LhARA linear optics documentation

N. Dover, K.R. Long, M. Maxouti

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 are 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 design 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 $\boldsymbol{i}$, $\boldsymbol{j}$ and $\boldsymbol{k}$ 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, $\boldsymbol{r}_0$, momentum, $\boldsymbol{p}_0$, and energy, E_0, of the reference particle at position s:

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

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 $p_0 = |\boldsymbol{p}_0|$.

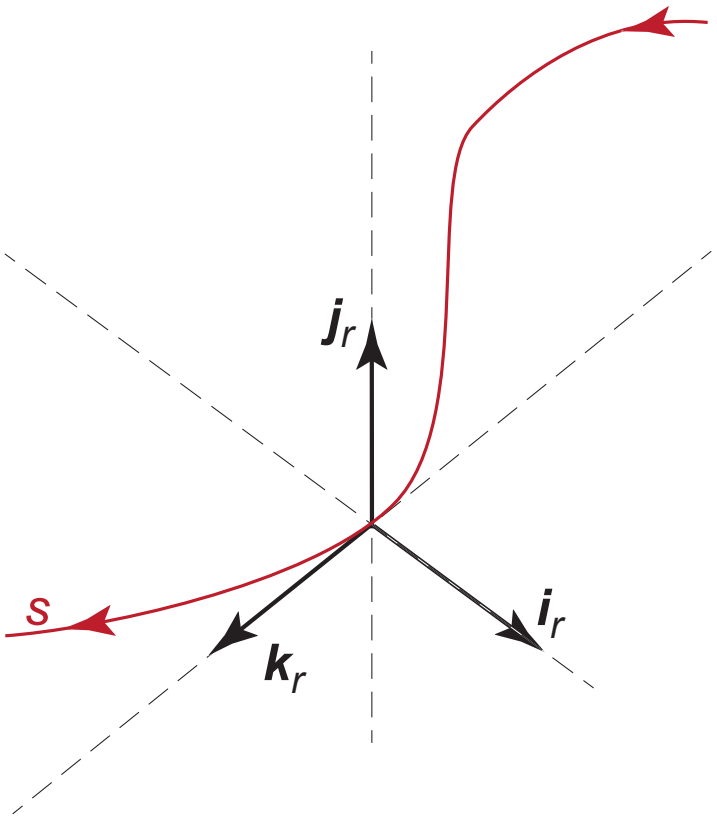

Figure 1: Reference particle local coordinate system. The trajectory of the reference particle is shown as the red line. The distance the reference particle has travelled, measured from the origin of coordinates in the laboratory frame, is labelled s. The origin of the "reference paricle local coordiante (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 $\boldsymbol{i}_r$, $\boldsymbol{j}_r$, and $\boldsymbol{j}_r$.

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 $\boldsymbol{k}_r$. 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 $\boldsymbol{i}_r$) 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 $\boldsymbol{j}_r = \boldsymbol{k}_r \times \boldsymbol{i}_r$.

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.

2.3 Transforming to and from reference particle local coordinates to laboratory coordinates

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

$$\boldsymbol{R}_0(s) = \mathbf{0}\,. \tag{3}$$

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

$$\boldsymbol{r}(s) = \boldsymbol{r}_0(s) + \boldsymbol{\delta r}(s)\,; \tag{4}$$

where:

$$\boldsymbol{\delta r}(s) = \underline{\underline{R}}(s)\boldsymbol{R}(s)\,;\text{and} \tag{5}$$

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

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

$$\begin{aligned} \boldsymbol{i}_r &= \begin{pmatrix} i_{rx} \\ i_{ry} \\ i_{rz} \end{pmatrix}\,; \\ \boldsymbol{j}_r &= \begin{pmatrix} j_{rx} \\ j_{ry} \\ j_{rz} \end{pmatrix}\,;\text{and} \\ \boldsymbol{k}_r &= \begin{pmatrix} k_{rx} \\ k_{ry} \\ k_{rz} \end{pmatrix}\,. \end{aligned} \tag{6}$$

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

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

3 Phase space and trace space

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.

Relativistic mechanics exploits four-vector position, $\underline{\mathcal{R}} = (\boldsymbol{r}, ct)$), and four-vector momentum $\underline{\mathcal{P}} = (c\boldsymbol{p}, E)$. 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.

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.

3.1 Phase space

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

$$\begin{bmatrix} \boldsymbol{r} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \\ \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} \end{bmatrix} \tag{8}$$

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 $(x_{\,\mathrm{RPLC}}, y_{\,\mathrm{RPLC}}, z_{\,\mathrm{RPLC}})$ and momentum $p_{\,\mathrm{RPLC}}$ with components $(p_{\mathrm{x}\,\mathrm{RPLC}}, p_{\mathrm{y}\,\mathrm{RPLC}}, p_{\mathrm{z}\,\mathrm{RPLC}})$. Taking the momentum of the reference particle in the laboratory frame to be p_0, the trace-space coordinates are given by:

$$\boldsymbol{\phi} = \begin{pmatrix} x_{\,\mathrm{RPLC}} \\ x\prime_{\,\mathrm{RPLC}} \\ y_{\,\mathrm{RPLC}} \\ y\prime_{\,\mathrm{RPLC}} \\ z_{\,\mathrm{RPLC}} \\ \delta_{\,\mathrm{RPLC}} \end{pmatrix} ; \tag{9}$$

where:

$$x\prime_{\,\mathrm{RPLC}} = \frac{\partial x}{\partial s} = \frac{cp_{x\,\mathrm{RPLC}}}{cp_0} ; \tag{10}$$

$$y\prime_{\,\mathrm{RPLC}} = \frac{\partial y}{\partial s} = \frac{cp_{y\,\mathrm{RPLC}}}{cp_0} ; \tag{11}$$

$$z_{\,\mathrm{RPLC}} = \frac{s}{\beta_0} - ct = \frac{\Delta s}{\beta_0} ; \text{and} \tag{12}$$

$$\delta_{\,\mathrm{RPLC}} = \frac{E}{cp_0} - \frac{1}{\beta_0} = \frac{\Delta E}{cp_0} . \tag{13}$$

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 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:

$$\boldsymbol{\phi}_{\text{end}} = \underline{\underline{T}}\, \boldsymbol{\phi}_{\text{start}} \,; \tag{14}$$

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

$$s_{\text{end}} = s_{\text{start}} + \delta s \,; \tag{15}$$

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].

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:

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

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

$$\delta s = l \,. \tag{17}$$

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:

$$g_x = \frac{\partial B_{qx}}{\partial x} = g_y = \frac{\partial B_{qy}}{\partial y} = g \,; \tag{18}$$

where the field in the quadrupole, $\boldsymbol{B_q}$, 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:

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

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:

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

4.3 Solenoid

The trajectory of a beam particle through a solenoid is determined by the magnetic field strength, $\boldsymbol{B}_s$, 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 $\boldsymbol{B}_s = (0, 0, B_{s0})$, where the solenoid axis lies along the z_{RPLC} axis. The solenoid field strength parameter is then given by:

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

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 may be written:

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

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

$$\delta s = l_s \, . \tag{25}$$

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 electostatic 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:

$$k_G = \frac{e}{2\epsilon_0}\frac{m_p\gamma}{p^2}n_e \, ; \tag{26}$$

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:

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

The increment in the reference particle trajectory is:

$$\delta s = l_G \, . \tag{28}$$

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

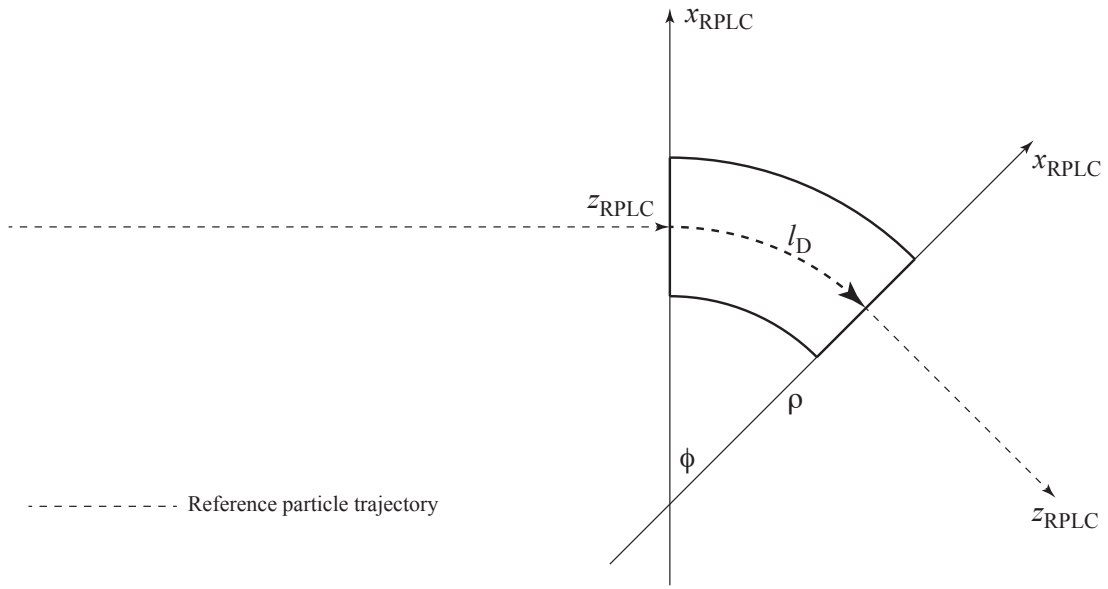

Figure 2: Schematic representation of the passage of the reference particle through a sector dipole. The outline of the sector dipole is shown by the solid black lines. The trajectory of the reference particle is shown as the dashed line. The length of the reference-particle trajectory inside the field 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 $\boldsymbol{j}_{\mathrm{RPLC}}$, i.e. $\boldsymbol{B}_D = (0, B_{D0}, 0)$. No edge focusing is considered.

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

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

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

$$p_0 = B_{D0}\rho\,; \tag{30}$$

so:

$$k_D = \frac{1}{\rho}\,; \tag{31}$$

and the angle ϕ is given by:

$$\phi = \frac{l}{\rho}\,. \tag{32}$$

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

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

The increment in the reference particle trajectory is:

$$\delta s = l_D \, . \tag{34}$$

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 $\varepsilon_{\max}$. The model kinetic-energy spectrum of the TNSA model presented in [4] is given by:

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

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, $\varepsilon_{\max}$, 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:

$$\varepsilon_{max} = X^2 \varepsilon_{i,\infty} \, ; \tag{36}$$

where X is obtained by solving:

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

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, a practical approach is taken. First, the cumulative probability $\Gamma(\varepsilon)$ is obtained by integrating equation 35 over ε and normalising the resulting cumulative probability such that $\Gamma(\varepsilon_{max}) = 1$. A value for the kinetic energy, ε, is chosen 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 $\Gamma(\varepsilon)$ then a new value for ε is chosen and the process repeats. Alternatively, if η is less than $\Gamma(\varepsilon)$ then 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

$$\sigma(\varepsilon) = 20^\circ - (\varepsilon_{max} - \varepsilon) \times 15 \, ; \tag{38}$$

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	$\frac{fE_{laser}}{T_e}$	-
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	$m_e c^2[\sqrt{1 + \frac{I\lambda^2}{1.37\times10^{18}}} - 1]$	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	$B = r_0 + dtan(\theta)$	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	$(\frac{Zk_BT_e}{m_i})^{\frac{1}{2}}$	m/s
Z	Ion charge number	1	-
k_B	Boltzmann constant	1.380649×10^{-23}	$m^2kgs^{-2}K^{-1}$
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	$2Zm_e c^2\sqrt{\frac{fP_{laser}}{P_R}}$	MeV
t_0	Ballistic time	$\frac{B}{v(\infty)}$	s
$v(\infty)$	Ballistic velocity	$\sqrt{\frac{2\varepsilon_{i,\infty}}{m_i}}$	m/s

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 38.

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).

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

Method	Argument	Return	Comment
`getinstances()`		List of instances of class	
`setDebug(Debug)`	Boolean		Sets flag to generate debug print-out
`getDebug()`		Boolean debug flag	If true, generate debug print-out
`setAll2None()`			Set all instance attributes to `None` at start of instanciation.

6.1 `BeamLineElement`

6.1.1 Parent class

6.1.1.1 Instanciation

The call to instanciate the `BeamLineElenent` class is:

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

The arguments are translated into instance attributes as described in section 6.1.1.2 and defined in table 3.

6.1.1.2 Instance attributes and access methods

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 instanciate 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 azimutal 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.

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);
```

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

Set method	Get method	Comment
`setName(Name)`	`getName()`	Set/get name of beam-line element.
`setrStrt(rStrt)`	`getrStrt()`	Set/get laboratory $[x, y, z]$ position of entrance.
`setvStrt(vStrt)`	`getvStrt()`	Set/get RPLC $[\theta, \phi]$ of principal axis.
`setdrStrt(drStrt)`	`getdrStrt()`	Set/get "error" displacement.
`setdvStrt(dvStrt)`	`getdvStrt()`	Set/get "error" deviation in $[\theta, \phi]$.
`setRot2LbStrt()`	`getRot2LbStrt()`	Set/get rotation matrix from RPLC axes to laboratory.
	`getStrt2End()`	Get displacement vector start to end in laboratory coordinates.
	`getRot2LabStrt()`	Get rotation matrix from RPLC to laboratory at start.
	`getRot2LanEnd()`	Get rotation matrix from RPLC to laboratory at end.
	`getTransferMatrix()`	Get transfer matrix set in derived class.

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

Method	Argument(s)	Return	Comment
`OutsideBeamPipe(R)`	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.
`Transport(V)`	6×1 np.ndarray	6×1 np.ndarray	Transport 6D trace-space vector, `V`, accross element. Final trace-space vector returned.
`Shit2Local(V)`	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.
`Shit2Laboratory(U)`	6×1 np.ndarray	6×1 np.ndarray	Transform 6D phase-space vector, `U`, from laboratory coordinates to trace-space coordaintes in the RPLC frame. Trace-space vector in RLPC frame returned.

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

Method	Argument(s)	Return	Comment
`cleaninstances()`			Delete (using "del") all instances of the `BeamLineElement` class. Reset `instances` list.
`removeInstance(inst)`	Instance of BLE		Remove instance `inst` and remove from list of instances of `BeamLineElement`.

References

[1] G. Aymar, T. Becker, *et al.*, "LhARA: The Laser-hybrid Accelerator for Radiobiological Applications," *Frontiers in Physics* **8** (2020) . https://www.frontiersin.org/articles/10.3389/fphy.2020.567738.

[2] The LhARA consortium, "The Laser-hybrid Accelerator for Radiobiological Applications," Tech. Rep. CCAP-TN-01, The Centre for the Clinical Application of Particles, Imperial College London, 2020. https://ccap.hep.ph.ic.ac.uk/trac/raw-attachment/wiki/Communication/Notes/CCAP-TN-01.pdf.

[3] A. Wolski, *Beam dynamics in high energy particle accelerators*. Imperial College Press, 57 Shelton Street, Covent Garden, London WC2H 9HE, 2014.

[4] J. Fuchs, P. Antici, *et al.*, "Laser-driven proton scaling laws and new paths towards energy increase," *Nature Physics* **2** (01, 2006) .

[5] J. Schreiber, F. Bell, *et al.*, "Analytical Model for Ion Acceleration by High-Intensity Laser Pulses," *Physical review letters* **97** (08, 2006) 045005.

[6] P. Casolaro, L. Campajola, G. Breglio, S. Buontempo, M. Consales, A. Cusano, A. Cutolo, F. Di Capua, F. Fienga, and P. Vaiano, "Real-time dosimetry with radiochromic films," *Scientific Reports* **9** (03, 2019) .

A Set-up and run

Introduction

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

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://g
}
```

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:

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/activat` 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`".

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.

`11-Parameters`: contains the parameter set used to specifiy 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.