

# FLUKA Combinatorial Geometry

21st FLUKA Beginners' Course ALBA Synchrotron (Spain) April 8-12, 2019

#### Introduction

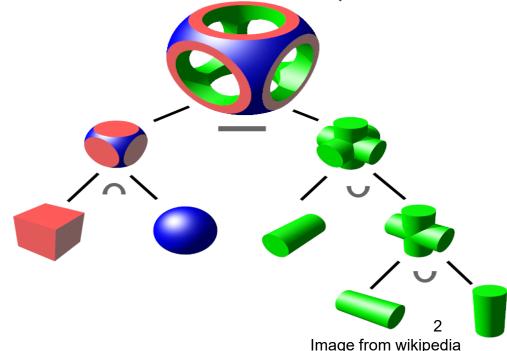
#### Principle of Combinatorial Geometry

Basic objects called bodies (such as cylinders, spheres, parallelepipeds, etc.) are combined to form more complex

objects called regions

This combination is done using Boolean operations:

Math	Operation	FLUKA
U	Union	I
$\cap$	Intersection	+
_	Subtraction	-



#### Introduction

Initially, FLUKA Combinatorial Geometry was similar to the package developed at ORNL for the neutron and gamma-ray transport program Morse (M.B. Emmett ORNL-4972 1975.

In the original CG (Morse) bodies were convex solid bodies (i.e. finite portions of space completely delimited by surfaces of first or second degree, i.e. planes or quadrics)

The present FLUKA CG package has been highly improved:

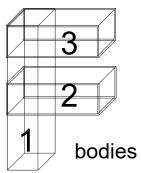
- addition of "infinite bodies"
- possibility of using body and region names instead of numbers and getting rid of alignment rules,
- availability of parentheses
- expansion and roto-translation of bodies
- comments
- repetition of patterns (lattices)
- □ voxels

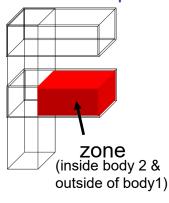
#### **Basic Concepts**

Four concepts are fundamental in the FLUKA CG:

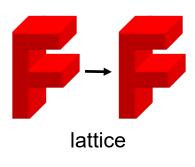
1

- Bodies: basic convex objects, plus infinite planes (half-spaces), infinite cylinders (circular and elliptical), and generic quadric surfaces (surfaces described by 2<sup>nd</sup> degree equations)
- Zones: sub-regions defined only via bodies intersection and subtraction
- Regions: defined as Boolean operations on bodies (union of zones)
- Lattices: duplication of existing objects (translated & rotated),
   will be explained in a separate lecture











Use of "infinite bodies" is encouraged: input are less error-prone and tracking is faster and more accurate.

#### Combinatorial Geometry Input

CG input must respect the following structure:

```
GFOBFGIN card
   VOXELS card (optional, see advanced geometry lecture)
   Geometry title (and reading format options)
       Body data
   END card
       Region data
   FND card
   LATTICE cards (optional, see advanced geometry lecture)
   Region volumes (optionally requested by a flag in the Geometry title,
                         used together with the SCORE command)
GFOFND card
```

Reminder for txt format input files: an asterisk (\*) in the 1<sup>st</sup> column comments the line

#### **GEOBEGIN** card

| Combon |

WHAT(1) not used

WHAT(2) set accuracy parameter - use with extreme care!

WHAT(3) logical unit for the geometry input.

Geometry input can be read from file; should be >20.0

WHAT(4) logical unit for the geometry output

Log feature; should be >20.0; Default is standard output

WHAT(5) Parenthesis optimization level (see FLUKA manual)

WHAT(6) not used

SDUM COMBNAME or COMBINAT

COMBNAME selects name based format, COMBINAT fixed format

Default: COMBINAT (!)

Is overwritten by WHAT(5) of a possible GLOBAL card

## Geometry input format

- The input file format for the geometry is different from the one adopted anywhere else in FLUKA (i.e. the number and length of the input fields is different)
- Different formats can be used (due to backward compatibility)
  - Fixed format
    - Alignment is mandatory
    - Bodies and regions are identified by numbers (rather than names), this makes geometry editing more difficult
  - Name based format
    - It is the recommended format
    - It is NOT the default!

#### Name based format

It has many advantages, the main are:

- input parameter alignment is not necessary
- bodies and regions are identified by names
- possible to edit the input sequence without affecting the region description (e.g. inserting a new body)
- parentheses can be used to perform complex Boolean operations in the description of regions.

Name based format input is used for both body and region

It is activated

either by a GLOBAL command at the beginning of the input file or putting SDUM = COMBNAME in the GEOBEGIN card



# Bodies

#### **Bodies**

- Each body divides the space into two domains: inside and outside.
- 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, delimited by a PLAne

■ 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**ipsoid of revolution

■ QUA: QUAdric

Other (deprecated) bodies: ARB, RAW, WED, BOX
 Do not use them, because they can cause rounding problems

#### **Bodies**

- The input for each body consists of:
  - the 3-letter code indicating the body type (RPP, ZCC...)
  - a unique "body name" (alphanumeric identifier, 8 character maximum, case sensitive)
  - a set of geometrical quantities defining the body (the number depends on the body type, see next slides)
- Different items can extend over as many lines as needed (Maximum 132 characters per line accepted)
- Different items have to be separated by one or more blanks, or by one of the separators , /;:
- Each body divides the space in two. Inside and Outside
   The normal vector points towards Outside

#### Infinite half-space parallel to coordinate axis

There are 4 kinds of infinite half-spaces

Three are delimited by planes perpendicular to the coordinate axes:

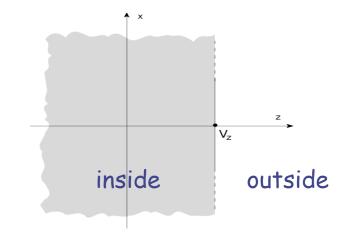
- 1. Delimited by a plane  $\perp$  to the x-axis. Code: YZP
- 2. Delimited by a plane  $\perp$  to the y-axis. Code: XZP
- 3. Delimited by a plane  $\perp$  to the z-axis. Code: XYP

All defined by a single number:

```
Vx (resp. Vy, or Vz),
coordinate of the plane on the
corresponding perpendicular axis
```

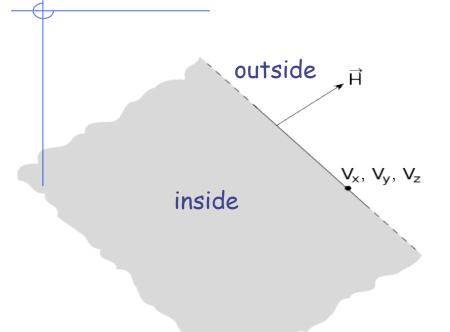
Points for which:

$$x < Vx$$
 (resp.  $y < Vy$ , or  $z < Vz$ ) are "inside the body"





#### Arbitrarily orientated infinite half-space: **PLA**



A PLA defines the infinite half space delimited by a generic plane

A PLA is defined by 6 numbers:

Hx, Hy, Hz (vector  $\bot$  to the plane, arbitrary length);

Vx, Vy, Vz (any point lying on the plane)

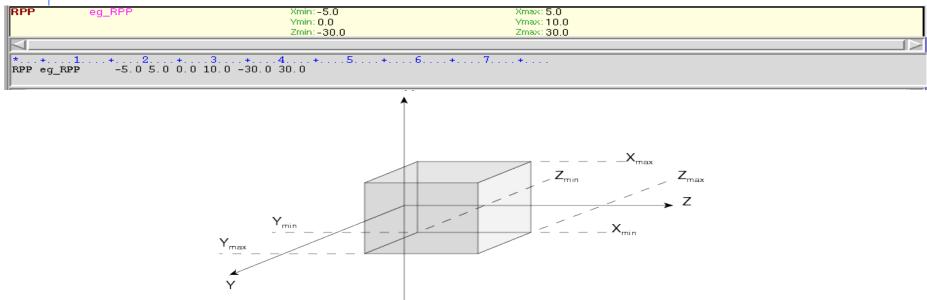
The half-space "inside the body" is that from which the vector is pointing (i.e. the vector points "outside").

PLA	eg_PLA	Nx: 0.0	Ny: 1.0	Nz: 1.0	
		×:1.	y: 2.	z: 3.	
abla					
*+	1 + 2 +		+ 7 +		
PLA eg_1	PLA 0.0 1.0 1.0 1.	2. 3.			
J					10
					13

#### Rectangular Parallelepiped: RPP

An RPP has its edges parallel to the coordinate axes It is defined by 6 numbers in the following order:

 $X_{min}$ ,  $X_{max}$ ,  $Y_{min}$ ,  $Y_{max}$ ,  $Z_{min}$ ,  $Z_{max}$ 



## Rectangular Parallelepiped: RPP

```
RPP
                                              Xmin: -5.0
                                                                                   Xmax: 5,0
            eg_RPP
                                              Ymin: 0.0
                                                                                   Ymax: 10.0
                                              Zmin: -30.0
                                                                                   Zmax: 30.0
    +....1....+....2....+....3....+....4....+....5....+....6....+....7....+....
                 -5.0 5.0 0.0 10.0 -30.0 30.0
```

An RPP definition extends over one single card in default fixed format, or over two cards in high-accuracy body fixed format Example in fixed format (the comment lines shown are allowed input lines):

```
+20.0
              -20.0
                                   -50.0
                                              +50.0
                                                         -38.5
                                                                    +38.5
RPP
```

\* (a parallelepiped centered on the origin)

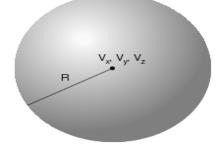
#### High-accuracy fixed format

#### Sphere

Sphere: SPH

A SPH is defined by 4 numbers:

Vx, Vy, Vz (coordinates of the centre), R (radius)



SPH	eg_SPH	×: 0.0 B: 10.0	y: 0.0	z: 0.0		
*+	*+1+2+3+4+5+6+7+					
SPH eg_SI	SPH eg_SPH 0.0 0.0 0.0 10.0					

#### Circular cylinder

#### Right circular cylinder: RCC

An RCC can have any orientation in space

Limited by a cylindrical surface and two plane faces  $\perp$  to its axis.

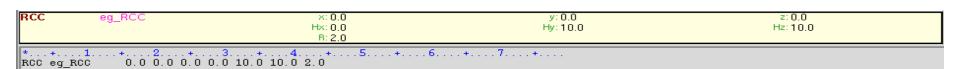
Each RCC is defined by 7 numbers:

Vx, Vy, Vz (centre of one face);

Hx, Hy, Hz (vector corresponding to the cylinder height, pointing

toward the other face);

R (cylinder radius).



 $V_x, V_v, V_z$ 

## Infinite cylinders

Infinite Circular Cylinder parallel to coordinate axis:

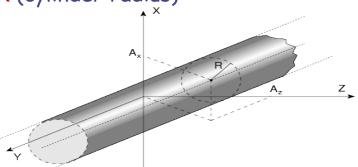
XCC, YCC, ZCC

Each XCC (YCC, ZCC) is defined by 3 numbers:

Ay, Az for XCC

(Az, Ax for YCC, Ax, Ay for ZCC) (coordinates of the cylinder axis),

R (cylinder radius)



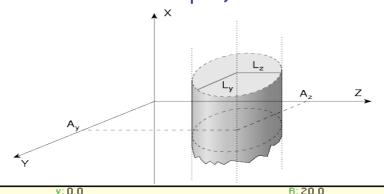
• Infinite Elliptical Cylinder parallel to coordinate axis:

XEC, YEC, ZEC

Each XEC (YEC, ZEC) is defined by 4 numbers: Ay, Az for XEC

(Az, Ax for YEC, Ax, Ay for ZEC) (coordinates of the cylinder axis); Ly, Lz for XEC

(Lz, Lx for YEC, Lx, Ly for ZEC) (semi-axes of the ellipse)



#### Arbitrary generic quadric: QUA

A QUA allows to insert a quadric surface This is defined by a  $2^{nd}$  degree equation F(x,y,z) = 0

Each QUA is defined by 10 numbers:

 $A_{xx}$ ,  $A_{yy}$ ,  $A_{zz}$ ,  $A_{xy}$ ,  $A_{xz}$ ,  $A_{yz}$ ,  $A_{x}$ ,  $A_{y}$ ,  $A_{z}$ ,  $A_{0}$  corresponding to the equation:

$$A_{xx} x^2 + A_{yy} y^2 + A_{zz} z^2 + A_{xy} xy + A_{xz} xz + A_{yz} yz + A_{xz} x + A_{yz} yz + A_{zz} x + A_{yz} yz + A_{zz} x + A_{yz} yz + A_{zz} x + A_{zz} x$$

A QUA definition extends over two cards in default fixed format, and over 4 cards in high-accuracy body fixed format.

# Regions

### Concept

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

	Union	Subtraction	Intersection
Name based format		_	+
Fixed format	OR	_	+
Mathematically	U	_	$\cap$

Regions but must be of homogeneous material composition.



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

#### Regions

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

or

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

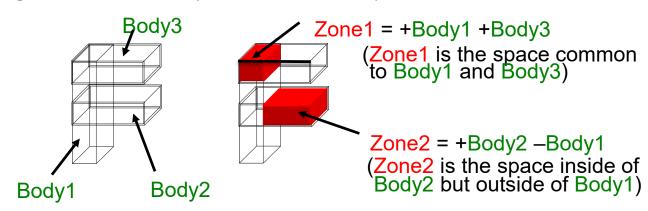
- REGNAME is the region "name"
   alphanumeric identifier, 8 character maximum, case sensitive
   Must start by an alphabetical character
- NAZ See next slide
- "boolean-zone-expression" See next slides

#### Regions

- NAZ (Number of Adjacent Zones) is a rough estimate of the number of zones a particle can enter when leaving the current region zones (5 by default). What actually matters is the NAZ sum over all regions, defining the size of the *contiguity list*
- While tracking, the program searches in the contiguity list for the neighbor zones of each zone. If the zone is not yet in the list, the whole geometry is scanned and it is added to the list with its neighbor zones
- When the NAZ limit is reached (i.e. the list is full) the code prints a warning: GEOMETRY SEARCH ARRAY FULL. This is not lethal: the calculation continues but with a reduced efficiency
- If you have more than 1000 regions, you must issue a GLOBAL card putting in WHAT(1) a higher limit (not beyond 10000)

# Boolean zone expressions (+/- operators)

- Zones are defined by intersections and/or subtraction of bodies
  - Zones are a described by a sequence of one or more bodies each being preceded by its + or - sign
  - +body: only the inner part of the body can belong to the zone (means that the zone being described is fully contained inside this body)
  - -body: only the outside of the body can belong to the zone (means that the zone being described is fully outside this body)





Zones must be finite: normally in the description of each zone

## Combining zones (| operator)

- The I (or OR) operator is used as a Boolean union operator in order to combine zones
- Such combination of zones forms a region
  - In its simplest form a region just consist of one zone
  - Regions are not necessarily simply connected, i.e. they can consist of zones which are not
    contiguous
  - On the other hand, zones belonging to the same region can be partially overlapping

#### Example:

In name based format one can also use parenthesis to form more complex Boolean operations

In evaluating the expressions, the highest operator precedence is given to parentheses, followed by +, - and the | operator

## Special Region: The Black Hole

All particles entering a black-hole are absorbed (they vanish)

FLUKA geometry MUST be embedded into a BLCKHOLE region (to avoid tracking particles to infinity)

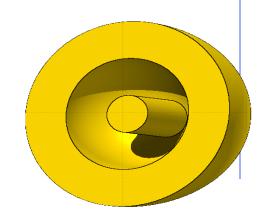
The outer surface of the BLCKHOLE region must be a single closed body (e.g. a sphere).

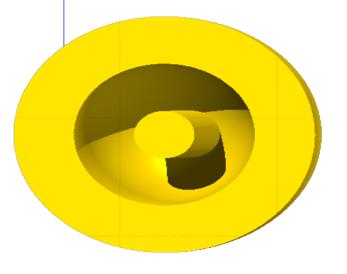
Further black-hole regions can be defined by the user if desired **BLCKHOLE region:** has material **BLCKHOLE assign to it** 

# Example

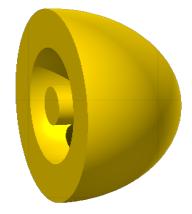
## Geometry Example

Target made of Gold

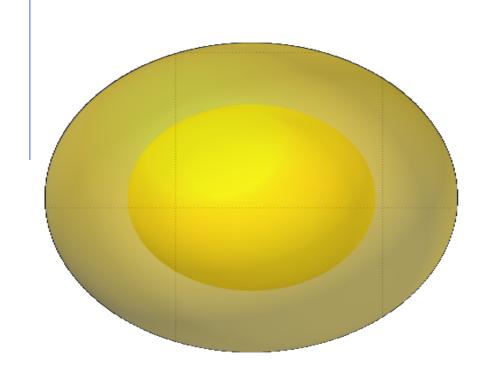


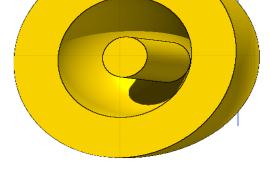


## How do we build it?



Geometry example: Target Bodies



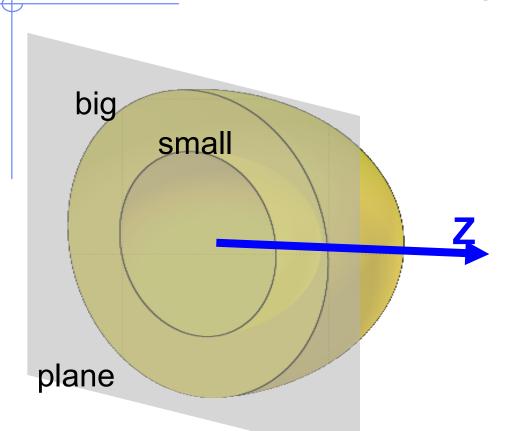


2 spheres: big, small

IN big

**OUT** small

Geometry example: Target Bodies



U:V

2 spheres: big, small IN big OUT small

1 infinite plane ⊥ Z OUT plane

VOID

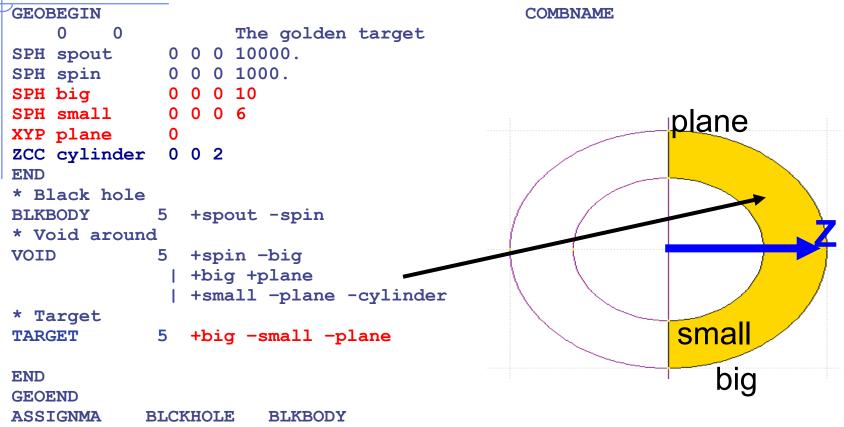
TARGET

ASSIGNMA

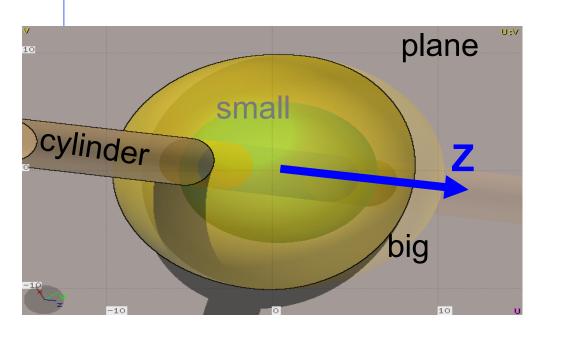
**ASSIGNMA** 

**VACUUM** 

GOLD



Geometry example: Target Bodies



2 spheres: big, small IN big OUT small

1 infinite plane ⊥ Z OUT plane

1 infinite cylinder // Z IN cylinder

VOID

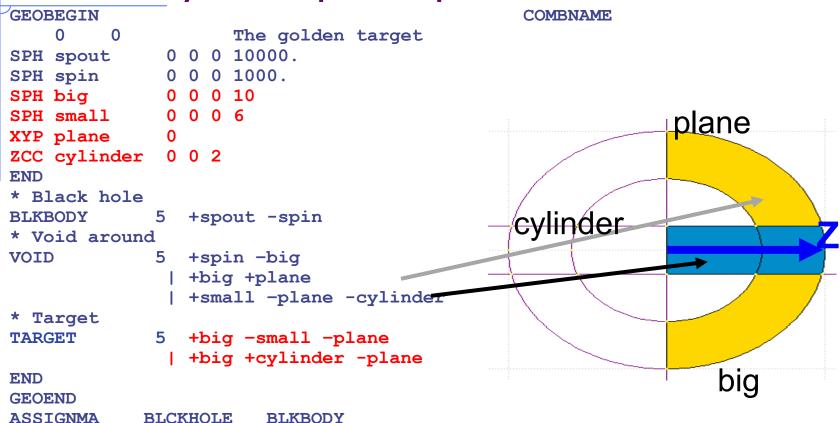
TARGET

ASSIGNMA

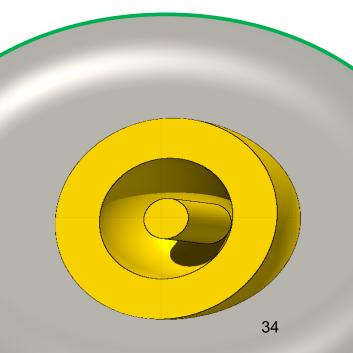
**ASSIGNMA** 

**VACUUM** 

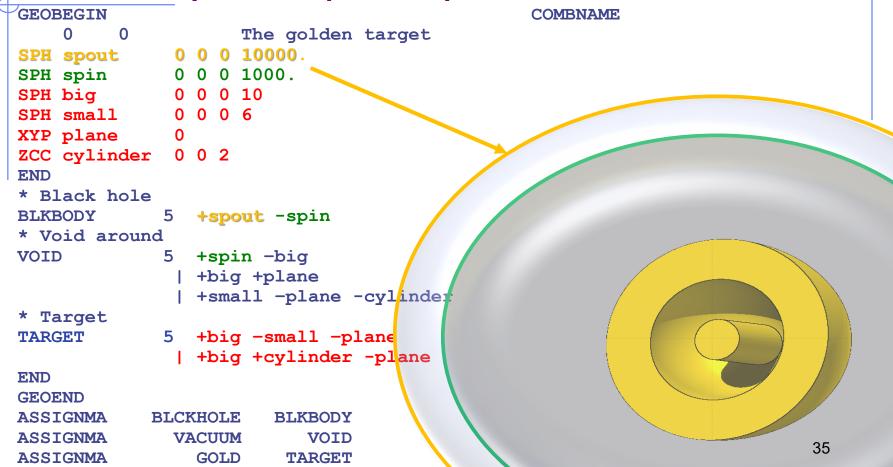
GOLD



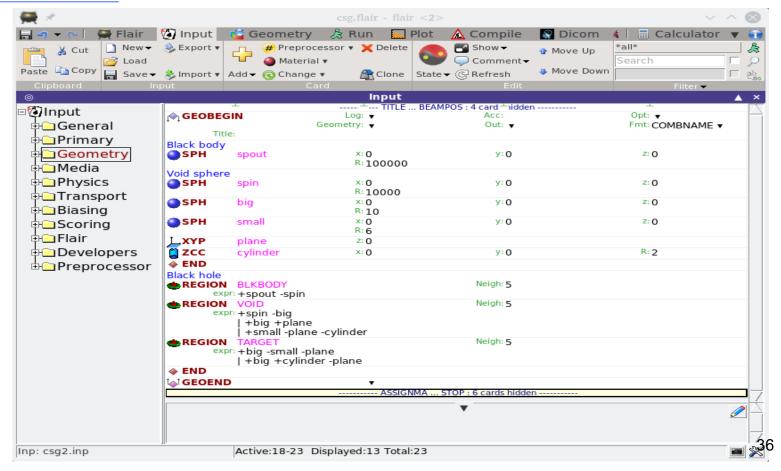
```
GEOBEGIN
                   The golden target
SPH spout 0 0 0 10000.
SPH spin
             0 0 0 1000.
SPH big
             0 0 0 10
SPH small
             0 0 0 6
XYP plane
ZCC cylinder
             0 0 2
END
* Black hole
BLKBODY 5 +spout -spin
* Void around
VOID
            5 +spin -big
               +big +plane
               +small -plane -cylinder
* Target
TARGET
            5 +big -small -plane
             | +big +cylinder -plane
END
GEOEND
ASSIGNMA
           BLCKHOLE
                      BLKBODY
ASSIGNMA
             VACUUM
                         VOID
ASSIGNMA
               GOLD
                       TARGET
```



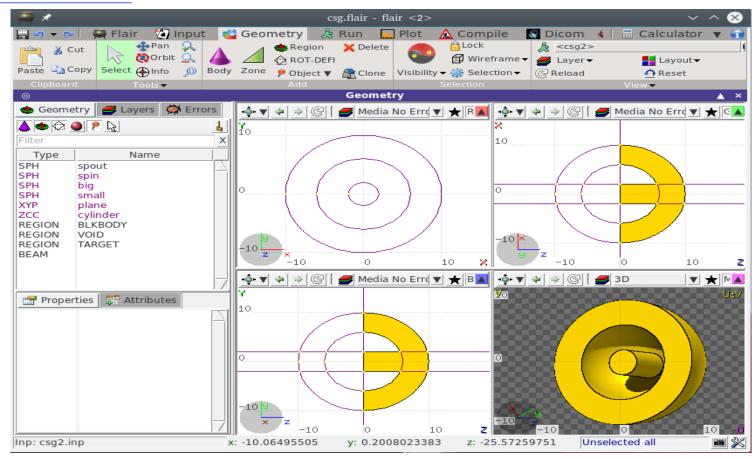
**COMBNAME** 



# Geometry example: input Flair



### Geometry example: input Flair



# Remarks

### **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 bodies make the 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, TRC), and for direction cosines of bodies with slant surfaces. The name based format or the high-accuracy fixed format should always be used in these cases.

### **Precision Errors**

Modeling assumptions

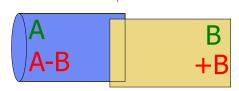
RCC RCC B

#### Avoid touching surfaces!

When floating point operations are involved

Use cutting surface B instead

Or force partial overlap of bodies



PLA

### Tracking accuracy

- □ FLUKA uses systematically double precision mathematic (i.e. 16 significant digits)
- □ GEOBEGIN's WHAT(2)\*10<sup>-6</sup>cm is the *absolute accuracy (AA)* requested for tracking and boundary identification
- □ The *relative accuracy (RA)* achievable in double precision is of the order of 10<sup>-14</sup>-10<sup>-15</sup>.
- □ AA should be larger than RA\*L, being L the largest coordinate value in the considered problem, i.e. the whole geometry size (The outer blackhole shell containing the system does not count)
- □ For very large and very small geometries, you may, respectively, need to increase or decrease the WHAT(2).

## **Geometry Errors and Debugging**

### **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 position does not belong to any region
   An error message will be printed in the .err file with the particle position
- IMPORTANT! It will not stop if a particle position belongs to more than one region. It will accept the first region it finds but the results will completely unreliable!!

### **Geometry Errors**

#### Further types of errors

- Problem space not enclosed by a black body region
- Never start a primary particle along a surface. You could get a geometry error even if the geometry is correct because FLUKA cannot determine the region
- Precision errors
- Lattice replica ←→ basic cell mismatch (see advanced geometry lecture)

#### Debugging Tools

- GEOEND card with the DEBUG option
- Error messages during simulation in the .err file
- Geometry plotting by Flair

   (automatically invoking the PLOTGEOM card)
- FLAIR geoviewer
- Simplegeo

### Debugging with FLUKA

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

```
\begin{array}{lll} \text{WHAT}(1) = X_{\text{max}} & \text{WHAT}(2) = Y_{\text{max}} & \text{WHAT}(3) = Z_{\text{max}} \\ \text{WHAT}(4) = X_{\text{min}} & \text{WHAT}(5) = Y_{\text{min}} & \text{WHAT}(6) = Z_{\text{min}} \\ \text{SDUM} = \text{DEBUG} & \end{array}
```

Second Card

WHAT(1)=Nx WHAT(2)=Ny WHAT(3)=Nz 
$$SDUM = 8$$

GEOEND GEOEND		Zmax Nz	Xmin	Ymin	Zmin	DEBUG &	
to GEOEND	DEBUG ▼ Xmin: Ymin: Zmin:		Yn	nax: nax: nax:		NX: NY: NZ:	

WARNING! The program stops if too many errors are found A message will be issued on the output unit

### Debugging with FLUKA

- If no error is found, no .err file will be created
- REMINDER: If the debugger does not find any error it does not mean that the geometry is error free!
- One has to test, changing the GEOEND settings especially for critical and complicated regions
- 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

# Spare Slides

### Geometry TITLE card

This card has no keyword, it is the line that follows the GEOBEGIN card (unless voxels are used) and its format is (215, 10X, A60)

The card gets three inputs: IVLFLG, IDBG, TITLE

IVLFLG (Input Volumes FLAG) triggers the normalization of the quantities scored in regions by the option SCORE

IVLFLG=  $0 \rightarrow$  no normalization applied

IVLFLG= 3 → results divided by region volumes given before GEOEND. Volume value for each region must be provided, format: (7E10.5).

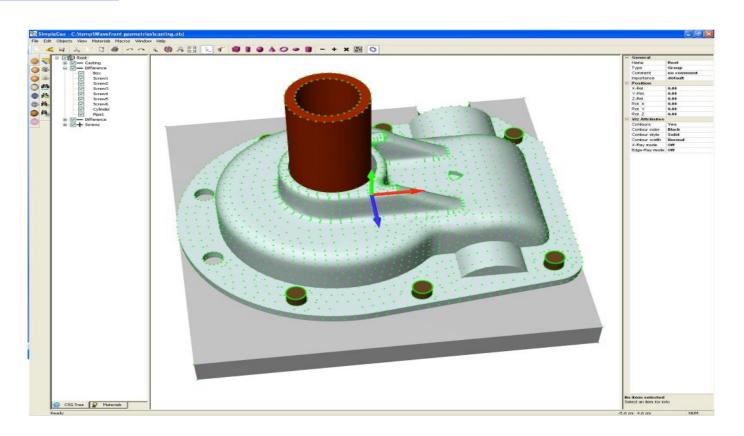
IDBG select different kinds of geometry fixed format input:

IDBG = 0 : default fixed format

IDBG = -10 or -100: high accuracy fixed format



### Auxiliary program: SimpleGeo



## Auxiliary program: SimpleGeo

- SimpleGeo is an interactive solid modeler which allows for flexible and easy creation of the models via drag & drop, as well as on-the-fly inspection
- Imports existing geometries for viewing
- Creating new geometries from scratch
- Export to various formats (FLUKA, MCNP, MCNPX)
- Download, Tutorials, etc.:
   http://theis.web.cern.ch/theis/s