#### III GEANT4 INTERNATIONAL AND GPU PROGRAMMING SCHOOL

Catania, Italy 9 – 13 November 2015

# Detector description: materials and geometry

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#### Introduction

Mandatory user classes in a Geant4:

- G4VUserDetectorConstruction
- G4VUserPhysicsList
- G4VUserPrimaryGeneratorAction

Materials, Volumes, Sensitive detectors and Fields to be used in the simulation must be defined in the G4VUserDetectorConstruction class

#### Part I: Units & materials

- System of units & constants
- Definition of elements
- Materials and mixtures
- NIST database

#### **Units in Geant4**

#### Don't use default units!

When specifying dimensions, always\* multiply by an appropriate unit:

G4double width = 12.5 \* m; G4double density = 2.7 \* g/cm3;

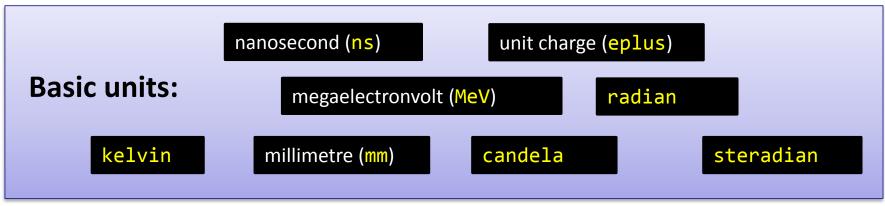
Most common units are defined in CLHEP:

G4SystemOfUnits.hhCLHEP/SystemOfUnits.hh

- You can define new units (later)
- Output data in terms of a specific unit:
  - **divide** a value by the unit:

G4cout << dE / MeV << " (MeV)" << G4endl;

#### **System of Units**



- All other units derived from the basic ones.
- Useful feature: Geant4 can select the most appropriate unit to use
  - specify the category for the data (Length, Time, Energy, etc...):

G4cout << G4BestUnit(StepSize, "Length");</pre>

**StepSize** will be printed in km, m, mm or ... fermi, depending on its actual value

#### How to define a new unit

• New units can be defined directly as constants, or (suggested way) as a G4UnitDefinition:

G4UnitDefinition(name, symbol, category, value);

• Example (speed):

G4UnitDefinition("km/hour", "km/h", "Speed", km/(3600\*s));

- The new category "Speed" will be registered in the kernel in G4UnitsTable (if not present)
- To print the list of units:
  - From the code:

G4UnitDefinition::PrintUnitsTable();

– At run-time, as UI command:

/units/list

#### Materials

- Different kinds of materials can be defined:
  - isotopes <> G4Isotope
  - elements <> G4Element
  - molecules<> G4Material
  - compounds and mixtures <> G4Material
- Attributes associated:
  - temperature, pressure, state, density
- **G4Isotope** and **G4Element** describe properties of the *atoms*:
  - Atomic number, number of nucleons, mass of a mole, shell energies, crosssections per atoms, etc...
- **G4Material** describes the *macroscopic* properties of the matter:
  - temperature, pressure, state, density
  - Radiation length, absorption length, etc...
- **G4Material** is used by tracking, geometry and physics

#### **Elements and isotopes**

• Isotopes...

G4Isotope(const	G4String&	name,	
	G4int	Z,	// atomic number
	G4int	n,	<pre>// number of nucleons</pre>
	G4double	a );	<pre>// mass of mole</pre>

• ...can be assembled into elements as follows:

<b>G4Element</b>	(const	G4String&	name,	
	const	G4String&	symbol,	// element symbol
		G4int	nIso );	<pre>// n. of isotopes</pre>

<pre>G4Element::AddIsotope(G4Isotope* iso,</pre>	// isotope
G4double relAbund);	<pre>// fraction of atoms</pre>

#### **Materials of one element and molecules**

• Single element material:

```
G4double z, a, density;
density = 1.390*g/cm3;
a = 39.95*g/mole;
G4Material* lAr = new G4Material("liquidAr", z=18, a, density);
```

• A molecule material (composition by number of atoms):

```
a = 1.01*g/mole;
G4Element* elH = new G4Element("Hydrogen", symbol="H", z=1., a);
a = 16.00*g/mole;
G4Element* elO = new G4Element("Oxygen", symbol="O", z=8., a);
density = 1.000*g/cm3;
G4Material* H2O = new G4Material("Water", density, ncomponents=2);
H2O->AddElement(elH, natoms=2);
H2O->AddElement(elO, natoms=1);
```

#### **Compounds and mixtures**

• Composition by fraction of mass:

```
a = 14.01*g/mole;
G4Element* elN = new G4Element(name="Nitrogen",symbol="N", z= 7., a);
a = 16.00*g/mole;
G4Element* elO = new G4Element(name="Oxygen",symbol="0", z= 8., a);
density = 1.290*mg/cm3;
G4Material* Air = new G4Material(name="Air", density, ncomponents=2);
Air->AddElement(elN, 70.0*perCent);
Air->AddElement(elO, 30.0*perCent);
```

• Composition of compound materials:

#### **Example: gas**

- It may be necessary to specify temperature and pressure
  - (dE/dx computation affected)

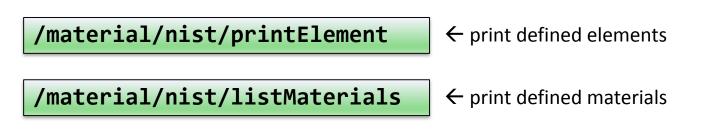
- <u>Absolute vacuum does not exist</u>: gas at very low density !
  - Cannot define materials composed of multiple elements through Z or A, or with  $\rho=0$

#### **Use the NIST material database**

- No need to predefine elements and materials
- Retrieve materials from NIST manager:

```
G4NistManager* manager = G4NistManager::Instance();
G4Material* H2O = manager->FindOrBuildMaterial("G4_WATER");
G4Material* air = manager->FindOrBuildMaterial("G4_AIR");
G4Material* vacuum = manager->FindOrBuildMaterial("G4_Galactic");
```

• UI commands:



#### **NIST Material Data-Base in Geant4**

- NIST database for materials is imported inside Geant4 <u>http://physics.nist.gov/PhysRefData</u>
- UI commands specific for handling materials
- The best accuracy for the most relevant parameters guaranteed:
  - Density
  - Mean excitation potential
  - Chemical bounds
  - Element composition
  - Isotope composition
  - Various corrections

Z	А	m	error	(%)	$A_{eff}$		
====	=======	======					
14	Si 22		3453	(22)			
	28.08						
			.02552	(21)			
			.011546	(21)			
			.004107	(11)			
			.992330	(3)			
			.98670476	(17)			
			.9769265327	· · ·		92.2297	(7)
		29 28	.97649472	(3)		4.6832	(5)
		30 29	.97377022	(5)		3.0872	(5)
		31 30	.97536327	(7)			
		32 31	.9741481	(23)			
		33 32	.978001	(17)			
		34 33	.978576	(15)			
		35 34	.984580	(40)			
		36 35	.98669	(11)			
		37 36	.99300	(13)			
		38 37	.99598	(29)			
		39 39	.00230	(43)			
		40 40	.00580	(54)			
		41 41	.01270	(64)			
		42 42	.01610	(75)			
				( - )			

- Natural isotope compositions
- More than 3000 isotope masses

#### **NIST materials in Geant4**

===							
###	### Elementary Materials from the NIST Data Base						
Z	Name	ChFormula	<pre>density(g/cm^3)</pre>	I(eV)			
===			========				
1	G4_H	H_2	8.3748e-05	19.2			
2	G4_He		0.000166322	41.8			
3	G4_Li		0.534	40			
4	G4_Be		1.848	63.7			
5	G4_B		2.37	76			
6	G4_C		2	81			
7	G4_N	N_2	0.0011652	82			
8	G4_0	0_2	0.00133151	95			
9	G4_F		0.00158029	115			
10	G4_Ne		0.000838505	137			
11	G4_Na		0.971	149			
12	G4_Mg		1.74	156			
13	G4_A1		2.6989	166			
14	G4_Si		2.33	173			

- NIST Elements:
  - H -> Cf ( Z = 1 -> 98 )
- NIST compounds:
  - e.g. "G4\_ADIPOSE\_TISSUE\_IRCP"
- HEP and Nuclear materials:
  - e.g. Liquid Ar, PbWO
  - It is possible to build mixtures of NIST and user-defined materials

N Name	ChFormula	density(g	/cm^3)
======= 13 G4 Ad	ipose_Tissue	======= 0.92	===== 63.2
1	0.119477		
6	0.63724		
7	0.00797		
8	0.232333		
11	0.0005		
12	2e-05		
15	0.00016		
16	0.00073		
17	0.00119		
19	0.00032		
20	2e-05		
26	2e-05		
30	2e-05		
4 G4_Air		0.001204	479 85.7
6	0.000124		
7	0.755268		
8	0.231781		
	0.012827		
2 G4_CsI		4.51	553.1
	0.47692		
55	0.52308		

#### Part II: Geometry

- Construction
  - Basic concepts
  - Basic implementation
- Detailed description
  - Solids
  - Logical volumes
  - Physical volumes
  - Regions
- Tools for geometry check
- (Magnetic) fields

#### **Geometry – implementation basics**

Implement a class inheriting from the abstract base class
 G4VUserDetectorConstruction:

```
class MyDetector : public G4VUserDetectorConstruction
{
   public:
      virtual G4VPhysicalVolume* Construct(); // required
      virtual void ConstructSDAndField(); // optional
      // ...
};
```

• Create an instance in the main program:

```
MyDetector* detector = new MyDetector();
runManager->SetUserInitialization(detector);
```

- Note: split the implementation into more classes & methods! (good programming practice)
  - especially for complex geometries!
- Note: there is no explicit deletion of MyDetector! Run manager does that automatically.

#### G4VUserDetectorConstruction

- Method Construct()
  - Define materials
  - Define solids and volumes of the geometry
  - Build the tree hierarchy of volumes
  - Define visualization attributes
  - Return the world physical volume!
- Method ConstructSDAndField()

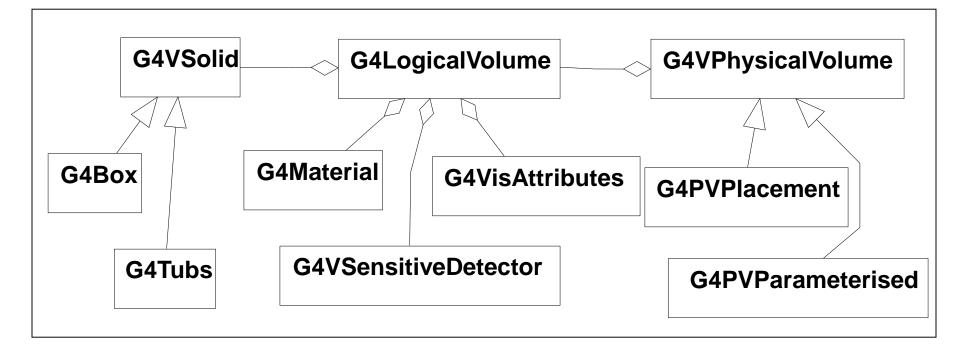


- Assign magnetic field to volumes / regions
- Define sensitive detectors and assing them to volumes —

#### ► G4VUserDetectorConstruction.hh

#### **Detector geometry components**

- Three conceptual layers
  - G4VSolid: shape, size
  - G4LogicalVolume: material, sensitivity, magnetic field, etc.
  - G4VPhysicalVolume: position, rotation

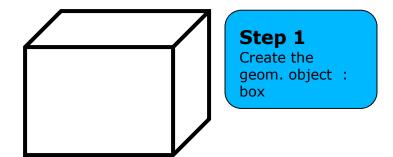


#### **Define detector geometry**

• Basic strategy

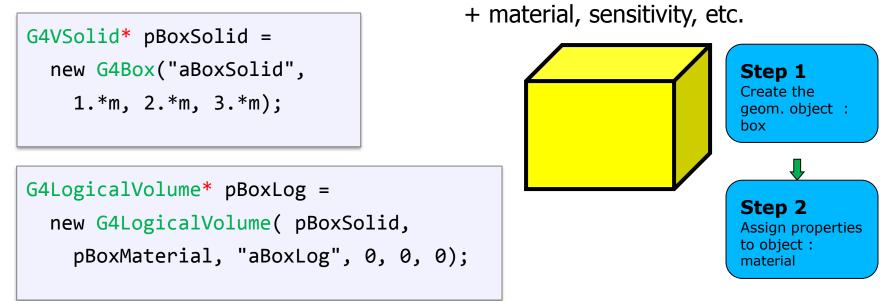
G4VSolid\* pBoxSolid =
 new G4Box("aBoxSolid",
 1.\*m, 2.\*m, 3.\*m);

Solid : shape and size

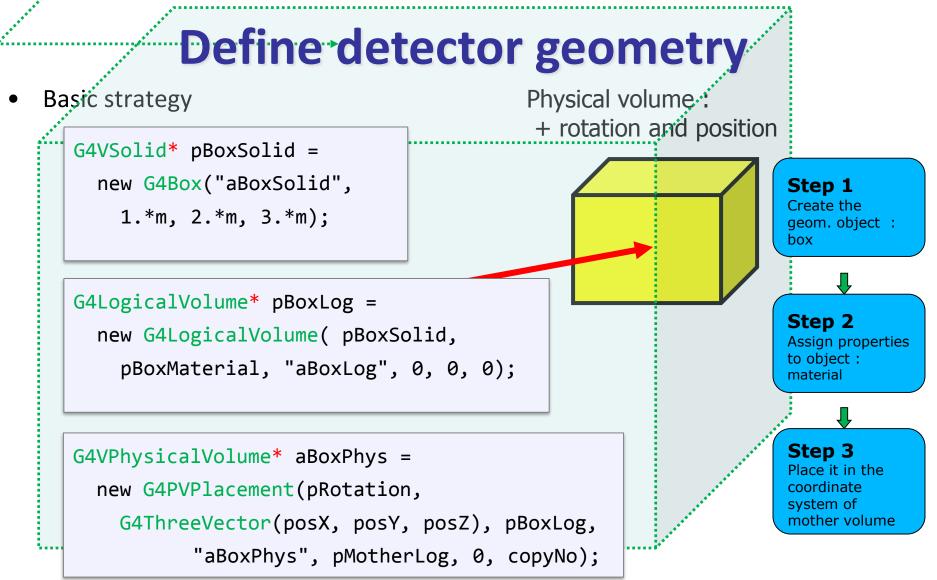


#### **Define detector geometry**

• Basic strategy



Logical volume :

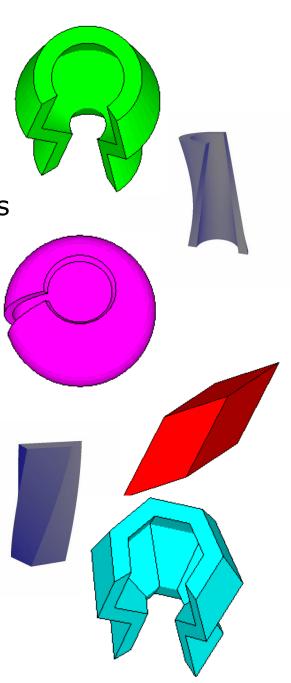


- A unique physical volume which represents the experimental area must exist and fully contains all other components
  - The world volume

# Solids

Solids defined in Geant4:

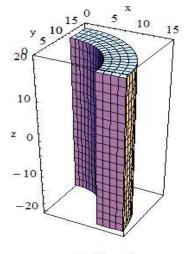
- CSG (Constructed Solid Geometry) solids
  - G4Box, G4Tubs, G4Cons, G4Trd, ...
- Specific solids (CSG like)
  - G4Polycone, G4Polyhedra, G4Hype, ..
  - G4TwistedTubs, G4TwistedTrap, ...
- BREP (Boundary REPresented) solids
  - G4BREPSolidPolycone, G4BSplineSurface, ...
  - Any order surface
- Boolean solids
  - G4UnionSolid, G4SubtractionSolid,

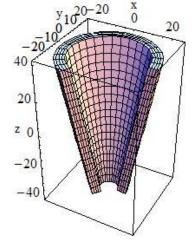


#### CSG: G4Tubs, G4Cons

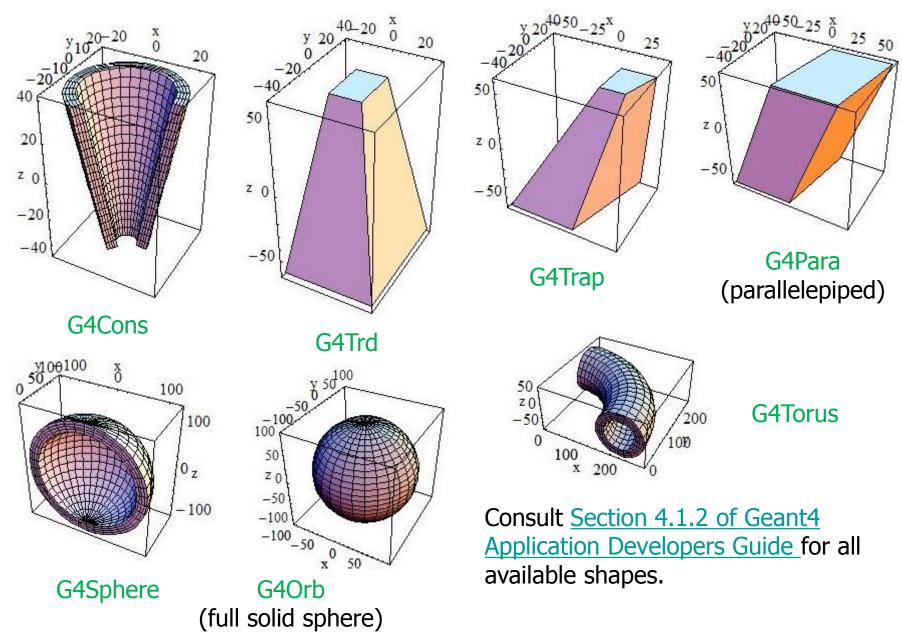
G	4Tubs(const	G4String&	pname,	//	name
	· ·				inner radius
		G4double	pRmax,	//	outer radius
					Z half length
					starting Phi
		G4double	pDphi);	//	segment angle

G4Cons(const	G4String&	pname,	//	name
	G4double	pRmin1,	//	inner radius -pDz
	G4double	pRmax1,	//	outer radius -pDz
	G4double	pRmin2,	//	inner radius +pDz
	G4double	pRmax2,	//	outer radius +pDz
	G4double	pDz,	//	Z half length
				starting Phi
	G4double	pDphi);	//	segment angle





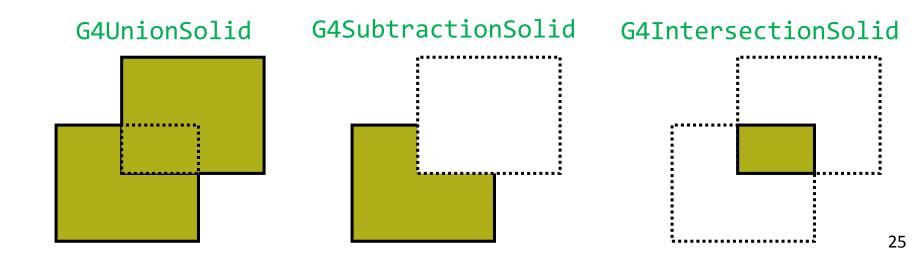
#### **Other CSG solids**



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#### **Boolean Solids**

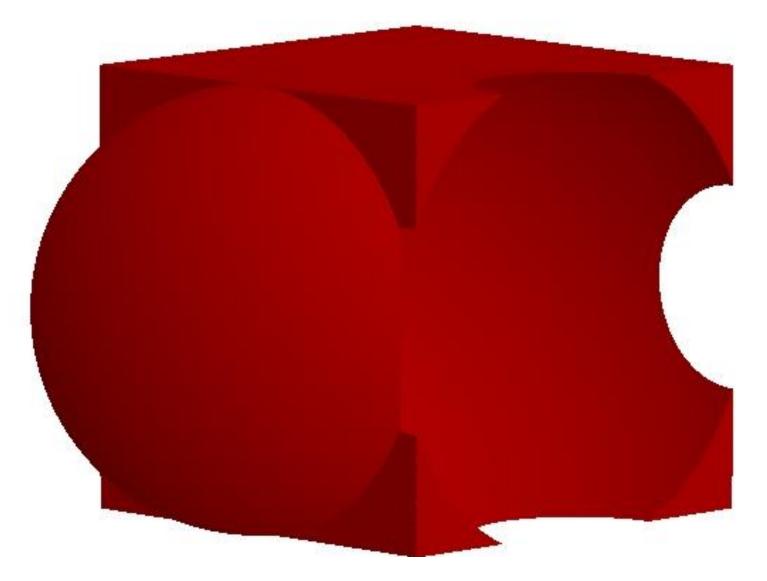
- Solids can be combined using boolean operations:
  - G4UnionSolid, G4SubtractionSolid, G4IntersectionSolid
  - Requires: 2 solids, 1 boolean operation, and an (optional) transformation for the 2<sup>nd</sup> solid
  - 2<sup>nd</sup> solid is positioned relative to the coordinate system of the 1<sup>st</sup> solid
  - Result of boolean operation becomes a solid. Thus a third solid can be combined with the resulting solid of first operation.
- Solids to be combined can be either CSG or other Boolean solids.
- <u>Note</u>: tracking cost for the navigation in a complex Boolean solid is proportional to the number of constituent CSG solids



#### **Boolean Solids - example**

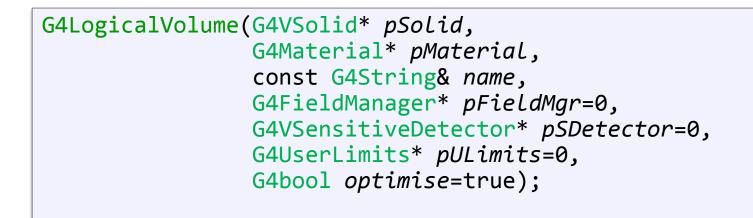
```
G4VSolid* box = new G4Box("Box",50*cm,60*cm,40*cm);
G4VSolid* cylinder =
    new G4Tubs("Cylinder",0.,50.*cm,50.*cm,0.,2*M PI*rad);
G4VSolid* union =
    new G4UnionSolid("Box+Cylinder", box, cylinder);
G4VSolid* subtract =
    new G4SubtractionSolid("Box-Cylinder", box, cylinder,
        0, G4ThreeVector(30.*cm,0.,0.));
G4RotationMatrix* rm = new G4RotationMatrix();
rm->RotateX(30.*deg);
G4VSolid* intersect =
    new G4IntersectionSolid("Box&&Cylinder",
        box, cylinder, rm, G4ThreeVector(0.,0.,0.));
```

#### **Boolean Solids**



Alternative: Unified solids (Geant4 10.0)

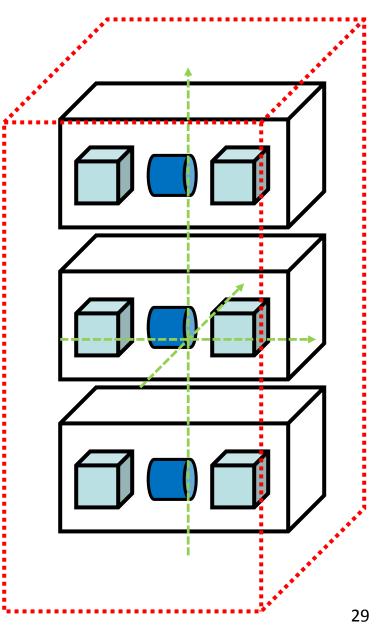
#### **G4LogicalVolume**



- Contains all information of volume except position:
  - Shape and dimension (G4VSolid)
  - Material, sensitivity, visualization attributes
  - Position of daughter volumes
  - Magnetic field, User limits
- <u>Physical volumes of same type can share a logical volume</u>.
- The pointers to solid and material must not be null!

#### **Geometrical hierarchy**

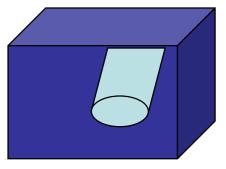
- It forms a tree.
- There is just one physical **world volume** forming a root of the tree:
  - The world volume defines the global coordinate system. The origin of the global coordinate system is at the center of the world volume
  - Position of a track is given with respect to this coordinate system
  - It contains all other volumes (with no protruding!)
- One logical volume can be placed more than once.
- One or more volumes can be placed in one mother volume.
- There must be no overlapping or protrusion.
- G4LogicalVolume carries the information about daughter volumes => if it is placed more than once, all daughters by definition appear in each physical instance



# **Physical Volumes**

A physical volume is a positioned instance of a logical volume inside a another logical volume (the mother volume).

• G4PVPlacement: a single positioned volume Note that a Placement Volume can still represent multiple detector elements, if several copies exist of the mother logical volume



G4PVPlacement

- Repeated Volumes: a single physical volume represents multiple copies of a volume within its mother volume
  - G4PVReplica (= simple repetition)
  - G4PVParameterised (= more complex)
    - G4PVDivision

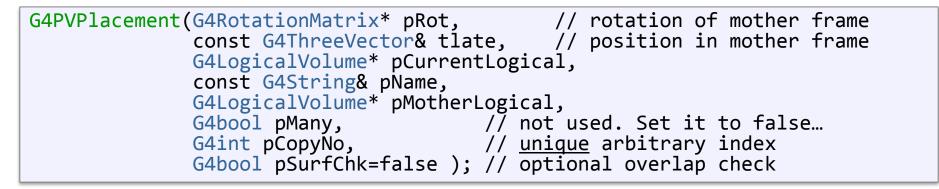
**G4PVParameterised** 

#### **G4PVPlacement**

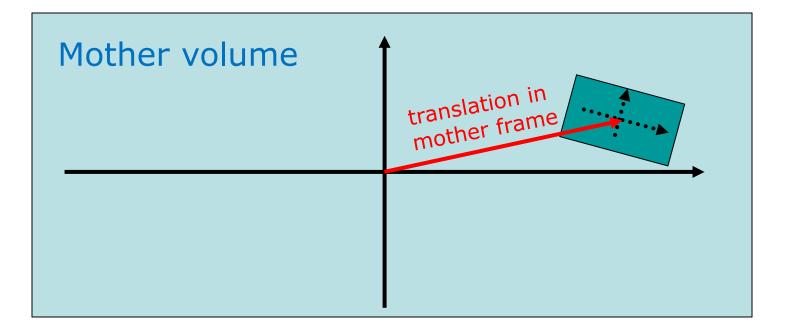
- Single volume positioned relatively to the mother volume
  - In a frame rotated and translated relative to the coordinate system of the mother volume
- Four constructors:
  - logical OR physical volume as mother
  - active OR passive transformation of the coordinate system

#### **G4PVPlacement**

#### Rotation <u>of</u> mother frame ...

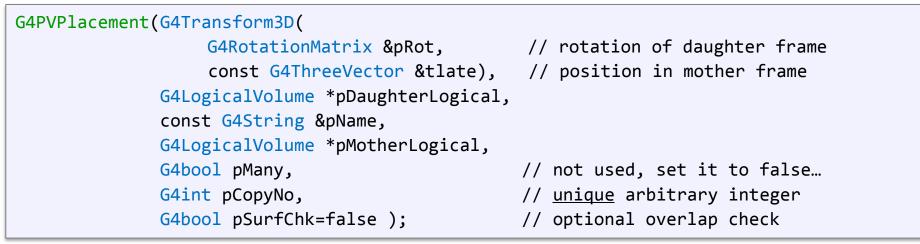


• Single volume positioned relatively to the mother volume (passive transformation)

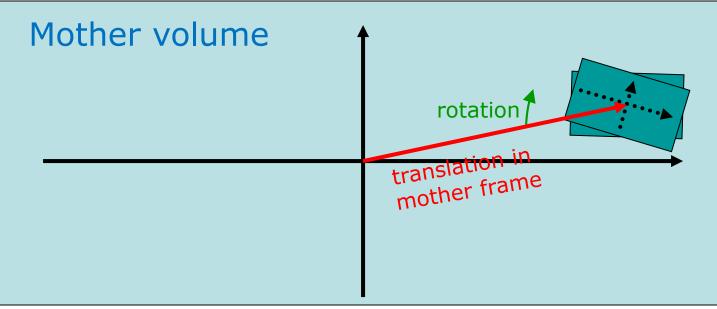


#### **G4PVPlacement**

#### Rotation <u>in</u> mother frame ...



Single volume positioned relatively to the mother volume (active transformation)



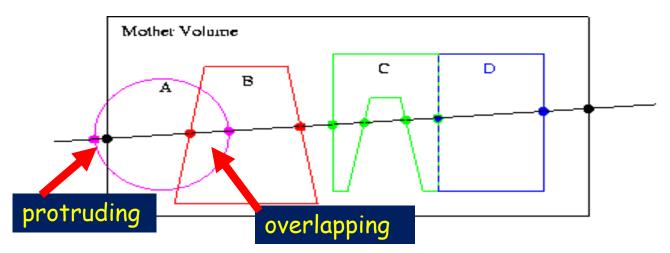
#### Regions

- A **region** is a collection of related logical volumes collected together independent of the geometry tree
- A region may have its unique
  - Production thresholds (cuts)
    - If a region in the mass geometry does not have its own production thresholds, those of the default region are used (i.e., may not be those of the parent region).
  - User limits
    - Artificial limits affecting to the tracking, e.g. max step length, max number of steps, min kinetic energy left, etc.
    - Limits assigned to logical volumes have priority though
  - Fast simulation manager
  - Field manager

Please note :

 World logical volume is recognized as the default region. User is not allowed to define a region to the world logical volume.

#### **Problems in geometry**



- Geant4 does not allow malformed geometries, neither protruding nor overlapping.
  - The behavior of navigation is unpredictable for such cases!
- Overlap become an important issue in complex geometries.
- There are tools for detecting wrong positioning:
  - Optional checks at construction
  - Kernel run-time commands
  - Graphical tools (DAVID, OLAP)

## **Tools for geometry checking**

• Constructors of G4PVPlacement and G4PVParameterised have an optional argument "pSurfChk".

G4PVPlacement(G4RotationMatrix\* pRot, const G4ThreeVector &tLate, G4LogicalVolume \*pDaughterLogical, const G4String &pName, G4LogicalVolume \*pMotherLogical, G4bool pMany, G4int pCopyNo, G4bool pSurfChk=false);

If this flag is true, overlap check is done at the construction:

some number of points are randomly sampled on the surface of creating volume.

This check requires lots of CPU time, but it is worth to try at least once.

Built-in run-time commands to activate verification tests for the user geometry:
 /geometry/test/run or /geometry/test/grid\_test

to start verification of geometry for overlapping regions based on a standard grid setup, limited to the first depth level

/geometry/test/recursive\_test

applies the grid test to all depth levels (may require lot of CPU time!)

/geometry/test/line\_test

to shoot a line along a specified direction and position

#### **Tools for geometry checking**

```
void MGManagerDetectorConstruction::CheckOverlaps()
                                                                                    Source
{
  G4PhysicalVolumeStore* thePVStore = G4PhysicalVolumeStore::GetInstance();
  G4cout << thePVStore->size() << " physical volumes are defined" << G4endl;
  G4bool overlapFlag = false;
  G4int res = 1000;
  G4double tol = 0.; // tolerance
  for (size t i=0; i<thePVStore->size(); i++)
  {
      overlapFlag = (*thePVStore)[i]->CheckOverlaps(res,tol,fCheckOverlapsVerbosity)
           overlapFlag;
  }
  if (overlapFlag)
      G4cout << "Check: there are overlapping volumes" << G4endl:
}
Checking overlaps for volume BeamLineSupport ... OK!
                                                                                  Output
Checking overlaps for volume BeamLineCover ... OK!
Checking overlaps for volume BeamLineCover2 ... OK!
Checking overlaps for volume VacuumZone ... OK!
Checking overlaps for volume FirstScatteringFoil ... OK!
   ----- WWWW ------ G4Exception-START ------ WWWW -
*** G4Exception : GeomVol1002 issued by : G4PVPlacement::CheckOverlaps()
Overlap with volume already placed !
         Overlap is detected for volume BrassTube2
         with HoleNozzleSupport volume's
         local point (12.6381,12.8171,-25.1867), overlapping by at least: 3.5 mm
*** This is just a warning message
        WWWW -----
                        This method can be called at any point after run->Initialize();
```

#### **Navigation in fields**

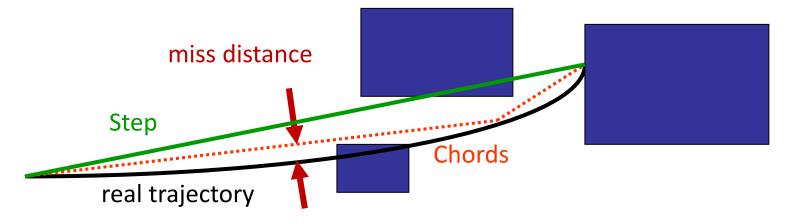
- In order to propagate a particle inside a field (e.g. magnetic, electric or both), we integrate the equation of motion of the particle in the field
  - Most common approach: Runge-Kutta (RK) method
  - RK methods of different orders are available (most common: 4th)
  - In specific cases, other solvers can also be used
- Geant4 breaks up this curved path into linear chord segments:



- Chord segments are determined so that they closely approximate the curved path; they're chosen so that their sagitta is small enough
  - The *sagitta* is the maximum distance between the curved path and the straight line

## Navigation in fields (2)

- Chords are used to interrogate the Navigator
  - to see whether the track has crossed a volume boundary
  - one step can consist of more than one chord



- Correctness of the navigation can be tuned by setting parameters:
  - miss distance: upper bound for sagitta
  - **delta intersection:** max error at intersection
  - **delta one step:** max error in position in general
- Setting the values too low has bad impact on CPU!

#### **Example: Uniform magnetic field**

In the MyDetector::ConstructSDAndField() method:

• Create the field itself:

G4MagneticField\* magField = new G4UniformMagField(G4ThreeVector(1.\*Tesla, 0., 0.));

• Register the field to the global field manager:

```
G4FieldManager* globalFieldMgr =
    G4TransportationManager::GetTransportationManager()
    ->GetFieldManager();
globalFieldMgr->SetDetectorField(magField);
```

• Crete a chord finder for it:

globalFieldMgr->CreateChordFinder(magField);

#### **Example: Non-uniform magnetic field**

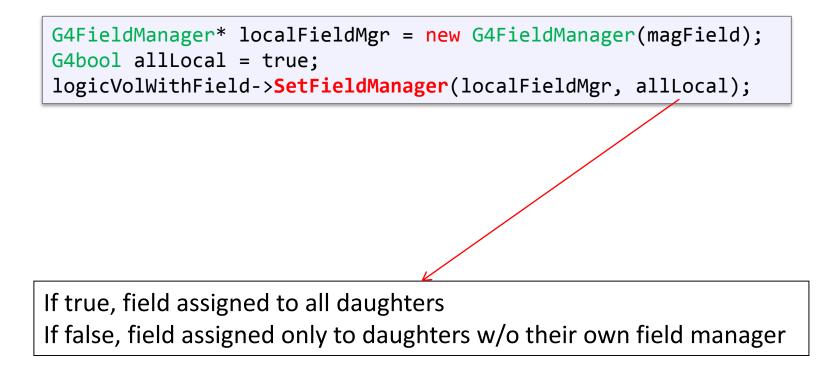
- Create a class, derived from G4MagneticField
  - override the GetFieldValue method:

```
void MyField::GetFieldValue(
    const G4double point[4], G4double *field) const
{
    // Artificial example
    G4double k = 1 * tesla / m;
    field[0] = k * point[1];
    field[1] = k * point[0];
    field[2] = 0;
}
```

- Then follow as in the uniform field case
- Note: point as well as field values are in global coordinates!

#### Assign a field to a logical volume

- It is possible to describe a field for a specific logical volume (and its daughters):
  - Create a local **G4FieldManager** and attach it to the logical volume:



#### Conclusion

- Geant4 has very broad range of capabilities for geometry description:
  - extensible set of units
  - complex hierarchy of volumes
  - many types of solids and their combinations
  - material description down to isotope level
  - magnetic (and other) field description

That's all, let's get practical!

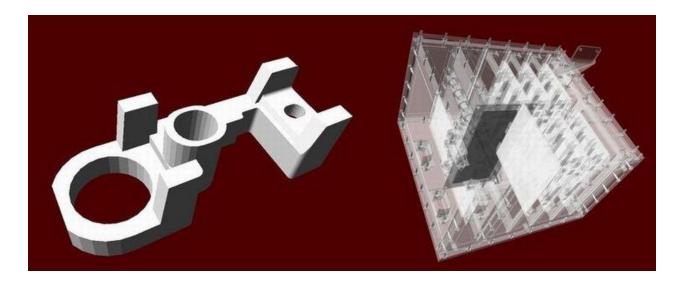
### Optional Advanced Additional... ...Topics

### **GDML / CAD**

- GDML is a XML-based format that enables to describe many aspects of geometry
  - you can load the geometry from external file
  - you can also save the geometry to an external file
  - includes materials, solids, logical & physical volumes

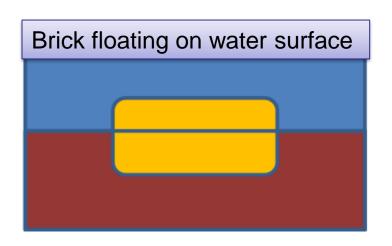
examples/extended/persistency/gdml

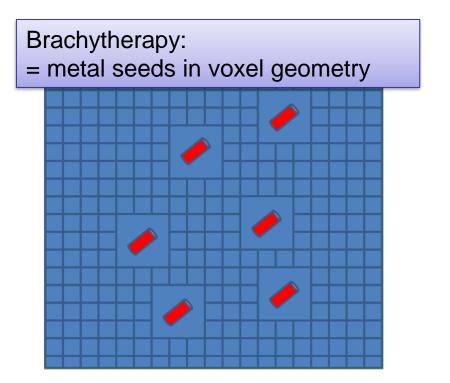
• To import **CAD**, you can construct the geometry using the G4TessellatedSolid class, see documentation.



#### **Parallel worlds**

- Implementation is complex (not to be covered here)
- Advantages for construction & navigation
- Two examples:





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