Materials and Geometry

Davide Chiappara
University of Padova (UNIPD)
Istituto Nazionale di Fisica Nucleare (INFN)

Mandatory User's classes – v1

Initialisation classes

Invoked at the initialisation

G4VUserDetectorConstruction
G4VUserPhysicsList

Action classes

Invoked during the execution loop

G4VUserPrimaryGeneratorAction

G4UserRunAction
G4UserEventAction
G4UserTrackingAction
G4UserStackingAction
G4UserSteppingAction

Note: Geant4 basic types

Aliases for the **primitive data types** to provide cross-platform compatibility:

G4double, **G4float**, **G4int**, **G4bool**, **G4long**

Enhanced version of string called **G4String**

inherits from **std::string** ⇒ all methods and operators

several additional methods

G4ThreeVector is a three-component class corresponding to a real physics vector (example later)

```
G4ThreeVector dimensions {1.0, 2.0, 3.0 };
```

Please, use these types for best compatibility (e.g. **G4int** instead of int, etc., **G4ThreeVector** when it makes sense etc.)

Part I: Units and 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** library (included in Geant4):

- ▶ CLHEP/SystemOfUnits.h
- ▶ G4SystemOfUnits.hh

You can define new units (not shown here)

Output data in terms of a specific unit:

divide a value by the unit

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

System of units

Basic units:

- nanosecond (ns)
- unit charge (eplus)
- megaelectronvolt (MeV)
- radian
- kelvin
- millimetre (mm)
- candela
- steradian

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");
```

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

Materials

Different levels of material description:

isotopes → **G4Isotope**
elements → **G4Element**
molecules, 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, cross-sections 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

Making elements

Isotopes can be assembled into elements

```
G4Isotope (const G4String& name,
                 G4int      z,      // atomic number
                 G4int      n,      // number of nucleons
                 G4double   a );    // mass of mole
```

Not number of neutrons!

Do not forget unit (g/mole)

… building elements as follows:

```
G4Element (const G4String& name,
           const G4String& symbol, // element symbol
           G4int      nIso );      // n. of isotopes

G4Element::AddIsotope(G4Isotope* iso,  // isotope
            G4double relAbund); // fraction of atom per volume
```

Otherwise, create **G4Element** with natural isotopic abundance:

```
G4Element (const G4String& name,
           const G4String& symbol,
           G4int      z,    // atomic number
           G4double   a );  // mass of mole
```

Do not forget unit (g/mole)

Elements and compounds

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);
```

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);
```

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="O", 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 mixtures

```
G4Element* elC   = …;    // define “carbon” element
G4Material* SiO2 = …;   // define “quartz” material
G4Material* H2O = …;    // define “water” material
density = 0.200*g/cm3;

G4Material* aerogel = new G4Material("Aerogel", density, ncomponents=3);
aerogel->AddMaterial(SiO2,fractionmass=62.5*perCent);
aerogel->AddMaterial(H2O, fractionmass=37.4*perCent);
aerogel->AddElement (elC, fractionmass= 0.1*perCent);
```

An example: a gas

Necessary to specify temperature and pressure
affect **dE/dx** calculations, thermal scattering

```
G4double density = 27. * mg/cm3;
G4double temperature = 325. * kelvin;
G4double pressure = 50. * atmosphere;

G4Material* CO2 = new G4Material("CO2Gas", density,
    ncomponents=2, kStateGas, temperature, pressure);
CO2->AddElement(C, natoms = 1);
CO2->AddElement(O, natoms = 2);
```

Absolute vacuum does not exist: gas at very low ρ !
Cannot define materials with ρ=0

```
G4double rho = 1.e-25*g/cm3;
G4double pr = 3.e-18*pascal;
G4Material* Vacuum = new G4Material(“interGalactic",Z, A,
rho, kStateGas, temperature, pr);
```

NIST material database

No need to predefine elements and materials

Retrieve elements and 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");
G4Element* Si = manager->FindOrBuildElement("Si");
```

UI commands:

```
/material/nist/printElement
```
← print defined elements

```
/material/nist/listMaterials
```
← print defined materials

▶ G4NistManager.hh

NIST material database

NIST database for materials is imported inside Geant4

http://physics.nist.gov/PhysRefData

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		A	m	error	(%)	A_{eff}
14	Si	22	22.03453	(22)		28.0855(3)
		23	23.02552	(21)		
		24	24.011546	(21)		
		25	25.004107	(11)		
		26	25.992330	(3)		
		27	26.98670476	(17)		
		28	27.9769265327	(20)	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

https://geant4-userdoc.web.cern.ch/UsersGuides/ForApplicationDeveloper/html/GettingStarted/materialDef.html#access-to-geant4-material-database

NIST materials

NIST elementary materials:

H → Cf (Z = 1 → 98)

NIST compounds:

e.g. “G4_ADIPOSE_TISSUE_IRCP”

HEP and Nuclear materials:

e.g. Liquid Ar, PbWO

Possible to build **mixtures** of NIST and user-defined materials

```
=====================================
###  Elementary Materials from the NIST Data
==================================
 Z Name  ChFormula       density(g/cm^3)  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_O   O_2            0.00133151      95
9   G4_F                  0.00158029      115
10  G4_Ne                 0.000838505     137
11  G4_Na                 0.971           149
```

```
==================================
###   Compound Materials from the NIST Data Base
==================================
 N Name      ChFormula        density(g/cm^3)  I(eV)
==================================
13  G4_Adipose_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                          0.00120479    85.7
             6    0.000124
             7    0.755268
             8    0.231781
            18    0.012827
2  G4_CsI                          4.51          553.1
            53    0.47692
            55    0.52308
```

Part II: Geometry

- *Basic concepts*
- *Implementation*
- *Tools for geometry checking*

Describe your Detector

- A detector geometry is made of a number of volumes
  - The largest volume is called **World** volume
    - It **must** contain all other volumes
- Derive your own concrete class from **`G4VUserDetectorConstruction`** abstract base class
  - Implementing the pure virtual method **`Construct()`**:
    - Define shapes/solids required to describe the geometry
    - Construct all necessary materials
    - Construct and place volumes of your detector geometry
    - (Define "sensitivity" properties associated to volumes)
    - (Associate magnetic field to detector regions)
    - (Define visualization attributes for the detector elements)

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 and methods! (good programming practice)

especially for complex geometries!

Note2: you should not delete the **MyDetector** instance! 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**!

▶ `G4VUserDetectorConstruction.hh`

Method **`ConstructSDAndField()`**

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

Three Conceptual Layers

G4VSolid

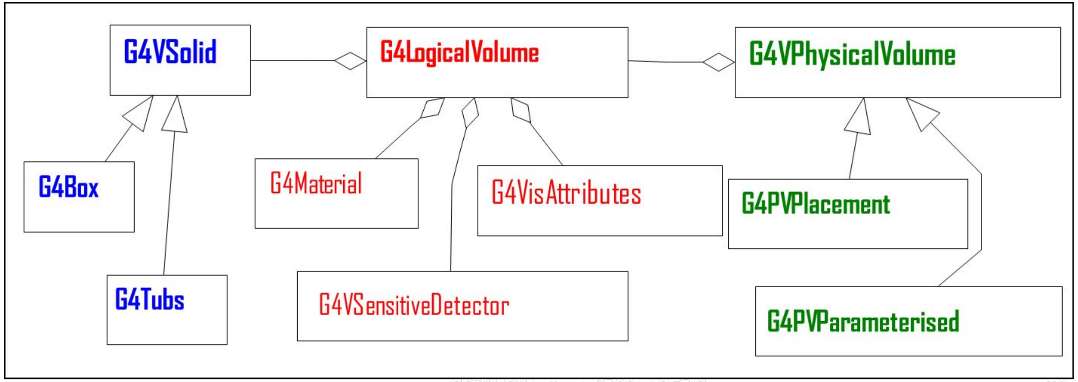
Shape, *size*

G4LogicalVolume

Hierarchy of volumes, *material*, *sensitivity*, magnetic field

G4VPhysicalVolume

Position, *rotation*. The same logical volume can be *placed many times* (repeated modules)



Define Detector Geometry

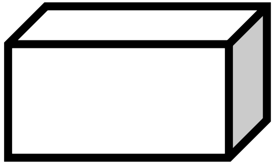
Basic strategy

```
G4VSolid* pBoxSolid =

  new G4Box("aBoxSolid",

        1.*m, 2.*m, 3.*m);
```

Solid: shape and size.



Step 1
Create the geom. object: box

Step 2
Assign properties to object : material

Define Detector Geometry

Basic strategy

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

```
G4LogicalVolume* pBoxLog =
   new G4LogicalVolume( pBoxSolid,
   pBoxMaterial, "aBoxLog", 0, 0, 0);
```

Logical volume : + material, sensitivity, etc.

Step 1
Create the geom. object: box

Step 2
Assign properties to object : material

Define Detector Geometry

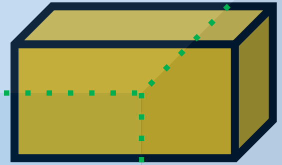
Basic strategy

```
G4VSolid* pBoxSolid =
   new G4Box(“aBoxSolid”,
          1.*m, 2.*m, 3.*m);
```

```
G4LogicalVolume* pBoxLog =
    new G4LogicalVolume( pBoxSolid,
    pBoxMaterial, “aBoxLog”, 0, 0, 0);
```

```
G4VPhysicalVolume* aBoxPhys =
     new G4PVPlacement(pRotation,
     G4ThreeVector(posX, posY, posZ), pBoxLog,“aBoxPhys”,
      pMotherLog, 0, copyNo);
```

Physical volume : + rotation and position



Step 1
Create the geom. object: box

Step 2
Assign properties to object : material

Step 3
Place it in the coordinate system of mother volume

Solids

CSG (Constructed Solid Geometry) solids

G4Box, G4Tubs, G4Cons, G4Trd, …

Analogous to simple GEANT3 CSG solids

Specific solids (CSG like)

G4Polycone, G4Polyhedra, G4Hype, …

G4TwistedTubs, G4TwistedTrap, …

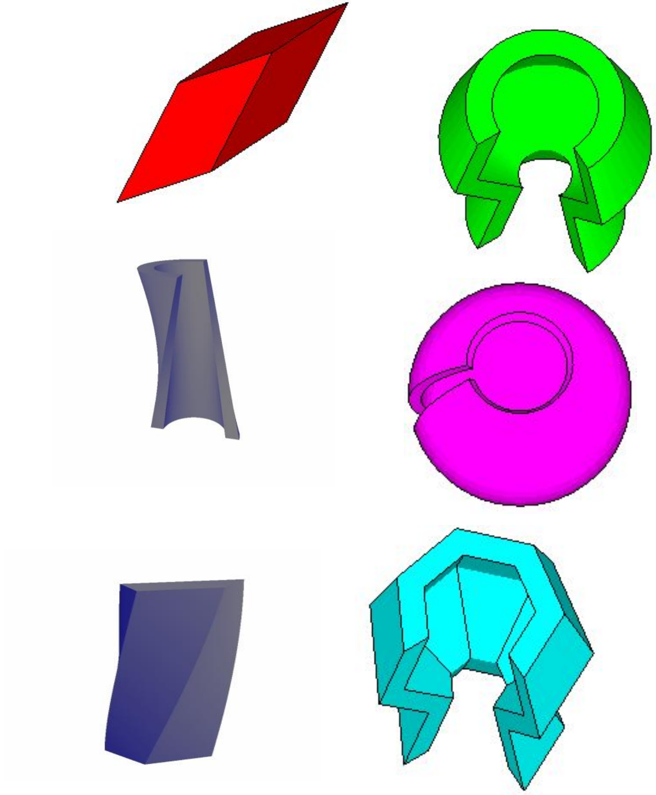
BREP (Boundary REPresented) solids

G4BREPSolidPolycone, G4BSplineSurface, …

Any order surface

Boolean solids

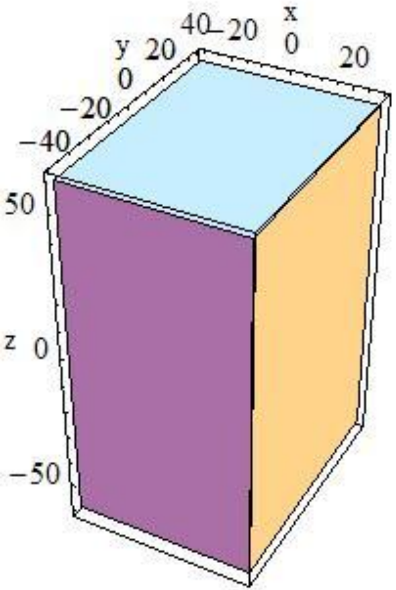
G4UnionSolid, G4SubtractionSolid, …



CSG: G4Box

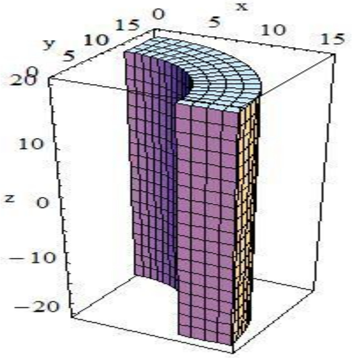
```
G4Box(const G4String& pname,   // name
              G4double  pX, // half-length in X
              G4double  pY, // half-length in Y
              G4double  pZ, // half-length in Z);
```

Note the half-length!

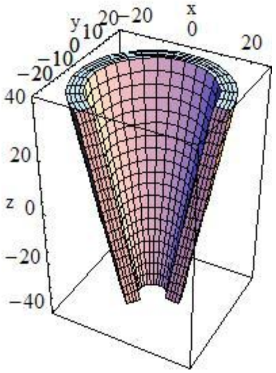


CSG: G4Tubs & G4Cons

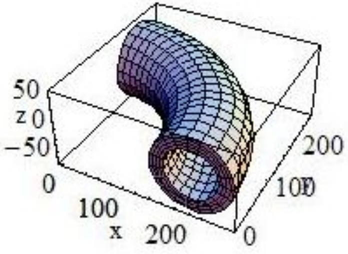
```
G4Tubs(const G4String& pname,   // name
             G4double  pRmin,   // inner radius (0)
             G4double  pRmax,   // outer radius
             G4double  pDz,     // Z half! length
             G4double  pSphi,   // starting Phi (0)
             G4double  pDphi);  // segment angle (twopi)
```



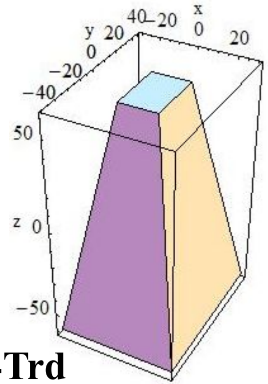
```
G4Cons(const G4String& pname,   // name
             G4double  pRmin1,  // inner radius -pDz
             G4double  pRmax1,  // outer radius -pDz
             G4double  pRmin2,  // inner radius +pDz
             G4double  pRmax2,  // outer radius +pDz
             G4double  pDz,     // Z half length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



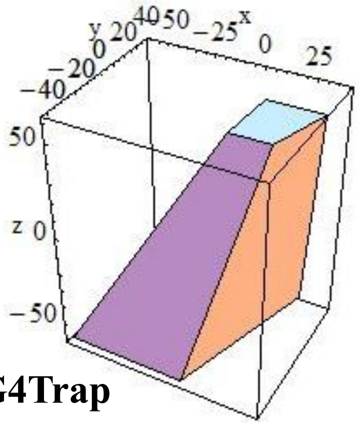
Other CSG Solids



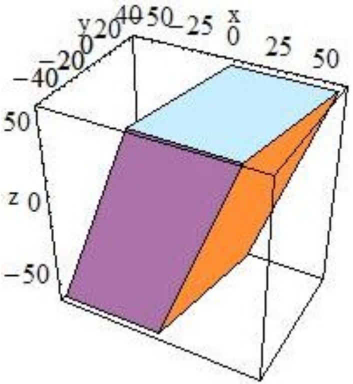
G4Torus



G4Trd

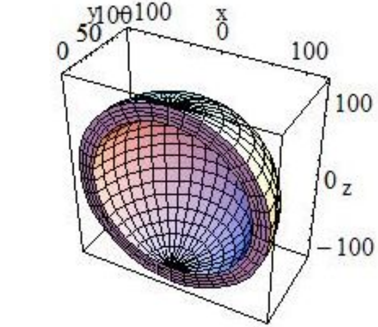


G4Trap

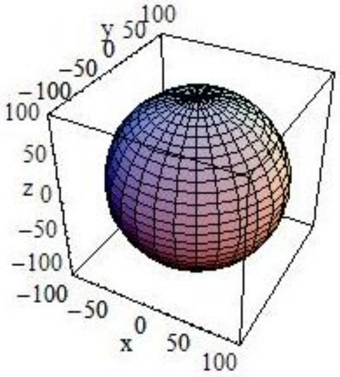


G4Para
(parallelepiped)

G4Sphere



G4Orb
(full solid sphere)



Check **Section 4.1.2** of Geant4 Application Developers Guide for all available shapes

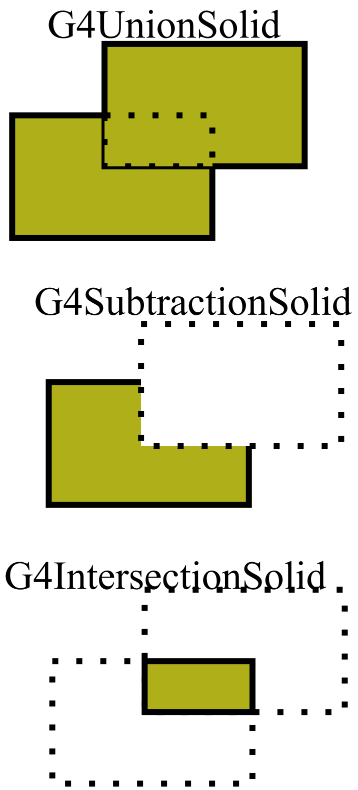
Boolean Solids

Solids can be **combined** using **boolean operations**:

- `G4UnionSolid`, `G4SubtractionSolid`, `G4IntersectionSolid`
- Requires: 2 solids, 1 boolean operation, and an (optional) transformation for the 2nd solid
- 2nd solid is positioned relative to the coordinate system of the 1st solid
- Result of boolean operation becomes a solid → re-usable in a boolean operation

Solids to be combined can be either CSG or other Boolean solids

Note: tracking **cost** for the navigation in a complex Boolean solid is proportional to the number of constituent CSG solids



Boolean Solids - an Example

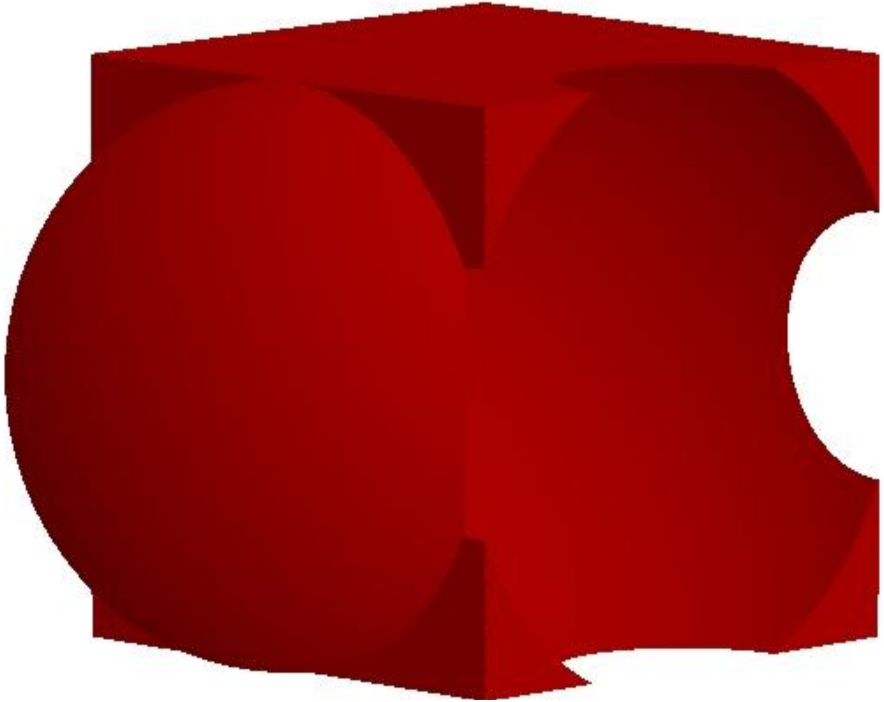
```
G4VSolid* box = new G4Box("Box",50*cm,60*cm,40*cm);
G4VSolid* cylinder =
    new G4Tubs("Cylinder",0.,50.*cm,50.*cm,0.,twopi);

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 Solid - Example



Logical Volumes

Contains all information of volume **except position:**

- Shape and dimension (**`G4VSolid`**)
- Material, sensitivity, visualization attributes
- Position of daughter volumes
- Magnetic field, User limits

Physical volumes of same type **can share** a logical volume.

The pointers to solid and material must be **not nullptr**

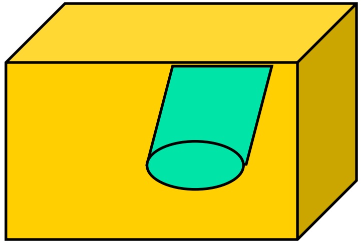
```
G4LogicalVolume(G4VSolid* pSolid,
                G4Material* pMaterial,
                const G4String& name,
                G4FieldManager* pFieldMgr=0,
                G4VSensitiveDetector* pSDetector=0,
                G4UserLimits* pULimits=0,
                G4bool optimise=true);
```

optional

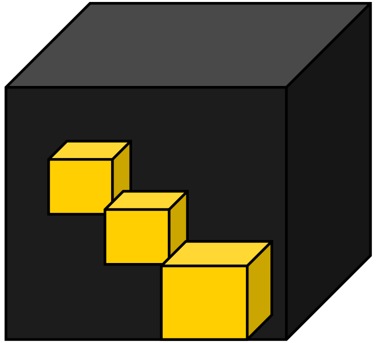
Physical Volumes

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

- Placement (**`G4PVPlacement`**)
  - it is **one** positioned volume
- Repeated: a volume placed **many times**
  - can represent any number of volumes
  - reduces use of memory
  - **`G4PVReplica`** (= simple repetition)
  - **`G4PVParameterised`** (= more complex pattern)
    - **`G4PVDivision`**



placement



repeated

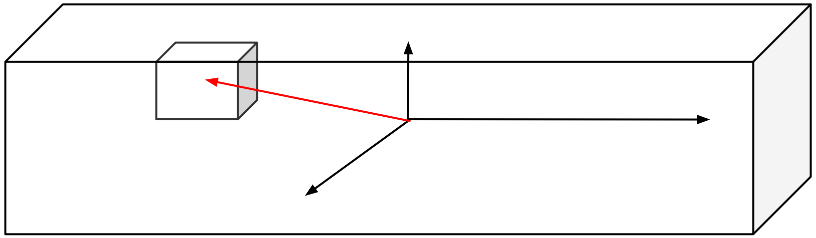
Geometry Hierarchy

A volume is placed in its mother volume

- Position and rotation of the daughter volume is described with respect to the local coordinate system of the mother volume
- The origin of the mother's local coordinate system is at the center of the mother volume
- Daughter volumes cannot protrude from the mother volume
- Daughter volumes cannot overlap

The logical volume of mother knows the daughter volumes it contains

- It is uniquely defined to be their mother volume



Geometry Hierarchy

One logical volume can be placed **more than once**. One or more volumes can be placed in a mother volume

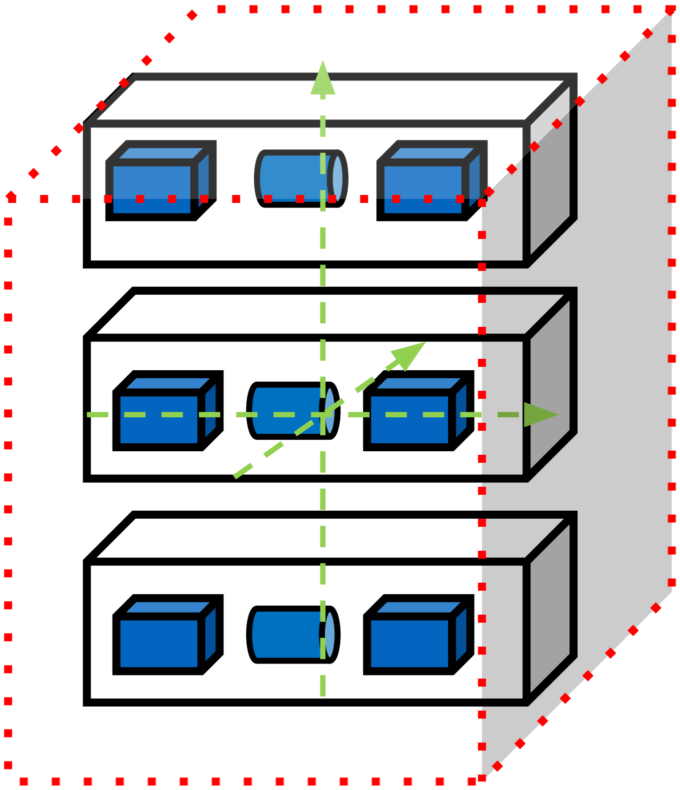
The mother-daughter relationship is an information of **`G4LogicalVolume`**

- If the mother volume is placed more than once, all daughters by definition appear in each placed physical volume

The **world volume** must be a unique physical volume which fully contains all other volumes (root volume of the hierarchy)

- 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 the global coordinate system



G4PVPlacement

Single volume positioned **relatively** to the mother volume

- In a frame rotated and translated relative to the coordinate system of the mother volume

A few variants available:

- Using `G4Transform3D` to represent the direct rotation and translation of the solid instead of the frame (*alternative constructor*)
- specifying the mother volume as a pointer to its physical volume instead of its logical volume

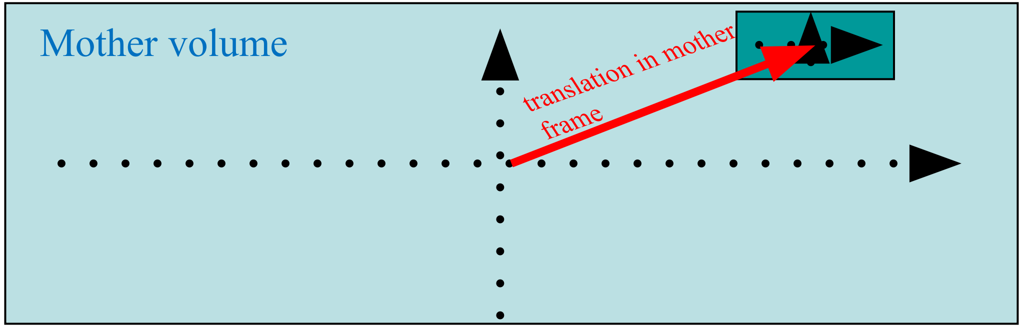
Four constructors available

- **logical** OR **physical** volume as mother
- **active** OR **passive** transformation of the coordinate system

G4PVPlacement: Rotation **of** mother frame …

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

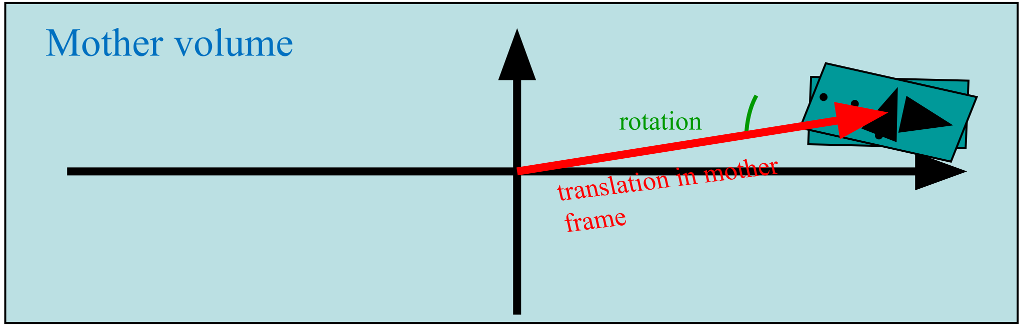
```
G4PVPlacement(G4RotationMatrix* pRot,          // rotation of mother frame
              const G4ThreeVector& tlate,     // position in mother frame
              G4LogicalVolume* pCurrentLogical,
              const G4String& pName,
              G4LogicalVolume* pMotherLogical,
              G4bool pMany,                   // not used. Set it to false…
              G4int pCopyNo,                  // unique arbitrary index
              G4bool pSurfChk=false );        // optional overlap check
```



G4PVPlacement: Rotation **in** mother frame …

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

```
G4PVPlacement(G4Transform3D(
                   G4RotationMatrix &pRot,          // rotation in daughter frame
                   const G4ThreeVector &tlate),     // position in mother frame
              G4LogicalVolume *pDaughterLogical,
              const G4String &pName,
              G4LogicalVolume *pMotherLogical,
              G4bool pMany,                        // not used, set it to false…
              G4int pCopyNo,                       // unique arbitrary integer
              G4bool pSurfChk=false );             // optional overlap check
```



Bird's eye on repeated volumes

Placement volume (**`G4PVPlacement`**): one positioned volume

- One physical volume represents one "*real*" volume

Repeated volume: a volume placed many times

- One physical volume represents any number of "*real*" volumes
  - Reduced *use of memory*
  - Very convenient for *large voxelized* geometries
- Parametrized (repetitions w.r.t. copy number)
  - **`G4VPVParameterisation`**
- Replicas and Divisions (**`G4PVReplica`**, **`G4PVDivision`**)

Note: a repeated volume is **not equivalent** to a loop of placements

- All placements of the loop exists individually in the memory

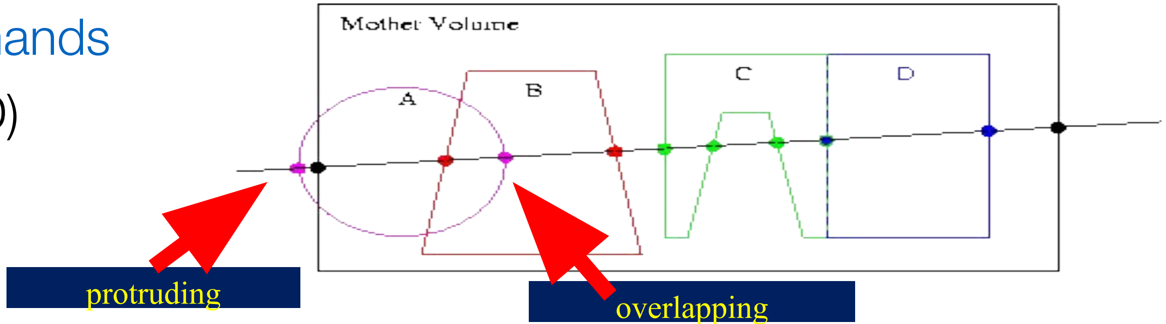
Geometry Problems

Geant4 does not allow for **malformed geometries**, neither protruding (daughter/mother) not overlapping (sisters)

- The behavior of navigation is **unpredictable** for such cases

The problem of detecting overlaps between volumes is bounded by the complexity of the solid models description

- Utilities are provided for detecting wrong positioning
  - Optional checks at construction
    - Kernel run-time commands
    - Graphical tools (DAVID)



Tools for Geometry Check

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**

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

/geometry/test/recursive_test for all depth levels (CPU intesive!)

Tools for Geometry Check

Source

```
void MyDetectorConstruction::CheckOverlaps()
{
  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;
}
```

Output

```
Checking overlaps for volume BeamLineSupport ... OK!
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-

Regions

A **region** is a **sub-set** of the geometry

It may have its specific

- Production thresholds (cuts)
- User limits
  - Artificial limits affecting to the tracking, e.g. max step length, max number of steps, min kinetic energy left, etc.
- Field manager

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

===> Task1

Link to the Tasks:

http://geant4.lns.infn.it/pavia2023/task1/index.html

Task 1 - Geometry

- Defining and using materials
- Constructing a volume using solids, logical and physical volumes
- Magnetic fields