https://doi.org/10.46813/2022-139-103 APFRFQ – A SIMULATION ENVIRONMENT FOR THE DEVELOPMENT OF HIGH-CURRENT LINEAR ION ACCELERATORS WITH RF FOCUSING

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Presented is an interactive environment, APFRFQ, for calculating linear accelerators based on rf field focusing of different types, namely, alternating phase focusing (APF), rf quadrupole focusing (RFQ) and a combination of previous two methods (APF&RFQ). The APFRFQ environment is capable of performing the following tasks in the interactive mode: setting the parameters of the accelerating gaps, calculating the accelerating-focusing channels of linear accelerators taking into account the real geometry of the electrodes, performing numerical simulation of particle dynamics in the calculated channels with the space charge forces taking into account, matching the input parameters of the beam with the given six-dimensional phase distribution and the accelerating structure.

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INTRODUCTION

When designing a high-power ion linear accelerator, one of the major tasks is to choose a proper technique for beam focusing depending on the accelerated ion type, the required energy range and the accelerated current value. In this case, the main parameters of the accelerating-focusing channel are bound to be optimal for the current task and calculated for the real structure geometry in a detailed numerical simulation of the beam dynamics taking into account the space charge forces. So, the designing of any accelerator starts with the choice of the focusing technique, then follows the specification of the main parameters and geometry of the accelerating channel, and then comes numerical simulation of the particle dynamics along the entire accelerating channel including matching sections between accelerating ones.

Considering the complexity of the problem, in the last 20-30 years, many scientific accelerating centers have begun to actively develop numerical tools for the particle dynamics simulation in the charged particle linacs. At NSC KIPT, the development of the numerical programs for the accelerating-focusing channel calculations and particle dynamics investigations proceeded simultaneously with the designing and construction of ion linacs. Much attention was given to the accelerators based on rf focusing, in particular, alternating phase focusing (see Refs. [1 - 6]).

Our experience in the calculation of acceleratingfocusing channels of a linac based on rf focusing demonstrated that all the stages for linac channels' development and beam dynamics simulation in these channels should be combined into a single numerical environment. This numerical environment should include both well-known, well-developed and formalized methods for radial and phase stability of charged particle motion and the possibility to heuristically analyze methods for stable localization of an accelerated beam in a linac channel that have not been proposed before. It is this approach that was used to develop a numerical simulation environment APFRFQ, which includes the most effective numerical methods and algorithms that have been tested in the calculation of various versions of ion linacs based on rf focusing.

1. DESCPTION OF THE CODE. MAIN METHODS AND ALGORITHMS

1.1. NUMERICAL INTEGRATION OF MOTION EQUATIONS OF CHARGED PARTICLES WITH TAKING INTO ACCOUNT THE SPACE CHARGE

Incorporated into the numerical simulation environment APFRFQ is the macroparticle method (see Ref. [7]). The method is as follows. Let us consider a classic physical system consisting of a large number of particles. The assignment of all coordinates and velocities fully determines the state of the system, and the knowledge of their interaction laws determines further evolution of this system. However, the number of particles in the system can be enormous which makes it impossible to give a detailed description of such a system using physical particles. In this case, the real physical system is divided into groups of large particles, each of which consists of a large number of real particles. Such a group is called a 'macroparticle'. The charge and mass of such a macroparticle is the sum of charges and masses of its constituent particles, and the coordinates and velocities are their average values.

Let a particle bunch consists of *N* macroparticles, each macroparticle has initial coordinates \mathbf{x}_i and velocities \mathbf{v}_i . The motion equation

$$\cdot \frac{d}{dt} (\gamma m_i \mathbf{v}_i) = \mathbf{F}_i \,. \tag{1}$$

Here m_i is mass of the macroparticle, γ is the Lorentz factor, F_i is the force acting on the macroparticle:

$$\mathbf{F}_i = \mathbf{F}_i^{int} + \mathbf{F}_i^{ext} \,. \tag{2}$$

Here \mathbf{F}_{i}^{int} is the force acting on the *i*th macroparticle from other macroparticles, and \mathbf{F}_{i}^{ext} is the force acting on the *i*th macroparticle from the rf field. The calculation of the interaction force can proceeding from the formalism either of long-range or short-range action. From a physical point of view, these two approaches are equivalent but for the computer simulation they result in different numerical algorithms. In the former case, the force acting on the macroparticle is directly calculated from Eq.(1) using the Coulomb law

$$\mathbf{F}_{i}^{int} = \sum_{i \neq j} \mathbf{F}_{ij}, \quad \mathbf{F}_{ij} = \frac{q_i q_j (\mathbf{x}_i - \mathbf{x}_j)}{4\pi\varepsilon_0 \left|\mathbf{x}_i - \mathbf{x}_j\right|^3}.$$
 (3)

Here x_i , x_j , q_i , q_j stand for the position and charge of the i^{th} and j^{th} macroparticle respectively.

In the latter case, the force and potential are continuous and their relation is

$$\mathbf{F} = -q\nabla\varphi \,. \tag{4}$$

The force acting on the i^{th} macroparticle is calculated according to

$$\mathbf{F}_{i}^{int} = \mathbf{F}(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_{i}}, \quad \varphi = \varphi(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_{i}}, \quad \nabla^{2}\varphi = \frac{-\rho}{\varepsilon_{0}}. \quad (5)$$

Here φ is the electrostatic potential, ρ stands for the charge density, ε_0 is the electric constant.

Usually, the first numerical approach is referred to as PP (particle-particle), while the second one is known as PM (particle-mesh). Numerically, the PP-method is the simplest. The leap-frog finite difference approximation of Eq. (1) has the following form

$$\frac{\mathbf{x}^{n+1} - \mathbf{x}^{n}}{DT} = \mathbf{v}^{n+\frac{1}{2}}, \quad m\gamma \frac{(\mathbf{v}^{n+\frac{1}{2}} - \mathbf{v}^{n-\frac{1}{2}})}{DT} = (\mathbf{F}_{i}^{int} + \mathbf{F}_{i}^{ext}). \quad (6)$$

Here DT is the time step, n is the time step number, v denotes the particle velocity. The particle position is updated at every integer time step, while the momentum is evaluated at every half-integer time step. To track the beam evolution, multiple repetition of the cycle over time is required.

Fundamentally, the time step cycle in the PM method differs from the time step cycle of the PP method in the way of calculating the force. In the PM method, the force is calculated in the following steps:

1. Distribute the charge over the grid.

2. Solve the Poisson equation using the fast Fourier transform (FFT algorithm).

3. Calculate the force using the grid potential.

4. Interpolate the force at the particle position.

Let us consider the difference between two methods (PP and PM).

In the PP method, the force is calculated directly without interpolation or descretization of the space domain. However, the data calculation for a single time step requires ~ N_p^2 computer operations, N_p being the macroparticle number. So, the reasonable number of macroparticles in a simulation is several thousand. Nowadays, computers with multi-core processors, on the one hand, and parallelization of computational processes, on the other hand, enable the number of macroparticles in the simulation to be tens of thousands.

In the PM method, the number of operations is proportional to N_p on steps $N \ge 1$, 3 and 4, while on the step $N \ge 2$ it is proportional to the grid node number (see Ref. [7]). Thus, a simulation model could consist of hundreds of thousands macroparticles. But at the same time, the accuracy of calculating the particle interaction force is less than in the PP method. This is primarily due to descretization of the computational domain and force 104 evaluation by numerical differentiation of the grid potential (step N_2 3). Note that in this method the Poisson equation is solved by the FFT algorithm. The integration domain should have a simple form – a cylinder or rectangular cuboid with the Dirichlet, Neumann or periodic boundary conditions for the potential. There should be no conductors within the domain. The necessity of boundary 'closure' in the PM method results in the following. In the transverse plane at a certain distance, it is necessary to introduce an artificial boundary condition. Usually, this boundary condition for the cylindrical geometry takes the form

$$\left. \varphi(r) \right|_{r=r} = 0, \tag{7}$$

in Cartesian coordinates it is

$$\varphi(x, y)\Big|_{\substack{x=\pm r_a\\y=\pm a}} = 0, \qquad (8)$$

where r_a is the channel aperture radius.

In the longitudinal direction, the boundary conditions are periodic, with a bunch period $\beta\lambda$

$$\varphi(z) = \varphi(z + \beta \lambda) \,. \tag{9}$$

Here $\beta = v/c$, v is the particle velocity, c stands for

the speed of light, λ is the accelerator operating wavelength. These boundary conditions are convenient when used in the accelerator initial part, when the beam occupies a significant part of the high-frequency period. In the medium energy range, the beam phase extent is about ~30° implying that in the longitudinal direction it occupies no more than 10% of the entire computational domain (Fig. 1,b, columns 2 and 3). Since in the FFT algorithm the grid spacing must be constant, the main number of grid nodes falls on the empty space. Thus, in the case of charged particle beams, the PM method is not always effective. Moreover, the use of the PM algorithm when simulating the initial part of the accelerator can lead to serious errors, for example, when calculating RFQ structures. Although the beam occupies almost the entire period when injected into the RFQ structure, a so-called 'focus' situation occurs several times during beam formation as a result of phase motion, when the beam density increases sharply in the vicinity of the synchronous particle and becomes poorly resolvable for the grid method. At the same time, the processes within such 'foci' of an intense beam largely determine the further evolution of the beam. The use of the PP method makes possible avoiding this kind of difficulty.

Regarding the PP method, let us make the following remark. The use of point charges when calculating the interaction force of particles can lead to non-physical 'heating' of the beam. The fact is that if the distance between two point charges is small, there arises a situation of pair 'collision'. However, in real beams, the conditions of 'collisionlessness' are usually satisfied, since the mean free path of particles without Coulomb collisions is much greater than the beam dimensions. To suppress the collisions, the macroparticle is given the shape of a finite charged sphere with a total charge q and radius a/2. In what follows, the force of interaction of two particles will be calculated by the following formulas as in Ref. [7]:

$$F(r) = \frac{q^2}{4\pi\varepsilon_0} \frac{1}{r^2}, \quad r \ge a,$$

$$F(r) = \frac{q^2}{4\pi\varepsilon_0 a^2} \left(\frac{8r}{a} - 9\frac{r^2}{a^2} + 2\frac{r^4}{a^4}\right), \quad r \le a,$$
(10)

where r stands for the distance between particle centers.

1.2. CALCULATION OF QUASI-STATIC FIELDS IN THE STRUCTURES OF THE LINEAR ION ACCELERATOR BY THE AUXILIARY CHARGES METHOD

To calculate fields in real structures, a method for calculating fields is used, which is a variation of the method of integral equations – the method of auxiliary charges (ACM) (see Ref. [8]). According to this method, the quasi-electrostatic field potential is represented as a superposition of the fields of point charges located outside the considered domain. The values of N charges are evaluated from the boundary conditions at N points on the electrode surface. Setting the magnitude of the charges inside the electrodes is equivalent to using a certain charge density on the surface of the electrodes. In 3D geometry the potential is expressed by (in CGS system of units)

$$\varphi(x, y, z) = \sum_{i=1}^{N} \frac{q_i}{\sqrt{(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2}} .$$
(11)

Here x_i , y_i , z_i are the point charge coordinates.

If we choose *N* points on the electrode surface then assuming that at each point with the coordinates $x_{i'}$, y_i , z_i is given the potential $\varphi(x', y', z')$, the charge q_i is calculated by

$$\sum_{i=1}^{N} \frac{q_i}{\sqrt{(x_j - x_i)^2 + (y_j - y_i)^2 + (z_j - z_i)^2}} = \varphi(x_j, y_j, z_j)$$
(12)
i, *j* = 1, 2,..,*N*.

If the problem is axisymmetrical, the potential is evaluated in the following way:

$$\varphi(r,z) = \sum_{i=1}^{N} q_i \frac{4r_i K(k_i)}{R(r,z)}, \quad K(k) = \int_0^{\pi/2} \frac{d\varphi}{\sqrt{1-k^2 \sin^2 \varphi}}, \quad (13)$$
$$k_i = \frac{2\sqrt{rr_i}}{R(r,z)}, \quad R(r,z) = \sqrt{(r+r_i)^2 + (z-z_i)^2}.$$

Here r_i and z_i are the cylindrical coordinates of the point charge, *K* denotes the complete elliptic integral of the first kind. The system of equations for q_i calculation takes the form

$$\sum_{i=1}^{N} q_{i} \frac{4r_{j}K(k_{ij})}{R_{i}(r_{j}, z_{j})} = \varphi(r_{j}, z_{j}) \quad i, j = 1, 2...N,$$

$$k_{ij} = 2 \frac{\sqrt{r_{j}r_{i}}}{R(r_{i}, z_{j})}.$$
(14)

This method for solving 3D quasi-electrostatic problems when the electrodes have a complex shape has been implemented in the program RFQFLD (see Refs. [9, 10]). The RFQFLD code is capable to calculate the fields in RFQ structures with semicircular electrodes modeled according to the sinusoidal or trapezoidal law for periodic and non-periodic structures, as well as for the section of transverse matching – 'bell'. The quasi-electrostatic fields are calculated with the quadrupole symmetry taking into account

$$\varphi(x, y, z) = \varphi(x, -y, z) = \varphi(-x, y, z).$$
(15)

In the longitudinal direction, there are several typical cases of boundary conditions and three of them are:

1. The boundary conditions for the initial part of the accelerator take the form:

$$\varphi(x, y, z)\Big|_{z=0} = 0, \quad \frac{\partial \varphi(x, y, z)}{\partial z}\Big|_{z=Lp} = 0. \quad (16)$$

Here z=0 is the longitudinal coordinate of the resonator wall location, L_p is the matching section length.

2. For the grouping section, when the structure is irregular, the boundary conditions must take into account the adjacent cells` influence

$$\frac{\partial \varphi(x, y, z)}{\partial z} \bigg|_{z=0} = 0, \quad \frac{\partial \varphi(x, y, z)}{\partial z} \bigg|_{z=L_{\tau}} = 0, \quad (17)$$

where z=0, as the origin, corresponds either to the cross-section coordinate at the point of maximum deflection of electrodes from the axis (an RFQ structure) or to the coordinate of the drift tube half-length (a drift tube structure), $L_s=L_{i.1}+L_i+L_{i+1}$, L_i is the length of the accelerating cell in which the field is calculated, $L_{i.1}$ and L_{i+1} are the adjacent cell lengths. In the drift tube structure, these boundary conditions are valid if the length of the drift tubes is small and the fields in adjacent gaps are different.

3. In quasi-regular structures, the effect of adjacent gaps can be neglected and the field in one cell can be calculated with the following boundary conditions

$$\frac{\partial \varphi(x, y, z)}{\partial z} \bigg|_{z=0} = 0, \quad \frac{\partial \varphi(x, y, z)}{\partial z} \bigg|_{z=L_{t}} = 0. \quad (18)$$

The influence of the resonator walls due to their considerable distance from the calculation domain is not taken into account

$$\varphi(r)\big|_{r\to\infty} = 0, \quad r = \sqrt{x^2 + y^2}.$$
 (19)

In the ACM method, it is very important to optimize the arrangement of auxiliary charges relative to the electrode surface so that the boundary conditions are fulfilled with the greatest accuracy at all points on the surface. From previous experience in simulation, the distance of auxiliary charges to the electrode surface should be equal to or slightly larger than the distance between the points on the electrode surface, in which the boundary conditions are set.

The error in the field calculations is estimated in the following way. Let $\tilde{\varphi}$ be a harmonic function which approximates the solution φ at the boundary *M* with the accuracy ε , i.e., the condition $|\varphi - \tilde{\varphi}| < \varepsilon$ is fulfilled. Then, by virtue of the maximum principle for a harmonic function, the solution error will not exceed ε at any point in the analyzed area.

Since in the ACM method the field sources (i.e., point charges) and observation points are separated, the singularity problem is completely absent. An attractive aspect of this method is the ability to accurately calculate the field strength, including on the electrode surface, without resorting to the procedure of numerical differentiation of the potential, using the expressions

$$\mathbf{E}(x) = \frac{1}{4\pi\varepsilon_0} \sum_{j=1}^{N} \frac{q_j(\mathbf{x} - \mathbf{x}_j)}{\left|\mathbf{x} - \mathbf{x}_j\right|^3},$$
(20)

where $\mathbf{E}(\mathbf{x})$ is the electric field strength at the point \mathbf{x} , q_j is the point charge located at the point x_j . Later, the RFQFLD code was modified by adding options for field calculations in axisymmetric and quadrupole gaps.

It is worth mentioning some advantages of the ACM method over the grid methods:

1. In the case of open boundaries, there is no need to `close` them artificially. The open boundary conditions are met automatically.

2. The solution is sought only in the area where it is needed. In particular, when calculating the beam dynamics, it is necessary to know the electric field distribution in the region of its interaction with the charged particle beam, i.e., only in the near-axis area.

3. The solution is highly accurate, including the electrode surface.

4. Simple coding.

1.3. FEATURES OF THE SIMULATION ENVIRONMENT APFRFQ

New methods implemented into the program are the following:

First is the method to construct an irregular (quasiperiodic) accelerating channel as a set of separate consistent focusing periods. In this case, the focusing periods themselves may differ from each other by the number of accelerating gaps, the phase distribution of synchronous particles and the accelerating field amplitudes along the gaps, the gap parameters, the diameter of the channel aperture, etc.

Second novelty is the 'local stability' method, which allows calculating the radial stability of motion not only in the vicinity of a synchronous particle, but also for nonequilibrium particles trapped in the acceleration mode along the longitudinal motion, taking into account their phase motion for channels with real distribution of accelerating fields and Coulomb forces. Moreover, the similar analysis can be carried out for any group of focusing periods, including the entire accelerating structure.

Next is the method to match the input parameters of the beam that has an arbitrary six-dimensional phase distribution to the parameters of any (irregular) accelerating structure when the space charge should be taken into account.

2. SOME EXAMPLES OF THE APFRFQ CODE APPLICATION

To illustrate the capabilities of the APFRFQ code, let us consider two practical examples of the development of linear accelerators based on rf field focusing without the use of external focusing devices, namely: the pre-stripping section of the multi-charged ion accelerator MILAC (see Ref. [11]) and the linear accelerator of helium ions (see Ref. [12]).

Nowadays, the initial part of MILAC accelerator includes a high-voltage injector with the output energy 33 keV/u and a pre-stripping section with grid focusing POS-15 for acceleration of heavy ions with mass-tocharge ratio $A/q \le 15$ up to 0.975 MeV/u. The presence of the grid focusing section drastically limits the accelerated current, from 10 mA at the section input to 40 μ A at the output.

The accelerating part of the pre-stripping section consists of two segments: the first segment is based on the RFQ structure and the structure based on combined alternating-phase and quadrupole rf focusing (CRFF) makes the second one.

The parameters for the RFQ section are: energy ranges 0.006...0.1 MeV/u, beam capture efficiency reaches $\ge 80\%$ under acceleration mode at input current of 10 mA (A/q = 20). At the same time, the reduction in the injection energy allows a significant increase in the injector reliability.

The CRFF section has a mixed focusing period: the pattern is FOOODDOOOF for the energy range 0.1...0.4 MeV/u (where F is the accelerating period with the focusing quadrupole that focuses in the transverse direction (say, along the *X*-coordinate), D denotes the defocusing quadrupole segment, and O represents the axisymmetric accelerating gap) and FOOOOODDOOOOOF for energies 0.4...1.0 MeV/u. For this section, the beam capture efficiency reaches almost 100% under the acceleration mode that far exceeds the same parameter for the grid focusing segment (0.4%).

Fig. 1,a presents the control panel view of the APFRFQ development environment. The control panel allows setting the accelerating period parameters, calculating the accelerating-focusing channels with actual geometry of the electrodes, and simulating the beam dynamics taking into account the space charge. The simulation results, i.e., the beam phase portrait, vertical and horizontal profiles of the beam, are displayed on the computer screen in real time. Some screenshots for the simulation of the MILAC pre-stripping section are shown in Fig. 1,b as an example.

The accelerating channel of the helium ion accelerator for the output energy 4 MeV was calculated by the means of APFRFQ. The injection current was 30 mA, the design output current - 10 mA. During the accelerating structure manufacture and its subsequent tuning, it was not possible to maintain the specified values of the field strength in the accelerating gaps. The re-calculated value of the accelerated ion current at the accelerating section output, taking into account the real geometry of the channel and the experimentally measured amplitude values of the rf field, was 6 mA. However, as there was no matching line between the injector and the accelerating structure, the experimentally measured current at the structure output was 0.9 mA. Fig. 2 gives the calculated input and output parameters of the beam dynamics simulations for the helium ion accelerator including the matching line. The input beam current was 30 mA, the output -4.5 mA.



Fig. 1. The main control panel of the APFRFQ environment (a); phase portrait, vertical and horizontal beam profiles (b): 1) at the entry-point of the RFQ structure; 2) at the entrance to the CRFF structure;
 3) at the output of the CRFF structure



Fig. 2. Parameters of helium ion beam for the channel with output energy of 4 MeV at 30 mA injection current: input (a); output (b)

CONCLUSIONS

The presented interactive environment, APFRFQ, for calculating linear accelerators with RF focusing is capable of making calculations of linac channels of any complexity not only for the well-known methods of ensuring stability of charged particle beam acceleration by RF field, but also to investigate the most common case of RF focusing, namely, the combination of alternating-phase focusing and RF quadrupole one. As the APFRFQ code has a modular architecture, it is flexible and could be easily updated for a new research.

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АРFRFQ – СЕРЕДОВИЩЕ ЧИСЕЛЬНОГО МОДЕЛЮВАННЯ ДЛЯ РОЗРОБКИ ВЕЛИКОСТРУМОВИХ ЛІНІЙНИХ ПРИСКОРЮВАЧІВ ІОНІВ З ФОКУСУВАННЯМ ВЧ-ПОЛЕМ

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Представлено APFRFQ – середовище чисельного моделювання для розробки великострумових лінійних прискорювачів з фокусуванням ВЧ-полем: змінно-фазовим фокусуванням (APF), ВЧ-квадрупольним фокусуванням (RFQ) та комбінацією згаданих фокусувань (APF&RFQ). Інтегроване середовище APFRFQ дозволяє в інтерактивному режимі вирішувати наступні задачі: задавати параметри прискорювальних зазорів, розраховувати прискорювально-фокусувальні канали лінійного прискорювача з урахуванням реальної геометрії електродів, проводити числове моделювання динаміки частинок у каналах, що були розраховані, з урахуванням сил об'ємного заряду, узгоджувати вхідні параметри пучка із заданим шестивимірним фазовим розподілом та прискорювальною структурою.

АРFRFQ – СРЕДА ЧИСЛЕННОГО МОДЕЛИРОВАНИЯ ДЛЯ РАЗРАБОТКИ СИЛЬНОТОЧНЫХ ЛИНЕЙНЫХ УСКОРИТЕЛЕЙ ИОНОВ С ФОКУСИРОВКОЙ ВЧ-ПОЛЕМ

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Представлена APFRFQ – среда численного моделирования для разработки сильноточных линейных ускорителей с фокусировкой ВЧ-полем: переменно-фазовой фокусировкой (APF), ВЧ-квадрупольной фокусировкой (RFQ) и их комбинацией (APF&RFQ). Интегрированная среда APFRFQ позволяет в диалоговом режиме выполнять следующие задачи: задавать параметры ускоряющих зазоров, рассчитывать ускоряюще-фокусирующие каналы линейных ускорителей с учетом реальной геометрии электродов, проводить численное моделирование динамики частиц в рассчитанных каналах с учетом сил объемного заряда, осуществлять согласование входных параметров пучка с заданным шестимерным фазовым распределением и ускоряющей структурой.