Consiglio Nazionale delle Ricerche

A small FORTRAN program for assessment of alignment tolerance in arbitrary sequences of flat mirrors

A. Simonetto

FP19/03   August 2019

ISTITUTO DI SCIENZA E TECNOLOGIA DEI PLASMI

Via R. Cozzi 53 - 20125 Milano (Italy)

Disclaimer

This report only represents the opinion of the author(s) at the time of writing.

1. INTRODUCTION

Mirrors are a common component in THz and sub-THz quasi-optical systems. The system designer always faces the need to specify alignment tolerances for manufacturing, but computing the impact of misalignments using commercial programs can be tedious, requiring lots of simulations.

This program tries to alleviate the burden by performing a Montecarlo analysis for an arbitrary sequence of flat mirrors, specified with the positions of the central axis reflection points in a single reference frame. It is somewhat similar to [1].

The first point is the position of the source, the last an arbitrary point on the axis of the output beam. Source and mirrors are assumed to have random errors in orientation, with a uniform distribution function within the specified tolerance.

All mirrors are assumed flat, which is of course a crude approximation, but for tolerance calculations of converging mirrors it usually provides a useful guidance. The error made with this approximation becomes smaller and smaller as tolerances are reduced, and results can be used as a starting point for more accurate simulations with commercial programs.

The program also computes the polarization and its dependence on alignment tolerances.

It is freeware and available in Fortran 90 source form at ISTP (former IFP) website alongside this report. Users are kindly requested to cite this report in their papers.

2. CONCEPTS

2.1 OPTICAL SYSTEM REPRESENTATION

An optical system of flat mirrors is represented as an ordered sequence of 3D *points* in a single Cartesian reference frame. Each point identifies an *element*. The first and last points in the sequence specify the location of the *source* and the direction of the *output ray* of the optical systems, while the other elements are the centres of the *mirrors*. Each element (except the output ray) has a user-specified angular tolerance.

2.2 REFLECTION AND POLARIZATION

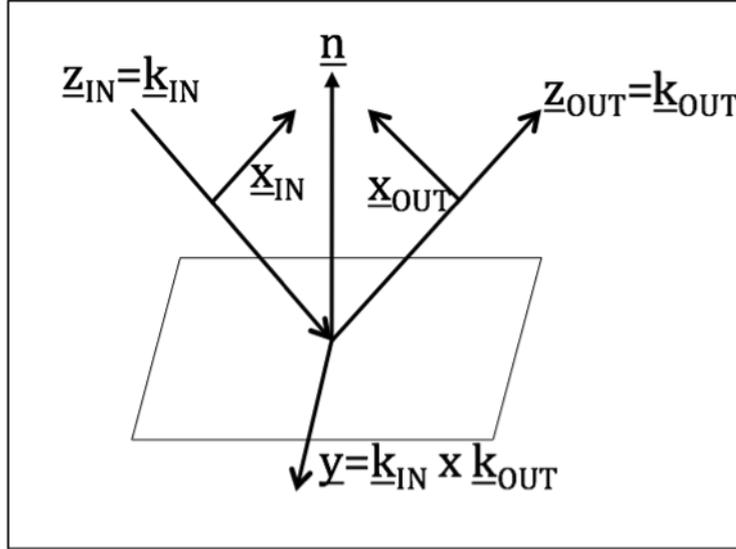Reflection at a mirror is easily represented in an intrinsic reference frame, shown in Figure 1.

Figure 1: intrinsic reference frame for reflection at a mirror

The axes of the reference frames (x_{IN}, y, k_{IN}), (x_{OUT}, y, k_{OUT}) are defined as:

$$\underline{k}_{i,IN} = \frac{\underline{P}_i - \underline{P}_{i-1}}{\left|\underline{P}_i - \underline{P}_{i-1}\right|}$$

$$\underline{k}_{i,OUT} = \underline{k}_{i+1,IN} \tag{1}$$

$$\underline{y} = \frac{\underline{k}_{IN} \times \underline{k}_{OUT}}{\left|\underline{k}_{IN} \times \underline{k}_{OUT}\right|} \tag{2}$$

$$\underline{x}_{IN} = \underline{y} \times \underline{k}_{IN}$$

$$\underline{x}_{OUT} = \underline{y} \times \underline{k}_{OUT} \tag{3}$$

where $\underline{P}_i$ are the position vectors of the user-input points.

Using this reference frame, the boundary conditions for specular reflection can be written very simply, so that the incident and reflected fields can be written as:

$$\underline{E}_{IN} = E_x \underline{x}_{IN} + E_y \underline{y}$$

$$\underline{E}_{OUT} = E_x \underline{x}_{OUT} - E_y \underline{y} \tag{4}$$

The input polarization at element 1 (input aperture) must be specified by the user in the intrinsic reference frame for reflection at the first mirror, and is computed for the rest of the optical system.

Another reference frame, very useful for describing misalignments, is shown in Figure 2. The y axis is of course the same as in Figure 1, whereas the others are defined as

$$\underline{n} = \frac{\underline{k}_{OUT} - \underline{k}_{IN}}{\left|\underline{k}_{OUT} - \underline{k}_{IN}\right|} \tag{5}$$

$$\underline{u} = \underline{n} \times \underline{y} \tag{6}$$

One can also write $\underline{k}_{OUT}$ in this new reference frame:

$$\underline{k}_{OUT} = \underline{k}_{IN} - 2\underline{n}\left(\underline{k}_{IN} \bullet \underline{n}\right) \tag{7}$$

And this relation shall be useful

$$\left|\underline{k}_{OUT} - \underline{k}_{IN}\right|^2 = 2\left(1 - \underline{k}_{IN} \bullet \underline{k}_{OUT}\right) \tag{8}$$
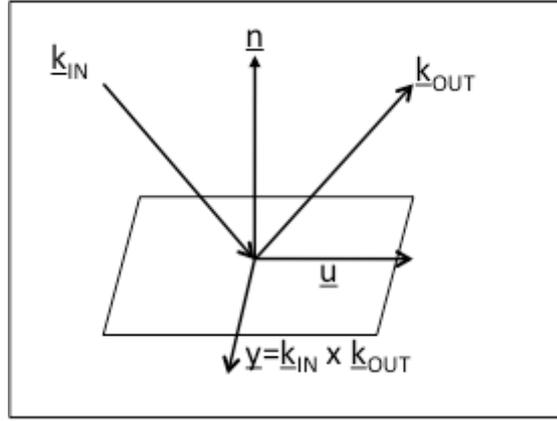
2

Figure 2: second reference frame at mirror

3. POSITIONING TOLERANCES

The orientation of any element (except the last, which is not a physical component) of the chain is assumed to have a random perturbation with a flat distribution within a cone of user-specified half-angle.

The program computes the collective impact of the random set of perturbations on the direction of the output beam and the point of incidence on every mirror.

The distribution of pseudo-random numbers is uniform (i.e. flat) on the (0-1) interval. To obtain a uniform distribution over a disk of unit radius (the base of the cone), one can use a random number to specify the polar angle, but the distribution of radii must then increase linearly from the centre of the disk, to compensate for the decrease in angular density of points specified with standard polar coordinates (r,φ).

This can be easily obtained using a pair of random numbers ran_1, ran_2 combined with

$$\begin{cases} r = ran_1 + ran_2 & \left(ran_1 + ran_2\right) \le 1 \\ r = 2 - ran_1 - ran_2 & \left(ran_1 + ran_2\right) > 1 \end{cases} \tag{9}$$

to obtain a random number r in the [0,1] interval with the required linear distribution.

The point (R,φ) on the base of the cone is thus

$$R = r \tan\theta$$
$$\varphi = 2\pi ran_3 \tag{10}$$

where θ is the user-specified angular tolerance.

The random perturbation can be used to write a new orientation for all optical elements

$$\underline{n}'_i = \beta\left[\underline{n}_i + \Delta\underline{n}_i\right] \tag{11}$$

where the scalar β accounts for re-normalization.

Similarly, the direction of the source is perturbed

$$\underline{k}'_{1,OUT} = \underline{k}'_{2,IN} \equiv \left[\underline{k}_{2,IN} + \Delta\underline{k}_{IN}\right]\alpha \tag{12}$$

where the scalar α accounts for re-normalization.

The ray path through the optical system changes as a consequence of perturbations and so do the points of incidence on mirrors and the polarization.

The polarization is computed easily using (1) to (4) with perturbed (primed) quantities, and so is the ray path, using (7).

The change in reflection point on the i-th mirror can be written as

$$\Delta\underline{x}_{i,OUT} = \Delta\underline{x}_{i-1,OUT} + L\left[\left(\underline{k}'_{i,IN} - \underline{k}_{i,IN}\right) \bullet \underline{y}_i\right]\underline{y}_i + L\left[\left(\underline{k}'_{i,IN} - \underline{k}_{i,IN}\right) \bullet \underline{u}\right]\underline{u} =$$

$$= \Delta \underline{x}_{i-1,OUT} + L\left(\underline{k}'_{i,IN} \bullet \underline{y}_i\right)\underline{y}_i + L\left[\left(\underline{k}'_{i,IN} - \underline{k}_{i,IN}\right) \bullet \underline{u}\right]\left(\underline{u} \bullet \underline{k}_{i,OUT}\right)\underline{k}_{i,OUT} +$$

$$+ L\left[\left(\underline{k}'_{i,IN} - \underline{k}_{i,IN}\right) \bullet \underline{u}\right]\left(\underline{u} \bullet \underline{x}_{i,OUT}\right)\underline{x}_{i,OUT} \tag{13}$$

where L is the distance from the previous element (source or mirror).
The two relevant components of the position error are

$$\Delta \underline{x}_{i,OUT} \bullet \underline{y}_i = \Delta \underline{x}_{i-1,OUT} \bullet \underline{y}_i + L\left(\underline{k}'_{i,IN} \bullet \underline{y}_i\right) \tag{14}$$

$$\Delta \underline{x}_{i,OUT} \bullet \underline{x}_{i,OUT} = \Delta \underline{x}_{i-1,OUT} \bullet \underline{x}_{i,OUT} + L\left[\left(\underline{k}'_{i,IN} - \underline{k}_{i,IN}\right) \bullet \underline{u}\right]\left(\underline{u} \bullet \underline{x}_{i,OUT}\right) \tag{15}$$

In order to provide an acceptable graphical representation, the polarization (assumed linear) is converted into the angle ψ between $\underline{E}$ and $\underline{x}_{OUT}$ (positive as usual in the direction from $\underline{x}_{OUT}$ to $\underline{y}$). The polarization scattering due to misalignments is represented as the difference between the perturbed and nominal polarization (in the -90 to +90 deg range).
The change in ray direction is represented with the angles made by the perturbed and nominal output ray directions in the (unperturbed) $\underline{x}_{OUT}\underline{k}_{OUT}$ and $\underline{y}_{OUT}\underline{k}_{OUT}$ planes

$$\theta_{i,x} = \arctan \frac{\underline{k}'_{i,OUT} \bullet \underline{x}_{i,OUT}}{\underline{k}'_{i,OUT} \bullet \underline{k}_{i,OUT}} \tag{16}$$

$$\theta_{i,y} = \arctan \frac{\underline{k}'_{i,OUT} \bullet \underline{y}_{i,OUT}}{\underline{k}'_{i,OUT} \bullet \underline{k}_{i,OUT}} \tag{17}$$

4. HISTOGRAMS AND MOMENTS

The histograms (normalized to unit sum) of (14-15), (16-17) and of the polarization angle are computed and written to disk.
The program is designed to allow a very large number of random perturbations. Data analysis is therefore implemented by necessity without storing all results.
Histograms have a pre-defined number of bins, and the extent of full-range deviation must be (conservatively) estimated beforehand.
Predicted maximum ranges in the program are

$$\Delta \theta_i = \tau \times 2^i$$
$$\Delta x_i = L_{i-1} \tan\left(\Delta \theta_{i-1}\right) \tag{18}$$

for the maximum angular deviation of the i-th element and the displacement in the point of incidence. In eq. (18), τ is the input tolerance, L_{i-1} the distance between i-1th and i-th elements.
The 50, 67, 95% probability regions are computed from the histograms by finding the levels $l(P)$ for which

$$P = \sum_{h(i,j)>l(P)} h(i,j) \tag{19}$$

where P is the required value (.50,.67,.95) and $h(i,j)$ is the normalized histogram.
The levels $l(P)$ are written to disk in order to allow plotting contours in the histogram. For a single-number assessment, the quantities

$$\sqrt{\frac{1}{\pi}A(P)} \tag{20}$$

are computed, with $A(P)$ the area of the domain where the histogram satisfies $h(i,j)>l(P)$. They represent an equivalent radius for the given probability confidence areas.

Histograms of the last element (the point on the output ray) -which are undefined- are copied from the previous one in the chain and rotated into a reference frame chosen by the user, instead of the intrinsic reference frame of Figure 1 for the mirror of interest that is used for all other histograms: the histogram is computed in the reference frame given by

$$\underline{z} = \underline{k}_{last,OUT}$$

$$\underline{y} = \frac{\underline{z} \times \underline{X}}{\left|\underline{z} \times \underline{X}\right|} \tag{21}$$

$$\underline{x} = \underline{y} \times \underline{z}$$

where $\underline{k}_{last,OUT}$ is the unperturbed unit vector of the output ray direction, $\underline{X}$ is the user-defined vector.

Moments are useful estimators of a distribution, and they are computed while instances of random perturbations are generated. The only approximation is using the sum instead of an integral. The quantities, as implemented in the program, are:

$$M_1(\Delta w) = \sum_{i,j} \Delta w(i,j) h(i,j) \tag{22}$$

$$M_2(\Delta w) = \sum_{i,j} \left[\Delta w(i,j)\right]^2 h(i,j) \tag{23}$$

$$M_3(\Delta w) = \sum_{i,j} \left[\Delta w(i,j)\right]^3 h(i,j) \tag{24}$$

where Δw is the variation in quantity w (polarization or angle or position), and separate moments are computed for x,y directions if w is a 2D quantity. The first moment (the average) is always zero in theory, and its value is an estimate of the numerical error due to discreteness of Montecarlo analysis.

One should note that the model is linear for small tolerances (i.e. for all practical cases), and the deviation from reference is zero-mean by definition (excluding the small numerical error due to Montecarlo analysis). Thus, there is no need to run the program more than once, since all results can be easily re-scaled.

In particular, moments (22-24) scale with 1st, 2nd, 3rd power of tolerance. The radius of the probability confidence areas (20) is proportional to tolerance, and so are the domains of histograms.

5. PROGRAM STRUCTURE

This section is only intended for those wishing to make modifications to the program and can be safely skipped by everyone else. The program is heavily commented, so this section is kept to a minimum.

The program reads a text file `opticalsystemv1.txt`, which contains all inputs and writes results on several output files.

Several PARAMETER constants are used for array dimensioning:
- MAXMIR=10: maximum number of elements (i.e. source+ mirrors+ output ray)
- NBINS=101: number of bins in each dimension of the histogram

The optical system is represented with an array, `points(3,MAXMIR)`, containing the user-input coordinates in an ordered list of length `nelem` ($\leq$MAXMIR); `points(:,1)` is the position of the source; `points(:,nelem)` is a point on the trajectory of the output ray.

Using these data, all the local coordinate systems are computed, together with distances between mirrors.

The former data, with the user-provided input polarization, are used to compute the polarization along the optical system.

Then the computation of random perturbations is performed in a double loop, the inner with a fixed 1000 limit, the outer chosen by the user.

6. PROGRAM USAGE

6.1 INPUT DATA

The program reads a single (text) file of parameters, named `opticalsystemv1.txt`. A sample is shown below.

```
0.001    ;tolerance [rad]
100      ;# of thousands of random cases (10000=1E6)
1. 0.    ;x,y components of input E(local reference frame);need not be normalized
0.238  0.954  0.180  ; X axis direction in wanted out reference frame
0.950155E+01  0.201000E+00  0.500111E+01 ;sequence of points [any unit]
(...)
0.649689E+01  0.986725E-01  0.376874E+01
empty line
```

In a more formal specification

Line number	Parameter(s)
1	angular tolerance [rad]
2	number of wanted perturbation instances divided by 1000
3	x,y components of electric field at first mirror (in intrinsic reference frame: x is in the plane of incidence, y is perpendicular to it, z is along beam axis). Need not be normalized
4	x,y,z components of a vector (in a user-chosen reference system) representing the direction of the x axis in a reference frame of choice for representing output histograms. Need not be normalized.
5	x,y,z coordinates (in the same reference frame used for specifying line 4, any unit of length) of the source
6ff	x,y,z coordinates (in the same reference frame used for specifying line 4, same unit of length as line 5) of the point of incidence on each mirror
last line	empty line, to make sure the previous line is read

Table 1: structure of input file and explanation of parameters.

The user may choose to avoid assessing random errors, which is simply done by setting 0 as the tolerance, and use the program to compute the nominal polarization.

6.2 OUTPUT FILES

All output files are tab-separated text files with header.
unperturbed.txt
This is a list (with header line) with the following information on each line:
- point number: label of the element, from 1 (source) to the total number
- output polarization [deg]: polarization after the element under consideration. For last point it is the output polarization. Frame of reference for polarization is the one shown in Figure 1, with the angle measured from x_{OUT} axis and the positive direction from x_{OUT} to y.
- components (1..3) of x_{OUT} axis in the reference frame used for specifying inputs.

- components (1..3) of $\underline{y}$ axis in the reference frame used for specifying inputs.
- components (1..3) of $\underline{z} = \underline{k}_{OUT}$ axis in the reference frame used for specifying inputs.

anghist<n>.txt

For element $<n>$ (n>1), histogram of deviation from reference beam direction. For the last element, *nelem*, the histogram is the same as for *nelem-1*, but with axes *x,y* referred to the reference frame specified by the user.

The format of each file is compatible with GNUPLOT:
- header line with real min, max values for deviations (i.e. positions of last non-empty bins) and bin size in both directions (identical)
- sequence of x,y,hist(x,y) along first row
- empty line
- sequence of x,y,hist(x,y) along second row
- empty line
- ...

xhist<n>.txt

For element $<n>$ (n>1), histogram of variation in position of point of incidence. Format is the same as for `anghist<n>.txt`.

polhist<n>.txt

For element $<n>$ (n>1), histogram of polarization angle. Format is similar to the other histograms:
- header line with real min, max values for deviations (i.e. positions of last non-empty bins) and bin size in both directions (identical)
- sequence of $\Delta\psi$,hist($\Delta\psi$)

moments.txt

This is a list (with header line) with the following information on each line:
- element number
- first moment in x direction for deviation in point of incidence
- first moment in y direction for deviation in point of incidence
- first moment in x direction for deviation from reference beam direction
- first moment in y direction for deviation from reference beam direction
- first moment for polarization angle
- <same sequence for second moments>
- <same sequence for third moments>

summary.txt

This is a list (with header line) with the following information on each line:
- element number
- x,y,z coordinates of (user-input) reference point of incidence.
- polarization angle [deg] in intrinsic reference frame
- modulus of maximum variation in polarization angle [deg]
- second moment of variation in polarization angle [deg^2]
- modulus of maximum variation along *x* in reference beam direction [deg]
- second moment of variation along *x* in reference beam direction [deg^2]
- same for *y*
- modulus of maximum variation along *x* in position of point of incidence [same units as user input]

- second moment of variation along *x* in position of point of incidence [same units as user input^2]
- same for *y*

erbars.txt

This is a list (with header line) with the following information on each line:
- element number
- equivalent radius (eq.20) of 95% confidence area of probability in variation in position of point of incidence
- same for 67% and 50% probability
- equivalent radius (eq.20) of 95% confidence area of probability in deviation from reference beam
- same for 67% and 50% probability

levels.txt

This is a list (with header line) with the following information on each line:
- element number
- contour level for 95% probability in variation of point of incidence
- same for 67% and 50% probability
- contour level for 95% probability in deviation from direction of reference beam
- same for 67% and 50% probability

gnuplotcmd.txt

This is a `gnuplot` script for plotting individual histograms on postscript files. The typical output is shown in Figure 3 below.

The script file contains:

```
set terminal  postscript color  landscape "Helvetica" 12
set view map
set size ratio 1.
set style data linespoints
set key off
unset surface
set contour base
set pm3d
set key off
set cntrparam levels discrete   <95% level> ,  <67% level> ,  <50% level>
set xrange [ <-range> :  <+range> ]
set yrange [ <-range> :  <+range> ]
set xlabel "theta_x [rad]" (or "x [.]")
set ylabel "theta_y [rad]" (or "y [.]")
set title "Center ray angular deviation[rad]@tol=<tolerance>rad; levels=50,67,95%
probability"
set output 'anghist<#>.ps' (or 'xhist<#>.ps')
splot "anghist2.txt" using 1:2:3 (or "xhist<#>.ps")
(...)
```

The last 8 commands are repeated for every 2D histogram file.

Center ray deviation [.]@tol= 1.00000000000000002E-003 rad; levels=50,67,95% probability
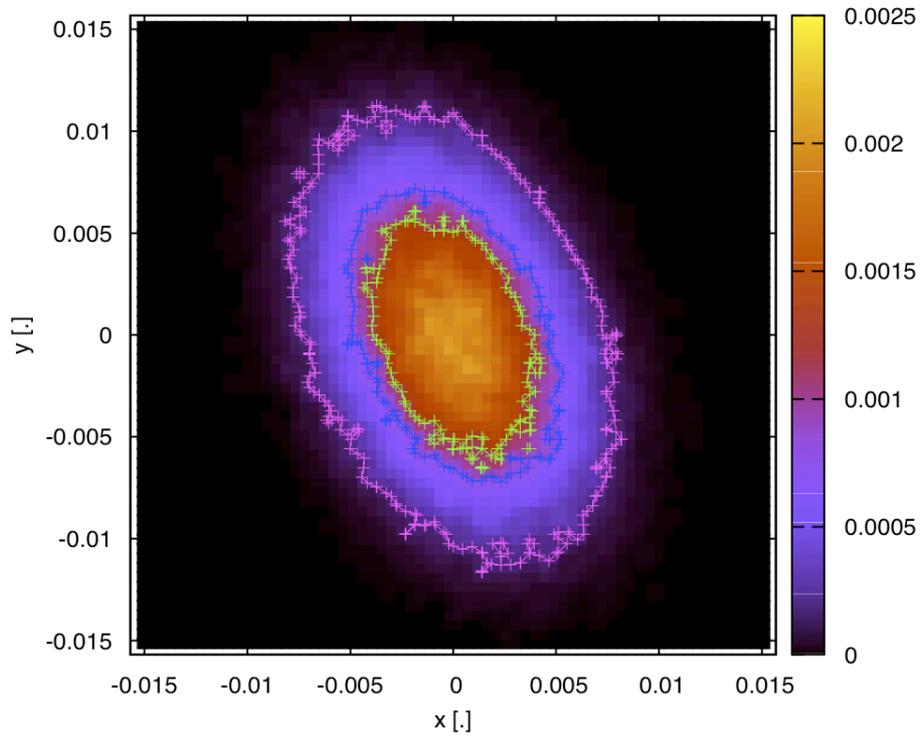
Figure 3: typical plot of histogram in variation of position of point of incidence, resulting from executin of the program-generated _gnuplot_ script. Axes units are shown with dots because they are unknown to the program, being a user choice.

8. REFERENCES

[1] A. Simonetto *A program for performance assessment of corrugated waveguide transmission lines*, IFP Internal Report FP18/1

9