

FLUKA Combinatorial Geometry

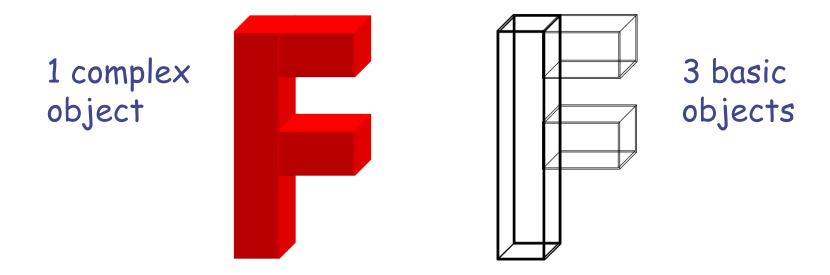
FLUKA Beginner's Course

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: union, intersection, and 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).

It was based on the original combinatorial geometry by MAGI (Mathematical Applications Group, Inc., W. Guber et al, MAGI-6701 1967).

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

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!

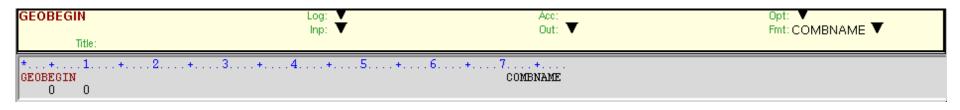
Name based format

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



Basic Concepts

Four concepts are fundamental in the FLUKA CG:

- Bodies: basic convex objects, plus infinite planes, infinite cylinders, and generic quadric surfaces
- 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

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)

FLUKA has been extended to include: infinite cylinders (circular and elliptical), planes (half-spaces), and generic quadrics (surfaces described by 2nd degree equations)

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

Basic Concepts: 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

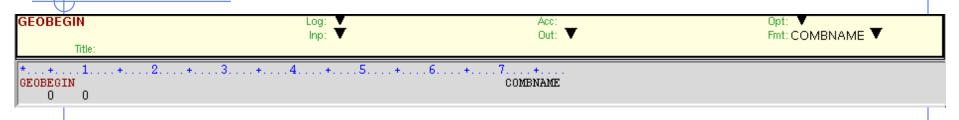
Combinatorial Geometry Input

CG input must respect the following structure:

```
VOXELS card (optional, see advanced geometry lecture)
Geometry title (and reading format options)
Body data
END card
Region data
END 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)
GEOEND card
```

Reminder for txt format input files: an asterisk (*) in the 1st column comments the line

GEOBEGIN card



- 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 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



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: ELLipsoid 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 , / ;:

All values are in cm!

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:

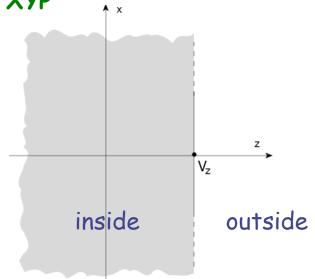
- 1. Delimited by a plane \perp to the x-axis. Code: YZP
- 2. Delimited by a plane \bot to the y-axis. Code: XZP
- 3. Delimited by a plane \perp to the z-axis. Code: XYP

All defined by a single number:

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

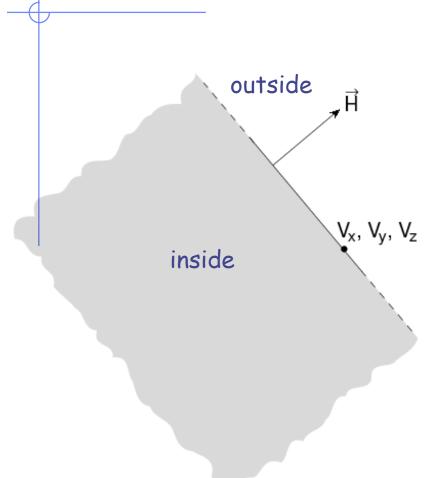
Points for which:

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



ı	XYP		_eg_XYF	'			Z: 10.0				
		+1. eg_XYP		. 2 +. 0	3	+4	+	5 +	6 4	7	+

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)

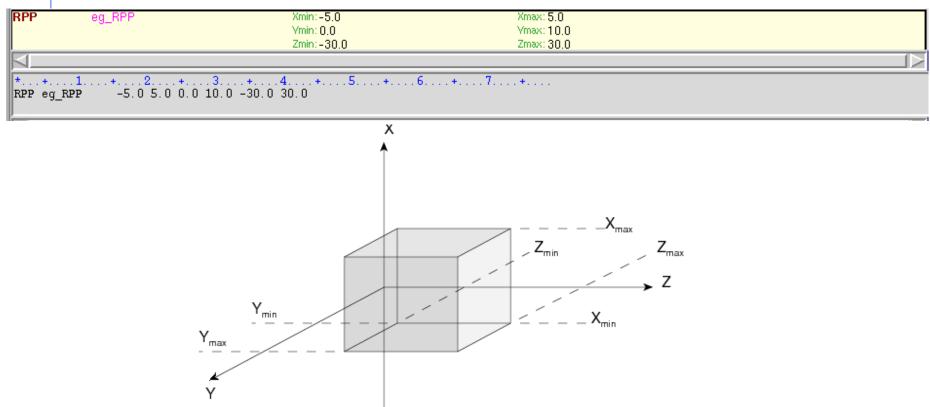
The half-space "inside the body" is that from which the vector is pointing (i.e. the vector points "outside").

PLA	eg_PLA[Nx: 0.0 x: 1	Ny: 1.0 v: 2	Nz: 1.0 z: 3
abla			· -	
*+. PLA eg	1+2+ PLA 0.0 1.0 1.0 1	. 3 + 4 + 5 + 6 . 2. 3.	+ 7 +	

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} (min and max coordinates delimiting the parallelepiped)



Rectangular Parallelepiped: RPP

```
Xmin: -5.0
                                                                                   Xmax: 5.0
RPP
            eg_RPP
                                              Ymin: 0.0
                                                                                   Vmax: 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):

```
*...+....5...+....6....+....7....+.
         -20.0
              +20.0
                     -50.0
 RPP
                            +50.0
                                  -38.5
```

* (a parallelepiped centered on the origin)

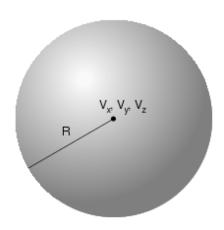
High-accuracy fixed format

Sphere

Sphere: SPH

A SPH is defined by 4 numbers:

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



SPH	eg_SPH	x: 0.0 R: 10.0	y: 0,0	z: 0.0		
*+	*+1+2+3+4+5+6+7+					
SPH eg_S	SPH eg_SPH 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.

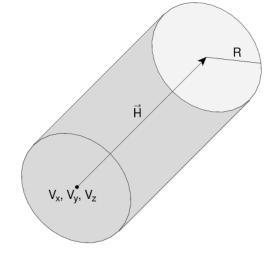
Each RCC is defined by 7 numbers:

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

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

toward the other face);

R (cylinder radius).



RCC	eg_RCC	×: 0.0	y: 0.0	z: 0,0	
	3=	Hx: 0.0	Hy: 10.0	Hz: 10.0	
		R: 2.0			

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),

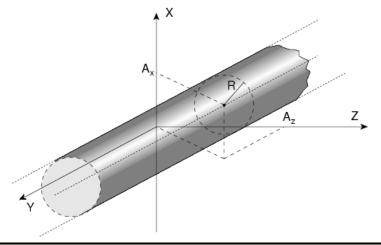
R (cylinder radius)

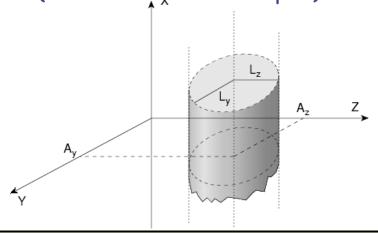
Infinite Elliptical Cylinder parallel to coordinate axis: XEC, YEC, ZEC

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)





ZCC eg_ZCC x: 0.0 y: 0.0 y: 0.0 R: 20.0

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:

$$A_{xx} x^2 + A_{yy} y^2 + A_{zz} z^2 + A_{xy} xy + A_{xz} xz + A_{yz} yz + A_{xx} x + A_{yy} y + A_{zx} x + A_{0} = 0$$

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	I	_	+
Fixed format	OR	_	+
Mathematically	U	_	\cap

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

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

Regions

or

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

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)

Regions Boolean expression

- zones are defined by intersections and/or subtraction of bodies, each body being preceded by its + or - sign
- (OR) operators are used to join zones
- In evaluating the expressions, the highest operator precedence is given to parentheses, followed by +, - and the | operator
- Parentheses are available in name based format (use with care!)
- If one line is not sufficient, any number of continuation lines can be added
- Blanks are ignored

Meaning of + and - operators

If a body number (or name) appears in a zone description preceded by a + operator, it means that the zone being described is wholly contained inside the body.

If a body number appears in a zone description preceded by a - operator, it means that the zone being described is wholly outside the body.

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

Meaning of the + and – operators

Target 5 +Outer +CutPlane

- * (the above region is the part of space common to bodies Outer and
- * CutPlane)

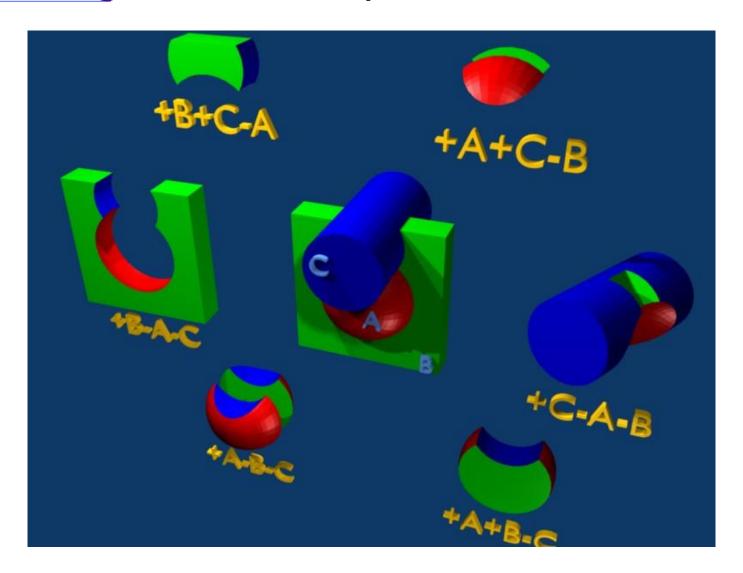
Regex 5 +Red -Blue -Green +Yellow

- * (the above region is the part of space common to body Red and Yellow,
- * excluding however what is inside body Blue and what is inside Green)

Air 5 +Room

* (the latter region coincides entirely with body Room)

Meaning of + and - operators



Meaning of the | (OR) operator

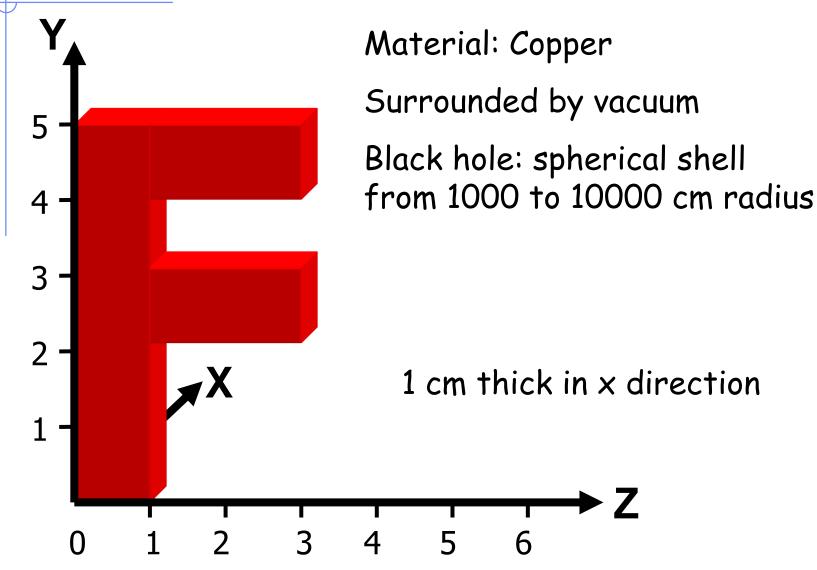
The I (or OR) operator is used as a Boolean union operator in order to combine zones (sub regions partially overlapping or not).

Zones are formed as body intersections or subtractions as previously explained

The regions are formed by the union of these zones.

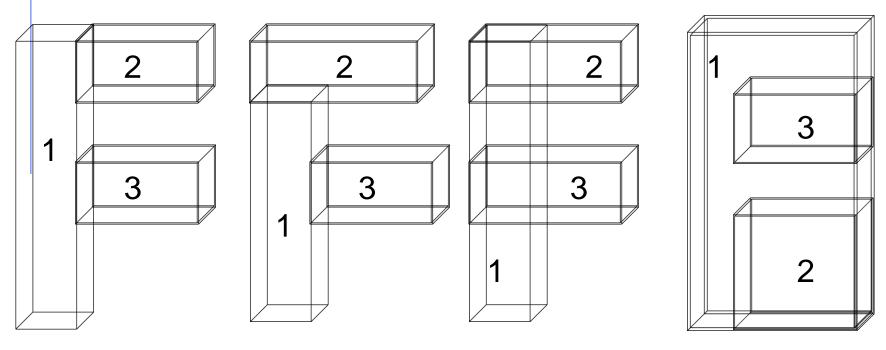
Examples:

Geometry Example "F" shaped target



Geometry example "F": Bodies

Several possibilities for bodies, e.g.:



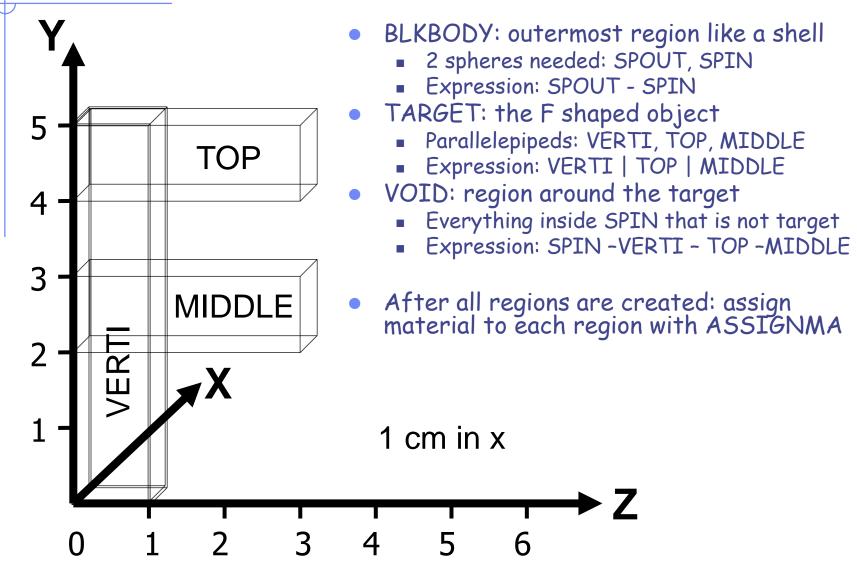
(A) Separated bodies

bodies

(B) Separated (C) overlapping (D) subtraction

The 4 options are equivalent. We will use C.

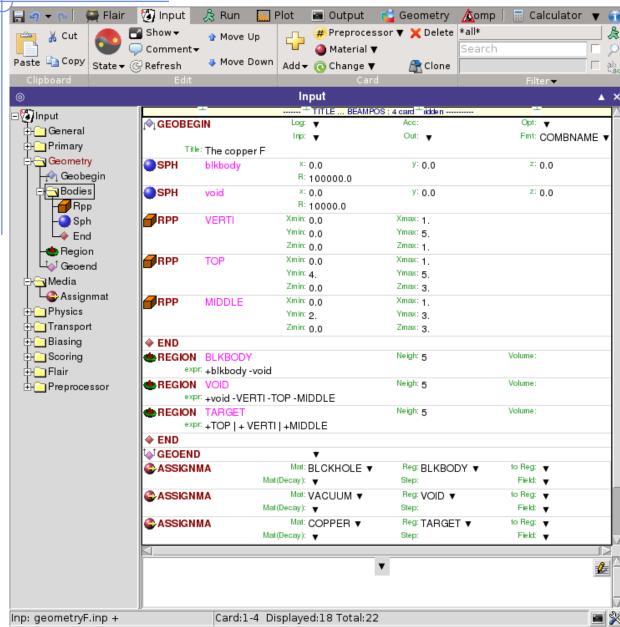
Geometry example "F": REGIONS



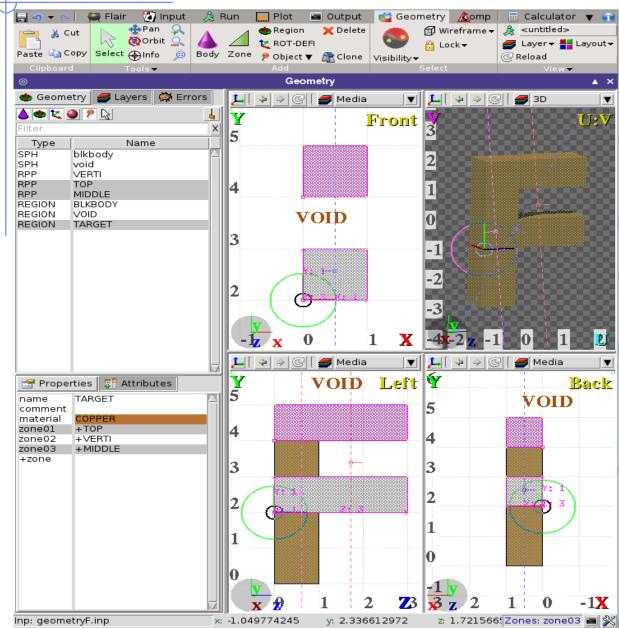
Geometry example "F": input file

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

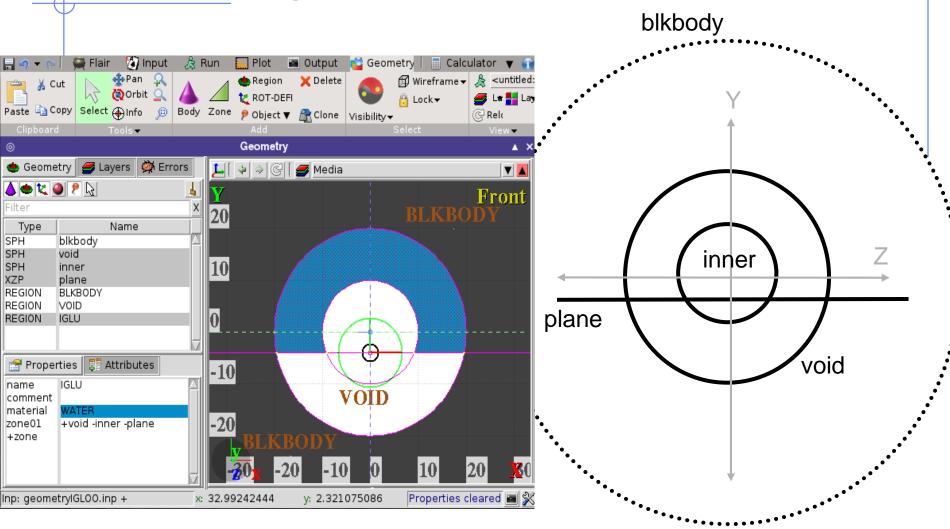
Geometry example "F": input Flair



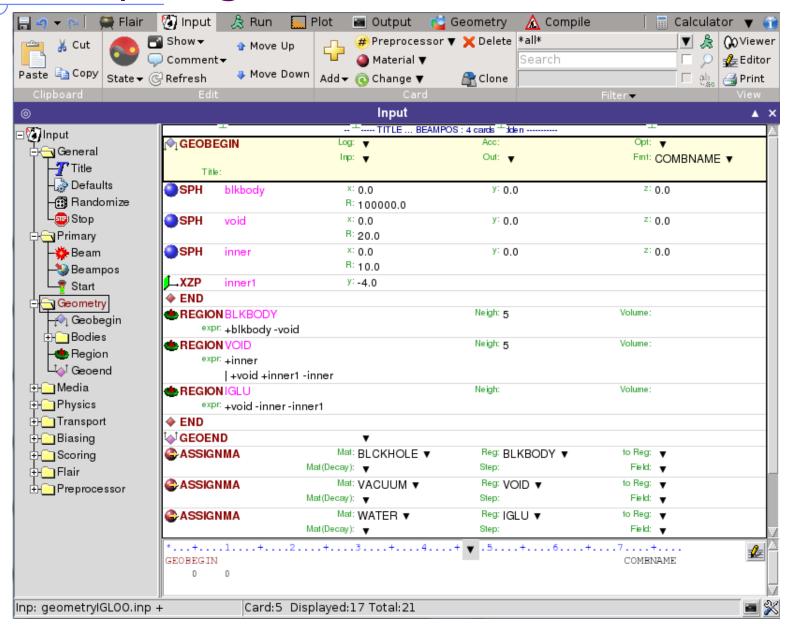
Geometry example "F": input Flair



Example: Igloo



Example: Igloo



Remarks

Important Notes

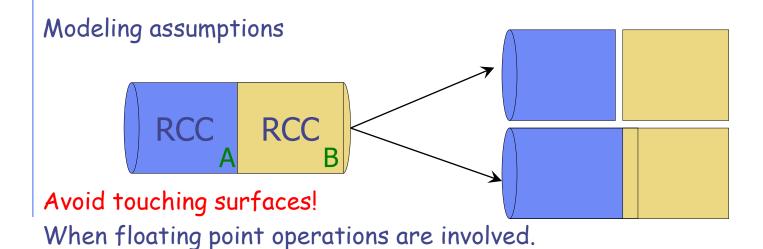
Whenever it is possible, the following bodies should be preferred:

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.

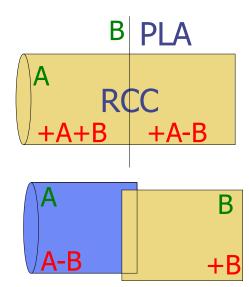
 Always use as many digits as possible in the definition of the body parameters, particularly for body heights (RCC, REC, TRC), and for direction cosines of bodies with slant surfaces. The name based format or the high-accuracy fixed format should always be used in these cases.

Precision Errors



Use cutting surface B instead

Or force partial overlap of bodies



Tracking accuracy

- □ FLUKA uses systematically double precision mathematic (i.e. 16 significant digits)
- □ GEOBEGIN's WHAT(2)*10⁻⁶cm 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^{-14} - 10^{-15} .
- □ 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) default value of 0.0001.

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
 (handled through a dedicated Flair frame)
- Error messages during simulation in the .err file
- Geometry plotting by Flair

 (automatically invoking the PLOTGEOM card)
- FLAIR Geometry Editor (very powerful! See dedicated lecture)
- 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

GEOEND GEOEND	Ymax Ny	Zmax Nz	Xmin	Ymin	Zmin	DEBUG &
Ģ †GEOEND	DEBUG Xmin: Ymin: Zmin:	∀	Xmax: Ymax: Zmax:		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 ****
```

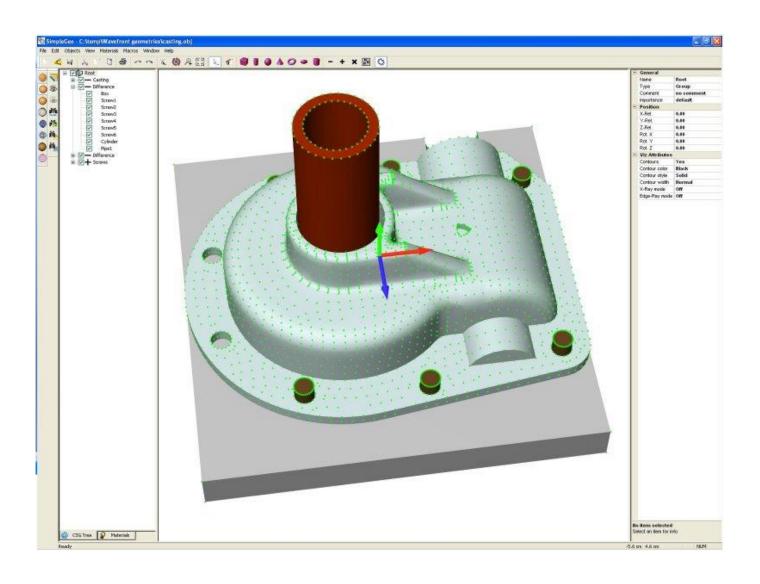
Point is contained in more than one region

```
**** is contained in more than 1 region ****

**** (regions: 6 7) ****
```

Not contained in any region **** is not contained in any region

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/simplegeo
- Operating system: Windows only

