RIBO: RADIOACTIVE ION BEAM OPTIMISER USER MANUAL

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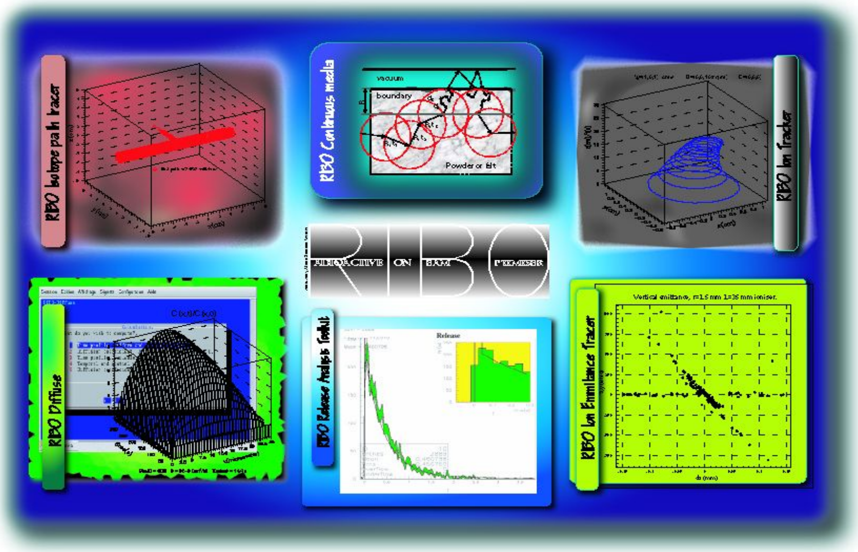
RIBO Isotope path tracer
RIBO Continuous media
RIBO Ion Tracker
RIBO
RADIOACTIVE ION BEAM OPTIMISER
RIBO Diffuse
RIBO Release Analysis Toolkit
RIBO Ion Emmitance Tracer
vacuum
boundary
Powder or felt
Release
Vertical emittance, r=1.5 mm 1=35 mm ioniser.

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Preface

Currently the nuclear chart includes around 3000 nuclides, distributed as β^+, β^- and α-emitters, stable and spontaneously fissioning isotopes. A similar amount of unknown nuclei belongs to the so-called *terra incognita*, the uncertain region contained also within the proton, neutron and (fast) fission driplines and thereby stable against nucleon emission. The exploration of this zone is to be assisted by the use of radioactive ion beams (RIB) and could provide a new understanding of several nuclear properties. Moreover, besides pointing at crucial questions such as the validity of the shell model, the dilute matter and the halo structure, challenging experiments outside nuclear physics are also attended, e.g., explanations of the nucleosythesis processes that may justify why the matter in the universe has evolved to present proportions of elements, and which represents a major challenge to nuclear physics.

These, together with other fascinating research lines in particle physics, solid state physics and medicine, demand utterly exotic and intense ion beams for which a global optimization of all relevant phenomena in beam formation has to be coherently conducted. As a response to this request, a Monte Carlo simulation code has been written, to integrate diffusion and effusion under various pressure flows and conditions, including the transport through continuous media and enabling diffractive and surface dependent effects, emulating ionization in surface and plasma ion sources and, finally, reproducing the movement of ions under electro-magnetic fields.

Chapter 1

Monte Carlo code. RIBO user manual.

1.1 RIBO, a MC code for isotope release optimization. Overview.

The Radioactive (or Rare) Ion Beam Optimiser, RIBO, is a scientific Monte Carlo simulation program focused on the optimization of radioactive ion beam production. It tracks the paths of atoms through ISOL targets, from generation (not included, this step should be calculated with codes like MCNPX [3], MARS [4, 5], FLUKA [6, 7]...) to ionization and extraction. It includes the following models:

Features of RIBO

- Diffusion from slabs, fibers or powder.
- Diffusion in 3D structures, with custom options.
- Heat transfer in 3D multi-body set-ups, including conduction, radiation, cooling, heat deposition ...
- Effusion in the molecular flow and the intermediate regime. Cosine law.
- Effusion through porous media.

- Effusion with multiple path-passage conditions, and surface-crossing sense detection.
- A**b**sorption (condensation) to the walls. Definition of cold spots.
- A**d**sorption-desorption on the walls (temporary retention). Frenkel sampling.
- Specular effusion.
- Custom collisions.
- Effusion through crystal systems (vibrations)[1].
- Effusion through systems with moving walls (valves).
- Effusion through systems with translucent walls (grids, leaks. . .).
- Surface ionization.
- Plasma ionization.
- Ion recombination.
- Ion transport in electric and magnetic fields. Emittance plots.

Other models are in consideration and could be implemented as a result of the common effort of a community of prospective users. Developments should be centralized through RIBO's web-page:

www.cern.ch/ribo

In addition a number of applications that help writing the input file and to analyze the output data[2] are being developed (and stored in $[tools]$)

[1]Under development.
[2]A set of PAW-based applications is under development.

1.2 Setup.

1.2.1 Description of files.

The RIBO code is distributed and backed by a number of FORTRAN files, data libraries and text files. The present distribution spans over the following files:

- DIFFUSE PACKAGE For diffusion calculations only (fancy options).

  . D.f, diffuse.e, diffuse.o, diffuse.sh, functC.f, license.pdf, README, timeN.f

- MONTE CARLO For typical (simple) diffusion and all effusion calculations.

  [data] Cond.dat, init.dat, plion.dat, sion.dat, Urz.dat, valves.dat, workf.dat, README

  [docs] effusion.pdf (dvi, tex), MANUAL, ...

  [batchinputs] Several runtime batch files.

  [targets] Several input files.

  [objects] diffuse3D.o, init.o, plION.o, powder.o, space.o, explicitEM.o, main.o, povray.o, readUrz.o, surfION.o

  [tools] 3D-view.sh, convgeom.f, make.sh, trajectory.sh, rotate.f, translate.f

  [sources] Bn.f, customcollision.f, customsource.f, emittance.f, math.f, readEfield.f, userprint.f, custom3D.f

  . license, README, version, ribo.stop (create it to stop current run), ribo.seed (contains an integer number that is used as seed, otherwise RIBO generates its own).

Moreover, for the graphical options (*Diffuse.sh*, *3D-RIBO.sh* and *trajectory.sh*) the two free programs are required:

1. Physics Analysis Workstation [8].

2. Persistence of Vision, Povray [9].

1.2.2 Installation.

Execute the make.sh script in $[tools]$ if you need to recompile. Otherwise no installation is required.

Then you should enable execution permission on the executable file that has been created:

```
> chmod +x RIBO
```

Finally you should edit your bash profile to include the path of the executable file or you can run it from the installed directory simply typing:

```
>./RIBO
```

Depending on the shell and configuration, typing ’bash’ or ’sh’ before ’RIBO’ may also work.

Once installed, in order to use the program, an input file has to be created. The following instructions explain how to do this. Alternatively, you can test the installation with the input files stored in $[targets]$. Give the name of the file and `RIBO` will search for in the directory $[targets]$, if failed, in $[inputs]$, and otherwise in the directory from which you are executing RIBO. Results will be stored in an output file whose name will be of your choice. Before doing a first test, it should be reminded that naming an output file with an existing file name will overwrite the old one.

1.3 Input file.

The input file contains the information of the geometric arrangement of the target, the starting properties and nature of atoms and the end conditions. Choices about the physical models to be employed and determination of the output modes are decided interactively at run time.

The input file is organized in four (or five) cards[3] each of them grouping different sets of information. Every card is initiated by a key word which must not be changed (it is case sensitive) followed by a line that explains the inputs to come. The explaining line can be edited but not deleted. The next lines contain the core information of the card, like the coefficients of the equations of the surfaces or the logic of the cells. Extra line spacing within a card or between cards is authorized since the program skips blanc spaces. Concerning the columns of text, there are no constraints on the horizontal spacing of elements within a line. However, an even arrangement of elements in columns helps to clarify the input file and to find possible mistakes.

The first two cards give the entire geometry of the system (walls and volumes) through which particles will effuse. This means that outer elements where atoms cannot reach shall not be described (e.g. if particles effuse through a tube only the inner bore is given as input; the outer surface defining the core is omitted). First comes the card **Surfaces**, corresponding to the walls of the system. Second, the card **Cells** describes the elementary cells that are enclosed by the given surfaces.

Third, the **Source** card, which contains all information about the initial state of the atoms (position, speed, mass) and fourth the card **Tally**, which gathers the end conditions of the simulation.

[3]This term of the computing jargon, comes from the days when punch cards where inserted in early computers to transmit a set of data.

1.3.1 *Surfaces* card.

This card contains all the information of the walls (surfaces) that bound the effusion paths of atoms. In some Monte Carlo codes [6, 7] these are known as *bodies*.

The program works internally with the equations of quadrics[4], which are introduced in the *Surfaces* card. The first lines look like this:

```
Surfaces
n  RC  T  X2  Y2  Z2  XY  XZ  YZ  X  Y  Z  C
third line
fourth line
...
```

The third, fourth, fifth . . . , (n+2)th line have the information of the surfaces 1, 2, 3 . . . , n. In each of these lines the **first column** corresponds to the surface number, 1, 2, 3 . . . Numbering should be done in consecutive jumps of 1 unity starting with 1. The **second** entry may contain several parameters about the surface nature:

- the *roughness coefficient* (RC), only relevant if Phong [10] reflections are active ([11] chapter 3.2.3), is stored in the integer part.
- the *absorption probability* is contained in the decimal part of *positive* numbers[5].
- the *opacity* of the surface is expressed in the decimal part when the number is *negative*. For example -0.35 means that 65% of the particles fly *through* this surface. This is only possible for interfaces between regions.

The temperature (T) - in Kelvin - of the surfaces is stored in the **third** entry. The remaining nine columns fully define any surface of second degree

Toroids have to be approached by several cylinders

[4] $c_{x^2} \cdot x^2 + c_{y^2} \cdot y^2 + c_{z^2} \cdot z^2 + c_{xy} \cdot x \cdot y + c_{xz} \cdot x \cdot z + c_{yz} \cdot y \cdot z + c_x \cdot x + c_y \cdot y + c_z \cdot z = C$

[5] e.g. 200.05 would mean that the surface is not diffusive (RC=200 $\sim$ Aluminum) and that its absorption coefficient is 0.05 (5 $\%$ of the impacting atoms condense to the surface).

(quadric). The family of *quadrics*comprises planes, cylinders, cones, spheres, hyperboloids...With this base of surfaces almost any arbitrary shape can be approached with a moderate consumption of memory and computation time. Smooth bends of tubes could have been modeled in a single surface: a toroid. However, these belong to fourth degree surfaces (quartics), for which 33 parameters are needed. This is too costly and rather unmanageable, which means that such surfaces must be implemented in pieces.

A plane with an equation x = 1 could be implemented as (geometric entries):

```
0 0 0 0 0 0 1 0 0 1
```

The last number corresponds to the independent term (C). Naturally, any proportional equation would be equivalent, e.g:

```
0 0 0 0 0 0 -25 0 0 -25
```

A sphere centered at the origin of radius R would be $x^2 + y^2 + z^2 = R^2 = C$, thus:

1 1 1 0 0 0 0 0 0 R^2

If the sphere is centered at x_0, y_0, z_0 then, the equation transforms to $(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = 3^2$, hence:

1 1 1 0 0 0 -2x_0 -2y_0 -2z_0 $(R^2 - {x_0}^2 - {y_0}^2 - {z_0}^2)$

Similarly, ellipsoids and cylinders can be implemented. Moreover, arbitrarily oriented figures may be obtained by applying the rotation equations over the coordinates. For instance, an ellipsoid with an axis **a** in the x, y plane forming an angle α with respect to the x coordinate can be introduced by applying a rotation α_z; $\hat{x}$ is replaced by $cos(\alpha) \cdot x + sin(\alpha) \cdot y$ and $\hat{y}$ by $sin(\alpha) \cdot x - cos(\alpha) \cdot y$. Therefore: $a^2 cos(\alpha) \cdot x + sin(\alpha) \cdot y^2 + b^2 sin(\alpha) \cdot x - cos(\alpha) \cdot y^2 + c \cdot z^2 = 1$

It should be remarked that the number of surfaces accepted by RIBO is unlimited, but, naturally, if simplifications conduct to less elements, then the CPU power requirements will be lower and results will be obtained faster.

Unlimited number of objects

At this point some prospective users might be thinking that the level of complication involved in writing the input file is fairly high. Responding to the demands of the first groups that have been exposed to these explanations, a routine called **convgeom** has been written to assist in the generation of the *Surfaces* card.

When executing **convgeom**, the user is asked to choose a surface type, it can be a plane (P), a sphere (S), a Cylinder (C), an ellipsoid (SQ), a cone (K) or a general quadric equation (GQ). Depending on this first choice, RIBO then asks to specify the radius, or the position of the plane, or the orientation of the plane/cylinder, or the radii of the ellipsoid. Then, the user can decide to rotate the surface by specifying the two Euler angles (or equivalently the two angles of the new $\hat{x}$ axis) and to make a translation. Finally the temperature of the surface is introduced and then the user can continue to define the second surface, and so on. The program writes into the input file the Surfaces card, including the headers.

For example:

```
> convgeom
 what is the input file name?
INPUT
 surface number 1
 P:plane,S:Sphere,C:Cylinder,K:cone,SQ:ellipse,GQ:gen
P
 YZ (PX), XZ (PY), XY (PZ), AX+BY+CZ=D (P)
PX
 position?
1
 eq:    0.  0.  0.  0.  0.  0.  1.  0.  0.  1.
 rotation? give polar angles of new x vector
 (polar,azimuthal)=(90,0) ==> no rotation
```

```
90 45
 rotation    90.  45.
 (alpha, beta)=    0.   0.   0.   0.   0.   0.   0.707107   0.707107   0.   1.
 translation?give x0,y0,z0
1 1 0
  (x0,y0,z0)=    1.   1.   0.
 X(x0,y0,z0)=    0.   0.   0.   0.   0.   0.   0.707107   0.707107   0.   2.414214
 what is the temperature of the surface[K]?
2000
 add surface? (Y/N)
Y

 surface number 2
 P:plane,S:Sphere,C:Cylinder,K:cone,SQ:ellipse,GQ:gen\
C
 Radius=?
2
 CX, CY, CZ?
CX
 eq:    0.   1.   1.   0.   0.   0.   0.   0.   0.   4.
 rotation? give polar angles of new x vector
 (polar, azimuthal)=(90,0) ==> no rotation
90 30
 rotation    90.  30.
 X(alpha, beta)=    0.250000   0.750000   1. -0.866025   0.   0.   0.   0.   0.   4.
 translation?give x0,y0,z0
0 0 0
 X0   0.250000   0.750000   1. -0.866025   0.   0.   0.   0.   0.   4.
 (x0,y0,z0)=    0.   0.   0.
 X(x0,y0,z0)=    0.250000   0.750000   1. -0.866025   0.   0.   0.   0.   0.   4.
 what is the temperature of the surface[K]?
1500
 add surface? (Y/N)
N
```

The generated input file would look like:

```
Surfaces
n   RC    T     x2     y2    z2     xy     xz    yz      x        y       z    c
1  0.5  2000.   0.     0.    0.      0.     0.    0.  0.707107 0.707107   0.   1.
```

```
2   0.5   1500.   0.25   0.75   1. −0.866025   0.   0.   0.   0.   0.  4.
```

It would now remain to define the cells.

1.3.2 *Cells* card.

This card includes the logic expressions that assemble the previously defined surfaces into the delimiting elements that enclose *cells* (these are referred to as **regions** in e.g. FLUKA [6] or GEANT4 [12]). Surfaces may extend infinitely, and therefore bounds are required to define real elements, thus the mechanism of cells. It should be stressed that cells are **finite** subspaces. This card has the following structure:

```
Cells
n  S1  S2  S3 ...
third line
fourth line
...
```

The third, fourth, fifth...(n+2)th lines correspond to the definition of the cells, 1,2,3 ...n, whose first element is precisely the cell number. The following columns define the cell volume in terms of the bounding surfaces. The MC code understands the cells as an intersection of the subspaces divided by a collection of surfaces; the boolean union operation is not defined; regions that require such an operator have to be split into several cells.

Boolean logics based on intersections

As an example of a simple cell, cell 1 comprises the volume over the plane 1, under the plane 2 and inside the sphere 3 then. The corresponding third line in the cells card is:

```
1  1  -2  -3
```

The recommended methodology consists in sketching the geometry and numbering the surfaces and cells onto this drawing. In some cases the concept *under* or *over* is not clear - like with oblique planes - then the guiding concept is the normal (unitary) vector at the surface; if the cell is to the side of the normal of the surface then the sign is positive, otherwise it is negative. This may again seem to lead to dubious cases. It should then be reminded that the gradient of the surface at a given point unambiguously defines the normal vector.

Sign defined by the gradient

Remarks:

† The MC code does NOT impose any restriction to the maximum number of cells of a given problem nor on the number of limiting surfaces of a given cell.

† The cells definitions have to be completed with zeros up to the maximum cell degree.

† The zeros in the cells definitions have to be put at the end.

† Cells are 'convex' elements; They are exclusively defined with the boolean intersection operator, and not with the union one.

The effort done with **convgeom** is directed to achieve the importation of geometry files whose format is compliant to other MC codes (e.g. MCNPX [3]). This shall enable to write the input files under those formats and to benefit from the plotting options offered by them.

1.3.3 Birth of particles, the *Source* card.

Predefined sources, *Source* card (input file card)

Maximum 15 entries for the source

The *Source* card has up to 1+14 entries that describe the source atoms, their starting position and the velocity distribution.The first entry is a character that encodes the geometric distribution shape of the generated atoms[6], The following vector of 14 numbers gives details of the source: mass number (A) ($S(1)$), temperature ($S(2)$), semi-angle -α- of aperture of the luminous cone ($S(3)$) with respect to the central direction of emission ($S(4)$, $S(5)$, $S(6)$), the birth coordinates centroid ($S(7)$, $S(8)$, $S(9)$), and details regarding the shape of the distribution. Coordinates from S(7) to S(14) are explained below:

1. **P**oint source. Only three geometric parameters are needed: x_0, y_0, z_0.

2. **S**pherical source. Like the point source with a radius: x_0, y_0, z_0, R.

3. **B**ox source. Particles are sampled within a parallelepiped centered at x_0, y_0, z_0, with sides of *full* lengths L_x, L_y, L_z and oriented in space with the angles θ, φ.

4. **T**arget generation. The starting position is sampled inside a cylinder centered at x_0, y_0, z_0, of radius R, *full* length L_x, Gaussian radial dispersion $sigma$, and angles of $\hat{n}$ θ, φ.

   Some remarks have to be made at this stage:

† A **C**ylinder category has not been included because random cylindrical birth distributions are a special case of **T**arget with $sigma = 0$.

[6]This character (P, S, B, or T) may have an attached prefix of the type Inum or A num, to force generation of *num* positively charged *I*ons or negative *A*nions, for example, I2S notes generation of ++ ions within a Sphere. For more information see section 1.3.3

† All angles -aperture cone and axis orientation- should be given in degrees.

† The atom temperature (in Kelvin) expresses the energy (velocity) of the atoms. The actual initial velocity will be sampled from the Maxwell Boltzmann distribution for that temperature. If the speed is unknown, then a good value is that of the wall temperatures since thermalization should fully have taken place after a few hundred collisions. If, instead, the speed is precisely known, then just input the value (in meters per second) preceded by the negative symbol, e.g -300.0 corresponds to exactly 300 m/s.

† The central angle of emission is indeed a velocity (unitary) directing vector. However, normalization is **not** required, it is done internally, e.g., 2 1 1 (not normalized) can be given instead of 0.8165 0.4082 0.4082 (normalized but not fully precise).

† For isotropic generation $\alpha = 180\,^{\circ}$, for focused beams $\alpha = 0$. In no case it can be omitted.

† Dimensions are expected, like elsewhere, in cm. If the axis of the cylinder is $\hat{x}$, then (θ, φ) = (90$\,^{\circ}$,0). If the cylinder has its axis in $\hat{y}$ then, (θ, φ) = (90$\,^{\circ}$,90$\,^{\circ}$), if it is in $\hat{z}$, then (θ, φ) = (0,*). Note that these rotations only affect the geometry of generation and not the velocity vectors. This means, in particular, that angles like (-90$\,^{\circ}$,0) or (0,-90$\,^{\circ}$) would also be valid for the two examples just shown. In these trivial examples this does not matter, but, for more complicated cases the parity property avoids errors of 'sign'.

† In total, for the point source 1+6+3 data are needed, 1+6+4 for spheres and 1+6+8 for the rest.

A simulation for a given source gives way to various sets of events (collisions, flight paths…). If these events are sorted into histograms, the resulting distributions can be added and subtracted to those of other simulations. This permits to reproduce almost any source by performing additions and subtractions from the elementary sources. Thus, e.g. the flight path of atoms born in a cylindric ring can be obtained by subtracting the pondered flight path distribution of a small cylindric source to that of a bigger one. Normalization has to take into account the volume of the respective sources and the number of histories[7]. As a first step, all histograms could be normalized to unity and then they could be weighted proportionally to the spatial volume of the sources. Analogue procedures are possible for complicated velocity spectra.

Particle birth within a cell (runtime option).

Another possibility to work with more elaborate sources is to force generation inside a given cell. This option is offered at runtime:

```
.................................................
|  ...source limited to a cell? give cell number.   |
|      celln > 0 ==> generation limited to volume   |
|        defined by celln                           |
|      celln = 0 ==> do not constrain to a cell     |
|      celln < 0 ==> just generate a geometry plot  |
___________________________________________________
```

A basic delimiting source is needed every time. The primary container source, chosen between *Point*, *Sphere*, *Target* and *Box* should include the entire source cell. If the introduced cell number is '0' then the method remains inactive. If it

[7]In Monte Carlo jargon, each individual repetition is called *history*, and the whole group of histories is called *simulation*, whose *size* will be the number of histories.

is negative, then `RIBO` will not do any simulation, it will just generate a plot of the geometry (see 1.9). Otherwise particles will be sampled exclusively inside the selected cell. This method can be universally used, e.g., an infinite sphere containing a dodecahedron, but in order to perform efficient simulations the volume of the primary source ought to match the cell dimensions as closely as possible (this is similar to the concept of **the rejection sampling technique** [13]). For instance, sampling the birth of atoms homogeneously inside the volume of a $\frac{1}{4}$-sector of a cylinder - cell **2** in the example below - can be carried out first by defining a source cylinder C of the same radius and then by using the cell delimiter command. The efficiency of the method corresponds to the fraction of the cylinder sector (here it is 25 $\%$).

```
Surfaces
n   RC    T    X2   Y2   Z2   XY   XZ   YZ   X   Y   Z   C
1   0.5   298  0    0    0    0    0    0    1   0   0   0
2   0.5   298  0    0    0    0    0    0    1   0   0   10
3   0.5   298  0    1    1    0    0    0    0   0   0   1
4   0.5   298  0    0    0    0    0    0    0   1   0   0
5   0.5   298  0    0    0    0    0    0    0   0   1   0
Cells
n   S1   S2 ...
1   1    -2   -3   4    5
2   1    -2   -3   4    -5
3   1    -2   -3   -4   5
4   1    -2   -3   -4   -5
Source
Type M    T     Alpha  nx   ny   nz   x    y    z    L    s    th   phi
C    40   298   180    1    0    0    5    0    0    10   0    0    0
Tally
S   Nmax   Tmax   Tpmax
2   1000   110    101
```

. . . The cell-delimited source command is more powerful than the composition (additions or subtractions) of simulations and can simulate more complicated distributions; e.g., a ring can be simulated by both ways but a cylinder sector is only produced by the cell restriction, as just shown.

Customized sources (programmable option).

The instructions given up to this point already offer a a fairly high control of the geometry distribution of the starting atoms and also give the possibility to choose the initial speed, the direction and the semi-aperture angle of an isotropic emission cone. However, the user may want to define fancier distributions: correlation of velocity and position coordinates, speed distributions, position dependent weights. . . the possibilities are infinite. Responding to these potential needs the open source routine "customsource.f" found in the directory SOURCES allows to create user define source distributions. This subroutine deals with the following (I/O) variables: x,y,z,ux,uy,uz,tp,SOURCE, where "SOURCE" is the vector that stores the parameters introduced in the input file in the card 'Source'. Thus the user can specify whichever dependency g(x,y,z,ux,uy,uz,tp,SOURCE). For instance, for a discrete generation profile over "y" where the probabilities are:

```
**    pill   position_y   production   probability  Probability
**     1        2.08         2.85          0.19         0.19
**     2        4.22         2.63          0.17         0.36
**     3        6.36         2.41          0.16         0.51
**     4        8.49         2.20          0.14         0.66
**     5       10.61         1.98          0.13         0.78
**     6       12.73         1.76          0.11         0.90
**     7       14.83         1.55          0.10         1.00
```
8

Then the user should write the following instructions in "customsource.f":

```
      a=rand(zero)
      IF (a.gt.0.9) THEN
        y=14.83
      ELSE IF (a.gt.0.78) THEN
        y=12.73
      ELSE IF (a.gt.0.66) THEN
        y=10.61
```
9

```
      ELSE IF (a.gt.0.51) THEN
        y= 8.49
      ELSE IF (a.gt.0.36) THEN
        y= 6.36
      ELSE IF (a.gt.0.19) THEN
        y= 4.22
      ELSE
        y= 2.08
      END IF
```

WARNING!! *Remember that any changes in the source files will take place only after having recompiled. The compilation instruction appears in the README file on the* `RIBO` *distribution and can be performed with the script* $[tools]$/*make.sh*

Reading source events from a file.

The user can also read values from the file 'init.dat' in the DATA directory of the `RIBO` distribution. This file must have been previously generated by another run with `RIBO` or by any other program, e.g. FLUKA. The file init.dat can have whatever format you wish as long as the reading instructions in "customsource.f" are coherent with the data in the file. The variables to play with are the 6-space coordinates + starting time. For example, to read x,y,x,ux,uy,uz,tp from init.dat, just uncomment the following line in "customsource.f" and recompile.

```
*        read(9,*)x,y,z,ux,uy,uz,tp
```

Sampling ions.

(see also section 1.3.3) Unless otherwise specified particles are initially neutral atoms that may later on ionize and recombine. However, `RIBO` offers two ways to control the charge state of the initial particle:

1. The first argument of the SOURCE card (see section 1.3.3) can be expanded with a prefix to indicate the ionic state of the particle. For instance:

- for neutral particles randomly generated within a *sphere*, the letter **S** is used as the first argument of the SOURCE card.
- if we want to sample positively ionized atoms of charge + within the same Sphere, use **IS** or **I1S** as the first argument.
- for ions of charge n+ use **InS**
- for ions of charge n- use **AnS**

2. the charge of the particle can be specified in the user modifiable routine *customsource.f* (see section 1.3.3) by assigning a value to the variable *ion*. e.g.
   - ion=2 for ++
   - ion=0 (default)
   - ion=- for -

1.3.4 The *Tally* (end) card.

The end conditions are preceded by a line with the word *Tally*. There are four inputs, the first and last are relative to the individual histories and the two intermediate fix the end conditions for the global simulation. Up to now, an end Tally would look like this (still valid):

Simple Tally card.

```
Tally
S   Nmax   Tmax  Tpmax
3    6000   750    10
```

The text and the case of the first line are unmodifiable, the second line is indicative and should not be omitted although it can be edited at the user taste. The first number in the last line indicates the surface used as detector for the atoms[12]. When atoms reach this surface, the history is completed and a new atom is simulated. The fourth number alternatively terminates the current history if the individual flight time reaches a certain threshold[13]. Setting a low threshold can be useful to have a fast scan of a rapid release peak, sparing the long simulations of the tails of the release distributions. For release fitting purposes, however, the threshold should be high, in order to avoid annoying normalization issues.

The second number displays the number of histories (size of the simulation) and the third one the maximum elapsed time. The simulation is finished as soon as any of these two events takes place: maximum time OR maximum number of atoms (histories).

WARNING: Make sure that you don't use tabulators in the Tally card

Complex Tally card.

In addition to the options provided in *Simple Tally Card*, the user can specify several *sequences* each of them composed of 1 or more conditions (every condition is a surface crossing). When ALL the conditions within any of the sequences are accomplished then the particle reaches the end. The user can do the following:

1. Specify to have various end surfaces (that is to say, several trivial *sequences* each composed by a single condition). This is logic **OR**, introduced by means of the character |).

   e.g. 10 **OR** 20 → `( 10 | 20 ) 6000 750 10`.

   The particle will stop when it first reaches 10 or 20 or when its elapsed time

[12]Several detectors and forced paths can be used with the *Complex Tally card*, described just after.

[13]Unlike the other threshold times, this one is not CPU time, but physical flight time.

exceeds 750 s or when the total CPU time for the simulation is greater than 6000 s.

2. Follow only the paths that first go through/hit a surface **and** then through another one (and so on).
   e.g. first through surface 10 **AND** then through 20 → `( 10 20 ) 6000 750 10`.
   Note that the order matters.

3. Specify the sense[14] of passage through a surface (±).
   e.g. end only when it crosses 10 positively → `+10 6000 750 10`.

4. Impose several crossings before termination (particular case of option 2.).
   e.g. Stop after crossing *surface 20* 3 times
   → `( 20 20 20 ) 6000 750 10`.

Some remarks should be made at this point:

† Parenthesis are needed to delimit the boolean definition of end surfaces.

† `( S1 | S2 ) Nmax Tmax Tpmax` is equivalent to
`( S2 | S1 ) Nmax Tmax Tpmax`

† `( -S1 | +S2 ) Nmax Tmax Tpmax` is equivalent to
`S1 Nmax Tmax Tpmax`

† `( S1 S2 ) Nmax Tmax Tpmax` is NOT equivalent to
`( S2 S1 ) Nmax Tmax Tpmax`

[14]The sign criteria is the gradient to the surface

† `( S1 S2 | S2 S1 ) Nmax Tmax Tpmax` means that both S1 and S2 have to be crossed, but the sequence is irrelevant.

† **WARNING: Make sure you don't use tabulators in the Tally card**

How to stop the simulation at any time.

The second and third cards in the *Tally* section determine the maximum number of histories and the maximum CPU elapsed time, whichever happens first. There's yet another way to stop a simulation at any time before any of the two other events take place. By simply creating a file called 'ribo.stop' in the running directory the simulation will stop after the current particle has been tracked. Note that in linux systems an empty file named *'ribo.stop'* can be created by simply typing the command *'touch ribo.stop'* in a command line.

1.3.5 Options card (New 2009 Feature).

Some parameters to control the simulations are accepted at the end of the input file. Each line will refer to a different control. The structure is the following: CONTROL value Where 'CONTROL' is a seven character keyword and 'value' is the number associated to that variable. For the time being only one external parameter EMAGFAC has been implemented. This is a factor that multiplies the internally calculated step-size used in the electromagnetic transport of ions. For example: EMAGFAC 2.0 will make the steps twice as long.

1.4 Data files

Most RIBO problems can be answered by writing or modifying an already existing *input file* and running RIBO on that file. The *input file* has information of the geometry and properties of the system, the source of particles and the scoring. Section 1.3 contains detailed instructions on how to write the input file. Most likely, beginners will not require to fully master the use of the different *data files* of RIBO, however it is advised to read through the following paragraphs in order to gain some understanding on the structure of the code and the *data files* that come along with the RIBO distribution.

1.4.1 $[data]/Cond.dat$ file

The file $[data]/Cond.dat$ is required by the `Diffuse3D` module for 3D-(heat or particle) diffusion calculations. This file, explained in 2.2.1 contains the information about the diffusion parameter, desorption time, emissivity and volumetric specific capacity (at constant pressure). An sample file comes with the RIBO distribution, in the DATA folder.

1.4.2 $[data]/heattable.dat$ file

The $[data]/heattable.dat$ file is not directly read by RIBO, but it is a useful reference to write the Cond.dat file for for 3-D heat transfer calculations.

1.4.3 $[data]/init.dat$ file

The $[data]/init.dat$ file is a good location to store starting conditions (e.g. position, speed and time) that will be read by `RIBO` at particle generation. For more information see in 1.3.3.

1.4.4 $[data]/plion.dat$ file

The $[data]/plion.dat$ file is used for *plasma ionization*. `RIBO` computes the electron impact direct ionization probability in an ionic plasma by folding the flux and effective energy of the source electron beam with the according cross sections. The cross sections are picked by the subroutine **plION** from the data file *plion.dat*, which contains the cross sections (1E-1 micro-barn) in several ion gases and for different state charges. More information is given in 1.7.3. Major development is expected in this area.

1.4.5 $[data]/sion.dat$ and $[data]/workf.dat$ file

The $[data]/sion.dat$ and $[data]/workf.dat$ files are related to *surface ionization*. `RIBO` computes the probability that a given neutral isotope will be positively ionized when striking a certain surface. The data required to decide on single surface ionization events are the ionization work function and ionic statistical weights, Wi,g0, g+,g- for the projectile atom Z (stored in $sion.dat$ and the substrate work function, written in $[data]/workf.dat$.

1.4.6 $[data]/valves.dat$ **file**

In some circumstances a few walls in the system are not static all the time. This is the case when a valve is present in the system. In order to deal with these objects RIBO reads over the file $[data]$/valves.dat and obeys the instructions thereby provided. This file contains a table where every line describes the opening and closing sequences of a wall that communicates two contiguous cells. More information is provided in 1.5.2.

1.5 Effusion models.

1.5.1 Collisions

The collision model is chosen at run-time. Custom collisions can be defined in a dedicated subroutine (see 1.10.1). Several events/considerations are taken into account during or after a collision:

Absorption at the surface

Upon colliding, the code checks if the particle should be permanently retained at the surface. If absorption has been activated (see section 1.7.3 to learn more how to activate this feature) then, after each collision with the walls, the code will check if the particle condenses in the surface. In order to do so, a uniform random number is compared to the absorption probability on the surface, which should have previously been introduced in the input file as the decimal part of the second input number of each surface (the integer part corresponds to the roughness parameter). This is further explained in section 1.3.1.

Adsorption at the surface

The particle may stick on the impinged surface for a limited time. In `RIBO` t_S represents either the average retention time or the parameter of the exponential Frenkel law. This parameter is given at runtime or in the custom collision subroutine (see section 1.10.1).

Reflection

Unless absorbed, the particle will bounce off the surface with and angle sampled from the collision law that is given by the user at runtime.

Energy Change

In general terms the atoms thermalize with the system. `RIBO` assumes that the atom gets the surface energy after the first collision. During runtime the user can opt to sample the energy of the outgoing particle from the corresponding Maxwell-Boltzmann law (at the temperature of the wall) or simply assign the average energy of this law. The second option is an excellent approximation as long as the number of collisions is high, which is usually the case.

Surface ionization

If activated during runtime, the atom may ionize when hitting certain surfaces (defined during runtime). The surface ionization probability is determined as explained in 1.4.5.

Recombination

In `RIBO` any ion hitting a surface will recombine into a neutral atom.

1.5.2 Special cases

Collisions with residual gas.

RIBO contains a simple hard-sphere statistical model to compute the interaction of *neutral atoms* with residual gas. The user needs to define a pressure level at runtime to activate this feature.

Translucent walls, grids and gas leaks.

RIBO allows defining translucent walls. Those have a certain probability to let particles through them. This feature is useful to implement fine grids without having to go through a tedious geometrical implementation of all orifices. The *opacity* of a *wall dividing two regions*[15] is expressed as a negative number in the second argument of a surface definition (the first argument after the surface number label). For example:

```
1 -0.35 2000 0 0 0 0 0 0 1 0 0 1
```

means that the first surface of the geometry (a Z=1 plane at 2000 K) has an opacity of 35%, thus a transparence of 65%.

Effusion through moving walls (valves).

In some circumstances a few walls in the system are not static all the time. This is the case when a valve is present in the system. In order to deal with these objects RIBO reads over the file $[data]$/valves.dat and obeys the instructions thereby provided. This file contains a table where every line describes the opening and closing sequences of a wall that communicates two contiguous cells. These walls would

[15] This feature is impossible for walls between a cell and the outer space

normally behave as virtual boundaries in the sense that they limit different regions (so they belong to the boolean logic definition) but particles do not *bounce* with them but rather they *cross* them.

The user must therefore specify the closing time ("start_time") together with the ramp time to close (fast valves may close in about 0.005 s), the respective opening time ("end_time") and opening ramp time, the surface number of the boundary that is going to lose its transparency and the area where it is acting, that is, the two cells that it is communicating/isolating.

For example, the "gate" 1 that communicates cell(1) with cell(2) and cell(1) with cell(3) can be closed in the interval t=(0-10)s between cell(1) and cell(3) and then open up there and close between cell(1) and cell(2).

```
                   __________                       __________
       t: 0-10 s  |          |         t:10-... s  |          |
          ________|          |             ________|          |
         |        :          |            |        |          |
         |  (2)  1:          |            |  (2)  1|          |
         |________:          |            |________|          |
                  |          |                     |          |
                  |   (1)   2|    ===>             |   (1)   2|
          ________|          |             ________|          |
         |        |          |            |        :          |
         |  (3)  1|          |            |  (3)  1:          |
         |________|          |            |________:          |
                  |          |                     |          |
                  |__________|                     |__________|
```

The corresponding definition would be:

```
start_time  t_ramp  end_time  t_ramp  surface   cell1   cell2
     0         0        10       0       1        1       3
     10        0         0       0       1        1       2
```

REMARKS:

† If *end_time* is smaller than *start_time* then the program assumes that the wall will no longer open after *start_time*.

† The surface that acts as a valve needs to be defined in the input file and it must divide two existing regions.

† The user must specify between which cells the wall will be acting (the order is irrelevant).

† The user can define up to 10 moving wall events.

† A wall can appear in several lines if there are several events concerning that wall.

† If the *end_time* is smaller than the *start_time* then the program assumes that in fact, the end time is infinite.

1.6 Pseudo random sequence. Random seed.

In absence of a 'ribo.seed' file, RIBO takes care of the random number initialization. Thus, any two runs are different unless the user provides a common random seed (integer) number in a file called 'ribo.seed', at the execution path.

1.7 Executing RIBO

1.7.1 The Isotope RElease Simulator, IRES

RIBO can be run on-line from a server at www.targisol.csic.es for simplified geometries and through a GUI front-end that permits easy operation of the code.

The server contains a wide compendium of release data (diffusion coefficients and sticking times) which is used in combination with this on-line version. The server administrator requires registration. Note, however, that the RIBO version installed in IRES is seriously outdated.

1.7.2 Express Execution with a batch file.

One of the most useful tools is the execution through a batch file. This file permits to execute the program routinely without having to reintroduce the interactive options.

When RIBO is executed all runtime options are automatically recorded in a file whose default name is ’batch’. If the user then wishes to re-simulate the system, it will be enough to type the *.exe file with ’<batch’ at the end, which means that all interactive data will be taken from the batch file.

The potential of this methodology is vast; a user could edit the batch file, change some input parameters (probably also the output file name) and save it as batch1, then repeat for different parameters for batch2. . . Finally, a script like:

```
{
RIBO < batch1
RIBO < batch2
⋮
}
```

or even a script with a loop, could produce an enormous amount of data.

Before going deep into the runtime options, you may want to test your RIBO distribution by running one of the batch files stored in the folder $[batchinputs]$

1.7.3 Runtime options.

At run time the user interacts with the program in order to define the input and output file names, the type of output, the models to be used and the options that shape out the results of the simulations.

In the first place the user introduces the file name of the **input file** and of the *output file*[16]. The input file name needs no particular extension, usually *.t is used, getting at the fact that the file describes a *t*arget, but *.inp or any other choices are also accepted. **WARNING:** The string of the input file should not be longer than 20 characters.

```
  Name of the input file?
rectangle.t
```

The name of the **output file** again needs no particular extension, *.out is quite intuitive (*.o should be avoided as it may lead to confusion between the output files and the object (assembled) files). **WARNING:** The string of the output file should not be longer than 20 characters.

```
  Name of the output file?
 (Beware it will overwrite the existing file)
results/rectangle.o
```

The code used to ask whether a histogram was to be made.

† This option is now obsolete!!

If the user wishes to intersect the domain covered by *Source* (see 1.3.3) with the volume restricted by a given cell, it is then asked to specify the cell identifier. If the source is to be limited (*intersected*) to the *union* of several cells (e.g. 10),

[16]RIBO searches for the input file in $[targets]$, $[inputs]$, and in running directory, with this priority order.

the user needs give the number of cells followed by '.1' (i.e. '10.1') in order to tell RIBO the inserted number is not the index of a single cell (e.g. '10' would mean that generation is restricted to a single cell and that the cell is number 10). Otherwise (no cell restriction), the value '0' should be typed.

```
| SOURCE CUSTOMIZATION:                                  |
| - You can edit the file [sources]/customsource.f       |
|     and then recompile with [tools]/make.sh            |
| - Additionally you can use the data file init.dat      |
|   by uncommenting "read..." in customsource.f          |
| - And you can restrict generation to a cell...         |
|       celln < 0 ==> just generate a geometry plot      |
|       celln = 0 ==> do not constrain to a cell         |
|       celln > 0 ==> generation restricted to cells     |
|       * INTEG   ==> generation limited to volume       |
|              defined by celln e.g. 5 ==> generation    |
|              will take place only within cell # 5      |
|       * INTEG.1 ==> generation limited to volume       |
|              defined by as many cells as integer       |
|               part, e.g. 12.1 ==> twelve delimiting    |
|               cells (numbers will be asked later)      |
__________________________________________________________
```

The following module activates the ionization mode and termination mode. Depending on the choice additional parameters will be demanded.[17]

```
__________________________________________________________

| SPECIAL EVENTS, TERMINATION                            |
| Please choose among these options:                     |
|   1: Crossing of end surface (1st card in "Tally")     |
|      No ionizations in the system.                     |
|   2: Atoms can be ionized in a PLASMA ion source       |
|      Histories (of atoms and ions) end when            |
```

[17]Laser ionization could be available in the future. The fourth option is not really an ionization mechanism, it is used to map the distribution of radioactive atoms stuck in the walls as a consequence of prolonged sticking.

```
|       they cross the end_surface detector              |
|    3: Atoms can be ionized in a SURFACE ioniser        |
|       Histories (of atoms and ions) end when           |
|       they cross the end_surface detector              |
|    4: Atoms can be absorbed in the walls. Trajec-      |
|       tories end at absorption or when crossing        |
|       the end surface                                  |
|  OR SEVERAL combined effects:                          |
|   23: Like options (1), 2 and 3                        |
|   24: Like options (1), 2 and 4                        |
|   34: Like options (1), 3 and 4                        |
| 234: Like options (1), 2, 3 and 4                      |
|    Please make your choice now                         |
'________________________________________________________'
```

As a function of the previous choice four options are then possible:

1. If RIBO is run *without* ionization, then no more data will be required at this point and the program will continue to collect the runtime parameters.

2. If ionization is activated, then the code will ask into how many cells the ion source expands. Please, consult the example at 3.1.3 to learn more.

Configuring the ion source

   - If *Plasma* ionization has been chosen, then the RIBO code will start by asking which are the indexes of all the ionizing cells, then it will demand the the flux of electrons and the program **plION** will take charge of the calculation of the electron impact direct ionization cross section subsequently asking for the energy of the electron beam, the species to be ionized and the sought ion state[18].

   - If *Surface* ionization is chosen, then the program will ask for the cell index of the first ion cell and for its corresponding surface ionizers,

[18]The database (plion.dat) should be consulted to see if the wished ion is tabulated.

then it will do the same for the second ion cell and so on. Next a program called **surfION** will be launched and it will ask which is the number of the surface that corresponds to the ionizer , and then it will demand the atomic numbers of the projectile and of the substrate, or, in their default, the work function, their mass number and the type of compound (Boride, Carbide, Element. . .).

3. If absorption has been activated, then, after each collision to the walls, the code will check if the particle condenses in the surface. In order to do so, a uniform random number is compared to the absorption probability on the surface, which should have previously been introduced in the input file, in the decimal part of the second input of each surface (the integer part corresponds to the roughness parameter) as explained in 1.3.1.

Activating absorption in the walls

From the fan of phenomena implemented in RIBO, after having decided about ionization, the user is asked to specify which of the remaining steps will be included in the simulation.

```
SELECT MODE:
  1: Diffusion.
  2: Effusion.
  3: Diffusion+Effusion.
recommended 2
  4: Conductance calculator (Clausing Coefficient).
  5: Diffusion3D. -- ALPHA VERSION !!
  6: Heat transfer (cond.+rad.). -- ALPHA VERSION !!
```

1: Diffusion This option uses the second Fick law, analytically integrated from the 1st law for simple cases like foils, cylinders (fiber) or spheres (powder) in uniform conditions. More elaborated descriptions based in finite integration of 1st law are provided by option 5 (see also chapter 2. or by the program `Diffuse`, explained on page 106. Note also that even if diffusion is not explicitly asked for (like in option 2), the output file computes the total release efficiency for effusion and diffusion, for a range of diffusion time constants (refer to section 1.11.2 on page 59.

If the user only wants to simulate Diffusion (this cannot be the case if Ionization is activated), then an ulterior option asks whether it will be in-grain or inter grain diffusion or both.

```
Diffusion/Powder.effusion/Both [D/P/B]?
```

In any case, one can obtain average parameters only or delay distributions[19].

```
CHOOSE THE OUTPUT MODE:(recommended 13)
 1: Only average figures
 2: Diffusion delay distribution
```

2: Effusion The recommended and standard option is '2' because diffusion can be simulated separately with **diffprof**. If only effusion is chosen (in addition or not to ionization), then the alternatives thereby available are those shown in example 3, 3.1.3.

3: Diffusion+Effusion This option combines the first two. The advantage is that the final release times (diffusion+effusion) are obtained without need of convolving an analytical diffusion formula with a fitted histogram of effusion. The drawback is that diffusion is sampled, and therefore it includes a stochastic, artificial error.

4: Conductance calculator (Clausing Coefficient) This option estimates the conductance between two sections in terms of the Clausing coefficient. For

[19]Required if time histograms are to be plotted.

technical reasons, the surfaces cannot coincide with the *endsurface* defined in the *Tally* card.

```
1: Only average figures
Introduce the beginning and ending surfaces
```

5: Diffusion3D. – ALPHA VERSION !! This uses the combinatorial geometry to define a 3D grid for a finite-difference finite-method integration of Fick's first Law. This allows to compute diffusion from arbitrary geometries, including distinct regions with different diffusing coefficients and other fancy effects. Chapter 2 introduces this module.

Extracting conductances for analytic vacuum calculations

6: Heat transfer (cond.+rad.). – ALPHA VERSION !! This is like option 5. but for heat diffusion (conduction). The different with respect to 5, is that in the surface of the objects instead of *atomic desorption*, *heat radiation* takes place. This option could be useful for coarse heat calculations of your target.

The next alternative concerns the physic model to be used for the reflection of atoms from the walls. Specular reflection (S) may be used to represent reflections of light in systems of mirrors, Lambertian reflections (B) follow the cosine model and thermalize the energy of the projectile to that of the surface, and exact reflections (D) include information of the crystal lattice and of its vibrations. The last choice, (C) custom, activates the user routine $[sources]$/customcollisions.f, explained in detail in 1.10.1 on page 47.

Reflection models

```
________________________________________________
| ........... COLLISION MODEL I ............... |
| What model for the treatment of the collisions? |
|    S: Specular(E<<)                             |
|   B: B=Knudsen-Lambert (recommended cosine law) |
|   D: Debye, semi-classic (under development)   |
|   C: Custom                                     |
| .............................................. |
|   BACK: Go back to previous menu                |
__________________________________________________
|  For option "C", Custom, modify the subroutine  |
| [sources]/customcollision.f at your convenience |
|  and recompile using [tools]/make.sh            |
__________________________________________________
```

During runtime the user can decide between having the energy of the reflected particles sampled from the Maxwell-Boltzmann distribution or fixing its energy to the average of the distribution. The second option saves CPU time while preserving precise results if the number of collisions is high enough (central theorem of the limit for normal distributions), but it may give way to notorious statistical errors in situations where few collisions take place.

```
__________________________________________________
| ...........  COLLISION MODEL II  ............ |
| Use average energy or sample from coll. law     |
|   Y: Use average energy (recommended)           |
|   N: Sample from collision law (slower)         |
| .............................................. |
|   BACK: Go back to previous menu                |
__________________________________________________
```

Including temporary sticking

It has been shown that the number of collisions suffered by each particle in its path to the exit of the system (or before ionization) can be included among other output numbers. Nonetheless, in some circumstances it may be interesting to specify sticking in the release times. The user can provide a positive ts, which will be used as an exact fix number, or a negative number (ts<0), which will serve to sample a sticking time upon every collision from the exponential law $p(t) = \frac{exp(\frac{-t}{|ts|})}{|ts|}$.

The same comment about the CPU-speed vs. accuracy done for energy sampling applies here (it is only worthwhile for a small number of collisions). Note that the user-routine $[sources]$/customcollision.f can cope with more complex schemes, e.g. desorption time depends on the surface and on the position. In particular, this allows to define **cold-spots**.

```
 ----------------------------------------------------
 |  Sticking time[s]?                                |
 |  > 0 ==> every collision delays exactly ts [s]    |
 |  = 0 (recommended). The output file includes a    |
 |     post-analysis with several hypothetic ts      |
 |     Use 0 for noble gases                         |
 |  < 0 ==> sample from law P(t)=exp(-t/ts)/ts       |
 |     It slows down calculations. Only necessary    |
 |     if the number of collisions is low            |
 ----------------------------------------------------
 |  For ts=ts(X,surface), see examples 4, 5 in the   |
 |    user routine customcollision.f                 |
 ----------------------------------------------------
```

The following step decides if the module for continuous media shall be used. If there is no continuous porous material (only slabs or empty system, etc.) then the option 'S' shall be used. The choice between powder and fiber is only relevant when diffusion is included in the calculation.

Selecting target filling

```
target filling: Slabs Fibers or Powder [S/F/P]?
```

If 'F' or 'P' are chosen then the program will need to know the average flight path of atoms in the Fiber or Powder. It will also ask for the probe spheres that should be used as macro steps for faster calculation.

The pressure inside the system is introduced in order to enable collisions between gas atoms.

residual pressure

```
 _____________________________________________________
| ....... COLLISION WITH RESIDUAL NUCLEI ........ |
|  Residual pressure [torr]? (0.75 torr = 100 Pa) |
| P <= 0 ==>  molecular flow (ideal vacuum)       |
| P >  0 ==>  collisions with residual gas        |
|  (if you do not know it but you know the mean   |
|  free path type anything > 0 now)               |
 _____________________________________________________
```

If no more input is given, the program will estimate the mean free path between atom collisions from statistical considerations. Alternatively, if the mean free path is known, it should be provided.

```
|                                                 |
|     RRRR   EEEEE   SSSS   GGGG   AAA     SSSS   |
|     R   R  E       S      G      A   A  S       |
|     RRRR   EEEE     SSS   G GG   AAAAA   SSS    |
|     R  R   E           S  G   G  A   A      S   |
|     R   R  EEEEE  SSSS    GGG   A   A  SSSS    |
|-------------------------------------------------|
- STARTING MODULE FOR INTERACTIONS BETWEEN ATOMS -


 _____________________________________________________
| .......COLLISION WITH RESIDUAL NUCLEI II ....... |
|  INTRODUCE A NUMBER n, IF ...                   |
| n > 0 ==>  n = ATOM DIAMETER [pm]               |
|  - Some indicative values [pm] are:             |
|  He:62;Ne:76;Ar:142;Kr:176;Xe:216;Rn:240;N2:374 |
|  - Consider also diameter ~= 2 x 1.4 x A^{1/3}  |
| n < 0 ==> |n| = -MEAN_FREE_PATH [cm] in "vacuum"|
| n = 0 ==> RIBO will estimate the MEAN_FREE_PATH |
 _____________________________________________________
```

In case of ionic transport, the emittance is computed with the program *emittance.f*. The central axis has to be modified to match the particularities of each case. The output is written in *emit.map*.

```
*****************************************************************************
****    EEEEE  M   M  II  TTTTT  TTTTT   AAA    N   N   CCCC  EEEEE     *****
****    E      MM MM  II    T      T    A   A   NN  N  C      E         ****
****    EEEE   M M M  II    T      T    AAAAA   N N N  C      EEEE      ***
****    E      M   M  II    T      T    A   A   N  NN  C      E         ****
****    EEEEE  M   M  II    T      T    A   A   N   N   CCCC  EEEEE     *****
******************************************************************************
*         The RIBO project , MARIO SANTANA LEITNER 2000-2006
*-----------------------------------------------------------------------------

      SUBROUTINE emittance(epsilon,X3,U3)
        real*8 X3(3),U3(3)                                                  ! i
        real*8 epsilon(2)                                                   ! o
        real*8 R(2),Pi                                                      ! a
***********************************************************************
*                 CUSTOMIZE THIS FUNCTION TO FIT YOUR PROBLEM         *
*   USAGE:  print emittance maps in a given cross section f           *
*                                                                     *
*   VARIABLES:                                                        *
*              INPUT                                                  *
*     X3(3)  --------  Absolute position (x,y,z)[cm]                  *
*     U3(3)  --------  Velocity {ux,uy,uz} of the ion [m/s]           *
*            AUXILIARY                                                *
*     R(2)   --------                                                 *
*     Pi     --------  3.141592...                                    *
*             OUTPUT                                                  *
*     epsilon(2) ---   Emittance in perpendicular directions          *
*     R(2)   --------  Transverse position of the beam axis [cm]      *
*                                                                     *
***********************************************************************
*
        Pi=3.14159257
*    Modify this according to the exit axis and position
        R(1)=X3(1)-0.0
        R(2)=Z3(3)-1.0
*    Safeguard condition
        IF (U3(3).eq.0.0) THEN
          write(6,*)'Warning:extraction axis perpendicular to velocity'
          U3(3)=1E-12
        END IF
        write(4,'(1X,F8.4,F9.5,F8.4,F9.5)')R(1),U3(1)/U3(3),R(2)
     $            ,U3(2)/U3(3)
        epsilon(1)=epsilon(1)+10*R(1)*1000*atan(U3(1)/U3(3))/Pi
        epsilon(2)=epsilon(2)+10*R(2)*1000*atan(U3(2)/U3(3))/Pi
      END$
```

At this point the program has all necessary elements to pursue simulations, eventually including in-grain diffusion in slabs, particles or fibers, inter-grain diffusion through powders or fibers, effusion in molecular or intermediately pressurized systems, with mirror like walls, diffusive walls or crystals, and ionization in plasma chambers or surface ionizers. After preprocessing some messages will appear in the screen and simulations will start. The connectivity matrix will be stored in a file called CCONM and the results will be stored in the output file.

1.8 Debugging running errors.

1.8.1 Introduction.

Running a Monte Carlo code is similar to programming: every little thing that is overlooked contains a potential bug and it will most likely induce an error at some point. The time required to detect and to fix the bug will exceed the amount of work needed to avoid such flaws from the beginning. This general recommendation concerns specially the implementation of the geometry. It is strongly advised to take some time to do a sketch of the system as it will be modeled, drawing and labeling each surface and marking the cells. Eventually this step may already help to rise some questions about the optimality of the target and often new configurations are immediately suggested. Moreover, the sketch helps to attain a logic numbering of surfaces and of cells, this will in turn aid to write the input file and also to introduce future modifications. Once the input file completed, it should be reread, cross checking with the sketch, counting the number of cells and surfaces, verifying that no space is undefined or multiply defined. If the file has been correctly tabulated, a fast glance will spot typing errors from the irregularities in the columns of data.

As what concerns the systematics, another advice is to make several stages before reaching the full complexity of the problem. This enables to progressively correct mistakes; for instance, first one can implement the system of tubes with a simple source (point source), then, after debugging, insert the target material (foils or powder. . .), and, only after proper running, implement a more complex source, etc. If this were done in one go, it would be harder to disentangle the individual causes of the overall errors.

If a major error has been produced the program will terminate, complaining about some input/output error. If this happened it could be due to any of these causes:

- Some of the lines needed have been forgotten (like the card names or the explanatory lines).
- A coefficient in the cells definition has been omitted, typically some zero, or the roughness coefficient, or the independent term.
- All cells do not have the same number of elements; some cell has not been completed with zeros.
- The source type is not compatible with the number of source parameters (missing orientation angles or particle mass, or temperature . . .).

- An additional line has been written somewhere (line breaking is not authorized).

Once the input file is ’digested’ by the program, it is preprocessed and a message summarizes the geometry, telling the number of surfaces, the number of cells and the maximum number of surfaces that contour a cell.

```
————————————————————— number of cells: 2
——— highest number of walls in a cell: 6
———————————————————— number of bodies: 7
..................
```

The MC code then assembles the geometry, thereby networking the cells that have a common interface, and then it saves the result into an array. By doing so, each time that RIBO verifies whether a particle migrates from the current cell to any neighboring region (this happens after every collision), the amount of checks needed is reduced to the number of connecting cells, listed in the connectivity matrix (computed only one, at the beginning). That matrix, printed separately in the file **CCONM** condenses a lot of information of the geometry of the system and therefore it aids to cross-check the *Cells* and the *Surfaces* cards of the input file. The file contains a column with several groups of integer numbers; every group starts by the cell number and it is followed by those cells that have a common interface with that given cell[28]. The CCONM matrix of the followed example has only two groups (there are only two cells):

```
1
2

2
1
```

[28]This does by far not mean that these cells are actually touching.

The first group says that cell number 1 (first line) is connected to cell number 2 (second line), the second group says that cell number 2 (third line) is connected to cell number 1 (fourth line). This case is quite trivial but it helps to underline two properties:

- The connectivity matrix is symmetric.
- All groups should at least have two elements so that no cell is isolated from the rest[29]. Every row of the connectivity matrix must have at least two numbers different from zero.

If the source of particles were entirely located outside the system or if the cell source contained some errors, then a message on the screen would clearly warn the user:

```
Error in source card, source out of cell domain?
```

This may happen due to an incorrect implementation of the source or to some flaw in the definition of the geometry of the system.

In some cases the errors of geometry are detected by a routine of `RIBO` that casts a message on the screen like:

```
GEOMETRY ERROR!
check cell 2 or surface 4
```

However, many errors are not traced by the code; a vast geometry case compiler is still a pending task for future upgrades of the program.

For the time being one more tool is available for debugging purposes. At run-time, option 7 gives the opportunity to track a particle from birth to termination. This tracking can be made effective in three subsequent choices:

[29]If that were the case an error message would show on screen and in the CCONM file.

```
Choose one option
 1:coordinates x,y,z
 2:cell history
 3:surface history
```

Normally this is enough to detect persistent geometry mistakes.

In addition to all this, the user can change the end surface and choose closer surfaces (e.g. instead of having the gage at the end of a complex tubular system, it can be first put at the end of the beginning section and then pushed forward to next section, etc.) to ease the detection of the errors of geometry.

1.8.2 Typical error situations/messages

Source error

```
...Reading the "source" settings...
invalid number: incomprehensible list input
apparent state: unit 1 named inputfile.t
last format: list io
lately reading direct formatted external IO
Aborted
```

Reason: † Too few parameters in Source card.

Input file error: surfaces not read.

```
READING INPUT FILE
 temp.t
 ...
   1) reading surfaces...
list in: end of file
apparent state: unit 1 named temp.t
last format: list io
lately reading direct formatted external IO
Aborted
```

Reason: † You wrote ’cells’ instead of ’Cells’.

Input file error: apparent error in source.

```
Post-processing geometry...
  DONE
 RUNNING...
 x,y,z   0.302196309   0.00917545272 -0.146321036
 Error in source card, source out of cell domain?
```

Reason:

† You forgot a mandatory comment line, e.g. after 'Surfaces', or after 'Cells'.

† You defined a source that falls completely off the geometry.

Input file reading error

```
...Reading the "source" settings...
invalid number: incomprehensible list input
apparent state: unit 1 named inputfile.t
last format: list io
lately reading direct formatted external IO
Aborted
```

Reason:

† You did not exactly spell 'Surfaces'.

† You misspelled the name of the input file.

Error in the cells definitions

```
reading geometry...
 ...storing surfaces (bodies)...
     ...storing cells (regions)...
invalid number: incomprehensible list input
apparent state: unit 1 named temp.t
last format: list io
lately reading direct formatted external IO
Aborted
```

Reason: † Missing elements in the region definition.

1.9 Making 3D model views.

Making a 3D view of the target geometry is one of the fastest options to find out bugs in the geometry and to become aware of the target proportions. This is now possible through *3D-RIBO* and *Povray*. The first program executes `RIBO` and halts it when the Povray compliant geometry file (*.pov) is created. Next *Povray* is called and the image file (*.tga) is created.

```
> 3D–view input.t 1
```

The flat *1* specifies that the image file will be a thumbnail. *2* or *3* would produce images with higher resolution.

The intermediate *.pov file is a text document with the combinatorial geometry in Povray format. This file can be edited to include fancy features, e.g. roughness and special optical effects. Then, 3-D can be run by specifying the proper file extension.

```
> 3D–view input.pov 1
```

1.10 User defined subroutines

`RIBO` includes a growing number of routines that the user can change and customize. It goes without saying, that important user developments will be gladly accepted and acknowledged, in this way, `RIBO` will grow and the whole community will benefit.

Presently these are the routines available in $[sources]$:

1.10.1 User defined collisions, *customcollision.f*

This routine is called if the user answers ’C’ in the runtime question about the collision model.

```
      SUBROUTINE CustomColl(X3,grad3,T,A,surn,celln,rc,ts,tde,U3,COL7)
       integer*4 surn,celln                                          ! i
       real*8 X3(3),grad3(3),rc,T,A,ts                               ! i
       real*8 U3(3),COL7(7),tde                                      ! i/o
       real*8 SU3(3),SV3(3),SW3(3)                                   ! a
       real*8 phi,alpha,cosphi,n,k,V3scaV3,norm,a1,b1,c1,v,t0        ! a
*********************************************************************
*                                                                   *
*     WRITTEN BY:                                                   *
*                        MARIO SANTANA LEITNER, 2006                *
*                                                                   *
*-------------------------------------------------------------------*
*                                                                   *
*              CUSTOMIZE THIS FUNCTION TO FIT YOUR PROBLEM          *
*   USE:  transport problems with special physics for the collisions *
*                                                                   *
*   HIGHLIGHTS:                                                     *
*           - customized law, as a function of impinging angle      *
*           - desorption time sampled from Frenkel Law              *
*           - simulation of COLD spots                              *
*           - desorption function of temperature (position)         *
*                                                                   *
*   ACTIVATE USE THROUGH option 'C' at RUNTIME to the QUESTION:     *
*     'What kind of treatment of the collisions?'                   *
*     'S=Specular(E<<),B=Knudsen-Lambert,D=Debye,C=Custom           *
*                                                                   *
*   VARIABLES:                                                      *
*               INPUT                                               *
*     X3(3)   ------- Absolute position at collision point (x,y,z) [cm] *
*     grad(3) ------ Surface gradient (normal) at collision point   *
*                           always pointing inwards and normalized. *
*     T        ------ Starting energy of the atom [k] (source card) *
*     A        ------ Atomic mass [uam] (source card of input file) *
*     abs(surn)  --- Surface number (from input file)               *
*     surn     ------  position from which the particle hits or crosses  *
*                        the surface:                                    *
*                        <0 ==> 'inside' (-gradient)                     *
*                        >0 ==> 'outside' (+gradient)                    *
*     celln    ------  Present number of cell (region)                   *
*     rc      -------  First parameter of the surface after surface      *
*                          index number (e.g. roughness coefficient)     *
*     ts      -------  Average sticking time per collision (if it is ~   *
*                         constant all-over, it is normally define as 0  *
*                         in the runtime options. The output file then   *
*                         includes a sensitivity analysis for values     *
*                         other than 0.                                  *
*             I/OUT                                                      *
*     U3(3)   -------  Incoming/Outgoing velocity, ux,uy,uz of the atom  *
*                         [m/s]                                          *
*     COL7(7) ------   Counter for the type of collision for each history *
*                          1: Maxwell type 1                             *
*                          2: Maxwell type 2                             *
*                          3: Mirror-like                                *
*                          4: Debye (semi-classic)                       *
*                          5: Custom 1                                   *
*                          6: Custom 1                                   *
*                                                                        *
*     tde     -------  Particle desorption time [s]. Normally desorption *
*                         time in the collisions is taken into account   *
*                         at the end of each history as "ts*COLL".       *
*                         If you use a special desorption time distri-   *
*                         bution, (examples 4, 5), update the value of   *
*                         tde (as shown in those examples).              *
*           AUXILIARY                                                    *
*     SU3(3),...----   Base of auxiliary vectors to build up reflection  *
*     phi,alpha...--   Auxiliary angles to build reflected direction     *
*     ...                                                                *
*            EXTERNAL                                                    *
*     rand    -------  Seed for random generation                        *
*                                                                        *
*   NOTES:                                                               *
*     - Check available mathematical functions in math.f                 *
*     - Surface ionization is done separately                            *
*      -                                                               *
*                                                                      *
************************************************************************
*
*
*----------------------------------------------------------------------*
*  EXAMPLE 1, Snell reflection if rc>0.5, otherwise perpendicular      *
*----------------------------------------------------------------------*
*       IF (rc.gt.0.5) THEN
*         k = V3scaV3(grad3,U3) ! k = grad3(1)*U3(1)+grad3(2)*U3(2)+grad3(3)*U3(3) < 0
*         U3(1) = U3(1) - 2 * k * grad3(1)  !
*         U3(2) = U3(2) - 2 * k * grad3(2)
*         U3(3) = U3(3) - 2 * k * grad3(3)
*         COL7(5) = COL7(5) + 1.0
*       ELSE
*         U3(1) = grad3(1)
*         U3(2) = grad3(2)
*         U3(3) = grad3(3)
*         COL7(6) = COL7(6) + 1.0
*       END IF
*
*----------------------------------------------------------------------*
*  EXAMPLE 2, If the incidence angle is within a cone of 60\deg around *
*      the surface normal, then reflect isotropically within that cone, *
*      otherwise use mirror-like reflections                           *
*----------------------------------------------------------------------*
*
*       cosphi = V3scaV3(U3,grad3)/(norm(U3)*norm(grad3))  ! cos(phi)=a * b / |a|*|b| < 0
*       IF (cosphi.lt.0.5) THEN                            ! (phi>60\deg)
*         k = V3scaV3(grad3,U3) ! k = grad3(1)*U3(1)+grad3(2)*U3(2)+grad3(3)*U3(3)
*         U3(1) = U3(1) - 2 * k * grad3(1)
*         U3(2) = U3(2) - 2 * k * grad3(2)
*         U3(3) = U3(3) - 2 * k * grad3(3)
*         COL7(5) = COL7(5) + 1.0
*       ELSE                                               ! (|phi|>60\deg)
*         CALL isotropic(grad3,U3,60)                      ! defined in math.f
*         COL7(6) = COL7(6) + 1.0
*       END IF
*
```

```
*-----------------------------------------------------------------------*
*  EXAMPLE 3 , Poth (or Phong) model.                                   *
*       The particle is reflected with a cosine^n law around the        *
*       mirror-like reflected direction.                                *
*       n depends on the roughness                                      *
*-----------------------------------------------------------------------*
*
*         n = exp(rc*5.887)                              ! rc->0 ==> very rough
*         cosphi = V3scaV3(U3,grad3)/(norm(U3)*norm(grad3)) ! cos(phi)=a b / |a|*|b| < 0
*C----- Sample the alpha from "cos(alpha)**n" by REJECTION
*         alpha = asin(rand()*cosphi)                    ! alpha uniform ...
*         DO WHILE (rand().ge.(cos(alpha))**(n-1.0))     ! ...between 0 and 90-phi
*           alpha = asin(rand()*cosphi)
*         END DO
*C----- Now sample the azimuthal angle, beta by INVERSE transformation
*         beta=rand()*2*3.14159265
*C----- Now build up local base and get exit vector U3
*         CALL surfaceBase(SU3,SV3,grad3)
*         a1 = SIN(alpha) * COS(beta)
*         b1 = SIN(alpha) * SIN(beta)
*         c1 = COS(alpha)
*         U3(1) = a1 * SU3(1) + b1 * SV3(1) + c1 * grad3(1)
*         U3(2) = a1 * SU3(2) + b1 * SV3(2) + c1 * grad3(2)
*         U3(3) = a1 * SU3(3) + b1 * SV3(3) + c1 * grad3(3)
*         CALL renorm(U3)
*         COL7(5)=COL7(5)+1.0
*
*-----------------------------------------------------------------------*
*  EXAMPLE 4 , if incidence angle > 60 ==> mirror-like , no sticking    *
*       Otherwise , cosine law reflection + maxwell-Boltzmann thermali- *
*       zation + sticking time ~ exp(-t/t0) , t0=1E-5s                  *
*-----------------------------------------------------------------------*
*
*         cosphi = V3scaV3(U3,grad3)/(norm(U3)*norm(grad3)) ! cos(phi)=a b / |a|*|b|
*         IF (cosphi.lt.0.5) THEN                        ! (phi>60\deg)
*           k = V3scaV3(grad3,U3) ! k = grad3(1)*U3(1)+grad3(2)*U3(2)+grad3(3)*U3(3)
*           U3(1) = U3(1) - 2 * k * grad3(1)
*           U3(2) = U3(2) - 2 * k * grad3(2)
*           U3(3) = U3(3) - 2 * k * grad3(3)
*          COL7(5) = COL7(5) + 1.0
*        ELSE                                          ! (phi>60\deg)
*          CALL cosineLaw(grad3,U3)                    ! existing function
*          CALL Boltzmann(U3,T,A,mode)                 ! existing function
*C-----Now adding updating total desorption time per particle, tde:
*          tde = tde + ts * log(1/rand())              ! ts provided at runtime
*          COL7(6) = COL7(6) + 1.0
*        END IF
*-----------------------------------------------------------------------*
*  EXAMPLE 5, Sample the VELOCITY vector (angle,speed) with the cosine  *
*      Law and and M-B thermalization.                                  *
*      USE customized STICKING, as a function of position, X3, surface  *
*      and with a distribution function (do not just use average value) *
*      of the type : exp(-t/ts)/ts, ts=1E-5s                             *
*      The dependence with position is, e.g.:  t0 = ts * (1 + 1.25*z)   *
*      The surface (surn = 5) is a COLD SPOT where: t0 = ts * 100.0     *
*-----------------------------------------------------------------------*
*
*        CALL cosineLaw(grad3,U3)                      ! existing function
*        CALL Boltzmann(U3,T,A,mode)                   ! existing function
*C-----Now adding updating total desorption time per particle, tde:
*        IF (surn.eq.5) THEN
*          t0 = 100.0 * ts
*        ELSE
*          t0 = ts * ( 1 + 1.25 * X3(3))
*        END IF
*        tde = tde + t0 * log(1/rand())                ! Frenkel Law
*        COL7(1) = COL7(1) + 1.0                       ! CosineLaw counter
**       WARNING: use a positive ts, with a negative time you would be applying
**         the exponential law twice!
      END
```

1.10.2 User defined desorption in powder, *powderdesorption.f*

Very often the number of collisions in the powder is very large and therefore desorption becomes important for most isotopes. If the mean sticking time in the powder differs from that elsewhere or if it changes from one region of powder to another, the user can customize the user routine $[sources]/$powderdesorp.f in order to meet the particular requirements.

```
      SUBROUTINE powderdesorption(COLPOW, celln, tdep, ts)
       integer*4 celln                                          ! i
       real*8 COLPOW, ts                                        ! i
       real*8 tdep                                              ! i/o
       external rand
***********************************************************************
*                                                                     *
*     WRITTEN BY:                                                     *
*                        MARIO SANTANA LEITNER, 2006                  *
*                                                                     *
*---------------------------------------------------------------------*
*                                                                     *
*                 CUSTOMIZE THIS FUNCTION TO FIT YOUR PROBLEM         *
*   USE:  add customized desorption time within a powder cell         *
*   NOTE: normally at the end of the history, the amount ts * (COLP)  *
*             is added if tdep is zero                                *
*          don't try to sample from distributions (i.e. Frenkel) because *
*             here we check after a bunch of collisions (actually when the *
*             particle exits the powder cell), and NOT after each     *
*             collision. This will not imply any big error (central limit *
*             theorem)                                                *
*   HIGHLIGHTS:                                                       *
*             - simulation of COLD spots                              *
*                                                                     *
*   THIS ROUTINE IS ALWAYS READ THROUGH                               *
*                                                                     *
*   VARIABLES:                                                        *
*               INPUT                                                 *
*      celln    ------ Cell (region) (from input file)                *
*     COLLPOW  ----- Number of collisions in the powder cell in the   *
*                            last passage through                     *
*      ts       -------- average sticking time per collision          *
*                            (given at runtime)                       *
*               I/OUT                                                 *
*      tdep     -------- Particle elapsed desorption time spent in powder *
*                            domains [s]                              *
*              EXTERNAL                                               *
*      rand    -------- Seed for random generation                      *
*                                                                       *
*************************************************************************
*
*-----------------------------------------------------------------------*
*  EXAMPLE 1, cells 1,3,5 contain powder, the first one is warmer than *
*     the second and that one is warmer than the third                 *
*-----------------------------------------------------------------------*
*        IF (celln.eq.1) THEN
*          tdep = tdep + 1.0*ts
*        ELSE IF (celln.eq.3) THEN
*          tdep = tdep + 2.0*ts
*        ELSE IF (celln.eq.5) THEN
*          tdep = tdep + 3.0*ts
*        END IF
      END
```

1.10.3 User defined source distributions, *customsource.f*

This routine, called at particle generation is explained in 1.3.3, on page 16.

1.10.4 User defined output printing files *userprint.f*

This routine is called at the end of each particle history. It allows the user to print in whatever relevant information in units 21-25[76]

```
      SUBROUTINE userprint(ofile,td,tp,ts,tPo,tde,tdep,COL,COLP,COL6,U3,
     &     X3,X03,ocell,celln,ion,ads,survec,endvec)
       character*20 ofile                                          ! i
       integer*4 ocell,celln,ion,ads,survec(11),endvec(11)         ! i
       real*8 X03(3),X3(3),U3(3)                                   ! i
       real*8 COL,COLP,COL6(6),td,ts,tde,tdep,tPo,teff,tp,tT       ! i
       real*8 V3scaV3,norm,eve                                     ! a
       external rand                                               ! e
*************************************************************************
```

[76]The data will be stored in the files *21.out* to *25.out* in the directory from which `RIBO` is run.

```
*                                                                    *
*     WRITTEN BY:                                                    *
*                          MARIO SANTANA LEITNER, 2006               *
*                                                                    *
*--------------------------------------------------------------------*
*                CUSTOMIZE THIS FUNCTION TO FIT YOUR PROBLEM         *
*   USAGE:   print values after each history, eg. x,y,z,teff         *
*                                                                    *
*   VARIABLES:                                                       *
*                INPUT                                               *
*     ofile    --------- Output file                                 *
*     ocell    --------- Cell where particle was born                *
*     celln    --------- Cell where particle trajectory ends         *
*     ion      --------- Ionic state: 0 = neutral, 1 = ionized       *
*     ads      --------- Adsorption:  0 = none, 1 = particle was adsorbed  *
*     endvec(11) ---  Tells which of the paths (you can put up to 11)  *
*                          has been first completed. In normal cases   *
*                          (a single end surface) this is not relevant *
*     survec(11) ---  Tells which is the end surface                 *
*     X03(3)--------- Absolute position at starting point (x0,y0,z0)[cm] *
*     X3(3)    --------- Absolute position at end point (xf,yf,zf)[cm]   *
*     U3(3)    --------- End velocity {ux,uy,uz} of the atom [m/s]       *
*     COL      --------- Total number of collisions outside powder/particle *
*     COLP     --------- Total number of collisions inside powder/particle  *
*     COLP6(6) -----  Collisions of type i per particle              *
*     td       --------- Diffusion release time [s]                  *
*     ts       --------- Sticking time per collision [s/coll]        *
*     tde      --------- Particle elapsed desorption time spent in surfaces *
*                          other than those of the powder [s]        *
*     tdep     --------- Particle elapsed desorption time spent in powder  *
*                          cells [s]                                 *
*     tPo      --------- Flight time in the powder [s]               *
*     teff     --------- Flight time outside the powder [s]          *
*     tp       --------- Total effusion time:                        *
*                          tp = teff + tPo + ts * (COL+COLP)         *
*     tT       --------- Total release time per particle:            *
*                          tT = tp + td                              *
*            AUXILIARY                                               *
*     eve      --------- Event index:                                *
*                          eve = ion + 2 * ads                          *
*      ...                                                              *
*            EXTERNAL                                                   *
*      rand    -------  Seed for random generation                      *
*                                                                       *
*   OUTPUT UNITS                                                        *
*      - UNITS 21-25 are available for the user                         *
*                                                                       *
*************************************************************************
*
*
*-----------------------------------------------------------------------*
**   EXAMPLE 1: write to unit 21 the final and initial radius in a      *
**      cylinder oriented with axis z                                   *
*-----------------------------------------------------------------------*
*
*         write(21,FMT='(1X,2F9.6)') sqrt(X3(1)**2+X3(2)**2),
*      $        sqrt(X03(1)**2+X03(2)**2)
*
*-----------------------------------------------------------------------*
**   EXAMPLE 2: write to unit 22 the number of collisions of each type  *
*-----------------------------------------------------------------------*
*
*         write(21,FMT='(1X,8F9.2)')COL,COLP,COL6
*      $        sqrt(X03(1)**2+X03(2)**2)
      END
```

1.10.5 Other user defined routines

The RIBO distribution includes some other user customizable FORTRAN functions and subroutines. Indeed, the directory $[sources]$ contains also the open routines for the 3-D diffusion calculations of 3D GRID, explained in chapter 2, and printed in 2.3.

1.11 Output file.

The output file contains information about the run, average numbers and variables linked with every history. Its shape depends on the requests made by the user during execution, but in general terms these elements can be out-marked:

- *Heading*. It includes authoring information and specifies the input file name and path.

- *Individual scores*. This section may contain the global and fractioned release time and total number of collisions for every simulated atom. This usually constitutes the core goal of the simulations since it permits to reconstruct the intrinsic release functions.

- *Average figures of the release speed*. This group of data includes the average release time, the relative time consumption in the diffusion and effusion phases, the amount of in-grain versus inter-grain diffusion time... In presence of ionic fluxes, this output is divided in two groups, for ions and for neutral atoms. This allows assessing the impact of ionization in the effusion path and extraction efficiency.

- *Fitting of events* to a release function (see section 1.11.1)

- *Estimated release fractions* for given parameters and for conditions other that the ones specified, i.e. different sticking times and diffusion time constants (explained in section 1.11.2).

- *Average effusion time in each cell*. It permits to see which elements are slowing down effusion.

- Average number of collisions to each surface. This array provides clues on the potential chemical selectivity of each surface, or on its surface ionization power.

- *Statistics of the free flight*: average distance between two consecutive collisions, average flight path from birth to ionization or up to extraction…

- *Statistics of the effusion in a powder or fiber* (if present): average free flight path, number of collisions…

- Report of the effect of the residual gas: average free path between two collisions with a gas atom and average number of collisions per history.

- *Summary of the ionization scores*: ionization probability, estimate of the ionization efficiency and error margin.

- *Module integrating computation times*.

- *Authoring*.

Some modules deserve a dedicated explanation. For all the rest examples will illustrates a complete output file presenting almost all modules.

1.11.1 Fitting of events to a release function.

Unless otherwise specified, the code prints at run time, the starting (x,y,z) and final conditions (diffusion time *td*, effusion in powder *tPo*, effusion elsewhere *tf*, number of collisions in the powder *COLP*, number of collisions elsewhere *COL*, and ionic state) of each history. If the user wanted to build up a release distribution function out of the data, then the histogram option could be of help. However, the ideal histogram binning depends of the distribution itself (unknown at the beginning) and of the quality of the results (statistics), and therefore fitting the histogram to a smooth function may then become problematic.

Indeed, very often the ultimate goal is to obtain an analytic function that describes the release distribution probability (intrinsic release function), *R(t)*. Thus, it may be useful to deduce this function without having to go through the cumbersome procedure of producing a histogram of the data and fitting a curve to it.

`RIBO` contains a release function fitting functionality that is based on the so-called "statistical momenta" of the distribution. The method is the following. For every history the code updates a variable that contains the, e.g., average 'flight time', $\langle tf \rangle$. For every new particle *n* this figure can be updated in this way:

$$\langle tf \rangle_n = \frac{n-1}{n} \cdot \langle tf \rangle_{n-1} + \frac{tf_n}{n} \tag{1.1}$$

Thus, the code can compute $\langle tf \rangle$ without need of storing $tf_1,\ tf_2,\ldots,tf_n$. The same can be done for the higher order momenta, $\langle tf^2 \rangle,\ \langle tf^3 \rangle\ldots$ and for other magnitudes, like tPo, $tf + tPo$,...

Now, if we believe that the release function behaves simply as a decaying exponential $f_1(t) = C \cdot exp(t/t_1)$, we can find the value of C and t_1 easily by computing the momenta of $f(t)$ and equalizing to those of the real distribution. Moreover, we impose that the distribution is normalized. The parameters thereafter obtained are printed in the output file, for example, for the flight time[91], a possible result can be:

```
1) T = FLIGHT_TIME_IN_VACUUM-----------------------
 M1      M2      M3      M4      M5
```

[91]The same is done for the *flight time in the powder/fiber*(if any) and for the *total effusion time*.

```
0.2379 0.3249 0.4003 0.4643 0.5182

 Fit to T(i,t) = exp(-t/t1)/t1:
  t1=   0.23786
 error O(2)[%]: -7.17366
 error O(3)[%]:-25.86393
 Fit to T(i,t) ~ (1-exp(-t/t1))*exp(-t/t2):
  t1=   0.04672
  t2=   0.19999
 error O(3)[%]:   7.83485
 error O(4)[%]:  -1.87617
```

The meaning of the results is:

† `M1,..,M1` are the five momenta for the free flight time ($\sqrt[n]{\langle {t_{flight}}^n \rangle}$) obtained from the distribution. In this category the flight time spent within a powder or felt mesh is not considered (it is counted in "2) T = FLIGHT_TIME_IN_POWDER –...").

† A first fit to a simple decaying exponential $f_1(t_1)$ is done, the fit parameter being `t1`.

† `error O(2)[%]` is the relative error between the predicted M2 (from f_1) and the real one. Idem for `O(3)`

† Idem for the second function $f_2(t_1, t_2)$.

† Diffusion is not included here because its function is in principle known [14].

1.11.2 Computation of release fractions.

The individual delays for every history are printed in the output file, as well as the particle state (atom or ion, extracted or absorbed) and starting coordinates, so that the user can compute the the release fraction as a function of whichever parameter, e.g. diffusion time constant, sticking time, starting z coordinate . . .

Moreover, the output file includes a set of tables with the estimated release fraction for the input parameters (diffusion coefficient, sticking time) for different half-lives as well as for a variety of other diffusion and sticking time constants.

Briefly, the way to obtain these values, consisted in recording on-line a covariance matrix with the statistical momenta of the *effusion flight time* ($tf + tPo$) and of the *number of collisions* ($COLP + COL$) (and crossed terms) up to degree 3. Then, for any sticking time t_s, a 2-exponential effusion release function like $f_2(t_1, t_2; t)$ could be fitted (let us now call it $E(t_1, t_2, t_s; t)$) in the way described in 1.11.1. The global release function $R(t)$, would result from folding diffusion[92] and effusion:

$$R(t) = D(\tau_D, geometry; t) \bigotimes E(t_1, t_2, t_s; t) \tag{1.2}$$

And the release fraction for a half-life $T_{1/2}$ would be:

$$RF(T_{1/2}) = \int_0^t R(t) \cdot exp(-t/(ln(2) \cdot T_{1/2})) \cdot dt \tag{1.3}$$

This is equivalent to making the Laplace transform $\mathfrak{L}$ of RF:

$$RF(T_{1/2}) = \mathfrak{L}\left(RF(t)\right) \circ \left(s = \frac{1}{ln(2) \cdot T_{1/2}}\right) \tag{1.4}$$

The key point is that the Laplace transform of a convolution of two functions ($D \bigotimes E$) is the product of the Laplace transforms of each function, so the global

[92]Which depends on the diffusion time constant τ_D and the geometry (foil, fiber, particle)

release fraction RF is the product of the diffusion release fraction DRF and the effusion release fraction ERF:

$$RF(T_{1/2}) = DRF(T_{1/2}) \cdot ERF(T_{1/2}) \tag{1.5}$$

`RIBO` computes DRF($\tau_D, geometry, T_{1/2}$) and ERF($t_1, t_2, t_s; T_{1/2}$) from the analytic functions and it prints out the results in tables. For example:

```
                   |-------------------- ts(s) -------------------|
tao_d[s]   0.10E+0  0.0E+0  0.1E-8  0.1E-7  0.1E-6  0.1E-5  0.1E-4
------------------------------------------------------------------
 T_1/2[s]   DRF[%]  RF(ts1) RF(ts2) RF(ts3) RF(ts4) RF(ts5) RF(ts6)
 0.1E-2     7.727    0.000   0.000   0.000   0.000   0.000   0.000
 0.3E-2    13.126    0.007   0.007   0.007   0.006   0.003   0.000
 0.6E-2    18.198    0.036   0.036   0.035   0.031   0.014   0.001
 0.1E-1    23.022    0.116   0.116   0.114   0.102   0.046   0.003
 0.3E-1    37.213    1.214   1.212   1.201   1.096   0.552   0.046
 0.6E-1    48.936    4.329   4.326   4.294   3.995   2.247   0.225
 0.1E+0    58.506    9.598   9.592   9.536   9.005   5.584   0.678
 0.3E+0    78.059   33.413  33.402  33.302  32.325  24.677   5.327
 0.6E+0    87.058   53.647  53.637  53.541  52.597  44.483  14.564
 0.1E+1    91.622   67.231  67.222  67.143  66.364  59.327  25.862
 0.3E+1    96.960   86.780  86.776  86.738  86.364  82.766  57.048
 0.6E+1    98.441   93.026  93.024  93.003  92.797  90.770  73.942
 0.1E+2    99.051   95.719  95.718  95.705  95.575  94.298  82.933
 0.3E+2    99.673   98.533  98.533  98.528  98.483  98.036  93.739
 0.6E+2    99.830   99.256  99.256  99.254  99.231  99.004  96.784
 0.1E+3    99.893   99.548  99.548  99.546  99.533  99.396  98.046
```

Chapter 2

3-D Diffusion module.

2.1 Brief physical introduction

The diffusion of atoms within a solid, and the conduction of heat both follow the Fick's Law:

$$\vec{J_{\hat{n}}} = a \cdot na\vec{bla}_{\hat{n}} U \tag{2.1}$$

Where U is the concentration ($[\frac{par}{cm^3}]$) or the temperature ($[K]$) and $\vec{J_{\hat{n}}}$ is the flux of particles ($[\frac{par}{cm^2 s}]$) or of heat power ($[\frac{J}{s}]$) in the direction determined by $\hat{n}$. The constant a corresponds either to the diffusion coefficient D ($[\frac{cm^2}{s}]$) or to the thermal conductivity k ($[\frac{W}{s\ K}]$).

`RIBO` divides the space in finite units of volume dV (voxels), the dimensions ($dV = dx_i^3$) of which are determined by the user. Each voxel will be labeled with its initial concentration (or temperature) and the cell number to which it belongs (if any). Time is discretized in time steps (the length is adjusted dynamically). Each voxel exchanges atoms (or heat) in the direction $\hat{i}$ through the interface area $dA_i = dx_j \cdot dx_k$ that communicates to the next voxel. This is done by mass diffusion (or head conduction) flows, or by desorption (or radiation[1]) if the communicating voxel belongs to vacuum.

For a given voxel i, j, k, the balance of U in the interval dt, expressed in Cartesian coordinates is:

$$dU = (g + d + s) \cdot dt \tag{2.2}$$

Where:

- g is the source term:

$$g = \begin{cases} \frac{par}{cm^3\ s} & \text{for atomic diffusion} \\ \frac{J}{cm^3\ s} & \text{for heat calculations} \end{cases} \tag{2.3}$$

- d is the diffusion or conduction flow term:

$$\sum_{i=x,y,z} \breve{a} \frac{\{U_{i+} - 2U_i + U_{i-1}\}}{dx_i} \cdot dA_i \cdot \frac{dt}{dV} \tag{2.4}$$

  The constant $\check{D}$ is the mass or heat diffusion coefficient ($[\frac{cm^2}{s}]$). Note that the thermal diffusion coefficient is obtained in terms of other more familiar parameters:

$$\check{D} = \frac{k}{Cp \cdot \rho} = \frac{conductivity[\frac{W}{cm\ s}]}{Specific\ Capacity\ [\frac{W\ s}{g\ K}] \cdot Density\ [\frac{g}{cm^3}]} \tag{2.5}$$

  The user is asked to split up the geometry in cells enclosed by quadrics. The mass diffusion / heat transfer properties of each cell must be defined by the user in the data file $[data]/Cond.dat$ (see 2.2.1 on page 65).

[1]Convection is not considered in this version, but it could be easily included.

- s is the surface term, which appears only in those voxels in the boundary between a cell and the vacuum. This term has the following meaning:

$$s = \begin{cases} d \cdot (1 - exp(dt/t_d))\,[\frac{par}{cm^3\ s}] & \text{atomic desorption for surfaces} \\ \varepsilon(T) \cdot \sigma_{SB} \cdot (T^4 - T_0^4) \cdot \frac{dA}{Cp \cdot \rho \cdot dV}\,[\frac{K}{s}] & \text{T = U, heat radiation} \end{cases} \tag{2.6}$$

  Where, for atomic desorption t_d is the average desorption time ($[s]$), and for heat radiation, $\varepsilon(T)$ is the emissivity (0-1), σ_{SB} is the Stephan-Boltzmann constant ($5.6703 \cdot 10^{12}[\frac{W}{K^4 cm^2}]$), U is the temperature T ($[K]$) of the voxel and T_0 is the average temperature 'seen' by the boundary voxel.[2]

  By applying the equation 2.2, the Concentration / Temperature in every voxel $C\,(i, j, k, 1)$[3] can be monitored over time.

2.2 Instructions of use

In order to run a 3D (atomic or thermal) diffusion problem, the following steps have to be cleared.

1. Retrieve the conduction, desorption and/or radiation constants, transform them into S.I, except length units (in $[cm]$), and fill in the $[data]/cond.dat$ file, as explained in 2.2.1.

2. Write the input file to describe the geometry of the system using combinatorial geometry. Note that you must fill in all the cards and fields in the standard way for effusion calculations (*Surfaces, Cells, Source and Tally*), even if you are not going to need them all.

[2]The function *dTrad.f* is open for the user to customize the expression of the radiation as well as the temperature dependency of ε, $\varepsilon(T)$.

[3]$C\,(i, j, k, 2)$ contains the cell index of the voxel $\{i, j, k\}$.

3. Adjust the source routines to match your specific requirements:

    - Customize the initial concentration (or temperature) distribution by modifying the file $[sources]/CSTART.f$, as explained in 2.3.1 (page 68).
    - If needed, introduce time-space-direction dependences in the diffusion parameter by editing the routine $[sources]/Dijkt.f$, printed in 2.3.3 (on page 70).
    - Edit the file $[sources]/gener.f$ (page 69) to add time-space-region dependent sources (or sinks) of atom concentration (or heat).
    - For heat transfer calculations, modify the subroutine $[sources]/radia.f$ (see sec 2.3.4, on page 72) to adjust the radiation function to your problem.
    - Customize the printing routine $[sources]/userPRINT3D.f$ (see section 2.3.5) to print the necessary information.

4. Recompile the `RIBO` distribution with the script provided in $[tools]/make.sh$

5. Run `RIBO` and provide the right run-time options, discussed in 3.1.4.

2.2.1 $[data]/Cond.dat$ file

The file $[data]/Cond.dat$ contains the information about the diffusion parameter, desorption time, emissivity and volumetric specific capacity (at constant pressure). The first 6 lines of the file are explanatory and should not be removed. The code should find the valid information starting exactly in row 7. The **first column**

(i) contains the cell number (celln). The **columns 2, 3, 4** have the information on the diffusion parameter $\check{D}$ ($\frac{cm^2}{s}$), either as the diffusion coefficient D, or the conductivity normalized to the specific capacity and to the density. In any case, the diffusion parameter can depend on the variable U (Concentration or Temperature). In every voxel (see eq. 2.2) the code will compute the diffusion parameter as:

$$\hat{D} = \hat{D0} + \hat{DU} \cdot U + D\hat{U}U \cdot U^2 \tag{2.7}$$

Column 5 has the information on the average desorption time ($[s]$) for atomic diffusion or the emissivity, ε, for photon radiation. Special temperature dependence laws $\varepsilon(T)$ should be introduced in $[sources]/dTrad.f$. See YYY

Columns 6, 7 and 8 Contain the specific heat capacity in $[\frac{W\ S}{cm^3\ K}]$. Three coefficients can be provided, like for $\check{D}$.

```
|   3-D DIFFUSION   (MASS/HEAT) DATA           RESPECT FORMAT !!
|   D(T)[cm2/s] = D0 + DC * C + DCC * C^2;      K(T)[W/cmK]= k0 + KT * T + KTT * T^2
|  Cp(T)[J/Kcm^3] = Cp0 + CpT * T + CpTT * T^2; t_desorption [s]; eps = emissivity 0,1
+-------------------------------------------------------------------------------------
  i    D0|K0  DC|KT   DCC|KTT  t_des|eps  - | Cp0  - | CpT  - | CpTT
-------------------------------------------------------------------------------------
  1     2.70   0.0      0.0       0.25    170.0     0.0      0.0
  2     2.49   0.0      0.0       0.19     58.0     0.0      0.0
```

2.2.2 Activating 3-D diffusion calculations

The user should give the following answers to activate 3D diffusion calculations (see example in 3.1.4),

1. **inputfilename**

2. **outputfilename**

3. **cello** cell to which generation is limited. Type 0 if you don't need any restriction here.
4. **1**
5. **inmode 5** for atomic diffusion) or **6** for heat transfer.
6. **output printing mode 8** average numbers, **9** print full grid, **C** custom.
7. **Xmin Ymin Zmin** Low edge coordinates of the 3D window. Vacuum will occupy the outer space.
8. **DX DY DZ** Lengths of the sides of the 3D window box.
9. **NX NY NZ** Number of bins in each direction.
10. **Termination condition and value**

2.3 User defined functions and subroutines

The file $[sources]/custom3D.f$ contains a set of functions and subroutines that can be edited to fit specific requirements in 3D diffusion problems. For the time being, the included objects are:

1. *CSTART.f* to specify the starting profile of concentration or temperature.
2. *gener.f* to define outer sources or sinks of atoms or heat.
3. *Dijkt.f* to customize the diffusion coefficient (spatial or time dependence).
4. *radia.f* to adapt the radiation function.
5. *userPRINT3D.f* to determine the entities to be printed.

2.3.1 Customizing the starting distribution of Concentration or Temperature, *CSTART.f*

```
      FUNCTION CSTART(R,celln,inmode)
        real*8 R(3),CSTART                                        ! i
        character*12 inmode                                       ! i
        integer*4 celln                                           ! i
        real*8 C0                                                 ! a
**********************************************************************
*               CUSTOMIZE THIS FUNCTION TO FIT YOUR PROBLEM          *
*                       USAGE: 3D diffusion problems                 *
* The starting Concentration / Temperature may depend on the coordinates *
*          e.g.  C0 = 273                                            *
*                C0 = 273 * ( R(1) + R(2) )                          *
*          It can also depend on the material (celln), or on both   *
*     Variables:                                                     *
*         - R(3): absolute coordinates, x,y,z [cm] of the volume voxel *
*         - CSTART: Starting concentration / Temperature             *
*         - celln: number of the cell                                *
*         - inmode: (5) ==> mass diffusion problem (6) ==> heat transfer *
**********************************************************************
        IF (celln.ge.1) THEN
          IF (inmode.eq.'5') THEN
            C0 = 1.0
          ELSE IF (inmode.eq.'6') THEN
            C0 = 500.0 ! starting temperature
          END IF
        ELSE                    ! outer space
          IF (inmode.eq.'5') THEN
            C0 = 0.0
          ELSE IF (inmode.eq.'6') THEN
            C0 = 298.0
          END IF
        END IF
        CSTART = C0
      END
```

2.3.2 Defining source and / or sink terms, *gener.f*

```
      FUNCTION gener(R,C0,t,PAR,Dbq,ncell,celln,inmode)
        integer*4 ncell,celln                                         ! i
        character*12 inmode                                           ! i
        real*8 R(3),C0,t,PAR(5),Dbq(7,ncell)                          ! i
        real*8 dV,CpRho                                               ! a
        real*8 gener                                                  ! o
*****************************************************************************
*      Customize this function to include heat or mass sources              *
*        that depend on the position X, or/and time, or/and                 *
*             the concentration, celln, emissivity, ...                     *
*****************************************************************************
*   VARIABLES:                                                              *
*        R(3) = coordinates (x,y,z)[cm]            DO NOT MODIFY VALUE!     *
*          C0 = Concentration [par/cm^3] | Temperature [K]                  *
*           t = elapsed time [s]                                            *
*      PAR(1) = dV = dx * dy * dz [cm^3]  Useful to normalize generation    *
*      PAR(2) = concentration/temperature at point X  [cm^-3 | T]           *
*      PAR(3) = celln                                                       *
*      PAR(4) = t_desorption/emissivity [s | W/cm^2*K^4]                    *
*      PAR(5) = dt [s]                                                      *
*      inmode = 5 mass diffusion | 6 heat transfer                          *
*    ---------------------------------------------------------------        *
*      Dbq(1) =  D0 [cm^2/K^0 s] | k0  [W/cm K^1]                           *
*      Dbq(2) =  DC [cm^2/K^1 s] | kT  [W/cm K^2]                           *
*      Dbq(3) = DCC [cm^2/k^2 s] | kTT [W/cm K^3]                           *
*      Dbq(4) =          t_s [s] | Eps [W/K^4]  !YYY Eps(T)...              *
*      Dbq(5) =                - | Cp0*rho  [W s/cm3 K^1]                   *
*      Dbq(6) =                - | CpT*rho  [W s/cm3 K^2]                   *
*      Dbq(7) =                - | CpTT*rho [W s/cm3 K^3]                   *
*       ncell = number of cells of the geometry                             *
*...........................................................................*
*       CpRho = Cp*Rho [W s/K cm^3]                                         *
*****************************************************************************
*   UNITS of gener                                  gener                   *
*      For MASS TRANSFER:                 dV                                *
*        need : par / (cm^3 * s)--------------> par / s                     *
*      For HEAT TRANSFER:            (dV/CpRho)                             *
*         need :   J / (cm^3 * s)--------------->  K / s              *
*   EXAMPLES:                                                          *
*      1) constant generation of particles, 1E5 (par/cm3 s)           *
*            gener [par/s] = 1E5 * dV                                  *
*      2) constant heat generation: (1kW/cm^3)                         *
*         ===> gener [K/s]   = 1000 * dV / (CpRho)                     *
************************************************************************
*   NOTE:                                                              *
*         The generation may depend on time and on X, ...              *
************************************************************************
        dV = PAR(1)   ! [cm^3]
        gener = 0.0
        IF (inmode.eq.'5') THEN        ! 3D mass diffusion
*         gener = 1E4 * dV                  ! [par/s]
        ELSE IF (inmode.eq.'6') THEN ! 3D heat transfer
          CpRho = (Dbq(5,celln))
     $           + (Dbq(6,celln) * T)
     $           + (Dbq(7,celln) * T * T)
          IF (celln.eq.1) THEN
* EXAMPLE 10 kW / cm^3 deposited in cell = 1:
            gener = 10000.0 / CpRho   ! [W/cm^3]-->[K/s]
          END IF
        END IF
      END
```

2.3.3 User defined mass/heat diffusion coefficients, *Dijkt.f*

```
      FUNCTION Dijkt(I,X,t,N,C,Dbq,ncell,inmode)
        integer*4 N(3),I(3),ncell                                  ! i
        character*12 inmode                                        ! i
        real*8 C(300,300,300,2),X(3),Dbq(7,ncell),t                ! i
        integer*4 celln                                            ! a
        real*8 CorT,CpRho,k                                        ! a
        real*8 Dijkt                                               ! o
************************************************************************
*                  CUSTOMIZE THIS FUNCTION TO FIT YOUR PROBLEM         *
************************************************************************
```

```
*                          written by MSL, 2006                                 *
*********************************************************************************
*     This function computes the DIFFUSION coefficient | CONDUCTIVITY          *
*     for a given voxel (that corresponds to position X), and depending        *
*     on the CONCENTRATION | TEMPERATURE, parsed constants Dbq and cell        *
*     number                                                                   *
*   VARIABLES:                                                                 *
*    case           (MASS) transfer              (HEAT) transfer               *
*   ---------------------------------------------------------------------      *
*   inmode:              = 5                |              =6                  *
*    CpRho:                                 |  Cp*Rho [W s/K cm^3]             *
*        k:                                 |  conductivity [W/K cm]           *
*    Dijkt: Diffusion coeff.(D)[cm^2/s]     |  k/(Cp*Rho) [cm^2/s]             *
*     C...:    {concentration,celln}        |   {Temperature,celln}            *
*      Dbq:      diffusion constants        |  conductance/emiss. (Cond.dat)   *
*        t:                        elapsed time [s]                            *
*     N(3):                number of divisions in {x,y,z}                      *
*     I(3):                   voxel identifier {i,j,k}                         *
*     X(3):              position of center of voxel {x,y,z}                   *
*    ncell:              total number of regions in geometry                   *
*   ---------------------------------------------------------------------      *
*   NOTES:                                                                     *
*     A quadratic law D(C) and k(T) are assumed, but other laws can be         *
*     implemented in this function                                             *
*********************************************************************************
*     The user may introduce fancy features now, for example:                  *
*     1) Time dependency of diffusion coefficient                              *
*        Dijkt = ... * sin(t)                                                  *
*     2) X-dependency of diffusion coefficient                                 *
*     ...                                                                      *
*********************************************************************************
        celln = NINT(C(I(1),I(2),I(3),2))
        IF (inmode.eq.'5') THEN
          IF (celln.eq.0) THEN
          Dijkt = 0.0
          ELSE
           CorT = C(I(1),I(2),I(3),1)   ! Concentration
          Dijkt = (Dbq(1,celln))
     $          + (Dbq(2,celln) * CorT)
     $          + (Dbq(3,celln) * CorT * CorT)
          END IF
        ELSE IF (inmode.eq.'6') THEN
          IF (celln.eq.0) THEN
          Dijkt = 0.0
          ELSE
           CorT = C(I(1),I(2),I(3),1)  ! Temperature
               k = (Dbq(1,celln))
     $          + (Dbq(2,celln) * CorT)
     $          + (Dbq(3,celln) * CorT * CorT)
          CpRho = (Dbq(5,celln))
     $          + (Dbq(6,celln) * CorT)
     $          + (Dbq(7,celln) * CorT * CorT)
          Dijkt = k / CpRho
          END IF
        END IF
      END
```

2.3.4 Customized heat radiation (and convection) function, *radia.f*

```
      FUNCTION radia(i,M,T,C,N,R,PAR,Dbq,dA,ncell)
        integer*4 i,ncell,N(3)                                            ! i
        real*8 M(3),T,PAR(5),dA(3),Dbq(7,ncell),C(300,300,300,2),R(3)     ! i
        real*8 emissivity,sigSB,eps,T0,dV,radia,CpRho,norm                ! a
        integer*4 celln                                                   ! a
***********************************************************************
*     THIS SUBROUTINE checks if we are in a heat radiation problem    *
*       (inmode=6) and, if so, it computes the radiated power Qr [W]  *
*       as a function of the emittance (eps), the exposed area dA(i)  *
*       and the temperature difference (T=C0,T0=external)             *
*     VARIABLES:                                                      *
*            i = exposed area normal vector {i,j,k}                   *
*         M(3) = material of neighboring cell (should be vacuum, M=0) *
*            T = Temperature of the voxel [K]                         *
*          C...= Temperature{i,j,k,celln}                             *
*         N(3) = number of divisions in {x,y,z}                       *
*        X(3) = position of center of voxel {x,y,z}                   *
*      PAR(1) = dV = dx * dy * dz [cm^3]  Useful to normalize generation *
*      PAR(2) = concentration/temperature at point X  [cm^-3 | T]     *
*      PAR(3) = celln                                                 *
*      PAR(4) = t_desorption/emissivity [s | W/cm^2*K^4]              *
*      PAR(5) = dt [s]                                                *
*   ---------------------------------------------------------         *
*      Dbq(1) =  D0 [cm^2/K^0 s] | k0  [W/cm K^1]                     *
*      Dbq(2) =  DC [cm^2/K^1 s] | kT  [W/cm K^2]                     *
*      Dbq(3) = DCC [cm^2/k^2 s] | kTT [W/cm K^3]                     *
*      Dbq(4) =           t_s [s] | Eps [W/K^4]  !YYY Eps(T)...       *
*      Dbq(5) =                -  | Cp0*rho  [W s/cm3 K^1]            *
*      Dbq(6) =                -  | CpT*rho  [W s/cm3 K^2]            *
*      Dbq(7) =                -  | CpTT*rho [W s/cm3 K^3]            *
*.....................................................................*
*       dA(3) = dA(i) is the perpendicular area for normal i [cm^2]   *
*       CpRho = Cp*Rho [W s/K cm^3]                                   *
*          T0 = ambient temperature [K]                               *
*       sigSB = Stephan-Boltzmann constant = 5.6703E-12 [W/cm^2*K^4]   *
***********************************************************************
*      CUSTOMIZATION                                                  *
*        - replace eps by a function of temperature eps(T)            *
*        - replace T0 by the ambient temperature or by the temperature *
*             of enfolding cells, e.g T0=C(10,4,9,1)                  *
***********************************************************************
         celln = NINT(PAR(3))
         IF (M(i).lt.1E-14) THEN
           CpRho = (Dbq(5,celln))
     $            + (Dbq(6,celln) * T)
     $            + (Dbq(7,celln) * T * T)
           dV    = PAR(1)                          ! [cm3]
           sigSB = 5.6703E-12                      ! [W/K^4 cm^2]
           emissivity = PAR(4)                     ! [-]
           eps = sigSB * emissivity                ! [W/K^4 cm^2]
           T0    = 298.0                           ! [K] ambient temperature
***********************************************************************
*      EXAMPLE: heat3D.t                                              *
*      - The solid W sphere sees the inner side of the outer Ta spheric *
*        shell. C(10,90,90,1) corresponds to the temperature in a point *
*         of the Ta inner side. The spheric symmetry allows to leave that *
*         same reference point for whatever position                      *
*       - The Ta spheric shell (celln=2) sees, in the inside, the W       *
*         sphere C(31,90,90,1) and, in the outside, the open air, T=298   *
***************************************************************************
          IF (celln.eq.1) THEN          ! W sphere
            T0  = C(10,90,90,1)         ! Temperature of inner face of Ta shell
          ELSE IF (celln.eq.2) THEN     ! Ta shell
            IF (norm(R).le.4.40) THEN ! inner face
            T0  = C(31,90,90,1)         ! ==> ~ Surface temperature of the W sphere
            ELSE                        ! outer face
            T0 = 298.0                  ! ==> Sky temperature
            END IF
          END IF
          radia = eps * ((T0**4)-(T**4)) * dA(i) / (CpRho*dV)
***************************************************************************
*       EXAMPLE 2     CONVECTION                                          *
*       - Note that you can also include convection                       *
*         First define the variable "conv" and the parameter "constant"    *
*       - Uncomment these lines:                                          *
*           conv = constant * (TO - T)                                    *
*           radia = eps * ((T0**4)-(T**4)) * dA(i) / (CpRho*dV) + conv    *
***************************************************************************
        ELSE
          radia = 0.0
        END IF
      END
```

2.3.5 Customized the printout values, *userPRINT3D.f*

```
      SUBROUTINE userPRINT3D(t,N,C,C0,nbin,Cmax,Imax,Rmax,cellmax,
     $           Cmin,Imin,Rmin,cellmin,sum,sum0)
        integer*4 N(3),Imax(3),Imin(3),cellmax,cellmin              ! i
        real*8 C(300,300,300,2),C0(300,300,300,2),Cmax,Cmin,nbin     ! i
        real*8 t,sum,sum0                                            ! i
        real*8 Rmax(3),Rmin(3),fmax,fmin,Cav,fav                     ! i
        integer*4 i                                                  ! a
      logical fileNOTyetOPEN                                            ! a
**********************************************************************
*              CUSTOMIZE THIS FUNCTION TO FIT YOUR PROBLEM            *
**********************************************************************
*                        written by MSL, 2006                         *
**********************************************************************
*   VARIABLES:                                                        *
*      - t:      Elapsed time [s]                                     *
*      - N(3):   Number of bins in each direction x,y,z               *
*      - C(300,300,300,2): two values for each voxel                  *
*            C(300,300,300,=2): material index (region number)        *
*            C(300,300,300,=1): Concentration | Temperature           *
*      - C0(300,300,300,2): stores the values of C at t=0             *
*      - Cmax(Cmin): Highest(Lowest) Concentration | temperature      *
*      - Imax(Imin): Pointers {i,j,k} of the voxel with Cmax(Cmin)    *
*      - Rmax(Rmin): Coordinates of the voxel of Cmax(Cmin) {x,y,z} [cm] *
*      - cellmax(cellmin): the voxel of Cmax(Cmin) belongs to celln...  *
*      - nbin:   number of voxels belonging to a cell                 *
*      - sum:    sum of concentrations/temperatures at time t         *
*      - sum0:   sum of concentrations/temperatures at time 0         *
**********************************************************************
*   EXAMPLE 1
*      - Print the evolution of the matrix C (lot of memory!!):
**
*        DATA fileNOTyetOPEN / .TRUE. /
*        IF ( fileNOTyetOPEN ) THEN
*        fileNOTyetOPEN = .FALSE.
*        OPEN(UNIT=26,FILE='26.out')
*        write(6,*)'Creating file unit 26'
*        END IF
**
*        write(6,*)C
**********************************************************************
*
      END $
```

Chapter 3

Examples of RIBO use.

3.1 Examples.

3.1.1 First example. Geometry issues.

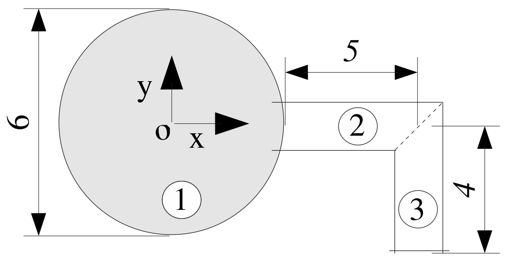

Figure 3.1: A simple example consisting on a bulb full of He at 300 K connected to a pipe of 1 cm diameter with a bend of 90 °.

The first example consists on bulb full felt with He at 300 K and connected to a pipe of 1 cm diameter with a bend of 90 °. Dimensions are shown in fig.3.1. It is indeed a simple geometry, but attention has to be paid to define the correct subspaces unambiguously. For that sake auxiliary planes are needed. In fig.3.2. surface 2 is an auxiliary plane that will help to define the second cell, if it was not used, the program could not logically decide between the real cell and the dotted one. In fact, it would allow transmission of particles both to the right and to the left. The same is valid for the crossing of pipes at the surface 4. The *Surfaces* card

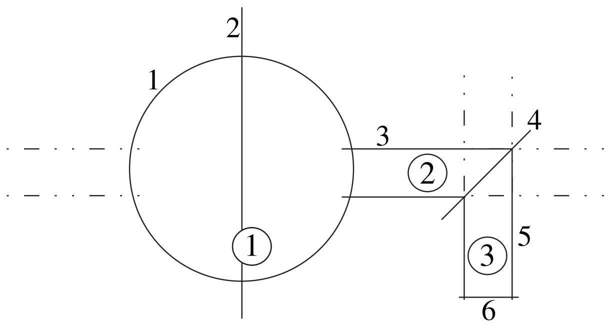

Figure 3.2: Surfaces and cells for the first example. Auxiliary surfaces are needed to define the correct subspaces.

would be something like this:

Surfaces

n	rc	T	x2	y2	z2	xy	xz	yz	x	y	z	C
1	0.5	300	1	1	1	0	0	0	0	0	0	9
2	0.5	300	0	0	0	0	0	0	1	0	0	0
3	0.5	300	0	1	1	0	0	0	0	0	0	0.25
4	0.5	300	0	0	0	0	0	0	1	-1	0	8
5	0.5	300	1	0	1	0	0	0	-16	0	0	-63.75
6	0.5	300	0	0	0	0	0	0	0	1	0	-4

And the *Cells* card would read as:

Cells

n	S1	S2	S3	S4
1	-1	0	0	0
2	1	2	-3	4
3	-4	-5	6	0

The *Source* card, for a homogeneous distribution in the sphere should be:

Source

Type	M	T	Alpha	nx	ny	nz	x	y	z	L	s	th	phi
S	4	300	180	1	0	0	0	0	0				

3.1.2 Second example. Bigger files.

A more realistic example for the field of radioactive ion beams is that of a target made of thin foils. Fig.3.3 sketches a target with a SPIRAL Christmas-tree-like shape [1, 2], intended to dissipate the energy of the beam in steps. Surfaces 1, 2 and 3 are planes and 4 and 5 cylinders; they delimit the target container and the transfer line (cells 1 and 2, respectively). The sixth surface is a cone and the remaining surfaces 1 $\div$ n are planes; these surfaces enclose the target slabs (of thickness d) and the spacing between them (δ between two consecutive front faces). The *Surfaces* card would look something like this (the symbols L1,

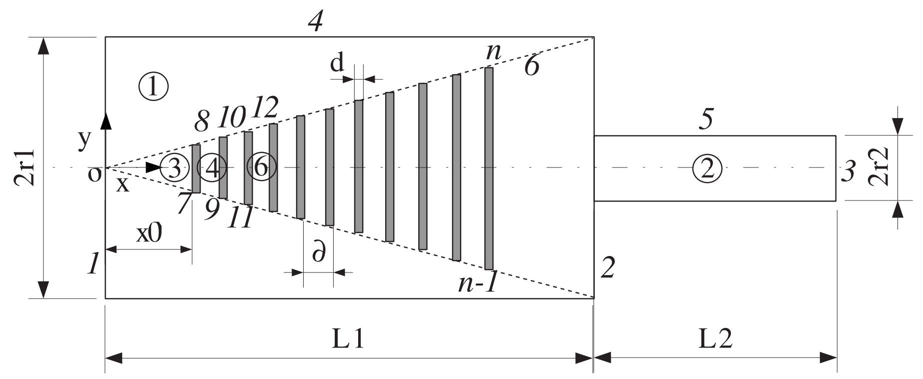

Figure 3.3: Sketch of a GANIL-SPIRAL type target [1, 2].

L2... should have to be replaced by numeric values):

Surfaces

n	rc	T	x2	y2	z2	xy	xz	yz	x	y	z	C	
1	0.5	300	0	0	0	0	0	0	1	0	0	0	plane
2	0.5	300	0	0	0	0	0	0	1	0	0	L1	plane
3	0.5	300	0	0	0	0	0	0	1	0	0	L2	plane
4	0.5	300	0	1	1	0	0	0	0	0	0	$r1^2$	big cylinder
5	0.5	300	0	1	1	0	0	0	0	0	0	$r2^2$	small cylinder
6	0.5	300	$-(r1/L1)^2$	1	1	0	0	0	0	0	0	0	containing cone
7	0.5	300	0	0	0	0	0	0	1	0	0	x0	first foil front
8	0.5	300	0	0	0	0	0	0	1	0	0	x0+d	first foil back

```
9   0.5  300  0  0  0  0  0  0   1  0  0   x0+δ    second foil front
10  0.5  300  0  0  0  0  0  0   1  0  0   x0+d+δ  second foil back
⋮
```

The *Cells* card would look more or less like this (if the number of elements is big, the best method is to use a spreadsheet to generate surfaces and cells):

```
Cells
n   S1   S2   S3   S4
1    1   -2   -4    6   container outside target zone
2    2   -3   -5    0   Transfer line and/or ionizer
3   -6    1   -7    0   cone peak
4   -6    7   -8    0   space between foils 1 and 2
5   -6    8   -9    0   space between foils 2 and 3
⋮
```

3.1.3 Third example, *test.inp*.

In the standard distribution of files an example input file called *test.inp* and a possible output file called *test.out* are provided. In this section all steps will be thoroughly described: input file, runtime options and interpretation of the output file. Thus, the user shall be able to test the system and to get acquainted to most functions of `RIBO`. Once results are recovered, experiencing with the input file and runtime options is encouraged so as to gain a total control of the program prior to real-case usage.

Input file

The details of the problem are found in the input file:

```
Surfaces
#   RC    T    X2  Y2  Z2  XY  XZ  YZ  X   Y   Z   C
1   0.5   298  0   0   0   0   0   0   1   0   0   −1.5
2   0.5   298  0   0   0   0   0   0   1   0   0   5
3   0.5   298  0   0   0   0   0   0   1   0   0   10
```

1

```
4    0.5   298    0     0    0    0    0    0    0    1    0    −1
5    0.5   298    0     0    0    0    0    0    0    1    0    1
6    0.5   298    0     0    0    0    0    0    0    0    1    −1
7    0.5   298    0     0    0    0    0    0    0    0    1    1
8    0.5   298    0.25  1    1    0    0    0    0    0    0    0.25
9    0.5   2000   0     1    1    0    0    0    0    0    0    0.249
Cells
#     S1    S2     ..
1     −8    0      0     0    0    0    0
2     8     1      −2    4    5    6    −7
3     2     −3     −9    0    0    0    0
Source
Type  M     T      Alfa  nx   ny   nz   X    Y    Z    R
S     7     298    180   −1   0    0    0    0    0    0.999
Tally
S     max   Tmax   Tpmax
3     300   750    10
```

The primary source that is used here is a sphere, the radius of which equals the maximum radius of the ellipsoid. The cell-limited option will be chosen at runtime.

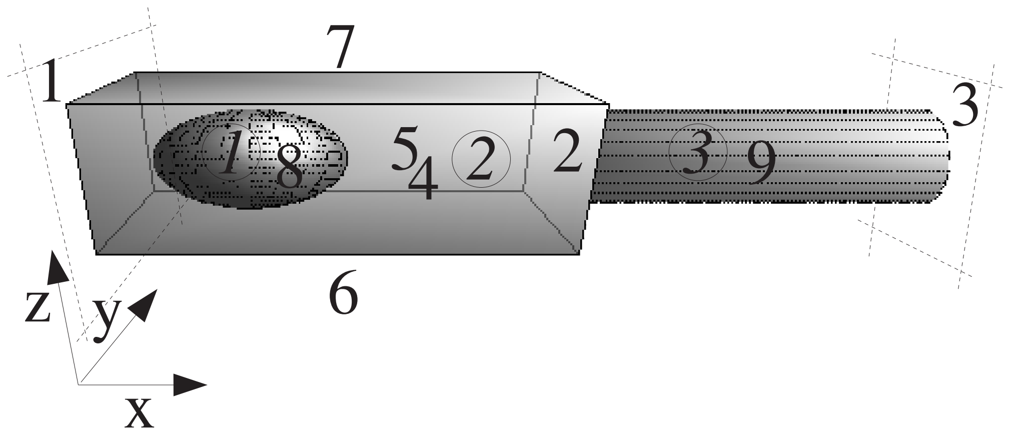

Figure 3.4: The target and ion source of example 3.

Runtime options

The sequence of interactions with the program at runtime is screen printed below. Some comments are interpolated:

The ion source may span over multiple cells

```
...
  ________________________________________________________________
 |    RRR                II         BBB            OO             |
 |    R   R              II         B   B        O    O           |
 |    RRR      adio -    II   on    BBB    eam   O    O   ptimi - |
 |    R   R   active     II         B   B        O    O   ser     |
 |    R   R              II         BBB            OO             |
  ________________________________________________________________
                                                 2000-2006 MSL

                          WELCOME !!

     ***********************************
     ** Program Licensed exclusively to:
     **     READER
     ***********************************
   version 30-06-06
   full version

 Name of the input file?
test.inp
 ifile=test.inp
 Name of the output file?
   (Beware it will overwrite this file!)
test.out
 READING INPUT FILE test.inp                ...
    1) reading surfaces...
    2) reading cells...
  ---------------------------- number of cells: 3
  ---  highest number of walls in a cell: 7
  --------------------------- number of bodies: 9
 .................
 ...reading tally
 3         300      750       10
```

```
Nmax,tmax,tpmax 300   750.   10.
reading geometry...
...storing surfaces (bodies)...
    ...storing cells (regions)...
 INPUT FILE HAS BEEN READ SUCCESSFULLY
________________________________________________________

| SOURCE CUSTOMIZATION:                                 |
| - You can edit the file [sources]/customsource.f     |
|    and then recompile with [tools]/make.sh            |
| - Additionally you can use the data file init.dat     |
|   by uncommenting "read..." in customsource.f         |
| - And you can restrict generation to a cell...        |
|       celln < 0 ==> just generate a geometry plot     |
|       celln = 0 ==> do not constrain to a cell        |
|       celln > 0 ==> generation restricted to cells    |
|       * INTEG   ==> generation limited to volume      |
|             defined by celln e.g. 5 ==> generation    |
|             will take place only within cell # 5      |
|       * INTEG.1 ==> generation limited to volume      |
|             defined by as many cells as integer       |
|              part, e.g. 12.1 ==> twelve delimiting    |
|              cells (numbers will be asked later)      |
________________________________________________________

1
________________________________________________________

|  SPECIAL EVENTS, TERMINATION                          |
|  Please choose among these options:                   |
|   1: Crossing of end surface (1st card in "Tally")|
|      No ionizations in the system.                    |
|   2: Atoms can be ionized in a PLASMA ion source      |
|       Histories (of atoms and ions) end when          |
|       they cross the end_surface detector             |
|   3: Atoms can be ionized in a SURFACE ioniser        |
|       Histories (of atoms and ions) end when          |
|       they cross the end_surface detector             |
|   4: Atoms can be absorbed in the walls. Trajec-      |
|       tories end at absorption or when crossing       |
|       the end surface                                 |
|  OR SEVERAL combined effects:                         |
 |   23: Like options (1), 2 and 3                     |
 |   24: Like options (1), 2 and 4                     |
 |   34: Like options (1), 3 and 4                     |
 | 234: Like options (1), 2, 3 and 4                   |
 |    Please make your choice now                      |
 '_____________________________________________________|
3
 how many ionising cells? max is 3
1
 cell number of ion cell number 1
3
 how many ionising surfaces in cell 3
1
 Ionizer surface number 1 in ion cell 1
9
```

After giving the name of the input and output file, we asked to restrict the source to cell number 1 (the ellipsoid) and activated simulations with a surface ioniser. The ionising surface is the cylinder 9, belonging to the cell 3, the extraction tube

```
 .------------------------------------------------
 |                                                |
 |   SSSS  U   U  RRR    FFFF  II   OOOO   N   N  |
 |  S      U   U  R  R   F     II  OO  OO  NN  N  |
 |   SSS   U   U  RRRP   FFF   II  O    O  N N N  |
 |      S  UU UU  R R    F     II  OO  OO  N  NN  |
 |  SSSS    UUU   R  R   F     II   OOOO   N   N  |
 |------------------------------------------------|
 |                                                |
 | This program computes the probability of sur-  |
 | face ionization after each single atom-surface |
 | collision. Theory summarized in KOE2000 p.223> |
 | is used. Parameters are the ionization work    |
 | function and ionic statistical weights, Wi,g0, |
 | g+,g- for an atom Z. They are stored in the    |
 | outer database sion.dat. The substrate work-   |
 | function is stored in workf.dat.               |
 |                                                    |
 |    written by Mario Santana Leitner. CERN 2003    |
 |---------------------------------------------------|
 Nmax1, Nmax2= 102 27
 atom:
  element (Z)? (0 if you want to define parameters)
3
 substrate:
  element (Z)? (0 if you want to define parameters)
74
  0:element;1:Boride;2:Carbide;3:Oxide;4:CeCompound
0
 gplus,gzero,gminus,Wf,Wi,Ae   1.   2.   1.   4.54   5.39   0.62
 T?[K]
2000
 positive surface ionization
 alphaS=   0.00360563289
 negative surface ionization
 alphaS=   6.61641972E-11
 betaS=   0.003592679
 ----------- ELECTROMAGNETIC ION TRANSPORT----------

  You are dealing with ions, which "see" the EM-
    fields, external or internal (plasma fields,...)
  IF you DO NOT know these fields, but you have a
    rough idea about the extraction efficiency of the
    ions from the source, you can give this number
    as well as the estimated extraction time [ms]
     e.g:  0.3  1E-3  would mean that 30 % of the
    initially ionised atoms, make it to the outlet
     as ions. The rest recombine. The process takes
     about 1 microsecond in all.
  IF you know these fields, you can edit explicitly
    transport the ions, by editing the functions:
    readEfield.f, Bn.f functions, emittance.f
   AND answering -1 0 now.
  ..............................................
 Ion extract. efficiency [0-1], extract. time [ms]?
0.2 1E-3
```

SURFION starts and we type the atomic number of the effusing atoms and of the ioniser substrate. We select the temperature of the surface and its composition (pure chemical element), and SURFION determines that the most likely event is positive surface ionisation and prints out the corresponding individual probabilities. Then, the module for the IONIC TRANSPORT asks whether we want an explicit EM transport (then we would need to customize the routines readEfield.f and Bn.f...) or rather we will estimate the extraction with an average extracting efficiency and an associated extracted time. We opt for the second and introduce the two values.

```
 SELECT MODE:
   1: Diffusion.
   2: Effusion.
   3: Diffusion+Effusion.
 recommended 2
   4: Conductance calculator (Clausing Coefficient).
   5: Diffusion3D. -- ALPHA VERSION !!
   6: Heat transfer (cond.+rad.). -- ALPHA VERSION !!
2
 ____________________________________________________
 |  CHOOSE THE OUTPUT MODE: (standard is 3)       |
 |     1: Only average figures                      |
 |     3: Print all relevant events (standard)      |
 |     4: Like 3 + individual desorption times      |
 |     5: Effusion time AND velocity direction      |
 |     6: Particle tracking options (x,cell,surf.)  |
 |     7: Only events in the POWDER/FIBER           |
 |    C: Use [sources]/userPRINT.f routine          |
 ____________________________________________________
3

 ____________________________________________________
 | ...........  COLLISION MODEL I  .............. |
 | What model for the treatment of the collisions? |
 |    S: Specular(E<<)                              |
|   B: B=Knudsen−Lambert (recommended cosine law) |
|   D: Debye, semi−classic (under development)   |
|   C: Custom                                    |
| .............................................. |
|   BACK: Go back to previous menu               |
__________________________________________________

|  For option "C", Custom, modify the subroutine  |
| [sources]/customcollision.f at your convenience |
|  and recompile using [tools]/make.sh            |
__________________________________________________

B

__________________________________________________

| ...........   COLLISION MODEL II   ............ |
| Use average energy or sample from coll. law    |
|   Y: Use average energy (recommended)          |
|   N: Sample from collision law (slower)        |
| .............................................. |
|   BACK: Go back to previous menu               |
__________________________________________________

Y
__________________________________________________

| ........... COLLISION MODEL III   ............ |
|  Sticking time[s]?                             |
|  > 0 ==> every collision delays exactly ts [s]  |
|  = 0 (recommended). The output file includes a  |
|     post−analysis with several hypothetic ts    |
|     Use 0 for noble gases                      |
|  < 0 ==> sample from law P(t)=exp(−t/ts)/ts     |
|     It slows down calculations. Only necessary  |
|     if the number of collisions is low         |
|................................................|
|  For ts=ts(X,surface), see examples 4, 5 in the |
|    user routine customcollision.f              |
__________________________________________________

0
...Reading the "source" settings...
```

We then select to run in mode 2 (standard option), to have the standard individual output 3, and choose the normal collisions (cosine law, thermalization without sampling and no initial sticking time).

```
...Reading the "source" settings...
  -----------------------------------------------
 |                                               |
 |          M   M  EEEEE   SSSS  H   H           |
 |          MM MM  E      S      H   H           |
 |          M M M  EEEE    SSS   HHHHH           |
 |          M   M  E          S  H   H           |
 |          M   M  EEEEE  SSSS   H   H           |
 |-----------------------------------------------|
  -- STARTING MODULE FOR e/diFFUSION IN POWDER --
 How many cells contain powder? e.g. 2
1
 what is the cell number of the powder cell #  1
1
 v=  949.3955
 mean free path in powder/fiber[um]?
  e.g. UC powder 15, ZrO2 fiber 250
15
 sphere probe radius[um](step path)? e.g. 800
  recommended: 6 x mean free path
90
 sampling a limiting residence time in powder...
 DONE, tmax_sphere_of_powder[ms]=  0.0110181198
 Characterization of macrocollisions in powder:
  Generating time and angle probability functions
  ... this may take some minutes ...
 ---------------Most likely macro step---------------
  pmax=  7427. (  0.7427 %)
  bin: 1 6 12 6 tm[s],thitax,alphav,thitav[deg]
  6.05996603E-07  123.75  345.  123.75
 ----------------------------------------------------
 DONE
```

Next, we specify that there is only one region containing powder, cell number 1. We give the mean free path in the powder and the size of the macro steps. MESH samples 100000 macrosteps to fill a 4D-grid that will serve to sample paths within the powder.

```
 ________________________________________________________
 | ....... COLLISION WITH RESIDUAL NUCLEI ........ |
 |  Residual pressure [torr]? (0.75 torr = 100 Pa) |
 | P <= 0 ==>  molecular flow (ideal vacuum)        |
 | P >  0 ==>  collisions with residual gas         |
 |  (if you do not know it but you know the mean    |
 |  free path type anything > 0 now)                |
 ________________________________________________________
1E-4
  0.0001
  -------------------------------------------------
 |                                                 |
 |     RRRR   EEEEE   SSSS   GGGG   AAA    SSSS    |
 |     R   R  E       S      G      A   A  S       |
 |     RRRR   EEEE    SSS    G GG   AAAAA   SSS    |
 |     R  R   E          S   G   G  A   A      S   |
 |     R   R  EEEEE  SSSS    GGG    A   A  SSSS    |
 |-------------------------------------------------|
 - STARTING MODULE FOR INTERACTIONS BETWEEN ATOMS -

 ________________________________________________________
 | .......COLLISION WITH RESIDUAL NUCLEI II ....... |
 |  INTRODUCE A NUMBER n, IF ...                     |
 | n > 0 ==>  n = ATOM DIAMETER [pm]                 |
 |  - Some indicative values [pm] are:               |
 |  He:62;Ne:76;Ar:142;Kr:176;Xe:216;Rn:240;N2:374 |
 |  - Consider also diameter ~= 2 x 1.4 x A^{1/3}  |
 | n < 0 ==> |n| = -MEAN_FREE_PATH [cm] in "vacuum"|
 | n = 0 ==> RIBO will estimate the MEAN_FREE_PATH |
 ________________________________________________________
0
 Free mean path between collisions with gas[cm],l,T,d,P:
  3587.8078  298.  44.  0.0001
 DONE.
 DONE
 READING data/valves.dat file for moving walls
  no valves active in the system
 Post-processing geometry...
  DONE
 END OF INITIALIZATION. SIMULATION STARTS!!
 RUNNING...
 N, Nion, Nabs,<dist>[m]   50. 8 0   1.15077824
 N, Nion, Nabs,<dist>[m]   100. 16 0   1.30160217
 N, Nion, Nabs,<dist>[m]   150. 22 0   1.42556459
```

```
N, Nion , Nabs,< dist >[m]   200. 32 0   1.37736645
N, Nion , Nabs,< dist >[m]   250. 36 0   1.34756701
N, Nion , Nabs,< dist >[m]   300. 41 0   1.37057745
closing ...
...fitting release function to statistical momenta
DONE. Results are stored in: test.out
```

Finally, RESGAS asks us for the residual pressure. Normally we would say 0. Here, however, we say it is 1E-4 torr. We ask the code to compute the free mean path from the pressure. Then `RIBO` *endsup the preparatory phase and starts the simulation. At the completion of a bunch of 50 particles it prints to screen the number of simulated particles, the number of extracted ions, the number of surface absorptions (here zero) and the mean effusion flight path.*

Output file interpretation

The resulting output file displays the following information (comments are interpolated).

```
results after processing input file:test.inp
______________________________________________________

preprocessing cpu time[s]=  327.
|-------------------------------------------------------|
|      event = 0 neutral particle                       |
|            = 1 ionised particle                       |
|            = 2 neutral particle absorbed              |
|            = 3 ionised particle absorbed              |
| x0, y0, z0 = birth coordinates                        |
|      ocell = starting cell (region)                   |
|         td = diffusion time in bulk [s]               |
|        tPo = effusion time in powder/felt [s]         |
|       COLP = number of collisions in powder/felt      |
|        COL = number of collisions elsewhere           |
|       teff = Flight time outside the powder [s]       |
|        tde = Total desorption time in vacuum [s]      |
|       tdep = Total desorption time in powder [s]      |
|         tp = Total effusion time [s]                  |
|                tp = teff + tPo + tde + tdep           |
|         tT = Total release time per particle [s]      |
|                tT = tp + td                           |
|       tdep = desorption time in the powder [s]        |
|-------------------------------------------------------|
event   x0      y0      z0      td       tP0       COLP       COL    teff      tT
  0   4.579   1.000  -0.009  0.00000  0.00228  144017.6     56.0  -0.00142  0.00086
  0   4.284   0.399   1.000  0.00000  0.00006    3644.3    314.0   0.00540  0.00546
  0   4.760   1.000   0.484  0.00000  0.00114   72076.3     76.0   0.00020  0.00133
 ***
  0   4.946  -0.440   1.000  0.00000  0.00872  551768.6    142.0  -0.00623  0.00249
  1   4.388  -0.472  -1.000  0.00000  0.00001     803.0    117.0   0.00211  0.00213
  0   4.193   1.000  -0.402  0.00000  0.00357  225838.4     36.0  -0.00290  0.00067
  0   3.952  -1.000  -0.951  0.00000  0.00008    4792.8    118.0   0.00198  0.00206
  1   3.891  -0.548  -1.000  0.00000  0.00043   27154.5    132.0   0.00191  0.00234
  1   4.316   0.185   1.000  0.00000  0.00420  265829.4    124.0  -0.00222  0.00198
 ***
 ***
```

The first part contains the table with the individual events. Out-coming particles are labeled with 1 (ions) or 0 (neutral atoms). The caption explains the different columns. e.g. by multiplying COL and COLP with an average sticking time one can get the total desorption time.

```
 ----------GENERAL FIGURES FOR NEUTRAL ATOMS----------
Average intrinsic delay time[s]=  0.0050
Slowest particle took  0.0338[s]
 Average particle time consumption:
  0.0000[%Diffusion]  100.0000[%Effusion]
 - - - - - - - - - - - - - - - - -
AVERAGE DELAY in POWDER[s]:  0.0035
 DIFFUSION DISTRIBUTED AS:
     0.0000% grain diffusion
   100.0000% intergrain
 ----------GENERAL FIGURES FOR IONISED ATOMS----------
Average intrinsic delay time[s]=  0.0049
Slowest particle took  0.0292[s]
 Average particle time consumption:
  0.0000[%Diffusion]  100.0000[%Effusion]
 - - - - - - - - - - - - - - - - -
AVERAGE DELAY in POWDER[s]:  0.0035
 DIFFUSION DISTRIBUTED AS:
     0.0000% grain diffusion
   100.0000% intergrain
```

This part of the output gives the effusion to diffusion and vacuum to powder time share. Since effusion was not explicitly activated (mode 1 or mode 3), 100 % of the release time is due to effusion. Obviously the average intrinsic delay time is bigger than the average delay in the powder (because it includes it).

```
 ------------------------------------------------
 *********   EFFUSION OF NEUTRAL ATOMS   *********
 - - - - - - - - - - - - - - - - - - - - - - - -
 EFFUSION IN VACUUM (excluding powder/fiber):
  TOTAL:   806.
Average free path[m]=    1.4589
 Distance between collisions:
   average=    1.6666[cm]
   highest maximum=    6.8559[cm]
 Average number of collisions=  87.5384615
  100.%b1   0.%b2   0.%D   0.%S
   b1: Stuck particles. Emitted thermally
   b2: Surface stuck particles. Thermally emitted
   D: Inelastic scattering. Debye surface phonons
   S: Almost elastic scattering. Specular reflection
 - - - - - - - - - - - - - - - - - - - - - - - -
 EFFUSION IN POWDER:
Average path[m]=    3.3238
  69.496[%] of total path
 Average collisions in the powder=  221586.217
  99.961[%] of total
 Distance between collisions in powder:
  average free mean path 14.99998[um]
 - - - - - - - - - - - - - - - - - - - - - - - -
 RESIDUAL GAS:
   Mean free path[m]:    3587.808
   Average # of collisions with residual atoms:      0.04
 ------------------------------------------------
 *********   EFFUSION OF IONISED ATOMS   *********
 - - - - - - - - - - - - - - - - - - - - - - - -
 EFFUSION IN VACUUM (excluding powder/fiber):
  TOTAL:   194.
Average free path[m]=    1.3579
 Distance between collisions:
   average=    1.6671[cm]
   highest maximum=    6.7662[cm]
 Average number of collisions=  81.4536082
  100.%b1   0.%b2   0.%D   0.%S
   b1: Stuck particles. Emitted thermally
   b2: Surface stuck particles. Thermally emitted
   D: Inelastic scattering. Debye surface phonons
   S: Almost elastic scattering. Specular reflection
 - - - - - - - - - - - - - - - - - - - - - - - -
 EFFUSION IN POWDER:
Average path[m]=    3.3322
  71.047[%] of total path
 Average collisions in the powder=  222144.447
  99.963[%] of total
 Distance between collisions in powder:
  average free mean path 14.99998[um]
 - - - - - - - - - - - - - - - - - - - - - - - -
 RESIDUAL GAS:
  Mean free path[m]:   3587.808
  Average # of collisions with residual atoms:     0.06
```

These two tables tell about the effusive path of the atoms and ions (when they were still neutral) in the tubes and inside the powder. It also prints the number of collisions with residual gas at the pressure that was specified at runtime

```
 STATISTICAL DATA
-------------------------------------------------

   Moment(T,i)=(<T^i>)^{1/i} [s]

 1) T = FLIGHT_TIME_IN_VACUUM------------------------
  M1     M2     M3     M4     M5
0.0015 0.0021 0.0027 0.0033 0.0038

 Fit to T(i,t) = exp(-t/t1)/t1:
  t1=  0.00154
 error O(2)[%]: -6.48439
 error O(3)[%]:-12.50578
 Fit to T(i,t) ~ (1-exp(-t/t1))*exp(-t/t2):
  t1=  0.00026
  t2=  0.00133
 error O(3)[%]: 14.89847
 error O(4)[%]: 21.85320

 2) T = FLIGHT_TIME_IN_POWDER------------------------
  M1     M2     M3     M4     M5
0.0034 0.0058 0.0079 0.0099 0.0118

 Fit to T(i,t) = exp(-t/t1)/t1:
  t1=  0.00343
 error O(2)[%]: 29.08787
 error O(3)[%]: 50.57320
 Fit to T(i,t) ~ (1-exp(-t/t1))*exp(-t/t2):
  t1= -0.00136
  t2=  0.00527
 error O(3)[%]:-30.52552
 error O(4)[%]:-44.10240

 3) T = TOTAL_EFFUSION_TIME (FLIGHT+STICKING)---
  M1     M2     M3     M4     M5
0.0050 0.0069 0.0089 0.0108 0.0126

 Fit to T(i,t) = exp(-t/t1)/t1:
  t1=  0.00498
 error O(2)[%]: -2.79223
 error O(3)[%]: -4.74298
 Fit to T(i,t) ~ (1-exp(-t/t1))*exp(-t/t2):
  t1 =   0.00031
  t2 =   0.00469
 error  O(3)[%]:   6.63791
 error  O(4)[%]:   8.99565
```

These are the momenta up to order 5 of the flight time in vacuum, in powder and the number of collision. With this information you can in principle build up many fitting functions. The code uses them to make fits based in exponential functions

```
 RELEASE  FRACTION  COMPUTATIONS
------------------------------------------------

 GIVEN  CONDITIONS:
==================

    T_1/2      ERF[%]
  ____________________

   0.1E-2        9.10
   0.3E-2       26.98
   0.6E-2       43.95
   0.1E-1       57.26
   0.3E-1       80.48
   0.6E-1       89.25
   0.1E+0       93.27
   0.3E+0       97.66
   0.6E+0       98.82
   0.1E+1       99.29
   0.3E+1       99.76
   0.6E+1       99.88
   0.1E+2       99.93
   0.3E+2       99.98
   0.6E+2       99.99
   0.1E+3       99.99
______________________________________________________________________________

 OTHER  CONDITIONS:
==================


                       |------------------------ts(s)------------------------|
  tao_d[s]    0.10E+0   0.0E+0   0.1E-8   0.1E-7   0.1E-6   0.1E-5   0.1E-4
  __________________________________________________________________________

   T_1/2[s]    DRF[%]   RF(ts1)  RF(ts2)  RF(ts3)  RF(ts4)  RF(ts5)  RF(ts6)
   0.1E-2      7.727     0.703    0.766    0.000    0.000    0.000    0.000
   0.3E-2     13.126     3.542    3.571    5.056    0.000    0.000    0.000
   0.6E-2     18.198     7.999    7.934    8.056    0.000    0.000    0.000
   0.1E-1     23.022    13.183   13.039   12.337    0.000    0.000    0.000
   0.3E-1     37.213    29.948   29.730   28.073   29.377    0.000    0.000
   0.6E-1     48.936    43.674   43.484   41.919   35.257    0.000    0.000
   0.1E+0     58.506    54.570  54.417  53.112  45.217   0.000   0.000
   0.3E+0     78.059    76.231  76.154  75.476  69.799  67.202   0.000
   0.6E+0     87.058    86.027  85.983  85.590  81.998  66.568   0.000
   0.1E+1     91.622    90.969  90.940  90.688  88.299  73.938   0.000
   0.3E+1     96.960    96.729  96.718  96.628  95.740  88.315  84.216
   0.6E+1     98.441    98.323  98.318  98.272  97.815  93.645  75.731
   0.1E+2     99.051    98.980  98.977  98.949  98.672  96.048  80.286
   0.3E+2     99.673    99.649  99.648  99.639  99.545  98.627  90.955
   0.6E+2     99.830    99.818  99.818  99.813  99.766  99.301  95.061
   0.1E+3     99.893    99.886  99.886  99.883  99.855  99.574  96.924

                      |-------------------- ts(s) --------------------|
  tao_d[s]    0.10E+1   0.0E+0  0.1E-8  0.1E-7  0.1E-6  0.1E-5  0.1E-4
 ----------------------------------------------------------------------
   T_1/2[s]   DRF[%]   RF(ts1) RF(ts2) RF(ts3) RF(ts4) RF(ts5) RF(ts6)
   0.1E-2      2.481     0.226   0.246   0.000   0.000   0.000   0.000
   0.3E-2      4.279     1.155   1.164   1.648   0.000   0.000   0.000
   0.6E-2      6.020     2.646   2.624   2.665   0.000   0.000   0.000
   0.1E-1      7.727     4.425   4.377   4.141   0.000   0.000   0.000
   0.3E-1     13.126    10.564  10.487   9.902  10.362   0.000   0.000
   0.6E-1     18.198    16.241  16.170  15.588  13.111   0.000   0.000
   0.1E+0     23.022    21.473  21.413  20.900  17.793   0.000   0.000
   0.3E+0     37.213    36.342  36.305  35.982  33.275  32.037   0.000
   0.6E+0     48.936    48.357  48.332  48.111  46.092  37.418   0.000
   0.1E+1     58.506    58.088  58.070  57.909  56.384  47.213   0.000
   0.3E+1     78.059    77.872  77.864  77.791  77.076  71.099  67.799
   0.6E+1     87.058    86.954  86.949  86.909  86.504  82.817  66.975
   0.1E+2     91.622    91.557  91.554  91.528  91.271  88.844  74.264
   0.3E+2     96.960    96.937  96.936  96.927  96.836  95.943  88.480
   0.6E+2     98.441    98.429  98.428  98.424  98.377  97.919  93.738
   0.1E+3     99.051    99.044  99.044  99.041  99.013  98.735  96.107
   ***
   ***
```

The exponential fitting functions are Laplace-Transformed and folded with the diffusion release efficiency for several diffusion parameters. The global release efficiency factor, as a function of the half-life and sticking coefficient [s] are printed in tables. Every table corresponds to a different diffusion time constant.

```
  ----------------------------------------------
|      average  effusion  time  in  each  cell [%]      |
|          cell                 <time  share>           |
              1                     10.344
              2                     88.634
              3                      1.022
|----------------------------------------------|
  ----------------------------------------------
| average   number   of   events   in   each  surface   |
| surface  <collisions> <absorptions> <eff[%]> |
     1         6.948         0.000         0.000
     2         4.101         0.000         0.000
     3         0.000         0.000         0.000
     4        19.103         0.000         0.000
     5        19.083         0.000         0.000
     6        19.267         0.000         0.000
     7        19.514         0.000         0.000
     8         0.000         0.000         0.000
     9         0.000         0.000         0.000
|----------------------------------------------|
 ----------------------------------------------
|                   CONNECTIVITY                |
|       ocell  ---> ecell         share         |
|           1            3        1.0010        |
|----------------------------------------------|
```

These 3 tables tell about the effusion time share in the different regions (1), the number of collisions and absorptions in each surface (2) (no particle collides *with last surface because they are forced to* cross *it) and the connectivity between the starting regions and the end region (3) (In this case they are all born in cell 1 because we forced that, and they all die when crossing surface 9, which belongs to cell 3.*

```
 --------------------------------------------------
SURFACE IONIZATION
surface collision ionization probability:   0.003592
 ionization efficiency= 19.40000[%]
 relative error=  6.44565[%]
 "IMPLICIT" ION TRANSPORT
 Ion extraction efficiency:  0.2
 (this factor is included in ionization eff)
 Ion extraction time[s]:  0.001
 (this factor is included in teff)
____________________________________________________
```

In presence of ion sources, `RIBO` *prints the ionization efficiency and the parameters linked to the transport of the ions.*

```
____________________________________________________

Number of histories[N]=  1000.  CPU time[s]=  130.
CPU_time/history=  0.13[s/history]
CPU_time/collision=  0.00184250808[s/collision]
===================================================
```

Duration of the simulation.

Connectivity matrix.

In this case the matrix of candidate links between cells is very simple:

```
1
2

2
1
3

3
2
```

This means that the first cell is only connected to the second (it is indeed so because it is embedded in the latter one), that the second source is connected not only to the first but also to the third one and that the third cell is only linked to the cell number two.

Data analysis.

The results stored in the output file can be analyzed in various manners depending on the specific needs of the problem. Usually the individual parts are imported into a worksheet in order to plot histograms with the possibility to observe the influence of several parameters on the delay time. Whence, a first column of results may contain the diffusion time, and this may be modified proportionally as a function of η. In the same way, the effusion time vector may be adjusted to a particular speed of atoms (proportional to $T^{0.5} \cdot M^{-0.5}$) and the sticking time vector will be obtained by multiplying the array that stores the number of collisions by the individual sticking times.

The array of results shall be divided in equally sized groups in order to compute separate calculations, merge them and compare them. This procedure provides information about the variance of the results.

3.1.4 Example of use of the 3D-Diffusion, 3D GRID: heat3D.t.

The `RIBO` distribution includes an example of the use of the 3-D diffusion package. The input file $[targets]/heat3D.t$ describes a simple case where a spherical target of W with a diameter of 3 cm is irradiated with a beam that deposits 10 $\frac{kW}{cm^3}$ uniformly over the sphere. The sphere is under vacuum and exchanges heat with a spheric heat screen that encloses the W target. The screen is made of Ta, it has an inner diameter of 4 cm and an outer diameter of 4.5 cm. The starting temperature of the W target is 500 K, while the shield is at room temperature. The example shows how to compute the evolution of the temperature of target and shield. Figure 3.4 describes the main parameters linked with this example:

Input file

The input file for this example is very simple. There are 3 quadrics (the three spheres that describe the radius of the target and the inner and outer radius of the shield) and 2 cells, one for the target and one for the shield.

The details of the problem are found in the $[targets]/heat3D.t$

```
Surfaces
#   RC    T     X2   Y2   Z2   XY   XZ   YZ   X    Y    Z     C
1   0.5   298   1    1    1    0    0    0    0    0    0     9.00
2   0.5   298   1    1    1    0    0    0    0    0    0    16.00
3   0.5   298   1    1    1    0    0    0    0    0    0    20.25
Cells
#   S1    S2    ..
1   −1    0
```

```
2     2       −3
Source
Type  M       T       Alfa  nx   ny   nz   x    y    z    R
S     90      298     180   −1   0    0    0    0    0    3
Tally
S     max     Tmax    Tpmax
3     50000   750     10
```

In the present version, the values of the Source card have no effect in the results for 3D-diffusion, but still, **it is compulsory to fill in all fields**. As for the Tally cards, for the moment only the third one (Tmax) is used in 3D-diffusion, having essentially the same meaning as for effusion simulations.

As for the data files, the simulation reads the specific capacity, conductivity and emissivity from $[data]/Cond.dat$. The example printed in 2.2.1 and included in the RIBO distribution already contains the values for W (cell 1) and Ta (cell 2). Note that this table can be refined by filling in the fields that show a dependence of first and second order with respect to the temperature (or concentration). Moreover, if the temperature of the system varies a lot, you may also want to introduce the variation of the emissivity with the temperature. You can easily do that by editing the function *radia* in the $[sources]/custom3D.f$ file.

Custom routines

The specific options (10 $\frac{kW}{cm^3}$, radiation function, starting temperatures...) are already implemented in the open source functions and subroutines in $[sources]/custom3D.f$. You are invited to look through them and identify the different choices.

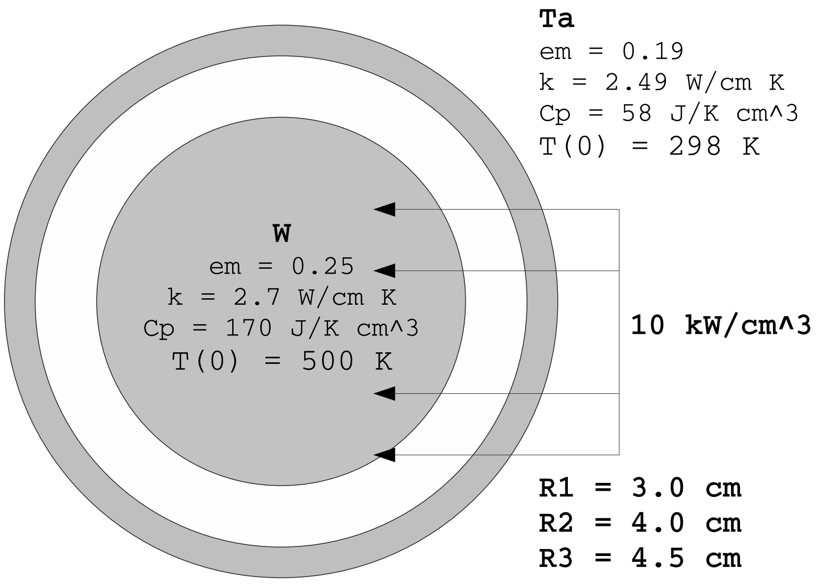

Figure 3.5: The spherical W target and the Ta screen.

Runtime options

† *NOTE*: The input values are stored in the batch file $[batchinputs]/heat3D.batch$.

```
 ____________________________________________________________
|    RRR               II        BBB          OO             |
|    R  R              II        B  B       O    O           |
|    RRR    adio-      II   on   BBB   eam  O    O  ptimi-   |
|    R  R   active     II        B  B       O    O  ser      |
|    R  R              II        BBB          OO             |
 ____________________________________________________________
                                            2000-2006 MSL


                          WELCOME !!

   ************************************
   ** Program Licensed exclusively to:
   **   READER
   ************************************
 version 30-06-06
```

```
  full version


 Name of the input file?
heat3D.t
 ifile=heat3D.t
 Name of the output file?
  (Beware it will overwrite this file!)
heat3D.out
 READING INPUT FILE heat3D.t              ...
   1) reading surfaces...
   2) reading cells...
 ------------------------ number of cells: 2
 --- highest number of walls in a cell: 2
 ----------------------- number of bodies: 3
 .................
 ...reading tally
 Nmax,tmax,tpmax 50000  750.  10.
 reading geometry...
 ...storing surfaces (bodies)...
     ...storing cells (regions)...
  INPUT FILE HAS BEEN READ SUCCESSFULLY
 ___________________________________________________________
 | SOURCE CUSTOMIZATION:                                   |
 | - You can edit the file [sources]/customsource.f        |
 |     and then recompile with [tools]/make.sh             |
 | - Additionally you can use the data file init.dat       |
 |   by uncommenting "read..." in customsource.f           |
 | - And you can restrict generation to a cell...          |
 |   ...source limited to a cell? give cell number.        |
 |       celln > 0 ==> generation limited to volume        |
 |         defined by celln                                |
 |       celln = 0 ==> do not constrain to a cell          |
 |       celln < 0 ==> just generate a geometry plot       |
 ___________________________________________________________
1
```

This part is standard. As for any simulation, the code asks for the input file name and the output file name. Then, as usual, it gives the chance to restrict the initial *distribution of particles (*CSTART.f, *2.3.1) to one of the cells defined in the input file.*

```
 _______________________________________________________
 |  SPECIAL EVENTS, TERMINATION                         |
 |  Please choose among these options:                  |
 |   1: Crossing of end surface (1st card in "Tally")|
 |      No ionizations in the system.                   |
 |   2: Atoms can be ionized in a PLASMA ion source     |
 |      Histories (of atoms and ions) end when          |
 |      they cross the end_surface detector             |
 |   3: Atoms can be ionized in a SURFACE ioniser       |
 |      Histories (of atoms and ions) end when          |
 |      they cross the end_surface detector             |
 |   4: Atoms can be absorbed in the walls. Trajec-     |
 |      tories end at absorption or when crossing       |
 |      the end surface                                 |
 |  OR SEVERAL combined effects:                        |
 |  23: Like options (1), 2 and 3                       |
 |  24: Like options (1), 2 and 4                       |
 |  34: Like options (1), 3 and 4                       |
 | 234: Like options (1), 2, 3 and 4                    |
 |   Please make your choice now                        |
 '______________________________________________________'
1
 SELECT MODE:
   1: Diffusion.
   2: Effusion.
   3: Diffusion+Effusion.
 recommended 2
   4: Conductance calculator (Clausing Coefficient).
   5: Diffusion3D. -- ALPHA VERSION !!
   6: Heat transfer (cond.+rad.). -- ALPHA VERSION !!
6
 ____________________________________________________
 |  CHOOSE THE OUTPUT MODE: (standard is 3)        |
 |     8: Only average figures                       |
 |     9: Print full matrix evolution (SPACE!!)      |
 |    C: Use the custom routine YYY                  |
 ____________________________________________________
8
```

The first of the questions has no impact in our future decisions. We answer 1. The next question is crucial. We choose 6, because we are dealing with a heat transfer problem. This triggers a preselected number of output formats, 8 (standard), 9 (full) and C, custom (please consult section 2.3.5)

```
  -----------------------------------------------
 |                                               |
 |    3333  DDDD      GGGG  RRRR   II  DDDD      |
 |        3 D   D    G      R   R  II  D   D     |
 |     333  D   D    G GGG  RRRR   II  D   D     |
 |        3 D   D    G   G  R  R   II  D   D     |
 |    3333  DDDD      GGGG  R   R  II  DDDD      |
 |-----------------------------------------------|
 | DEFINING 3D WINDOW FOR THE CALCULATIONS       |
 | 1) starting vertex xmin,ymin,zmin[cm]?        |
 |     e.g: -10 -10 -5                           |
-4.5 -4.5 -4.5
 | 2) what are the full widths x,y,z [cm]?       |
 |     e.g:  10  10  5                           |
 |-----------------------------------------------|
9.0 9.0 9.0
 | 3) number of divisions in x,y,z? e.g: 10 10 20 |
 |-----------------------------------------------|
180 180 180
```

The module 3D takes over. The user must define the 3D window where heat transfer will act. Vacuum will replenish the remaining space. The first data input are the coordinates of the lower corner Xmin, Ymin, Zmin. The 3D box will be defined by writing the 3 amplitudes deltaX, deltaY, deltaZ. Finally, the space will be evenly discretized in parallelepipeds when the number of divisions in each dimension is *given. Here we are in a symmetrical case so the number of division in each dimension is the same.*

† *WARNING*: The maximum dimension of the matrix is 300 300 300 !!

```
   INITIALISING GRID... PLEASE WAIT
 _____________________________________________

   Number of voxels outside vacuum 1814368.
   Maximum value at t = 0      500.000
   Minimum value at t = 0        0.000
   Average value at t = 0     398.7524
 _____________________________________________


 ________________________________________________________
  | ...............  END CONDITION  .................|
  |  What is the end condition for the 3 D problem? |
  |  (Give condition number and associated value)   |
  |   - 1  tmax[s]    e.g. 1   20                   |
  |      means "stop␣when␣elapsed␣time␣=␣20␣s"       |
  |   - 2  average/average(0)  e.g. 2   0.2         |
  |      means "stop␣when␣average␣Temperature␣␣␣␣␣␣␣␣|
␣|␣␣␣␣␣decreases␣down␣to␣0.5␣of␣the␣initial␣value" |
  |   - 3  Tmin[K]    e.g. 3   350                  |
  |      means "stop␣when␣minimum␣Temperature␣␣␣␣␣␣␣␣|
␣|␣␣␣␣␣goes␣below,␣or␣grows␣up␣to␣Tmin"            |
  |   - 4  Tmax[K]    e.g. 4   1700                 |
  |      means "stop␣when␣maximum␣Temperature␣␣␣␣␣␣␣␣|
␣|␣␣␣␣␣goes␣below,␣or␣grows␣up␣to␣Tmax"            |
  |   - 5  #_of_steps     e.g. 5   1000             |
  |      means "stop␣after␣1000␣time␣steps"          |
  |   - 6  |(dT/T)max/dt|  e.g. 6   1E-6            |
  |      means "stop␣when␣the␣maximum␣relative␣T␣␣␣␣␣|
␣|␣␣␣␣␣change␣per␣unit␣time␣goes␣below␣1E-6/s␣␣␣␣␣␣|
␣|␣␣␣␣␣(biggest␣change␣<␣1%␣in␣10000␣s)"           |
  |.................................................|
  |  NOTE:                                          |
  |   - Whatever condition, the computation will be |
  |     terminated if the computation time exceeds  |
  |     CPUmax [s] (4th entry in "Tally", input file |
________________________________________________________

 ------Read Cond.dat matrix, found matrix is:-----
  2.700    0.000    0.000    0.250 170.000    0.000    0.000
 2.490    0.000    0.000    0.190   58.000    0.000    0.000
 ________________________________________________________

  INITIALISING TIME STEPS...
  RUNNING...
    time[s]      Cmax     IM       XM          YM          ZM          Cmin    Im        Xm      ...
   0.000000    500.0000   1    -2.9750    -0.3750    -0.0750    298.0000   2    -4.4750   ...
   0.136000    508.0000   1    -2.9250    -0.3750    -0.0750    298.0000   2    -4.4750   ...
   * * *
   * * *
   1.052380    561.9047   1    -1.9250    -0.0750    -0.0250    297.4828   2    -2.5250   ...
   1.097014    564.5302   1    -1.8750    -0.0750    -0.0250    293.7514   2    -2.5250   ...
CALCULATION FINISHED!
DONE. Results are stored in: heat3D.out
```

Ribo initialises the 3D grid. It then asks for the termination condition. In this case the simulation will finish when the maximum temperature reaches 700 K, or when the computational time reaches Tmax = 750 s

Output file interpretation

The resulting output file displays the following information:

```
results after processing input file:heat3D.t
 ________________________________________________________

 preprocessing cpu time[s]=  15.
|--------------------------------------------------------|
 |        time = elapsed time [s]                         |
 |        Cmax = Maximum value (it can be multiple)       |
 |          IM = cell to which Cmax belongs               |
 | {XM,YM,ZM} = coordinates of one of the Cmax            |
 |        Cmin = Minimum value (it can be multiple)       |
 |          Im = cell to which Cmin belongs               |
 | {Xm,Ym,Zm} = coordinates of one of the Cmin            |
 |      <C(t)> = Average value of C                       |
 |  <C(t)/C0> = Relative increase or decrease <C>         |
|----------------------------------------------------------------|
   time[s]    Cmax    IM      XM    ...    Cmin     Im      Xm   ... <C(t)/C0> <C(t)>
  0.000000  500.0000  1   -2.9750 ... 298.0000  2   -4.4750 ... 1.0000    398.752
  0.136000  508.0000  1   -2.9250 ... 298.0000  2   -4.4750 ... 1.0100    402.743
  0.274078  516.1242  1   -2.2750 ... 297.9584  2   -3.0750 ... 1.0202    406.794


     *          *
     *          *

  1.046866  561.5804  1   -1.9250 ... 293.8229  2   -2.5750 ... 1.0770    429.468
  1.052380  561.9047  1   -1.9250 ... 297.4828  2   -2.5250 ... 1.0774    429.630
  1.097014  564.5302  1   -1.8750 ... 293.7514  2   -2.5250 ... 1.0807    430.940
-----------------------------------------------------------------
Number of steps= 50  CPU time[s]=  765.
CPU_time/step=    15.3[s/step]
CPU_time/sim_time=  693.922836[s_CPU/s_diffusion]
=================================================


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ISOLDE-CERN,  2001-2009
```

The output file for these type of calculations is rather simple to interpret. In output mode 8, the elapsed diffusion time is printed in the ***first column****. The highest found temperature, the cell and the coordinates of a voxel with such temperature (there may be many with the same value) are printed in* ***columns 2-6****. The same information is displayed in* ***columns 7-11*** *for the minimum value. Finally, the* ***fore-last column*** *tells about the ratio of the average Temperature at time t, and that at time 0, and the* ***leftmost column*** *shows the evolution of the average temperature with time. The file ends with some numbers related to the computational speed.*

The primary source that is used here is a sphere, the radius of which equals the maximum radius of the ellipsoid. The cell-limited option will be chosen at runtime.

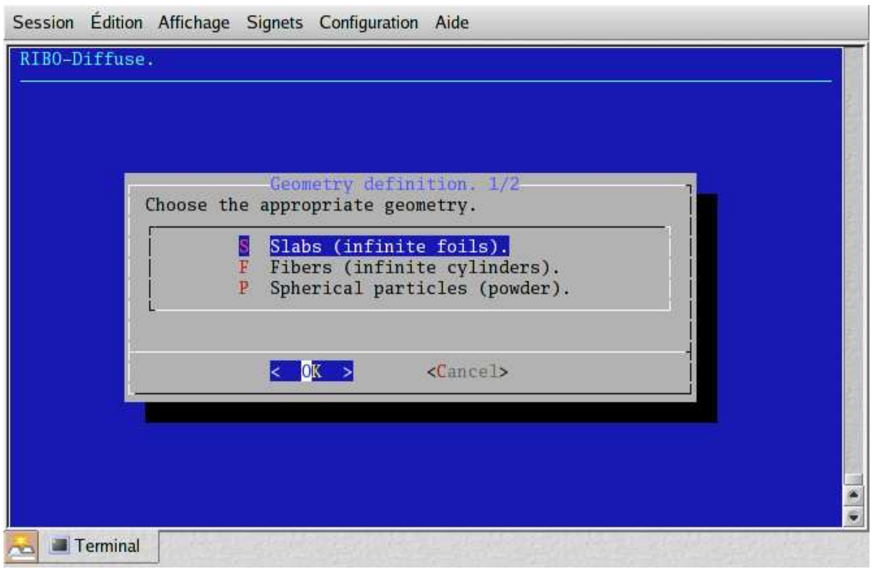
Chapter 4

RIBO-Diffuse. A diffusion toolkit.

DIFFUSE is a bash shell script that manages the core FORTRAN program DIFFUSE.F. It computes diffusion profiles analytically (through the infinite series provided by Fujioka [14] and the second law of Fick [15]) and, for one-dimensional geometries under variable and/or non-homogeneous conditions, numerically (first law of Fick). Additionally, it may compute the diffusion coefficient provided that a release fraction is known at any given time. More details can be found in [11], 2.5.1.

Running DIFFUSE is trivial because it is fully interactive. Fig.4 shows the first and second menu choices. In fig.4.1(a) options **1,3,5** permit to plot the drop of total concentration in the slab as a function of time. **5** additionally shows the space dependency (2-D graph). In any of the cases, it is necessary to install PAW [8] to have the functions plotted. Otherwise, the user can take the output data, written in the file *profile.dat* and use his favorite data analyzing program. **2** and **4** invert the diffusion function to extract the Diffusion coefficient from a fixed diffusion release situation.

Based on the chosen option, DIFFUSE poses the following questions:

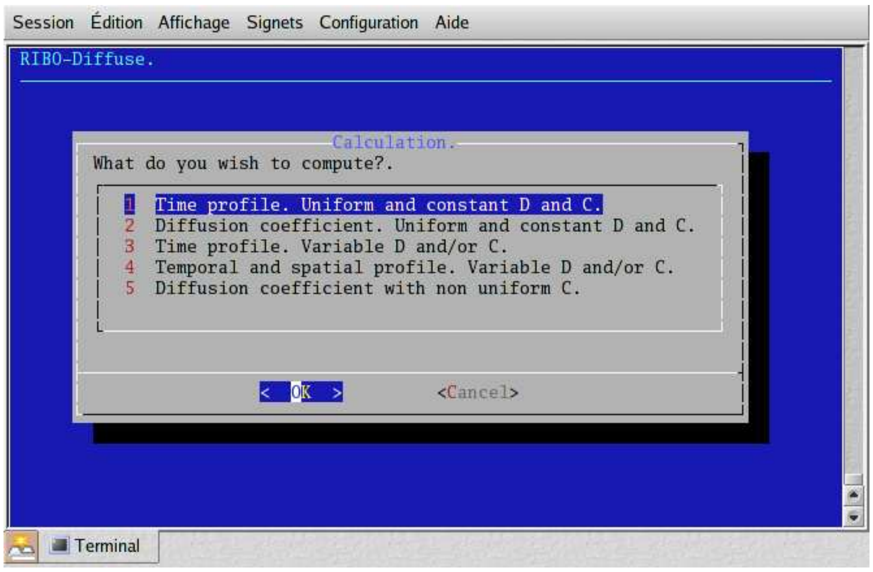


```
RIBO-Diffuse.

Geometry definition. 1/2
Choose the appropriate geometry.

        S  Slabs (infinite foils).
        F  Fibers (infinite cylinders).
        P  Spherical particles (powder).
```

(a) First choice of DIFFUSE.



```
RIBO-Diffuse.

Calculation.
What do you wish to compute?.

   1  Time profile. Uniform and constant D and C.
   2  Diffusion coefficient. Uniform and constant D and C.
   3  Time profile. Variable D and/or C.
   4  Temporal and spatial profile. Variable D and/or C.
   5  Diffusion coefficient with non uniform C.
```

(b) Options for 1-D calculations.

Figure 4.1: Screen captures of the interactive DIFFUSE program.

Insert the number of space nodes

A good compromise between precision and speed of computation would be between 10 and 1000.

Insert the diffusion coefficient [cm2/s]

The units are specified, $[\frac{cm^2}{s}]$

Fractional concentration
Insert the remaining concentration.

e.g. 0.5 would mean that 50 % has diffused out.

Insert the lapse length [s].

It refers to the final time, or the time at which the fractional concentration is measured.

Time definition.
Insert the printing time grid (number intervals).

The time steps for the diffusion calculations are adjusted internally to keep the system stable, but the time steps are often much too small to have them all printed. Thus, the user specifies what should be the time binning.

For the present status of the program, the user needs to introduce the wished time dependencies directly in the corresponding subroutines.

```
      SUBROUTINE timeN(N,i,m,t,dt,a)
        real*8 N(m,2),t,dt,tao,pulse,a,x
        integer*4 i,m
* decay law
        tao=0.097                                              1
*         tao=27.0
*         N(i,1)=N(i,1)*exp(-log(2.0)*dt/tao)
* pulsing source
        x=(a/m)*i
```

```
         pulse=0.5
         IF (mod(t,pulse).lt.1.0001*dt.and.t.gt.pulse) THEN
           N(i,1)=N(i,1)+functC(x,a)*1
         END IF
       END
```

For time dependencies, or

```
      FUNCTION functC(x,a)
        real*8 x,a
        x=a-x
        functC=1*exp(-x*10.0/a)*(1-exp(-x*1.0/a))
        x=a-x
        functC=1*sin(x*3.1415927/a)**2
        functC=1
      END
```

For space variations of the concentration or, finally:

```
       FUNCTION D(i,m,a,t,Dc)
         real*8 x,a,t,Dc,r
         integer*4 i,m
         x=da*(i-0.5)
*         D=Dc*sin(x*3.1415927/a)*exp(-t/100)
         D=Dc
*         r=0.999
*         D=((1+r)-(2*r)*(x/a))*Dc
         IF (t.le.1) THEN
*            D=7.7778*Dc
         END IF
       END
```

For space and time variations in D.

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