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IMPROVEMENTS TO PARMILA*

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Summary

PARMILA[1] is an internationally accepted standard for Monte Carlo simulation of linac and transport line performance. We discuss several modifications and improvements to this code. A generalized magnet routine allows the simulation of electrostatic and magnetic quadrupoles, solenoids, sextupoles, and octupoles. Optional inclusion of linear fringe fields and/or geometric aberrations is provided for in the quadrupole transformation. The dipole routine has been replaced with a more accurate algorithm. The accelerating gap transformation has been replaced by a set of implicit equations which accurately describe the relativistic particle behavior in the presence of longitudinal and transverse electric fields described by a set of 6 weighted Fourier moments (transit time factors). A simple model allows these moments, in turn, to be approximated from the cell geometry and the usual T and S functions. A number of added convenience features - interactive disk storage and retrieval of particle coordinates, individual particle input and observations, an interactively callable test for particle longitudinal stability, and an automated quadrupole tuning procedure - all add to the code's versatility, convenience, and strength as a design tool.

Dipoles

In the dipole subroutine, BEND, both the vertical edge focusing and the central region tracking algorithms have been changed. For an edge angle β with vertical focusing, the effect of edge focusing is modeled by the transformation[2]

$$\begin{aligned} x' &= x_0' + (x_0/\rho)\tan\beta \\ y' &= y_0' - (y_0/\rho)\left[\tan\beta - (0.5 + \tan^2\beta)(g/\rho_0)\sec\beta\right] \end{aligned} \tag{1}$$

In Eq. (1), x_0, x_0', y_0, y_0' refer to the initial horizontal position and divergence and vertical position and divergence. The particle radius of curvature, ρ, is the ratio of the rigidity ($B\rho$) to the magnetic field strength (B_0), while ρ_0 is the synchronous particle radius of curvature, and g is the magnet gap.

The transformation in the central region is that used in DECAY TURTLE.[3] For a bend angle ϕ,

$$\begin{aligned} x &= (x_0 + \rho_0)\cos\phi + \rho[\cos\theta_2 - \cos(\theta_1 + \phi)] - \rho_0 \\ x' &= \tan\theta_2 \\ y &= y_0 + y_0'\rho[\phi + \theta_1 - \theta_2]\cos\theta_1 \\ y' &= y_0'\cos\theta_1/\cos\theta_2 \quad , \end{aligned}$$

where

$$\begin{aligned} \theta_1 &= \tan^{-1}(x_0') \\ \sin\theta_2 &= \sin(\theta_1 + \phi) - \left[(x_0 + \rho_0)/\rho_0\right]\sin\phi \quad . \end{aligned} \tag{2}$$

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To extend the generality of effects which can be treated, we have added a coordinate rotation capability to the low energy beam transport (LEBT) routine. A rotation by angle θ about the z axis before the bend and by $-\theta$ after the bend, for example, simulates the effect of a bend at angle θ with respect to the horizontal.

Generalized Beam Optics

A new routine, MAGNET, has been written to allow quite general treatment of the effects of solenoids, magnetic and electrostatic quadrupoles, sextupoles, and octupoles.

Solenoids

The solenoid transformations were taken from Banford.[4] The element is divided into N sections. Entrance and exit fringe transforms

$$\begin{aligned} x' &= x_0' \pm y_0/2\rho \\ y' &= y_0' \mp x_0/2\rho \end{aligned} \tag{3}$$

are applied in the first and last calls. In between, there are N sequential transforms through the constant central field regions

$$\begin{aligned} x' &= x_0'\cos(L/N\rho) + y_0'\sin(L/N\rho) \\ y' &= -x_0'\sin(L/N\rho) + y_0'\cos(L/N\rho) \\ x &= x_0 + x_0'\rho\sin(L/N\rho) + y_0'\rho\left[1 - \cos(L/N\rho)\right] \\ y &= y_0 - x_0'\rho\left[1 - \cos(L/N\rho)\right] + y_0'\rho\sin(L/N\rho) \end{aligned} \tag{4}$$

where L is the solenoid length. Between sections, space charge calculations can be performed.

Quadrupoles

The first order equations of motion in a horizontally focusing quadrupole are

$$\begin{aligned} x'' + K_q x &= 0 \\ y'' - K_q y &= 0 \end{aligned} \tag{5}$$

with

$$K_q = \begin{cases} B'/(B\rho) & \text{for magnetic quad} \\ \gamma q e E'/(\gamma + 1)\,AW & \text{for electrostatic quad} \end{cases} \tag{6}$$

In Eq. (6), B' and E' are the magnetic and electric field gradients, W is the particle kinetic energy per nucleon, and A is the atomic mass number. For constant K_q, the first order solutions to Eq. (5) are well known. In order to allow for a more realistic behavior of K_q, we have added the option for a piecewise linear behavior of $K_q(s)$ over the fringe field regions. Equation (5) may then be solved exactly in terms of Airy functions.[5] The third order expansion of that solution has been implemented.

If third-order geometric aberrations are included, Eqs. (5) become [6]

$$x'' + K_q x = \tfrac{1}{2} K_q \left[-3xx'^2 - xy'^2 + 2x'yy'\right]$$

$$+ K'_q xyy' + \tfrac{1}{4} K''_q (xy^2 + x^3/3) \qquad (7)$$

$$y'' - K_q y = \tfrac{1}{2} K_q \left[3yy'^2 + x'^2 y - 2xx'y'\right]$$

$$- K'_q xx'y - \tfrac{1}{4} K''_q (x^2 y + y^3/3)$$

Equation (7) is solved approximately by treating the right hand side as a small perturbation on the orbits predicted by Eq. (5). A Green's function integral approach is used. For example, the perturbation Δx obtained in passage through a short section, L, of magnet is approximated as

$$\Delta x = L \int_0^L f_x(s)\, ds - \int_0^L s\, f_x(s)\, ds \qquad (8)$$

and $\Delta x' = d(\Delta x)/dL$. Results in the y plane follow with $K_q \rightleftarrows -K_q$ and $x \rightleftarrows y$. The force terms f_x are the right hand side of Eq. (7) with $x = x_0 + sx'_0$, $y = y_0 + sy'_0$, $x' = x'_0$, and $y' = y'_0$.

Sextupoles and Octupoles

Higher order magnetic multipoles are treated as pure, hard-edged fields. The magnetic field of a 2(n+1) order multipole is

$$\underset{\sim}{B} = \left[B_0\, a/(n+1)\right] \underset{\sim}{\nabla} (r/a)^{n+1} \sin (n+1)\, \theta \qquad (9)$$

where B_0 is the pole-tip field at radius a, and (r,θ) are the cylindrical transverse coordinates. The coordinate transformation is then given as a drift length plus a perturbation, i.e., $x = x_0 + Lx'_0 + \Delta x$ with Δx obtained as in Eq. (8). For a sextupole, $f_x(s) = K_s(x^2 - y^2)$, $f_y(s) = 2K_s xy$ with $K_s = B_0/(B\rho a^2)$; the octupole forces are $f_x(s) = -K_0 x\,(3y^2 - x^2)$ and $f_y(s) = K_0 y\,(3x^2 - y^2)$ with $K_0 = B_0/(B\rho a^3)$.

Gap Transformation

In an accelerator gap, particles follow an orbit through a nonlinear space- and time-dependent electric field. PARMILA models this process by a series of three transformations: a free (unaccelerated) drift to the gap center, a single point transformation, and another free drift. A lack of documentation for the "as received" point transformation has led us to carry out a detailed, self-consistent derivation. The resulting algorithm differs from that supplied with PARMILA.

We use the following physical approximations:

1) The effective electric field which causes particle acceleration is

$$E_z(z,\underset{\sim}{r}) = \left[1 + (\pi r/\beta_s \lambda)^2\right] E_z^0(z)$$
$$\underset{\sim}{E}_t(z,\underset{\sim}{r}) = -\tfrac{1}{2}\, \underset{\sim}{r}\, (\partial/\partial z)\, E_z^0 \qquad (10)$$

2) In small correction terms, the particle velocity, β, may be replaced by $\bar{\beta} = \tfrac{1}{2}(\beta_{in} + \beta_{out})$.

3) The point transformation at the gap center, expressed in terms of the particle coordinates there, is unaffected by the presence of space charge or focusing.

The relativistic equations of motion, in the absence of space charge or focusing, are

$$dW/dz = (q/A)eE_z\left[z, \underset{\sim}{r}(z)\right] \cos\left[\frac{2\pi}{\lambda}\int_0^z \frac{d\xi}{\beta(\xi)} + \phi_0\right]$$

$$d\phi/dz = (2\pi/\lambda)\,(\beta^{-1} - \beta_s^{-1}) \qquad (11)$$

$$(d/dz)\,(\beta\gamma\, d\underset{\sim}{r}/dz) = (qe/Am\beta c^2)\, \underset{\sim}{E}_t\left[z, \underset{\sim}{r}(z)\right]$$
$$\times \cos\left[\frac{2\pi}{\lambda}\int_0^z \frac{d\xi}{\beta(\xi)} + \phi_0\right]$$

In Eq. (11), W is the particle kinetic energy per nucleon, ϕ is its phase, $\underset{\sim}{r}(z)$ its transverse displacement when it reaches longitudinal position z. The particle velocity is βc, $\beta_s c$ is the synchronous velocity, λ is the wavelength of the rf accelerating field, and ϕ_0 the particle phase at the gap center.

Using the approximations above, these equations can be integrated through a linac cell extending from $z = -\ell_1$ to $z = \ell_2$ with $z = 0$ at the gap center. In the absence of space charge and focusing, we find

$$\phi_{out} = \phi_{in} + \ell_1 \phi'_{in} + \ell_2 \phi'_{out} + C\Big[T'(\sin\phi_s - \sin\phi_0) + S'(\cos\phi_s - \cos\phi_0)\Big]$$

$$W_{out} = W_{in} + (q/A)\, eV_g \Big\{\Big[T - 2\pi(\bar{\beta}_s/\bar{\beta} - 1)\, T' + (\pi r_0/\bar{\beta}_s\lambda)^2\, T - (2\pi^2/\bar{\beta}_s\lambda)\, \underset{\sim}{r}_0 \cdot \underset{\sim}{r}'_0\, S'\Big] \cos\phi_0$$
$$+ \Big[S + 2\pi(\bar{\beta}_s/\bar{\beta} - 1)\, S' + (\pi r_0/\bar{\beta}_s\lambda)^2\, S - (2\pi^2/\bar{\beta}_s\lambda)\, \underset{\sim}{r}_0 \cdot \underset{\sim}{r}'_0\, T'\Big] \sin\phi_0\Big\}$$

$$\begin{pmatrix} \underset{\sim}{r}_{out} \\ \underset{\sim}{r}'_{out} \end{pmatrix} = \begin{pmatrix} 1 & \ell_2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \dfrac{(1-\frac{1}{2}\mathcal{A})^2 + \frac{1}{4}\mathcal{B}\mathcal{C}}{\mathcal{D}} & (\beta\gamma)_{in}\, \dfrac{\mathcal{C}}{\mathcal{D}} \\ \left(\dfrac{1}{\beta\gamma}\right)_{out} \dfrac{\mathcal{B}}{\mathcal{D}} & \dfrac{(\beta\gamma)_{in}}{(\beta\gamma)_{out}}\, \dfrac{(1+\frac{1}{2}\mathcal{A})^2 + \frac{1}{4}\mathcal{B}\mathcal{C}}{\mathcal{D}} \end{pmatrix}$$
$$\times \begin{pmatrix} 1 & \ell_1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \underset{\sim}{r}_{in} \\ \underset{\sim}{r}'_{in} \end{pmatrix}$$

where

$$C = 2\pi qeV_g / Am\bar{\beta}_s^2\, \bar{\gamma}_s^3\, c^2$$

$$\mathcal{A} = (qeV_g/Am\bar{\beta}^2\, \bar{\gamma}\, c^2)\Big\{\Big[T - 2\pi(\bar{\beta}_s/\beta)\, T'\Big] \cos\phi_0 + \Big[S + 2\pi(\bar{\beta}_s/\bar{\beta})\, S'\Big] \sin\phi_0\Big\}$$

$$\mathcal{B} = (\pi qeV_g/Am\bar{\beta}^2 c^2 \lambda)\Big\{\Big[S + 2\pi(\bar{\beta}_s/\bar{\beta} - 1)\, S'\Big] \times \cos\phi_0 - \Big[T - 2\pi(\bar{\beta}_s/\bar{\beta} - 1)\, T'\Big] \sin\phi_0\Big\}$$

$$\mathcal{C} = -(qeV_g\lambda/Am\bar{\beta}^2\bar{\gamma}^2 c^2)\Big[S' \cos\phi_0 + T' \sin\phi_0\Big]$$

$$\mathcal{D} = 1 - \tfrac{1}{4}(A^2 + \mathcal{B}\mathcal{C}) \tag{12}$$

Eqs. (12) are an implicit transformation since they involve, e.g., the gap-center values

$$\phi_o = \phi_{in} + \ell_1 \phi'_{in} + C\left[T'_{\frac{1}{2}}(\sin\phi_s - \sin\phi_o) + S'_{\frac{1}{2}}(\cos\phi_s - \cos\phi_o)\right] \tag{13}$$

$$\underset{\sim}{r}_o = \tfrac{1}{2}(\underset{\sim}{r}_{in} + \ell_1 \underset{\sim}{r}'_{in} + \underset{\sim}{r}_{out} - \ell_2 \underset{\sim}{r}'_{out})$$

$$\bar{\beta}\bar{\gamma}\,\underset{\sim}{r}'_o = \tfrac{1}{2}\left[(\beta\gamma)_{in}\underset{\sim}{r}'_{in} + (\beta\gamma)_{out}\underset{\sim}{r}'_{out}\right] .$$

In these expressions, V_g is the voltage across the gap, while the transit time factors are

$$\begin{aligned}
T &= V_g^{-1}\int_{-\ell_1}^{\ell_2} E_z^o \cos\omega t_s(z)\,dz \\
S &= -V_g^{-1}\int_{-\ell_1}^{\ell_2} E_z^o \sin\omega t_s(z)\,dz \\
T' &= V_g^{-1}\int_{-\ell_1}^{\ell_2} (z/\beta_s\lambda)\,E_z^o \sin\omega t_s(z)\,dz \\
S' &= -V_g^{-1}\int_{-\ell_1}^{\ell_2} (z/\beta_s\lambda)\,E_z^o \cos\omega t_s(z)\,dz \\
T'_{\frac{1}{2}} &= V_g^{-1}\int_{-\ell_1}^{0} (z/\beta_s\lambda)\,E_z^o \sin\omega t_s(z)\,dz \\
S'_{\frac{1}{2}} &= -V_g^{-1}\int_{-\ell_1}^{0} (z/\beta_s\lambda)\,E_z^o \cos\omega t_s(z)\,dz \quad ,
\end{aligned} \tag{14}$$

where

$$t_s(z) = c^{-1}\int_0^z d\xi/\beta_s(\xi) \quad .$$

A simple parametric model

$$E_z^o = (a + b\,z)\,\Theta(z_1 - |z|) \tag{15}$$

may be used to approximate T', S', $T'_{\frac{1}{2}}$, and $S'_{\frac{1}{2}}$ in terms of T and S. Here, Θ is the Heaviside step function, while a, b, z_1 are parameters to be fit to V_g, T, and S.

Convenience Features

PARMILA is being used to optimize ANL's heavy ion fusion test bed program, especially in the design of low-beta linacs and final transport systems. We have added a number of features (coordinate storage, individual particle I/O, tests for longitudinal stability and automated tuning) to facilitate interactive parameter variation and testing.

Coordinate Storage

Coordinate storage is useful if one wishes to use the beam coordinates at some point in a system as the starting coordinates in iteratively studying a succeeding section of that system. A command has been added which replaces the initial coordinate array, COR, with the contents of the final array CORD. The initial coordinates may first be stored on - and later recalled from - disk memory.

Individual Particle I/O

Individual particle coordinate input and observation is often useful; a few rays carefully placed in phase space can characterize the entire beam behavior. We have added the capability to explicitly enter the initial ray coordinates and to observe the final coordinates at the interactive terminal.

Test for Longitudinal Stability

From the approximate longitudinal equation of motion of a particle under constant average accelerating field and in the presence of space charge forces, it is easy to show [7] that ϕ will execute stable oscillations provided

$$\phi_2 \leq \phi \leq \phi_1$$

and

$$|W - W_s| \leq \left[-(qeE/2\pi A)\sin\phi_s\,\beta^3\gamma^3\lambda mc^2\,(1-k)\right]^{\frac{1}{2}} \times \left[(\phi_1 - \phi_s)^2 - (\phi - \phi_s)^2 + \frac{(\phi_1 - \phi_s)^3 - (\phi - \phi_s)^3}{3(1-k)\phi_s}\right]^{\frac{1}{2}}$$

where

$$\begin{aligned}
\phi_1 &= -(1 - 2k)\,\phi_s \\
\phi_2 &= (2 - k)\,\phi_s
\end{aligned} \tag{16}$$

In Eq. (16), ϕ_s and W_s are the synchronous phase and kinetic energy, and k is the ratio of space charge to gap defocusing forces. A command has been added which checks all particles according to the criteria in Eq.(16). The average accelerating field and the beam current and shape (used to determine k) are optionally either input with the command or calculated from the next cell description and the rms beam parameters.

Automated Tuning

Our technique for optimizing the quadrupole gradients in a linac is to force the rms emittance ellipses in the x-x' and the y-y' planes to make equal but opposite tilt angles with the x and y axes at the "neutral" positions midway between horizontally and vertically focusing magnets. A Newton's method interactive search has been implemented to find the gradient values which satisfy this criterion.

References

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