III. GIOS INPUT FILE FORMAT

Contents

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GIOS uses the method of transfer matrices, all elements of which are described by algebraic expressions. Each optical element is characterized by one transfer matrix. All transfer matrices are multiplied resulting in an overall transfer matrix. The elements that can be used are: a field–free drift distances, magnetic or electrostatic quadrupoles, hexapoles, octupoles or multipoles, a magnetic or electrostatic sector fields, acceleration regions, solenoids, etc.

GIOS uses either parallelogram–like (mainly for spectrometer designs) or elliptical phase–space areas (mainly for accelerator or beam line designs). "Homogeneous" space–charge forces can be taken into account.

GIOS determines "normalized aberration coefficients" (see section 4.1 and section 4.3 of part III) which all assume an upright rectangular or an upright elliptical phase–space distribution at the object and postulate each optical system to be amended by "virtual object lenses" in order to allow initial oblique phase–space distibutions and still provide an easy to interprete definition of image aberations.

GIOS provides easy to read graphical presentations of the ion–optical system under consideration including individual particle trajectories or calculated beam properties like for instance a beam–envelope for the complete system or parts thereof. At desired z–locations GIOS also determines contour–line intensity plots for a plane formed by two phase–space coordinates, for instance x,y or x,a, taking into account all upstream apertures.

The output of GIOS is written onto a file called "GIOSOUT.DAT". The input of GIOS must be on a file "GIOSIN.DAT" to which the selected input file is copied automatically. The possibilities to structure the "GIOSIN.DAT" file are outlined below.

$\boxed{\text{The first line of this file } \underline{\textbf{must}} \text{ always be a "title line".}}$

$\boxed{\text{The last line } \underline{\textbf{must}} \text{ read: "END" ;}}$

In between are the GIOS–commands each of which must start on a new line. A GIOS–command can extend over several 72 character lines and must end with (␣;), i.e. a semicolon preceded by a blank space. All characters behind the (;) symbol are regarded as comment. A line starting with a (;) symbol is a comment line. Each command must start with two or three characterizing words each of which is represented by its first letter only. A blank space (␣) is the word limiter.

1 General Input Commands

As soon as a GIOS–command is identified by its characterizing words a string of default numbers is attached to it. The numbers contained in the command then change these default numbers one by one. In case there are fewer numbers given than contained in the default string, the leftover default values remain valid.

The first line in GIOSIN.DAT [see title line (section 1.1)] must be present. The second, third and/or fourth lines (see sections 1.2, 1.3, 1.4) can be omitted, in which case the default definitions will be used. If the second, third or fourth command lines appear more than once, the latest command will override any prior one.

1.1 The Title Line

The Title line in GIOSIN.DAT is a string of up to 80 characters chosen by the user. This title should identify the present example and distinguish it from all others. It should be changed for every calculation performed for instance by a date and a running number so that the file can be identified later. The given title will be repeated in the final output.

1.2 Choosing Appropriate Lengths Units [LU]

All distances in z–direction are given in longitudinal units (LLU) and all distances in x– and y–directions in transversal units (TLU). The lengths of the LLU and TLU units (as given in meters) can be defined by the command:

R(eference) **L**(ength) <LLU in m> <TLU in m> ;
example: R L 100.0 0.01 ;
default: R L 1.000 1.00 ;

To avoid confusion, it is most advisable to always keep the same LLU and TLU for all calculations performed in a period of some weeks. If no strong reasons speak against this, it is recommended to **use only the default definitions** of LLU and TLU in which case both length units are measured in meters.

1.3 Selecting a Momentum–Deviation instead of an Energy–Deviation [M]

The chromatic properties of a particle beam are usually described by

1. δ_K (in GIOS: D) with $K/q = (K_0/q_{)}0(1+\delta_K)$ and
2. δ_m (in GIOS: G) with $m_0/q = (m_{00}/q_0)(1+\delta_m)$

(see Eqs. (1) of section III). However, by the command:

M(omentum) ;

the definition of δ_m is changed to δ_p (in GIOS: P) with $p/q = (p_0/q_0)(1+\delta_p)$.

1.4 Selecting the Calculation Order of the Optics Calculation [CO]

The highest order to which calculations will be performed can be chosen by the command:

C(alculation) **O**(rder) < x–order> < y–order> ;
example: C O 3 3 ;
default: C O 1 1 ;

The first number (1,2 or 3) describes the calculation order for the x–direction and the second number (1,2 or 3) describes the calculation order for the y–direction. In order to save computer time and reduce the length of the GIOSOUT.DAT file it is recommended to keep both numbers as small as possible.

2 Commands that Describe the Initial Particle Beam

If any of the beam defining commands (see in sections 2 and 3) appear more than once, the last command overrides all previous ones.

2.1 Choosing a Reference Particle that Can Move along the Optic Axis

2.1.1 Defining the Initial Reference Particle of a system [RP]

The characteristic parameters of the reference particle are defined by the command:

R(eference) **P**(article) <energy K_{00} in MeV> ; <rest mass m_{00} in mass units> <charge $\overline{q}$ in charge units e > ;
example: R P 100 4 1 ;
default: R P 1 1 1 ;

One mass unit is 1/12 of one ^{12}C–atom or 931.49433 MeV[1]. The charge of one electron is (–e), i.e. 1.602177*10^{-19}Asec[2].

In principle GIOS assumes always nonrelativistically fast particles for its calculations, though, to first order all calculations are performed correctly also for arbitrarily fast particles. However, for purely magnetic systems, GIOS calculates correctly to all orders if

1. the particle mass m_{old} is arbitrarily increased to a new mass m_{new} with usually $m_{new} \geq 1000 m_{old}$ while, in order to keep the momentum of the particle constant the energy K_{old} must be reduced to $K_{new} = (K_{old}/m_{new})(m_{old} + K_{old}/1863.003)$. Here all m are in mass units amu and all K are in MeV. The potential drops of all "dipole sheets" or "acceleration columns" must be reduced accordingly.

2. all GIOS calculations are performed with a momentum–deviation δ_p (see section 1.3) instead of an energy deviation δ_K, so that GIOS calculates and shows corrrect momentum dispersions and chromaticities. The also calculated and shown mass–dispersions and mass–chromaticities,howeve, become meaningless since in this case they relate to the arbitrarily chosen mass number m_{new}.

2.1.2 Changing the Reference Particle within a system [CR]

The characteristic parameters of the reference particle can be changed at some position z by the command:

C(hange) **R**(eference_Particle) <energy K_{00} in MeV> ; <rest mass m_{00} in mass units> <charge $\overline{q}$ in charge units e >
example: C P 100 4 1 ;

[1]Note that one proton has a rest mass of 1.0073 amu and one electron of 0.00054858 amu.

[2]In case of very energetic particles their magnetic rigidity – often also called their $B\rho$–value – is given as $\overline{\chi}$ in "Tesla meters" or as $\tilde{\chi}$=299.79246$\overline{\chi}$ in "MeV/c". In both cases one can determine the corresponding particle energy for $\overline{q}$-times charged particles as K=-931.502m_0+$\sqrt{(931.502 m_0)^2 + (\overline{q}\tilde{\chi})^2}$.

If the here demanded new energy $K_{00,new}$ differs from the prior one $K_{00,old}$ it is assumed that a dipole sheet exists across which the particle energy changes from $K_{00,old}$ to $K_{00,new}$[3]. Besides the possibility to describe the action of a dipole sheet in a GIOS input file, it should be noted that in case of an optical system, in which space–charge forces do not vanish, it also is necessary to newly define the beam current downstream from every assumed dipole sheet. (If the dipole sheet would accelerate particles from a potential K_1/q_0 to a potential K_2/q_0, the beam current would change from I_0 to $I_0\sqrt{K_1/K_2}$.)

2.2 Defining the Initial Phase–Space Distribution of a Beam

2.2.1 Parallelogram–like Phase–Space Areas [PX, PY]

An upright rectangular xa–phase–space area is defined by the command:

P(arallelogram–like) **X**(–direction) <source half width x_{00} in TLU> $<\tan\alpha_{00}$ or $a_{00}>$ with $\alpha_{00}>$ <distance ℓ_x to the next angle–limiting aperture in LLU> ;
example: P X 0.001 0.01 1.0 ;
default: P X 0.001 0.01 0.0 ;

Note also that $\tan\alpha_{00} = \pm d_x/\ell_x$ with $2d_x$ being the diameter of the next angle limiting aperture.

Analogous definitions are necessary for the yb–phase–space area.

example: P Y 0.01 0.002 1.0 ;
default: P Y 0.001 0.01 0.0 ;

Note that usually $\ell_x \neq \ell_y$ and that $\ell_x = 0$ or $\ell_y = 0$ are interpreted as $\ell_x = \infty$ or $\ell_y = \infty$.

2.2.2 Elliptical Phase–Space Areas [TX, TY]

An upright elliptical xa–phase–space area is defined by the command:

T(wiss_parameter) **X**(–direction) $<\alpha_{Tx}><\beta_{Tx}$ in TLU> $<\varepsilon_x = x_{00}a_{00}$ in TLU> ;
example: T X 0.500 0.001 0.000001 ;
default: T X 0.001 0.001 0.000001 ;

Analogous definitions are necessary for the yb–phase–space area.

example: T Y 0.3 0.001 0.0000005 ;
default: T Y 0.001 0.001 0.000001 ;

[3]In case very energetic particles their magnetic rigidity – often also called their $B\rho$–value – is given as $\overline{\chi}$ in "Tesla meters" or as $\tilde{\chi} = 299.79246\overline{\chi}$ in "MeV/c". In both cases one can determine the corresponding particle energy of $\overline{q}$-times charged particles as $K = -931.502m_0 + \sqrt{(931.502m_0)^2 + (\overline{q}\tilde{\chi})^2}$.

2.2.3 Maximal Energy–, Mass–, or Momentum–Deviations [DP]

For some plot–commands and for the **P**(RINT) **N**(UMERICAL ...)–command one should define how large δ_K, δ_m or δ_p are assumed to be. The corresponding command is:

D(eviation) **P**(arameter)< δ_m or δ_p > < δ_K in units> ;
example: D P 0.02 0.01 ;
default: D P 0 0 ;

If δ_m, δ_p or δ_k are given as 0.01 then they are all 1%

2.3 Taking Space–Charge Forces into Account [BC, BN]

Space–charge calculations are initiated by the commands:

B(eam) **C**(urrent) < I in Ampere>
B(eam) **N**(ew_current) < I in Ampere>

which define the beam current I_i at z_i. In case of bunching I_{i+1} is larger than I_i and in case of debunching I_{i+1} is smaller than I_i. In between, the actual current I is linearly interpolated. If not specified otherwise at the end of the optical system, it is assumed as default that a BN$< I >$–command is included with $< I >$ being the value defined in the BC$< I >$–command or the last BN$< I >$–command.

3 Description of the Optical System under Consideration

3.1 Field–Free Regions [DL]

The simplest optical element is a field–free region defined by the command:

D(rift) **L**(ength) <length L in LLU> ;
example: D L 1.0 ;

3.2 Rotationally Symmetric Lenses

3.2.1 A Thin Lens [TL]

A simple device is also a thin lens of focal length f_x and f_y in x– and y–directions. This thin lens is defined by the command:

T(hin) **L**(ens) < f_x^{-1} in LLU^{-1} > < f_y^{-1} in LLU^{-1} > <identifier> ;
example: T L 1.0 1.0 1 ;

The <identifier> here has one of the following two meanings:

- 1: an electrostatic thin lens (in which case the lens chromaticity relates to an energy–to–charge deviation)
- 2: a magnetic thin lens (in which case the lens chromaticity relates to a momentum–to–charge deviation)

3.2.2 A Z–Pinch–Plasma–Lens [ZP]

A Z–Pinch Plasma–Lens has equal focusing forces in both the $x-$ and the $y-$directions.

Z(pinch) **P**(lasma–lens) <effective length ℓ of lens in LLU> $<B_Q$ in T at pole tip$>$ <aperture radius G_0 in TLU> ;
example: Z P 0.2 1.0 0.02 ;

3.2.3 An Accelerating Column [AC]

An accelerating column here is assumed to feature an in z–direction accelerating electrostatic field of length ℓ which will change the particle energy[4]. and thus also the angles of inclination of particle trajectories.

A(ccelerating) **C**(olumn) <effective length ℓ of column in LLU> $<E$ in kV/mm$>$ <aperture radius G_0 in TLU> ;
example: A C 0.5 1.0 0.05 ;

In case of an optical system, in which space–charge forces do not vanish, it also is necessary to newly define the beam current downstream from the accelerating column. (If the accelerating column under consideration accelerates particles from a potential K_1/q_0 to a potential K_2/q_0, the beam current would change from I_0 to $I_0\sqrt{K_1/K_2}$.)

3.2.4 Fringing Fields for an Accelerating Column [FF]

To third order, fringing field integrals for accelerating columns are effective only for its focal length not its third–order image aberrations. This fringing field is defined by the command:

F(ringing) **F**(ield) <table#> $< I_1 = (I_{1B}) = G_0^{-2}[\int\int(E/E_0)^2 dz dz - I_{4A} z_b G_0 - z_b^2/2] >$ $< I_2 = (I_{4A}) = G_0^{-1}[\int(E/E_0)^2 dz - z_b] >$ $< I_3 = (I_{5A}) = G_0 \int(E'/E_0)^2 dz >$ $< I_4 = (-I_{6A}) = -\int z(E'/E_0)^2 dz >$ $< I_5 = (I_{9A}) = G_0^{-2}\{\int[(E/E_0)^2 \int(E/E_0)dz]dz - z_b^2/2\} >$; $< I_6 = (-I_{10A}) = -\int[(E'/E_0)^2 \int(E/E_0)dz]dz >$
example: F F 0 0.209 -0.0768 0.0552 -0.33 ;
default: F F 1 ; .

with $E_0 = E_z(z_b)$ being the accelerating field in the main field region as well as $E = E_z(z)$ and $E' = \partial E_z(z)/\partial z$ denoting this field strength and its z–derivative at an arbitrary position along the optic axis.

For <table#>=0 the numerical values of all fringing–field integrals must be listed.
For <table#>$\neq$0 the fringing–field integrals are taken from GIOS_FF.DAT. Note that

- z is the coordinate along the optic axis and that

[4] In case very energetic particles their magnetic rigidity – often also called their $B\rho$–value – is given as $\overline{\chi}$ in "Tesla meters" or as $\tilde{\chi} = 299.79246\overline{\chi}$ in "MeV/c". In both cases one can determine the corresponding particle energy of q-times charged particles as $K = -931.502m_0 + \sqrt{(931.502m_0)^2 + (q\tilde{\chi})^2}]$

- G_0 is the aperture radius of the last opening in the accelerating column.
- All integrals must be taken from z_a outside to z_b inside the main–field regions.

Note here that the fringing–field integrals are only small corrections, so that usually approximate values of I_1, I_2, I_3, I_4 I_5, I_6, are satisfactory and that reasonably good results can be obtained if a set of standard fringing–field integrals is used, determined from a realistic fringing–field distribution, i.e. a field distribution in which Laplace's equations are valid everywhere. One such realistic fringing–field distribution is that for a relatively long accelerating column of aperture $2G_0$ whose fringing field is not modified by any other electrode. The fringing–field integrals that correspond to such a situation are listed in the file $GIOS_F F.DAT$ under #1. In case one has more information about fringing–field distributions that really exist one can obtain the corresponding fringing–field integrals from GIOS also (see section XXX). The use of these new, more accurate fringing–field integrals, however, most probably will modify the earlier results only very slightly.

Note that a fringing field **can only be situated** between a field–free region and an acceleration column.

3.2.5 A Magnetic Solenoid Lens [SL]

A magnetic solenoid here is assumed to feature a longitudinal magnetic flux density in z–direction.

S(olenoid) **L**(ens) <effective length ℓ of solenoid in LLU> $< B$ in Tesla$>$ <aperture radius G_0 in TLU> ;
example: M S 0.5 1.0 0.05 ;

3.2.6 Fringing Fields for a Solenoid [FF]

To third order, fringing field integrals for a solenoid are effective only for its focal length not its third–order image aberrations. This fringing field is defined by the command:

F(ringing) **F**(ield) <table#> $< I_1 = (I_{1B}) = G_0^{-2}[\iint(B/B_0)^2 dzdz - I_{4A} z_b G_0 - z_b^2/2] >$ $< I_2 = (I_{4A}) = G_0^{-1}[\int(B/B_0)^2 dz - z_b] >$ $< I_3 = (I_{5A}) = G_0 \int(B'/B_0)^2 dz >$ $< I_4 = (-I_{6A}) = -\int z(B'/B_0)^2 dz >$ $< I_5 = (I_{9A}) = g_0^{-2}\{\int[(B/B_0)^2 \int(B/B_0)dz]dz - z_b^2/2\} >$; $< I_6 = (-I_{10A}) = -\int[(B'/B_0)^2 \int(B/B_0)dz]dz >$
example: F F 0 0.209 −0.0768 0.0552 −0.33 ;
default: F F 1 ; .

with $B_0 = B_z(z_b)$ being the solenoidal flux density in the magnet coil as well as $B = B_z(z)$ and $B' = \partial B_z(z)/\partial z$ denoting this flux density and its z–derivative at an arbitrary position along the optic axis.

For <table#>=0 the numerical values of all fringing–field integrals must be listed.
For <table#>≠0 the fringing–field integrals are taken from GIOS_FF.DAT. Note that

- z is the coordinate along the optic axis and that
- G_0 is the aperture radius of the solenoid.
- All integrals must be taken from z_a outside to z_b inside the main–field region.

Note here that the fringing–field integrals are only small corrections, so that usually approximate values of I_1, I_2, I_3, I_4 I_5, I_6, are satisfactory and that reasonably good results can be obtained if a set of standard fringing–field integrals is used, determined from a realistic fringing–field distribution, i.e. a field distribution in which Laplace's equations are valid everywhere. One such realistic fringing–field distribution is that for a relatively long solenoid of aperture $2G_0$ whose fringing field is not modified by any other ferromagnetic parts. The fringing–field integrals that correspond to such a situation are listed in the file $GIOS_FF.DAT$ under #1. In case one has more information about a fringing–field distributions that really exists one can obtain the corresponding fringing–field integrals from GIOS also (see section XXX). The use of these new, more accurate fringing–field integrals, however, most probably will modify the earlier results only very slightly.

Note that a fringing field can **only be situated** between a field–free region and an acceleration column.

3.3 Multipoles

3.3.1 A Magnetic Multipole [MM]

A general magnetic multipole, i.e. a superimposed quadrupole, hexapole and octopole, is defined by the command

M(agnetic) **M**(ultipole) <effective length ℓ of multipole in LLU> < B_Q in T at pole tip> < B_H in T at pole tip> < B_O in T at pole tip> <aperture radius G_0 in TLU> ;
example: M M 0.2 1.0 0 0 0.2 ;

B_Q, B_H and B_O here are the quadrupole–, hexapole– and octopole–components of the magnetic flux density. For positive values of B_Q, B_H and B_O positively charged ions positioned at positive x–values are driven towards the optic axis.

This multipole–command is also applicable for a pure quadrupole, hexapole or octopole. However, to save computer time, it is advisable to use in such cases the following commands:

3.3.2 A Magnetic Quadrupole [MQ]

A pure magnetic quadrupole is defined by the command:

M(agnetic) **Q**(uadrupole) <effective length ℓ of quadrupole in LLU> < B_Q in T at pole tip> <aperture radius G_0 in TLU> ;
example: M Q 0.2 1.0 0.02 ;

3.3.3 A Magnetic Hexapole [MH]

A pure magnetic hexapole is defined by the command:

M(agnetic) **H**(exapole) <effective length ℓ of hexapole in LLU> < B_H in T at pole tip> <aperture radius G_0 in TLU> ;
example: M H 0.2 0.5 0.02 ;

3.3.4 A Magnetic Octopole [MO]

A pure magnetic octopole is defined by the command:

M(agnetic) **O**(ctopole) <effective length ℓ of octopole in LLU> < B_O in T at pole tip> <aperture radius G_0 in TLU> ;
example: M O 0.2 0.6 0.02 ;

3.3.5 An Electrostatic Multipole [EM]

An electrostatic multipole is defined by the command:

E(lectrostatic) **M**(ultipole) <effective length ℓ of multipole in LLU> < V_Q in kV at electrode> < V_H in kV at electrode> < V_O in kV at electrode> <aperture radius G_0 in TLU> ;
example: E M 0.1 1.0 0 0 0.03 ;

V_Q, V_H and V_O here are the quadrupole–, hexapole– and octopole–components of the electrode potential. For positive values of V_Q, V_H, V_O positively charged ions positioned at positive x–values are driven towards the optic axis.

Analogously to the magnetic case the multipole–command is also possible for a pure quadrupole, hexapole or octopole. However, to save computer time it is advisable to use in such cases the following commands:

3.3.6 An Electrostatic Quadrupole [EQ]

A pure electrostatic quadrupole is defined by the command:

E(lectrostatic) **Q**(uadrupole) <effective length ℓ of quadrupole in LLU> < V_Q in kV at electrode> <aperture radius G_0 in TLU> ;
example: E Q 0.1 1.0 0.03 ;

3.3.7 An Electrostatic Hexapole [EH]

A pure electrostatic hexapole is defined by the command:

E(lectrostatic) **H**(exapole) <effective length ℓ of hexapole in LLU> < V_H in kV at electrode> <aperture radius G_0 in TLU> ;
example: E H 0.2 0.3 0.03 ; .

3.3.8 An Electrostatic Octopole [EO]

A pure electrostatic octopole is defined by the command:

E(lectrostatic) **O**(ctopole) <effective length ℓ of octopole in LLU> < V_O in kV at electrode> <aperture radius G_0 in TLU> ;
example: E O 0.2 0.8 0.03 ; .

3.3.9 Fringing Fields for a Magnetic or Electrostatic Multipole, Quadrupole or Hexapole [FF]

To third order, fringing fields for multipoles are effective only for their quadrupole– or hexapole–component. This fringing field is defined by the command:

F(ringing) **F**(ield) <table#> $< I_1 = (I_{1A}) = G_0^{-2}[\int\int(g/g_0)dzdz - z_b^2/2] >$ $< I_2 = (I_{2A}) = G_0^{-3}\{\int[z\int(g/g_0)dz]dz - z_b^3/3\} >$ $< I_3 = (I_{3A}) = G_0^{-3}\{\int[\int(g/g_0)dz]^2dz - z_b^3/3\} >$ $< I_4 = (I_{4A}) = G_0^{-1}[\int(g/g_0)^2dz - z_b] >$ $< I_5 = (I_{1B}) = G_0^{-2}[\int\int(g/g_0)^2dzdz - I_{4A}z_bG_0 - z_b^2/2] >$ $< I_6 = (I_{5A}) = G_0\int(g'/g_0)^2dz >$ $< I_7 = (I_{6A}) = \int z(g'/g_0)^2dz >$ $< I_8 = (I_{8A}) = \int\int(g'/g_0)^2dzdz - I_{5A}z_b/G_0 >$ $< I_9 = (I_{11A}) = G_0^{-4}\{\int[\int(g/g_0)dz][\int\int(g/g_0)dzdz]dz - I_{1A}z_b^2G_0^2/2 - z_b^4/8\} >$ $< I_{10} = (I_{11B}) = G_0^{-4}\{\int z[\int(g/g_0)dz]^2dz - z_b^4/4\} >$ $< I_{11} = (I_{12A}) => $ $< I_{12} = (I_{12B}) => $;
example: F F 0 0.209 -0.0768 0.0552 -0.33 ;
default: F F 1 ; .

with $g_0 = g(z_b)$ being the radial field gradient in the main field region as well as $g = g(z)$ and $g' = \partial g(z)/\partial z$ denoting this field gradient and its z–derivative at an arbitrary position along the optic axis.

For <table#>=0 the numerical values of all fringing–field integrals must be listed.
For <table#>$\neq$0 the fringing–field integrals are taken from GIOS_FF.DAT. Note that

- z is the coordinate along the optic axis and that
- G_0 is the aperture radius of the multipole.
- All integrals must be taken from z_a outside to z_b inside the main–field regions.

Note here that the fringing–field integrals are only small corrections, so that usually approximate values of I_1, I_2, I_3, I_4 I_5, I_6, I_7, I_8 I_9, I_10, I_11, I_12 are satisfactory and that reasonably good results can be obtained if a set of standard fringing–field integrals is used, determined from a realistic fringing–field distribution, i.e. a field distribution in which Laplace's equations are valid everywhere. However, before the system is finally built, one should perform calculations with fringing–field distributions that are as accurate as possible, obtained from measurements or precise 2D or better–calculations. The fringing–field integrals from any such fringing–field distribution can be obtained from GIOS also (see section XXX). The use of these new, more accurate fringing–field integrals will modify the earlier results slightly to first– and second–order. In most any case, however, these modifications can be counterbalanced by slightly varying the geometry or some quadrupole and in critical cases some hexapole parameters in the optical system under consideration.

Note that a fringing field can **only be situated** between a field–free region and a multipole or quadrupole or hexapole.

3.4 Thin Lens Quadrupole Doublets [MD, ED]

A magnetic or electric doublet is approximated by thin lenses. It is possible to choose three focusing systems:

- a point–to–parallel focusing system
- a stigmatic focusing system
- an astigmatic focusing system.

The doublet must be defined in a block (see section 7.1) with the **B U** and the **B E** commands. The first quadrupole is defocusing in x–direction if the 'sign' of the block name is negative. There are four such doublet commands

M(agnetic) **D**(oublet) <block name> <identifier>; **M**(agnetic) **D**(oublet) <-block name> <identifier>;
E(lectric) **D**(oublet) <block name> <identifier>; **E**(lectric) **D**(oublet) <-block name> <identifier>;
example: B U PART ; D L 0.4 ; E Q 0.2 0.05 ; D L 0.4 ; E Q 0.2 -0.05 ; D L 0.4 ; B E ; E D -PART S ;

There are three possible choices for the <identifier>

- P: **P**oint–to–parallel focusing system
- S: **S**tigmatic focusing system
- A: **A**stigmatic focusing system

3.5 Sector Fields

3.5.1 A Magnetic Sector Field [MS]

A magnetic sector field is defined by the command:

M(agnetic) **S**(ector_field)
<radius of deflection ρ_{B0} in LLU> <angle of deflection ϕ_0 in degrees>
<half air gap G_0 in TLU> $< n_{B1} >$ $< n_{B2} >$ $< n_{B3} >$;
example: M S 1.0 90 0.05 0.51 ;
default: M S 1.0 90 0.01 0 0 0 ;

The magnetic flux density in this sector field equals

$$B(x, y = 0) \quad = \quad B_0[1 - n_{B1}\left(\frac{x}{\rho_{B0}}\right) - n_{B2}\left(\frac{x}{\rho_{B0}}\right)^2 - n_{B3}\left(\frac{x}{\rho_{B0}}\right)^3 - \ldots] \, .$$

For first– and second–order calculations n_{B1} is defined for $-1 < n_{B1} < 1$. For third–order calculations n_{B1} is defined only for $0 < n_{B1} < 1$.

3.5.2 Fringing Fields for a Magnetic Sector Field [FF]

Fringing fields for magnetic sector fields are defined by the command:

F(ringing) **F**(ield) <table# > <entrance or exit angle ε in degrees> <relative curvature ρ_{B0}/R of effective field boundary> $< I_1 = (I_{1A}) = G_0^{-2}[\int\int(B/B_0)d\zeta d\zeta - \zeta_b^2/2] >$ $< I_2 = (I_{1B}) = G_0^{-2}[\int\int(B/B_0)^2 d\zeta d\zeta - I_{4A}\zeta_b G_0 - \zeta_b^2/2] >$ $< I_3 = (I_{4A}) = G_0^{-1}[\int(B/B_0)^2 d\zeta - \zeta_b] >$ $< I_4 = (I_{4B}) = G_0^{-1}[\int(B/B_0)^3 d\zeta - \zeta_b] >$ $< I_5 = (I_{5A}) = G_0 \int(B/B_0)^2 d\zeta >$ $< I_6 = (I_{6A}) = \int\zeta(B/B_0)^2 d\zeta >$ $< I_7 = (I_{9A}) = G_0^{-2}\{\int[(B/B_0)^2 \int(B/B_0)d\zeta]d\zeta - \zeta_b^2/2\} >$ $< I_8 = (I_{10A}) = \int[(B'/B_0)^2 \int(B/B_0)d\zeta]d\zeta >$ $< I_9 = (I_{2A}) = G_0^{-3}\{\int[\zeta \int(B/B_0)d\zeta]d\zeta - \zeta_b^3/3\} >$ $< I_{10} = (I_{3A}) = G_0^{-3}\{\int[\int(B/B_0)d\zeta]^2 d\zeta - \zeta_b^3/3\} >$ $< I_{11} = (I_{2B}) = G_0^{-3}[\int(B/B_0)^2\zeta^2 d\zeta - \zeta_b^3/3] >$;
example: F F 0 10.0 1.0 0.4853 −0.5145 −0.3027 ;
default: F F 1 0 0 ; .

with $B_0 = B_\eta(\zeta_b)$ being the η–component of the magnetic flux density in the main field region as well as $B = B_\eta(\zeta)$ and $B' = \partial B_\eta(\zeta)/\partial\zeta$ denoting the η–component of this flux density and its ζ–derivative at an arbitrary position along the optic axis.

In case of <table#>=0 the numerical values of all three fringing–field integrals must be listed. In case of <table#>≠0 the fringing–field integrals are taken from GIOS_FF.DAT. Note that

- ζ is a coordinate perpendicular to the effective field boundary,
- G_0 is the half magnet air gap,

- the integral I_5 must be taken from ζ_a to the effective field boundary, i.e. to ζ =0,
- the integrals I_1 and I_4 must be taken from ζ_a outside to ζ_b inside the main–field region.

Note here that the fringing–field integrals are only small corrections so that usually approximate values for I_1, I_4, I_5 are satisfactory and that reasonably good results can be obtained if a set of standard fringing–field integrals is used, determined from a realistic fringing–field distribution, i.e. a field distribution in which Laplace's equations are valid everywhere. However, before the system is finally built, one should perform calculations with fringing–field distributions that are as accurate as possible obtained from measurements or precise 2D or better 3D calculations. This will then modify the results slightly to first– and–second order where these modifications usually can be counterbalanced by varying the geometry or some quadrupole and hexapole parameters slightly.

Note that ε (see Fig. 4.8 in Ref. 7) is positive if the normal to the field boundary is further away from the center of curvature of the optic axis than the incoming or outgoing beam. Note further, that ρ_{B0}/R (see Fig. 8.6 in Ref. 7) is positive for a convex field boundary and negative for a concave one. Note also that a fringing field can only be situated between a field–free region and a magnetic sector.

3.5.3 A Magnetic Rectangle [MR]

A magnetic rectangle is defined by the command:

M(agnetic) **R**(ectangle) <length $\ell = \rho_{B0}\phi_0$ in LLU> <magnetic flux density B in T> <half air gap G_0 in TLU> <tilt angle $\bar{\varepsilon}$ in degrees> $< n_{B1} >$ $< n_{B2} >$ $< n_{B3} >$;
example: M R 1.0 0.58 0.05 ;
default M R 1.0 0.58 0.01 10 0 0 0 ;

In GIOS the **MR**–command invokes a **MS**–command for which the entrance and exit angles of a magnetic sector field, are both chosen to be $\varepsilon_1 = \phi_0/2 - \bar{\varepsilon}$ and $\varepsilon_2 = \phi_0/2 + \bar{\varepsilon}$. Usually, the magnetic flux density in a magnetic rectangle is homogeneous ($n_{B1} = n_{B2} = n_{B3} = 0$). However, if n_{B1}, n_{B2} and/or n_{B3} are non zero, a radially inhomogeneous magnetic sector field is assumed as defined above in section 3.4.1.

3.5.4 Fringing Fields for a Magnetic Rectangle [FF]

Fringing fields for magnetic rectangles are defined analogously to those for magnetic sector fields including the curvatures of the field boundaries. However, the entrance/exit angle must be omitted since the ($\bar{\varepsilon}$) are defined in the **MR**–command.

3.5.5 An Electrostatic Sector Field [ES]

An electrostatic sector field is defined by the command:

E(lectrostatic) **S**(ector–field) <radius of deflection ρ_{E0} in LLU> <angle of deflection ϕ_0 in degrees> <half electrode gap G_0 in TLU> $< n_{E1} > < n_{E2} > < n_{E3} >$;
example: E S 1.0 90 0.03 1 ;
default: E S 1.0 90 0.01 0 0 0 ;

where the toroidicity of the mid–equipotential surface of the sector field is determined by R_E (see Fig. 4.17 in Ref. 7) with

$$\frac{\rho_{E0}}{R_E} = n_{E1} + n_{E2}\left(\frac{x}{\rho_{E0}}\right) + \frac{n_{E3}}{2}\left(\frac{x}{\rho_{E0}}\right)^2 + \ldots$$

For first– and second–order calculations n_{E1} is defined for $-2 < n_{E1} < 2$. For third–order calculations n_{E1} is defined only for $0 < n_{E1} < 2$. Special cases are:

- cylindrical electrodes: $n_{E1} = n_{E2} = n_{E3} = 0$
- spherical concentric electrodes: $n_{E1} = -n_{E2} = n_{E3} = 1$
- toroidal electrodes, i.e. electrodes which intersect the xz– as well as the yz–planes in circles: $n_{E1} \neq n_{E2} \neq n_{E3} \neq 0$

3.5.6 Fringing Fields for an Electrostatic Sector Field [FF]

Fringing–field integrals for electrostatic sector fields (see # 19 in the FF-integral table) are defined by the command:

F(ringing) **F**(ield) <table# > <entrance or exit angle ε > <relative curvature ρ_{E0}/R of effective field boundary> $< I_1 = (I_{1a}) = G_0^{-2}[\int\int(E/E_0)d\zeta d\zeta - \zeta_b^2/2] >$ $< I_2 = (I_{1b}) = G_0^{-2}[\int\int(E/E_0)^2 d\zeta d\zeta - \zeta_b^2/2 - I_{4a}\zeta_b G_0] >$ $< I_3 = (I_{4a}) = G_0^{-1}[\int(E/E_0)^2 d\zeta - \zeta_b] >$ $< I_4 = (I_{4b}) = G_0^{-1}[\int(E/E_0)^3 d\zeta - \zeta_b] >$ $< I_5 = (I_{5A}) = G_0 \int(E'/E_0)^2 d\zeta >$ $< I_6 = (I_{6A}) = \int \zeta(E'/E_0)^2 d\zeta >$ $< I_7 = (I_{3A}) = G_0^{-3}\{\int[\int(E/E_0)]^2 d\zeta - \zeta_b^3/3\} >$ $< I_8 = (I_{3B}) = G_0^{-3}\{\int[\int(E/E_0)^2 d\zeta][\int(E/E_0)d\zeta]d\zeta - I_{4A}\zeta_b^2 G_0/2 - \zeta_b^3/3\} >$;
example: F F 0 0 0.09819 0.1217 −0.2404 −0.3781 0.72 −0.6924 0.03167 0.06924 ;
example: F F 1 0 0 ;

with $E_0 = E_\xi(\zeta_b)$ being the ξ–component of the electrostatic field strength in the main field region as well as $E_\xi = E_\xi(\zeta)$ and $E' = \partial E_\xi(\zeta)/\partial\zeta$ denoting the ξ–component of this field strength and its ζ–derivative at an arbitrary position along the optic axis. For the entrance angle ε **only** "0" is allowed up to now.

In case of <table#>=0 the numerical values of all fringing–field integrals must be listed explicitly. In case of <table#>≠0 the fringing–field integrals are taken from GIOS_FF.DAT. Note that

- ζ is a coordinate perpendicular to the effective field boundary and that
- G_0 is the half electrode gap.
- All integrals must be taken from ζ_a outside to ζ_b inside the main–field region.

Note here that the fringing–field integrals are only small corrections so that usually approximate results for I_{1a}, I_{1b}, I_{4a}, I_{4b}, I_5, I_6, I_7, I_8 are satisfactory and reasonably good results can be obtained if a set of standard fringing–field integrals is used, determined from a realistic fringing–field distribution, i.e. a field distribution in which Laplace's equations are valid everywhere. However, before the system is finally built, one should perform calculations with fringing–field distributions that are as accurate as possible obtained from measurements or precise 2D– or better 3D–calculations. This will then modify the results slightly to first– and second–order where these modifications usually can be counterbalanced by varying the geometry or some quadrupole and hexapole parameters slightly.

Note that ρ_{B0}/R is positive (or negative) for a convex (or a concave) field boundary. Note also that a fringing field can only be situated between a field–free region and a sector field.

3.6 A Wien Filter [WF]

A Wienfilter is defined by the command

W(ien) **F**(ilter) <length ℓ in LLU>
<radius of deflection ρ of optic axis in LLU> <magnetic flux density in T> <half magnet air gap G_{B0} in TLU> <half electrode distance G_{E0} in TLU> <radius R_B of magnetic flux lines in TLU> <radius R_E of mid–equipotential surface in TLU> <variation dR_B/dx of radius of magnetic flux lines> <variation dR_E/dx of radius of mid–equipotential surface> <height h$\leq 2G_{B0}$ of electrodes in TLU> <identifier1> <identifier2> ;
example: W F .3 0 .5 .01 .01 0 0 0 0 . 008 0 1 ;

If the <identifier 1> is 0 the height of the electrodes is assumed to be infinite. There are two choices for the <identifier 2>

- 0: the magnetic and the electrostatic fringing fields coincide
- 1: the electrostatic fringing field is inside a magnetic sector field,
  i.e. the electrodes end within the magnet.

3.7 Changing the Direction of Deflection [CB]

GIOS assumes that all sector fields deflect the particle beam in the negative x–direction, i.e. to the right, looking downstream. However, a change of the direction of deflection can always be invoked by the command:

C(hange) **B**(ending_direction) ;
example: C B ;

4 The Selection of GIOS Output

The GIOS output always starts by listing the corresponding input file. A message: "error card" in this listing indicates that something was wrong in the preceding line of the input file. Since GIOS has a finite capacity to store input–file entries (< 600), apertures (< 10), algebraic expressions (< 20), etc., some error messages may refer to storage limitations being exceeded, rather than disclose a fault in the format or syntax of the offending line.

The second portion of the output contains a compilation of the source– and particle–definitions and a detailed description of the optical system under consideration. In front and in back of each drift distance the floor coordinates U, V are listed together with the angle of the beam direction W. Note that the first sector field is always assumed to deflect to the right, i.e. towards negative V–values.

4.1 Changing Floor Coordinates [CF]

Usually the floor coordinates are U=V=W=0 initially. However, there is the possibility to change this presetting[5] by the command:

C(hange) **F**(loor-coordinates) <U in LLU> <V in LLU> <W in degrees> ;
example: F 0 5 -30 ;

At any position z_i, corresponding to the position z_i in the input file, the following printouts can be initiated which describe the transfer matrix of the system from z_0 to z_i or beam properties at z_i.

4.2 Printout of Transfer Matrices from z_0 to z_i [SC, NC]

For the printout of transfer matrices symplektic or nonsymplektic coordinates can be chosen in GIOS. If a nonsymplektic coordinate system is chosen, the beam inclinations relative to the optic axis are described by:

$$\mathrm{A} = p_x/p_z = \tan(\alpha) \qquad \mathrm{B} = p_y/p_z = \tan(\beta)$$

where p_x, p_y, p_z are the x, y, z components of the momentum of the particle under considerations. If a symplektic coordinate system is chosen, the beam inclinations are described by:

$$\mathrm{A} = p_x/p_0 = \sin(\alpha)\sqrt{\frac{(1+\delta_K)(1+\delta_m)}{1+\cos^2\alpha\tan^2\beta}} \qquad \mathrm{B} = p_y/p_0 = \sin(\beta)\sqrt{\frac{(1+\delta_K)(1+\delta_m)}{1+\cos^2\beta\tan^2\alpha}}$$

where p_0 is the momentum of the reference particle.

A symplektic coordinate system for the downstream system is chosen by the command

S(ymplektic) **C**(oordinate_system) ;

while a nonsymplektic coordinate system for the downstream system is chosen by the command

N(onsymplektic) **C**(oordinate_system) ;

As a default a nonsymplektic coordinate system is assumed.

[5]The **"C F"** command changes the initial U,V,W coordinates in the GIOS system printout as well as in the `BEAM_CUR.MTA` file and the corresponding system graph.

4.2.1 Printout of one System Transfer Matrix [PM]

A transfer matrix that connects the beam at z_0 and z_i is printed by the command:

P(rint) **M**(atrix) ;
example: P M ;

Note that the position z_i is described in LLU and the time the reference particle needed to arrive at this z_i is described in TU=μsec LLU/m. Thus TU is given in μsec if LLU is in meters. Note further that one overall tranfer matrix is automatically printed at the end of each GIOS calculation; therefore, a **PM**–command is needed only when intermediate results are desired.

4.2.2 Printout of the Magnitudes of Aberrations [PN]

The matrix elements $(r_i|x^k a^\ell y^m b^n \delta_K^o \delta_m^p)$ multiplied by $x_{00}^k a_{00}^\ell y_{00}^m b_{00}^n \delta_{K0}^o \delta_{m0}^p$, are determined and listed in the same fashion as transfer matrices by the command:

P(rint) **N**(umerical_trajectory_deviations) <identifier> ;
example: P N ;
example: P N E ;

There are three possible choices for the <identifier> (see ref. 19):

- P: parallelogram–like phase–space areas in (x, a) and (y, b) are assumed (default);
- E: elliptical phase–space areas in (x, a) and (y, b) are assumed;
- S: a "spherical" phase–space volume in (x, a, y, b) is assumed.

The **PN**–command provides a simple way to judge the relative importance of aberrations.

4.2.3 Printout of Couple Coefficients [PCC]

The derivatives of the image aberrations at the end of the optical system with respect to a ficticious multipole element at $z = z_i$ are calculated and listed in the same fashion as transfer matrices at $z = z_i$ by the command:

P(rint) **C**(ouple) **C**(oefficients) ;
example: P C C ;

4.2.4 Printout of the Positions of the Next Images, Pupils and Waists [PI]

The distances from z_i to the next image, waist and pupil are calculated by the command:

P(rint) **I**(mages_waists_pupils) ;
example: P I ;

4.2.5 Printout of Beam Diameters, Twiss Parameters and Phase Shifts [PE]

The beam envelopes and Twiss parameters at $z = z_i$ as well as the phase shift ψ_i between z_0 and z_i are printed or both parallelogram–like for elliptical phase–space areas by the command:

P(rint) **E**(envelope) ;
example: P E ;

4.3 A Printer Plot of the Focal Planes [PF]

A printer plot of the shape of the focal planes are produced by the command:

P(lot) **F**(ocal_Plane) <identifier> <shown maximal x–width in TLU> <shown maximal z–length in LLU> ;
example: P F E ;

There are two possible choices for the <identifier>:

- M: the angle– and energy–image curves are shown for ions of different masses;
- E: the angle– and mass–image curves are shown for ions of different energies.

If the maximal x– and z–widths are not given explicitly, they are chosen as default values such that the trajectories are included in the shown printer plot. For the calculations the energy–deviation δ_K and the mass–deviation δ_m are used as they were defined by the **DP**–command.

4.4 Plots of Beam Envelopes

4.4.1 Printer Plot of the Beam Envelope [PB]

A printer plot of the optical system under consideration is produced showing the calculated first–order envelope of the real beam (indicated is also a beam formed by trajectories that start from a point source under angles A and B) by the command:

P(lot) **B**(eam) <identifier> <number of printer lines> <shown maximal x–width in TLU> <shown maximal y–width in TLU>
example: P B 100 0.15 0.15 ;
example: P B E 100 0.05 0.05 ;
default: P B P 100 0.10 0.10 ;

There are two possible choices for the <identifier>:

- P: representing a parallelogram–like phase–space area;
- E: representing an elliptical phase–space area.

If the <identifier> is left off completely, GIOS assumes: <identifier>=P, if PX, PY were used at the beginning of the GIOS input or <identifier>=E, if TX, TY were used.

4.4.2 Graphic Output of System and Trajectories [PB]

A graphic output calculated to second– and third–order is obtained by a command very similar to the printer plot of 4.4.1 by:

P(LOT) **B**(EAM) <identifier> <length of plot in cm> <shown maximal x–width in TLU> <shown maximal y–width in TLU> <width of plot in cm> <N: number of plots> <plot resolution in z direction in cm> < x_0: number of trajectory starting points in the x–coordinate> < a_0: number of trajectory starting points in the a–coordinate> < g_0: number of trajectory starting points in the g–coordinate> < d_0: number of trajectory starting points in the d–coordinate> < y_0: number of trajectory starting points in the y–coordinate> < b_0: number of trajectory starting points in the b–coordinate> ;
example: P B 30 0.1 0.1 2 2 0.02 2 2 1 3 2 2 ;
example: P B E 40 0.1 0.1 2.5 2 0.03 2 2 1 3 2 2 ;

There are two possible choices for the <identifier>:

- P: representing a parallelogram–like phase–space area;
- E: representing an elliptical phase–space area.

If the <identifier> is left off completely, <identifier>=P, if PX, PY were used at the beginning of the GIOS input or <identifier>=E, if TX, TY were used. The calculation is performed to the order given in the "Calculation Order"–command.

When the number of graphs is set to $N = 1$, only the horizontal and vertical plots for the system with straightened optic axes are generated: "**beam_str.mta**". For $N = 2$ a realistic top–view with correct floor coordinates is shown in addition: "**beam_cur.mta**", as well as a graphic representation of the field strength of indifferent elements along the optic axis: "**fields.mta**". The total number of starting points of trajectories is distributed equally spaced within the initially defined phase–space areas x_0, a_0 or y_0, b_0 or within the range of masses (g_0) and energies (d_0) as defined in the "Deviation Parameter"–command. Note that the "**length of a plot**" can safely be ignored but must be included in the command. This number must be within 20 and 70. Note also that the total number of trajectories increases rapidly according to

$$n_x = x_0 * a_0 * g_0 * d_0 \quad and \quad n_y = y_0 * b_0 * g_0 * d_0 \ .$$

4.4.3 Graphic Output of Values of Arithmetic Functions [DF]

The value F(z) of a defined arithmetic expression is shown along the optic axis: "**func**.mta**".

D(raw) **F**(unctions) <arithmetic expression> <shown maximal x–width in TLU> <shown maximal z–width in LLU>
example: D F =R ;

4.4.4 Beam Plot of a Segment of the Optical System [PS]

To plot only a portion of an ion–optical system starting at z_i, one must use the command:

P(lot) **S**(egment) <identifier> <length of plot in cm> <shown maximal x–width in TLU> <shown maximal y–width in TLU> <width of plot in cm> <N: number of plots> <plot resolution in z direction in cm> < x_0: number of trajectory starting points in the x–coordinate> < a_0: number of trajectory starting points in the a–coordinate> < g_0: number of trajectory starting points in the g–coordinate> < d_0: number of trajectory starting points in the d–coordinate> < y_0: number of trajectory starting points in the y–coordinate> < b_0: number of trajectory starting points in the b–coordinate> ;
example: P S 30 0.1 0.1 2 2 0.02 2 2 1 3 2 2 ;
example: P S E 40 0.1 0.1 2.5 2 0.03 2 2 1 3 2 2 ;

The parameters are the same as for the "Plot_Beam"–commands of section 4.4.1 and 4.4.2. The plot terminates at the position z_i in the input file with the command:

P(lot) **S**(egment_end) ;

4.5 Plots of Intensity Distributions

4.5.1 Printer Plots of Intensity Distributions in Phase–Space [PP]

A printer plot of an intensity distribution in phase–space is initiated at z_i by the command:

P(lot) **P**(hase_space) (f,g) <identifier> <total number of particles> <f–dimension of plot> <g–dimension of plot> <total number of mass values> ;
example: $R = ((@, X) \uparrow 2 + (@, Y) \uparrow 2) \uparrow 0.5$); P P (R,D) P 1000 0.025 0.050 1 ;

The following choices are possible for either f or g in (f,g):

X = final X–position	x = initial X–position
A = final A–angle	a = initial A–angle
G = mass (quantized)	g = mass (quantized)
D = energy (quantized)	d = energy (continuous)
Y = final Y–position	y = initial Y–position
B = final B–angle	b = initial B–angle
T = final time	t = final time
N = ray counter (how many rays)	n = count in window

In addition, any other letter can be used if it has been defined upstream as an algebraic variable. The special expression $(@, k)$ may be used to substitute individual trajectory coordinates (i.e.; $k = X, A, G, D, Y, B, T$) into arithmetic expressions (see section 5.1) before plotting.

The total number of mass values are distributed equally over the mass widths defined in the "D(eviation) P(arameter)"–command.

There are three possible choices for the <identifier>:

- P: the initial distributions in f and g are chosen independently;
- E: only those (x,a) or (y,b) combinations are chosen which lie inside (x_{00},a_{00}) or (y_{00},b_{00}) ellipses;
- S: only those (x,a), (y,b) or (x,y) combinations are chosen which lie inside (x_{00},a_{00}), (y_{00},b_{00}) or (x_{00}, y_{00}) ellipses.

All parameters following (f,g) can be omitted. As default the <identifier> equals P and GIOS assumes 1000 particles and one mass; the size of the plot is chosen automatically by the program according to a first–order calculation.

4.5.2 Graphic Output of Intensity Distributions in Phase–Space [PQ, PP]

A graphic output "**pspace**.mta**" similar as the printer plot produced by the "P(lot) P(hase_space)"–command of section 4.5.1 is obtained by inserting the following command directly before the "P(lot) P(hase_space)"–command:

P(lot) **Q**(uality) <contour line of a times the maximum intensity> <contour line of b times the maximum intensity> <contour line of c times the maximum intensity> <contour line of d times the maximum intensity> <contour line of e times the maximum intensity> <contour line of f times the maximum intensity> ;
example: P Q .1 .3 .5 .7 .9 ; P P (x,y) 10000 .02 .10 3 ;

where for each number a,b,c,d,e,f a contour line is shown. An entry < 0.01 will default to a contour line at 0.05 and an entry > 0.99 will default to 0.95.

4.5.3 Defining Aperture Slits [AS]

In connection with the "P(lot) P(hase_space)"–command in section 4.5.1 and the graphics "P(lot) B(eam)"–command in sections 4.4.1 and 4.4.2, one can introduce up to 10 commands to simulate the effects of aperture slits positioned upstream at any z_i by the command:

A(perture) **S**(lit) <identifier> $< \pm d_x$ size in x–direction in TLU> $< \pm d_y$ size in y–direction in TLU> ;
example: A S S 0.01 0.01 ;

There are two possible choices for the <identifier>:

- P: a rectangular aperture is assumed of cross section $2d_x 2d_y$;
- E: an elliptical aperture is assumed of cross section $\pi d_x d_y$;

4.5.4 Defining Current Densities in the Beam [B]

In connection with the "P(lot) P(hase_space)"–command and the "P(lot) B(eam)"–command, one can define an initial particle–density distribution by the command:

B(eam) <identifier> <distance d_0 in TLU between center of distribution and optic axis> <half width g_0 in TLU of the distribution> <n, with $j = 1 - (g/g_0)^n$ defining the distribution with $g \leq g_0$ >
example: B X 0.005 0.003 2 ;

There are three possible choices for the <identifier>:

- X or Y in TLU ;
- A or B ;
- G or D in units of the reference mass m_{00} or energy K_0 .

If the command reads only BX, BY, BA, BB, BG, BD; a homogeneous distribution $n = \infty$ is assumed as default with g_0 being the maximal coordinate given in the initial phase space definitions PX or PY. When several PP–commands (see section 5.11) are used in the same GIOSIN.DAT–file, each PP–command may be preceded by a set of BEAM–commands to define a new and independent selection of trajectories for each graph.

4.5.5 Defining Beam–Shifts and Beam–Rotations [SR]

In connection with the "P(lot) P(hase_space)"–command one can shift and rotate the coordinate system at any z_i by the command:

S(hift) **R**(otate) < x–shift in TLU> < a–bend in RAD> < y–shift in TLU> < b–bend in RAD> <rotation Θ around the optic axis in degrees> ;
example: S R 0.01 0.01745 0 0 0 ;

The SR–command will be executed in the following order: firstly bends, secondly shifts and thirdly rotations.

For positive values of bends and shifts the optic axis is bent and shifted in the negative x– and y–directions. A positive value of Θ causes a righthand rotation of the xy–plane around the optic axis so that a point $x_1 = y_1 > 0$ becomes $x_2 > x_1$, $y_2 < y_1$ for small values of Θ. Note that the SR–command only modifies the phase–space graphs. Note especially that, though feasible in principle the SR–command does not modify the floor coordinates UV. When combining the SR–command and the CB–command be especially careful to count the bend angles all in the correct direction!

5 Arithmetic calculations

Arithmetic calculations are possible with standard functions (+), (−), (∗), (÷), (|), ABS (...), SIGN (...) and up to five levels of brackets.

5.1 The Definition of Arithmetic Expressions

The definition of a name for an arithmetic expression is performed by the command:

W(one–letter_name) = ... arithmetic expression ... ;
example: B=(X,AD)/((A,A)∗(X,D)) ;
example: A=2 ∗0.5 −F ;

In the second example F must have been defined upstream as an arithmetic expression.

The ... arithmetic expression ... may contain the following operators:

- constants [real numbers like 0.5 or 1.0 followed by at least one blank (␣)]
- names of other arithmetic expressions
- elements of the transfer matrix at z_i, for instance, (X,A), (Y,B), (X,AA), (X,AAD), ...
- coordinates of rays (see section 4.5.1), for instance, $(@, x)$, $(@, A)$,$(@, Y)$, ...
- names of variables (see section 6.4)

5.2 Using Algebraic Formulas

Use of a **prior defined** name of an arithemtic expression, i.e. an "algebraic variable" in a GIOS–command, is achieved by

... = W ...
example: D L =A ;

6 Selection of FIT Routines

6.1 The Interactive Fit [*INT]

For an "interactive fit" the first line in the GIOSIN.DAT file must read <u>only</u>:

∗**INT**(eractive)
example: ∗**INT** **DESIGN** 17A ... ... ;

and the second line must contain the title. Then one can stop, restart or cancel the optimisation procedure at any time as well as set variables and print–out parameters. A description of the possibilities is given in a menu on–line.

6.2 Varying the Length of a Field–Free Region to achieve an Image, a Pupil or a Waist [FI, FP, FW]

There are three commands which add a drift length ΔL to an existing system at z_i where ΔL is chosen such that an image, a waist or a pupil is achieved at $z = z_i + \Delta L$. These commands are:

F(it) **I**(mage) <identifier> < z_{max} in TLU> < z_{min} in TLU> ;
F(it) **W**(aist) <identifier> < z_{max} in TLU> < z_{min} in TLU> ;
F(it) **P**(upil) <identifier> < z_{max} in TLU> < z_{min} in TLU> ;

There are two possible choices for the <identifier>:

- X: a x–image, a x–waist, a x–pupil;
- Y: a y–image, a y–waist, a y–pupil.

6.3 Choosing a Fitting Algorithm [FS, FG]

There are two fitting algorithms installed in GIOS ("simplex" or "conjugated gradients") which are activated by the commands:

F(it) **S**(implex) <number of fit cycles> ;
F(it) **G**(radient) <number of fit cycles> ;
example: F G 10 ;
default: F S 25 ;

The number of fit cycles determines after how many iterations intermediate results are printed. For most optimisations it is recommended to use FS.

6.4 Selecting Variables [V]

Quantities which should be varied must be amended by

... **V**(w <lower limit> <higher limit>) ...

In case the lower and higher limits are omitted, these limits are assumed to be $-\infty$ and $+\infty$.

example: D L 1.0V(Z) ;
example: H = 1.0V(B 0.1 1.5) ; D L =H ;

The name w stands for an one–letter symbol that allows subsequent referencing (or coupling) to another variable. If there is no need for a back reference the one–letter symbol can be omitted.

example: D L 1.0V ;
example: D L 1.0V(0.75 1.25) ;

In case two variables have the same name, the variables are varied in the same or in the opposite direction if the names of the two variables have the same or the opposite sign, respectively. If the names of the two variables have opposite signs the variables are varied in opposite directions.

example: D L 1.0V(+C) ; or D L 1.0V(C) ;
example: D L 1.0V(+C) ; D L 1.0V(−C) ;

6.5 How to Cause some Matrix Elements to Attain Desired Values [F]

If it is desired that a certain matrix element takes up a goal value at z_i, one can use the command:

F(IT) (**f,g**) <goal_value> <weight> !a,b,c, ... ;
example: F (X,AA) 0 ;
example: F (X,A) 0 10000 !C,S ;

(f,g) here characterizes some matrix element. The symbols a,b,c are names of variables as defined in section 6.4.

The goal for the fitting routine is to minimize the sum of all $\Sigma\{[(f,g)-\text{goal\_value}]*\text{weight}\}^2$. In case that the weight factor has a negative sign, the fit routine stops as soon as the expression [abs((f,g)∗weight)] is smaller than [abs(goal_value)]. As default the goal value is assumed to be 0, the weight 1 and the list of variable names to include the names of all variable quantities.

6.6 How to Cause some Algebraic Variables to Attain Desired Values [FA]

In a similar manner that a matrix element can be postulated to attain certain values at z_i, one can postulate a certain algebraic variable to attain a goal value at z_i by the command:

F(it) **A**(lgebraic) <algebraic_variable> <goal_value> <weight>
example: F A A 0 ;
example: F A B 4.5 1000;

The symbols a,b,c are names of variables as defined in section 6.4.

The goal for the fitting routine is to minimize the sum of all
Σ{[<algebraic_variable> −goal_value] ∗weight}^{2}. In case the weight factor has a negative sign, the fit routine stops as soon as [abs(<algebraic_variable> ∗weight)] is smaller than [abs(goal_value)]. As default the goal value is assumed to be 0, the weight 1 and the list of variable names to include the names of all variable quantities.

6.7 How to Cause some Floor Coordinates to Attain Desired Values [FC]

There is also the possibility to postulate that the floor coordinates U,V or the angle W of the optic axis relative to its initial direction attain certain values by the command

F(it) **C**(oordinate) @ <goal_value> <weight> ;

@ stands for either U or V or W.

The goal for the fitting routine is to minimize the sum of all $\Sigma\{[C-\text{goal\_value}]*\text{weight}\}^2$. In case the weight factor has a negative sign, the fit routine stops as soon as [abs($(C - goal\_value)$∗weight)] is smaller than [abs(goal_value)]. As default the goal value is assumed to be 0, the weight 1 and the list of variable names to include the names of all variable quantities.

6.8 How to cause Beam Envelopes to attain certain Values [FE]

The first–order cross section of a beam can be fitted to a desired value by the command

F(it) **E**(nvelope) <identifier> **@** <goal value for beam cross section> <weight>;
example: F E E Y .01 999 ;

@ stands for either X or Y. There are two possible choices for the <identifier>:

- P: parallelogram–like phase–space areas (x, a) and (y, b) are assumed;
- E: elliptical phase–space areas (x, a) and (y, b) are assumed.

If the <identifier> is left off completely, **P** is chosen if **PX**, **PY** were used at the beginning of the GIOS input and **E** is chosen if **TX**, **TY** were used.

The goal for the fitting routine is to minimize the sum of all $\Sigma\{[@-\text{goal\_value}]*\text{weight}\}^2$. In case that the weight factor has a negative sign, the fit routine stops as soon as the expression [abs((@−goal_value)∗weight)] is smaller than [abs(goal_value)]. As default the goal value is assumed to be 0, the weight 1 and the list of variable names to include the names of all variable quantities.

7 Optical Systems Consisting of Repetitive or of Mirror–Symmetric Cells

7.1 The Definition of a Sub–System [BU, BE]

A BLOCK of a system is characterized by a name that consists of several letters and/or numbers. A block is defined by:

B(lock) **U**(nit) <block name> ;
. . .
. . .
B(lock) **E**(nd) ;

The block–name may consist of up to four letters. This command causes the command lines of the corresponding block to be stored and the transfer matrix of the block to be calculated. The fit commands in this BLOCK will be used only to calculate the transfer matrix of the block.

7.2 Using an Earlier Defined Block [IB]

The input command lines of a block defined in section 7.1 are included[6] in an optical system by one of the commands:

[6]Note that inside a **B**(lock) one can only

1. use the "C R" command if the reference energies at the entrance and exit of the block are identical
2. include an external accelerating matrix if it applies to the phase–space before the acceleration column.

I(nclude) **B**(lock) <block name> ;
I(nclude) **B**(lock) < −block name> ;

In the second case, the command lines of the block are included in reverse order[7]. This is useful for the design of mirror symmetric systems.

7.3 Storing the Transfer Matrix of a Block [WM]

The transfer matrix of a block as defined in section 7.1 is written to the file TAPE09.DAT by the command

W(rite) **M**(atrix) <block name> ;

For writing the system matrix of the entire system onto TAPE09.DAT, the block name must be "*" only. In this case the name of the matrix is taken from the first four characters of the title line.

7.4 Using the Stored Transfer Matrix of a Block [IM]

The transfer matrix of a block as defined in section 7.1 is included in an optical system by the command

I(nclude) **M**(atrix) <block name> ;

The matrix used here can either be defined in a "B(LOCK) U(NIT)"–command or it will be read from the file from TAPE09.DAT, if it had been written to the file TAPE09.DAT in a previous GIOS run .

7.5 Defining a System that Consists of Many Similar Sub–Systems [DS, DE]

In certain cases, some sub–system must be used repeatedly. This is achieved by the almost self–explanatory command:

D(o) **S**(equence) <number of cycles> ; . . . ; . . . ; **D**(o) **E**(nd) ;

8 Calculating Lists of Systems

8.1 Varying specified Quantities [DL]

To determine the dependence of an optical system from one of its quantities, one can use the command

[7] Note here that the "I M" command can not be used inside a reversed block.

```
D(ata) L(ist) <name of variable>
        <first value to be used as variable>
        <second value to be used as variable>
        <third value to be used as variable>
        < ... > ;
```

Here the variable of the given name takes up the listed numerical values, for each of which GIOS must calculate the optical system once. This variable must be defined in a preceding GIOS–command as

```
... < numerical value> D (<name of variable>)
```

The "D(ata) L(ist)"–command must be added at the end of the GIOS–input in the following manner:

```
title line
... ;
... ;
... ;
END ;
REPEAT
D L ... ;
D L ... ;
END ;
```

If more than one D L–command is found, GIOS calculates the optical system for all possible combinations of the corresponding variables [see also Example 4 in the Appendix].

As default there is no data output for a REPEAT–command.

8.2 Storing GIOS Results [WD]

In order to write specific GIOS results as a table on the file TAPE10.DAT one must use the command:

```
W(rite) D(ata) @ <identifier> ;
```

@ here stands for:

- the name of a variable,
- an algenraic expression,
- a matrix element (f,g) where the value of this matrix element is multiplied by the corresponding maximal values of X,A,G,D,Y or B defined in the PX, PY or TX, TY commands.

The <identifier> – here a name of the result – is written onto TAPE10.DAT. This file must later be read with a standard FORTRAN program.

9 Appendix

9.1 Comparison between GIOS, TRANSPORT and MARYLIE

We have compared to third order the results of GIOS, TRANSPORT and MARYLIE as far as magnetic quadrupoles and magnetic sector fields are concerned[8]. In these comparisons GIOS and MARYLIE were in very good agreement to third order including fringing field terms while there were differences already to lower orders between GIOS and TRANSPORT. For such comparisons, however, it should be noted that the description of particle trajectories in MARYLIE and in TRANSPORT are slightly different. In TRANSPORT the inclinations of ion trajectories are desribed by x'=p_x/p_z and y'=p_y/p_z, where p_x, p_y, p_z denote the x, y, z components of the momentum of the particle under consideration. In MARYLIE the inclinations of particle trajectories are described in by x'=p_x/p_0 and y'=p_y/p_0, i.e. in the so called "symplektic" form, with p_0 being the momentum of the reference particle. In GIOS both descriptions are allowed. In its standard form GIOS uses the "nonsymplektik" form used in TRANSPORT and as a nonstandard option the "symplektik" form used in MARYLIE. Note that the elements of a "symplektic" and a "nonsymplektic" transfer matrix should all agree except for the second order chromatic elements and for all third order elements.

In some instances the need arose to recalculate a TRANSPORT calculation by using GIOS. Since TRANSPORT neglects some of the fringing–field effects the results can not be identical though they usually are similar. Before starting such a recalculation by GIOS it is useful to use the GIOS description of fringing fields such that only the rough TRANSPORT approximation of fringing fields is used.

In case the ion optical system starts with an upright phase space, i.e. if one chooses in GIOS: Lx=Ly=∞ (with ∞ being written as 0 in the **"P X"** and **"P Y"** commands)one finds that:

1. for magnetic quadrupoles[9]. the results of the TRANSPORT command

   5.0 1.0 -8.03316 2.5

   can be simulated by GIOS, by describing in its nomenclature a correspondingly nonrealistic fringing field distribution by:

   ```
   F F 0 ;
   M Q 1.0 -0.803316 0.025 ;
   F F 0 ;
   ```

2. For magnetic sector fields the results of the TRANSPORT command

[8] Electrostatic elements are so far only described in GIOS but not in TRANSPORT or in MARYLIE

[9] Usually the neglection of fringing fields in TRANSPORT results in pole tip flux densities which are $\leq 1\%$ wrong. Such a deviation then must be corrected experimentally by varying the magnet currents in the finally built quadrupoles.

1.........5.39741
16.0 5 5
16.0 7 .35
2.0 10
4.0 2.61799 18
2.0 10

can be simulated by GIOS to second order by describing in its nomenclature a correspondingly nonrealistic fringing field distribution by:

```
R P 322014 238.0592 ;
F F 0 10 0 0 -.7 0 ;
M S 10 15 0.05 ;
F F 0 10 0 0 -.7 0 ;
```

The third order terms of TRANSPORT can be reproduced by GIOS only if the FF-commands are left off completely, i.e., if absolutely no fringing field effects are taken into account.

9.2 How to rerun a TRANSPORT–calculation by GIOS

When an ion-optical system has been optimized by TRANSPORT, it can be a good idea to further optimize it by GIOS, since then the fringing fields can better be taken into account. A certain problem arises, however, since the input data of TRANSPORT must be modified so that GIOS can calculate the same problem. Besides the need to describe the optical system, it here is necessary to change the σ_{ij}-description of the initial oblique phase-space ellipse in TRANSPORT to the initial oblique parallelogram-like phase-space area of GIOS with an inscribed phase-space ellipse. Assuming that one knows the values of

- $\sqrt{\sigma_{11}}$, $\sqrt{\sigma_{22}}$, r_{21} as well as ε_x
  with $\pi\varepsilon_x$ being the area of the xx' phase-space ellipse
- $\sqrt{\sigma_{33}}$, $\sqrt{\sigma_{44}}$, r_{43} as well as ε_y
  with $\pi\varepsilon_y$ being the area of the yy' phase-space ellipse

one should fill into the 3_{rd} and 4_{th} lines of the GIOS-input file:

1. in case one wants to use the standard GIOS description of a parallelogram-like phase-space area –into which an ellipse is inscribed with the ellipse being tangential to the parallelogram at the midpoints of all its sides–
   - P X $<\sqrt{\sigma_{11}}>$ $<\varepsilon_x/\sqrt{\sigma_{11}}>$ $<\frac{-1}{r_{21}}\sqrt{\frac{\sigma_{11}}{\sigma_{22}}}>$
   - P Y $<\sqrt{\sigma_{33}}>$ $<\varepsilon_y/\sqrt{\sigma_{33}}>$ $<\frac{-1}{r_{43}}\sqrt{\frac{\sigma_{33}}{\sigma_{44}}}>$
2. in case one wants to use the GIOS description of an elliptical phase-space area –around which a parallelogram with two upright sides is circumscribed–
   - T X $<r_{21}/\sqrt{1-r_{21}^2}>$ $<\sigma_{11}/\varepsilon_x>$ $<\varepsilon_x>$

- T Y $< r_{43}/\sqrt{1-r_{43}^2} >$ $< \sigma_{33}/\varepsilon_y >$ $< \varepsilon_y >$.

In order to compare the results of the TRANSPORT and the GIOS calculations one can make GIOS to also calculate the values of R=$\sqrt{\sigma_{11}}$, S=$\sqrt{\sigma_{22}}$, T=r_{21} and U=$\sqrt{\sigma_{33}}$, V=$\sqrt{\sigma_{44}}$, W=r_{43} by writing at the top of the list of elements in the GIOS-input file:

- X = $< \sqrt{\sigma_{11}} >$;
- E = $< \varepsilon_x >$;
- A = E/X ;
- Y = $< \sqrt{\sigma_{33}} >$;
- F = $< \varepsilon_y >$;
- B = F/Y ;

and at the end of the GIOS-input file, i.e. after the output transfer matrix has been determined, calculate the above required quantities via an arithmetic expression. An example, in which this is done, is added for illustrating purposes.

```
EXAMPLE OF HOW TO DETERMINE S11, S22, R21, S33, S44, R43
;ASSUME: SQRT(S11)=.005, SQRT(S22)=.002, R21=-.998, EPS=.0005
;ASSUME: SQRT(S33)=.002, SQRT(S44)=.004, R43=-.985, EPS=.0004
R P .1 100 1 ;
P X .005 .010 2.5050 ;
P Y .002 .200 0.5076 ;
C 0 3 3 ;
F S ;
;************************
X = .005 ;
E = .0005 ;
Y = .002 ;
F = .0004 ;
;************************
A = E/X ;
B = F/X ;
;-----------------------------------------------------------------------------
D L ...  ;
F F ...  ;
M Q ...  ;
F F ...  ;
D L ...  ;
;.......  ;
;.......  ;
;-----------------------------------------------------------------------------
R = (((X,X)*X)↑2 +((X,A)*A)↑2 )↑.5 ;
S = (((A,X)*X)↑2 +((A,A)*A)↑2 )↑.5 ;
T = (1 /(((X,X)*(A,X)*X*X +(X,A)*(A,A)*A*A)/E) ↑2 +1 )↑ -0.5 ;
U = (((Y,Y)*Y)↑2 +((Y,B)*B)↑2 )↑.5 ;
V = (((B,Y)*Y)↑2 +((B,B)*B)↑2 )↑.5 ;
W = (1 /(((Y,Y)*(B,Y)*Y*Y +(Y,B)*(B,B)*B*B)/F) ↑2 +1 )↑ -.5 ;
;
P N P ;
P N E ;
P N S ;
END ;
END
```