Romanian Reports in Physics, Vol. 60, No. 2, P. 235–249, 2008

NUMERICAL MODELLING OF EXPERIMENTS WITH LOW ENERGY ELECTRON BEAMS

M. RIZEA

"Horia Hulubei" National Institute of Physics and Nuclear Engineering
P.O. Box MG-6, RO-077125 Bucharest-Magurele, Romania
E-mail: rizea@theory.nipne.ro

(Received September 12, 2007)

Abstract. The problem of the beam diagnosis in electron accelerators by numerical simulation is considered and methods towards its solution are presented. In particular, we investigated an installation composed by a vacuum electron source, two axially symmetric magnetic lenses and two beam profile monitors. Using a set of input parameters and a previous computation of the magnetic field, we have obtained by numerical calculations the beam parameters at the electron source exit: emmitance and cross-over radius and position. In the mathematical formulation, the most important parts are the solution of a second order differential equation (the paraxial equation) and the minimization of a function with several variables. We have tried and compared different methods in order to find the optimal procedures. On their basis computer codes have been produced and used for practical applications.

Key words: electron beams, beam diagnosis, numerical modelling, several variable function minimization, differential equations of the form $y'' = f(x, y)$.

1. INTRODUCTION

Charged particle beams produced in linear accelerators are used in a large variety of scientific and industrial applications. The beam diagnosis is essential for the accelerator design. The determination of beam parameters by numerical modelling is very convenient, since it reduces substantially the technical effort and costs. The main components of such an installation are: the electron source, the magnetic lenses and the beam profile monitors (wire scanners). A magnetic lens consists of a coil of copper wires inside the iron pole pieces. A current through the coils creates a magnetic field in the bore of the pole pieces. The rotationally symmetric magnetic field is inhomogeneous in such a way that it is weak in the center of the gap and becomes stronger close to the bore. Electrons close to the center are less strongly deflected than those passing the lens far from the axis. The overall effect is that a beam of parallel electrons is focused into a spot (so-called cross-over). The focusing effect of a magnetic lens increases with the magnetic

field, which can be controlled via the current flowing through the coils. Previously, we have developed a computer code for the calculation of the magnetic field and of the flux density in such a magnetic lens, based on the finite element method (see [1]). Now, we continue with the determination of beam parameters at the electron source exit: emmitance and cross-over radius and position.

2. STATEMENT OF THE PROBLEM

We investigated an effective laboratory installation composed by a vacuum electron source, two axially symmetric magnetic lenses and two beam profile monitors. Using experimental data and mathematical description we find the beam characteristics by numerical fitting and optimization. The problem can be formulated as follows:

Given parameters

1. U [V] = beam acceleration potential, I_0 [A] = beam current;
2. $Vb1_{min}$, $Vb1_{max}$, $Vb2_{min}$, $Vb2_{max}$, V_{step} – lens polarization range;
3. dL_{M1} [mm], d_{M1M2} [mm] – displacements used in the monitors location determination;
4. a_1, b_{11}, b_{12}, b_{13}, b_{14}, b_{15} – coefficients of the fifth degree polynomial fitting the set of measured beam cross-section radii in the monitor M1 plane;
5. a_2, b_{21}, b_{22}, b_{23}, b_{24}, b_{25} – similar coefficients for the monitor M2;
6. ab_{max} [gauss], bb_{max} [gauss/V], σ [m] – parameters to fit the magnetic field;
7. W_1, W_2 – weights used in the definition of the function to be minimized;
8. *ftol* = minimization criterion – the iteration process stops when the difference between two successive minimum function values (as relative error) becomes less than this tolerance;
9. *tol* = accuracy parameter for the solution of the differential equation below.

Adjustable parameters

1. ϵ_0 [mm mrad] = root-mean-square (rms) beam emittance;
2. R_0 [mm] = radius of the cross-over;
3. z_0 [mm] = position of the cross-over.

Calculus flow

Let be

$$Vb_{inf} = \min(Vb1_{min}, Vb2_{min}), \quad Vb_{sup} = \max(Vb1_{max}, Vb2_{max}).$$

For trial values of ϵ_0, R_0, z_0 we perform the following steps:

1. Define

$$zm_1 = z_0 + dL_{M1}, \quad zm_2 = zm_1 + d_{M1M2}$$

For $V_i = Vb_{inf} + i * V_{step},\ i = 0, \ldots, I,\ V_I = Vb_{sup}$ do

2. If $Vb1_{min} \le V_i \le Vb1_{max}$ integrate

$$\frac{d^2R(z)}{dz^2} = -\frac{\eta B(z)^2 R(z)}{8U} + \frac{C_1 I_0}{U^{3/2} R(z)} + \frac{\varepsilon_0^2}{R(z)^3} \tag{2.1}$$

where

$$C_1 = \frac{1}{4\pi\alpha_0\sqrt{2\eta}} = 1.51676 \times 10^4,$$

$\eta = 1.76044 \times 10^{11}$ is the electron charge-to-mass ratio, α_0 is a dielectric constant and

$$B(z) = B_{max}(V_i) \exp\left(-\frac{(z - z_0)^2}{2\sigma^2}\right),$$

$$B_{max}(V) = (ab_{max} + bb_{max} \times V)/10^4$$

is the axial magnetic field.

The function $R(z)$ represents the root-mean-square beam radius and satisfies the paraxial equation (2.1) – see [2, 3].

The integration interval is $[0, zm_1]$ and the initial conditions are $R(0) = R_0$, $R'(0) = 0$.

3. Assign $P_i = R(zm_1)$.

4. Otherwise $P_i = 0$.

Similarly,

5. If $Vb2_{min} \le V_i \le Vb2_{max}$ integrate Eq. (2.1) on the interval $[0, zm_2]$ with the same initial conditions.

Assign $Q_i = R(zm_2)$.

6. Otherwise $Q_i = 0$.

7. Define $F_i = M1(V_i),\ G_i = M2(V_i),$ where

$$M1(V) = (a_1 + b_{11} * V + b_{12} * V^2 + b_{13} * V^3 + b_{14} * V^4 + b_{15} * V^5)/1000$$

$$M2(V) = (a_2 + b_{21} * V + b_{22} * V^2 + b_{23} * V^3 + b_{24} * V^4 + b_{25} * V^5)/1000.$$

8. Form

$$\chi^2 = W_1 \sum_{i=0}^{I} (F_i - P_i)^2 + W_2 \sum_{i=0}^{I} (G_i - Q_i)^2. \tag{2.2}$$

9. Obtain the set of parameters $\epsilon_0,\ R_0,\ z_0$ so that χ^2 be minimum.

More physical and technical details on this problem can be found in [4] and [5].

3. NUMERICAL SOLUTION

We have tried several methods, in order the find the most convenient procedures both for minimization and for differential equation integration.

3.1. MINIMUM FINDING

For the minimization of a function of several variables we used the following routines:

1. POWELL – Powell algorithm, using function values only (see [6, 7], section 10.5).
2. FMFP – SSP Package, Fletcher and Powell algorithm, using first derivatives (see [8]).
3. ADWP – CPC Program Library, Tsoulos and Lagaris algorithm for global optimization, using first derivatives (see [9]).
4. ADWU – CPC Program Library, Tsoulos and Lagaris algorithm for local minima, using first derivatives (see [10]).

When needed, the gradient components have been approximated by finite differences.

As input, the routines POWELL and FMFP require an initial vector as the first estimation of solution, while ADWP and ADWU require limits defining the intervals where the components of the solution are located.

Numerical tests showed that all routines give practically the same result. The difference consists in how close should be defined the first estimate. The greatest freedom is allowed by the routine POWELL. In addition, the method of Powell does not require the first derivatives, which in our case are not available (they can be only estimated numerically, which increases the computing time). For these reasons, we have chosen this method, which we shall briefly describe in the following.

Powell's Method

Given a function f of n variables the problem is to find n parameters x_1, x_2, …, x_n so that $f(x_1, x_2, ..., x_n)$ is a minimum. An idea is to change one parameter at a time. If we start at a point **P** in n-dimensional space and proceed from there in some vector direction **d**, then the function f can be minimized along the line **d** by some one-dimensional method. A multidimensional minimization will consist of sequences of such line minimizations. Different methods will differ only by how, at each stage, they choose the next direction **d** to try. A simple method could be: take the unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$, …, $\mathbf{e}_n$ as a set of directions. Using a one-dimensional method, move along the first direction to its minimum, then from there along the

second direction to its minimum, and so on, cycling through the whole set of directions as many times as necessary, until the function stops decreasing. In practice this procedure can fail to converge or requires many iterations. More appropriate directions should be chosen. Such a set consists of **non-interfering** directions with the special property that minimization along one is not damaged by subsequent minimization along another, so that not finishing search through the set of directions can be avoided. The so-called **conjugate directions** satisfy this condition. To define them let us note first that if we minimize a function along some direction **u**, then the gradient of the function must be perpendicular to **u** at the line minimum.

Next take some particular point **P** as the origin of the coordinate system with coordinates x_1, x_2, …, x_n. We note **x** the vector with these components. Then the function f can be approximated by its Taylor series

$$f(\mathbf{x}) = f(\mathbf{P}) + \sum_i \frac{\partial f}{\partial x_i} + \frac{1}{2}\sum_{i,j} \frac{\partial^2 f}{\partial x_i \partial x_j} + \ldots \approx c - \mathbf{bx} + \frac{1}{2}\mathbf{xHx} \tag{3.3}$$

where

$$c \equiv f(\mathbf{P}),\ \mathbf{b} \equiv -\nabla f\,|_{\mathbf{P}},\ \left[\mathbf{H}\right]_{ij} \equiv \frac{\partial^2 f}{\partial x_i \partial x_j}|_{\mathbf{P}}\ . \tag{3.4}$$

The matrix **H** whose components are the second partial derivatives of the function is called the Hessian matrix.

In the approximation of (3.3), one can easily calculate the gradient of f:

$$\nabla f = \mathbf{Hx} - \mathbf{b}. \tag{3.5}$$

When we move along some direction, the change in the gradient is then given by:

$$\delta(\nabla f) = \mathbf{H}(\delta\mathbf{x}). \tag{3.6}$$

Suppose that we have moved along some direction **u** to a minimum and now propose to move along some new direction **v**. The condition that motion along **v** not destroy our minimization along **u** is just that the gradient stay perpendicular to **u**, *i.e.*, that the change in the gradient be perpendicular to **u**. By equation (3.6) this means that

$$0 = \mathbf{u}\,\delta(\nabla f) = \mathbf{uHv}. \tag{3.7}$$

When (3.7) holds for two vectors **u** and **v**, they are said to be **conjugate**. When the relation holds pairwise for all members of a set of vectors, they are said to be a conjugate set. If one does successive line minimization of a function along a conjugate set of directions, then it is not needed to redo any of those directions. One pass of n line minimizations will find exactly the minimum of a quadratic

form like (3.3). For functions f that are not exactly quadratic forms, the process does not reach exactly the minimum; but repeated cycles of n line minimizations will converge rather quickly (quadratically) to the minimum.

Powell first discovered a direction set method that produces n mutually conjugate directions (see [6]). Each iteration of the procedure begins with a search down n linearly independent directions $\xi_1, \xi_2, \ldots, \xi_n$, starting from the best known approximation to the minimum, $\mathbf{P}_0$. Initially, these directions are chosen to be the coordinate directions (basis vectors). Next a new direction, ξ, is defined and the linearly independent directions for the next iteration are $\xi_2, \xi_3, \ldots, \xi_n, \xi$. The way in which ξ is chosen ensures that, if a quadratic is being minimized, after k iterations the last k of the n directions used for the $(k + 1)$ th iteration are mutually conjugate. After n iterations all the directions are mutually conjugate and in consequence the exact minimum of the quadratic is found.

An iteration of the basic procedure is as follows:

- For $i = 1, 2, \ldots, n$ calculate λ_i so that $f(\mathbf{P}_{i-1} + \lambda_i \xi_i)$ is minimum and define $\mathbf{P}_i = \mathbf{P}_{i-1} + \lambda_i \xi_i$.
- For $i = 1, 2, \ldots, n - 1$ replace ξ_i by ξ_{i+1}.
- Replace ξ_n by $\mathbf{P}_n - \mathbf{P}_0$.
- Choose λ so that $f(\mathbf{P}_n + \lambda(\mathbf{P}_n - \mathbf{P}_0))$ is a minimum and replace $\mathbf{P}_0$ by $\mathbf{P}_0 + \lambda(\mathbf{P}_n - \mathbf{P}_0)$.

This sequence is repeated until the function stops decreasing. Powell has also given an algorithm to find the minimum along a line, based on a quadratic defined by three function values. During the time, Powell's method was improved (see [7]) and it continues to be one of the best existing procedures for the minimization of a function of several variables without calculating derivatives.

3.2. DIFFERENTIAL EQUATION SOLUTION

Equation (2.1) is of the form $y'' = f(x, y)$. Numerical solution is possible by transforming the equation in a system of first order and then applying specific techniques (like classical Runge-Kutta). However, it is generally more efficient to apply techniques adapted to the particular form of the equation (without first derivative). We have investigated two types of such methods: Runge-Kutta-Nyström (1) and multi-step (2). Their main features will be presented below.

1. Runge-Kutta-Nyström method

Given the system of second-order differential equations

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y_0', \tag{3.8}$$

the explicit Runge-Kutta-Nyström (RKN) method obtains the solution at the point x_{n+1} in terms of the solution at the point x_n (separated by the step h) according the formulae

$$y_{n+1} = y_n + hy'_n + h^2 \sum_{i=1}^{s} \bar{b}_i f(x_n + c_i h, \hat{y}_i), \tag{3.9}$$

$$y'_{n+1} = y'_n + h \sum_{i=1}^{s} b_i f(x_n + c_i h, \hat{y}_i) \tag{3.10}$$

where

$$\hat{y}_i = y_n + c_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, \hat{y}_j), \quad i = 1, \ldots, s. \tag{3.11}$$

The RKN method is completely determined by means of the Butcher tableau

$$\begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ . & & & \cdots & \\ c_s & a_{s1} & a_{s2} & \ldots & a_{s,s-1} \\ \hline & \bar{b}_1 & \bar{b}_2 & \ldots & \bar{b}_{s-1} \quad \bar{b}_s \\ \hline & b_1 & b_2 & \ldots & b_{s-1} \quad b_s \end{array}$$

or, equivalently, by the quadruple ($\mathbf{c}$, $\mathbf{A}$, $\bar{\mathbf{b}}$, $\mathbf{b}$) where $\mathbf{c}, \bar{\mathbf{b}}, \mathbf{b} \in \mathbb{R}^s$, $\mathbf{A} \in \mathbb{R}^{s \times s}$ and s denotes the number of stages of the RKN method. The coefficients are determined from minimizing conditions of the local truncation error. If the error per step is of the order h^{p+1}, the total accumulated error has order h^p. Then the method is called of order p.

In practice embedded pairs of RKN methods are used, because they provide a convenient error estimation. An **embedded q(p) pair** of RKN methods is based on the RKN method ($\mathbf{c}$, $\mathbf{A}$, $\bar{\mathbf{b}}$, $\mathbf{b}$) of order q and another RKN method ($\mathbf{c}$, $\mathbf{A}$, $\bar{\mathbf{b}}^*$, $\mathbf{b}^*$) of order $p < q$. Some coefficients are common to both methods.

A local error estimation in the integration point $x_{n+1} = x_n + h$ is determined by the expressions

$$\delta_{n+1} = y_{n+1} - y^*_{n+1}, \quad \delta'_{n+1} = y'_{n+1} - y'^*_{n+1}. \tag{3.12}$$

$E_{n+1}(h) = \max\{\| \delta_{n+1} \|_\infty, \| \delta'_{n+1} \|_\infty\}$ represents the local error estimation to control step-size h for RKN processes by the formula (see [11]):

$$h_{new} = 0.9 h_{old} \left(\frac{Tol}{E_{n+1}(h_{old})} \right)^{1/(p+1)}, \tag{3.13}$$

where Tol is the maximum allowable error. If $E_{n+1}(h) < Tol$, then the step is accepted and a local extrapolation is performed: although one actually controls an estimate of the local error in the lower order solution, it is the higher order solution that is accepted at each point. If $E_{n+1}(h) \geq Tol$, then the step is rejected and the calculation is continued with the new step given by (3.13).

There are several formulae for such methods (see [12, 13]. In our calculations we have used the routine DOPRIN, based on an embedded pair of RKN methods of orders $7(6)$, due to Dormand and Prince (see [11]).

2. Multi-step Method

We have considered a class of four step methods, introduced in [14]. A four step method for the equation (3.8) has the form:

$$\begin{aligned} &a_0 y_{n+2} + a_1 y_{n+1} + a_2 y_n + a_3 y_{n-1} + a_4 y_{n-2} = \\ &= h^2 \left[b_0 f_{n+2} + b_1 f_{n+1} + b_2 f_n + b_3 f_{n-1} + b_4 f_{n-2} \right] \end{aligned} \tag{3.14}$$

where $f_i = f(x_i, y_i)$. The formula (3.14) connects the values at five consecutive points (the distance between the last and the first point is of four steps). Given four y values, by Eq. (3.14) one obtains the solution at a new point (either x_{n+2} for forward propagation or x_{n-2} for backward propagation).

Since Eq.(3.14) is homogeneous in the weights, one weight can be fixed from the beginning; we put $a_0 = 1$. The other nine weights are derived by imposing the two necessary and sufficient conditions for convergence, *i.e.* consistency and stability.

A numerical method is said to be **convergent** if the numerical solution approaches the exact solution as the step size h goes to 0.

The numerical scheme is **consistent** (mathematically correct) if its discrete operator (with finite differences) converges towards the continuous operator (with derivatives) of the differential equation for $h \to 0$ (vanishing truncation error). More precise, if ϵ_h is the local error (the difference between the result given by the method and the exact solution at each step), the consistency condition is:

$$\lim_{h \to 0} \frac{\epsilon_h}{h} = 0 \tag{3.15}$$

(the order of the method is greater than 0).

Stability means that the equation with finite differences which approximates the differential equation has no solutions growing indefinitely with the number of steps. We shall examine these conditions for our four step methods.

To determine the weights of the four step formula, we associate to Eq. (3.14) the functional

$$F[y(x);h] \equiv y(x+2h) + a_1 y(x+h) + a_2 y(x) + a_3 y(x-h) + a_4 y(x-2h) - \\ - h^2 \left[b_0 y''(x+2h) + b_1 y''(x+h) + b_2 y''(x) + b_3 y''(x-h) + b_4 y''(x-2h) \right] \tag{3.16}$$

and require that F identically vanishes for all x and h when $y(x)$ is any of the following eight functions:

$$1,\ x,\ x^2,\ x^3,\ x^4,\ x^5,\ x^6,\ x^7. \tag{3.17}$$

A linear system of eight equations for nine unknowns results, which admits a unique solution if one unknown is assumed given. We take $a_2 = -2q$, where q is a free parameter and we obtain the following set of weights:

$$a_0 = a_4 = 1, \quad a_1 = a_3 = q - 1, \quad a_2 = -2q, \\ b_0 = b_4 = \frac{17-q}{240}, \quad b_1 = b_3 = \frac{29+3q}{30}, \quad b_2 = \frac{111+97q}{120}. \tag{3.18}$$

Thus, the four step schemes form a one-parameter family. Each scheme in this family is identified by the value assigned to q and it will be abbreviated as $S(q)$.

If $y(x)$ admits Taylor series representation, we find that the local truncation error of the method $S(q)$ is

$$LTE(x;q) = \frac{31q-159}{60480} h^8 y^{(8)}(x) + O(h^{10}). \tag{3.19}$$

This expression shows that any $S(q)$ is consistent (its order is 7).

The stability condition imposes some restriction on the values of q. The scheme (3.14) is (zero) stable if no root of the characteristic equation

$$a_0\lambda^4 + a_1\lambda^3 + a_2\lambda^2 + a_3\lambda + a_4 = 0 \tag{3.20}$$

exceeds 1 in absolute value and the multiplicity of the roots of modulus 1 is at most two. The characteristic equation of $S(q)$ is

$$\lambda^4 + (q-1)\lambda^3 - 2q\lambda^2 + (q-1)\lambda + 1 = (\lambda-1)^2(\lambda^2 + (q+1)\lambda + 1) = 0 \tag{3.21}$$

and this shows that the mentioned conditions are satisfied only when $q \in (-3, 1]$.

The fact that the four step schemes form a family has practical consequences, allowing the increase of the computational efficiency. By combining different schemes we have the following possibilities:

- To reduce the number of iterations at each step, in the predictor-corrector mode of calculation.
- To generate the additional starting values when the initial data are given only at two points.
- To evaluate the local truncation error and to control it.
- To modify the step size (halving/doubling) during the integration process.

These facilities make the application of the four step methods flexible and efficient. The order is comparable to the RKN methods used in DOPRIN.

Concerning the starting values, the four step schemes need two values: $y(x_0)$ and $y(x_0+h)$. As normally $y(x_0)$ and $y'(x_0)$ are given as input, to obtain $y(x_0+h)$ one can use a truncated Taylor series (in accordance with the order of the scheme):

$$y(x_0+h)=y(x_0)+\sum_{k=1}^{8}\frac{y^{(k)}(x_0)}{k!}h^k. \tag{3.22}$$

The derivatives of orders $k>1$ result directly from the equation (3.8).

Comparative tests with DOPRIN and a code based on the four step schemes have shown that to reach the same accuracy DOPRIN is superior with respect to the total number of steps, while the four step procedure is better in terms of the number of function evaluations. For our equation (2.1) the routine DOPRIN proved to be a little bit faster and we preferred it in the generation of the χ^2 function (eq. 2.2).

4. APPLICATION

As an illustration of the described numerical procedure, we have considered a device with the following **input parameters**:

1. beam potential: $U=2.1\times10^4$ V; beam intensity: $I_0=0.42$ A

2. lens polarization range:

$$Vb1_{min}=2,\ Vb1_{max}=4.4,\ Vb2_{min}=2,\ Vb2_{max}=4.2,\ V_{step}=0.1$$

3. distances defining the monitors location: $dL_{M1}=0.185$ mm, $d_{M1M2}=0.200$ mm

4. parameters for the magnetic field representation (deduced from the numerical evaluation of the magnetic field): $ab_{max}=7.76$, $bb_{max}=46.335$, $\sigma=0.035$

5. weights: $W_1=1$, $W_2=1$

6. minimization tolerance: $ftol=10^{-8}$

7. accuracy of the solution of the differential equation: $tol=10^{-10}$.

The fitting coefficients a_1, b_{11}, b_{12}, b_{13}, b_{14}, b_{15}, respectively a_2, b_{21}, b_{22}, b_{23}, b_{24}, b_{25}, have been obtained from measured beam cross-section radii at the two monitors.

Initial values of unknown parameters:

$$\epsilon_0=10^{-4},\quad R_0=0.005,\quad z_0=0.06.$$

The successive iterations are shown in the Table 1.

Table 1

Values given by the minimization process

Iteration	ε_0^2	R_0	z_0	χ^2
0	0.100000E–07	0.500000E–02	0.600000E–01	2.3109577E–03
1	–0.126759E–07	0.395585E–02	–0.753830E–01	7.6353863E–04
2	–0.359997E–08	0.761546E–02	–0.196383E–01	4.1796627E–04
3	–0.436766E–08	0.909810E–02	–0.246454E–01	3.8259545E–04
4	–0.441185E–08	0.921419E–02	–0.243259E–01	3.8166121E–04
5	–0.441290E–08	0.924444E–02	–0.242494E–01	3.8161764E–04
6	–0.438277E–08	0.927009E–02	–0.241779E–01	3.8158980E–04
7	–0.417219E–08	0.932020E–02	–0.239968E–01	3.8142210E–04
8	–0.377366E–08	0.937339E–02	–0.237556E–01	3.8112684E–04
9	0.218594E–07	0.113847E–01	–0.116159E–01	2.7038194E–04
10	0.225626E–07	0.108193E–01	–0.114264E–01	2.5839637E–04
11	0.278103E–07	0.102816E–01	–0.117266E–01	2.4073796E–04
12	0.300168E–07	0.105039E–01	–0.132023E–01	2.2750250E–04
13	0.838213E–07	0.149652E–01	–0.146383E–01	1.2072823E–04
14	0.103167E–06	0.152228E–01	–0.156617E–01	9.7808828E–05
15	0.122627E–06	0.154245E–01	–0.158466E–01	9.2637653E–05
16	0.123397E–06	0.154765E–01	–0.158664E–01	9.2621850E–05
17	0.123406E–06	0.154769E–01	–0.158676E–01	9.2621834E–05
18	0.123399E–06	0.154765E–01	–0.158676E–01	9.2621833E–05

Final values:

$$\epsilon_0 = 0.35128 \times 10^{-3}, \quad R_0 = 0.15476 \times 10^{-1}, \quad z_0 = -0.15868 \times 10^{-1}.$$

One can see that the resulted parameters are stabilized to at least 5 digits. With these parameters one can integrate the paraxial equation to obtain root-mean-square beam radii at the monitors in terms of the lens polarization. Their variation is represented in the Fig. 1. The positions of the monitors are: $zm_1 = z_0 + dL_{M1} =$ 0.169 mm, $zm_2 = zm_1 + d_{M1M2} = 0.369$ mm.

To offer more details about the physical process, in Figs. 2 and 3 are shown the solutions of the paraxial equation (2.1) at the two extreme values of the each range of lens polarization.

5. CONCLUSION

In this paper, we have presented numerical procedures involved in the non-destructive diagnosis and the calculation of the beam evolution in low energy electron

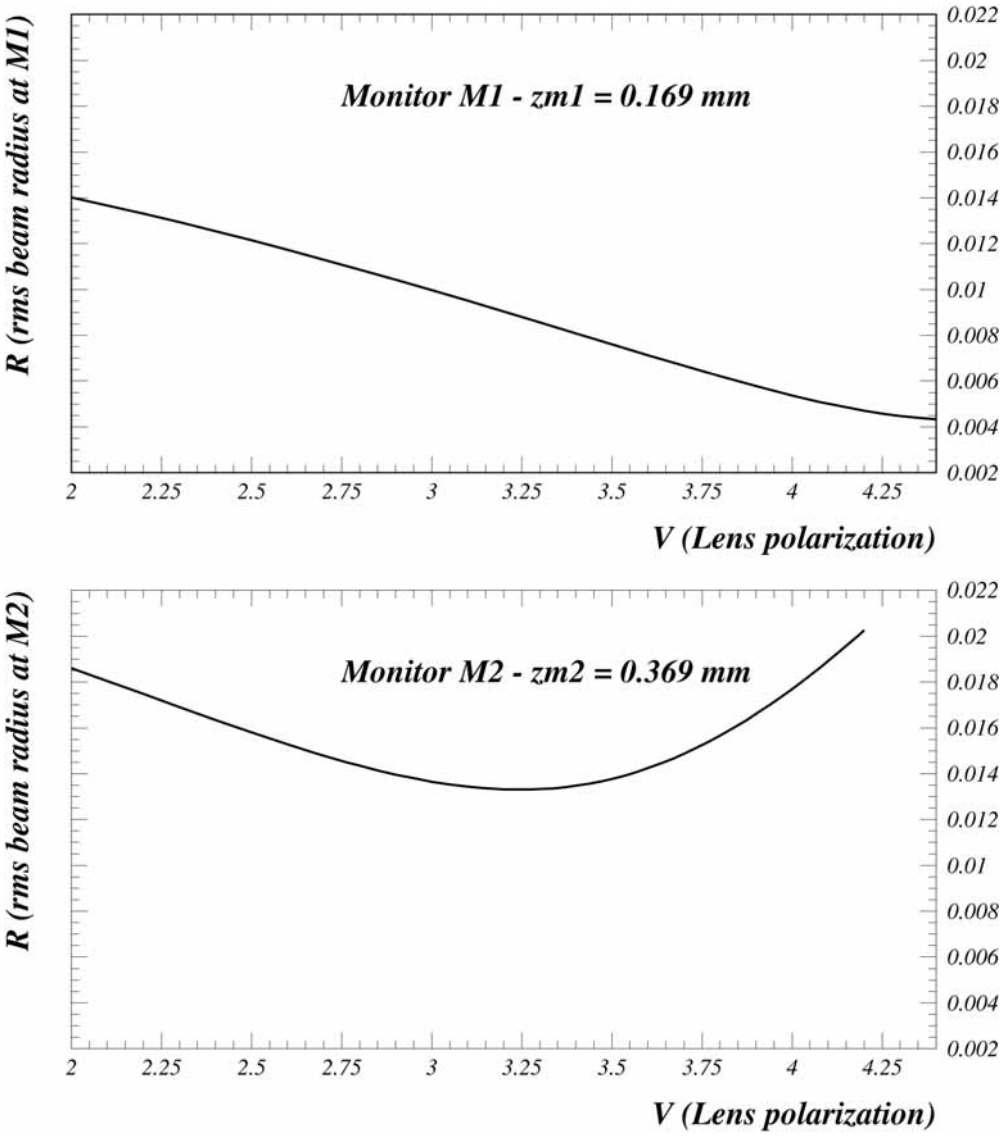

Fig. 1 – The root-mean-square beam radii (R) at the monitors in function of the lens polarization (V).

accelerators. The main mathematical problems have been the solution of a nonlinear differential equation and the minimization of a function of several variables. We have tried several methods, to retain the most appropriate combination for our purposes. To solve the differential equation we have used an embedded pair of Runge-Kutta-Nyström methods with error control and high accuracy, while for the minimization we have used Powell's method, which converges fast and do not require the calculation of gradient components. By the

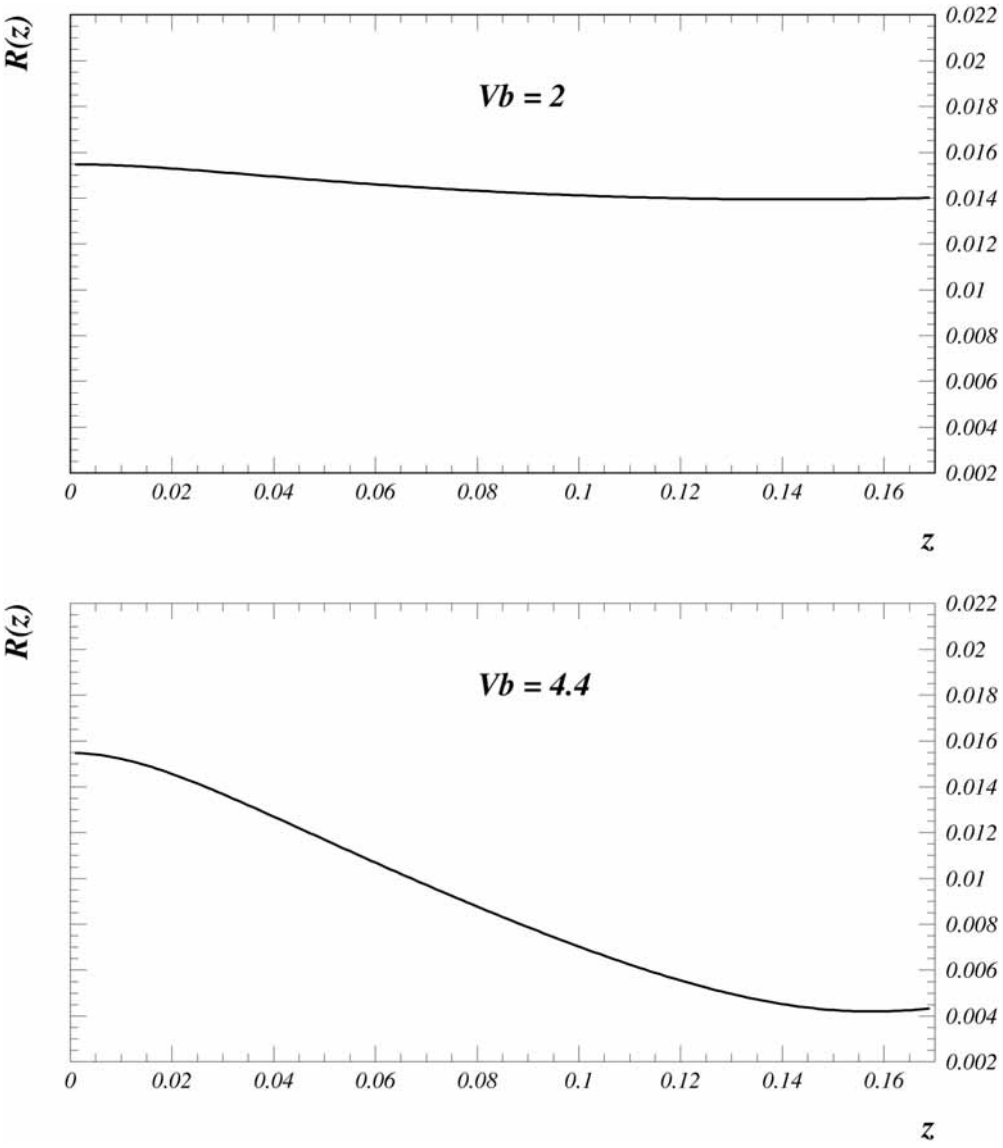

Fig. 2 – The solution $R(z)$ of the paraxial equation for $z \in [0, zm1]$.

described procedure important parameters can be found characterizing the beam at the electron source exit: emittance and cross-over radius and position. The knowledge of these elements is essential for the entire installation design. A reliable numerical description of the physical processes provides useful and low-cost information for practical applications. Corresponding computer codes have been produced and successfully tested, which can also be used for other configurations.

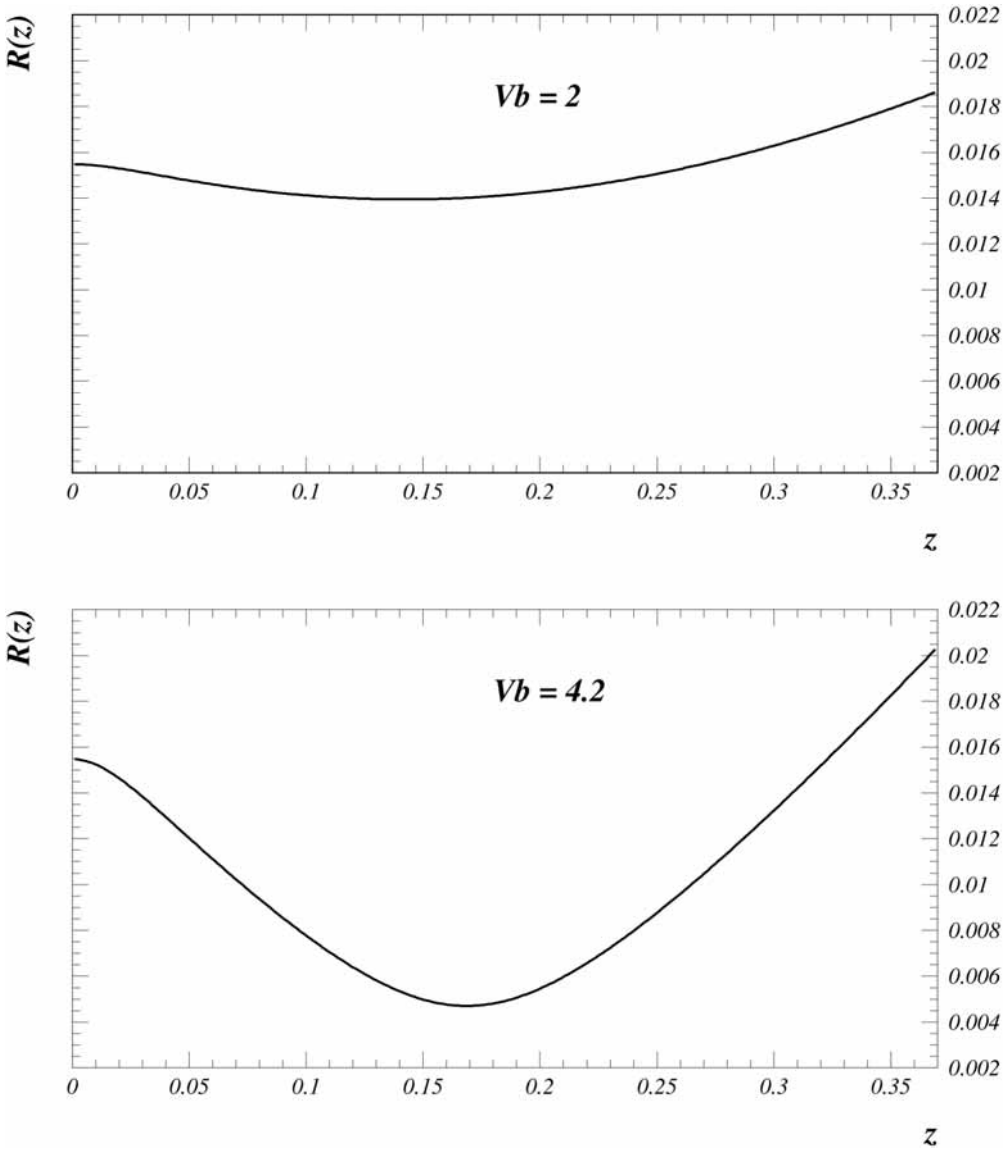

Fig. 3 – The solution $R(z)$ of the paraxial equation for $z \in [0, zm2]$.

Combining theoretical and experimental methods of high efficiency it is possible to optimize the irradiation devices with electron beams applied in technological processes, such as welding, hardening, cladding and surface alloying.

Acknowledgements. Thanks are due to Dr. Silvia Marghitu and to Dr. Octav Marghitu for valuable and stimulating discussions concerning the physical problem.

REFERENCES

1. M. Rizea, *The magnetic field calculation and the electron trajectory determination in computer aided design of unsaturated magnetic lenses*, Romanian Journal of Physics, **37** (1992) 1031–1051.
2. I. M. Kapchinskij, V. V. Valdimirskij, *Limitations of proton beam in strong focusing linear accelerator associated with the beam space charge*, Proc. Int. Conf. on High Energy Accelerators and Instrumentation, CERN (1959) 274–288.
3. P. Ciuti, *On the equation defining the profile of non-relativistic beams with space charge forces and finite emittance*, Nucl. Instr. Meth., **93** (1971) 295.
4. S. Marghitu, C. Dinca, M. Rizea, C. Oproiu, M. Toma, D. Martin, E. Iliescu, *Non-destructive beam characterization at an electron source exit*, Nucl. Instr. Meth. in Phys. Research B, **161**–**163** (2000) 1113–1117.
5. S. Marghitu, O. Marghitu, C. Oproiu, G. Marin, Fl. Scarlat, *Diagnosis and dynamics in a simple low energy medium current electron beam channel*, Nucl. Instr. Meth. in Phys. Research B, **217** (2004) 498–504.
6. M. J. D. Powell, *An efficient method for finding the minimum of a function of several variables without calculating derivatives*, Computer Journal, **7** (1964) 155–162.
7. W. H. Press, B. P. Flannery, S. A. Teukolsky, W. T. Vetterling, *Numerical Recipes*, Cambridge University Press, Cambridge (1986).
8. R. Fletcher, M. J. D. Powell, *A rapidly convergent descent method for minimization*, Computer Journal, **6** (1963) 163–168.
9. Ioannis G. Tsoulos, Isaac E. Lagaris, *Genetically Controlled Random Search: A global optimization method for continuous multidimensional functions*, Comput. Phys. Commun., **174** (2006) 152–159.
10. Ioannis G. Tsoulos, Isaac E. Lagaris, *MinFinder: Locating all the local minima of a function*, Comput. Phys. Commun., **174** (2006) 166–179.
11. E. Hairer, S. P. Norsett, G. Wanner, *Solving ordinary differential equations, Vol. I Nonstiff problems*, second ed., Springer Verlag, Berlin (1993).
12. J. R. Dormand, M. E. A. El-Mikkawy, P. J. Prince, *Families of embedded Runge-Kutta-Nyström formulae*, IMA J. Numer. Anal., **7** (1987) 235–250.
13. J. R. Dormand, M. E. A. El-Mikkawy, P. J. Prince, *High-order embedded Runge-Kutta-Nyström formulae*, IMA J. Numer. Anal., **7** (1987) 423–430.
14. L. Gr. Ixaru, M. Rizea, *Four step methods for* $y'' = f(x, y)$, J. Comput. Appl. Mathem., **79** (1997) 87–99.