MOMENT METHOD BEAM DYNAMICS CODE DEVELOPMENT: EXTENDED FOR RADIO FREQUENCY QUADRUPOLE SIMULATIONS[*]

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Abstract

A Radio Frequency Quadrupole (RFQ) enables acceleration of a continuous low-velocity hadron beam, combining velocity independent electric focusing and adiabatic bunching, resulting in high-current compact bunches with nearly 100% capture and transmission efficiency. Fast and accurate beam dynamics simulations are of paramount importance during the design, commissioning and operation of an RFQ. This article presents the implementation of an RFQ beam line element (BLE) into V-Code, a moment method beam dynamics simulation code with precision and efficiency advantages when calculating average or rms beam dimensions, projected emittances or total energy. Both the BLE implementation methods and a successful simulation of an exemplary section of the MYRRHA RFQ are discussed in this article.

INTRODUCTION

V-Code [1, 2] is a sixth order moment method Vlasov beam dynamics code, providing precise average and rms beam dimensions, projected emittances and total energy results. It is substantially faster than full particle in cell (PIC) codes, and outperforms macro-particle tracking algorithms with its precision. The Vlasov equation (Eq. 1) is time integrated, starting from an initial particle beam distribution and accounting for all acting internal and external forces along the particles' path. The initial particle bunch is expressed by a six dimensional phase space with longitudinal and transverse dynamics. Not only the average bunch coordinates and momenta, but also higher order correlation parameters up to the sixth order are enclosed in the phase space distribution function $f(\tau, \vec{r}, \vec{p})$, with equivalent time $\tau = ct$, speed of light c, time t, space coordinates $\vec{r}$ and normalized momentum ($\vec{p} = \vec{P}/mc$). $\gamma = E/mc^2$ is the normalized energy, with energy E and mass m, and $\vec{F}$ represents the electromagnetic forces from accelerator components, as well as space charge forces.

$$\frac{\partial f}{\partial \tau} + \frac{\partial f}{\partial \vec{r}} \frac{\vec{p}}{\gamma} + \frac{\partial f}{\partial \vec{p}} \frac{\vec{F}}{mc^2} = 0 \qquad (1)$$

The electromagnetic field distribution in V-Code can be described by a multipole expansion of field data from finite element (FE) or finite difference time domain (FDTD) field simulation results, enhancing the accuracy of the beam dynamics results compared to field data from analytical models.

Implementation of the RFQ as a new BLE in V-Code requires an accurate 3D RFQ model generation, field data extraction and a multipole field representation model with tuneability and error prediction.

RFQ 3D MODEL

The rods of an RFQ are arranged in a quadrupole geometry for transversal electric focussing of the beam, while the longitudinal modulation (vertical rods shifted out of phase by π) together with the RF induced currents in the rods yield accelerating electric fields at the bunch passage instance. The electromagnetic field distributions are calculated using CST Studio Suite [3]. The integrated Visual Basic for Applications (VBA) programming functionality allows to set up a COM based interface with MATLAB to support the setup of a custom RFQ model. Our VBA code is able to model RFQ rods with three different approaches: sinusoidal modulation algorithms, two- and four-term potential function based algorithms and functions fitted from tabulated data. Additionally, the user may specify radial matchers and transition cells (Fig. 1). Required parameters are minimum aperture a, modulation m, cell length, electrode cross section radius... A separate code is written to generate the stems for the RFQ.
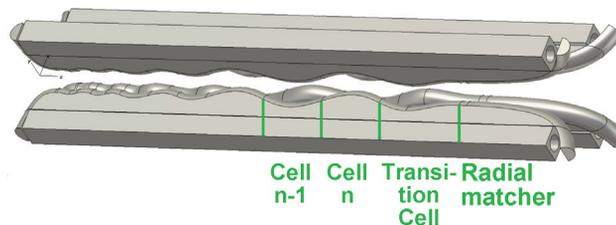

Figure 1: Exemplary short RFQ 3D model.

RFQ ANALYTICAL FIELD SOLUTION

Since the electrode gap is small compared to the RF wavelength and the electric field between the rods arrises from the potential difference between the rods, and not from the RF magnetic field contribution, a quasistatic approach is valid [4].

$$U(r, \theta, z, t) = \sin(\omega t + \phi) \Bigg[$$

$$\sum_{p=0}^{\infty} A_{0,2p+1} r^{2(2p+1)} \cos(2(2p+1)\theta) +$$

$$\sum_{n=1}^{\infty} \sum_{s=0}^{\infty} A_{n,s} I_{2s}(knr) \cos(2s\theta) \cos(knz) \Bigg] \qquad (2)$$

The scalar potential function $U(r, \theta, z, t)$ (Eq. 2) [8] characterizes the RF electric field distribution in an RFQ cell with length L (Fig. 2). r, θ, z are the polar coordinates, time t, $\omega/2\pi$ the RF frequency, ϕ the initial phase shift, p, s and n multipole component indices with restriction $n + s = 2p + 1$, I_{2s} the modified Bessel function, A_s and A_{ns} pole tip geometry dependent multipole coefficients in function of $m(z), a, k$ and V_0, with $m(z)$ the modulation parameter, minimum aperture a, electrode potential difference V_0, $k = 2\pi/2L$ with $2L = \beta_s\lambda$ the electrode modulation period, β_s the synchronous particle velocity and wave length λ. $\vec{E} = -\nabla U$ is the associated electric field strength.
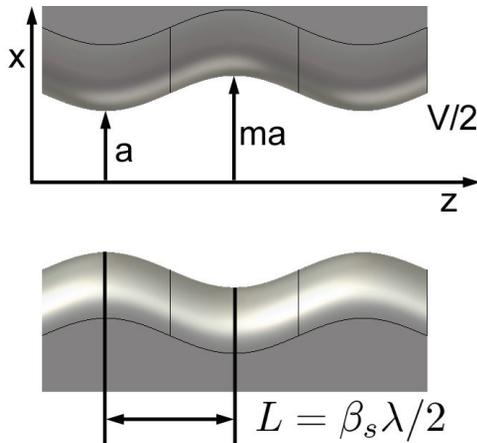

Figure 2: RFQ electrode tip geometry.

IDENTIFICATION USING 3D FE FIELD DATA

A contemporary RFQ design differs significantly from the idealized geometry for which Eq. 2 is available. Therefore 3D numerical field simulation is compulsory. Nevertheless Eq. 2 can be used to reconstruct the fields in V-Code, together with an identification of the multipole coefficients based on a nonlinear regression in MATLAB of Eq. 2 to the 3D numerical field data calculated in CST Studio Suite. These routines are available on a cell-by-cell basis for the two-, four- and eight-term coefficients. The eight-term potential function with multipole coefficients $A_{01}, A_{03}, A_{10}, A_{12}, A_{21}, A_{23}, A_{30}$ and A_{32}, is considered as sufficiently accurate [5], and is implemented in the beam dynamics code TRACK. A comparison of the mean square error (MSE) of the different fits confirms this (Table 1).

Table 1: MSE comparison of n-term multipole fits to field data of cell 76.

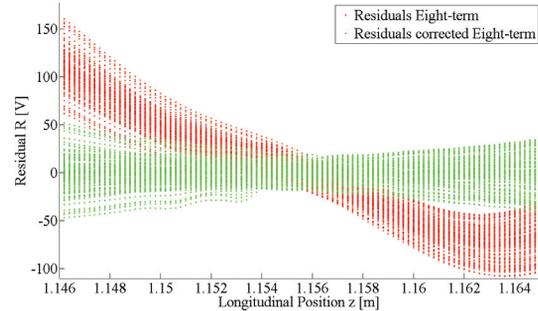| n-term	2	4	8	Corr. 8
MSE [V^2]	1056	276	267	196

Figure 3: Residual comparison between a regular eight-term and a corrected eight-term scalar potential function fitted to 3D FE/FDTD MYRRHA [6] RFQ data for a single cell using nonlinear regression.

An analysis of the fit residuals shows a longitudinal dependency pattern of the RFQ cell structures (Fig. 3), since the latter induce a longitudinal field asymmetry. This motivates the introduction of an additional correction polynomial enabling a more accurate field reconstruction in V-Code. For the MYRRHA RFQ the overal error of the standard eight-term potential of 1.00% is reduced to 0.25% for the corrected eight-term potential (Fig 4).
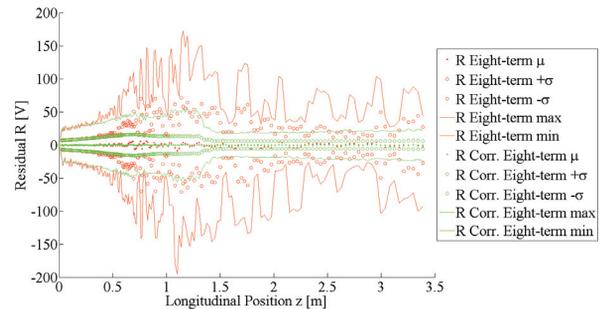

Figure 4: Residual comparison between a regular eight-term and a corrected eight-term scalar potential function fitted to 3D FE/FDTD MYRRHA [6] RFQ data.

IMPLEMENTATION IN V-CODE

The potential function (2), with a user-specified number of terms is implemented as an RFQ BLE in V-Code. The presence of Taylor-expandable Bessel functions and higher order derivable functions ($\cos(knz)$) makes Eq. 2 suitable for implementation in a moment method code. In a first stage the two-term potential function (Eq. 3), combined with an appropriate RF signal, is implemented in

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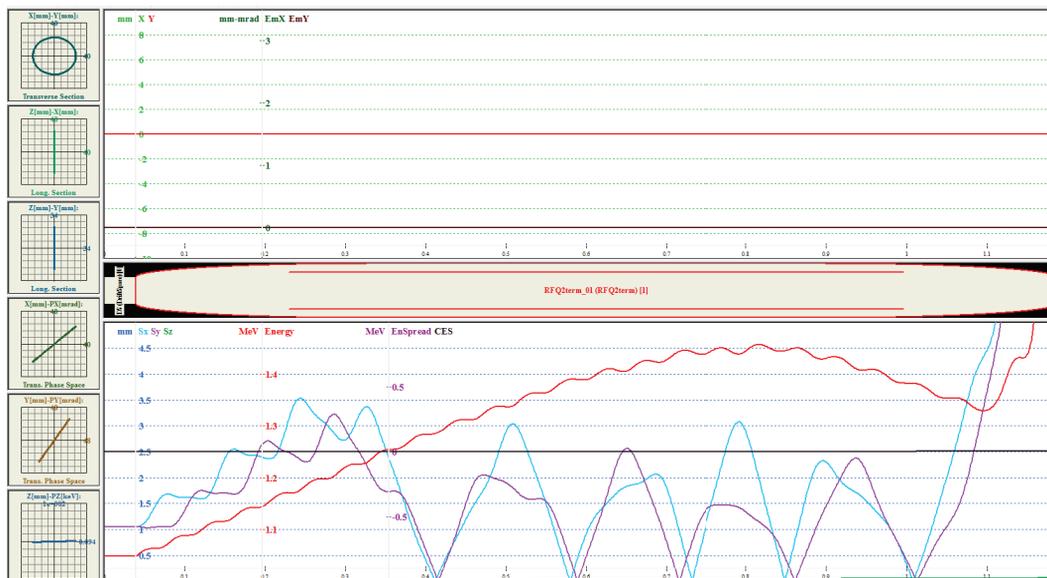**D06 Code Developments and Simulation Techniques**

Figure 5: V-Code two-term potential function simulation of the last 26 cells of the MYRRHA RFQ.

V-Code. $I_0(kr)$ is substituted with a sixth order Taylor expansion to preserve accuracy, leaving parameters A_{01}, A_{10} and $k = 2\pi/2L$ to be provided for every cell, together with the RF frequency, RF phase, rod orientation and field amplitude of the RFQ.

$$V(r, \theta, z) = A_{01}r^2 \cos(2\theta) + A_{10}I_0(kr)\cos(kz) \quad (3)$$

The two-term RFQ is implemented in V-Code as such that a future expansion with higher order terms and correction terms can be seamlessly integrated. Additionally the radial matchers and transition cells require an individual implementation prior to be added to the modulated RFQ fields.

EXAMPLE: MYRRHA RFQ

The beam dynamics of the last 26 cells of the accelerator section (≈ 1.1 m) of the MYRRHA RFQ were calculated in V-Code to validate the implementation (Fig. 5). An initial particle distribution energy of 1.05 MeV was determined based on the length of the first accelerating cell, together with the design frequency of 176 MHz, and a phase shift of -5°. The particle energy increases up to 1.45 MeV (design energy 1.5 MeV), and the bunch is successfully contained betweens the rods. At ≈ 1.1 m the beam diverges and is lost. The divergence is attributed to inaccurate initial particle bunch data and to the limited accuracy of the two-term potential function. It is expected that the (corrected) eight-term potential function will improve the focussing characteristics and keep the bunch in phase with the RF, boosting the energy to 1.5 MeV.

CONCLUSIONS AND OUTLOOK

The paper describes a semi-automatical 3D model generation of an RFQ with arbitrary rod modulation, the identification of a corrected 8-term analytical field model from 3D numerical field data and its usage as a new BLE in a moment method beam dynamics code. The new BLE extends fast and accurate beam dynamics calculations for LINACS incorporating an RFQ. The results indicate that a two-term potential description has an insufficient accuracy. Future work will upgrade to the corrected 8-term potential and add radial matcher and transit cell field reconstruction.

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