Body Transformations and Special Geometries

Beginners' FLUKA Course

Contents

- body transformations
- lattice
- voxels

Geometry directives

Special commands enclosing body definition:

$Start_xxx

.....

$End_xxx

where "xxx" stands for
“expansion“, "translat" or "transform"

They provide respectively a coordinate expansion/reduction, a coordinate translation or a coordinate roto-translation of the bodies embedded between the starting and the ending directive lines.

Directives in geometry: expansion/reduction

- $Start_expansion ... $End_expansion

  it provides a coordinate expansion (reduction) factor f for all bodies embedded within the directive

$Start_expansion 10.0
```
SPH Sphere 5.0 7.0 8.0 50.0
```
$End_expansion

transforms a sphere of radius 50 centered in (+5,+7,+8)
into a sphere of radius 500 centered in (+50,+70,-80)

Putting the body in its quadric form

$$A_{xx}\,x^2 + A_{yy}\,y^2 + A_{zz}\,z^2 + A_{xy}\,xy + A_{xz}\,xz + A_{yz}\,yz + A_x\,x + A_y\,y + A_z\,z + A_0 = 0$$

or
$$\begin{bmatrix} x & y & z & 1 \end{bmatrix} \begin{bmatrix} A_{xx} & A_{xy}/2 & A_{xz}/2 & A_x/2 \\ A_{xy}/2 & A_{yy} & A_{yz}/2 & A_y/2 \\ A_{xz}/2 & A_{yz}/2 & A_{zz} & A_z/2 \\ A_x/2 & A_y/2 & A_z/2 & A_0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix} = 0 \qquad \text{i.e.} \quad \mathbf{r}^T M_{QUA}\, \mathbf{r} = 0$$

the expansion/reduction matrix is $T = \begin{bmatrix} f & 0 & 0 & 0 \\ 0 & f & 0 & 0 \\ 0 & 0 & f & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

and the transformed body equation is $\mathbf{r}^T (T^{-1})^T M_{QUA}\, T^{-1}\, \mathbf{r} = 0$

Directives in geometry: translation

- $Start_translat ... $End_translat

  it provides a coordinate translation S_x,S_y,S_z for all bodies embedded within the directive

```
$Start_translat -5.0 -7.0 -8.0
SPH Sphere 5.0 7.0 8.0 50.0
$End_translat
```

transforms a sphere of radius 50 centered in (+5,+7,+8)
into a sphere of radius 50 centered in (0,0,0)

the translation matrix is $T = \begin{bmatrix} 1 & 0 & 0 & S_x \\ 0 & 1 & 0 & S_y \\ 0 & 0 & 1 & S_z \\ 0 & 0 & 0 & 1 \end{bmatrix}$

Directives in geometry: roto-translation

- $Start_transform ... $End_transform

  it applies a pre-defined (via ROT-DEFI) roto-translation to all bodies embedded within the directive

```
ROT-DEFI , 201.0, 0., +116.5650511770780, 0., 0., 0., cylrot
$Start_transform cylrot
QUA Cylinder 0.5 1.0 0.5 0.0 1.0 0.0 0.0 0.0 0.0 -4.0
$End_transform
```

transforms an infinite circular cylinder of radius 2 with axis {x=-z,y=0}
into an infinite circular cylinder of radius 2 with axis {x=z/3,y=0} (**clockwise rotation**)

the roto-translation matrix is $T = \begin{bmatrix} & & & S_x \\ & R & & S_y \\ & & & S_z \\ 0 & 0 & 0 & 1 \end{bmatrix}$

- it allows to rotate a RPP avoiding the use of the deprecated BOX !

- note that also the **inverse** transformation can be used T^{-1}

$Start_transform -cylrot

Directives in geometry: warnings

- $Start_expansion and $Start_translat are applied when reading the geometry → no CPU penalty (the concerned bodies are transformed once for ever at inizialization)

  $Start_transform is applied runtime → some CPU penalty

- One can **nest** the different directives *(at most one per type!)* but, no matter the input order, the adopted sequence is always the following:

  $Start_transform StupiRot

  $Start_translat -5.0 -7.0 -8.0

  $Start_expansion 10.0

  ```
  QUA WhatIsIt +1.0 +1.0 +1.0 0.0 0.0 0.0 -10.0 -14.0 -16.0 -2362.0
  ```

  $End_expansion

  $End_translat

  $End_transform

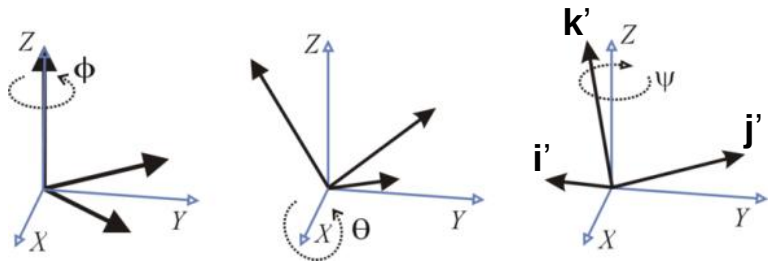
- Directives are not case sensitive (whereas roto-translation names are)

Identifying rotation angles

Let's define the orientation of a body in the space
by a system of 3 orthogonal versors **i'**, **j'**, **k'** , whose coordinates
are expressed with respect to the fixed reference frame X,Y,Z

Then **[i' j' k']** = $\begin{bmatrix} c_1c_3 - c_2s_1s_3 & -c_1s_3 - c_3c_2s_1 & s_2s_1 \\ c_2c_1s_3 + c_3s_1 & c_1c_2c_3 - s_1s_3 & -c_1s_2 \\ s_3s_2 & c_3s_2 & c_2 \end{bmatrix}$ (in the ZXZ convention)

where $c_1=\cos(\psi)$ $c_2=\cos(\theta)$ $c_3=\cos(\Phi)$ $s_1=\sin(\psi)$ $s_2=\sin(\theta)$ $s_3=\sin(\Phi)$



here $\Phi = 45^o$ $\theta = 30^o$ $\psi = -60^o$

The obtained Euler angles can be input as azimuthal angle of
three consecutive rotations (ROT-DEFI)

Lattice

FLUKA geometry has *replication* (lattice) capabilities

Only one *level is implemented* (no nested lattices are allowed)

- The user defines lattice positions in the geometry and provides transformation rules from the lattice to the prototype region:
  1. in the input with the ROT-DEFI card
  2. in a subroutine (lattic.f)

The lattice identification is available for scoring

Transformations include:

Translation, Rotation and Mirroring (the last only through routine).

WARNING:

Do not use scaling or any deformation of the coordinate system

Lattice

- The regions which constitute the elementary cell *(prototype)* to be replicated, have to be defined in detail
- The Lattices *(replicas/containers)* have to be defined as "empty" regions in their correct location.
  WARNING: The lattice region should map exactly the outer surface definition of the elementary cell.
- The lattice regions are declared as such with a LATTICE card at the end of the geometry input
- In the LATTICE card, the user also assigns lattice names/numbers to the lattices. These names/numbers will identify the replicas in all FLUKA routines and scoring
- Several basic cells and associated lattices can be defined within the same geometry, one LATTICE card will be needed for each set
- Non-replicas carry the lattice number **0**
- Lattices and plain regions can coexist in the same problem

LATTICE card

After the Regions definition and before the GEOEND card the user can insert the LATTICE cards

- WHAT(1), WHAT(2), WHAT(3)
  Container region range (from, to, step)
- WHAT(4), WHAT(5), WHAT(6)
  Name/number(s) of the lattice(s)
- SDUM

blank	to use the transformation from the lattic routine
ROT#nn	to use a ROT-DEFI rotation/translation from input
name	the same as above but identifying the roto-translation by the name assigned in the ROT-DEFI SDUM (any alphanumeric string you like)

Example

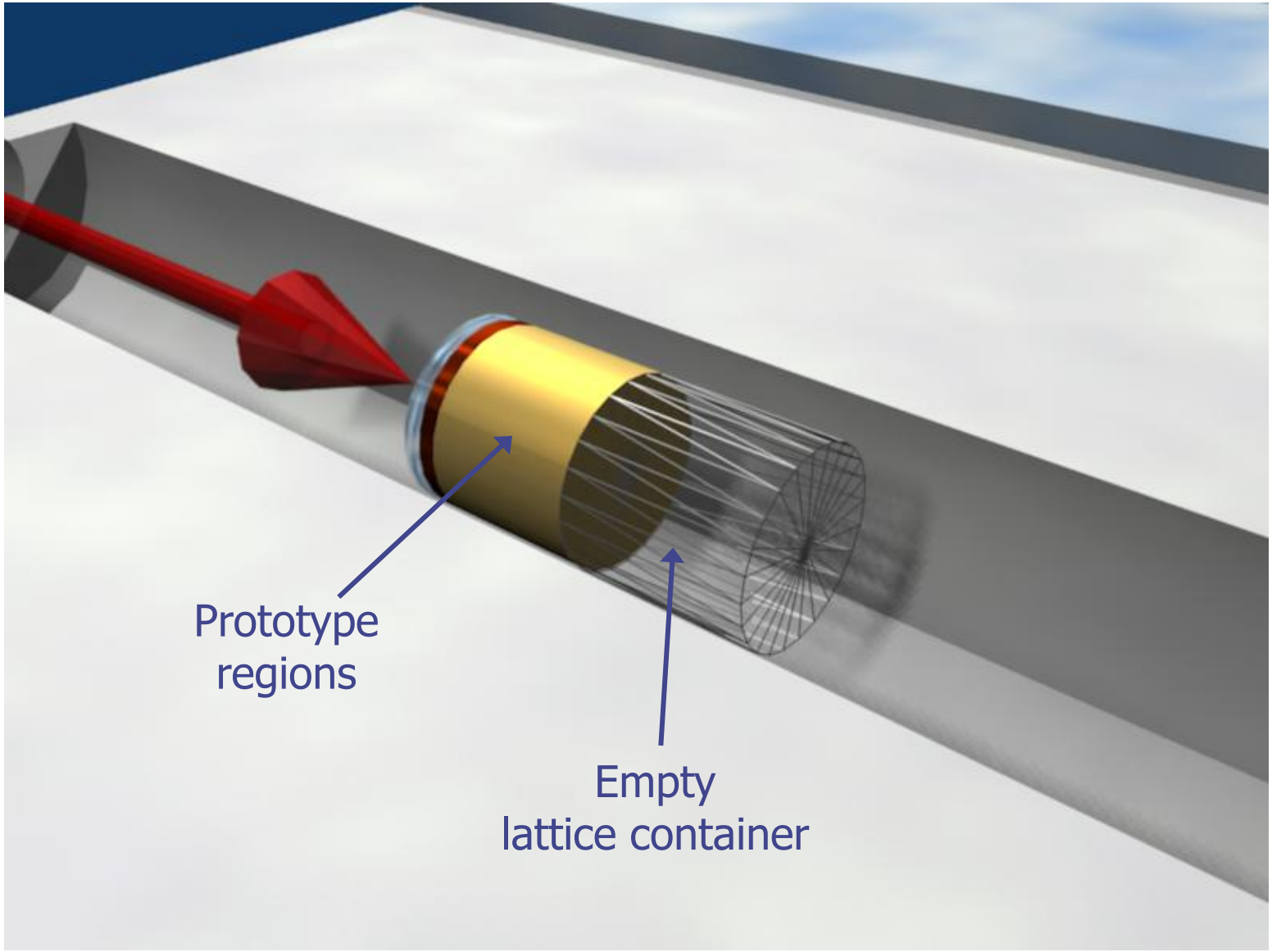

```
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+...
LATTICE       6.00000  19.00000              101.0000    114.00
```

Region # 6 to 19 are the "placeholders" for the first set replicas. We assign to them lattice numbers from 101 to 114

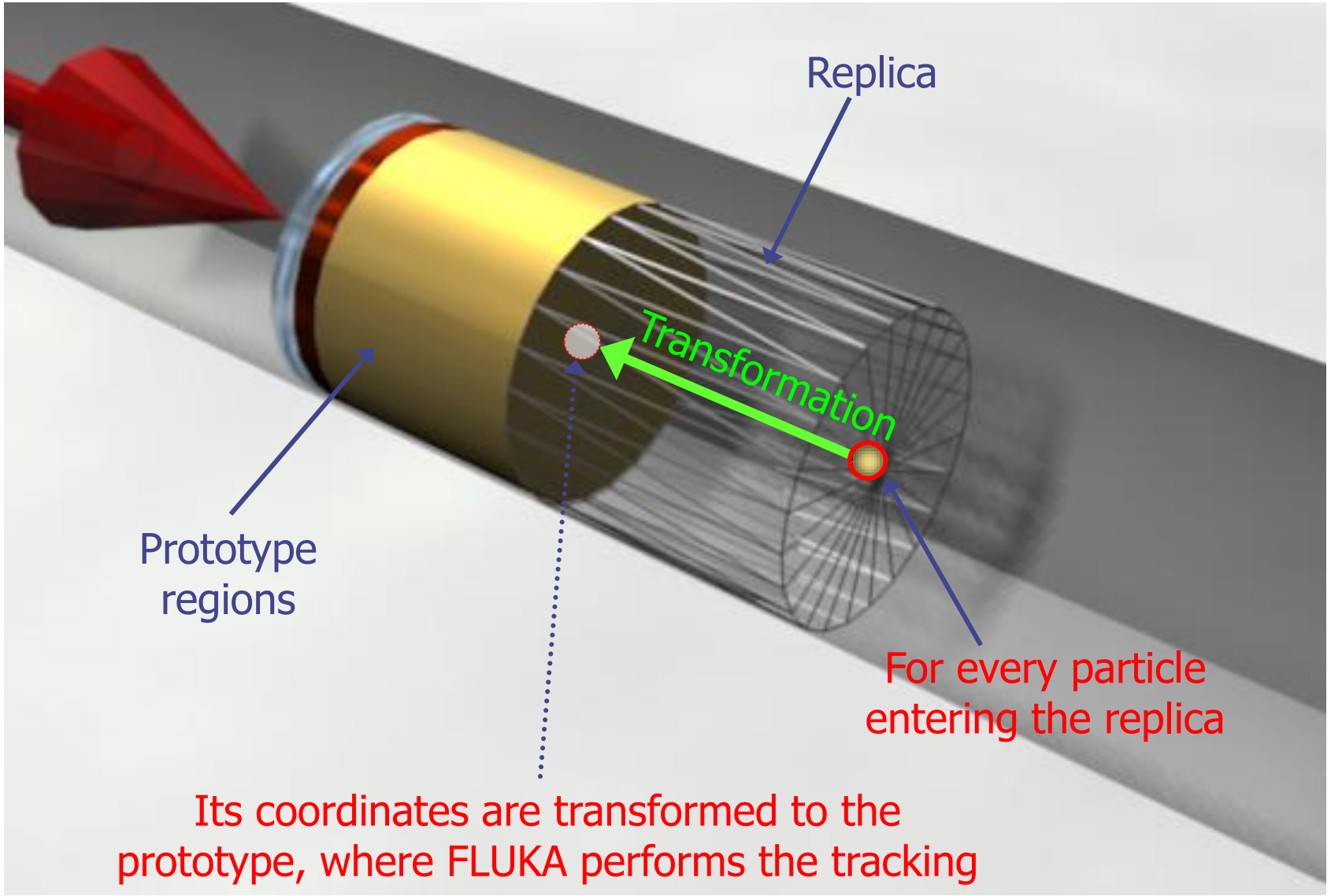
```
LATTICE        TARGR1                          TargRep                        1tra
```

TARGR1 is the container region using transformation *1tra*

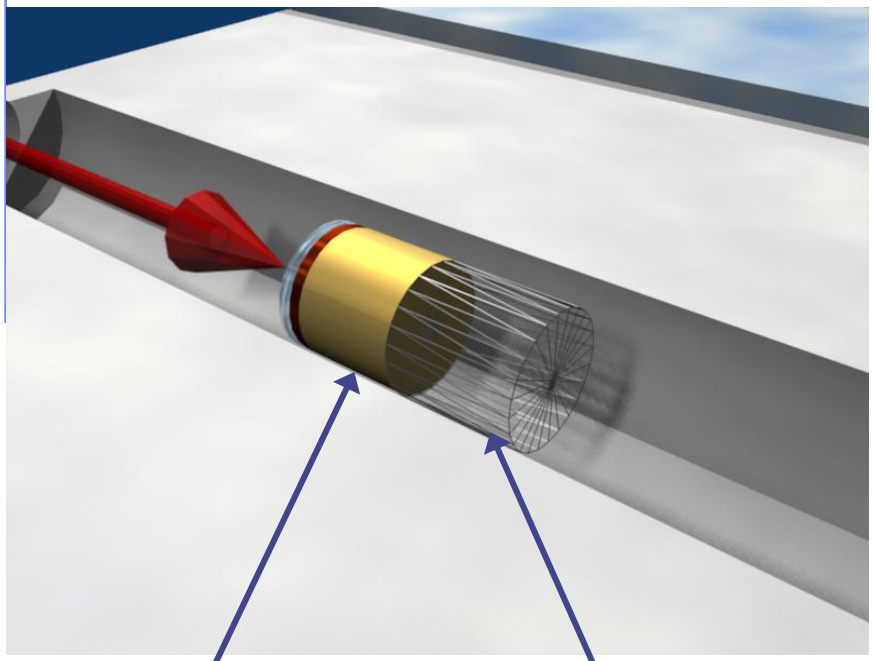
Example

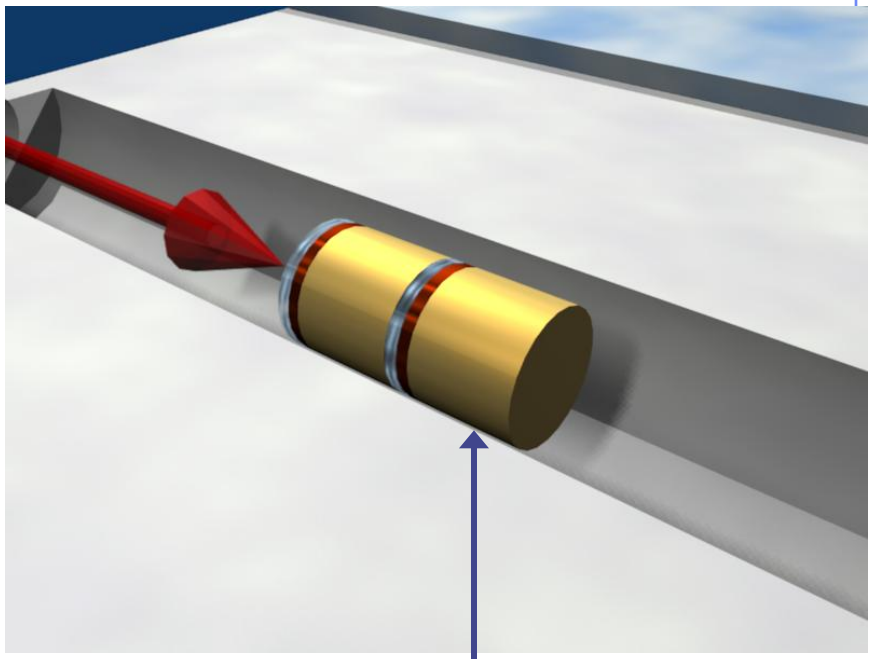


Example


Replica
Transformation
Prototype
regions
For every particle
entering the replica
Its coordinates are transformed to the
prototype, where FLUKA performs the tracking

Example





Prototype cell

Empty lattice cell

Final replica

Transformation by input

- Rotations/Translations can be defined with the ROT-DEFIni card
- Can be assigned to a lattice by name or with ROT#nnn SDUM in the LATTICE card
- ROT-DEFIni cards can be consecutive (using the same index or name) to define complex transformations

WARNING:

Since matrix multiplication is not commutative the order of the Rotation/Translation operations in 3D is important.

ROT-DEFIni

The ROT-DEFIni card defines roto-translations that can be applied to i. USRBIN, EVENTBIN, and ii. LATTICE. It transforms the position of the tracked particle i. before scoring with respect to the defined binning or ii. into the prototype with the order:

- First applies the translation
- followed by the rotation on the azimuthal angle
- and finally by the rotation on the polar angle.

$$\mathbf{X_{new} = M_{polar} \times M_{az} \times (X + T)}$$

WHAT(1): assigns a transformation index and the corresponding rotation axis

I + J * 100 or **I * 1000 + J**

I = index of rotation (WARNING: NOTE THE SWAP OF VARIABLES)

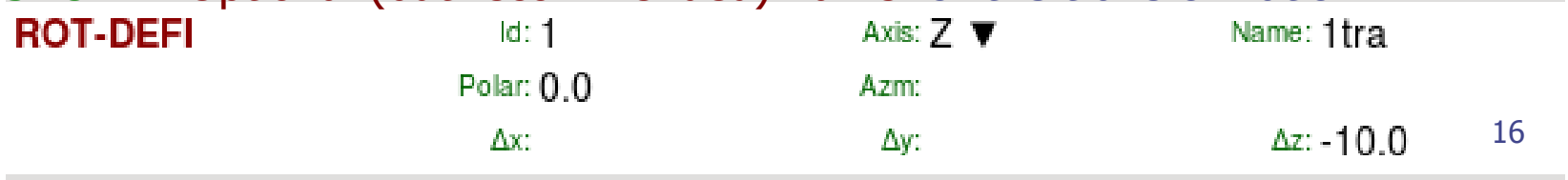
J = rotation with respect to axis (1=X, 2=Y, 3=Z)

WHAT(2): Polar angle of the rotation ($0 \leq \vartheta \leq 180^o$ degrees)

WHAT(3): Azimuthal angle of the rotation ($-180 \leq \varphi \leq 180^o$ degrees)

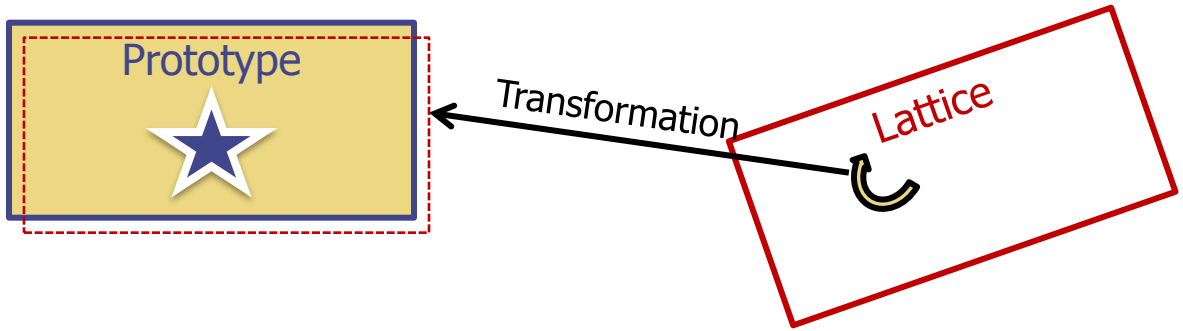
WHAT(4), WHAT(5), WHAT(6) = X, Y, Z offset for the translation

SDUM: Optional (but recommended) name for the transformation



Numerical Precision

- Due to the nature of the floating point operations in CPU, even if the transformation looks correct the end result could be problematic

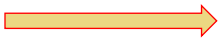


This small misalignment between lattice/transformation/prototype could lead to geometry errors

- Use as many digits as possible to describe correctly the prototype and lattice cells as well as the transformation.
  It is mandatory that the transformation applied to the container makes the latter EXACTLY corresponding to the prototype
- One can use a FREE and FIXED card before and after the ROT-DEFI to input more than 9 digits
- GEOBEGIN WHAT(2) allows to relax the accuracy in boundary identification (USE WITH CAUTION)

Lattice: Important remarks

- Materials and other properties have to be assigned only to the regions constituting the prototype.
- In all (user) routines the region number refers to the corresponding one in the prototype.
- The SCORE summary in the .out file and the scoring by regions add together the contributions of the prototype region as well as of all its replicas!
- The lattice identity can be recovered runtime by the *lattice number*, as set in the LATTICE card or available through the GEON2L routine if is defined by name
- In particular, the LUSRBL user routine allows to manage the scoring on lattices in the special USRBIN/EVENTBIN structure.



The USRBIN/EVENTBIN special binning

EVENTBIN or USRBIN with WHAT(1)=**8** :

Special user-defined 3D binning. Two variables are discontinuous (e.g. region number), the third one is continuous, but not necessarily a space coordinate.

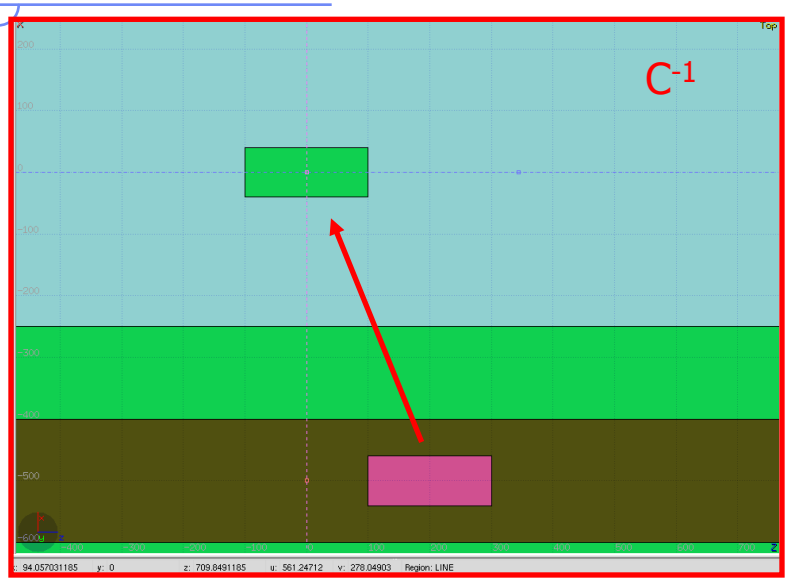
Variable	Type	Default	Override Routine
1st	integer	region number	MUSRBR
2nd	integer	lattice cell number	LUSRBL
3rd	float	zero	FUSRBV

Tips & Tricks

- Always remember that the transformation must bring the container onto the prototype and not viceversa!

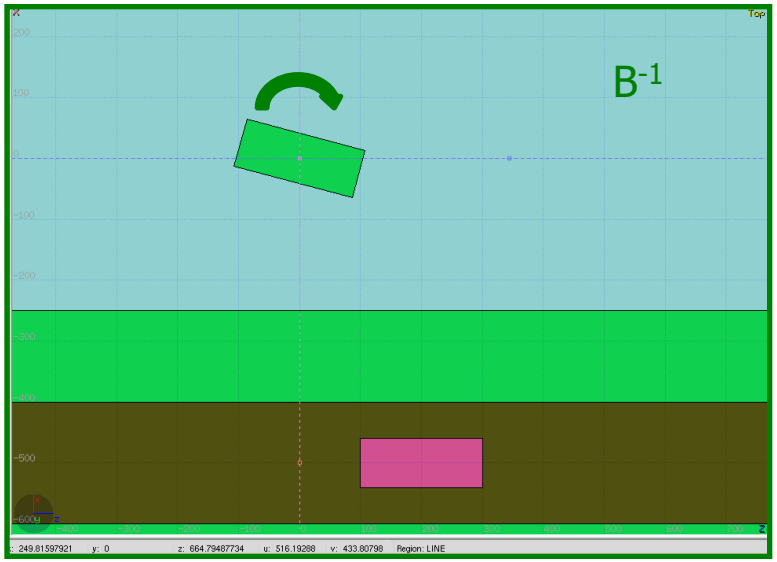
- You can always divide a transformation into many ROT-DEFI cards for easier manipulation.
- Rotations are always around the origin of the geometry, and not the center of the object.
  - To rotate an object, first translate the object to the origin of the axes
  - Perform the rotation
  - Move it by a final translation to the requested position.
    Of course with the inverse order since everything should apply to the replica
- In order to define the replica body, you can clone the body enclosing the prototype (assigning it a new name!) and apply to it the $Start_transform directive with the inverse of the respective ROT-DEFI transformation.

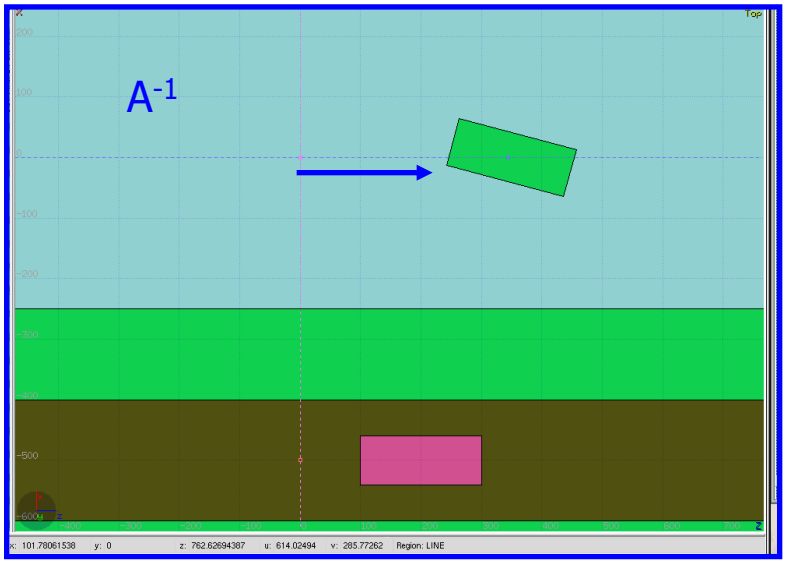
Tips & Tricks




```
GEOBEGIN
...
RPP CollProt -540.0 -460.0 -20.0 20.0 100.0 300.0
$start_transform –rotColl *
RPP CollRepl -540.0 -460.0 -20.0 20.0 100.0 300.0
$end_transform
...
GEOEND
ROT-DEFI, 1.0, 0.0, 0.0, 0.0, 0.0, -350.0, rotColl   [A]
ROT-DEFI, 201.0, 0.0, -15.0, 0.0, 0.0, 0.0, rotColl   [B]
ROT-DEFI, 1.0, 0.0, 0.0, -500.0, 0.0, 200.0, rotColl   [C]
```

* Remember: if R=CBA, then $R^{-1}=A^{-1}B^{-1}C^{-1}$



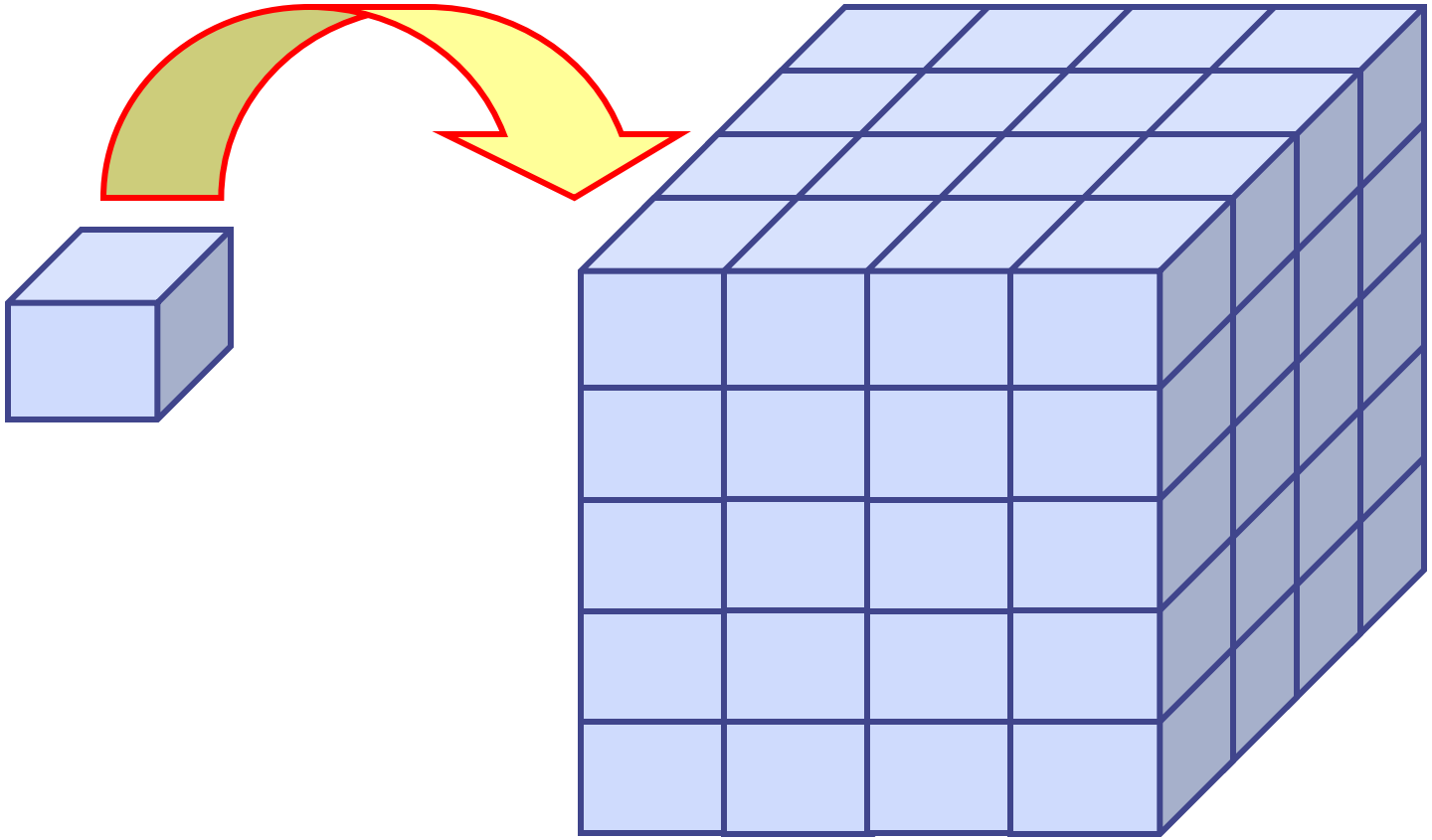


(Tips & Tricks)

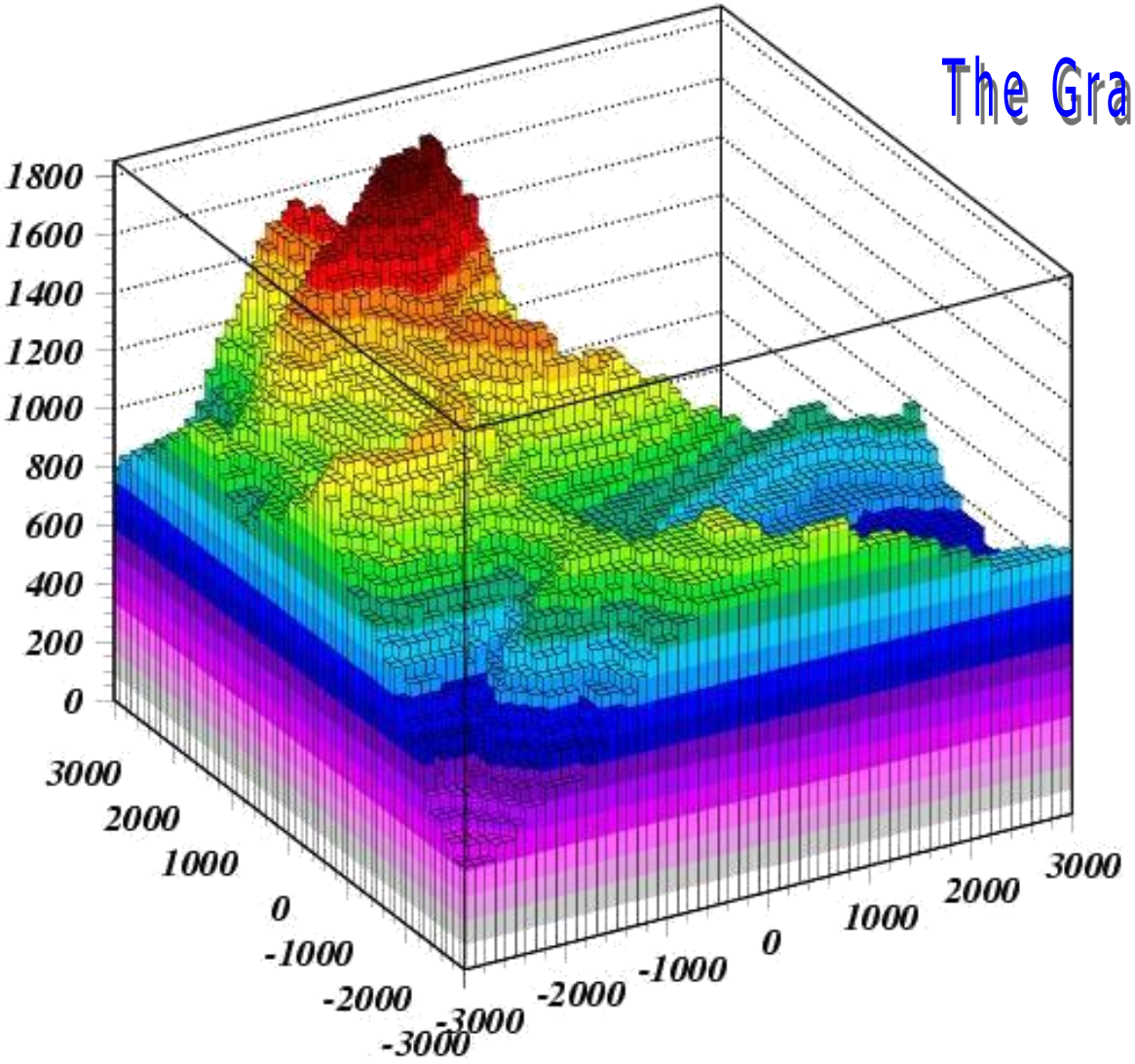
- The Geometry transformation editor in flair can read and write ROT-DEFI cards with the transformation requested
- An easy way of creating a replica and the associated transformation is the following:
  1. Select the body defining the outer cell of the prototype
  2. Clone it with (Ctrl-D) and change the name of the clones. Click on "No" when you are prompted to change all references to the original name.
  3. Open the Geometry transformation dialog (Ctrl-T)
  4. Enter the transformation of the object in the listbox
  5. Click on "Transform" to perform the transformation on the clone bodies
  6. Click on "Invert" button to invert the order of the transformation
  7. Enter a name on the "ROT-DEFIni" field and click "Add to Input" to create the ROT-DEFIni cards
  8. Now you have to create manually the needed regions and the LATTICE cards

The FLUKA voxel geometry

It is possible to describe a geometry in terms of “voxels”, i.e., tiny parallelepipeds (all of equal size) forming a 3-dimensional grid



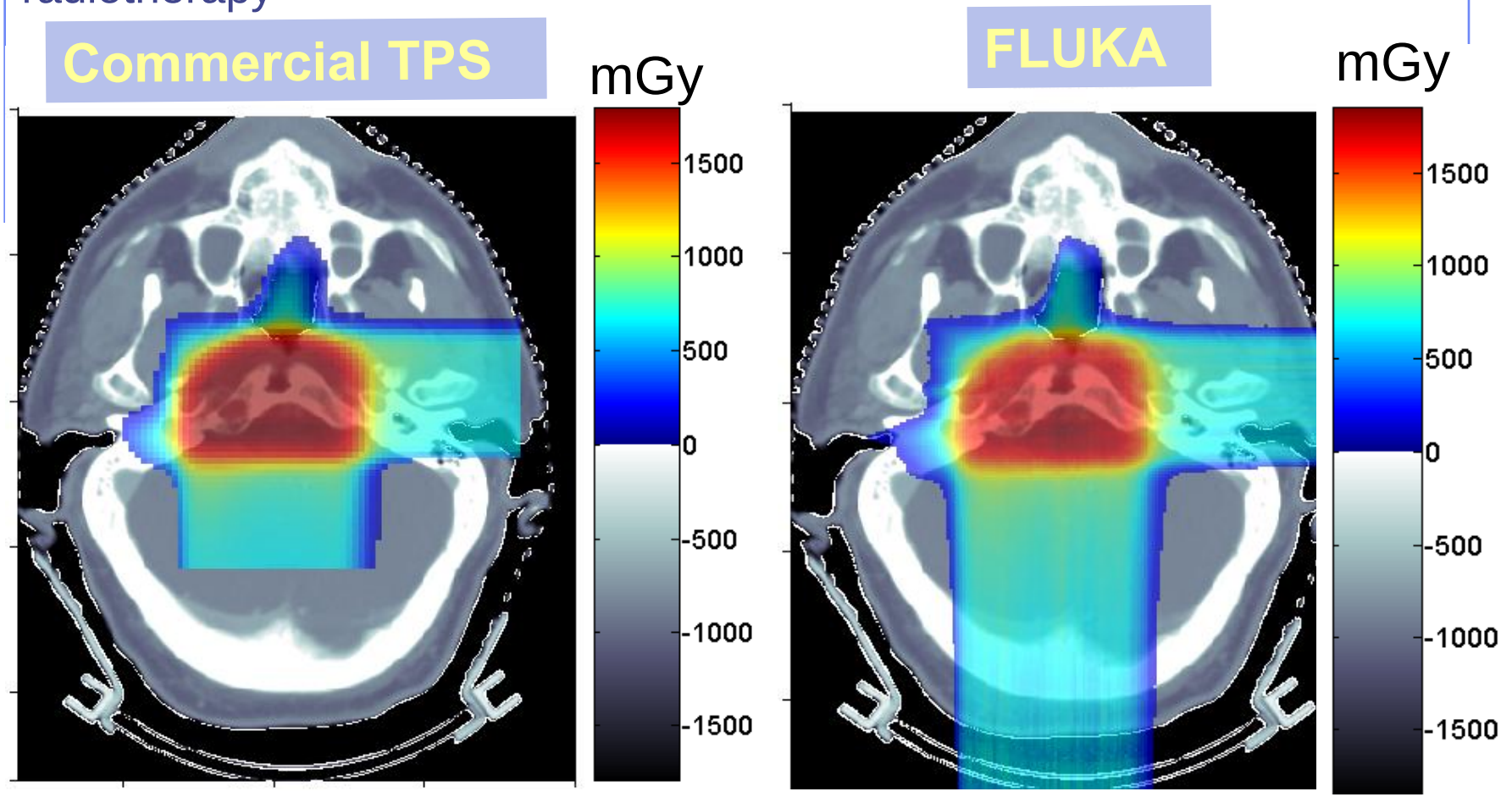
An example



The Gran Sasso in FLUKA

Another example, for medical applications

Voxel geometries are especially useful to import CT scan of a human body, e.g., for dosimetric calculations of the planned treatment in radiotherapy



[K. Parodi et al., 2007]

Concepts

- The CT scan contains integer values “Hounsfield Unit” reflecting the X-ray attenuation coefficient μ_x

$$HU_x = 1000\ (\mu_x - \mu_{H20})\ /\ \mu_{H20}\ ,\ \text{typically } -1000 \leq HU \leq 3500$$

- We will use loosely the word “organ” to indicate a group of voxels (or even more than one group) made of the same “tissue” material (same HU value or in a given HU interval)
- The code handles each organ as a CG region, possibly in addition to other conventional “non-voxel” regions defined by the user
- The voxel structure can be complemented by parts written in the standard Combinatorial geometry
- The code assumes that the voxel structure is contained in a parallelepiped. This RPP is automatically generated from the voxel information.

Procedure

- To describe a voxel geometry, the user must convert his CT scan or equivalent data to a format understood by FLUKA

- This stage should :
  - Assign an organ index to each voxel. In many practical cases, the user will have a continuum of CT values (HU), and may have to group these values in intervals
  - Each organ is identified by a unique integer ≤32767. The organ numbering does not need to be contiguous (i.e. “holes” in the numbering sequence are allowed.)
  - One of the organs must have number **0** and plays the role of the medium surrounding the voxels (usually vacuum or air).
  - The user assigns to each NONZERO organ a voxel-region number. The voxel-region numbering has to be contiguous and starts from 1.

Procedure

- The information is input to FLUKA through a special **unformatted** file *vxl containing:
  - The number of voxels along each coordinate axis
  - The number of voxel-regions, and the maximum organ number
  - The voxel dimension along each coordinate axis
  - A 3D matrix specifying the organ to which each voxel corresponds

    in Fortran list-oriented format, with the x coordinate running faster than y, and y running faster than z.

val(1)	corresponds to 1,1,1 == organ # of first voxel
…	…
val(N_x)	corresponds to N_x,1,1
val(N_x+1)	corresponds to **1**,**2**,1
…	…
val(2*Nx)	corresponds to N_x,2,1
…	
val(N_y*N_x)	corresponds to N_x,N_y,1
…	…
val(N_z*N_y*N_x)	corresponds to N_x,N_y,N_z == organ # of last voxel

  - A list of the voxel-region number corresponding to each organ

Input file: geometry description

Prepare the usual FLUKA input file.

The geometry is written like a normal Combinatorial Geometry input, but in addition a VOXELS card must be inserted right after the GEOBEGIN card and before the Geometry title card

- WHAT(1), WHAT(2), WHAT(3) = x, y, z coordinates chosen as the origin of the "voxel volume", i.e. the corner of a RPP extending from WHAT(1) to WHAT(1) + NX*DX, … and containing all the voxels
- WHAT(4) possible ROT-DEFI **transformation applying to the RPP**
- (WHAT(5), WHAT(6): not used)
- SDUM = name of the voxel file

  (extension will be assumed to be .vxl)

```
VOXELS      -20.0     -30.0     -40.0  transf                    ct
```

Input file: geometry description

One will have

- The usual list of NB bodies, not including the RPP corresponding to the "voxel volume" (see VOXELS card above). This RPP will be generated and added automatically by the code as the (NB+1) th body, with one corner in the point indicated in the VOXELS card, and dimensions NX*DX, NY*DY and NZ*DZ as read from the voxel file.
- The usual list of NR regions, with the space occupied by the body named VOXEL or numbered NB+1 (the "voxel volume") subtracted. In other words, the NR listed regions must cover the whole available space, except the space corresponding to the "voxel volume". This is easily obtained by subtracting the body VOXEL (or NB+1) in the relevant region definitions, even though this body is not explicitly input at the end of the body list.

```
* vacuum inside
VACI       5 +SHI +SHTB -SHBT -VOXEL
```

Voxel Regions

The code will automatically generate NO+2 additional regions, where NO = number of non-zero organs:

Name	Number	Description
VOXEL	NR+1	sort of a "cage" for all voxels. Nothing should ever be deposited in it. The user shall assign VACUUM to it.
VOXEL001	NR+2	containing all voxels belonging to organ number 0. There must be at least 2 of such voxels, but in general they should be many more. Typical material assignment to this region is air
VOXEL002	NR+3	corresponding to organ 1
VOXEL003	NR+4	corresponding to organ 2
VOXEL###	NR+2+NO	corresponding to organ NO

Voxel Material Assignment

The assignment of materials shall be made by the card ASSIGNMAt (and in a similar way for other region-dependent options) referring to the first NR regions in the usual way, and to the additional voxel regions using the correspondence to organs.

```
ASSIGNMA   BLCKHOLE    BLKH
ASSIGNMA    VACUUM     VACO
ASSIGNMA   ALUMINUM      AL
ASSIGNMA    VACUUM     VACI
ASSIGNMA    VACUUM    VOXEL
ASSIGNMA    VACUUM VOXEL001
ASSIGNMA TITANIUM VOXEL002
ASSIGNMA      AIR VOXEL003
ASSIGNMA   COPPER VOXEL004
ASSIGNMA  CALCIUM VOXEL005
ASSIGNMA   CARBON VOXEL006
ASSIGNMA      AIR VOXEL007
```

cage

0 Organ

6 "Non-zero" organs