

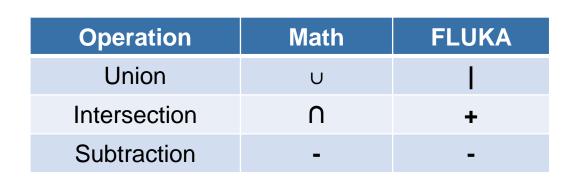
Geometry – Basic

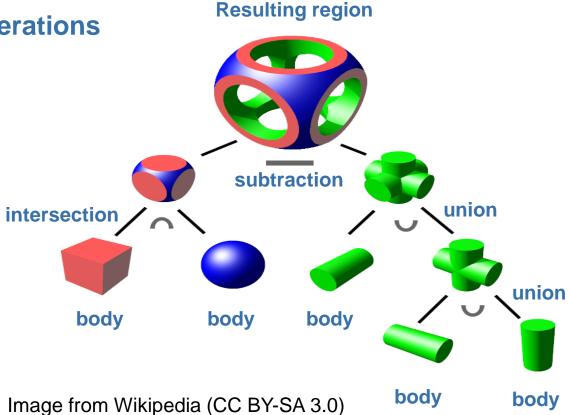
Introduction to the combinatorial geometry package in FLUKA

Beginner course – NEA November 2023

Introduction

- Principle of Combinatorial Geometry (CG)
 - 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**

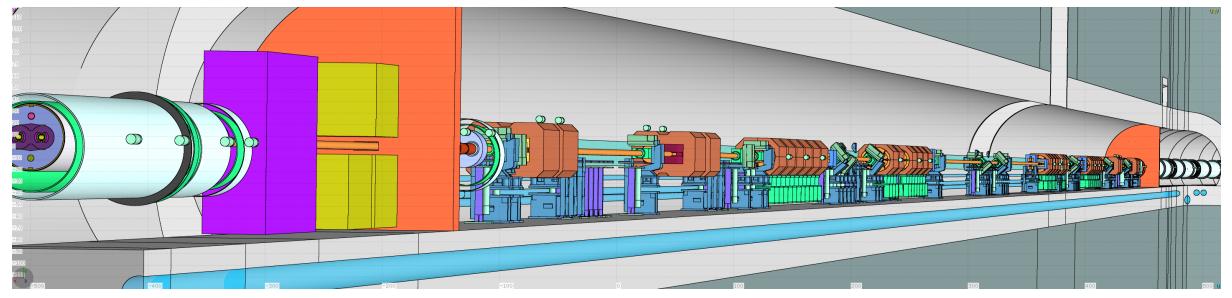






Introduction

- Combinatorial Geometry in FLUKA
 - Originally based on the geometry package for the neutron and gamma-ray transport program Morse developed at ORNL (M.B. Emmet ORNL-4972, 1975).
 - Many improvements have been incorporated over time, for example roto-translations of bodies, repetition of patterns, or voxels

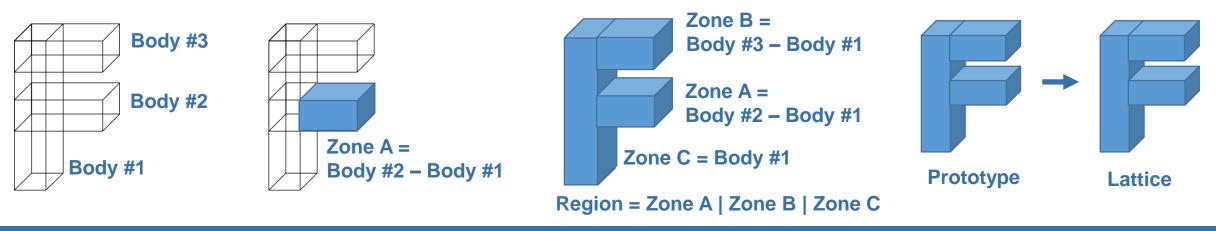


Example: LHC collimation insertion region built from the combination of bodies like planes, cylinders, cuboids, ...



Basic concepts and terminology

- Four concepts are fundamental in the FLUKA CG
 - Bodies: basic geometrical objects which are placed somewhere in the coordinate system
 - These include: **basic convex objects**, plus **infinite planes** (half-spaces), **infinite cylinders** (circular and elliptical), and **generic quadric surfaces** (surfaces described by 2nd degree equations)
 - **Zones**: sub-regions defined only via the intersection and subtraction of bodies
 - Regions: union of zones
 - In the simplest case a region consists of a single zone (no union operation needed in this case ...)
 - Lattices: duplication of existing objects (regions) confined in a container volume
 - Container can be translated and rotated, multiple duplications are possible



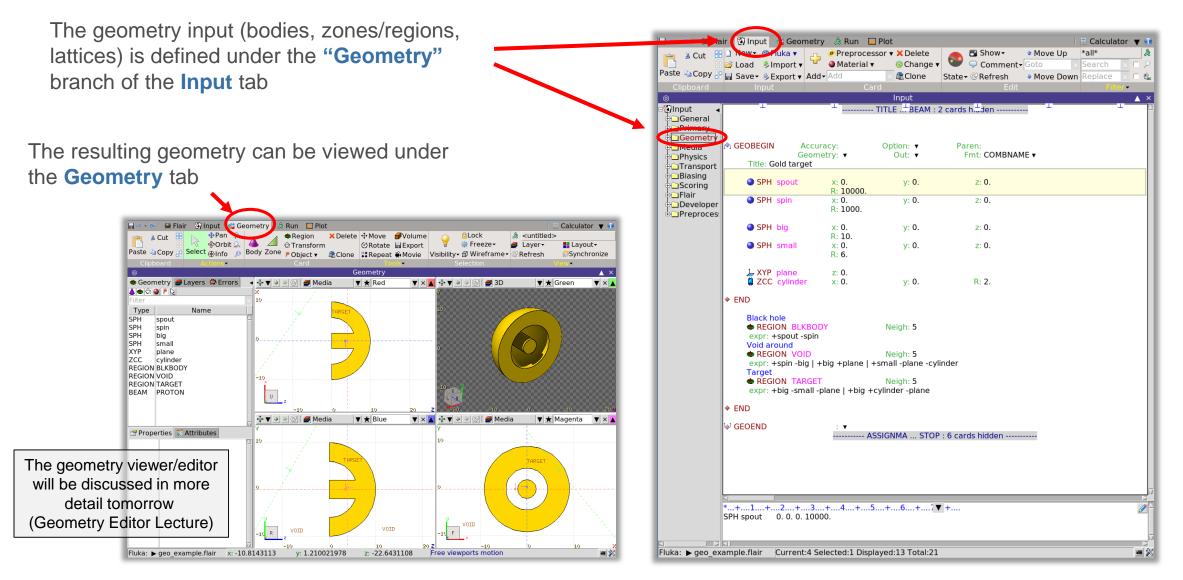


Geometry input

How to structure the geometry definition



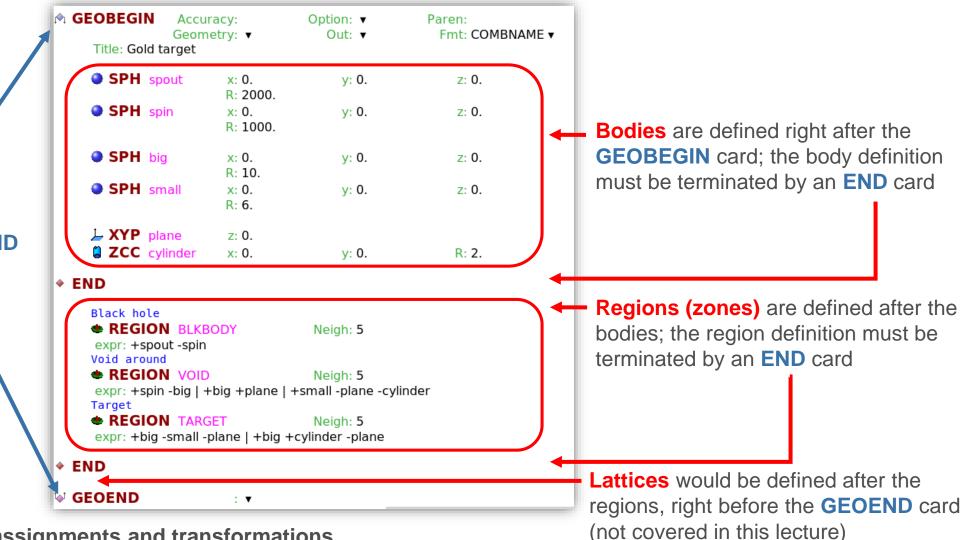
Geometry input in Flair





Structure of the geometry input

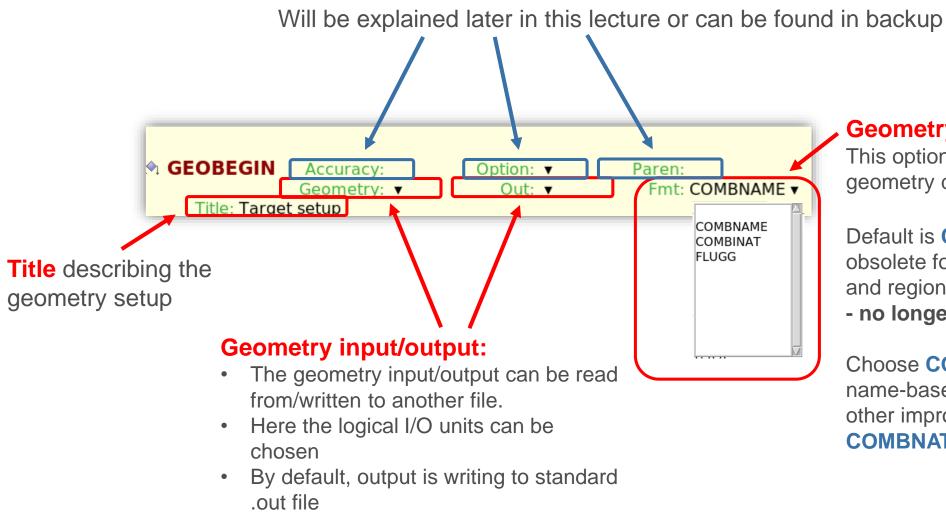
The geometry definition must be enclosed by the **GEOBEGIN** and **GEOEND** cards



Note: material definition/assignments and transformations are defined outside of GEOBEGIN-GEOEND



The GEOBEGIN card



Geometry input format:

This option allows choosing how the geometry description is formatted.

Default is **COMBNAT**, which selects an obsolete formatting style (e.g. bodies and regions are identified via numbers) - **no longer supported by Flair!**

Choose **COMBNAME**, which is the name-based format and also features other improvements compared to **COMBNAT**.



Bodies

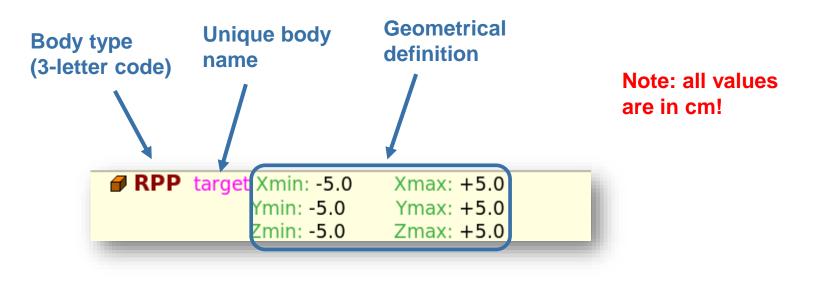
The basic objects of the FLUKA CG



Body definitions

- A body definition in FLUKA consists of:
 - A 3-letter code indicating the body type
 - A unique body name (alphanumeric identifier, 8 character maximum, case sensitive)
 - A set of geometrical quantities defining the body, e.g. the body dimensions and the position in the coordinate system (the numbers depend on the body type, see next slides)

GEOBEGIN Accur Geom Title: Gold target	racy: etry: ▼	Option: ▼ Out: ▼	Paren: Fmt: COMBNAME •
SPH spout	x: 0. B: 2000.	y: 0 .	z: 0.
• SPH spin	x: 0. R: 1000.	y: 0 .	Bodies
SPH big	x: 0. B: 10.	y: 0.	z: 0.
SPH small	x: 0. R: 6.	y: 0 .	z: 0.
 XYP plane ZCC cylinder 	z: 0. x: 0.	y: 0.	R: 2 .
END			
Black hole • REGION BLKB expr: +spout -spin Void around	ODY	Neigh: 5	
 REGION VOID expr: +spin -big + Target 		Neigh: 5 ⊦small -plane -cyl	inder
REGION TARG expr: +big -small -		Neigh: 5 cylinder -plane	
END			

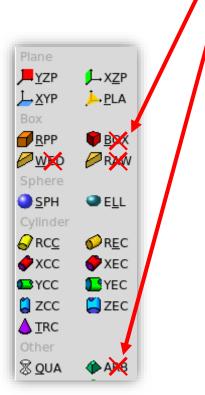




List of bodies

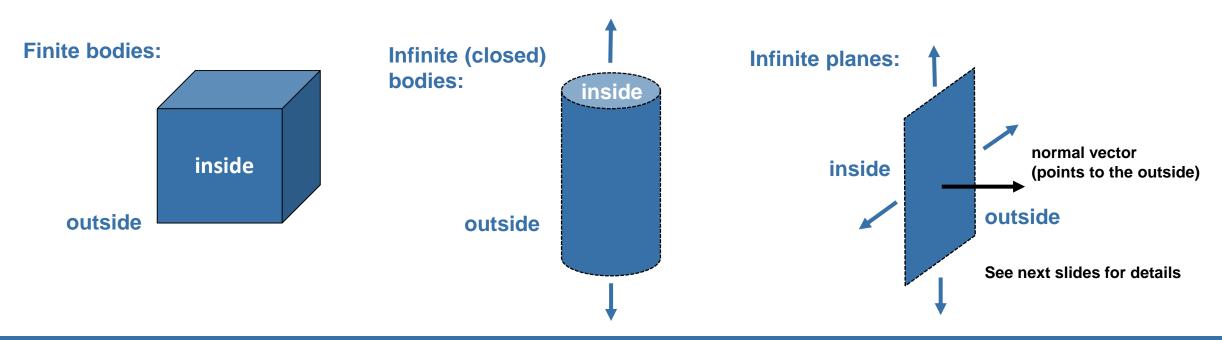
- Following bodies are presently available in FLUKA:
 - Planes
 - XYP, XZP, YZP: Infinite half space delimited by a coordinate plane
 - PLA: Generic infinite half-space, delimited by a PLAne
 - Boxes
 - RPP: Rectangular ParallelePiped
 - Sphere and spheroid
 - SPH: SPHere
 - ELL: ELLipsoid of revolution
 - Cylinders and cones
 - XCC, YCC, ZCC: Infinite Circular Cylinder, parallel to coordinate axis
 - RCC: Right Circular Cylinder
 - XEC, YEC, ZEC: Infinite Elliptical Cylinder, parallel to coordinate axis
 - REC: Right Elliptical Cylinder
 - TRC: Truncated Right angle Cone
 - Other
 - QUA: QUAdric

Note: BOX, WED, RAW, ARB are deprecated. Do not use them, because they can cause rounding problems.



Division of space

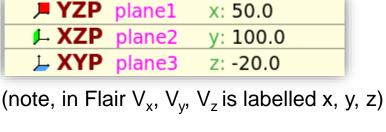
- Each body splits the space into two domains: inside and outside
 - This concept will be later used when defining zones and regions
 - **+body** refers to the volume **inside** of the body
 - -body refers to the volume outside of the body
 - The concept of inside and outside is applied to all bodies including infinite planes

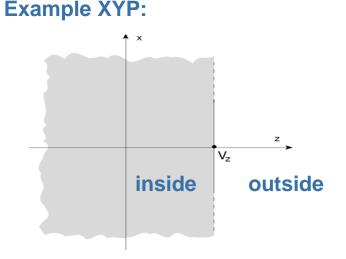




Infinite planes parallel to coordinate axes

- Divide space in two half spaces parallel to coordinate axes
 - Three possibilities:
 - Plane \perp to the x-axis \rightarrow 3-letter code: **YZP**
 - Plane \perp to the y-axis \rightarrow 3-letter code: **XZP**
 - Plane \perp to the z-axis \rightarrow 3-letter code: XYP
 - All defined by a single number (coordinate of the plane on the perpendicular axis):
 - x-coordinate V_x for YZP
 - y-coordinate V_v for XZP
 - z-coordinate V_z for XYP
 - Inside vs outside:
 - Points for which $x < V_x$ (resp. $y < V_y$, or $z < V_z$) are "inside the body"
 - Points for which $x > V_x$ (resp. $y > V_y$, or $z > V_z$) are "outside the body"





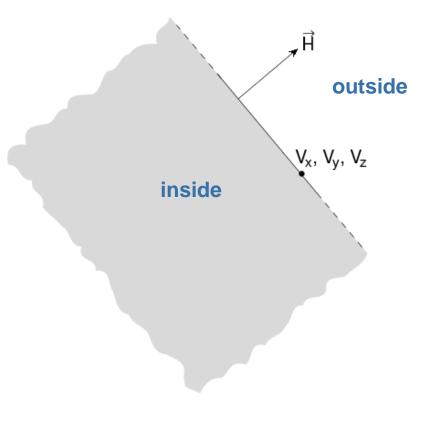


In Flair:

Arbitrarily orientated infinite plane

- Divides space in two arbitrarily oriented half spaces
 - 3-letter code: PLA
 - A PLA is defined by 6 numbers:
 - H_x , H_y , H_z (vector \perp to the plane, arbitrary length)
 - V_x , V_y , V_z (any point lying on the plane)
 - Inside vs outside:
 - The half-space "inside the body" is that from which the vector H_x, H_y, H_z is pointing (i.e. the vector points "outside").

In Flair:			(note, in F	lair H _x , H _y , H _z is la	abelled Nx, Ny, I	Nz)
	Þ PLA	plane4	Nx: 1.0 x: 0.0	Ny: 5.0 y: 3.0	Nz: 4.0 z: 2.0	

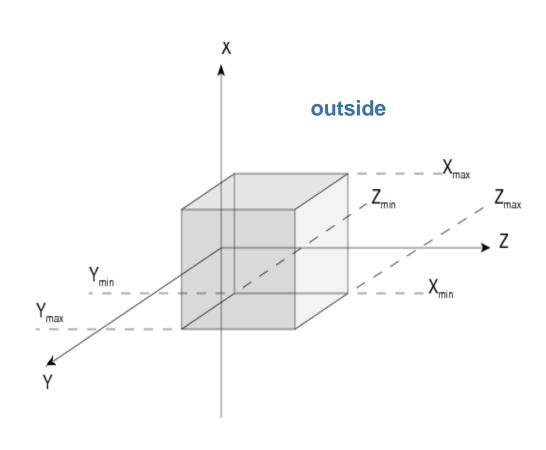




Rectangular parallelepiped

- Box with faces parallel to the coordinate axis
 - 3-letter code: RPP
 - A RPP is defined by 6 numbers:
 - X_{min} , X_{max} (positions of the two ZY faces of the RPP)
 - Y_{min} , Y_{max} (positions of the two XZ faces of the RPP)
 - Z_{min} , Z_{max} (positions of the two XY faces of the RPP)
 - Inside vs outside:
 - A point x, y, z is "inside the body" if it is contained in the RPP (i.e. X_{min} < x < X_{max} and Y_{min} < y < Y_{max} and Z_{min} < z < Z_{max})





💣 RPP	target Xmin: -5.0	Xmax: +5.0
	Ymin: -5.0	Ymax: +5.0
	Zmin: -5.0	Zmax: +5.0

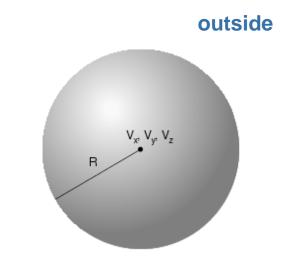


In Flair:

Sphere

- Sphere at arbitrary location
 - 3-letter code: SPH
 - A SPH is defined by 4 numbers:
 - V_x , V_y , V_z (origin of the sphere)
 - **R** (radius of the sphere)
 - Inside vs outside:
 - A point **x**, **y**, **z** is defined as "inside the body" if it is contained inside the sphere

In Flair:		(note,	in Flair \	V_x , V_y , V_z is labelled x,	y, z)
•	SPH	target1	x: 5.0 R: 4.0	y: 3.0	z: 8.0





Right circular cylinder

- Finite cylinder at arbitrary position and with arbitrary orientation, limited by a cylindrical surface and two plane faces \perp to its axis
 - 3-letter code: RCC
 - A RCC is defined by 7 numbers:
 - V_x, V_y, V_z (base of the cylinder, i.e., center of one cylinder face)
 - H_x, H_y, H_z (vector corresponding to the cylinder height, pointing to the center of the other face)
 - R (radius of the cylinder)
 - Inside vs outside:
 - A point x, y, z is defined as "inside the body" if it is contained inside the cylinder

In Flair: (note, in Flair V_x, V_y, V_z is labelled x, y, z) **RCC** target2 x: 5.0 y: 2.0 z: 8.0 Hx: 3.0 Hy: 3.0 Hz: 0.0 R: 2.0



R

outside

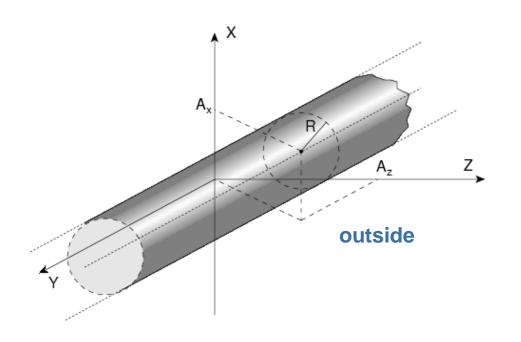
Ĥ

 V_x, V_y, V_z

Infinite circular cylinders

- Infinite circular cylinder parallel to one of the coordinate axis, at arbitrary position
 - Three possibilities:
 - Cylinder parallel to the x-axis \rightarrow 3-letter code: **XCC**
 - Cylinder parallel to the y-axis \rightarrow 3-letter code: **YCC**
 - Cylinder parallel to the z-axis \rightarrow 3-letter code: **ZCC**
 - An XCC/YCC/ZCC is defined by 3 numbers:
 - A_y, A_z for XCC, A_x, A_z for YCC, A_x, A_y for ZCC (coordinates of the cylinder axis)
 - R (radius of the cylinder)
 - Inside vs outside:
 - A point **x**, **y**, **z** is defined as "inside the body" if it is contained inside the cylinder

In Flair:	(note, in Flair	A_x, A_y, A_z is lab	elled x, y, z)
ACC cyl1	y: 4.0	z: 3.0	R: 1.0
Sec cyl2	z: 2.0	y: -5.0	R: 2.0
Sec cyl3	x: -3.0	y: 2.0	R: 5.0



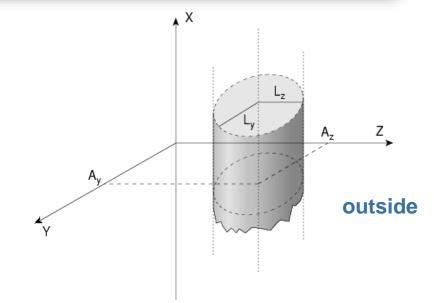


Infinite elliptical cylinders

- Infinite elliptical cylinder parallel to one of the coordinate axis, at arbitrary position
 - Three possibilities:
 - Cylinder parallel to the x-axis \rightarrow 3-letter code: **XEC**
 - Cylinder parallel to the y-axis \rightarrow 3-letter code: **YEC**
 - Cylinder parallel to the z-axis \rightarrow 3-letter code: **ZEC**
 - An XCC/YCC/ZCC is defined by 4 numbers:
 - A_y, A_z for XCC, A_x, A_z for YCC, A_x, A_y for ZCC (coordinates of the cylinder axis)
 - L_y, L_z for XCC, L_x, L_z for YCC, L_x, L_y for ZCC (semiaxes of the cylinder)
 - Inside vs outside:
 - A point **x**, **y**, **z** is defined as "inside the body" if it is contained inside the cylinder

In Flair: (note, in Flair A_x , A_y , A_z is labelled x, y, z)

🛛 🗢 XEC cyl4	y: 3.0	z: 2.0
	Ly: 2.0	Lz: 5.0
Sec 2015	z: 1.0	x: 0.0
	Lz: 3.0	Lx: 1.0
Sec 28	x: 4.0	y: -2.0
	Lx: 0.5	Ly: 1.0





Arbitrary generic quadric

- A quadric surface defined by a 2^{nd} degree equation F(x,y,z) = 0
 - 3-letter code: QUA
 - Each QUA is defined by 10 numbers:

$$\mathbf{C}_{\mathbf{x}\mathbf{x}}, \, \mathbf{C}_{\mathbf{y}\mathbf{y}}, \, \mathbf{C}_{\mathbf{z}\mathbf{z}}, \, \mathbf{C}_{\mathbf{x}\mathbf{y}}, \, \mathbf{C}_{\mathbf{x}\mathbf{z}}, \, \mathbf{C}_{\mathbf{y}\mathbf{z}}, \, \mathbf{C}_{\mathbf{x}}, \, \mathbf{C}_{\mathbf{y}}, \, \mathbf{C}_{\mathbf{z}}, \, \mathbf{C}_{\mathbf{0}}$$

• Corresponding to the equation:

$$C_{xx} x^2 + C_{yy} y^2 + C_{zz} z^2 + C_{xy} xy + C_{xz} xz + C_{yz} yz + C_x x + C_y y + C_z x + C_0 = 0$$

🕷 QUA target 👘	Cxx: -5.0	Cyy: 2.0	Czz: -3.0
	Cxy: 1.0	Cxz: -4.0	Cyz: 1.0
	Cx: 6.0	Cy: 8.0	Cz: 2.0
	C: -1.0	-	





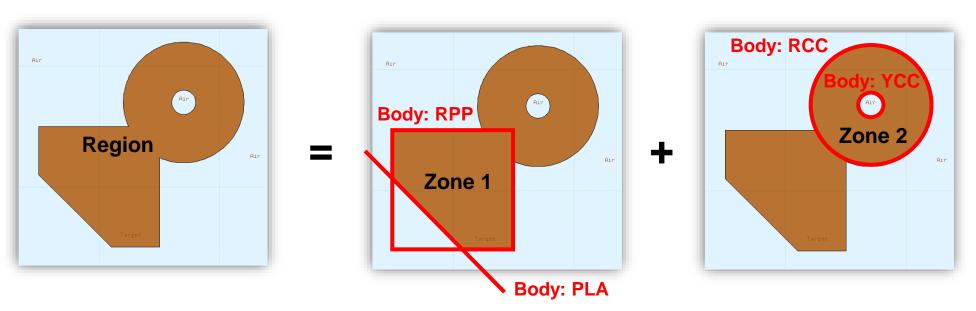
Regions (and zones)

Combining bodies to create your geometry model



Concept of zones and regions

- Regions are defined by combining FLUKA bodies using Boolean operations, more precisely:
 - Regions are obtained by the union of sub-regions (called zones); in the simplest case a region consists of a single zone
 - Zones are defined by intersections and/or subtractions of bodies (Boolean zone expressions)



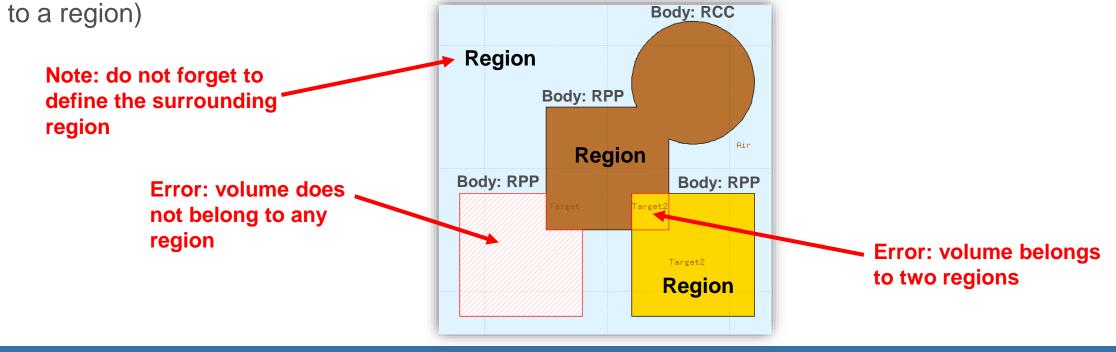
Zones belonging to the same region can overlap!!

On the other hand, zones belonging to the same region must not necessarily be connected.



Basic principles ...

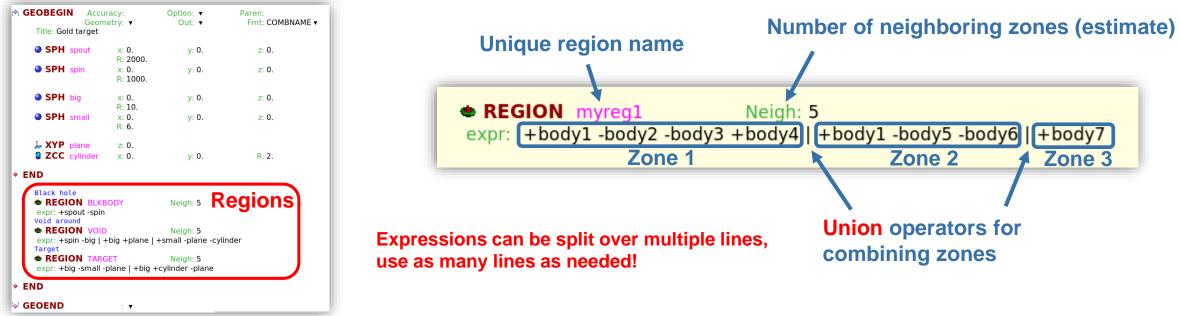
- ... when building geometries:
 - Zones and hence regions must be finite
 - Each point in space must belong to one (and only one) region
 - Note that also the region surrounding your principal geometry must be defined (e.g. air region)
 - Regions are of homogeneous material composition (i.e. only one material can be assigned





Region definitions

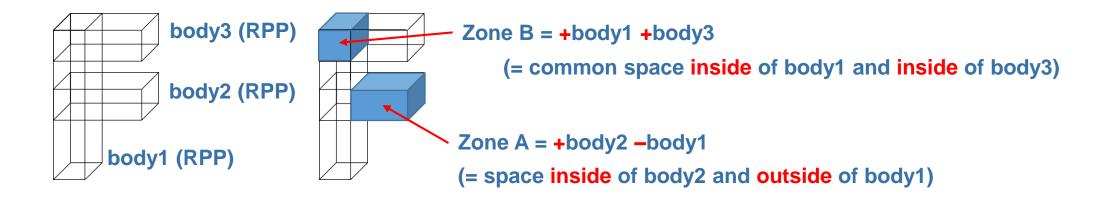
- A region definition in FLUKA consists of:
 - A unique region name (alphanumeric identifier, 8 character maximum, case sensitive, must start with an alphabetical character)
 - An estimate of the number of neighboring zones (see backup)
 - A single Boolean zone expression or a series of Boolean zone expressions combined via the union operator





Boolean zone expressions

- Zones are a described by a sequence of one or more bodies each being preceded by a + or - sign (remember: +/- means inside/outside a body)
 - +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)





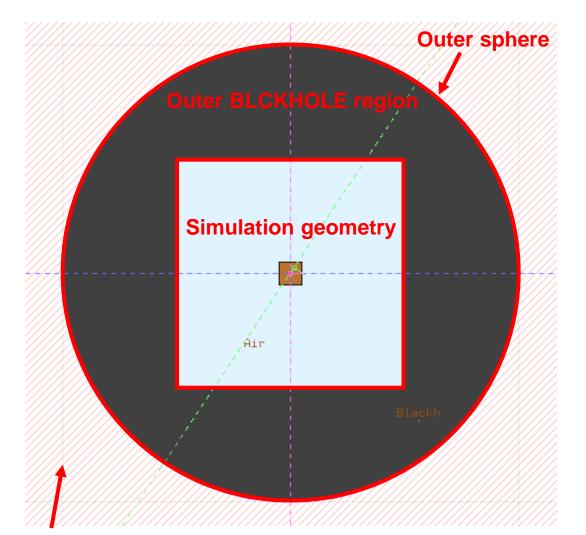
Parenthesis in region definitions

- Parentheses can be used to perform complex Boolean operations in the description of regions
- In evaluating the expressions, the highest operator precedence is given to parentheses, followed by +, - and the | operator
- Still, the extensive use of parenthesis is discouraged and can create unreadable and inefficient code
 - It is perfectly possible to implement (complex) geometries without using parenthesis
- In case you use parentheses, pay attention to the respective parameters on the GEOBEGIN card (optimisation level and runtime evaluation of parenthesis)
 - See backup for details



Special region: the outer black hole confinement

- FLUKA defines a special material called BLCKHOLE:
 - BLCKHOLE is an **all-absorbing material**
 - Particles vanish when entering a region filled with BLCKHOLE
- The entire geometry must be embedded in a region filled with BLCKHOLE
 - This avoids tracking particles to infinity
 - The outer surface of this BLCKHOLE region must be a single closed body (e.g. a sphere)



Outside of the BLCKHOLE enclosure, the region can remain undefined!



Tracking accuracy

- The tracking accuracy parameter can be adjusted on the GEOBEGIN card
 - Defines absolute accuracy used for tracking and boundary identification (in units of 10⁻⁶ cm)
 - Should be larger than A_r*L , where:
 - L is the largest coordinate value in the geometry (without BLCKHOLE confinement)
 - A_r is the relative accuracy achievable in double precision (~10⁻¹⁴-10⁻¹⁵).
 - By default, FLUKA tries to guess the parameter based on the second biggest body in your geometry (assuming the biggest one is the BLCKHOLE confinement)
 - Can be overwritten by explicitly setting the parameter on GEOBEGIN

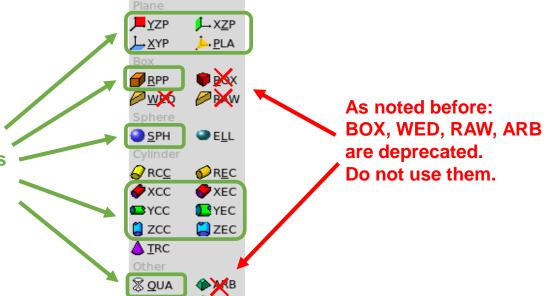




Tracking speed

- Number of bodies per zone:
 - If the number of bodies *per zone definition* becomes large this slows down the tracking
 - Rather segment in more zones than using too many bodies per zone (rule of thumb: not more than 10 bodies per zone definition)
 - Overlapping zones (for the same regions) can even be beneficial since particles may remain longer in one zone
- Recommendations on the use of bodies:

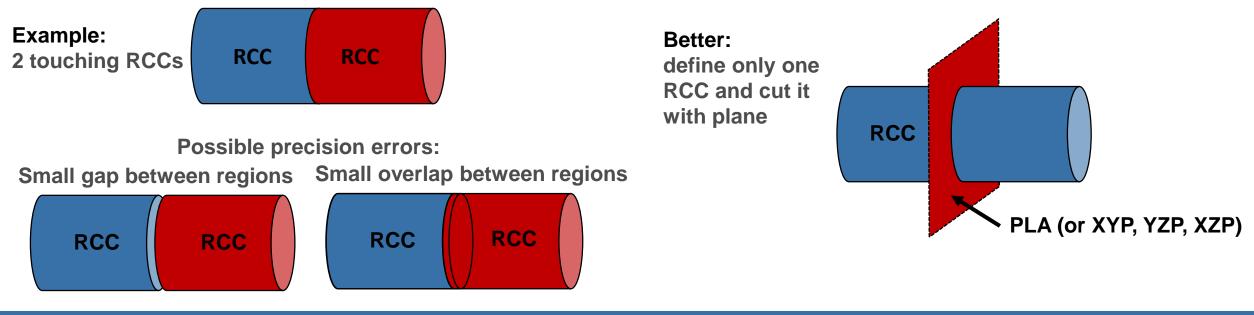
Prefer the bodies shown in green – tracking is faster since unnecessary boundary intersection calculations are avoided when the particle step is shorter than the distance to the region boundary.





Precision errors in region definitions

- Always use as many digits as possible in the definition of body parameters
 - Particularly for body heights (RCC, REC, TRC)
- Avoid touching surfaces when floating point operations are involved
 - For the above bodies, the position of the opposite face is calculated using the height vector
 - This can lead to precision errors during tracking in case two such bodies touch each other





 V_x, V_y, V_z

Geometry example and debugging

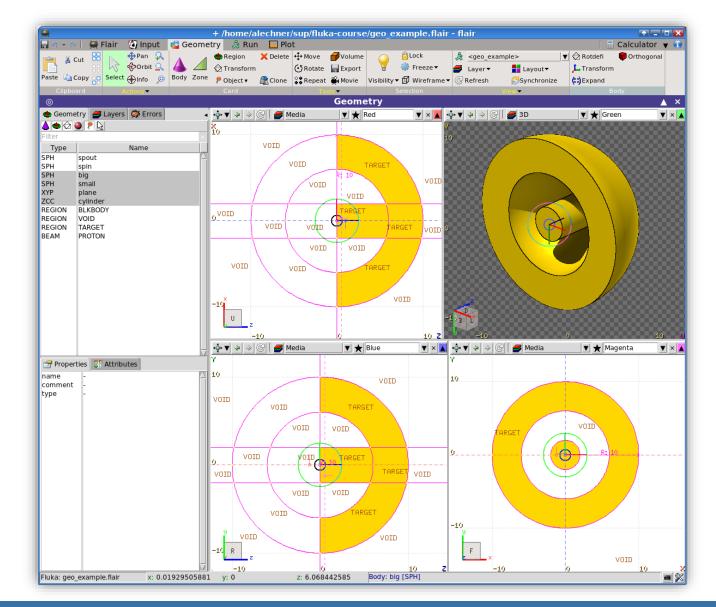
A practical example and how to detect geometry errors



Target made of gold – how to build it?

• Steps:

- Create enclosing BLCKHOLE region
- Create target region
- Create void region around the target



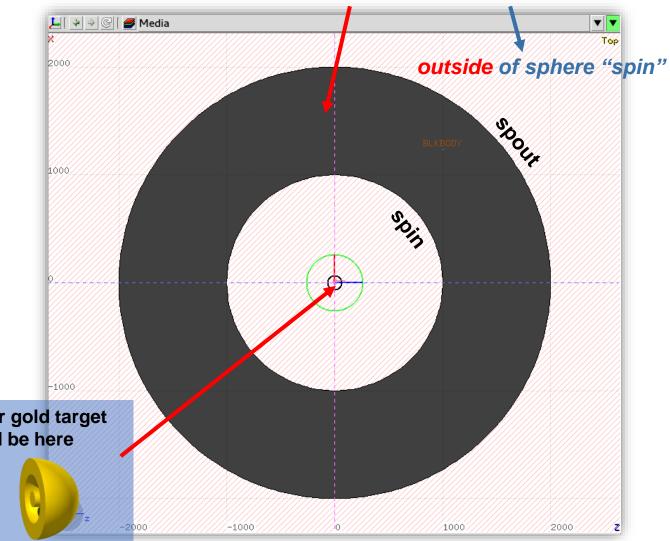


Step 1: surrounding BLCKHOLE region

inside of sphere "spout"

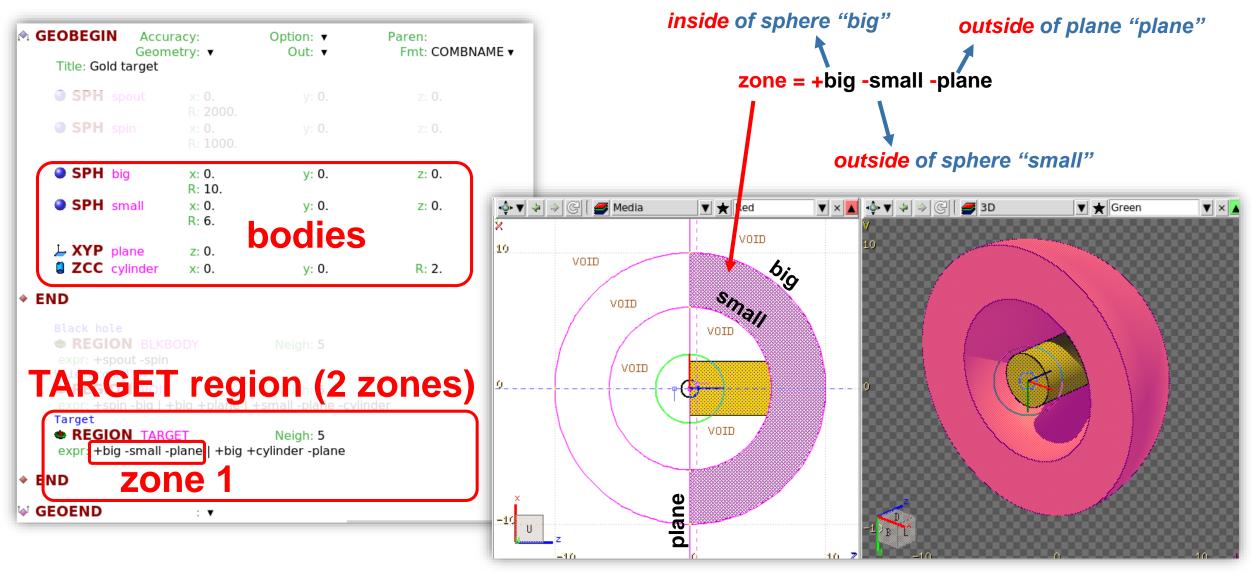
zone = +spout -spin

SPH spout	x: 0. R: 2000.	y: 0 .	z: 0.	
SPH spin	x: 0. R: 1000.	y: 0 .	z: 0.	
SPH big	x: 0. R: 10.	y: 0.	z: 0.	
SPH small	x: 0. R: 6.			
XYP plane ZCC cylinder			R: 2.	
			on (1 zo	one)
Black hole Black hole REGION BLKE expr: +spout -spin		Neigh: 5		
 REGION VOID 		Neigh: 5 small -plane -cylin	der	
expr: +spin -big · Target				



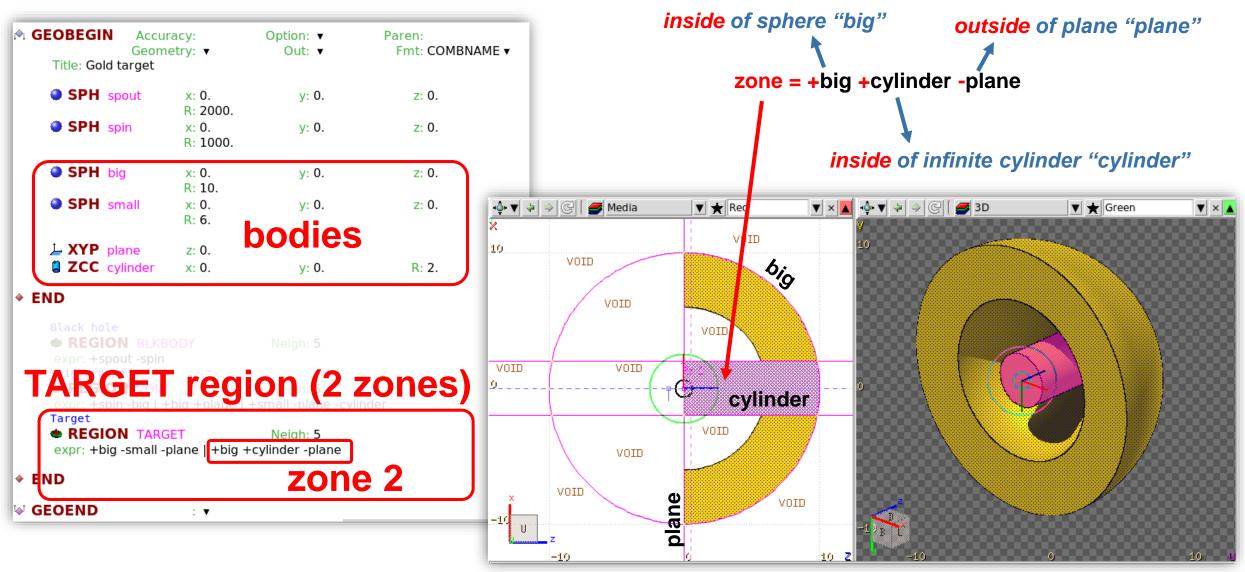


Step 2: Gold target – zone 1





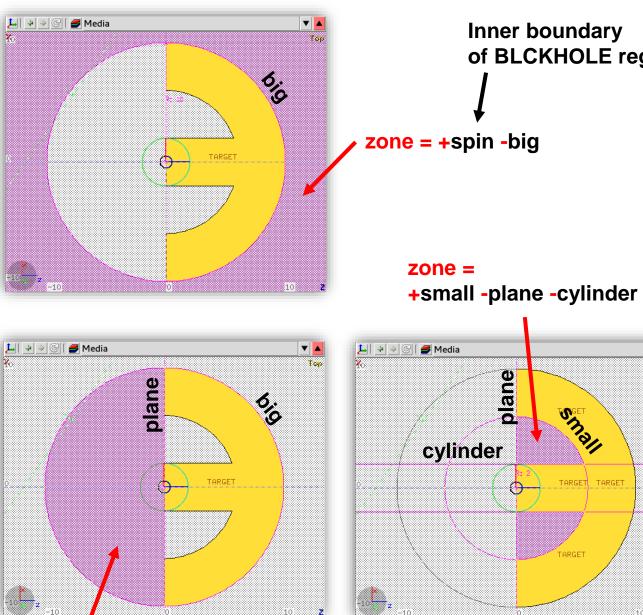
Step 2 (cont.): Gold target – zone 2



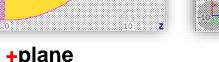


Step 3: the VOID region

GEOBEGIN Accur	acy: etry: ▼	Option: V	Paren:
Title: Gold target		DOUI	es ^{Emt:} COMBNAM
SPH spout	x: 0. R: 2000.	y: 0 .	z: 0.
SPH spin	x: 0. R: 1000.	y: 0 .	z: 0.
SPH big	x: 0. R: 10.	y: 0.	z: 0.
SPH small	x: 0. R: 6.	y: 0 .	z: 0.
XYP plane ZCC cylinder	z: 0. x: 0.	y: 0 .	R: 2.
END			
Black hole REGION BLKB expr: +spout -spin	ODY	Neigh: 5	
	big +plane	Neigh: 5 +small -plane -cylin	der
REGION TARG expr: +big -small -p	ET blane +big -	VOID r	egion
END		(3 zone	es)
GEOEND	: 🔻		



zone = +big +plane





10

z

Inner boundary

plane

of BLCKHOLE region

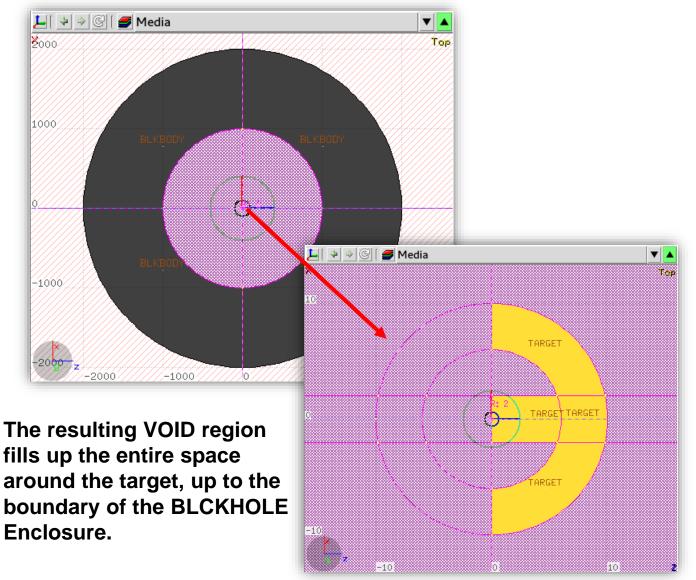
small

ARGET

TARGET TARGET

Step 3 (cont.): the VOID region

GEOBEGIN Accur Geom Title: Gold target	racy: etry: ▼	Option: • btodi	Paren: COMBNAME •
SPH spout	x: 0. R: 2000.	y: 0 .	z: 0.
SPH spin	x: 0. R: 1000.	y: 0 .	z: 0.
SPH big	x: 0. R: 10.	y: 0 .	z: 0.
SPH small	x: 0. R: 6.	y: 0 .	z: 0.
XYP plane ZCC cylinder	z: 0. x: 0.	y: 0 .	R: 2.
+ END		,	
Black hole REGION BLKB expr: +spout -spin	ODY	Neigh: 5	
Void around • REGION VOID expr: +spin -big +		Neigh: 5 +small -plane -cyli	nder
REGION TARG expr: +big -small -	ET plane +big +	VOID r	egion
◆ END		(3 zone	es)
GEOEND	: 🔻	`	•





Some remarks on 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:** the code **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 be completely unreliable.

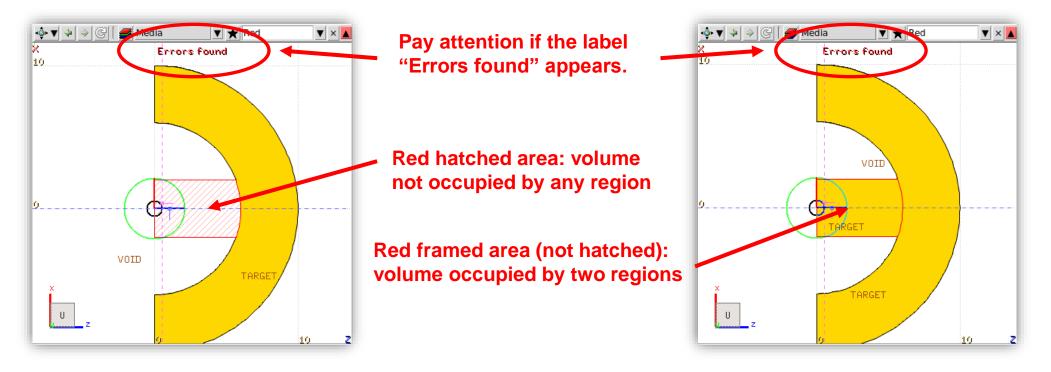
• Further types of errors:

- Problem space not enclosed by a BLCKHOLE 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 (see remarks on the choice of bodies in the previous section)
- Lattice replica and basic cell mismatch (see advanced topics)



Debugging of geometry errors

- Inspect the .err file for relevant messages
- Use the Flair geoviewer
 - Note that errors are only detected if they are within the view planes (i.e., if they are outside the viewed planes, they are not shown)





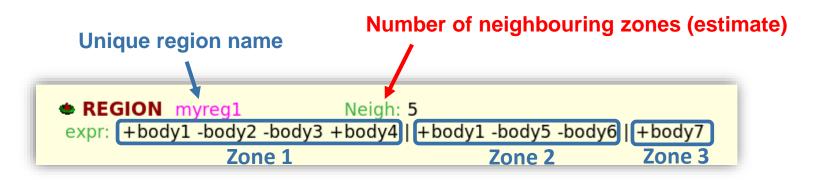
Backup



The number of adjacent zones (REGION card)

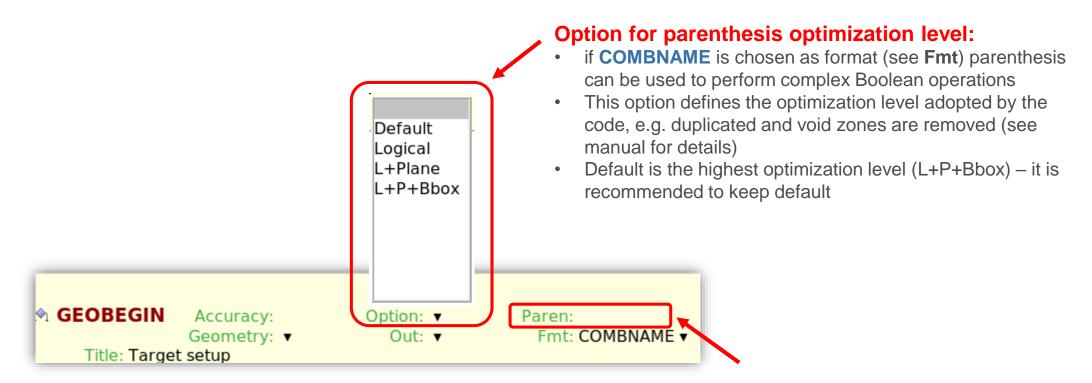
• "Neigh" parameter on the REGION card:

- 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 sum over all regions, defining the size of the contiguity list. Note: for many simulation cases, the default value is fine.
- While tracking, the program searches in the contiguity list for the neighboring 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 neighboring zones.
- When the 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).





Parenthesis-related settings on GEOBEGIN card



Option for selecting runtime parenthesis evaluation:

 Depending on the chosen factor, parenthesis are not expanded during initialization but at runtime



