optimal accelerator parameters has to come by with a thorough research of structures suiting the experimenter physicist, and can be divided into the following steps:

I. *Basic modeling.*

✓ aligning the succession of structure optimality criteria based on the existing systems;

✓ selection and classification of optimization parameters and influences, i. e. constructing a vector of operating parameters and operating functions;

✓ creating a physical and mathematical model of the whole focusing system suiting all the possibilities and expectations of the experimenter physicists.

II. *Research of the constructed models, parameters and quality criteria functionals.*

✓ linear model adjustment, which result is the local optimum set for selected criteria of the system;

✓ rejection of solutions not suiting the researcher's additional criteria, some of which could be admission satisfactions, realization possibilities and so on;

✓ including of additional effects in the scope of the linear model, such as fringing fields, self-charge etc;

✓ the account of nonlinear effects with the purpose of consecutive rejection of the local minima found at the previous stages.

As a result of performance of the given list of actions, the researcher receives a final set of acceptable decisions from which final customer carries out a choice based on additional, weakly-formalized criteria such as cost, technological realization restrictions of the given decisions.

The above told implies that the problem has to satisfy multiple criteria. At the same time, many of those criteria are contradicting (antagonistic), therefore antagonism account problem instantly appears, by means of the weight factors, indicators or any other.

The ideology described above is considered in the present paper on an example of a probe forming system (see [Lebed, 2002]).

2 Physical Backgrounds

Among the big family of beam lines, the special place is occupied by ion-optical systems, to which, in particular, micro- and nanoprobes concern. Under an ion-optical system we understand a system intended for transferring a beam from one part of the space to another (transportation), in which the basic attention is given to the formation of cross-section phase characteristics of the beam (focusing).

Figure 1 presents an example of a nanoprobe.

Distances between lenses, lense lengths, distance from objective to target ('working distance'), 'pre-distance' and fields created by lenses serve as the controls in systems of this type. At the same time, a num-

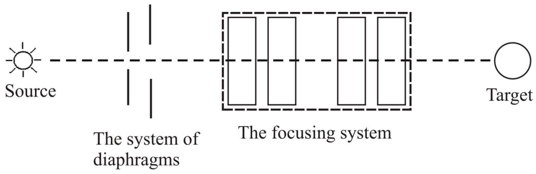

Figure 1. An exemplary structure of probe forming system.

ber of parameters, such as, for example, lense lengths, remain fixed after the construction of the beam line or demand considerable expenses for customization, and the other part can be subsequently corrected via adjustment.

Physical controls can be divided on two categories:

— control parameters (lengths, distances, diaphragm characteristics);

— control functions (functions describing field distribution along the optical axis of the system).

However, often, by choosing operation functions from some class (for example, from piecewise-constant) it is possible to carry out a transition from the control functions to the system elements parameters.

When designing the given kind of beam lines, it is necessary to consider the following complex of quality functionals and restrictions:

1. The criteria defining focusing characteristics.
2. Aperture restrictions.
3. Additional restrictions (for example, fixation of distance between lenses).
4. Luminosity of the beam line.

There are various approaches to the methodology of the formation of these functionals and the account of restrictions. The matter is, in some cases it is favourable to consider this or that restriction as a functional component, and in others – to include it in the list of restrictions in the form of equalities or inequalities.

Criteria defining focusing characteristic. Criteria defining focusing characteristics serve as the basic criteria for ion-optical systems. For nanoprobes where the target size of a beam on a target must be of an order of several nanometers, the requirements for beam compression factor can reach up to 100 and more times. Approaches to definition of what to understand as a size of a beam on a target are various, therefore different quality functionals arise. Figure 2 shows some of such approaches. We then consider the given approaches and rule out the functionals.

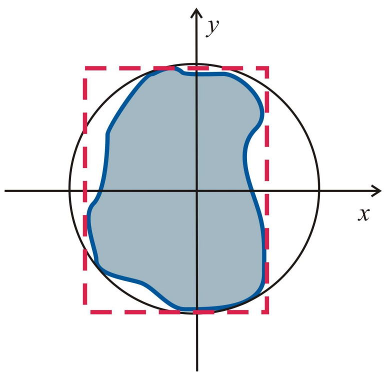

Figure 2. Different focusing criteria examples.

1. The circle of the least radius comprising a projection of a beam phase portrait to the axis plane can act as a functional defining the beam size on a target. Then the focusing problem can be formulated as follows:

finding $\inf\limits_{U\in\mathcal{U}} \sup\limits_{\mathcal{M}}(x^2+y^2)$, where $\mathcal{M}$ is a projection of a beam phase portrait, and $\mathcal{U}$ is a set of admissible controls.

2. The area occupied by a beam on a target:

finding $\inf\limits_{U\in\mathcal{U}} S(x,y)$, where $S(x,y)$ — area of a projection of a beam phase portrait to the axis plane.

3. The greatest deviation of one of the coordinates of a beam phase portrait projection:

finding $\inf\limits_{U\in\mathcal{U}} \max(\sup\limits_{\mathcal{M}} x, \sup\limits_{\mathcal{M}} y)$.

Possible cases are when the deviation of one of the coordinates is less critical than of the other, i. e. the beam section can have the oblong form. In this case it is necessary to add the corresponding weight factor into the current criterion.

Aperture restrictions. Aperture restrictions are the natural restrictions of ion-optical systems, and are defined by system composition.

1. For a square-shaped vacuum tube the following restrictions can be used:

$\sup\limits_{s\in[s_0,s_T]} |x(s)| \le x_{max}-\varepsilon,\ \sup\limits_{s\in[s_0,s_T]} |y(s)| \le y_{max}-\varepsilon,$

where s is the optical axis of the beam system, x_{max} and y_{max} represent the distance between the optical axis and aperture, ε is the minimal allowed distance between the beam and the aperture.

2. In the case of round-shaped aperture, the restriction can be formulated in terms of cylindric coordinates as follows:

$\sup\limits_{s\in[s_0,s_T]} |r(s)| \le r_{max}-\varepsilon,\ r(s)=\sqrt{x(s)+y(s)}.$

Often though, the restrictions can be more complex. In the examples demonstrated above, $x_{max}, y_{max}, r_{max}$ can be not constant but some given functions of s.

Additional restrictions. When constructing beam lines depending on their purpose, additional limitations often arise, that are related to some specifics of the system. For example, the minimal distance between control elements, driven by technological reasons, or the given distance between certain lenses, can be selected as one of the limitations in order to have a future possibility of installing additional modules.

Luminosity of the beam line. Other than focusing, another important factor is the amount of focused particles hitting a target, which defines the luminosity. The system has to have maximum acceptance, i. e. the phase space bandwidth, in order to provide high luminosity:

$\sup\limits_{U\in\mathcal{U}} \sup\limits_{V\in\mathcal{V}} \int\limits_{\mathcal{M}} f(\vec{X})d\vec{X}$, where $\vec{X}=(x,x',y,y')$ is the vector of the basic phase variables, $f(X)$ is the particle distribution function, $\mathcal{U}$ is the set of admissible controls, and $\mathcal{V}$ is the set of collimator system parameters. Depending on the starting distribution of the base

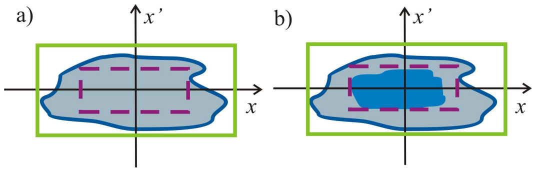

Figure 3. Acceptance examples.

phase set, certain acceptance values can be accepted. For instance, Figure 3 shows an acceptance outlined with a thick line, providing full preservation of the particles getting absorbed by the focusing system input. In the case of the uniform distribution of particles of the basic set (see Fig. 3a), the acceptance represented by thick broken line provides a 50% particle pass-through, which is unacceptable in most cases. However, if the distribution is nonuniform (see Fig. 3b) and the acceptance is at 95%, such values suit quite well.

Thus we are in the need to minimize a set of functionals at a time, which, in general form, could be represented with one using α_i and P_i weights, the selection of which defines the level of significance of a criterion:

$I(\vec{B},\vec{U}) = \sum_{i=1}^{k} \alpha_i I_i^{2P_i}(\vec{B},\vec{U}),$

where $\mathcal{B}$ is the control parameters set, $\mathcal{U}$ is the control functions set, $\vec{B} \in \mathcal{B}, \vec{U} \in \mathcal{U}$.

As stated before, the selection of the control functions set defining the controlling field from a certain appropriate class allows us to introduce parameters. So instead of $[\mathcal{B},\mathcal{U}]$ we will be using the pair $[\mathcal{B},\mathcal{B}_u]$ where $\mathcal{B}_u$ is the set parameters describing the controlling field.

3 Mathematical model of beam control system

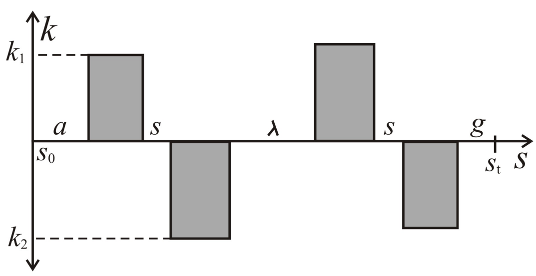

Figure 4. Russian quadruplet focusing system.

Let's consider a so-called "russian quadruple" [Andrianov, Dymnikov and Osetinsky, 1978] as an example, which allows to form beams with high degrees of compression. For the given system of quadrupoles (see Fig. 4) energy supply symmetry conditions are satisfied:

$$k(s) = -k(s_t - s), \quad s \in [s_0, s_t], \tag{1}$$

where s — parameter of length along an optical axis of the system, s_0, s_t — an initial and an end points accordingly, $k(s)$ is a gradient distribution function.

The particle motion equations in the linear approximation have the following appearance:

$$\begin{aligned} x'' + k(s)x = 0, \quad x' = dx/ds, \\ y'' - k(s)y = 0, \quad y' = dy/ds. \end{aligned} \tag{2}$$

The solution of the given equation system can be written down with the use of matrix propagator of the system $\mathbb{R}(s|s_0)$:

$$\vec{X}(s) = \mathbb{R}(s|s_0)\vec{X}_0, \quad \vec{X}_0 = \vec{X}(s_0), \tag{3}$$

Usually, focusing systems have a necessary constraint set up on the point-to-point beam transference (see, for example, [Andrianov, Dymnikov and Osetinsky, 1978]), which, in linear approximation, equals to:

$$r_{12} = r_{34} = 0, \tag{4}$$

where r_{12}, r_{34} — the elements of $\mathbb{R}(s_1|s_0)$.

The matrix $\mathbb{R}(s|s_0)$ can be presented as following:

$$\mathbb{R}(s_t|s_0) = \mathbb{R}_g \mathbb{M}(s_1|s_0)\mathbb{R}_a, \tag{5}$$

where $\mathbb{R}_g$, $\mathbb{M}(s_1|s_0)$, $\mathbb{R}_a$ — matrixes corresponding to passage of the working distance, focusing system and pre-distance accordingly.

Taking (1) into account for identity of transfer matrixes in planes $\{x, x'\}, \{y, y'\}$ it is enough (see [Andrianov, Edamenko, Chernyshev and Tereshonkov, 2008]) for the following condition to satisfy:

$$m_{11} = m_{22}, \tag{6}$$

where m_{11}, m_{22} — the elements of $\mathbb{M}(s_1|s_0)$.

In a nonlinear case, the equation of particle motion have much more difficult appearance. In the assumption of monochromaticity of a beam, let's write out the equation with the third order decomposition:

$$\begin{aligned} x'' + kx = &- \frac{3}{2}kxx' - \frac{1}{2}kxy'^2 + kx'yy' + \\ &+ k'xyy' + \frac{1}{12}k''x^3 + \frac{1}{4}k''xy^2 + \mathcal{O}(5), \\ y'' - kx = &\frac{3}{2}kyy' + \frac{1}{2}kyx'^2 - ky'xx' - \\ &- k'yxx' - \frac{1}{12}k''y^3 - \frac{1}{4}k''yx^2 + \mathcal{O}(5). \end{aligned} \tag{7}$$

In this case, the solution is:

$$\vec{Z}(s) = \mathbb{R}^{11}(s|s_0)\vec{Z}_0 + \mathbb{R}^{13}(s|s_0)\vec{Z}_0^{[3]}. \quad (8)$$

where $\vec{Z}^{[3]}$ — the third order Kronecker degree of a phase vector $\vec{Z}$.

4 Optimization methods

When solving optimization problems, a researcher may encounter difficulties with picking a method fully appropriate for the given problem. The high-quality implementation of the properly selected method or method aggregates allows finding the desired solution with the least computing costs.

4.1 The problem definition

While describing fringing fields, a transition from functions to parameters can be made. Thus, the selection of a function approximately describing a given fringing field and its parametrical representation is made at the same time.

Consequently, after we have the appropriate quality functionals and restrictions, the following problem of nonlinear programming can be formulated:

find $\inf\ I(\vec{B}, \vec{B}_u)$,

limited by the equations: $h_i(\vec{B}, \vec{B}_u) = 0,\ i = 1, \ldots, m$,

and inequalities: $g_i(\vec{B}, \vec{B}_u) \geq 0,\ i = m+1, \ldots, p$.

Here $I(\vec{B}, \vec{B}_u)$, $h_i(\vec{B}, \vec{B}_u)$ and $g_i(\vec{B}, \vec{B}_u)$ could be either linear or nonlinear functions.

As the basic method class of nonlinear programming problem solving we can outline the following:

— methods using derivatives;
— direct methods;
— statistical methods.

Gradient methods have proved themselves to be good among derivative-classes for some types of functionals. However, the using of such methods requires inclusion of all the limitations into a functional, which, considering the given antagonism, leads to it's over-complication. Additionally, the calculation of complex functional derivative may also pose additional difficulties.

Calculations have shown that sliding tolerance method using deformed polyhedron (see [Himmelblau, 1975]) shows high efficiency as a direct method. The main idea of this method lies in building and adjusting a multi-dimensional polyhedron on each step, that approaches the optimum while being in a certain neighbourhood of the restriction satisfaction area. While approaching the solution, this neighbourhood shrinks down and the restrictions are precisely satisfied when the sought point is reached. This method stands out thanks to its feature allowing us to choose between the inclusion of restrictions into the very minimizing functional with various weight coefficients, as well as their taking into account while building the restriction satisfaction area.

While using statistical methods, the problem of working out the limitations, considering their nonlinear structure, also arises, just like for the derivative-using ones. Usually, statistical methods don't tend to have a high convergence speed and become inappropriate for finding the global minimum when a certain high amount of parameters is reached. However, they can aid well in the task of getting initial approximations for other optimization methods.

The author's method requires:

— the using of random search for getting initial approximations and the selection of areas suspicious to be enclosing the optimum;
— the further minimization of the said approximations using the sliding tolerance method.

4.2 Global optimization

The solving of a nonlinear programming problem is a problem of global optimization. Usually, under global optimization, a search of one best decision giving a global minimum to the quality functional is understood. However, at the decision of real physical problems on beam lines designing, the given approach is impracticable. This is connected with impossibility of accurate formalization of all the quality criteria, with construction of a uniform functional with limited number of parameters and realization of its global minimization in comprehensible time. The search of the demanded decision is a creative process and assumes obligatory presence of the person competent in the given area, capable to appropriately place priorities of various quality criteria by carrying out some numerical experiments, to estimate a possibility of realization and reliability of the found decisions.

In the present paper, under global optimization, we understand the consecutive process, allowing to receive a limited set of decisions optimum in a certain sense, their gradual rejection on a number of additional criteria, their research on satisfaction to admissions and realization possibility. The result of the given process is a small set of decisions on the basis of which the experimenter carries out a definitive choice of the decision for realization based on cost, reliability and convenience of the realization criteria.

The given process is mostly iterative. Varying different parameters that define the importance of some quality criteria, as well as entering of various criteria into the functional or their consideration in the form of restrictions and the use of personal experience in analysis of the results approaches the researcher to the required decision. Thus, the big role in the given process is played by the presence of the qualitative software and tools, allowing to carry out the necessary calculations and represent the received results in the form convenient for the analysis.

5 Solution to the task

The calculations were made using the Maple applied algebra package as well as the custom software (see Fig. 5).

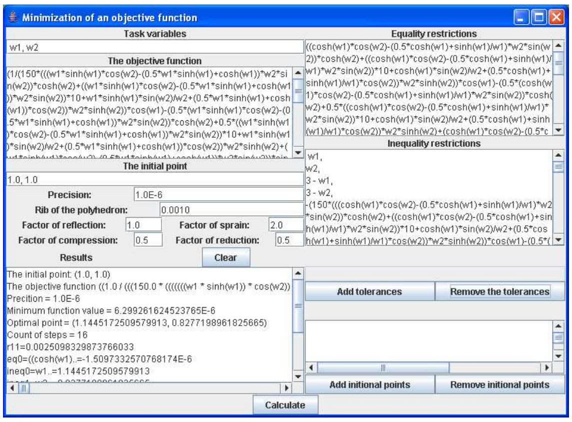

Figure 5. Custom software package screenshot.

Let us analyze the possible solutions for the system considered above (see Fig. 4). The controlling parameters vector in this case is $\vec{B} = (s, \lambda, a, g; k_1, k_2)$. Let's then apply a number of limitations onto the controlling parameters as follows: $a = 150$, $g = 1$, $\lambda = 2$, $s = 0.5$.

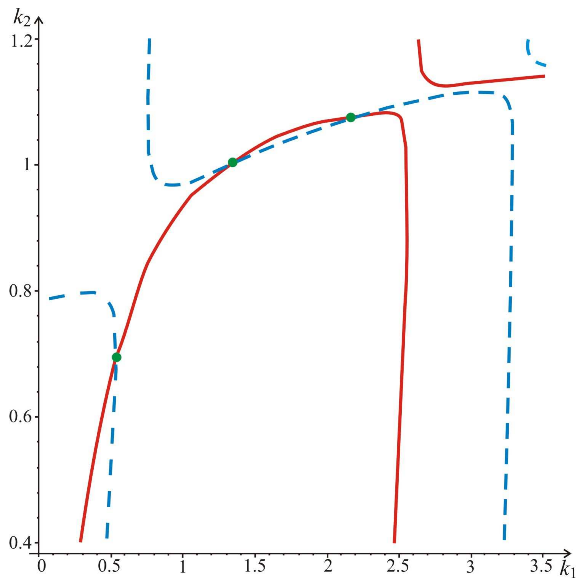

Figure 6. Load curves and working distance length restriction $g = 1$.

Figure 6 shows graphs representing the satisfaction of (6), as well as the load curves (solid line) and the working distance length restriction $g = 1$ (broken line). The corresponding intersection points are marked as follows: K^1 = (0.54345, 0.69629), K^2 = (1.37421, 1.00696), K^3 = (2.23405, 1.07949).

The following beam compression factors correspond with the aforementioned points in the scope of our linear model: $r_{11}(K^1)$ = -0.0352203, $r_{11}(K^2)$ = 0.0061025, $r_{11}(K^3)$ = 0.0087011.

Regarding the compression factors, the most interesting is the point K^2. Note, however, the stability of this solution regarding the deviation of control fields from the values set. Figures 7, 8, 9 plot the corresponding values, with solid line representing K^1, broken line — K^2, and dotted line — K^3.

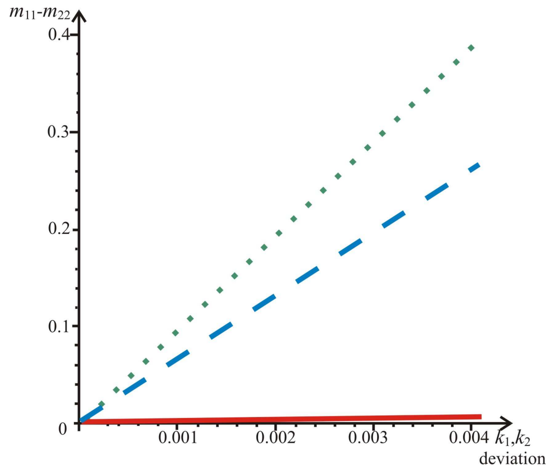

Figure 7. Load curves condition brakes given the deviations of k_1, k_2.

Figure 7 shows that, for the two solutions found, a minor deviation from the optimal parameters (k_1, k_2) leads to a major break of condition (6), which may also lead to the point-to-point focusing condition break.

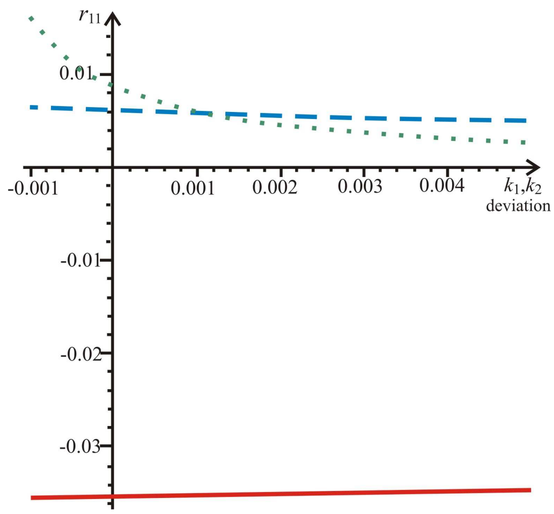

Figure 8. Beam compression factor values given the deviations of k_1, k_2.

Figure 8 represents the change of the beam compression factor when the (k_1, k_2) parameters deviation takes place. Inside the neighborhood of the solutions K^1 and K^2 there is a stable enough conservation of the compression factor value. K^3 shows a major deviation of the compression factor while the certain minor parameter deviation takes place (see Fig. 9).

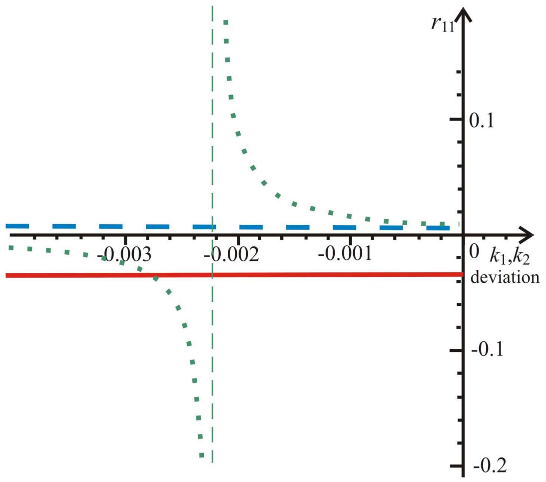

Figure 9. Unlimited derating of the beam compression factor given the deviations of k_1, k_2.

Therefore, at this stage we have the screening of the solution K^3. The two remaining solutions require further analysis for satisfying additional criteria such as fringing fields (see [Tereshonkov, Andrianov, 2008], for example) and nonlinear effects (see, for example, [Andrianov, Edamenko and Tereshonkov, 2008]), as well as influence of parameter deviation sensitivity of the condition (6) to the solution K^2.

6 Conclusion

In the present paper, the methodology of modeling and finding the optimal parameters for beam lines with high beam compression requirements, based on multi-objective analysis, is considered. The given methodology aims for solving the problem of taking into account many, and often contradicting, criteria of quality, consequently considering them. The linear model building and analysis, followed by the inclusion of additional limitations and criteria, leads to the shrinking of a set of solutions down to a finite fixed set, appropriate enough for the selection of a certain solution to be realized.

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