Nuclear Instruments and Methods in Physics Research A 851 (2017) 20–28

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Development of a relativistic Particle In Cell code PARTDYN for linear accelerator beam transport

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ARTICLE INFO

Keywords:
Particle in Cell
Beam dynamics

ABSTRACT

A relativistic Particle In Cell (PIC) code PARTDYN is developed for the beam dynamics simulation of z-continuous and bunched beams. The code is implemented in MATLAB using its MEX functionality which allows both ease of development as well higher performance similar to a compiled language like C. The beam dynamics calculations carried out by the code are compared with analytical results and with other well developed codes like PARMELA and BEAMPATH. The effect of finite number of simulation particles on the emittance growth of intense beams has been studied. Corrections to the RF cavity field expressions were incorporated in the code so that the fields could be calculated correctly. The deviations of the beam dynamics results between PARTDYN and BEAMPATH for a cavity driven in zero-mode have been discussed. The beam dynamics studies of the Low Energy Beam Transport (LEBT) using PARTDYN have been presented.

1. Introduction

An Indian spallation neutron source (ISNS) has been proposed at RRCAT, Indore. ISNS consists of 1 GeV H- injector linac which injects a high current beam into an accumulator ring. As a part of the ongoing project, a PIC code for beam PARTicle DYNamics in Linear Accelerator PARTDYN has been developed to study the beam dynamics of the space charge dominated beam in the Low Energy Beam Transport (LEBT) and Medium Energy Beam Transport (MEBT) sections of the linac. PARTDYN can be used to simulate the z-continuous (2D) beam and bunched (3D) beam in the accelerator transport sections consisting of axially symmetric accelerating cavities, and magnetic focusing elements like quadrupoles, solenoids etc.

PIC is a standard technique for the transport of space charge dominated beam. The details of the PIC method can be found in references [1–3]. Apart from the space charge solver using the PIC technique, PARTDYN contains a particle distribution generation and particle tracking algorithm. PARTDYN is developed in MATLAB. MATLAB is a good platform for the fast development of the code but is too slow for non-vectored operations like the sequential 'for' loops which are often encountered in the code. This speed bottleneck can be removed by using the MEX files which are a way to call the C/FORTRAN routines directly from MATLAB.

In this paper we describe the algorithms used in the development of PARTDYN. We also discuss the validation of PARTDYN calculations with analytical results and compare the performance and the deviations of the code with other well developed codes like PARMELA [4] and BEAMPATH [3]. In future we would like to incorporate collision of beam ions with neutral gas using Monte Carlo technique in the 2D code for the study of space charge compensation. The space charge compensation method is used in the Low energy beam transport (LEBT) of the linac to reduce space charge induced emittance growth.

2. Physical modeling and equations of motion

The z-continuous beam is represented as a slice of macro-particles in the x-y plane on which the 2D space charge grid is superimposed. The boundaries of the grid correspond to the aperture of the transport channel. The bunched beam is represented by the collection of macro-particles on a three dimensional spatial grid. In the transverse direction the grid boundary is decided by the aperture and in longitudinal direction the grid extends over the bunch period=$\beta\lambda$. Where β is the beam's average relativistic parameter and λ is the free space wavelength of rf field. A macro-particle represents a group of particles in the real beam with same q/m ratio. The computation grid moves along with the beam centroid.

Initially the phase space is filled with macro-particles according to the type of distribution chosen. The particle trajectories are then integrated in the fields consisting of external electromagnetic fields and self-space charge fields. The space charge field is calculated at each

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http://dx.doi.org/10.1016/j.nima.2017.01.038
Received 31 May 2016; Received in revised form 18 January 2017; Accepted 18 January 2017
Available online 19 January 2017
0168-9002/

integration step using the Poisson solver and the macro-particles are thus transported self consistently over the length of transport section. The macro-particle is lost if it touches the boundaries of the aperture. If the particle leaves the grid longitudinally, its contribution to the space charge field is neglected. But its trajectory is computed with a space charge kick of a point charge at the beam centroid.

For the relativistic generalization **u**=γ**v** is used instead of **v**. the equations of motion are given by:

$$\frac{d\vec{x}}{dt} = \frac{\vec{u}}{\gamma},\ \frac{d\vec{u}}{dt} = \frac{q}{m}(\vec{E} + \frac{\vec{u}}{\gamma} \times \vec{B}), \qquad (1)$$

$$\gamma^2 = 1 + \frac{u^2}{c^2}$$

Where,q is charge and m is the rest mass of the particle, $\vec{x}$ and $\vec{u}$ refer to x,y and z components of position and velocity. The electric and magnetic fields in Eq. (1) are a combination of external fields $\vec{E_{ext}}$ and $\vec{B_{ext}}$, and space charge fields of the beam $\vec{E_{sc}}$. The integration is performed with a fixed time step Δt.

3. Initial loading of particles

For linear focusing and linear space charge density the courant-Snider(C-S) invariant of motion are given by [5]:

$$A_x^2 = \left(\sqrt{\beta_x}x' + \frac{\alpha_x x}{\sqrt{\beta_x}}\right)^2 + \left(\frac{x}{\sqrt{\beta_x}}\right)^2 A_y^2 = \left(\sqrt{\beta_y}y' + \frac{\alpha_y y}{\sqrt{\beta_y}}\right)^2 + \left(\frac{y}{\sqrt{\beta_y}}\right)^2 \qquad (2)$$

where, x, x', y, y' are the phase space coordinates of the particle and α_x, α_y, β_x, β_y are the TWISS parameters of the beam. A_x^2,A_y^2 define the areas of the phase space ellipses in x and y plane and thus are related to the beam emittances ε_x and ε_y. A distribution that is specified as a function of Courant-Snyder (C-S) invariants, is in equilibrium throughout the beam transport. But except the Kapchinskij-Vladimirskij (KV), any other function of C-S invariant produces a non-uniform space charge density and hence is not self-consistent. Nonetheless such distributions have elliptical symmetry and consequently are employed in linear focusing channels with longitudinal variations in focusing strengths. Consider the parameter F defined as a function of C-S invariants as:

$$F = A_x^2 + \nu A_y^2 \qquad (3)$$

where $\nu = \frac{\varepsilon_x}{\varepsilon_y}$ is the ratio of beam emittances.F is related to the emittance of the beam,F_0 being the total emittance of the beam. The different distributions defined as a function of parameter F are shown in Table 1.

Methods to generate such distributions can be found in references [3,6]. In this code we have used the ‘Inverse function’ method of [3] to generate the distributions. The same technique is used for the generation of bunched beam, wherein we make use of the above process for

Table 1
Definition of different phase space distributions.

Type of distribution	Definition $f(r)$
K V	$\frac{\nu}{\pi^2 F_0}\delta(F - F_0)$
Waterbag	$\frac{2\nu}{\pi^2 F_0^2}$
Parabolic	$\frac{6\nu}{\pi^2 F_0^2}\left(1 - \frac{F}{F_0}\right)$
Gaussian	$\frac{\nu}{\pi^2 F_0^2}\exp\left(-\frac{F}{F_0}\right)$

the transverse phase space and a separate C-S invariant parameter for the longitudinal space. It is known that the density projection of any distribution of C-S invariant in 6D phase space cannot produce a uniform ellipsoid bunch [6]. Hence unlike K-V, there is no distribution that is self-consistent with space charge in 3D real space. In 3D, a distribution which produces a uniform ellipsoid bunch and whose rms parameters can be readily calculated is the so called ‘TRACE-3D’ distribution [7]. This distribution is uniform in any of the 3 phase space coordinate (x,y,z), (x′,y′,z′), (x, y,z′) etc. It should be noted that TRACE-3D is not an equilibrium distribution even without space charge since it is not a function of C-S invariant or any other invariant of motion. Fig. 1 shows the phase space projections of the different distributions listed in Table 1. The different colored contours represent the varying densities of the distribution. The red color represents the highest density and blue the lowest. The real space projections of 2D Gaussian and TRACE-3D bunched beam are shown in Fig. 2.

4. Field solver

The space charge field of the beam is calculated by solving the Poisson's equation:

$$\nabla^2\phi = -\frac{\rho}{\varepsilon_0} \qquad (4)$$

where ϕ is the space charge potential and ρ is the space charge density of the beam. The computational space is first discretized using a rectangular/cylindrical grid in two and three dimensions for the continuous and bunched beams respectively. The space charge of macro-particles is distributed among the grid nodes using the ‘Area Weighing Method’ [1]. For the rectangular 2D case the charge of the nth particle is deposited on the neighboring 4 nodes as:

$$\rho_{i,j} = \rho_c\left(1 - \frac{|x_n - x_i|}{h_x}\right)\left(1 - \frac{|y_n - y_j|}{h_y}\right)\rho_{i+1,j} = \rho_c\left(\frac{|x_n - x_i|}{h_x}\right)\left(1 - \frac{|y_n - y_j|}{h_y}\right)\rho_{i,j+1} = \rho_c\left(1 - \frac{|x_n - x_i|}{h_x}\right)\left(\frac{|y_n - y_j|}{h_y}\right)$$
$$\rho_{i+1,j+1} = \rho_c\left(\frac{|x_n - x_i|}{h_x}\right)\left(\frac{|y_n - y_j|}{h_y}\right) \qquad (5)$$

where, x_i, y_i are the coordinates of the *(i,j)*th node from the origin, and x_n,y_n are the coordinates of the nth particle. h_x,h_y are mesh sizes. ρ_c is the charge density per cell related to current I by:

$$\rho_c = \frac{I}{\beta cNh_x h_y} \qquad (6)$$

Similar equations are used for the charge deposition of the particle on the neighboring 8 nodes of the 3D grid. Since the bunch has relativistic velocity in z direction, before the Poisson equation is solved, the grid is transformed in the bunch center of mass frame. The distance of the grid nodes in longitudinal direction is multiplied by the Lorentz factor γ, whereas the transverse grid spacing remains the same.

4.1. Poisson solver

A FFT based Green's function method is mostly used to solve the Poisson equation subject to open boundaries. This is true for the case in which the pipe radius is much larger than the beam transverse size. When the beam size is not too small, the effects of the conducting beam pipe have to be considered. For simple regular shaped boundary conditions like rectangular/cylindrical pipe, spectral methods utilizing Fourier expansion of the electrostatic potential may be used.

For the z-uniform beam, Poisson equation in 2D Cartesian coordinates is given by:

$$\frac{d^2\phi}{dx^2} + \frac{d^2\phi}{dy^2} = -\frac{\rho(x, y)}{\varepsilon_0} \qquad (7)$$