FLUKA Geometry

FLUKA Advanced Course

Contents

- combinatorial geometry and format recalls
- bodies
  - generic quadric
  - transformations and rotation concepts
- regions operators
  - problems and hints
  - parentheses
- lattice
- ancillary core routines
- dynamic objects
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Basic Concepts

Four concepts are fundamental in the FLUKA CG:

- **Bodies** - basic convex objects + infinite planes & infinite cylinders + generic quadric
- **Zones** - sub-region defined only with intersection and subtraction of bodies (used internally)
- **Regions** - are defined as boolean operations of bodies (union of zones)
- **Lattices** - duplication of existing regions (translated & rotated)

Input format

- The input format for the geometry is different from that adopted elsewhere in FLUKA, i.e. the number and length of the input fields is different.
- The recommended format is name based. For backward compatibility there are also other formats. **Name based format is not the default one!**

  Name based format input is used for both body and region if requested by COMBNAME in the GEOBEGIN card, or by a GLOBAL command at the beginning of the input file.

  One advantage of name based format is that alignment of the input parameters is not necessary. Bodies and regions are identified by **names**. Its main advantages, in addition to the freedom from strict alignment rules, are the possibility to modify the input sequence without affecting the region description (for instance, by inserting a new body) and the availability of parentheses to perform complex boolean operations in the description of regions.

- In fixed format alignment is mandatory. Bodies and regions are identified by **numbers** and not by names which makes creation and updating of the geometry difficult.

Input structure

FLUKA CG input must respect the following sequential order:

GEOBEGIN card
- **VOXELS** card *(optional)*
- Geometry title (and reading format options)
- Body data
- **$Start_**transformation *(optional)*
- Body data
- **$End_**transformation *(optional)*
- Body data
- **END** card *(automatically added by flair)*
- Region data
- **END** card *(automatically added by flair)*
- **LATTICE** cards *(optional)*
- Region volumes

(optionally requested by a flag in the Geometry title, used together with **SCORE**)

GEOEND card

Cards having a * in column 1 are treated as comments

GEOBEGIN card

The meanings of the WHAT and SDUM parameters are:

WHAT(1) flag for switching off geometry error messages: **don't touch!!**
Default = 0.0 (all geometry error messages are printed)

WHAT(2) used to set the **accuracy parameter**

WHAT(3) = logical unit for the geometry input.
If > 0.0 and different from 5, the name of the corresponding file must be input on the next card. Otherwise, the geometry input follows.

WHAT(4) = logical unit for the geometry output. If > 0.0 and different from 11, the name of the corresponding file must be input on the next card. Otherwise, geometry output is printed on the standard output.

WHAT(5) **Parenthesis optimization level**

WHAT(6) not used

SDUM = COMBNAME or COMBINAT
COMBNAME selects name based format, COMBINAT fixed format
Default: COMBINAT (!)
Can be overwritten by WHAT(5) of a possible GLOBAL card

Tracking accuracy

WHAT(2)*10^{-6}cm is the *absolute accuracy (AA)* requested for tracking, applying to boundary identification.

The *relative accuracy (RA)* achievable in double precision is of the order of 10^{-14}-10^{-15}.

So *AA* should be larger than *RR*L*, being *L* the largest coordinate value in the problem world (excluding the outer blackhole shell containing it), i.e. the whole geometry size.

For very large (e.g., Earth) and very small geometries, you may need to increase or decrease, respectively, the WHAT(2) default value of 0.0001.

Bodies

- Each body divides the space into two domains inside and outside. The outside part is pointed to by the normal on the surface.
- 3-character code of available bodies:
  - RPP: Rectangular parallelepiped
  - SPH: Sphere
  - XYP, XZP, YZP: Infinite half space delimited by a coordinate plane
  - PLA: Generic infinite half-space
  - XCC, YCC, ZCC: Infinite circular cylinder, parallel to coordinate axis
  - XEC, YEC, ZEC: Infinite elliptical cylinder, parallel to coordinate axis
  - RCC: Right circular cylinder
  - REC: Right elliptical cylinder
  - TRC: Truncated right angle cone
  - ELL: Ellipsoid of revolution
  - **QUA**: Generic quadric surface
- Other bodies ARB, RAW, WED, BOX
  - don't use them, they cause sometimes rounding problems

Important Notes

- Whenever it is possible, the following bodies should be preferred:

  PLA, RPP, SPH, XCC, XEC, XYP
  XZP, YCC, YEC, YZP, ZCC, ZEC,QUA

  These make tracking faster, since for them extra coding ensures that unnecessary boundary intersection calculations are avoided when the length of the next step is smaller than the distance to any boundary of the current region.
- Always **use as many digits as possible** in the definition of the body parameters, particularly for body heights (RCC, REC), and for direction cosines of bodies with slant surfaces. The free format or the high-accuracy fixed format should always be used in these cases.

Bodies input

The input for each body consists of

- the 3-letter code indicating the body type
- a unique body name
  (8 character maximum, alphanumeric identifier, case sensitive)
- a set of geometrical quantities defining the body
  (their number depends on the body type)

A maximum of 132 characters per line are accepted,
use extra lines if required

The different items, separated by **one or more blanks**, or
by one of the separators **, / ; :**
can extend over as many lines as needed.

All numbers are in cm!

Generic quadric: QUA

A QUA is the most generic quadric surface

It is defined by 10 coefficients in the following order:

$$\mathbf{A_{xx}\ A_{yy}\ A_{zz}\ A_{xy}\ A_{xz}\ A_{yz}\ A_x\ A_y\ A_z\ A_0}$$

corresponding to the equation

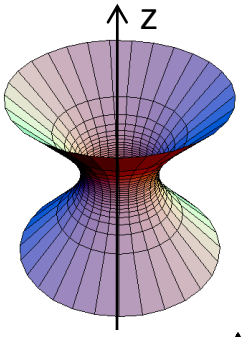
$$A_{xx}\,x^2 + A_{yy}\,y^2 + A_{zz}\,z^2 + A_{xy}\,xy + A_{xz}\,xz + A_{yz}\,yz + A_x\,x + A_y\,y + A_z\,z + A_0 = 0$$

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

For example:

```
QUA EllHyper 0.25 1.0 -4.0 0.0 0.0 0.0 0.0 0.0 0.0 -1
```

is an elliptic hyperboloid with axis equal to z

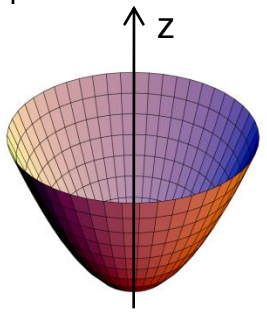



```
QUA Cylinder 0.5 1.0 0.5 0.0 1.0 0.0 0.0 0.0 0.0 -4.0
```

is an infinite circular cylinder of radius 2 with axis {z=-x,y=0}
(i.e. at -45º on the xz plane)

```
QUA EllParab 0.25 1.0 0.0 0.0 0.0 0.0 0.0 0.0 -1.0 0.0
```

is an elliptic paraboloid with axis equal to z



Directives in geometry:expansion(&reduction)

- $Start_expansion ... $End_expansion

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

$$\mathbf{r}'^{T} M_{QUA} \mathbf{r}' = 0 \qquad \mathbf{r} = T\,\mathbf{r}' \qquad T = \begin{bmatrix} f & 0 & 0 & 0 \\ 0 & f & 0 & 0 \\ 0 & 0 & f & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$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)

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

$$\mathbf{r}'^{T} M_{QUA} \mathbf{r}' = 0 \qquad \mathbf{r} = T\,\mathbf{r}' \qquad T = \begin{bmatrix} 1 & 0 & 0 & S_x \\ 0 & 1 & 0 & S_y \\ 0 & 0 & 1 & S_z \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

```
$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)

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

$\mathbf{r'}^T M_{QUA} \mathbf{r'} = 0$ $\qquad$ $\mathbf{r} = T\,\mathbf{r'}$ $\qquad$ $T = \begin{bmatrix} & R & & S_x \\ & & & S_y \\ & & & S_z \\ 0 & 0 & 0 & 1 \end{bmatrix}$

```
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**)

- 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, $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

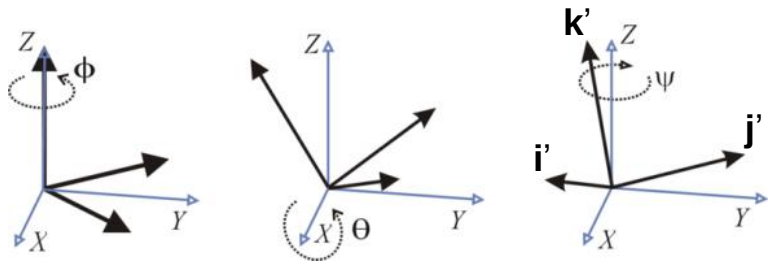
- Directives are not case sensitive (whereas roto-translation names are)

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

Regions (I)

Input for each region starts on a new line and extends on as many continuation lines as are needed. It is of the form:

REGNAME NAZ boolean-zone-expression | boolean-zone-expression | ...

- "*boolean-zone-expression*" is a sequence of one or more body names preceded by the operators **+** (intersection) or **–** (complement or subtraction). Several zone expressions can be combined by the union operator **|** . (A single boolean-zone-expression is admitted).
The operator precedence sequence is: first parentheses (see later), then **+** and **–** , last **|**.

- *REGNAME* is the region name (an arbitrary unique alphanumeric character string chosen by the user). The region name must begin by an alphabetical character and must not be longer than 8 characters.

Regions (II)

- *NAZ* is a rough guess for the number of zones which can be entered leaving the current region zones, it is 5 by default. What in fact matters is its **sum over all regions**, defining the size of the *contiguity list*.

At the beginning, to find the neighboring zones, the code searches over the whole geometry, but as the tracking proceeds, it learns the neighbors of each zone: if one is not yet in the contiguity list, it is added, making the calculation more and more efficient. When the above size limit is reached, the code prints a warning: GEOMETRY SEARCH ARRAY FULL. This is not lethal: the calculation continues but with a reduced efficiency. If the neighboring zone is not found in the contiguity list, the code will scan ALL zones.

If you have more than 1000 regions, you must issue a GLOBAL card putting in WHAT(1) a higher limit (not beyond 20000)

Operators

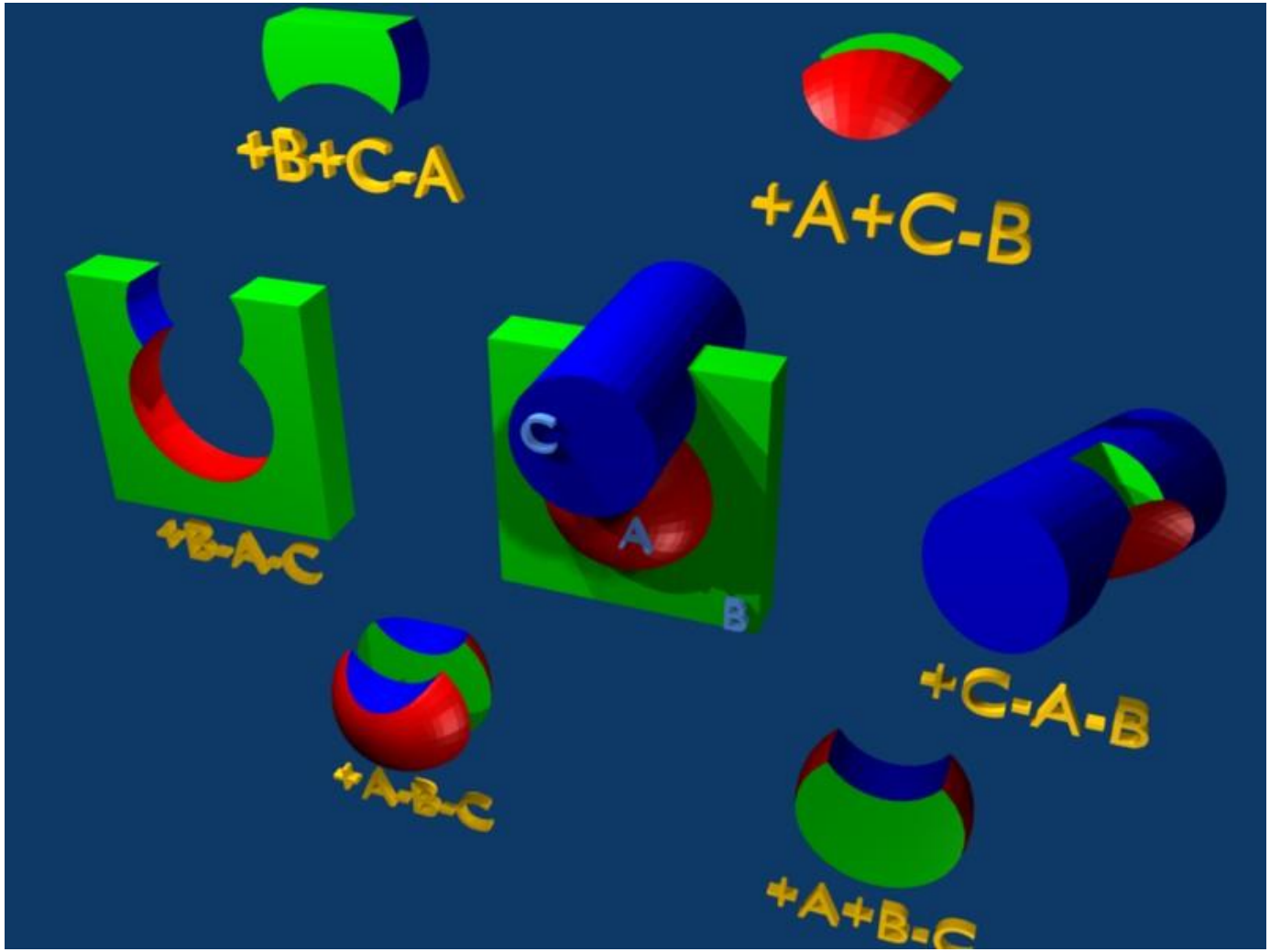
Regions are defined as **combinations of bodies** obtained by boolean operations:

	Union	Subtraction	Intersection
Named based	**|**	**–**	**+**
Fixed	*OR*	*–*	*+*
Mathematically	∪	−	∩

Regions are not necessarily simply connected (they can be made as the union of two or more non contiguous or partially overlapping zones) but must be of **homogeneous material composition**.

Zones must be finite: obviously, in the description of each zone and hence of each region the symbol **+** must appear at least once.

Illustration of the + and – operators



The Blackhole

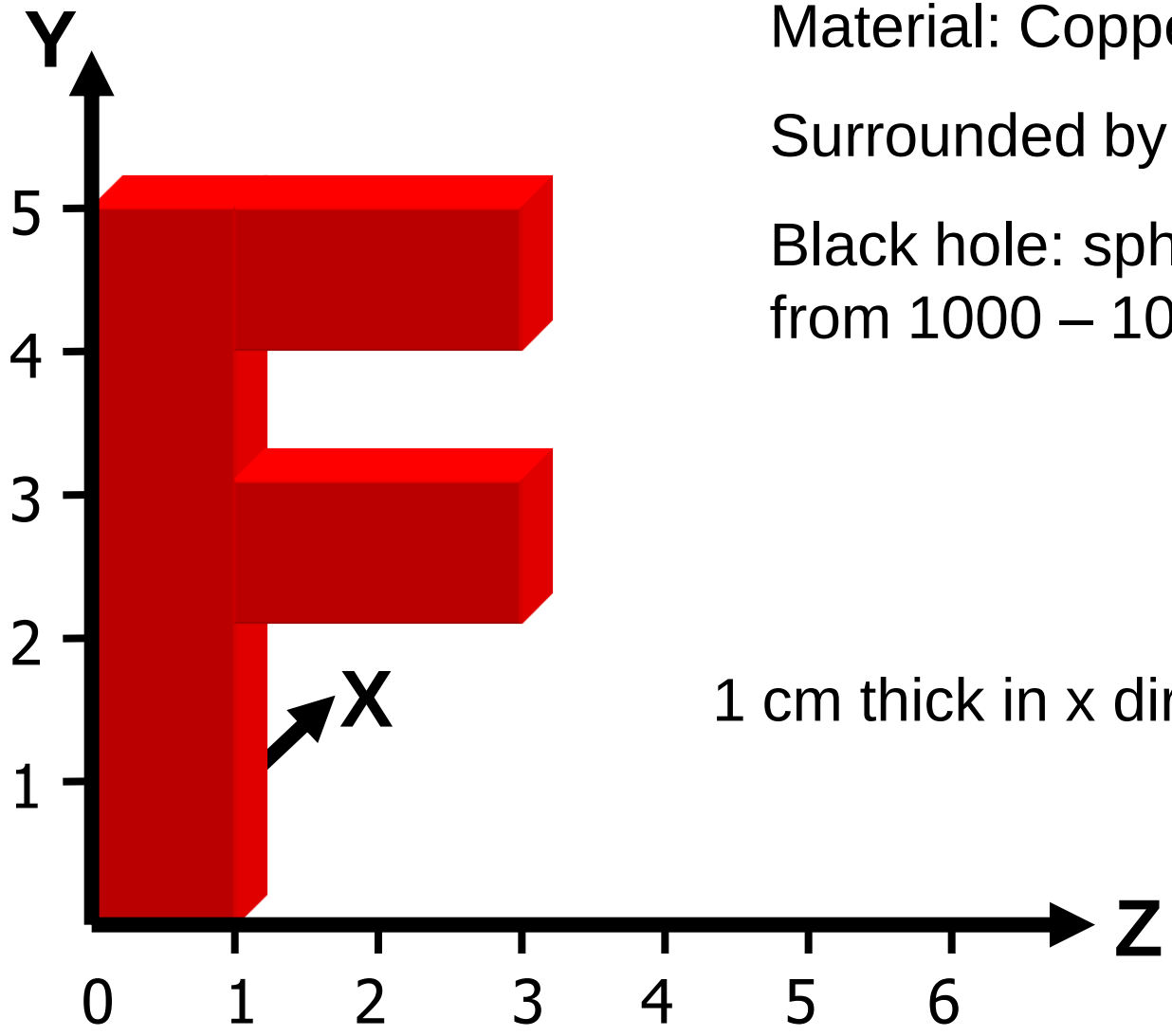
To avoid infinite tracking the particles must be stopped somewhere. This has to be insured by the user by defining a region surrounding the geometry and assigning the material BLCKHOLE to it.

All particles that enter the blackhole are absorbed (they disappear). Further blackhole regions can be defined by the user if necessary.

The blackhole is the outermost boundary of the geometry. Inside the blackhole region:

Each point of space must belong to one and only one region!

Geometry Example "F" shaped target



Material: Copper

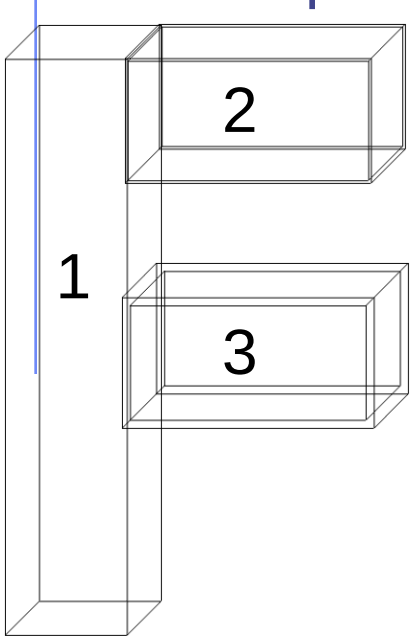
Surrounded by vacuum

Black hole: spherical shell from 1000 – 10000 cm

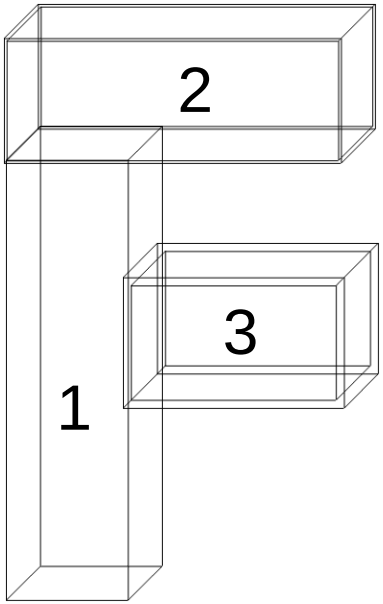
1 cm thick in x direction

Geometry example “F”: Bodies

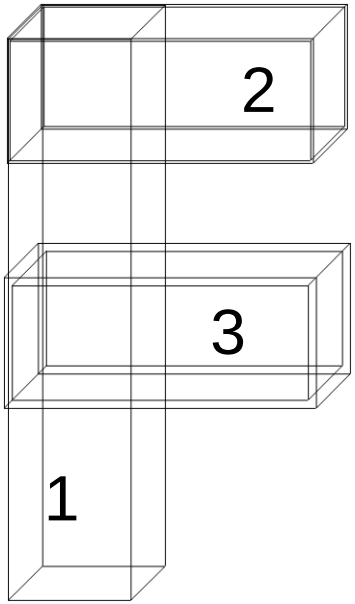
Several possibilities for bodies:



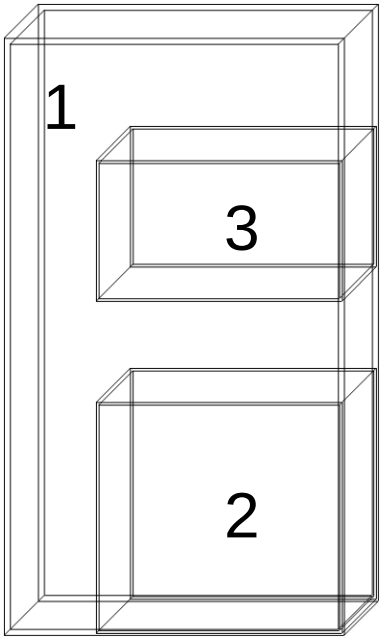
(A) 3 bodies



(B) 3 bodies



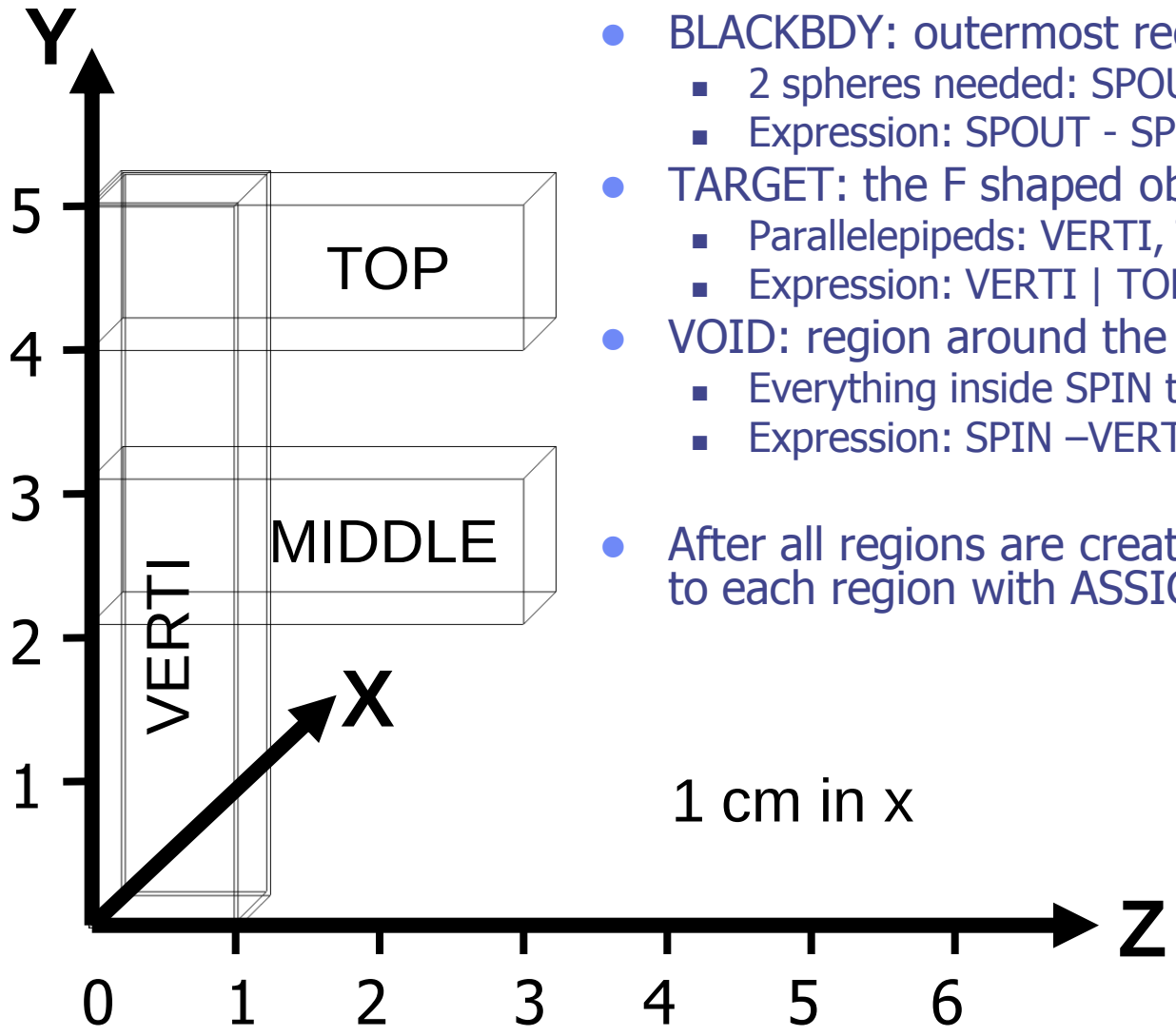
(C) overlapping



(D) subtraction

We will use C.

Geometry example "F": REGIONS



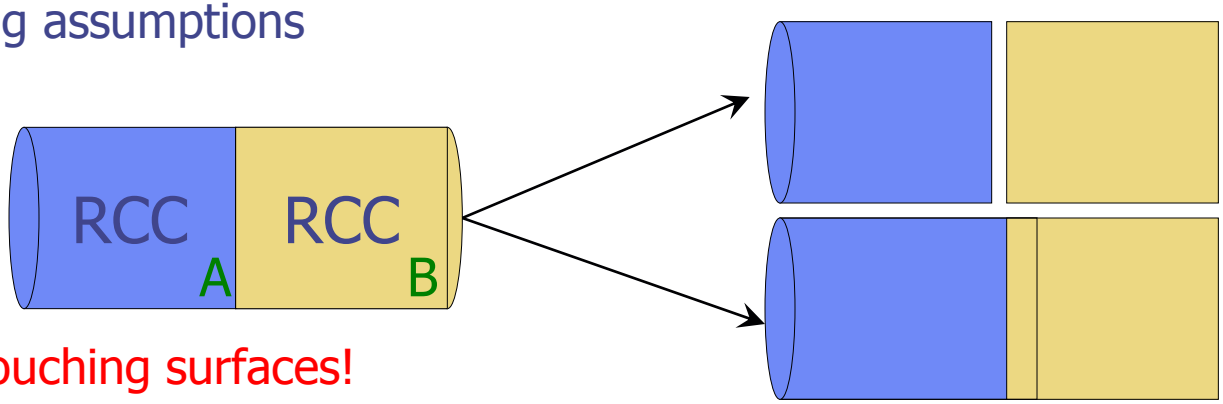
- BLACKBDY: outermost region like a shell
  - 2 spheres needed: SPOUT, SPIN
  - Expression: SPOUT - SPIN
- TARGET: the F shaped object
  - Parallelepipeds: VERTI, TOP, MIDDLE
  - Expression: VERTI | TOP | MIDDLE
- VOID: region around the target
  - Everything inside SPIN that is not target
  - Expression: SPIN –VERTI – TOP –MIDDLE
- After all regions are created: Assign material to each region with ASSIGNMA

Geometry example “F”: input file

```
GEOBEGIN                                                    COMBNAME
    0    0           The copper F
SPH SPIN         0.0 0.0 0.0 1000.
SPH SPOUT        0.0 0.0 0.0 10000.
RPP VERTI        0.0 1. 0.0 5. 0.0 1.
RPP TOP          0.0 1. 4. 5. 0.0 3.
RPP MIDDLE       0.0 1. 2. 3. 0.0 3.
END
* Black hole
BLKBODY       5  +SPOUT -SPIN
* Void around
VOID          5  +SPIN -TOP -VERTI -MIDDLE
* Target
TARGET        5 TOP | VERTI | MIDDLE
END
GEOEND
ASSIGNMA    BLCKHOLE   BLKBODY
ASSIGNMA      VACUUM      VOID
ASSIGNMA      COPPER    TARGET
```

Preventing precision errors

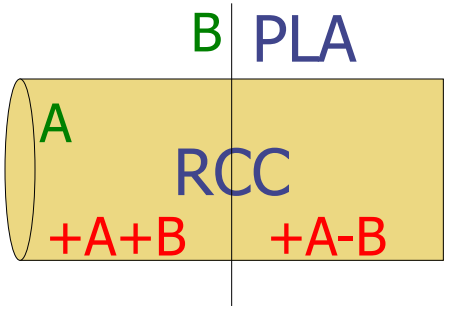
Modeling assumptions



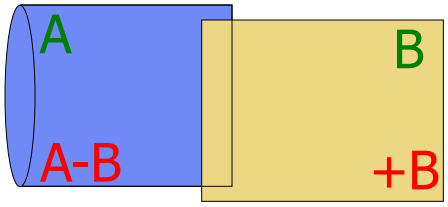
Avoid touching surfaces!

When floating point operations are involved

- Use cutting surfaces B instead.

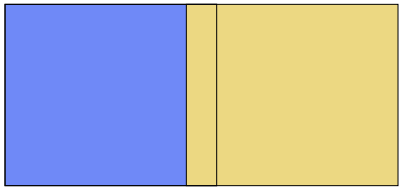


- Or force partial overlap of objects



Geometry errors

- During execution the code always needs to know the region where a particle is located at every step.
- The program will stop only if a particle's position does not belong to any region.
  It will issue an error message on the .err file with the particle position.
- IMPORTANT! It will not stop if a particle's position belongs to more than one region. It will accept the first region it finds but results will be meaningless!!



Debugging (I)

GEOEND card activates the geometry debugger.

Detects both undefined or multiple defined points in a selected X,Y,Z mesh

Two cards are needed

First card

WHAT(1)=X_{max} WHAT(2)=Y_{max} WHAT(3)=Z_{max}
WHAT(4)=X_{min} WHAT(5)=Y_{min} WHAT(6)=Z_{min}
SDUM = DEBUG

Second Card

WHAT(1)=Nx WHAT(2)=Ny WHAT(3)=Nz
SDUM = &

```
GEOEND      Xmax      Ymax      Zmax      Xmin      Ymin      Zmin DEBUG
GEOEND        Nx        Ny        Nz                                &
```

Debugging (II)

- If no error is found, no .err file will be created.
- Errors will be listed in the .err file in the form:

  **** Lookdb: Geometry error found ****
  **** The point: -637.623762 -244.554455 -96.039604 ****

  - Point is contained in more than one region

    **** is contained in more than 1 region ****
    **** (regions: 6 7) ****

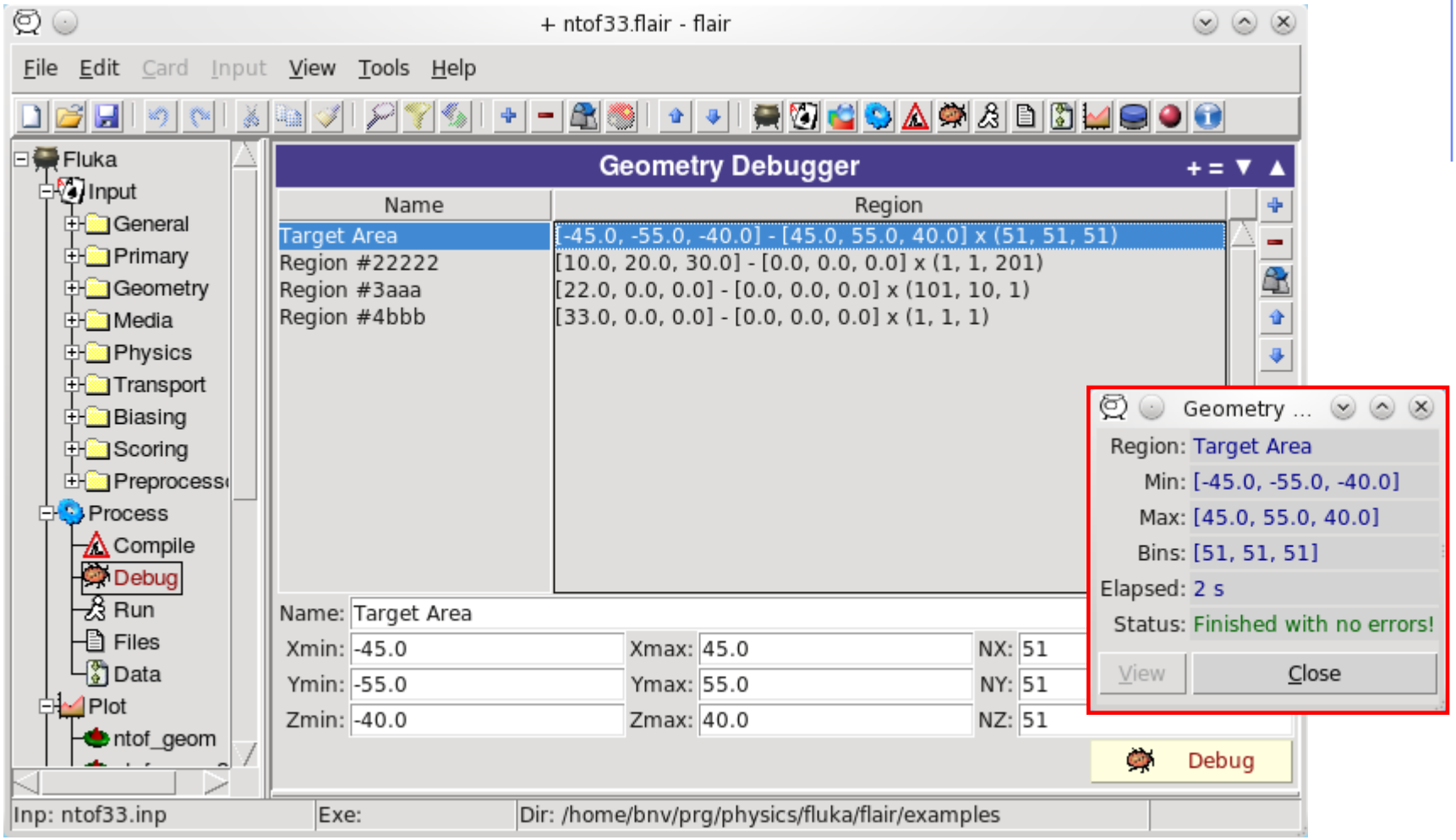
  - Not contained in any region

    **** is not contained in any region

- Exploit the geometry symmetry asking for 2D scans on planes
- Scan only the problematic areas
- Adopt as step length an irrational number in order to prevent from ending up on "special" points (i.e. boundaries)
- REMINDER: If the debugger doesn't find any error it doesn't mean that the geometry is error free!

Debugging (III)

It can be easily run through Flair

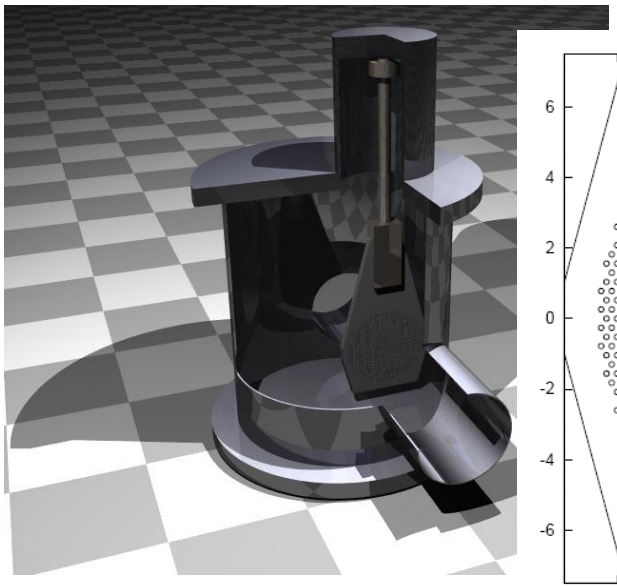


Some hints

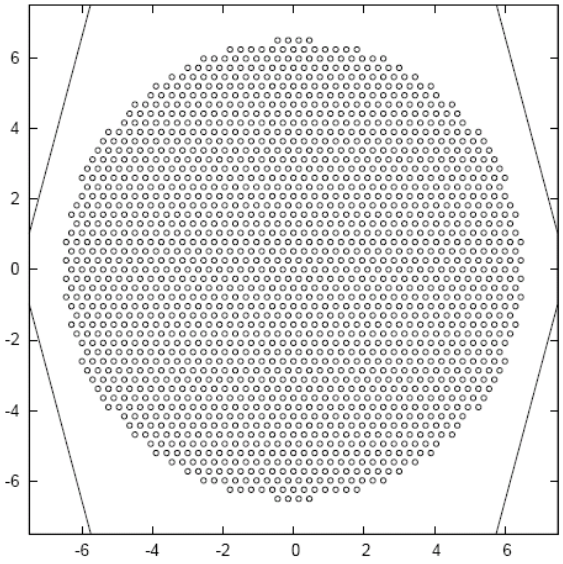
- **Never start a particle from a surface**. You could get a geometry error even if the geometry is correct because FLUKA cannot determine the region.
- FLUKA tries to correct this by moving the particle a bit.
- However if it happens too often the run will stop.
- To avoid this the starting point of the beam particle must be slightly moved
- **Never eject a particle along a surface** (for the same reason)

User optimization in region definition

A zone involving many bodies increases the tracking time, since the exiting conditions imply a respective number of checks

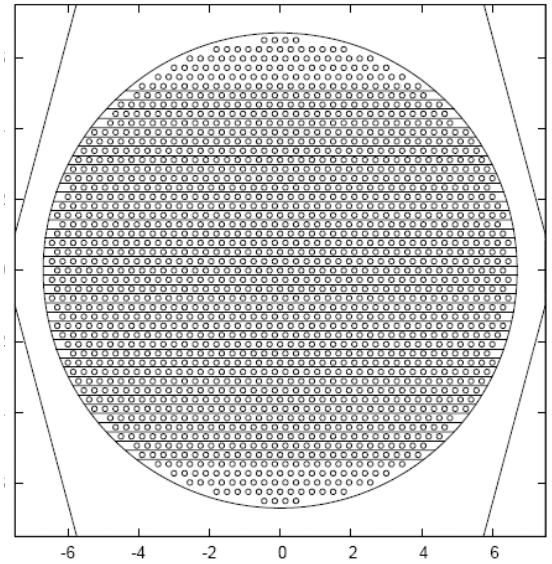


1731 holes



one zone with MANY bodies: large CPU time!

slices with <50 holes



many zones with much less bodies each: significant benefit

...ideally large zones (far boundaries) with few bodies (!)

⇒ prefer overlapping zones

Parentheses

Parentheses are grouping together combinations of bodies.
Parentheses can be used in name based format only.

Examples:

```
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7...
* Subtract from body2 regions regR03, regR04, regR05
regV02 5  +body2 - (+body4  -body3)
          - (+body6  -body5 |+body8 -body7) - body9 -body10
regR03 5 +body4  -body3
regR04 5 +body6  -body5 |+body8 -body7
regR05 5 +body9 | +body10
```

Nested parentheses are supported, however:

parentheses should be used with care since their expansion can generate a quickly diverging amount of terms. A partial optimization is performed on planes (aligned with the axes) and bounding boxes only

Parenthesis Expansion (I)

- Parentheses expansion is almost like converting
  from product of sums to sum of products
- Product operators are: **+**/**-**, Sum operator: **|**
- The final result will be an expression in the normal form. Unions of all possible combinations of the bodies in the expression!
- Initially the code removes all repeated terms:
  A + A = A
  A – A = ∅
  expA | expA = expA

Parenthesis Expansion (II)

Geometrical optimization can drastically reduce the number of zones

1. Elimination of same type of planes (XYP, XZP, YZP) inside a zone (product)
2. Optimization of zones based on the bounding boxes of the bodies.
   - Infinite objects have an infinite bounding box on some of the dimensions i.e. XYP, ZCC etc.
   - PLAnes do not have a bounding box
   - For each zone after the expansion, if the intersection of the bounding boxes is empty the zone is discarded

Lattice (I)

FLUKA geometry has *replication* (lattice) capabilities

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

[In a future release there will be the possibility of a second level]

- 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 should include:

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

WARNING:

Do not use scaling or any deformation of the coordinate system

Lattice (II)

- 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 Region 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

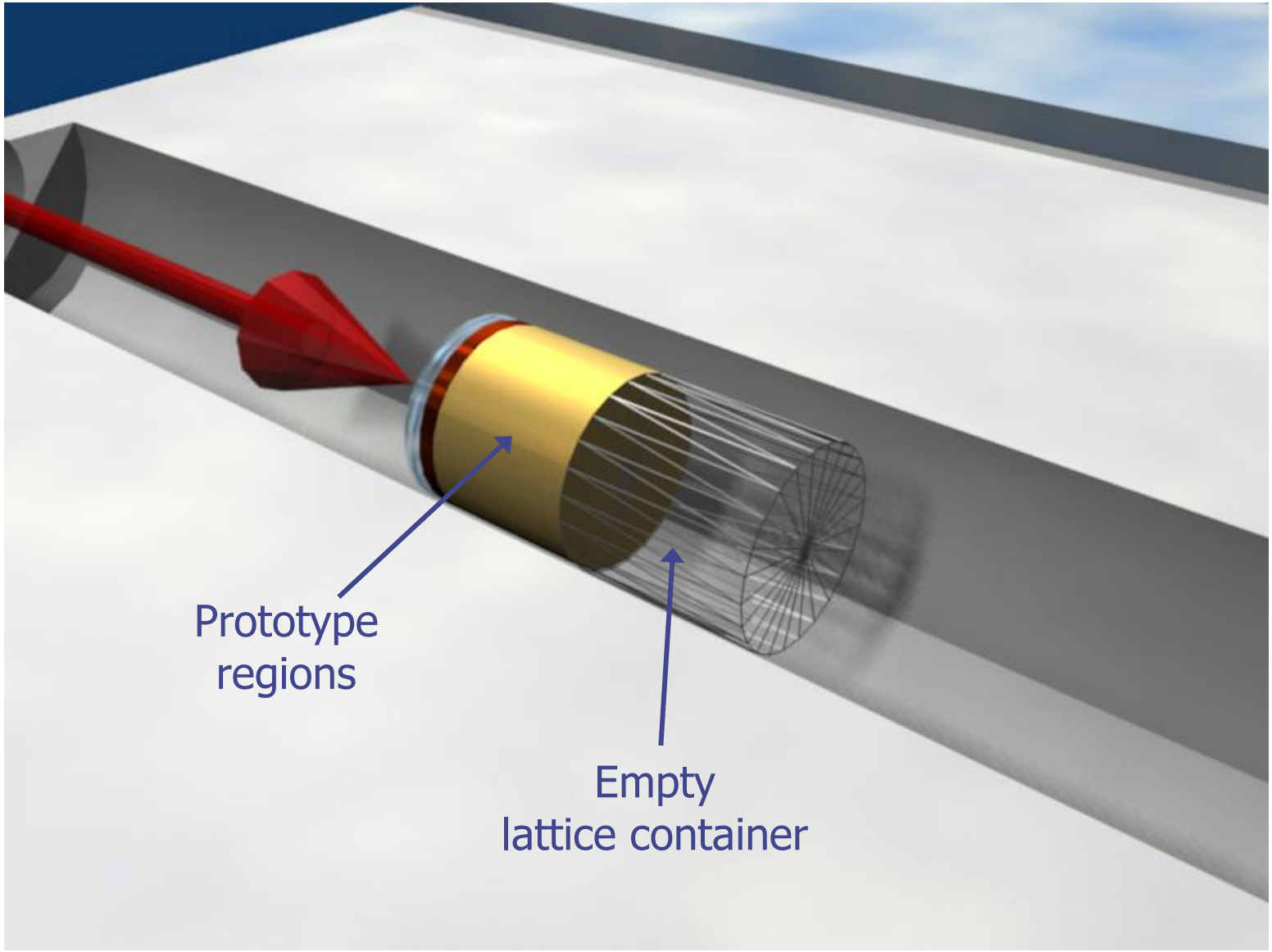

```
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+...
LATTICE       6.00000  19.00000              101.0000    114.00
```

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

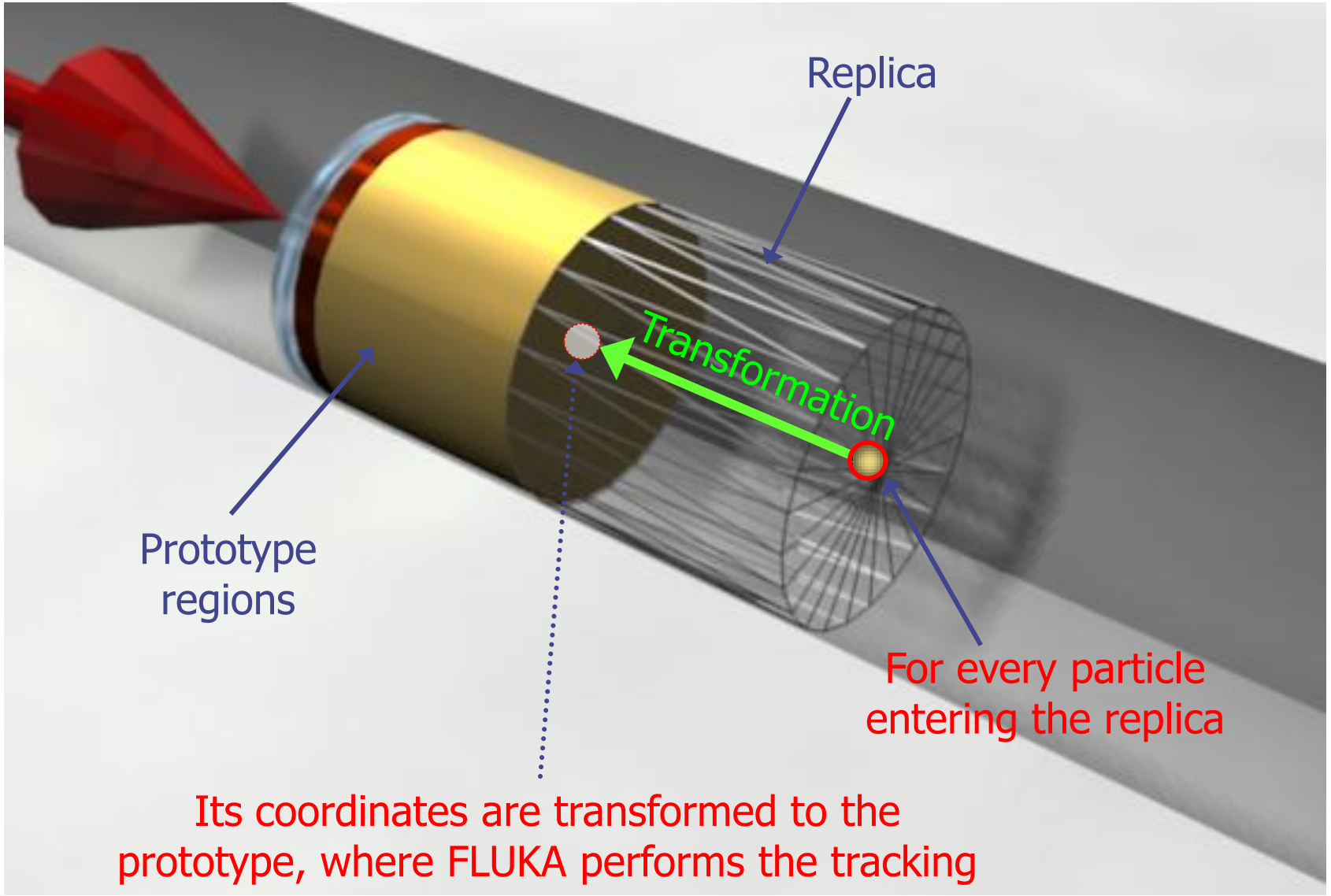
```
LATTICE        TARGR1                          TargRep                        1tra
```

TARGR1 is the container region using transformation *1tra*

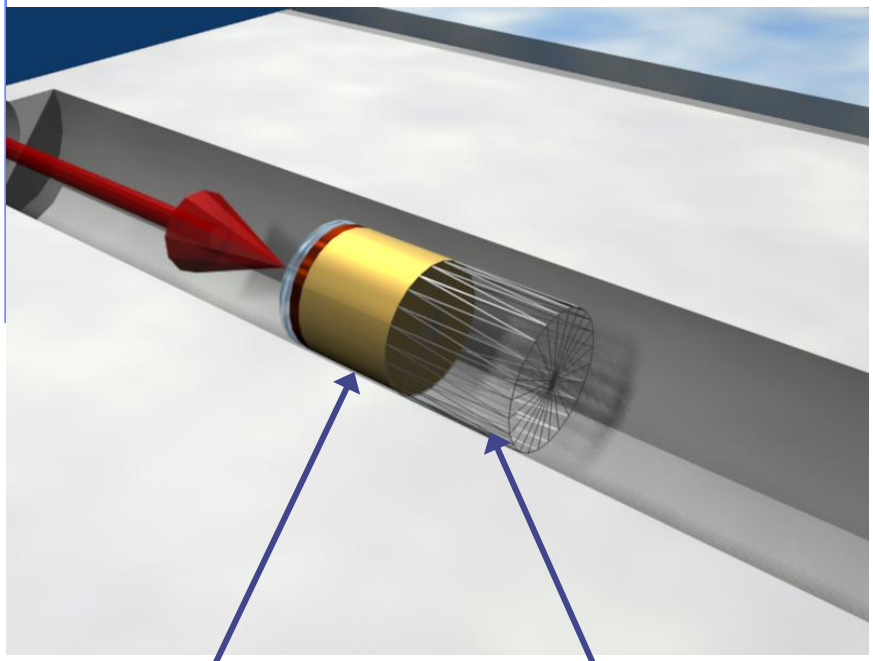
Example (I)

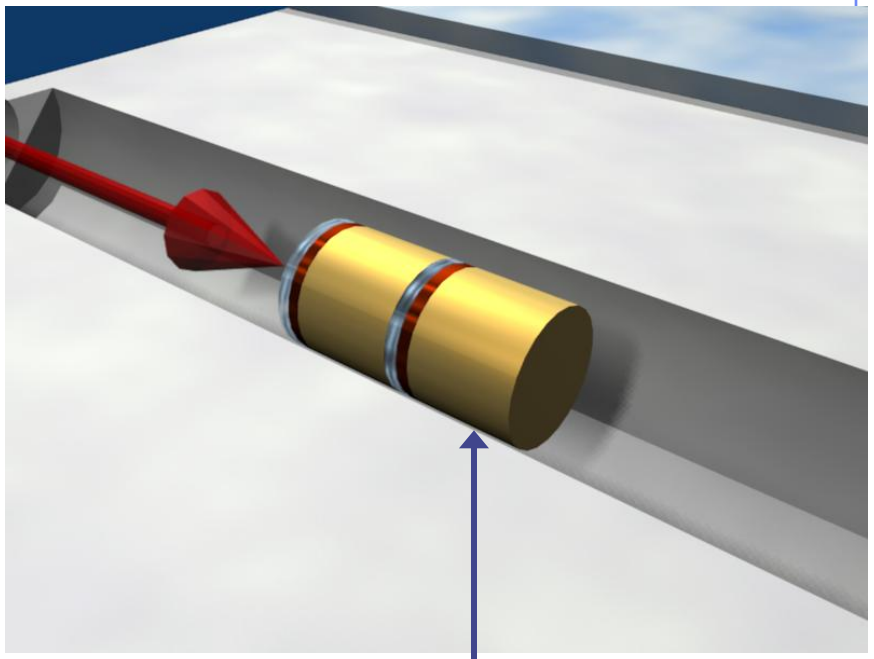


Example (II)


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

Example (III)





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 concatenated (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)

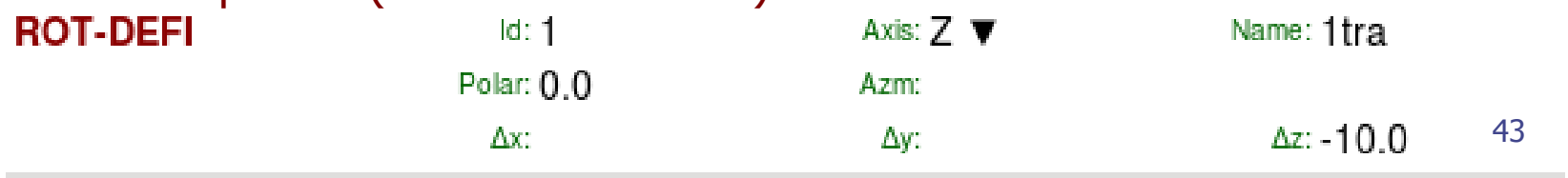
J = rotation with respect to axis (1=X, 2=Y, 3=Z)

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



The lattic routine (I)

- The actual transformation from the lattice cell (container) to the elementary cell (prototype) can also be provided through the lattic routine (if the LATTICE SDUM is left blank)

  The use of the routine is mandatory for mirroring, and turns out to be highly preferable in the case of a lot of replicas placed according to a simple arithmetical rule (e.g. segmented detectors). Otherwise, the use of the LATTICE and ROT-DEFI cards does not imply any particular limitation and offers the possibility of being combined with the $Start_transform directive for the container definition (see later) and with the use of ROTPRBIN for the roto-translation of USRBIN scoring grids.

SUBROUTINE LATTIC (XB, WB, DIST, SB, UB, IR, IRLTGG, IRLT, IFLAG)

- IRLTGG is the current lattice number (it can optionally be set in the LATTICE card), IR is the current region number
- XB,WB are vectors with the current particle position and direction
- the routine must give back SB,UB, i.e. position and direction *transported to the prototype*

The

ENTRY LATNOR (UN, IRLTNO, IRLT)

must provide the transformation for a vector representing a direction (no translation), applying to boundary normals (UN is both the in and out vector; IRLTNO is the current lattice number)

The lattic routine (II)

As an example, for the *10cm translation along z* shown in the previous slides:

```
LOGICAL LFIRST
DATA LFIRST / .TRUE. /
SAVE LFIRST, IREP
IF (LFIRST) THEN ! Find replica's lattice number
        CALL GEON2L('TargRep ', IREP, IERR)
        LFIRST = .FALSE.
END IF
IF ( IRLTGG .EQ. IREP ) THEN
        SB (1) = XB (1)
        SB (2) = XB (2)
        SB (3) = XB (3) – 10.0D0
        UB (1) = WB (1)
        UB (2) = WB (2)
        UB (3) = WB (3)
END IF
```

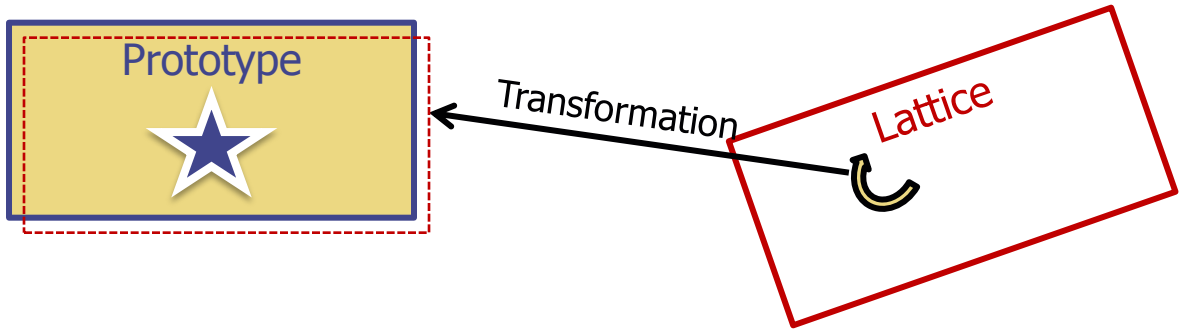
And the UN transformation is the identity

More complex cases can involve reflections and rotations.
For instance, for a reflection around the z axis :

```
UN (1) = UN (1)
UN (2) = UN (2)
UN (3) =-UN (3)
```

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

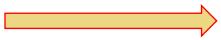


This small misalignment between lattice/transformation/prototype could lead to geometry errors

- 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	no default*	FUSRBV

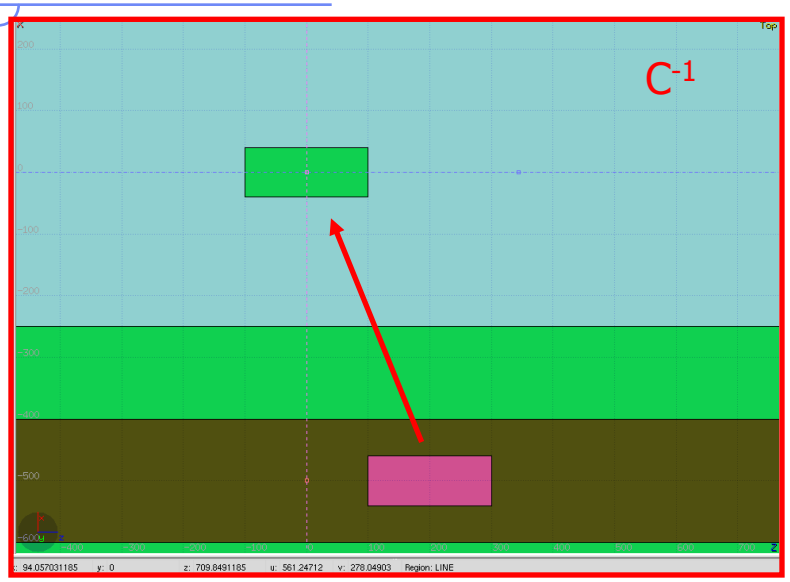
* Presently it returns 0

Tips & Tricks (I)

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

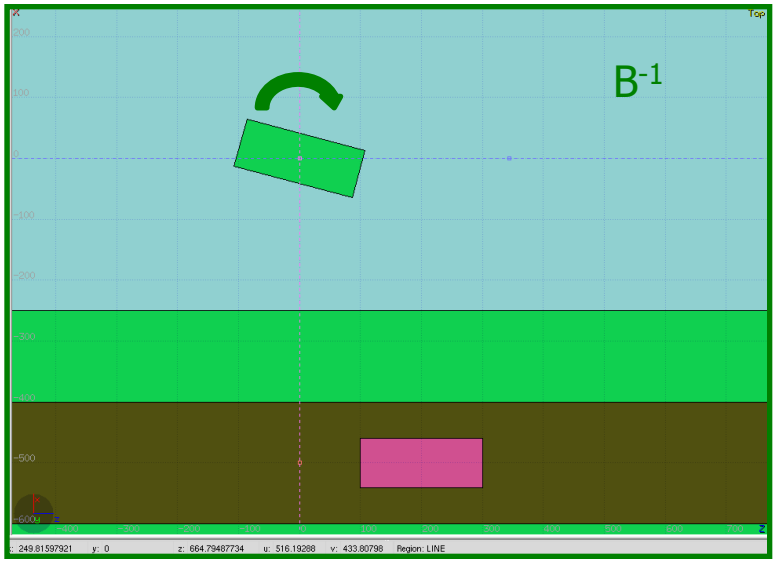
- You can always divide a transformation into many ROT-DEFI cards for easier manipulation.
- Rotations are always around the origin of the geometry, and not the center of the object.
  - To rotate an object, first translate the object to the origin of the axes
  - Perform the rotation
  - Move it by 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.

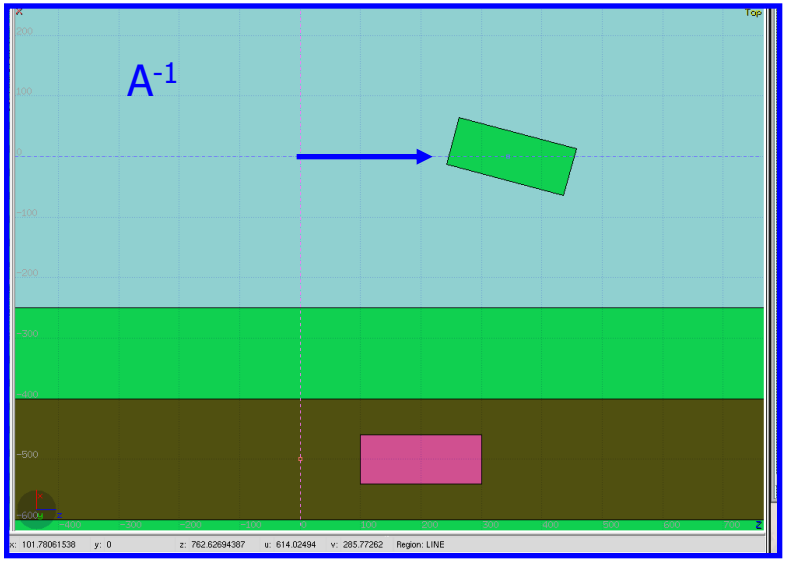
Tips & Tricks (II)




```
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 (III) using flair

- 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

Accessing ancillary core routines

- To convert the lattice/region name of interest into the respective number (and vice versa), use the following routines – giving back IERR=0 in case of success - :

```
CHARACTER*8 LATNAM
CALL GEON2L(LATNAM, NLATT, IRTLAT, IERR)      Lattice Name to Lattice #
CALL GEOL2N(NLATT, LATNAM, IRTLAT, IERR)      Lattice # to Lattice Name
```

IRTLAT is the returned index of the (possible) roto-translation associated

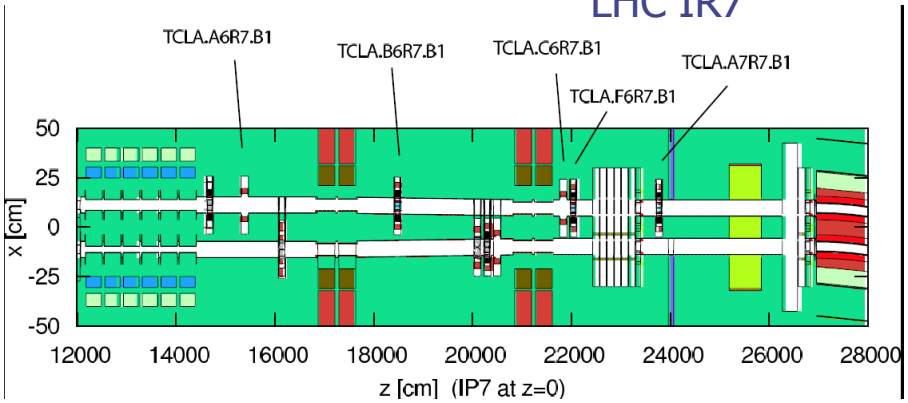
```
CHARACTER*8 REGNAM
CALL GEON2R(REGNAM, NREG, IERR)      Region Name to Region #
CALL GEOR2N(NREG, REGNAM, IERR)      Region # to Region Name
```

- It is always a good practice to call these functions only the first time the calling user routine is accessed and save the gotten info for later use

Object runtime readjustment (I)

- how to implement collimator replicas set at different apertures?

LHC IR7



- how to implement the actual rock thickness according to the muon incident direction?

[courtesy of M.Sioli, INFN]

Object runtime readjustment (II)

In the lattic (when entering a container) and source (as well as usrmed) user routines, it is possible to manipulate the body parameters

```
CHARACTER*8 BODNAM
CALL NM2BDY (BODNAM, IBODY, IERR)        Body Name to Body #
DIMENSION BDYPAR(NBDYPA)
BDYPAR(I)=...                  with I=1, NBDYPA
CALL RSTBDY (IBODY, ITYPE, BDYPAR, NBDYPA)
```

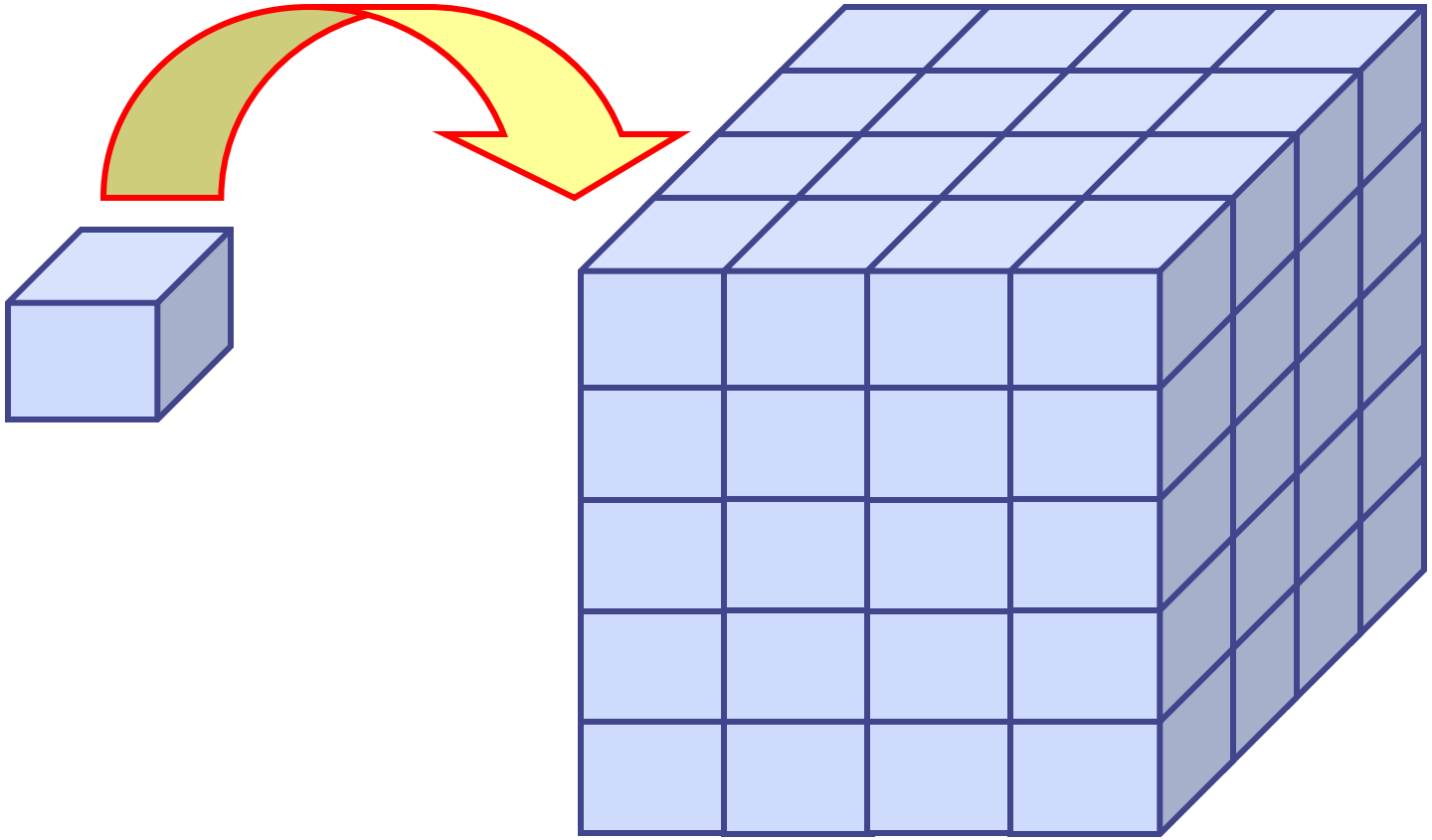
It forces recomputing distances only for IBODY

Body type	Type # [ITYPE]	# of parameters [NBDYPA]
ARB	1	30
SPH	2	4
RCC	3	7
REC	4	12
TRC	5	8
ELL	6	7
BOX	7	12
WED	8	12
RPP	9	6
ZCC	10	3

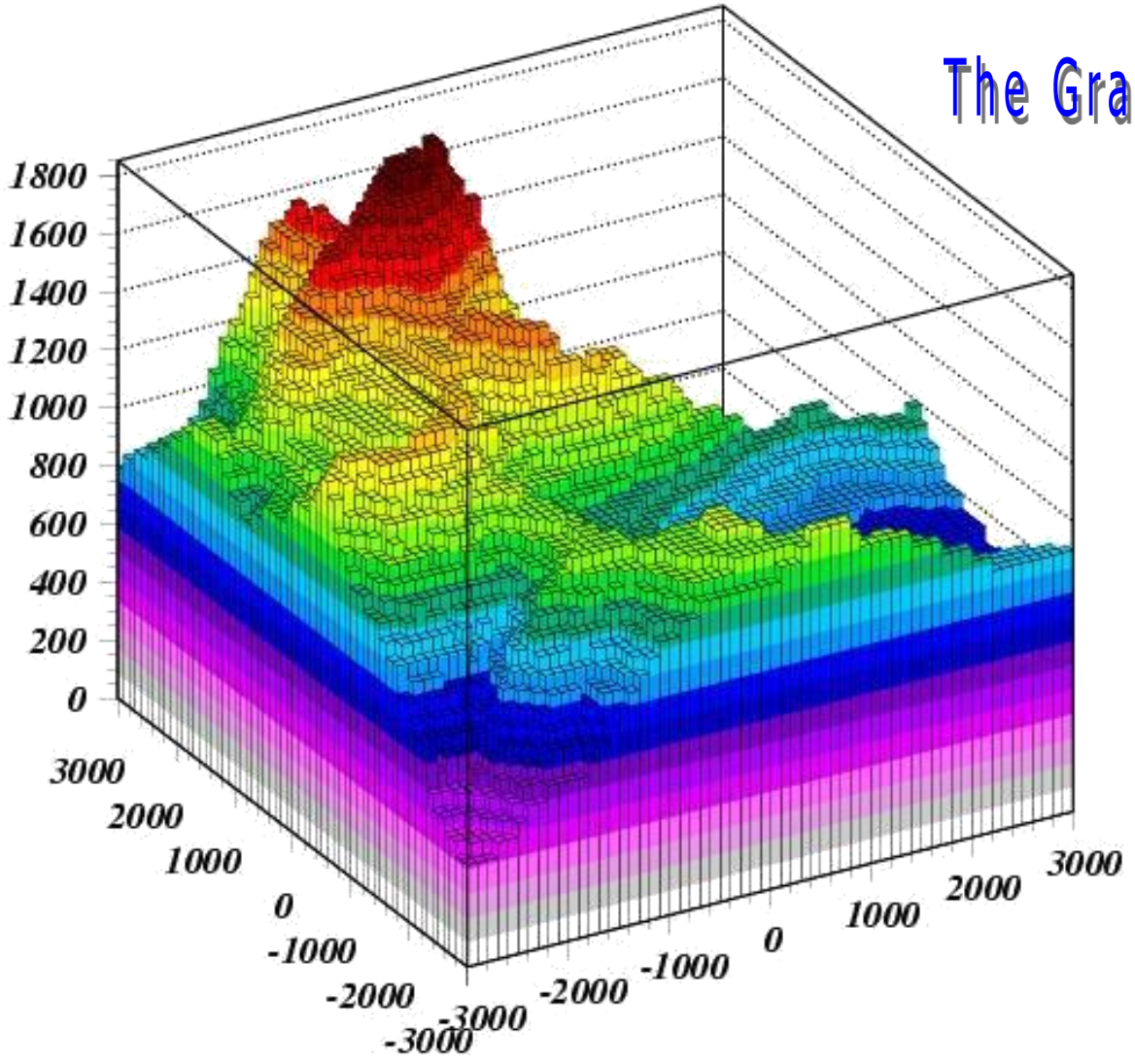
Body type	Type # [ITYPE]	# of parameters [NBDYPA]
ZEC	11	4
XYP	12	1
XZP	13	1
YZP	14	1
PLA	15	6
XCC	16	3
XEC	17	4
YCC	18	3
YEC	19	4
QUA	20	10

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

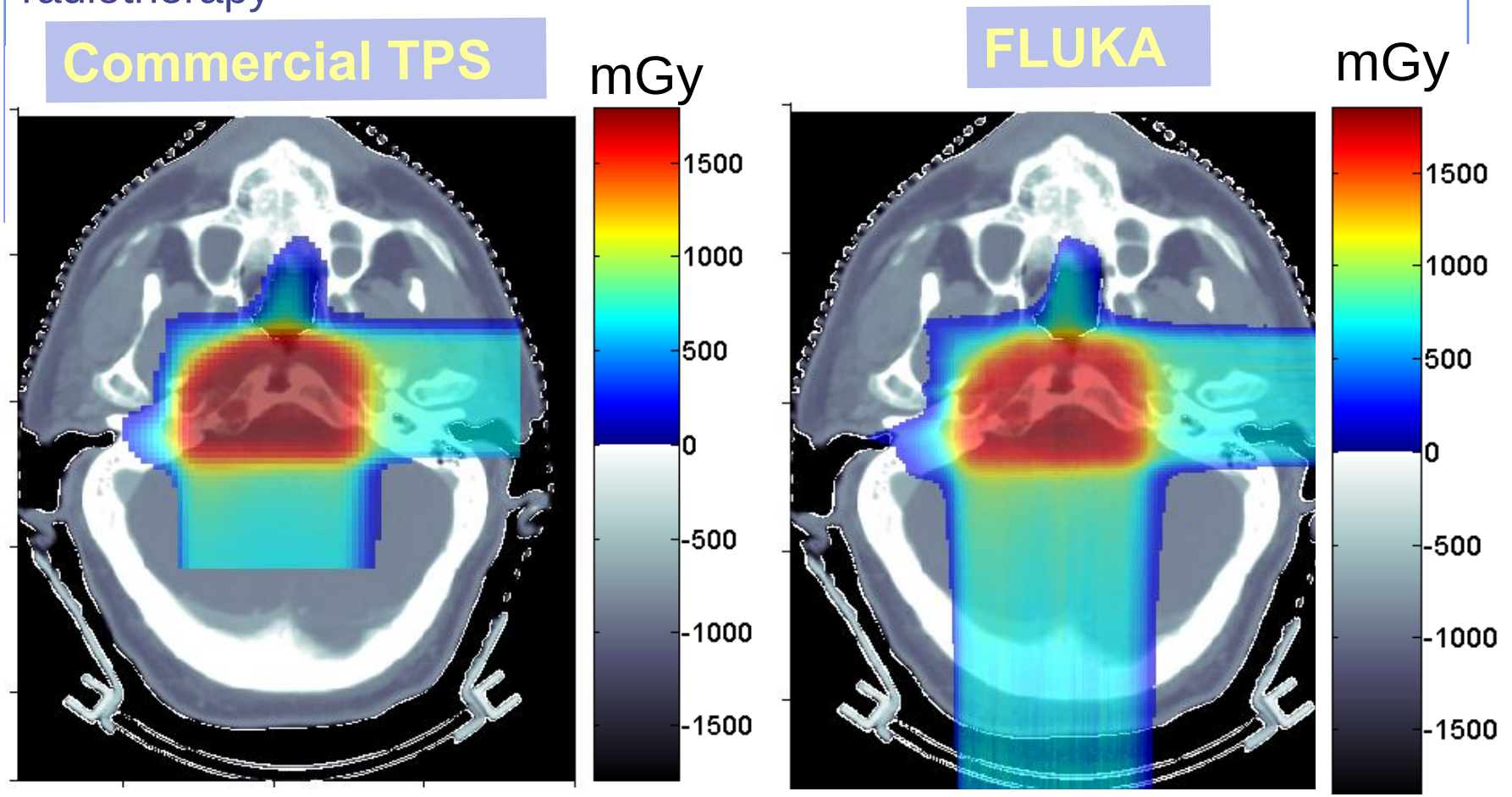


An example


The Gran Sasso in FLUKA
1800
1600
1400
1200
1000
800
600
400
200
0
3000
2000
1000
0
-1000
-2000
-3000
-3000
-2000
-1000
0
1000
2000
3000

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

- A CT scan contains integer values (Hounsfield Unit) reflecting the X-ray attenuation coefficient m_x

$$HU_x = 1000\ (m_x - m_{H20}) / m_{H20}$$

- 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 (I)

- 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 (II)

- 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

writect.f

```
      PROGRAM WRITECT
      IMPLICIT DOUBLE PRECISION ( A-H, O-Z )
*  COLUMNS: FROM LEFT TO RIGHT
*  ROWS: FROM BACK TO FRONT
*  SLICES: FROM TOP TO BOTTOM
      PARAMETER ( DX = 2.0D+00 )
      PARAMETER ( DY = 3.0D+00 )
      PARAMETER ( DZ = 4.0D+00 )
      PARAMETER ( NX = 20 )
      PARAMETER ( NY = 20 )
      PARAMETER ( NZ = 20 )
      DIMENSION CT(NX,NY,NZ)
      INTEGER*2 CT
      DIMENSION VXL(NX,NY,NZ)
      INTEGER*2 VXL
      CHARACTER TITLE*80
      DIMENSION IREG(1000), KREG(1000)
      INTEGER*2 IREG, KREG
*
      CALL CMSPPR
      DO IC = 1, 1000
         KREG(IC) = 0
      END DO
      OPEN(UNIT=30,FILE='ascii_ct',STATUS='OLD')
      READ(30,*) CT
*
*
      NO=0
      MO=0
```

Number and Dimensions of voxels

read the original CT scan

In this example, the organ number is simply set equal to the CT number for each voxel

For each voxel

```
      DO IZ=1,NZ
         DO IY=1,NY
            DO IX=1,NX
               IF (CT(IX,IY,IZ) .GT. 0) THEN
                 IO= CT(IX,IY,IZ)
                 VXL(IX,IY,IZ) = IO
                 MO = MAX (MO,IO)
                 DO IR=1,NO
                    IF (IREG(IR) .EQ. IO) GO TO 1000
                 END DO
                 NO=NO+1
                 IREG(NO)=IO
                 KREG(IO)=NO
                 WRITE(*,'(A,2I10)')' New number, old number: ', NO, IO
1000             CONTINUE
               END IF
            END DO
         END DO
      END DO
*     NO = number of different organs
*     MO = max. organ number before compacting
*
      WRITE(*,*) ' NO,MO',NO,MO
      OPEN(UNIT=31,FILE='ct.vxl',STATUS='UNKNOWN',FORM='UNFORMATTED')
      TITLE = 'Egg-like CT scan'
      WRITE(31) TITLE
      WRITE(31) NX,NY,NZ,NO,MO
      WRITE(31) DX,DY,DZ
      WRITE(31) VXL
      WRITE(31) (KREG(IC),IC=1,MO)
      STOP
      END
```

Assign organ IO to this voxel

If new organ: assign new region NO to organ IO

Write the file for FLUKA

Input file: geometry description (I)

- Prepare the usual FLUKA input file. The geometry must be written like for a normal Combinatorial Geometry input (in any of the allowed formats, as part of the normal input stream or in a separate *.geo file), but in addition must include:
  - VOXELS card as the first line, before the Geometry title card, with the following information:

    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), 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                        ct
```

Input file: geometry description (II)

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