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## THE PROGRAMME LIBRARY <br> FOR NUMERICAL SIMULATION <br> OF CHARGED PARTICLE DYNAMICS <br> IN TRANSPORTATION LINES

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## 1. Introduction

The programme library for numerical simulation of the charged particle beam transportation lines realized on IBM PC in Visual Basic code is presented. A number of computer codes has been developed earlier taking into account non-linear space charge fields in numerical simulations of charged particle beams [1,2,3,4,5,6,7].

The presented programme library is purposed for the numerical calculation and optimization of the beam dynamics in the transportation lines including various magnetic and electrostatic elements. The space charge influence on transverse beam dynamics is taken into account here. It is based on two different methods of mathematical simulation: the method of the distribution function moments $[8,9]$ and the particle-particle method (PP-method).

This paper presents analysis and study of charged particle beams for sources of multiple-charged ions and the averaged beam characteristics, such as the mean velocity and root-mean-square dimensions. The main advantage of the moment method is to describe beam dynamics faster in comparison with methods of multiparticle description.

The PP-Method is successfully used in investigation of detailed beam characteristics, distribution function of particles, ion transition from one charge state to another. This method is also helpful to consider nonlinearity of eigenfields of electrons and ions. It could be used to describe the motion of a dense medium, electrodynamics of the dense media and beams of charged particles.

Earlier the methods were applied to calculate and optimize the high intensity beam injection line for the Meson Factory of the Institute for Nuclear Research (Troitsk) [10]. Those methods and codes were used as a background for the new generation code library. The library is installed on the modern PC hardware and software to extend a number of available transportation line elements and make it comfortable in the interactive mode which provides an advanced graphical interface. The programme may be used for numerical simulation of dynamics of multicomponent beams with a real charged state distribution.

## 2. Moment Method Use for Beam Transportation Calculation

Let us define a second order moments matrix M of the distribution function
according to Ref [9] while considering the eigenfield nonlinearity:

$$
M^{I I}=\left(\begin{array}{ll}
M_{x x} & M_{x v}  \tag{1}\\
M_{x v}^{*} & M_{v}
\end{array}\right)
$$

$$
M_{i x}^{1, t}=\int_{f} x_{i} x_{j} d \vec{x} d \vec{v}, \quad \quad M_{i v}^{i, j}=\int_{f} x_{i} v_{j} d \vec{x} d \vec{v}
$$

$$
\begin{equation*}
M_{v}^{i j}=\int f v_{i} v_{j} d \vec{x} d \vec{v}, \quad i, j=1,2 . \tag{2}
\end{equation*}
$$

Here f is the beam distribution function, and $x_{i}, v_{j}$ are particle coordinates and velocities. The evolution of the matrix M under beam transportation through linear electromagnetic fields is defined by a set of equations [10]:

$$
\begin{align*}
& \frac{d M_{x x}}{d z}=M_{x v}+M_{x v}^{*}, \\
& \frac{d M_{x v}}{d z}=M_{v v}+M_{x x} B^{*}+M_{x v}^{*} A^{*},  \tag{3}\\
& \frac{d M_{v v}}{d z}=B M_{x v}+M_{x v}^{*} B^{*}+A M_{x v}+M_{x v} A^{*} .
\end{align*}
$$

where $z=v_{z} t$ and $v_{z}=\beta c$ are longitudinal coordinates and velocity, the matrix B includes external and space charge forces, matrix A includes external forces only (magnetic field defined by particle transverse motion is neglected), $M^{*}, A^{*}, B^{*}$ are transposed matrices M, A, B. The matrices A and B for typical magnetic and accelerating cavities have the following forms:

- Solenoid with axial magnetic field B:

$$
B^{e x t}=\frac{Z e}{2 \beta \gamma A m_{\rho} c^{2}} \frac{\partial B_{x}(z)}{\partial z}\left(\begin{array}{cc}
0 & 1  \tag{4}\\
-1 & 0
\end{array}\right), \quad A^{\text {at }}=\frac{Z e B_{z}(z)}{\beta \gamma A m_{\rho} c^{2}}\left(\begin{array}{cc}
0 & 1 \\
-1 & 0
\end{array}\right)
$$

- Quadrupole with gradient G :

$$
B^{e x t}=\frac{Z e G}{\beta \gamma A m_{p} c^{2}}\left(\begin{array}{cc}
-1 & 0  \tag{5}\\
0 & 1
\end{array}\right), \quad A^{e x}=0
$$

- Horizontal bending magnet (sector type):

$$
B^{e x t}=-\left(\frac{Z e B_{z}}{\beta \gamma A m_{p} c^{2}}\right)^{2}\left(\begin{array}{ll}
1 & 0  \tag{6}\\
0 & 0
\end{array}\right), \quad A^{e x t}=0,
$$

- Vertical bending magnet (sector type):

$$
B^{e n t}=-\left(\frac{Z e B_{z}}{\beta \gamma A m_{p} c^{2}}\right)^{2}\left(\begin{array}{ll}
0 & 0  \tag{7}\\
0 & 1
\end{array}\right), \quad A^{e x t}=0
$$

- Accelerating cavity:

$$
A^{e x t}=\frac{1}{\gamma} \frac{\partial \gamma}{\partial z}\left(\begin{array}{ll}
1 & 0  \tag{8}\\
0 & 1
\end{array}\right)
$$

The elements of moment matrix M for the horizontal bending magnet with the pole face rotation $\alpha$ and bending radius $\rho$ are transformed accordingly:

$$
\begin{align*}
M & =W^{*} M W, \\
& =\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
\frac{\tan \alpha}{\rho} & 0 & 1 & 0 \\
0 & -\frac{\tan \alpha}{\rho} & 0 & 1
\end{array}\right) \tag{9}
\end{align*}
$$

Matrix elements for a vertical bending magnet are changed to $-\alpha$.
In formulae (4)-(8) the values $Z e$ and $A m_{p}$ are ion mass and charge, respectively, $\gamma$ is a relativistic factor (for electrons $\mathrm{Z}=1$ and $\mathrm{Am}>m_{e}$, where $m_{e}$ is the electron mass).

Space charge forces in (3) are considered to be linear [10], [12]. In this case:

$$
\begin{equation*}
B^{s}=\frac{I}{\beta^{2} \gamma^{3} I_{A}} \frac{M_{x x}^{-1 / 2}}{S p M_{x x}^{1 / 2}} \tag{10}
\end{equation*}
$$

with Alfven current $I_{A}=\beta \gamma A m_{\rho} / Z e^{2}$. Matrix $M_{<x}^{1 / 2}$ is defined with conditions $M_{x x}^{1 / 2} M_{x x}^{1 / 2}=M_{x x}, M_{x x}^{1 / 2} M_{x x}^{-1 / 2}=E, \mathrm{E}$ is the unit matrix. Direct calculations are reduced to the elements of the matrices $M^{1 / 2}$ and $M^{-1 / 2}$ :

$$
\begin{aligned}
& M_{11}^{1 / 2}=\frac{M_{11}+\left[\operatorname{det} M_{x x}\right]^{1 / 2}}{\left(S p M_{x x}+2\left(\operatorname{det} M_{x x}\right)^{1 / 2}\right)^{1 / 2}}, \quad M_{22}^{1 / 2}=\frac{M_{22}+\left[\operatorname{det} M_{x x}\right]^{1 / 2}}{\left(S p M_{x x}+2\left(\operatorname{det} M_{x x}\right)^{1 / 2}\right)^{1 / 2}}, \\
& M_{12}^{1 / 2}=\frac{M_{12}+\left[\operatorname{det} M_{x x}\right]^{1 / 2}}{\left(S p M_{x x}+2\left(\operatorname{det} M_{x x}\right)^{1 / 2}\right)^{1 / 2}}, \quad M_{12}^{1 / 2}=M_{21}^{1 / 2}, \\
& M_{11}^{-1 / 2}=\frac{M_{22}^{1 / 2}}{\operatorname{det}\left(M^{1 / 2}\right)}, \quad M_{12}^{-1 / 2}=-\frac{M_{12}^{1 / 2}}{\operatorname{det}\left(M^{1 / 2}\right)}, \quad M_{22}^{-1 / 2}=\frac{M_{11}^{1 / 2}}{\operatorname{det}\left(M^{1 / 2}\right)}, \quad M_{21}^{1 / 2}=M_{12}^{1 / 2} .
\end{aligned}
$$

The solution of set (3) could be used to define averaged values of the beam (transverse beam sizes and velocities, cross term). The main advantage is a shorter calculation time for the main beam characteristics due to the particleless approach.

The approach of linear forces is correct for long beams with the constant transverse density of charged particles. Real particle distributions usually have nonlinear eigenfields that could be described with high order moments and , according to this, a high order set of equations. The approach of effective linearisation of transversal fields for a special kind of distribution function was introduced to solve the problem in the frames of second order moments.

## 3. Equations of Particle Motion in PP-Method

The set of equations of the particle motion in various external fields has the following form:

$$
\begin{align*}
& \frac{d^{2} x_{i}}{d s^{2}}=F_{x i}^{p}+\frac{Q}{\gamma^{2} n} \sum_{i=1}^{n} \frac{x_{i}-x_{j}}{r_{i j}^{2}} Z_{j}  \tag{12}\\
& \frac{d^{2} y_{i}}{d s^{2}}=F_{y i}^{p}+\frac{Q}{\gamma^{2} n} \sum_{i=1}^{n} \frac{y_{i}-y_{j}}{r_{i j}^{2}} Z_{j}
\end{align*}
$$

where $x_{i}, y_{i}$ are transverse coordinates for i 's particle, $Q=2 I / \beta^{3} \gamma I_{\text {cr }}, I$ is the linear current density of the beam, $\beta=v_{z} / c$ is the relative longitudinal velocity of any particle, c is the velocity of light, $\gamma=\left(1-\beta^{2}\right)^{-1 / 2}, I_{c r}=m_{p} c^{3} / e$ for ions and $I_{c r}=m_{e} c^{3} / e$ for electrons. The distance $r_{i j}$ between particles $I$ and j is: $r_{i j}^{2}=\left(x_{i}-x_{j}\right)^{2}+\left(y_{i}-y_{j}\right)^{2}$ if $r_{i j} \geq 2 a_{0}$ and $r_{i j}=2 a_{0}$ if $r_{i j}<2 a_{0}$, where $a_{0}$ is the radius of the particle, $n$ is the particle number. The forces $F_{x j}^{p}$ and $F_{y i}^{p}$ determine the particle interaction with external electromagnetic fields. In particular, when the external field is an axial symmetric magnetic field of any solenoid with induction $B_{z}(z)$, then

$$
\begin{align*}
& F_{x i}^{s}=Q_{1}\left(\frac{\partial y_{i}}{\partial z} B_{z}+\frac{1}{2} \frac{\partial B_{z}}{\partial z} y_{i}\right), \\
& F_{y i}^{s}=-Q_{1}\left(\frac{\partial x_{i}}{\partial z} B_{z}+\frac{1}{2} \frac{\partial B_{z}}{\partial z} x_{i}\right) . \tag{13}
\end{align*}
$$

All other elements of a typical transportation line could be written in the same manner, for example:
for a quadrupole with the gradient of the magnetic field $G(z)$ :

$$
\begin{align*}
& F_{x i}^{Q}=-Q_{1} G(z) x_{i}  \tag{14}\\
& F_{y i}^{Q}=-Q_{1} G(z) y_{i},
\end{align*}
$$

for a vertical bending magnet with the amplitude $B_{y}$ (sector type):

$$
\begin{align*}
& F_{x i}^{M}=-Q_{1}^{2} B_{y}^{2} x_{i},  \tag{15}\\
& F_{y i}^{M}=0,
\end{align*}
$$

for a horizontal bending magnet with the amplitude $B_{x}$ (sector type):

$$
\begin{align*}
& F_{x i}^{M}=0,  \tag{16}\\
& F_{y i}^{M}=-Q_{1}^{2} B_{x}^{2} y_{i} .
\end{align*}
$$

Here $Q_{1}=Z e / A m_{p} c^{2} \beta$ for ions and $Q_{1}=e / m_{e} c^{2} \beta$ for electrons. In these equations $Z e$ is the total ion charge, $m_{p,} m_{e}$ are the masses of proton and electron, respectively, $A$ is the atomic number of the ion. The values of the forces are equal to $F_{x i}^{f s}=F_{y i}^{f s}=0$ in the free space.

## 4. Beam Initial Data for the Distribution Function Moments and PP-Methods

The initial data for the method of distribution function moments and PPmethod are related to each other. The beam initial data are determined by the values of Twiss parameters ${ }_{x}, \alpha_{y}, \beta_{x}, \beta_{y}$ and emittances of the beam $\varepsilon_{x}, \varepsilon_{y}$ in transverse phase planes $x v_{x}, y v_{y}$, respectively. To unify the initial data, the RMS-dimensions and RMS-velocities of the beam are connected with the above parameters as follows:

$$
\begin{aligned}
& \overline{a_{x}^{2}}=\varepsilon_{x} \beta_{x}, \overline{a_{y}^{2}}=\varepsilon_{y} \beta_{y}, \overline{x v_{x}}=-\varepsilon_{x} \alpha_{x}, \overline{y v_{y}}=-\varepsilon_{y} \alpha_{y} \\
& \overline{v_{x}^{2}}=\left(\left(\overline{x v_{x}}\right)^{2}+\left(\overline{y v_{y}}\right)^{2}\right) / \overline{a_{x}^{2}}, \overline{v_{y}^{2}}=\left(\left(\overline{x v_{x}}\right)^{2}+\left(\overline{y v_{y}}\right)^{2}\right) / \overline{a_{y}^{2}}
\end{aligned}
$$

The beam parameters:

- total current (microA);
- type of beam: electron or ion; the beam in the first case has a charge, which is equal to the electron charge, in the other case, the beam is characterized by the ratio of the ion charge to the atomic number; and it is necessary to set the atomic number here.
- type of density distribution in the four-dimensional phase space; it is KapchinskyVladimirsky distribution in case if the method of distribution function moments is used.

Fig. 1 shows an example of User interface to determinate the beam parameters. This form appears in the monitor screen when User chooses the item "Inital Data" +

+ 'Beam's Parameters+Initial Data" in the main menu.



## Fig.1. The form for choosing the beam parameters

The initial data in PP-method are determined by the same values. There are four types of density distribution in the four-dimensional phase space: uniform, gaussian, water bag and parabolic distributions.It is possible to select one of them according to the best approximation of the conditions to solve this problem. The initial distribution of the particles in four-dimensional phase space, i. e. it's coordinates and velocities are calculated by special programmes using the random number generators. All of the above beam parameters are determined when the item "Initial Data" + "Beam's Parameters+Initial Data" is chosen in the main menu. A special form appears in the screen of the monitor as a result of choosing this item. One can see this form in Fig. 2.

User can determine the beam data by focusing the screen pointer to the text field and putting the needed values from the keyboard. The shift to the next text field is produced by clicking the key "Tab". It is necessary to click button "Cancel" and get rid of these data. The beam data will be inserted into the memory when User selects the button "Enter". This data may be written in a special file (see below).


Fig.2. The form to select and insert the beam parameters
The PP-method makes it possible to take into account a charge distribution and Coulomb interaction of all species. In this case the total current is distributed between different species if the beam has more than one ion species. The total current is distributed between different species, and the sum of their partial currents is always equal to the total current in this case. The charge distribution is determined in a special file under the name SPREAD.TXT and, could be corrected with any text editor. This distribution is plotted in the monitor screen and one can choose a number of charge states and the lowest and highest states from the complete charge states distribution according to the required accuracy of simulation. Simple mouse clicking is used for all interactive manipulations. The text field with a charge number changes the color when User clicks this field. The next mouse clicking makes the black color over all the region of selected charges. User interface for choosing the charge state is shown in Fig. 3.


Fig. 3. User interface for choosing the charge state
This picture could be printed by clicking the button "PRINT DISTRIBUTION" (see Fig. 3). The beam parameters may be written in a special file with extension "*.ind" (initial data) when User chooses the menu item "Initial data" + "Writing of Initial Data". User is able to indicate a path to this file and it's name in the WINDOWS dialogue regime is similar to "File" + "Save As". User can read this file choosing the menu item "Calculation of Channel" + "Reading Initial Data From Disk", if the initial beam parameters are invariable during the next programme runs.
5. User Interface for Setting Up Parameters of the Beam Transportation Line

Parameters of the transportation line are determined in the regime of a dialogue. There are two main forms aimed at this.

The first of them allows one to set up the total length of the transportation line, the total number of its elements, the diameter of the inner tube, the Z-coordinate and radius of the diaphragm. This form is presented in Fig. 4.


Fig. 4. User interface for setting up the parameters of transportation line
User can determine the parameters of the line elements with the second form. First of all, it is necessary to determine the type of eleme.nts. Both programmes can work with the following types of elements:

- solenoids,
- vertical dipole magnets,
- horizontal dipole magnets,
- quadrupoles, acceleration cavities,
- free spaces.

When User clicks the button "Enter" (see Fig. 4), then the form which is seen in Fig. 5, appears in the screen of the monitor and offers to User to set on a free space length before this element, the length of the element, it's aperture and value of the physical parameter of this element (the amplitude of the longitudinal field for the solenoid, the value of gradient for the quadrupole and so on).


Fig. 5. User interface to define element parameters

This dialogue continues until the number of the element is less than the total number of the elements. User can turn down this parameters by clicking the button "Cancel" if parameters of the element are wrong, else he can choose the button "Enter". User can click the button "Information" to get more information about the coincidence of the element parameters. The programme automatically returns to the main menu when the parameters of the last element of the transportation line are determined. User can write these data in a special file with extension "*.str" (structure) choosing the item of the main menu "Channel's structure"+"Writing channel's data". The transportation line structure could be restored by choosing the item "Calculation of channel" + "Reading channel's parameters from disk", if it is not necessary to change it during the next runs of the programme.

There are two possibilities for setting the external magnetic field of the solenoid in the programme. The components of the magnetic field are executed analytically when calculation of beam dynamics is fulfilled in paraxial approximation, so it is necessary to set only the amplitude of the longitudinal magnetic field. The components of the field can be set up while reading the file when the components of the magnetic field are represented by the table of values experimentally measured or calculated along the solenoid axis on different radii. Then the dialogue box will appear in the screen of the monitor if User chooses the item of the main menu "Reading data field from file". The file containing the field data with extension "*.dat" (field data) has a structure shown in Table 1:

Table 1

| R | z | Br | Bz |
| :---: | :---: | :---: | :---: |
| 11 | z1 | $\mathrm{Br}(\mathrm{r} 1, \mathrm{z} 1)$ | $\mathrm{Bz}(\mathrm{r} 1, \mathrm{z1})$ |
| r2 | z1 | $\operatorname{Br}(12, z 1)$ | $\mathrm{Bz}(\mathrm{r}, \mathrm{z} 1)$ |
| $\ldots$ | z1 |  |  |
| r1 | z2 | $\operatorname{Br}(\mathrm{r} 1, \mathrm{z2})$ | Bz(r1,z2) |
| r2 | z2 | $\mathrm{Br}(\mathrm{r} 2, \mathrm{z2})$ | $\mathrm{Bz}(\mathrm{r} 2, \mathrm{z} 2)$ |
| .... | z2 | .... | ..... |

The procedure provides linear interpolation of the external magnetic field into the point of a real particle position. The file with the field data is created and corrected in any text editor.

The picture of the channel geometry appears in the screen of the monitor when procedures of setting up parameters of the transportation line and initial beam data are finished. The main initial beam parameters are shown in special windows. Rectangular boxes in the top of this picture represent the elements of the transportation line. The numbers disposed over these boxes show the values of gradients, the amplitude of the magnetic field and so on. An example of this picture is shown in Fig. 6:


Fig. 6. Panel visualizing the beam dynamics calculation

## 6. User Interface for Transportation Line Calculations

User interface for the transportation line calculation with the method of moments of the distribution function is described in this paragraph. The transportation line could be calculated in two regimes:

- the transportation beam line is calculated for all it's elements without any stops up to the last element,
- the transportation beam line is calculated element by element with the stop after each element.
User has a possibility to exchange the position of the element along the line and the amplitude of the physical field of this element in the last case. This case will be realized if User chooses the item of the main menu "Channel's Run on Element". The beam envelopes appear on the panel to visualize the beam dynamics calculation in the both cases. The red line shows the envelope of the beam in horizontal direction, the blue - in the vertical one. The green line shows the amplitude of the longitudinal magnetic field via the distance.

The calculations go on until the right-hand end of the first element is reached. Then the calculations are stopped and the box with the question "Will you continue? Choose the answer!" and two buttons "Yes!" and "No!" appear. The calculations will be continued up to the right-hand side of the next element if User chooses "Yes". The background color of the top panel's part will be changed if User chooses "No". It means that the programme is ready to get new data from User. User can click the mouse pointer on the box of the elements and the foreground color of this box will be red. If User clicks the button "Insert" on the keyboard, then the box with the number
of this element, the old value of the field amplitude in this element will appear in the monitor screen. The empty string offers to User to set up a new value of the amplitude. The calculations will be continued from the right-hand end of the previous element or from the beginning of the transportation line when the first element parameters vary then User clicks the mouse pointer in the position of the element.

User is also able to alter the position of any element changing it's field amplitude. It is necessary to click the mouse pointer on the box of this element and click the buttons "->" or "<-" for moving the element to the right or to the left. The text box in the bottom of the monitor screen with the longitudinal coordinates of the left-hand end of the element will appear in the last case.

## 7. The Output Data

As it was described above, the beam envelopes in horizontal and vertical directions are shown in the monitor screen in the tempo of the transportation line calculation, if the method of the moments is selected. The real beam dimensions along the trace will be shown in the monitor screen if the PP-method is selected. In this case User can see the output Twiss parameters, the number of lost particles and emittances in the horizontal and vertical directions when the calculations are finished. There are three possibilities for User:

- the particle losses along the trace of the transportation line,
- the phase portrait and dimensions in the horizontal and vertical dimensions,
- the output current distribution.

User clicks the button with the corresponding superscription to make a choice (see Fig. 6).

The examples of the particle losses along the trace and phase portrait (the left hand picture) with the cross section of the beam are shown in Figs 7 and 8, respectively.

## 8. Conclusion

The programme library to calculate transportation lines of intense beam of charged particles is developed. There are two different methods for these calculations. The first of them, based on the method of moments for distribution function allows one to define the mean square root characteristics of the beam in interactive regime. Users can change the parameters of the transportation lines and choose a quasioptimal variant of these parameters during calculations. User interface in this case gives visualized results in the screen monitor in the real rate of calculations. The detailed characteristics of the beam behavior along the line axes may be calculated with PP-method when this variant of the transportation line is


Fig. 7. The particle losses along the trace of transportation.


Fig. 8. The phase portrait of circular beam in horizontal plane and it's cross section in the horizontal and vertical planes
chosen. The programme library may be used to calculate the electron and ion beams, the distribution of ion charge states and beam eigenfields could be taken into account.

Parameters of the transportation line and the main beam characteristics can be written in special files and then read again, that allows one to calculate and optimize the transportation line in a short period of time. The results of calculations can be printed and written in files from the programme.

The main disadvantage of the presented PP-method codes is the way of eigenfield calculation as a particle-particle Coulomb interaction. These eigenfield calculation requires a very long calculation time and limits the number of the test particles in the beam simulation. To introduce the Poisson equation into the procedure means to improve the situation and develop the library.
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