Some Problems of Global Optimization for Beam Lines

Serge Andrianov, Nikolay Edamenko,Eugeny Podzivalov

***Abstract*— Last year's an interest in microprobe beam lines has been increased sharply. This is explained by wide application region of similar facilities. The probe forming systems for generation of beams of nanometer size (so-called nanoprobe) require precise control of the beam characteristics. The heightened sensibility to control parameters deviations forces us to survey very careful mathematical and computer simulation before any manufacture. The nature of such systems as control systems leads us forming special methods and technologies for optimal control problem solution. Moreover, here we owe to realize a searching of a comprehensive set of performance criteria, makes detailed predictions on beam characteristics, possible configuration defects and critical elements, and gives indications for improvement. A path approaching an optimized configuration can thus be established based on well-defined quantitative criteria and special mathematical and computer models for micro- and nanoprobes as control systems. There are discussed some practical results.**

I. Introduction

Complexity of the most beam physics problems leads to the necessity to create effective and adaptive methods for numerical simulation (computing) including the optimization procedure. The process of ordering and accumulation of used knowledge, decomposition of the whole system into a set of simple subsystems (real and/or virtual) can guarantee good maintainability, reasonability, and extensibility of designed codes for the following computing. At this step a designer forms his understanding of practical problems under study. Obviously it is necessary to pay attention to classification and systematization of used knowledge about the problem. It should be noted that the deep mathematical formalization helps to create more adequate and effective mathematical models and tools. As a result of such investigation is a complex of mathematical models for beam lines under study, appropriate computer models and a set of special optimization methods. These investigating methods and tools must guarantee an appropriate solutions with necessary effectiveness and flexibility. Any beam line can be presented as a control system with a some set of control parameters and a set of control function. The control parameters describes such characteristics as drift and magnetic elements lengths, aperture and diaphragms sizes and so on. The control functions correspond to electromagnetic fields ensure a desired behavior of the beam. In particular, an essential part of any control element is fringe fields, which make an impact on beam characteristics. The complexity of beam dynamics leads us to necessity of very careful investigation such dynamical systems with control as beam lines. In the base of the suggested approach we put the matrix formalism for Lie algebraic methods (see, for example, [1]) and a concept of the LEGO-approach (see [2] and [3]) and can realize this optimization process [4] for searching of an appropriate set of optimal solutions. In another words we consider the problem of global optimization as a problem of search for a set of optimal solutions. This set gives the necessary information for a beam line designer for selection of necessary variants of beam line configurations.

Saint-Petersburg State University, Saint-Petersburg, 198504, Russia; e-mail: sandrianov@yandex.com

Let us consider basic levels of the modeling process in more detail [5]. On the first step we have to constrain a hierarchy of so called approximating models. These models inherits all essential properties of the system under study. This inheritance is realized the step-by-step conception [4]. On this step a designer defines a hierarchical sequence of problems. In particular he has to define necessary dynamical equations, beam line models and a set of control parameters and functions. On this step we should define a set of optimal criteria, which can lead us to the appropriate solution.

The next step is the step of mathematical models, which is augmented by necessary mathematical attributes and solution methods. In this paper we constrain our formal picture using the matrix formalism for Lie algebraic tools. This allows us to obtain solutions of dynamical motion equations and formulate practically all optimal demands using uniform conception. On this step we methodically use computer algebra methods and tools. In particular, in this case the designer can formulate both solutions and optimal criteria in the terms of elements of these block-matrices. The possibility to find symmetries and invariants admitted by the system allows us to enhance the effectiveness of our modeling process.

II. The Mathematical Backgrounds

Following to [1] we can write the motion equations for beam particles in the following form

$$\frac{d\mathbf{X}}{ds} = \sum_{k=0}^{\infty} \mathbb{P}^{1k}(\mathbf{U}; s)\mathbf{X}^{[k]}, \quad \mathbf{X}_0 = \mathbf{X}(s_0), \tag{1}$$

were $\mathbf{X}(s)$ is a current phase vector of a particle (at s measured along the beam line axis), $\mathbb{P}^{1k}(\mathbf{B}, \mathbf{U}; s|s_0)$ are two-dimensional block-matrices collected all nonlinear effects of k-th order and $\mathbf{B}$, $\mathbf{U}(s)$ are a vector of control parameters and a vector of control functions. The solution of the Eq. (1) can be written in the matrix form too

$$\mathbf{X}(\mathbf{U}; s|s_0) = \sum_{k=1}^{\infty} \mathbb{R}^{1k}(\mathbf{B}, \mathbf{U}; s|s_0)\mathbf{X}_0^{[k]}. \tag{2}$$

Here $\mathbb{R}^{11}(\mathbf{B}, \mathbf{U}; s|s_0)$ is a matrizant presenting the solution of the linear approximation model, $\mathbb{R}^{1k}(\mathbf{B}, \mathbf{U}; s|s_0)$, $k \geq 2$ collect all aberrations of k-th order.

A. Control Vector Presentation

As mentioned above we have two control vectors: the first vector is the vector of control parameters $\mathbf{B}$, and the second — the vector of control functions describing electromagnetic field along the beam line axis. Let us define this vector in more detail. The first group of parameters defines the geometrical parameters of the beam line — $\mathbf{B}_{\text{geom}}$, the second — the beam phase portrait characteristics $\mathbf{B}_{\text{beam}}$. The control vector-function $\mathbf{U}(s)$ one can substitute for a vector of control parameters $\mathbf{B}_{\text{force}}$ — parametric descriptions of the control functions $\mathbf{U}(s)$ (describing the deflecting and focusing forces acting in the beam line). This substitution should consider an approximating presentation for the electromagnetic field distribution using a special set of approximating function (see, for example, [6]). This approach allow beam line designers to select appropriate field distribution for the purpose of achievement of desired results. The similar proceeding allows us to formulate the problem of optimal control theory as a problem of nonlinear programming, which can be written in the form

$$\begin{aligned} &\inf \mathbf{F}(\mathbf{Y}), \quad \dim \mathbf{F} = r, \ \dim \mathbf{Y} = n, \\ &\mathbf{H}(\mathbf{Y}) = 0, \quad \dim \mathbf{H} = m \leq n, \\ &\mathbf{G}(\mathbf{Y}) \leq 0, \quad \dim \mathbf{G} = p, \end{aligned} \tag{3}$$

where r is a number of optimal criteria, $\mathbf{F}$ — a vector optimal criterion, the vector function $\mathbf{H}$ describes equality restrictions and the vector function $\mathbf{G}$ — inequality restrictions for the vector of control parameters $\mathbf{Y} = \{\mathbf{B}_{\text{geom}}, \mathbf{B}_{\text{beam}}, \mathbf{B}_{\text{field}}\}^{\mathrm{T}}$. As an example, we describe the method of replacement of control function $\mathbf{U}$ with a vector of control parameters $\mathbf{B}_{\text{field}}$. In the beam line theory the usual form of description for control field distribution functions there are used so-called square form functions (piecewise constant functions). In this case of piecewise presentation the vector $\mathbf{A}_{\text{field}}$ corresponds to "lengths and heights of steps" for an applicable square form function $U_{\text{field}}(s)$ — a component of the control vector $\mathbf{U}_{\text{field}}(s)$.

It should be noted that the corresponding selection of approximating functions has to satisfy to some special conditions guarantee the physical constraints. On the next step the designer can select functions which permit symbolic solutions of linearized motion equations (for example, sin, cos, Airy's functions) in general or using polynomials (for example, for sextupole lenses)

$$\frac{d\mathbf{X}}{ds} = \mathbb{P}^{11}(\mathbf{U}; s)\mathbf{X}, \quad \mathbf{X}_0 = \mathbf{X}(s_0), \tag{4}$$

B. A Dynamical Model

It should be note that the block-matrices $\mathbb{R}^{1k}(s|s_0)$ in the (2) can be evaluated for auxiliary kinds of dependencies $\mathbb{P}^{1k}(s|s_0)$ on s using the Magnus representation for a Lie map [5], generated by (4). Unfortunately only for a small set of functional dependencies of $\mathbb{P}^{11}(s)$ from s one can evaluate matrices $\mathbb{R}^{11}$. Fortunately there is a set of appropriate functions for which we can do it. Moreover these functions can be chosen as a basis for control field approximation (see, i. e. [6]). The set of these functions must be reduced, because for the nonlinear aberrations, described by (2), we must evaluate the nonlinear aberration matrices according to the following formulae

$$\mathbb{R}^{1k}(s|s_0) = \int\limits_{s_0}^{s} \mathbb{R}^{11}(s|\tau)\mathbb{P}^{1k}(\tau)\mathbb{R}^{kk}(\tau|s_0)d\tau, \tag{5}$$

where $\mathbb{R}^{kk} = \left(\mathbb{R}^{11}\right)^{[k]}$ is the Kronecker k-power of a matrix $\mathbb{R}^{11}$. The equalities can be also used in the case of approximation of control functions with polynomials (in the case of spline-approximation approach). For these cases we should use the coefficients of the corresponding approximation functions as components of the control vector $\mathbf{A}_{\text{field}}$ [6].

The evolution beam particles can be written not only in the form of linear and nonlinear motion equation (2) or (3) in the form of (2).

For the linear approximating model using (1) we can write the following equation for a single particle for the linear approximating model:

$$\mathbf{X}(s) = \mathbb{R}^{11}(\mathbf{B}_{\text{geom}}, \mathbf{B}_{\text{field}}; s|s_0)\mathbf{X}_0(\mathbf{B}_{\text{beam}}). \tag{6}$$

Taking into account (6) we can write for N beam particles the following equality:

$$\begin{aligned} \mathbb{M}^N(s) &= \mathbb{R}^{11}(\mathbf{B}_{\text{geom}}, \mathbf{B}_{\text{field}}; s|s_0)\mathbb{M}_0^N(\mathbf{B}_{\text{beam}}), \\ \mathbb{M}_0^N &= \{\mathbf{X}_0^1, \ldots, \mathbf{X}_0^N\}, \ \mathbf{X}_0^k \in \mathfrak{M}_0, \ \forall k = \overline{1, N}, \end{aligned} \tag{7}$$

where $\mathfrak{M}_0$ is an initial set occupied by beam particles at the initial moment s_0, the matrix $\mathbb{M}^N(s)$ describes the particle distribution at the moment s for N particles. This set can be presented using distribution function $f(\mathbf{X}, s)$ or so called envelope matrix $\mathbb{S}$. This matrix can be evaluated in the form

$$\mathbb{S}(s) = \mathbb{A}^{-1}(s),$$

where $\mathbb{A}(s)$ is a form matrix for an ellipsoid $\mathbf{X}^*\mathbb{A}\mathbf{X} \leq 1$ approximating the set $\mathfrak{M}(s)$, or

$$\mathbb{S}^{\text{rms}}(s) = \int\limits_{\mathfrak{M}(s)} f(\mathbf{X}, s)\mathbf{X}\mathbf{X}^* d\mathbf{X}.$$

The evolution of $f(\mathbf{X}, s)$ and σ-matrices (II-B) and (II-B) can be written in according the corresponding equalities [6]. For σ-matrix $\mathbb{S}$ evolution one can write:

$$\mathbb{S}(s) = \mathbb{S}^{11}(s) = \sum_{l=1}^{\infty}\sum_{j=1}^{\infty} \mathbb{R}^{1l}(s|s_0)\mathbb{S}_0^{lj} \left(\mathbb{R}^{1j}(s|s_0)\right)^*,$$

where

$$\mathbb{S}_0^{ik} = \int\limits_{\mathfrak{M}_0} f_0(\mathbf{X})\mathbf{X}^{[i]} \left(\mathbf{X}^{[k]}\right)^* d\mathbf{X}, f_0 = f(\mathbf{X}, s_0).$$

For distribution function we have [7]:

$$f(\mathbf{X},s)=\sum_{k=0}^{\infty}\mathbf{F}_k^*\mathbf{X}^{[k]},\ f_0(\mathbf{X})=\sum_{k=0}^{\infty}\left(\mathbf{F}_k^0\right)^*\mathbf{X}^{[k]}, \quad (8)$$

where

$$\mathbf{F}_0=\mathbf{F}_0^0,\ \mathbf{F}_k=\sum_{l=1}^{k}\left(\mathbb{T}^{kl}\right)^*\mathbf{F}_l^0,\ k\geq 1. \quad (9)$$

Here $\mathbb{T}^{ik}$ $(i\leq k,\ k\geq 2)$ can be evaluated under the generalized Gauss's algorithm:

$$\mathbb{T}^{11}=\left(\mathbb{R}^{11}\right)^{-1},\ \ \mathbb{T}^{kk}=\left(\mathbb{R}^{kk}\right)^{-1}=\left(\mathbb{R}^{11}\right)^{-[k]}, \quad (10)$$

and

$$\mathbb{T}^{ik}=-\mathbb{T}^{ii}\sum_{j=i+1}^{k}\mathbb{R}^{ij}\mathbb{T}^{jk},\ i<k,\ \mathbb{T}^{ik}\equiv\mathbb{O},\ i>k. \quad (11)$$

C. Optimization Criteria

In the previous subsection we consider the basic equalities in accordance with which dynamical beam evolution is propagated. The matrix formalism allows designers to formulate his criteria in terms of elements of introduced matrices. Let us describe some of them for the problem of focusing system design (here we base on high precision focusing systems with additional demands, see, for example, [6], [7]). Let us discuss some of these demands, which play one of the main role in a focusing system design. As a simplest model of such system we consider the system presented on Fig. 1, where a is a "pre-distance", g — a "working space". A collimating system can be consisted from several diaphragms, and a focusing system consists from several quadrupole lenses or solenoids, separated by drifts and a target system with sensors. This system can also (if it is necessary) enclose a deflecting system, which plays a role of scanning system.

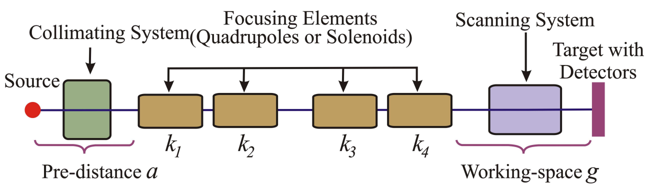

Fig. 1. The preliminary scheme for a focusing beam line

One of the standard demands is the so called condition — focusing "*point-to-point*". Here we mean that a point-source has to give the point-like image on the target of the beam line. This condition is similarly to the corresponding demand in the light optics. In the terms of elements of the matrizant $\mathbb{R}^{11}(s|s_0)$ this condition can be written in the form

$$r_{12}=r_{34}=0. \quad (12)$$

The equalities (12) can be solved relative to one of drift lengths. Usually this does for so called the length of working space g (see Fig. 1).

The second part of focusing criteria can be chosen in the following form

$$\inf_{\text{parameters set}}\left(r_{11}^2+r_{33}^2\right). \quad (13)$$

Analogue approach can be applied to other demands on our focusing system and, if it is necessary, for the scanning system. Let us consider (as an example of additional constraint) the invariance requirement for beam image. In another words here we mean the following condition: a round portrait of the initial beam image in the configuration space must get over a round portrait for a final image on the target. The focusing system for four quadrupoles with similar condition is well known as "russian quadruplet", but similar condition (it is very popular among physicists) can be generalized for any case of a focusing system configuration [5]. This demand can be presented in the following way

$$k(s)=-k(s_t-s),\quad m_{11}=m_{22}, \quad (14)$$

where $[s_0,s_t]$ is the full interval of our system, and m_{ik} are elements of the matrizant $\mathbb{M}^{11}$, where

$$\mathbb{R}^{11}_{\text{full}}=\mathbb{R}^{11}(s_t|s_0)=\mathbb{L}_g\mathbb{M}^{11}\mathbb{L}_a. \quad (15)$$

Here $\mathbb{L}_a$ and $\mathbb{L}_g$ are matrizants for drifts with lengths equal to a and g accordingly. The condition (14) leads us to the following equality for the full matrizant

$$\mathbb{R}^{11}_{\text{full}}=\begin{pmatrix}\mathbb{R}^{11}_x & \mathbb{O}\\ \mathbb{O} & \mathbb{R}^{11}_y\end{pmatrix},\ \mathbb{R}^{11}_x=\mathbb{R}^{11}_y. \quad (16)$$

As we mention above the length parameter g can be evaluated using (12). In this case we obtain the value g as a fractional rational function from m_{ik} and a. So we convert one of optimal conditions to the inequality constraint $g_{\text{techn}}\leq g\leq g_{\max}$, where $g_{\max}$ is a maximal value of the working space defined by the total system length L_{tot}.

Here we should note just usage of matrix formalism allows us to formulate practically all physical demands as mathematical object functions and corresponding limitations in terms of matrix elements of $\mathbb{R}^{11}$. This approach can be extended and for the case with fringe fields (as an essential part of any real control element).

The special role for focusing systems for micro-and nanoprobes play the problem of forming a given particle distribution function on the target. This problem is solved using nonlinear control elements, and also can be solved in terms of elements of our matrix presentation for an evolution operator of beam particles. In our notations we mean the matrices $\mathbb{R}^{11}$ and $\mathbb{R}^{13}$, among them the second matrix plays the main role. Indeed the equalities (8)–(11) give us to evaluate the metric for convergence of desirable and resulting on the target distribution functions in terms of matrix elements of $\mathbb{T}^{ik}$ and so $\mathbb{R}^{ik}$, $i\leq k,\ k\geq 2$.

So our physical optimization problem can be written as the nonlinear programming problem (3). The described concept of modeling allows to include and to extract control elements at all steps of the process using the LEGO-technology [3]. This leads us to the concept of structural optimization, according to this the designer obtains a possibility to search not only optimal parameters of the beam line but an optimal structure of the beam line.

III. Global Optimization for Beam Line Configuration

It is known that practically any problem connected with searching appropriate variants of beam line configurations can be formulated as a problem of optimal control theory. In another words a designer must make a choice anyway, including selection a geometry configuration, a type of focusing system (FODO-structure or solenoids sequence), type and structure of scanning facility (if it is necessary) and optimize linear and nonlinear parts of the beam line optics. It is necessary to note that the corresponding optimization problem is a multi-objective problem. Moreover, some of these optimal conditions are antagonistic (for example, the focusing and aperture demands). In some previous papers the authors suggested the optimization technique based on a step-by-step procedure [4], [5] for solving similar problems. Usually this approach leads us to a set of appropriate solutions, and demands as a next step a computational experiments for reduction of this set using some additional restriction conditions. So on the first step of the optimization process the designer must obtain a set of control parameters, which determine some appropriate solutions. Selecting the corresponding values as starting points he begin to study these solutions including some more realistic variants of electromagnetic fields in the control elements. In particular, here we should mention so called fringe fields as an intrinsic part of any control element in beam line facilities. Presentation of fringe fields in term of model function from some appropriate class of function [6] allows the designer not only to study effects induced by fringe fields, but to optimize their influence. It should be noted that the fringe field effect for nonlinear beam dynamic is much complicated as compared with this effect in the case of linear dynamics. So on this second step the primary control parameters set is widened at the expense of parameters for fringe fields model functions.

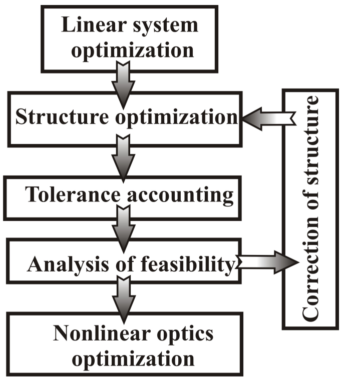

Fig. 2. The sequence of optimization steps.

The straightforward process is usually used on the step of linear optics design (see Fig. 2). On this step we use so called structure optimization, which is an automatic synthesis of beam line components, which guarantee the given properties of the desired beam line. Thus the structure optimization means optimization of a goal function (a weighted sum of partial goal functions) under some constraints, describing physical and geometrical restrictions. As a result of such procedure is a set of optimal structures for the beam line. The dynamical system of our beam line on this first step usually very simple: the control electromagnetic field is described by piecewise constant functions and space-charge forces are neglected. On the second step the designer must include in optimization process the additional parameters (see the note on fringe fields model functions) without changing the set of criteria and basic constraints on the set of control parameters.

A. Nonlinear Optimization

On the next step we should reject those variants, which are not appropriate in respect to their practical realization. As an example of similar reason we can indicate the problem of agreement with tolerance restrictions on all parameters. The corresponding analysis technique provides the beam line designer with powerful qualitative and quantitative tools for lattice studies. On the fourth step of our solution process the selected structure variants line up in a sequence of the most-appropriate options. It is necessary to note that on this step one of important role can play cost parameters. In the case of improper data we must input correction procedure and repeat our process of optimal structure selection. Further

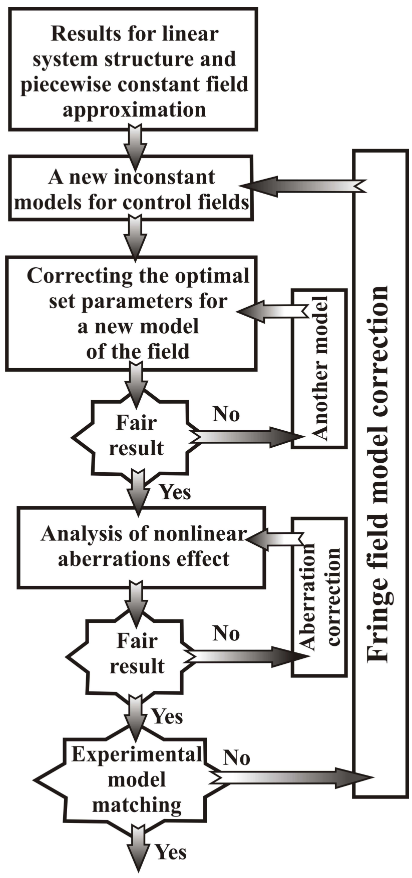

Fig. 3. The main steps of nonlinear optimization process

the designer must go on to the next step of nonlinear optimization process. Indeed the optimization process on this step is not so straightforward. This process reminds of the process of predictor–corrector one. In according to this the designer must correct his optimization process not only after finishing results receiving. For this purpose he use special analysis solvers, which help him to select nonlinear optimization strategy (see Fig. (3)). An additional demands and control parameters (i. e. for fringe field description) we must include additional demands that may conflict with each other. Here we must use a multi-objective optimizer, which can solve our problem by producing a population of best-ranked solutions on a multidimensional surface from which a set of appropriate solutions can be chosen by the designer.

B. A Concept of Hierarchical Sequence of Approximation Models

The above pointed approach is based on a concept of hierarchical sequence of approximation models [4], which can be built for an investigated beam line. Starting from linear dynamical model the designer must *step-by-step* include more and more complex effects. Here the main problem is to select the successive steps for similar process. Unfortunately here there can not suggest the universal procedure. We can be guided by our previous experience and, if it is possible, some experimental data.

C. An Optimal Solution Strategy

Above described problems can be solved using the matrix formalism for beam dynamic description on the one hand and a combination of different kind of solvers for nonlinear programming problems on the other hand. The previous papers (see references to this paper) we use such methods as a stochastic search (Monte-Carlo methods) on the initial step of the problem solution, direct methods without derivatives evaluation (in our case we use Himmelblau [8]). As we discussed above the traditional processes of designing and tuning any beam line then it is very difficult to model optimal structure taking into account all sufficient conditions of the different nature. Indeed often found solutions through trial and error and the designer can not chose the appropriate solutions. Her we describe a strategy of optimal solutions search, which was approved for different kind of beam line structures and destinations. In contrast to some published papers devoted to similar problems (see,for example, [9]) we search a set of optimal solutions according to the step-by-step concepts of optimization process [4]. For this goal we separate our problem on several stages: from linear approximation with piecewise constant distribution of the control field up to nonlinear approximation with variant fringe field distribution models. Let us point reasons of this suggested approach to beam line design process:
– a very nonlinear problem (even for linear approximation for beam dynamics) and many local optimums;
– a multi objective problem (typically the designer works to optimize more than one property simultaneously);
– the designer would like to find the optimal tradeoff. These reasons leads us to need usage of efficient and robust methods, which can "work" with many parameters and search for multi-objectives. A combination of above mentioned methods and multi-objective genetic algorithms (see, for example, [10]) allows us to obtain very close solutions. Moreover this permitted to obtain not only desirable results for required parameters, but and very important information about admissible tolerances for control parameters.

In the whole described approach can be formalized by the following algorithm.
Step 0 A quasi admissible set $\mathfrak{B}^0_{fin} \supset \mathfrak{B}_{fin}$ is constructed (according to the investigator's experience).
Step 1 A selected optimization method (see above) is used for optimal solution searching on the set: $\mathbf{B}^{opt}_0 \in \mathfrak{B}_{fin} \subset \mathfrak{B}^0_{fin}$.
Step 2 According to some strategy the new admissible set $\mathfrak{B}^1_{fin}$ is constructed.
Step 3 The optimization problem is solved on the set $\mathfrak{B}^1_{fin}$.
Step 4 This process is continued according described procedure by proceeding to the second Step.
...
Step N The whole optimization process if finished under the following condition implementation

$$\mathfrak{B}^N_{fin} = \mathfrak{B}_{fin}.$$

The optimal solution obtained $\mathbf{B}_{fin} \in \mathfrak{B}_{fin}$ is treated as required optimal solution.

As we mentioned above suggested optimization process allows getting the tolerance information automatically, and the designer can interrupt the optimal solutions searching on the suitable step, if he obtains the desired tolerance information.

IV. Conclusion

The discussed approach to global optimization based on the matrix formalism for Lie algebraic tools and LEGO-technology (both for description and solution levels) allows to create effective and comfortable computer tools both for beam dynamics and for optimization process. On the every step of the optimization process the designer obtains all necessary information for experimental verification (if it is possible) or computational experiments using alternative numerical methods and programm tools (for example, MAD X). The optimization process is controlled by the designer and permits to obtain useful additional information (i. e. tolerance estimations for control parameters). Described approach was tested on some different problems of beam physics and demonstrated undoubted effectiveness (see, [4]–[7], [10]).

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