

LhARA linear optics documentation

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1 Introduction

The LhARA [1, 2] linear optics package was written to allow rapid calculations to initiate more detailed studies of the LhARA beam lines and to be used as a tool to check issues as they arise. The package has been written in Python so that it is accessible and can readily be updated, modified and maintained. At present the code treats proton beams only.

The documentation presented here is designed to present the approximations and notation in a consistent form and to summarise the module, class and data structures that have been adopted.

2 Coordinate systems

2.1 Laboratory coordinate system

The origin of the LhARA coordinate system, the “laboratory coordinate system” or “laboratory reference frame”, is at the position of the laser focus at the laser-target interaction point. The z axis is horizontal and parallel to the nominal capture axis, pointing in the downstream direction. The y axis points vertically upwards and the x axis completes a right-handed orthogonal coordinate system.

Unit vectors along the x , y and z axes are \mathbf{i} , \mathbf{j} and \mathbf{k} respectively. The position of the reference particle, its momentum and energy are described as functions of the distance it has travelled from the origin of coordinates to its current position. The distance the reference particle has travelled is defined to be s , making the position, \mathbf{r}_0 , momentum, \mathbf{p}_0 , and energy, E_0 , of the reference particle at position s :

$$\begin{aligned} \mathbf{r}_0 &= \mathbf{r}_0(s); \\ \mathbf{p}_0 &= \mathbf{p}_0(s); \text{ and} \\ E_0 &= E_0(s). \end{aligned} \tag{1}$$

The magnitude of the reference particle velocity is v_0 and the relativistic parameters that determine the reference particle energy and momentum are:

$$\begin{aligned} \beta_0 &= \frac{v_0}{c}; \text{ and} \\ \gamma_0 &= \frac{1}{\sqrt{1 - \beta_0^2}}; \end{aligned}$$

where c is the speed of light. The time, t , at which the reference particle is at s is also a function of s :

$$t = t(s) = \frac{s}{v_0} = \frac{s}{c} \frac{E_0}{cp_0}; \tag{2}$$

where $p_0 = |\mathbf{p}_0|$.



Figure 1: Reference particle local coordinate system. The trajectory of the reference particle is shown as the red line. The distance the reference particle has travelled, measured from the origin of coordinates in the laboratory frame, is labelled s . The origin of the “reference particle local coordinate (RPLC) system is coincident with the position of the reference particle. The directions of unit vectors along each of three righthanded, orthogonal coordinate axes are shown as black arrows labelled i_r , j_r , and k_r .

2.2 Reference particle local coordinate system

A coordinate system defined relative to the position of the reference particle, the “reference particle local coordinate” (RPLC) system, may be defined using the direction in which the particle is travelling. The position of the particle defines the origin of the RPLC system, see figure 1. The tangent to the reference particle trajectory at s defines the z_r axis with unit vector k_r . In the laboratory frame, the presence of local electric or magnetic fields may cause the reference particle’s trajectory to change. In the neighbourhood of the particle, the curved trajectory may be described in terms of an arc of a circle. The x_r axis (with unit vector i_r) is then taken to be in the direction pointing away from the centre of the circle. The third coordinate axis, y_r , is defined to complete the right-handed orthogonal coordinate system; the unit vector along the y_r axis being given by $j_r = k_r \times i_r$.

The trajectory of the reference particle is a straight line as it traverses a drift space and a variety of beam-line elements. Examples of such beam-line elements include solenoids, quadrupoles, etc. The reference trajectory is also undeviated by passage through an accelerating cavity placed such that the accelerating field is parallel to the reference-particle trajectory.

The RPLC coordinate system at $s = 0$ is taken to coincide with the laboratory coordinate system. Beam-line elements are placed sequentially along the trajectory of the reference particle. The RPLC system at the entrance to a particular beam-line element is taken to coincide with the RPLC system defined at the exit of the beam-line

element after which it is placed.

40 2.3 Transforming to and from reference particle local coordinates to laboratory co-ordinates

In the RPLC system, the trajectory of the reference particle, \mathbf{R}_0 , is:

$$\mathbf{R}_0(s) = \mathbf{0}. \quad (3)$$

The position of a test particle in the RPLC frame, \mathbf{R} , is described with reference to the position of the reference particle. In the laboratory frame, the position of the test particle is:

$$\mathbf{r}(s) = \mathbf{r}_0(s) + \delta\mathbf{r}(s); \quad (4)$$

where:

$$\delta\mathbf{r}(s) = \underline{\underline{R}}(s)\mathbf{R}(s); \text{ and} \quad (5)$$

$\underline{\underline{R}}(s)$ is a rotation matrix that takes the RPLCs at s to the laboratory frame coordinates.

In the laboratory frame, the unit vectors \mathbf{i}_r , \mathbf{j}_r and \mathbf{k}_r are given by:

$$\begin{aligned} \mathbf{i}_r &= \begin{pmatrix} i_{rx} \\ i_{ry} \\ i_{rz} \end{pmatrix}; \\ \mathbf{j}_r &= \begin{pmatrix} j_{rx} \\ j_{ry} \\ j_{rz} \end{pmatrix}; \text{ and} \\ \mathbf{k}_r &= \begin{pmatrix} k_{rx} \\ k_{ry} \\ k_{rz} \end{pmatrix}. \end{aligned} \quad (6)$$

The rotation matrix, $\underline{\underline{R}}$, may now be written:

$$\underline{\underline{R}}(s) = \begin{bmatrix} i_{rx} & j_{rx} & k_{rx} \\ i_{ry} & j_{ry} & k_{ry} \\ i_{rz} & j_{rz} & k_{rz} \end{bmatrix}. \quad (7)$$

3 Phase space and trace space

45 The motion of particles passing through an accelerator is most often described using classical Hamiltonian mechanics; quantum mechanics being required only in particular cases such as the description of spin polarisation in a storage ring. In classical Hamiltonian mechanics the equations of motion are solved to give the evolution of the position, momentum, and energy as functions of a single independent parameter. The independent parameter is often taken to be time.

50 Relativistic mechanics exploits four-vector position, $\underline{\mathcal{R}} = (r, ct)$, and four-vector momentum $\underline{\mathcal{P}} = (c\mathbf{p}, E)$. In the Hamiltonian description of particle dynamics, these four vectors become functions of the independent variable, i.e. $\underline{\mathcal{R}} = \underline{\mathcal{R}}(t)$ and $\underline{\mathcal{P}} = \underline{\mathcal{P}}(t)$. In the laboratory system, the position of the reference particle along its trajectory is directly related to the time coordinate by $t = c\beta_0 s$. This allows s to be taken as the independent variable and for the motion of particles in the beam to be derived as function of s .

55 The 6D phase-space coordinates of a particle as a function of s are given by the position and momentum three vectors. The particle energy may be determined from the invariant mass and the time coordinate from the invariant interval between the origin and the the position represented by s .

The “trace-space” coordinates of a particle are defined relative to the reference particle. Usually, a beam is understood to contain particles which follow trajectories that differ rather little from that of the reference particle. Trace space is defined such that the position, “momentum”, and “energy” coordinates are small for particles which follow trajectories close to that of the reference particle. The utility of this approach is that trace-space coordinates may be used to perform Taylor expansions of the Hamiltonian which may readily be solved to yield a description of particle transport using functions that are linear in the trace-space coordinates.

The notation used for the 6D phase and trace spaces are defined in this section.

65 3.1 Phase space

The 6D phase-space vector is defined in terms of the three-vector position and three vector momentum as:

$$\begin{bmatrix} \mathbf{r} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \\ \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} \end{bmatrix} \quad (8)$$

The trajectory of the particle may be evaluated as a function of time or s .

3.2 Trace space

Trace space is defined to simplify the calculation of the trajectory of particles through the accelerator lattice and is derived from the phase space expressed in the RPLC frame. Consider a particle with position $(x_{\text{RPLC}}, y_{\text{RPLC}}, z_{\text{RPLC}})$ and momentum p_{RPLC} with components $(p_{x\text{RPLC}}, p_{y\text{RPLC}}, p_{z\text{RPLC}})$. Taking the momentum of the reference particle in the laboratory frame to be p_0 , the trace-space coordinates are given by:

$$\phi = \begin{pmatrix} x_{\text{RPLC}} \\ x'_{\text{RPLC}} \\ y_{\text{RPLC}} \\ y'_{\text{RPLC}} \\ z_{\text{RPLC}} \\ \delta_{\text{RPLC}} \end{pmatrix}; \quad (9)$$

where:

$$x'_{\text{RPLC}} = \frac{\partial x}{\partial s} = \frac{cp_{x\text{RPLC}}}{cp_0}; \quad (10)$$

$$y'_{\text{RPLC}} = \frac{\partial y}{\partial s} = \frac{cp_{y\text{RPLC}}}{cp_0}; \quad (11)$$

$$z_{\text{RPLC}} = \frac{s}{\beta_0} - ct = \frac{\Delta s}{\beta_0}; \text{ and} \quad (12)$$

$$\delta_{\text{RPLC}} = \frac{E}{cp_0} - \frac{1}{\beta_0} = \frac{\Delta E}{cp_0}. \quad (13)$$

Here $\Delta s = s - s_0$ and $\Delta E = E - E_0$, where s_0 and E_0 are the reference particle position and energy respectively; E and s are the energy and position of a particular particle in the beam.

4 Transfer matrices

A beam line may be described as a series of beam-line elements arranged one after the other. The problem of transporting a particle through the beam line may then be carried out as a series of steps through each of the elements in turn. Taking advantage of the trace space defined above, the transport of a particle across a particular beam-line element may be described in terms of a linear transformation:

$$\phi_{\text{end}} = \underline{\underline{T}} \phi_{\text{start}} ; \quad (14)$$

where ϕ_{start} is the trace-space vector at the start of the beam-line element and ϕ_{end} is the transformed trace-space vector at the end. The step across the beam-line element implies an increment, δs , to the s -coordinate given by:

$$s_{\text{end}} = s_{\text{start}} + \delta s ; \quad (15)$$

where s_{start} and s_{end} are the coordinate along the reference particle trajectory at the start and end of the beam-line element respectively. There are many excellent descriptions of the derivation of the transfer matrices, $\underline{\underline{T}}$, so only the results are quoted here. The notation used below is developed from that used in [3].

75 4.1 Drift

A “drift” space refers to a region in which the beam propagates in the absence of any electromagnetic fields. In a drift, particles propagate in straight lines, therefore:

$$\underline{\underline{T}}_{\text{drift}} = \begin{pmatrix} 1 & l & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & l & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{l}{\beta_0^2 \gamma_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} ; \quad (16)$$

where l is the length of the drift. The increment in the reference particle trajectory is:

$$\delta s = l . \quad (17)$$

4.2 Quadrupole

The passage of a beam particle through a quadrupole magnet may be described by specifying the field gradient, g , within the magnet and the length, l_q , of the quadrupole measured along its axis. The impact of a quadrupole on the trajectory of a particle in the xy plane is independent of the impact of the magnet on the particle's trajectory in the yz plane. In this sense quadrupole focusing in the xz and yz planes is said to be “uncoupled”.

If the field gradient along the x and y axes is identical, then:

$$g_x = \frac{\partial B_{qx}}{\partial x} = g_y = \frac{\partial B_{qy}}{\partial y} = g ; \quad (18)$$

where the field in the quadrupole, \mathbf{B}_q , has components $(B_{qx}, B_{qy}, 0)$.

In the “hard-edge” approximation, where the field falls to zero at the start and end of the quadrupole, the transfer matrix for a quadrupole focusing in the xz plane (a “focusing quadrupole”) may be written:

$$\underline{T}_{\text{Fquad}} = \begin{pmatrix} \cos(\sqrt{k_q}l_q) & \frac{\sin(\sqrt{k_q}l_q)}{\sqrt{k_q}} & 0 & 0 & 0 & 0 \\ -\sqrt{k_q}\sin(\sqrt{k_q}l_q) & \cos(\sqrt{k_q}l_q) & 0 & 0 & 0 & 0 \\ 0 & 0 & \cosh(\sqrt{k_q}l_q) & \frac{\sinh(\sqrt{k_q}l_q)}{\sqrt{k_q}} & 0 & 0 \\ 0 & 0 & \sqrt{k_q}\sinh(\sqrt{k_q}l_q) & \cosh(\sqrt{k_q}l_q) & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{l_q}{\beta_0^2\gamma_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}; \quad (19)$$

where:

$$k_q = \frac{gc}{p} \times 10^{-3}, \quad (20)$$

and c is the speed of light in metres per second, p is the magnitude of the momentum of the particle in MeV/c, and the field gradient, g , is given in T/m. As before, β_0 is the relativistic velocity of the reference particle and $\gamma_0 = (1 - \beta_0^2)^{-\frac{1}{2}}$. The increment in the reference particle trajectory is:

$$\delta s = l_q. \quad (21)$$

It is important to include a description of the effect of dispersion on beam transport through the LhARA beam line since the laser-driven proton and ion source provides a broad energy spectrum. Reference [3] provides two methods for the description of dispersion in a linear approximation. The first is to use the reference momentum to calculate the quadrupole focusing strength ($k_{0q} = \frac{gc}{p_0} \times 10^{-3}$) and to include terms in the expressions for x , x' , y , and y' dependent on δ . The second is to use equation 20 to calculate the effective quadrupole focusing strength. The second approach has been adopted here.

In the same notation, the transfer matrix for a quadrupole focusing in the yz plane (a “defocusing quadrupole”) may be written:

$$\underline{T}_{\text{Dquad}} = \begin{pmatrix} \cosh(\sqrt{k_q}l_q) & \frac{\sinh(\sqrt{k_q}l_q)}{\sqrt{k_q}} & 0 & 0 & 0 & 0 \\ \sqrt{k_q}\sinh(\sqrt{k_q}l_q) & \cosh(\sqrt{k_q}l_q) & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos(\sqrt{k_q}l_q) & \frac{\sin(\sqrt{k_q}l_q)}{\sqrt{k_q}} & 0 & 0 \\ 0 & 0 & -\sqrt{k_q}\sin(\sqrt{k_q}l_q) & \cos(\sqrt{k_q}l_q) & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{l_q}{\beta_0^2\gamma_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (22)$$

4.3 Solenoid

The trajectory of a beam particle through a solenoid is determined by the magnetic field strength, \mathbf{B}_s , within the solenoid and the length of the solenoid, l_s , measured along its axis. As the particle enters the solenoid, the fringe field imparts momentum transverse to the axis of the magnet. This results in the particle executing a helical trajectory, the axis of the helix being parallel to the solenoid axis. The sense of the rotation depends on the particle charge and the polarity of the field. The helical motion means that the evolution of the particle motion in the xz plane is coupled with the evolution of the particle motion in the yz plane.

In the “hard-edge” approximation, the magnetic field inside the magnet is given by $\mathbf{B}_s = (0, 0, B_{s0})$, where the solenoid axis lies along the z_{RPLC} axis. The solenoid field strength parameter is then given by:

$$k_s = \left[\frac{B_{s0}c}{2p} \times 10^{-3} \right]^2; \quad (23)$$

95 where B_{s0} is measured in T, p in MeV/c and c in m/s.

The transfer matrix for passage of a positive particle through a solenoid with field pointing in the positive z_{RPLC} direction may be written:

$$\underline{T}_{\text{Sol}} = \begin{pmatrix} \cos^2(\sqrt{k_s}l_s) & \frac{1}{2\sqrt{k_s}} \sin(\sqrt{k_s}l_s) & \frac{1}{2} \sin(2\sqrt{k_s}l_s) & \frac{1}{\sqrt{k_s}} \sin^2(\sqrt{k_s}l_s) & 0 & 0 \\ -\frac{\sqrt{k_s}}{2} \sin(2\sqrt{k_s}l_s) & \cos^2(\sqrt{k_s}l_s) & -\sqrt{k_s} \sin^2(\sqrt{k_s}l_s) & \frac{1}{2} \sin(2\sqrt{k_s}l_s) & 0 & 0 \\ -\frac{1}{2} \sin(2\sqrt{k_s}l_s) & -\frac{1}{\sqrt{k_s}} \sin^2(\sqrt{k_s}l_s) & \cos^2(\sqrt{k_s}l_s) & \frac{1}{2\sqrt{k_s}} \sin(2\sqrt{k_s}l_s) & 0 & 0 \\ \sqrt{k_s} \sin^2(\sqrt{k_s}l_s) & -\frac{1}{2} \sin(2\sqrt{k_s}l_s) & -\frac{\sqrt{k_s}}{2} \sin(2\sqrt{k_s}l_s) & \cos^2(\sqrt{k_s}l_s) & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{l}{\beta_0^2 \gamma_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (24)$$

As in the case of the quadrupoles, dispersion is accounted for using equation 23. The increment in the reference particle trajectory is:

$$\delta s = l_s. \quad (25)$$

4.4 Non-neutral (electron) plasma (Gabor) lens

A dense gas of electrons confined in a Penning-Malmberg trap provides an electric field that can be used to focus a positive ion beam. The electron gas is confined axially in the lens by an electrostatic potential created using a central anode of length l_G . The gas is confined radially using the uniform field of a solenoid. Assuming a uniform electron density, n_e , the focusing parameter, k_G , may be written:

$$k_G = \frac{e}{2\epsilon_0} \frac{m_p \gamma}{p^2} n_e; \quad (26)$$

100 where e is the charge on the electron, ϵ_0 is the permittivity of free space, and m_p is the proton mass. As in the case of the quadrupoles and solenoid, dispersion is accounted for using equation 26. The force on a particle passing through the electron gas is towards the axis of the lens and is proportional to the radial distance of the particle from the axis. Focusing is therefore cylindrically symmetric and does not couple motion in the the xz and yz planes.

In the “hard-edge” approximation, the electric field inside the lens falls to zero at the end of the electron gas and the contribution of the magnetic field used to confine the electron gas in the transverse direction has a negligible effect on particles passing through the lens. The transfer matrix for passage of a positive particle through the lens may be written:

$$\underline{T}_G = \begin{pmatrix} \cos(\sqrt{k_G}l_G) & \frac{\sin(\sqrt{k_G}l_G)}{\sqrt{k_G}} & 0 & 0 & 0 & 0 \\ -\sqrt{k_G} \sin(\sqrt{k_G}l_G) & \cos(\sqrt{k_G}l_G) & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos(\sqrt{k_G}l_G) & \frac{\sin(\sqrt{k_G}l_G)}{\sqrt{k_G}} & 0 & 0 \\ 0 & 0 & -\sqrt{k_G} \sin(\sqrt{k_G}l_G) & \cos(\sqrt{k_G}l_G) & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{l}{\beta_0^2 \gamma_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (27)$$

The increment in the reference particle trajectory is:

$$\delta s = l_G. \quad (28)$$

4.5 Dipole

The reference particle trajectory in the beam-line elements described above passes along the axis of the element. In contrast, a dipole bends the reference trajectory so that it describes the arc of a circle (see figure 2). The



Figure 2: Schematic representation of the passage of the reference particle through a sector dipole. The outline of the sector dipole is shown by the solid black lines. The trajectory of the reference particle is shown as the dashed line. The length of the reference-particle trajectory inside the field of the sector dipole is l_D . The x_{RPLC} and z_{RPLC} coordinate axes at the entry and exit of the sector dipole are shown. The radius of curvature of the reference particle-trajectory trajectory inside the magnet is ρ and the angle through which the x_{RPLC} is rotated is ϕ .

code provides for the transport through a “sector dipole” in the hard-edge approximation. In this case, the field within the magnet is taken to be constant and parallel to \hat{j}_{RPLC} , i.e. $\mathbf{B}_D = (0, B_{D0}, 0)$. No edge focusing is considered.

The passage of particles through a dipole may be described by defining the parameter, k_D :

$$k_D = \left[\frac{B_{D0}c}{p} \times 10^{-3} \right]^2. \quad (29)$$

The momentum of the reference particle is related to the curvature. ρ , by:

$$p_0 = B_{D0}\rho; \quad (30)$$

so:

$$k_D = \frac{1}{\rho}; \quad (31)$$

and the angle ϕ is given by:

$$\phi = \frac{l}{\rho}. \quad (32)$$

With these definitions the transfer matrix for passage through a dipole may be written:

$$\underline{T}_D = \begin{pmatrix} \cos(\phi) & \rho \sin(\phi) & 0 & 0 & 0 & \frac{\rho}{\beta_0} (1 - \cos(\phi)) \\ -\frac{\sin(\phi)}{\rho} & \cos(\phi) & 0 & 0 & 0 & \frac{\sin(\phi)}{\beta_0} \\ 0 & 0 & 1 & l & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -\frac{\sin(\phi)}{\beta_0} & -\frac{\rho}{\beta_0} (1 - \cos(\phi)) & 0 & 0 & 1 & \frac{l}{\beta^2 \gamma^2} - \frac{l - \rho \sin(\phi)}{\beta_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (33)$$

The increment in the reference particle trajectory is:

$$\delta s = l_D . \quad (34)$$

5 Source

A variety of options for the generation of the particle distribution at source are included in the package (see section ??). The principal, and the default, option is the target-normal sheath acceleration (TNSA) model presented in [4]. This model is summarised in this section.

5.1 Energy distribution

The typical kinetic energy spectrum produced in target-normal sheath acceleration falls rapidly with kinetic energy before dropping rapidly to zero above a maximum “cut off” energy ε_{\max} . The model kinetic-energy spectrum of the TNSA model presented in [4] is given by:

$$\frac{dN}{d\varepsilon} = \frac{n_{e0}c_s t_{laser} S_{sheath}}{\sqrt{2\varepsilon} T_e} \exp\left(-\sqrt{\frac{2\varepsilon}{T_e}}\right); \quad (35)$$

where N is the number of protons or ions produced per unit solid angle, ε is the ion kinetic energy in Joules, n_{e0} and T_e are the hot electron density and temperature respectively, c_s is the ion-acoustic velocity, t_{laser} is the duration of the laser pulse, and S_{sheath} is the effective area over which the TNSA mechanism takes place. The variables and the units in which they are expressed are presented in table 1.

Equation 35 is based on time-limited fluid models which are unable to predict the cut-off kinetic energy, ε_{\max} , accurately. The cut-off kinetic energy is taken to be that given by the model described in [5] where the time over which the laser pulse creates the conditions necessary for acceleration. The kinetic energy cut-off is given by:

$$\varepsilon_{max} = X^2 \varepsilon_{i,\infty}; \quad (36)$$

where X is obtained by solving:

$$\frac{t_{laser}}{t_0} = X \left(1 + \frac{1}{2} \frac{1}{1 - X^2} \right) + \frac{1}{4} \ln \left(\frac{1 + X}{1 - X} \right); \quad (37)$$

where t_0 is the time over which the ion acceleration may be treated as ballistic and $\varepsilon_{i,\infty}$ is given in table 1.

To generate the kinetic energy spectrum, the probability density function, $g(\varepsilon)$, is defined such that the probability, $\delta\mathcal{P}$, of a particle being generated in the interval $\varepsilon \rightarrow \varepsilon + \delta\varepsilon$ is given by:

$$\delta\mathcal{P} = g(\varepsilon) \delta\varepsilon. \quad (38)$$

$g(\varepsilon)$ can be written in terms of the differential spectrum given in equation 35 through the introduction of a normalisation constant \mathcal{N} :

$$g(\varepsilon) = \frac{1}{\mathcal{N}} \frac{dN}{d\varepsilon}. \quad (39)$$

The cumulative distribution function, $G(\varepsilon)$, is given by:

$$G(\varepsilon) = \int_0^{\varepsilon_{\max}} g(\varepsilon) d\varepsilon; \quad (40)$$

where the normalisation constant, \mathcal{N} , is set so that $G(\varepsilon_{\max}) = 1$. Carrying out the integration yields:

$$G(\varepsilon) = \frac{2}{\mathcal{N}} \frac{n_{e0}c_s t_{laser} S_{sheath}}{\sqrt{2T_e}} \sqrt{\frac{T_e}{2}} \left[1 - \exp\left(-\sqrt{\frac{2\varepsilon}{T_e}}\right) \right]. \quad (41)$$

Table 1: Parameters present in the TNSA analytical equation 35.

Parameter	Definition	Value	Unit
N	Ion number	-	-
ε	Ion kinetic energy	-	J
n_{e0}	Hot electron density	$\frac{N_E}{ct_{laser} S_{sheath}}$	pp/m^3
N_e	Accelerated electron number	$\frac{f E_{laser}}{T_e}$	-
E_{laser}	Laser energy	70	J
f	Energy conversion efficiency	$1.2 \times 10^{-15} I^{0.75}$, max=0.5	-
I	Laser intensity	4×10^{20}	W/cm^2
T_e	Hot electron temperature	$m_e c^2 [\sqrt{1 + \frac{I \lambda^2}{1.37 \times 10^{18}}} - 1]$	J
m_e	Electron mass	9.11×10^{-31}	Kg
c	Speed of light	3×10^8	m/s
λ	Laser wavelength	0.8	μm
t_{laser}	Laser pulse duration	28×10^{-15}	s
B	Radius of electron bunch	$B = r_0 + d \tan(\theta)$	m
S_{sheath}	Electron acceleration area	πB^2	m^2
r_0	Laser spot radius	$\sqrt{\frac{P_{laser}}{I \pi}}$, I in W/m^2	m
d	Target thickness	$400 - 600 \times 10^{-9}$	m
θ	Electron half angle divergence	0.436	rad
P_{laser}	Laser power	2.5×10^{15} , $P_{laser} = \frac{E_{laser}}{t_{laser}}$	W
c_s	Ion-acoustic velocity	$(\frac{Z k_B T_e}{m_i})^{\frac{1}{2}}$	m/s
Z	Ion charge number	1	-
k_B	Boltzmann constant	1.380649×10^{-23}	$m^2 kg s^{-2} K^{-1}$
m_i	Proton mass	1.67×10^{-27}	Kg
P_R	Relativistic power unit	$\frac{m_e c^2}{r_e} = 8.71 \times 10^9$	W
r_e	Electron radius	2.82×10^{-15}	m
$\varepsilon_{i,\infty}$	Maximum ion kinetic energy	$2Z m_e c^2 \sqrt{\frac{f P_{laser}}{P_R}}$	MeV
t_0	Ballistic time	$\frac{B}{v(\infty)}$	s
$v(\infty)$	Ballistic velocity	$\sqrt{\frac{2\varepsilon_{i,\infty}}{m_i}}$	m/s

The kinetic energy spectrum may now be obtained by choosing a value for ε using a probability distribution uniform over the range $0 < \varepsilon < \varepsilon_{max}$. A second random number, η , uniformly distributed on the range $0 < \eta < 1$ is then chosen. If η is greater than $G(\varepsilon)$, a new value for ε is chosen and the process repeats. Alternatively, if η is less than $G(\varepsilon)$, the value of ε is accepted.

5.2 Angular Distribution

The angular distribution of the flux of protons and ions produced by the TNSA mechanism may be described as a cone centred on the normal to the foil surface. The opening angle of the cone decreases as the ion energy considered increases.

The angular distribution of the particles at the laser-driven source has been approximated using a Gaussian distribution [6]. At low kinetic energy ($\varepsilon = 0$), the sigma ($\sigma(\varepsilon)$) of the gaussian distribution is taken to be 20° . $\sigma(\varepsilon)$ is assumed to decrease linearly with energy such that

$$\sigma(\varepsilon) = 20^\circ - (\varepsilon_{max} - \varepsilon) \times 15; \quad (42)$$

i.e. $\sigma(\varepsilon)$ decreases from 20° at $\varepsilon = 0$ to 5° at ε_{max} . The polar angle, θ , is then chosen from the gaussian distribution with sigma given by equation 42.

Finally, the azimuthal angle, ϕ , is chose from a distribution uniform over the range $0 < \phi < 2\pi$.

Maria, not sure what this means: A beam diameter of 10 microns has been used.

6 Module, class and data structures

The linear optics package has been written in object-oriented Python and is broken down in four principal modules:

- BeamLineElement: provides descriptions of the various beam-line elements required to build a description of the beam line. Each individual element, such as a drift, quadrupole, etc., is described in a class derived from the `BeamLineElement` parent class.
- BeamLine: provides code to assemble the elements into a coherent beam line. `BeamLine` is a singleton class to ensure that two beam lines can not be simulated in a single run of the package.
- Beam: provides code to calculate ensemble properties of the beam such as emittance, etc. The ensemble properties are stored as instance attributes of the `Beam` class.
- Particle: provides code to record beam particles at positions along the beam line. The module provides the singleton `ReferenceParticle` class derived from the `Particle` class.

Other modules: `BeamIO`, `LaTeX`, `PhysicalConstants`, `Report`, `Simulation` and `Utilities` support the principal modules or provide services. The data structure is implemented as attributes of the instances of the various classes. This section describes the implementation of the various modules, the classes of which they are composed, and how access to the data is provided.

Each class has methods by which to access a list of the class instances and a Boolean flag by which to generate debug print out (see table 2).

6.1 BeamLineElement

6.1.1 Parent class

6.1.1.1 Instantiation

The call to instantiate the `BeamLineElement` class is:

```
BeamLineElement(Name, rStrt, vStrt, drStrt)
```

Table 2: Methods by which to set and access class attributes.

Method	Argument	Return	Comment
<code>getInstances()</code> <code>setDebug(Debug)</code> <code>getDebug()</code> <code>setAll2None()</code>	Boolean	List of instances of class Boolean debug flag	Sets flag to generate debug print-out If true, generate debug print-out Set all instance attributes to <code>None</code> at start of instantiation.

The arguments are translated into instance attributes as described in section 6.3.2 and defined in table 3.

6.1.1.2 Instance attributes and access methods

155 Properties common to all beam-line elements are stored as instance attributes of the parent `BeamLineElement` class. The instance attributes are defined in table 3. The attributes are accessed and set using the methods defined in table 4.

Table 3: Definition of attributes of instances of the `BeamLineElement` class. The attributes marked * above the dividing line are required in the call to instantiate the element. The attributes marked † below the dividing line are calculated.

Attribute	Type	Unit	Comment
Name*	String		Name of beam-line element.
rStrt*	numpy.ndarray	m	$[x, y, z]$ position of entrance to element in laboratory coordinate system.
vStrt*	numpy.ndarray	rad	$[[i], [\theta, \phi]]$ (polar and azimuthal angles) of RPLC y and z axes ($i = 0, 1$ respectively) at start.
drStrt*	numpy.ndarray	m	“Error”, $[x, y, z]$, displacement of start from nominal position (not yet implemented).
dvStrt*	numpy.ndarray	rad	“Error”, $[[i], [\theta, \phi]]$, deviation in θ and ϕ from nominal axis (not yet implemented).
Strt2End†	numpy.ndarray		1×3 translation from start of element to end; in laboratory coordinates. Set in derived class.
Rot2LbStrt†	numpy.ndarray		3×3 rotation matrix that takes RPLC axes to laboratory axes at start.
Rot2LbEnd†	numpy.ndarray		3×3 rotation matrix that takes RPLC axes to laboratory axes at end. Set in derived class.
TnrsMtrx†	numpy.ndarray		3×3 transfer matrix. Set in derived class.

6.1.1.3 Processing methods

Table 5 presents the processing methods provided in the `BeamLineElement` class.

Table 4: Definition of access methods for the `BeamLineElement` class.

Set method	Get method	Comment
<code>setName (Name)</code>	<code>getName ()</code>	Set/get name of beam-line element.
<code>setrStrt (rStrt)</code>	<code>getrStrt ()</code>	Set/get laboratory $[x, y, z]$ position of entrance.
<code>setvStrt (vStrt)</code>	<code>getvStrt ()</code>	Set/get RPLC $[\theta, \phi]$ of principal axis.
<code>setdrStrt (drStrt)</code>	<code>getdrStrt ()</code>	Set/get “error” displacement.
<code>setdvStrt (dvStrt)</code>	<code>getdvStrt ()</code>	Set/get “error” deviation in $[\theta, \phi]$.
<code>setRot2LbStrt ()</code>	<code>getRot2LbStrt ()</code>	Set/get rotation matrix from RPLC axes to laboratory.
<code>setRot2LabStrt ()</code>	<code>getRot2LbStrt ()</code>	Set/get rotation matrix from RPLC to laboratory at start.
<code>setStrt2End (t)</code>	<code>getStrt2End ()</code>	Set/get displacement vector start to end in laboratory coordinates. <code>setStrt2End</code> takes 1 argument, <code>t</code> , a 1D <code>np.ndarray</code> containing the translation from the start to the end of the element in RPLC.
<code>setRot2LbEnd (R)</code>	<code>getRot2LbEnd ()</code>	Set/get rotation matrix from RPLC to laboratory at end. <code>setRot2LbEnd</code> takes 1 argument, <code>R</code> , a 2D <code>np.array</code> containing the rotation matrix to be set.
	<code>getTransferMatrix ()</code>	Get transfer matrix set in derived class.

6.1.1.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

`readElement (dataFILE)` and `writeElement (dataFILE)` ;

160 where `dataFILE` is the a file instance managed by `BeamIO`.

6.1.1.5 Utilities

Table 6 presents the utilities provided in the `BeamLineElement` class.

Table 5: Processing methods provided by the `BeamLineElement` class.

Method	Argument(s)	Return	Comment
<code>OutsideBeamPipe(R)</code>	Float	Boolean	Returns False if particle is inside beam pipe. If R , radial distance from z axis in RPLC, falls outside beam pipe, returns True.
<code>Transport(V)</code>	6×1 np.ndarray	6×1 np.ndarray	Transport 6D trace-space vector, V , across element. Final trace-space vector returned.
<code>Shit2Local(V)</code>	6×1 np.ndarray	6×1 np.ndarray	Transform 6D trace-space vector, V , from RPLC to laboratory coordinates. Phase-space vector in laboratory frame returned.
<code>Shit2Laboratory(U)</code>	6×1 np.ndarray	6×1 np.ndarray	Transform 6D phase-space vector, U , from laboratory coordinates to trace-space coordinates in the RPLC frame. Trace-space vector in RLPC frame returned.

Table 6: Utilities provided by the `BeamLineElement` class.

Method	Argument(s)	Return	Comment
<code>cleaninstances()</code>			Delete (using “del”) all instances of the <code>BeamLineElement</code> class. Reset instances list.
<code>removeInstance(inst)</code>	Instance of BLE		Remove instance <code>inst</code> and remove from list of instances of <code>BeamLineElement</code> .

6.1.2 Derived class: `Facility(BeamLineElement)`

6.1.2.1 Instantiation

165 The call to instantiate the `Facility` derived class is:

```
FacilityName, rStrt, vStrt, drStrt, dvStrt, p0, VCMV)
```

Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `Facility` arguments are translated into instance attributes as described in section 6.1.2.2 and defined in table 7.

170 6.1.2.2 Instance attributes and access methods

The instance attributes are defined in table 7. The attributes are accessed and set using the methods defined in table 8.

6.1.2.3 Processing methods

The `Facility` derived class has no processing methods.

Table 7: Definition of attributes of instances of the `Facility` (`BeamLineElement`) derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
p0	float	MeV	Kinetic energy of reference particle.
VCMV	float	m	Radius of vacuum-chamber mother volume. The radius defines edge of the volume at which a particle trajectory is terminated. It may be necessary to introduce a beam pipe later.

Table 8: Definition of access methods for the `Facility` derived class.

Set method	Get method	Comment
setp0 (Name)	getp0 ()	Set/get momentum of reference particle (in MeV).
setVCMV (VCMV)	getrVCMV ()	Set/get radius of vacuum chamber mother volume.

6.1.2.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

`readElement (dataFILE)` and `writeElement (dataFILE) ;`

175 where `dataFILE` is the a file instance managed by `BeamIO`.

6.1.2.5 Utilities

The `Facility` derived class has no utilities.

6.1.3 Derived class: `Drift` (`BeamLineElement`)

6.1.3.1 Instantiation

180 The call to instantiate the `Drift` derived class is:

`Drift (Name, rStrt, vStrt, drStrt, dvStrt, Length)`

Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `Drift` arguments are translated into instance attributes as described in section 6.1.3.2 and defined in table 9.

185 6.1.3.2 Instance attributes and access methods

The instance attributes are defined in table 9. The attributes are accessed and set using the methods defined in table 10.

6.1.3.3 Processing methods

The `Facility` derived class has no processing methods.

Table 9: Definition of attributes of instances of the `Drift (BeamLineElement)` derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
Length	float	m	Length of drift.

Table 10: Definition of access methods for the `Facility` derived class.

Set method	Get method	Comment
<code>setLength (Length)</code> <code>setTransferMatrix ()</code>	<code>getLength ()</code>	Set/get length of drift (in m). Set transfer matrix.

6.1.3.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

```
readElement (dataFILE)    and    writeElement (dataFILE) ;
```

190 where `dataFILE` is the a file instance managed by `BeamIO`.

6.1.3.5 I/o methods

The `Facility` derived class has no utilities.

6.1.4 Derived class: `Aperture (BeamLineElement)`

6.1.4.1 Instantiation

195 The call to instantiate the `Aperture` derived class is:

```
Aperture (Name, rStrt, vStrt, drStrt, dvStrt, ParamList)
```

Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `Aperture` arguments are translated into instance attributes as described in section 6.1.4.2 and defined in table 11.

200 6.1.4.2 Instance attributes and access methods

The instance attributes are defined in table 11. The attributes are accessed and set using the methods defined in table 13.

6.1.4.3 Processing methods

The `Aperture` processing method is defined in table 13.

6.1.4.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

```
readElement (dataFILE)    and    writeElement (dataFILE) ;
```

205 where `dataFILE` is the a file instance managed by `BeamIO`.

Table 11: Definition of attributes of instances of the `Aperture (BeamLineElement)` derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
<code>ParamList</code>	<code>[]</code>		List containing aperture parameters. The first parameter is an <code>int</code> and defines the aperture “Type”. The remaining elements in the parameter list are <code>floats</code> with meanings that depend on Type.
<code>ParamList[0]</code>	<code>int</code>		Type= 0; circular
<code>ParamList[1]</code>	<code>float</code>	<code>m</code>	Radius of circular aperture
<code>ParamList[0]</code>	<code>int</code>		Type= 1; Elliptical
<code>ParamList[1]</code>	<code>float</code>	<code>m</code>	Radius of elliptical aperture along x_{RPLC} axis
<code>ParamList[2]</code>	<code>float</code>	<code>m</code>	Radius of elliptical aperture along y_{RPLC} axis

Table 12: Definition of access methods for the `Facility` derived class.

Set method	Get method	Comment
<code>setApertureParameters (ParamList)</code>		Set aperture paramters. Sets Type and parameters depending on Type.
	<code>getType ()</code>	Get Type of aperture.
	<code>getParams ()</code>	Get aperture parameters.
<code>setTransferMatrix ()</code>		Set transfer matrix.

6.1.4.5 Utilities

The `Aperture` derived class has no utilities.

Table 13: Utilities provided by the `Aperture` derived class.

Method	Argument(s)	Return	Comment
<code>Transport (V)</code>	<code>np.ndarray</code>	<code>np.ndarray</code> or <code>None</code>	Transport trace-space vector V . If V falls outside of the aperture, return <code>None</code> .

6.1.5 Derived class: `FocusQuadrupole (BeamLineElement)`

6.1.5.1 Instantiation

210 The call to instantiate the `FocusQuadrupole` derived class is:

```
FocusQuadrupole(Name, rStrt, vStrt, drStrt, dvStrt, Length, Strength,
                kFQ)
```

215 Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `FocusQuadrupole` arguments are translated into instance attributes as described in section 6.1.5.2 and defined in table 14. The quadrupole `Length` is required together with either the field gradient, `Strength` (equation 18), or the quadrupole k parameter, `kFQ` (equation 20).

6.1.5.2 Instance attributes and access methods

The instance attributes are defined in table 14. The attributes are accessed and set using the methods defined in table 16.

Table 14: Definition of attributes of instances of the `FocusQuadrupole (BeamLineElement)` derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
<code>FQmode</code>	int		If 0, use particle momentum in calculation of transfer matrix; if 1, use reference particle momentum.
<code>Length</code>	float	m	Effective length of quadrupole.
<code>Strength</code>	float	T/m	Magnetic field gradient; required if <code>kFQ</code> is not given.
<code>kFQ</code>	float	m^{-2}	Quadrupole k paramter.

Table 15: Definition of access methods for the `FocusQuadrupole` derived class.

Set method	Get method	Comment
<code>setFQmode (FQmode)</code>	<code>getFQmode ()</code>	Set/get <code>FQmode</code> .
<code>setLength (Length)</code>	<code>getLength ()</code>	Set/get length.
<code>setStrength (Length)</code>	<code>getStrength ()</code>	Set/get strength (field gradient).
<code>setKfQ (Length)</code>	<code>getKfQ ()</code>	Set/get <code>kFQ</code> , quadrupole k parameter.
<code>setTransferMatrix ()</code>		Set transfer matrix.

6.1.5.3 Processing methods

The `FocusQuadrupole` processing method is defined in table 16.

Table 16: Utilities provided by the `FocusQuadrupole` derived class.

Method	Argument(s)	Return	Comment
<code>calcKfQ()</code>		float	Calculates <code>kFQ</code> if strength is specified.
<code>calcStrength()</code>		float	Calculates Strength if <code>kFQ</code> is specified.

6.1.5.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

`readElement(dataFILE)` and `writeElement(dataFILE)` ;

where `dataFILE` is the a file instance managed by `BeamIO`.

6.1.5.5 Utilities

225 The `FocusQuadrupole` derived class has no utilities.

6.1.6 Derived class: `DefocusQuadrupole` (`BeamLineElement`)

6.1.6.1 Instantiation

The call to instantiate the `DefocusQuadrupole` derived class is:

230 `DefocusQuadrupole(Name, rStrt, vStrt, drStrt, dvStrt, Length, Strength,`
`kDQ)`

Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `DefocusQuadrupole` arguments are translated into instance attributes as described in section 6.1.6.2 and defined in table 17. The quadrupole `Length` is required together with either the field gradient, `Strength` (equation 18), or the quadrupole k parameter, `kDQ` (equation 20).

6.1.6.2 Instance attributes and access methods

The instance attributes are defined in table 17. The attributes are accessed and set using the methods defined in table 19.

6.1.6.3 Processing methods

240 The `DefocusQuadrupole` processing method is defined in table 19.

6.1.6.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

`readElement(dataFILE)` and `writeElement(dataFILE)` ;

where `dataFILE` is the a file instance managed by `BeamIO`.

Table 17: Definition of attributes of instances of the `DefocusQuadrupole` (`BeamLineElement`) derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
DQmode	int		If 0, use particle momentum in calculation of transfer matrix; if 1, use reference particle momentum.
Length	float	m	Effective length of quadrupole.
Strength	float	T/m	Magnetic field gradient; required if kDQ is not given.
kDQ	float	m^{-2}	Quadrupole k paramter.

Table 18: Definition of access methods for the `DefocusQuadrupole` derived class.

Set method	Get method	Comment
<code>setDQmode(DQmode)</code>	<code>getDQmode()</code>	Set/get DQmode.
<code>setLength(Length)</code>	<code>getLength()</code>	Set/get length.
<code>setStrength(Length)</code>	<code>getStrength()</code>	Set/get strength (field gradient).
<code>setKDQ(Length)</code>	<code>getKDQ()</code>	Set/get kDQ, quadrupole k parameter.
<code>setTransferMatrix()</code>		Set transfer matrix.

6.1.6.5 Utilities

The `DefocusQuadrupole` derived class has no utilities.

Table 19: Utilities provided by the `DefocusQuadrupole` derived class.

Method	Argument(s)	Return	Comment
<code>calcKDQ()</code>		float	Calculates <code>kDQ</code> if strength is specified.
<code>calcStrength()</code>		float	Calculates <code>Strength</code> if <code>kDQ</code> is specified.

6.1.7 Derived class: `SectorDipole` (`BeamLineElement`)

6.1.7.1 Instantiation

The call to instantiate the `SectorDipole` derived class is:

```
SectorDipole(Name, rStrt, vStrt, drStrt, dvStrt, Angle, B)
```

Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `SectorDipole` arguments are translated into instance attributes as described in section 6.1.7.2 and defined in table 20.

The orientation of the RLPC coordinate axes with respect to those of the laboratory frame changes from the start of sector dipole to its end. Referring to figure 2, the vector, \mathbf{v}_{ES} , that translates the origin of the RLPC coordinate system at the start of the sector dipole to the origin of the RLPC coordinate system at its end is given by:

$$\mathbf{v}_{ES} = 2\rho_0 \sin\left(\frac{\phi}{2}\right) \begin{pmatrix} \sin\left(\frac{\phi}{2}\right) \\ 0 \\ \cos\left(\frac{\phi}{2}\right) \end{pmatrix}; \quad (43)$$

where ρ_0 is the radius of the circular locus of the trajectory of the reference particle. If the rotation matrix taking the RPLC axes at the start of the sector dipole to the laboratory coordinate axes is $\underline{\underline{R}}_S$, then the vector, $\mathbf{v}_{ES}^{\text{lab}}$, that translates from the start of the sector dipole to its end in laboratory coordinates is given by:

$$\mathbf{v}_{ES}^{\text{lab}} = \underline{\underline{R}}_S \mathbf{v}_{ES}. \quad (44)$$

The rotation matrix that transforms from the RPLC system at the end of the sector dipole to the laboratory coordinate system, $\underline{\underline{R}}_E$ is given by:

$$\underline{\underline{R}}_E = \underline{\underline{R}}_S \underline{\underline{R}}; \quad (45)$$

where:

$$\underline{\underline{R}} = \begin{pmatrix} \cos \phi & 0 & -\sin \phi \\ 0 & 1 & 0 \\ \sin \phi & 0 & \cos \phi \end{pmatrix}. \quad (46)$$

6.1.7.2 Instance attributes and access methods

The instance attributes are defined in table 20. The attributes are accessed and set using the methods defined in table 21.

6.1.7.3 Processing methods

The `SectorDipole` derived class has no processing methods.

Table 20: Definition of attributes of instances of the `SectorDipole (BeamLineElement)` derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
Angle	float	rad	Angle through which sector dipole bends positive reference particle.
B	float	T	Magnetic field.

Table 21: Definition of access methods for the `SectorDipole` derived class.

Set method	Get method	Comment
<code>setAngle (Angle)</code>	<code>getAngle ()</code>	Set/get bending angle.
<code>setB (B)</code>	<code>getB ()</code>	Set/get dipole magnetic field.
<code>setLength ()</code>	<code>getLength ()</code>	Set/get length of reference particle trajectory through sector dipole (arc length).
<code>setTransferMatrix ()</code>		Set transfer matrix.

6.1.7.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

```
readElement (dataFILE)    and    writeElement (dataFILE) ;
```

where `dataFILE` is the a file instance managed by `BeamIO`.

6.1.7.5 Utilities

The `SectorDipole` derived class has no utilities.

6.1.8 Derived class: `Solenoid (BeamLineElement)`

6.1.8.1 Instantiation

The call to instantiate the `Solenoid` derived class is:

```
Solenoid (Name, rStrt, vStrt, drStrt, dvStrt, Length, Strength, kSol)
```

Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `Solenoid` arguments are translated into instance attributes as described in section 6.1.8.2 and defined in table 22. The solenoid `Length` is required together with either the magnetic field strength, `Strength` or the solenoid k parameter, `kSol` (equation 23).

6.1.8.2 Instance attributes and access methods

The instance attributes are defined in table 22. The attributes are accessed and set using the methods defined in table 24.

6.1.8.3 Processing methods

The `Solenoid` processing method is defined in table 24.

Table 22: Definition of attributes of instances of the `Solenoid(BeamLineElement)` derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
Length	float	m	Effective length of solenoid.
Strength	float	T/m	Magnetic field gradient; required if kSol is not given.
kSol	float	m ⁻²	GaborLens k paramter required if Strength not given.

Table 23: Definition of access methods for the `Solenoid` derived class.

Set method	Get method	Comment
<code>setLength(Length)</code>	<code>getLength()</code>	Set/get length.
<code>setStrength(B)</code>	<code>getStrength()</code>	Set/get strength (solenoid magnetic field).
<code>setKSol(Length)</code>	<code>getKFQ()</code>	Set/get kSol, solenoid k parameter.
<code>setTransferMatrix()</code>		Set transfer matrix.

6.1.8.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

```
readElement(dataFILE)    and    writeElement(dataFILE);
```

where `dataFILE` is the a file instance managed by `BeamIO`.

6.1.8.5 Utilities

The `Solenoid` derived class has no utilities.

Table 24: Utilities provided by the `Solenoid` derived class.

Method	Argument(s)	Return	Comment
<code>calcKsol()</code>		float	Calculates <code>kSol</code> if strength is specified.
<code>calcStrength()</code>		float	Calculates <code>Strength</code> if <code>kSol</code> is specified.

275 6.1.9 Derived class: `GaborLens` (`BeamLineElement`)

6.1.9.1 Instantiation

The call to instantiate the `GaborLens` derived class is:

```
GaborLens(Name, rStrt, vStrt, drStrt, dvStrt, Bz, VA, RA, Rp, Length,
          kSol)
```

280 Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `GaborLens` arguments are translated into instance attributes as described in section 6.1.9.2 and defined in table 25. The `Gabor` lens `Length` is required together with either the parameters `Bz`, `VA`, `RA`, `Rp` correspond, respectively, to the parameters B_z , V_A , V_A and R_p defined in section 4.4, or `kSol`, the solenoid strength parameter of the equivalent solenoid (see section 4.4).

285 The effective electron number density inside the trap is calculated using either `Bz`, `VA`, `RA` and `Rp` or `kSol`.

6.1.9.2 Instance attributes and access methods

The instance attributes are defined in table 25. The attributes are accessed and set using the methods defined in table 26.

Table 25: Definition of attributes of instances of the `GaborLens` (`BeamLineElement`) derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
<code>Bz</code>	float	T	Effective length of Gabor lens.
<code>VA</code>	float	V	Effective length of Gabor lens.
<code>RA</code>	float	m	Effective length of Gabor lens.
<code>RP</code>	float	m	Effective length of Gabor lens.
<code>Length</code>	float	m	Effective length of Gabor lens.
<code>Strength</code>	float	T/m	Magnetic field gradient; required if <code>kSol</code> is not given.
<code>kSol</code>	float	m^{-2}	k parameter of the solenoid with the equivalent focusing strength.

6.1.9.3 Processing methods

290 The `GaborLens` derived class has no processing methods.

6.1.9.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

```
readElement(dataFILE)    and    writeElement(dataFILE);
```

where `dataFILE` is the a file instance managed by `BeamIO`.

Table 26: Definition of access methods for the `GaborLens` derived class.

Set method	Get method	Comment
<code>setBz(Bz)</code>	<code>getBz()</code>	Set/get magnetic field of the Penning-Malmberg trap.
<code>setVA(VA)</code>	<code>getVA()</code>	Set/get anode voltage of the Penning-Malmberg trap.
<code>setRA(RA)</code>	<code>getRA()</code>	Set/get radius of the anode of the Penning-Malmberg trap.
<code>setRP(RP)</code>	<code>getRP()</code>	Set/get magnetic effective radius of the plasma confined within the Penning-Malmberg trap.
<code>setLength(Length)</code>	<code>getLength()</code>	Set/get effective length of the lens.
<code>setStrength(Strength)</code>	<code>getStrength()</code>	Set/get k-parameter of the solenoid with the equivalent focal length.
<code>setElectronDenisty()</code>	<code>getElectronDenisty()</code>	Set/get electron density.
<code>setTransferMatrix()</code>		Set transfer matrix.

6.1.9.5 Utilities

The `GaborLens` derived class has no utilities.

6.1.10 Derived class: `CylindricalRFCavity` (`BeamLineElement`)

6.1.10.1 Instantiation

The call to instantiate the `CylindricalRFCavity` derived class is:

```
CylindricalRFCavity(Name, rStrt, vStrt, drStrt, dvStrt, Gradient,
                    Frequency, Phase)
```

Parent class arguments `Name`, `rStrt`, `vStrt`, `drStrt`, and `dvStrt` are described in section 6.3.2. These arguments are passed directly to `BeamLineElement`. The `CylindricalRFCavity` arguments are translated into instance attributes as described in section 6.1.10.2 and defined in table 27.

6.1.10.2 Instance attributes and access methods

The instance attributes are defined in table 27. The attributes are accessed and set using the methods defined in table 28.

6.1.10.3 Processing methods

The `CylindricalRFCavity` derived class has no processing methods.

6.1.10.4 I/o methods

Methods to read and write instance attributes to the files defined using the `BeamIO` package (see section ?? are provided. The calls are:

```
readElement(dataFILE)    and    writeElement(dataFILE);
```

where `dataFILE` is the a file instance managed by `BeamIO`.

Table 27: Definition of attributes of instances of the `CylindricalRFCavity` (`BeamLineElement`) derived class. All attributes are required in the call to instantiate the element.

Attribute	Type	Unit	Comment
Gradient	float	MV/m	Peak electric field gradient on axis.
Frequency	float	MHz	Resonant frequency.
Phase	float	rad	Phase cavity at time reference particle crosses centre of cavity, “linac convention”.
TransitTimeFactor	float		Transit time factor (equation ??).
V0	float	MV	Peak voltage.
alpha	float		α paramter defined in equation ??.
wperp	float		ω_{\perp} paramter defined in equation ??.
cperp	float		c_{\perp} paramter defined in equation ??.
sperp	float		s_{\perp} paramter defined in equation ??.
wprll	float		$\omega_{ }$ paramter defined in equation ??.
cprll	float		$c_{ }$ paramter defined in equation ??.
sprll	float		$s_{ }$ paramter defined in equation ??.

6.1.10.5 Utilities

The `CylindricalRFCavity` derived class has no utilities.

Table 28: Definition of access methods for the CylindricalRFCavity derived class.

Set method	Get method	Comment
setGradient (Gradient)	getGradient ()	Set/get peak electric field.
setFrequency (Frequency)	getFrequency ()	Set/get frequency.
setAngularFrequency (AngFreq)	getAngularFrequency ()	Set/get angular frequency.
setPhase (Phase)	getPhase ()	Set/get phase.
setWaveNumber (WaveNumber)	getWaveNumber ()	Set/get wavenumber.
setLength (Length)	getLength ()	Set/get Length.
setRadius (Radius)	getRadius ()	Set/get Radius.
setTransitTimeFactor (TransitTimeFactor)	getTransitTimeFactor ()	Set/get TransitTimeFactor.
setV0 (V0)	getV0 ()	Set/get peak voltage.
setalpha (alpha)	getalpha ()	Set/get alpha.
setwperp (wperp)	getwperp ()	Set/get wperp.
setcperp (cperp)	getcperp ()	Set/get cperp.
setsperp (sperp)	getsperp ()	Set/get sperp.
setwprll (wprll)	getwprll ()	Set/get wprll.
setcprll (cprll)	getcprll ()	Set/get cprll.
setsprll (sprll)	getsprll ()	Set/get sprll.
setmrf (mrf)	getmrf ()	Set/get mrf.
setTransferMatrix ()		Set transfer matrix.

6.2 BeamLine

BeamLine is a singleton class that sets up the beam line geometry and provides methods to track particles through the beam line using the transfer matrices defined in section 6.1. The beam-line geometry is provided in the form of a “csv” file read using pandas. The format of the “csv” file is defined in section ???. Alternatively, if a data file written using the BeamIO package is being read, the beam-line geometry is read from the top of the data file.

6.2.1 Instantiation

The call to instantiate the BeamLineElement class is:

```
BeamLine (BeamLineSpecificationCSVfile, readDataFile)
```

BeamLineSpecificationCSVfile is a the full path of the CSV file containing the beam-line specification. readDataFile is a boolean flag. If readDataFile is set to True, then the BeamLine instance will be created and the beam-line geometry will be read from the header of the BeamIO data file. If readDataFile is not set or is set to False, the beam-line geometry will be read from BeamLineSpecificationCSVfile.

6.2.2 Instance attributes and access methods

The instance attributes are presented in table 29 and the access methods are summarised in table 30.

Table 29: Definition of attributes of instances of the BeamLine class.

Attribute	Type	Comment
BeamLineSpecificationCSVfile*	path	Full path to beam-line specification file.
BeamLineParamPandasInstance	dataframe	Pandas data frame containing beam line parameters.
Element	list	List of instances of BeamLineElement class containing point cloud.

Table 30: Definition of access methods for the BeamLine class.

Set method	Get method	Comment
setSrcTrcSpc (SrcTrcSpc)	setSrcTrcSpc ()	Set trace space at source; SrcTrcSpc is represented as (1, 6) np.ndarray.
	getinsance ()	Get instance of BeamLine class.
	BeamLineSpecificationCSVfile ()	Get beam line specification csv file.
	(getBeamLineParamPandas)	Get pandas dat from containing beam line specification.
	getElement ()	get list of BeamLineElement instances.

6.2.3 Processing methods

Table 31 presents the processing methods provided in the BeamLine class.

6.2.4 I/o methods

Methods to read and write instance attributes to the files defined using the BeamIO package (see section ?? are provided. The calls are:

```
readElement (dataFILE)    and    writeElement (dataFILE) ;
```

where dataFILE is the a file instance managed by BeamIO. In addition the csv file containing the specification of the beam line is read in using the method:

```
csv2pandas (csvFILE) ;
```

where csvFILE (path) is the full path to the csv file.

6.2.5 Utilities

The BEamLine class has no utilities.

Table 31: Processing methods provided by the BeamLine class.

Method	Argument(s)	Return	Comment
addBeamLine()		Success	Loops through pandas data frame and manages parsing and instantiation of beam line elements defined in the specification csv file. Returns Success (bool) which is True if the beamline has been set up successfully and False otherwise.
addFacility()			Manages the extraction of parameters from the pandas data frame and the creation of the single Facility(BeamLineElement) object.
addSource()			Manages the extraction of parameters from the pandas data frame and the creation of the single Source(BeamLineElement) object.
parseFacility()		Name, K0, VCMVr	Parses pandas data frame to extract parameters. Returns the facility Name (string), the kinetic energy of the reference particle K0 (float) in MeV, and the vacuum chamber mother volume radius, VCMVr (float).
parseSource()		Name, Mode, Param	Parses pandas data frame to extract parameters. Returns Name (string), Mode (string), and Param (list) containing the parameters required to instantiate source Mode object.
addBeamLineElement(iBLE)			Adds BeamLineElement object iBLE to the list of BeamLineElement that make up the beam line.
checkConsistency()		Consistent	Checks the consistency of the beamline representation in memory with the representation in the specification csv file. Returns Consistent (bool) which is True if the beamline is consistent and False otherwise.
trackBeamn(NEvts, particleFILE)			Generates NEvts (int) particles and tracks them through the beam line.

The `Beam` class provides methods to calculate the parameters describing the beam passing through an instance of the `BeamLine` class. The covariance matrix is calculated at the various locations defined in the `BeamLine` instance. The calculation is performed either by calculating the covariance matrices particle by particle or by using transfer matrices to propagate the covariance matrix from the source. The latter (propagation of the covariance matrix) is not yet implemented.

6.3.1 Instantiation

The call to instantiate the `BeamElement` class is:

```
Beam(readDataFile, nEvtMax, outputCSVfile, beamlineSpecificationCSVfile)
```

`readDataFile`, the path to the BeamIO file containing the particles that form the beam, is required. `nEvtMax` (optional) defines the number of particles to be read; if it is not given, all particles in `readDataFile` will be read. A CSV file at `outputCSVfile` will be created containing a summary of the beam parameters if this parameter is given. `beamlineSpecificationCSVfile` (the full path of the CSV file containing the beam-line specification) is not required if version 2 or later of the BeamIO data-file format is being used. The optional argument is retained for backward compatibility.

6.3.2 Instance attributes and access methods

The instance attributes are presented in table 32 and the access methods are summarised in table 33.

Table 32: Definition of attributes of instances of the `Beam` class. The attributes marked * above the dividing line are required in the call to instantiate the element. The attributes marked † below the dividing line are calculated.

Attribute	Type	
<code>InputDataFile</code> *	path	Path to BeamIO data file
<code>nEvtMax</code> *	int	Maximum number of events to read
<code>outputCSVfile</code> *	path	Path to csv file in which summary of beam parameters is written
<code>beamlineSpecificationCSVfile</code> *	path	Path to csv file containing beamline specification. Kept for backward compatibility (version 1 only)
<code>Element</code> []	list	List of instances of <code>BeamElement</code> class
<code>Location</code> []†	str	Name of location
<code>s</code> []†	float	Sum of coordinates
<code>CovSums</code> [][]†	list	Sums required to calculate covariance matrix
<code>nParticles</code> []†	list	Number of particles at each location
<code>CovMtrx</code> [][]†	list	Covariance matrix by location
<code>sigmaxy</code> [][]†	list	RMS x and y by location
<code>emittance</code> [][]†	list	Emittance by location; calculated from <code>CovMtrx</code> . [<code>iloc</code>][0][0] α_x , [<code>iloc</code>][0][1] α_y
<code>Twiss</code> [][][]†	list	Twiss parameters by location. [<code>iloc</code>][0][0] α_x , [<code>iloc</code>][0][1] α_y , [<code>iloc</code>][1][0] β_x , [<code>iloc</code>][1][1] β_y , [<code>iloc</code>][2][0] η_x , [<code>iloc</code>][2][1] η_y

Table 33: Definition of access methods for the Beam class.

Set method	Get method	Comment
<code>setSrcTrcSpc (SrcTrcSpc)</code>	<code>setSrcTrcSpc ()</code>	Set trace space at source; SrcTrcSpc presented as (1, 6) np.ndarray.
	<code>getinsance ()</code>	Get instance of Beam class.
	<code>BeamSpecificationCSVfile ()</code>	Get beam line specification csv file.
	<code>(getBeamParamPandas)</code>	Get pandas dat from containing beam-line specification.
	<code>getElement ()</code>	get list of BeamElement instances.

6.3.3 Processing methods

355

Table 34 presents the processing methods provided in the Beam class.

6.3.4 I/o methods

Methods to read and write instance attributes to the files defined using the BeamIO package (see section ?? are provided. The calls are:

```
readElement (dataFILE)    and    writeElement (dataFILE) ;
```

where dataFILE is the a file instance managed by BeamIO. In addition the csv file containing the specification of the beam line is read in using the method:

```
csv2pandas (csvFILE) ;
```

where csvFILE (path) is the full path to the csv file.

6.3.5 Utilities

360

The BEamLine class has no utilities.

Table 34: Processing methods provided by the Beam class.

Method	Argument(s)	Return	Comment
<code>addBeam()</code>		Success	Loops through pandas data frame and manages parsing and instantiation of beamline elements defined in the specification file. Returns <code>Success</code> (bool) value if the beamline has been set up successfully, <code>False</code> otherwise.
<code>addFacility()</code>			Manages the extraction of parameters from the pandas data frame and the creation of the single <code>Facility(BeamElement)</code> instance.
<code>addSource()</code>			Manages the extraction of parameters from the pandas data frame and the creation of the single <code>Source(BeamElement)</code> instance.
<code>parseFacility()</code>		Name, K0, VCMVr	Parses pandas data frame to extract parameters. Returns the facility name, the kinetic energy of the reference particle, K0 (float) in MeV, and the vacuum chamber volume radius, VCMVr (float).
<code>parseSource()</code>		Name, Mode, Param	Parses pandas data frame to extract parameters. Returns Name (string), Mode (string), and Param (list) containing the parameters required to instantiate source <code>Mode</code> instance.
<code>addBeamElement(iBLE)</code>			Adds <code>BeamElement</code> instance to the list of instances of <code>BeamElement</code> that make up the beam line.
<code>checkConsistency()</code>		Consistent	Checks the consistency of the beamline representation in memory with the representation in the specification csv file. Returns <code>Consistent</code> (bool) which is <code>True</code> if the beamline is consistent and <code>False</code> otherwise.
<code>trackBeamn(NEvts, particleFILE)</code>			Generates <code>NEvts</code> (int) particles and tracks them through the beam line.

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A Set-up and run

Introduction

380 This section summarises the steps needed to set-up and run the linear optics simulation of the LhARA beam line. A summary of the tasks that the software suite performs will be documented in due course. The code has been developed in python; python 3 is assumed.

Getting the code

385 The linear optics package is maintained using the GitHub version-control system. The latest release can be downloaded from:

```
\centerline{
  \href{https://github.com/ImperialCollegeLondon/LhARALinearOptics.git}{https://o
}
```

390 Dependencies and required packages

The linear optics code requires the following packages:

- Python modules: `scipy` and `matplotlib`.

It may be convenient to run the package in a “virtual environment”. To set this up, after updating your python installation to python 3.9, execute the following commands:

```
395 1. python3 -m venv --system-site-packages venv
    • This creates the director venv that contains files related to the virtual environment.
2. source venv/bin/activate
3. python -m pip install pandas scipy matplotlib
```

To exit from the virtual environment, execute the command `deactivate`. The command `source venv/bin/activate` places you back into the virtual environment.

The Imperial HEP linux cluster provides python 3.9.18 by default.

Unpacking the code, directories, and running the tests

After downloading the package from GitHub, or cloning the repository, you will find a “`README.md`” file which provides some orientation and instructions to run the code. In particular, a bash script “`startup.bash`” is provided which:

- Sets the “`LhARAOpticsPATH`” environment variable so that the files that hold constants etc. required by the code can be located; and
- Adds “`01-Code`” (see below) to the `PYTHONPATH`. The scripts in “`02-Tests`” (see below) may then be run with the command “`python 02-Tests/<filename>.py`”.

410 Below the top directory, the directory structure in which the code is presented is:

`01-Code`: contains the python implementation as a series of modules. Each module contains a single class or a related set of methods.

`02-Tests`: contains self-contained test scripts that run the various methods and simulation packages defined in the code directory.

415 `11-Parameters`: contains the parameter set used to specify the various beam lines presently implemented.

The instructions in the `README.md` file should be followed to set up and run the code.

Running the code

Execute `startup.bash` from the top directory (i.e. run the bash command `source startup.bash`). This will:

- Set up `LhARAOpticsPATH`; and
- Add `01-Code` to the `PYTHONPATH`. The scripts in `02-Tests` may then be run with the command `python 02-Tests/<filename>.py`;
- Example scripts are provided in `03-Scripts`, these can be used first to “Run” the simulation and then to “Read” the data file produced. Example scripts are provided for the DRACO, LION, and LhARA Stage 1 beam lines.