

Materials and Geometry

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User Classes

Initialisation classes

Invoked at the initialization

- G4VUserDetectorConstruction
- G4VUserPhysicsList

Global: **only one instance** of them exists in memory, shared by all threads (**readonly**). Managed only by the **master** thread.

Action classes

Invoked during the execution loop

- G4VUserActionInitialization
 - G4VUserPrimaryGeneratorAction
 - G4UserRunAction (*)
 - G4UserEventAction
 - G4UserTrackingAction
 - G4UserStackingAction
 - G4UserSteppingAction

Local: an **instance** of each action class exists **for each thread**.

(*) Two RunAction's allowed: one for master and one for threads

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](#)

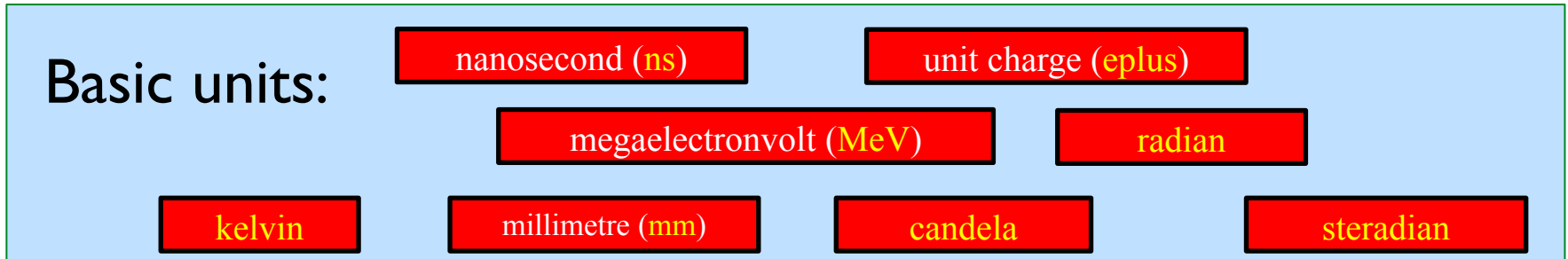
You can define new units (not shown here)

Output data in terms of a specific unit:

divide a value by the unit

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

System of units



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 $\rho=0$

```
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!**



Method **ConstructSDAndField ()**

Assign **magnetic field** to volumes / regions

Define **sensitive detectors** and assign them to volumes

▶ G4VUserDetectorConstruction.hh

Three Conceptual Layers

G4VSolid

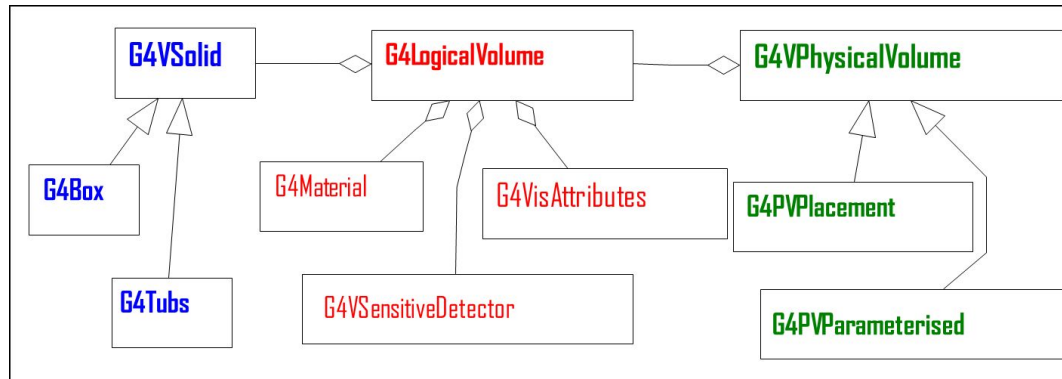
Shape, size

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

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

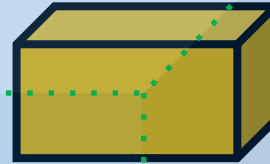
Basic strategy

```
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

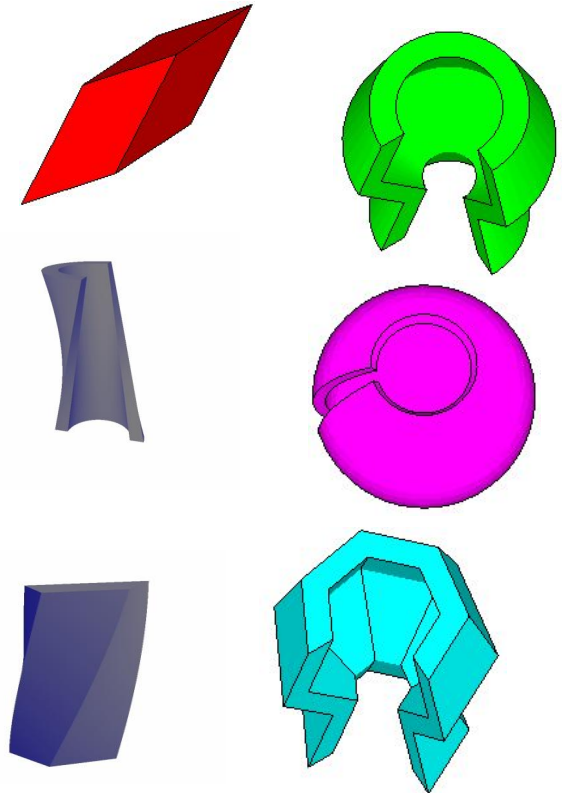
Solids

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

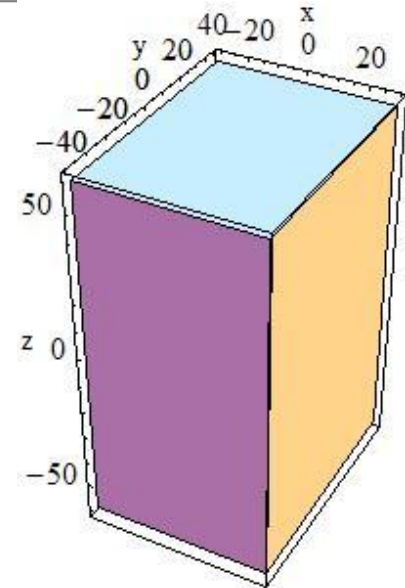
Boolean solids
G4UnionSolid, G4SubtractionSolid, ...



CSG: G4Box

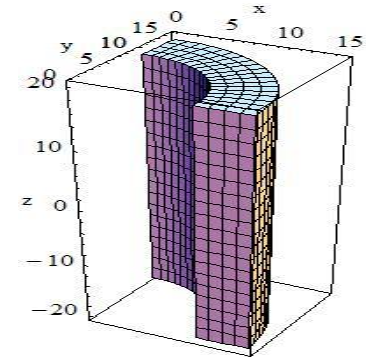
```
G4Box(const G4String& pname, // name  
      G4double pX, // half-length in X  
      G4double pY, // half-length in Y  
      G4double pZ, // half-length in Z);
```

Note the half-length!

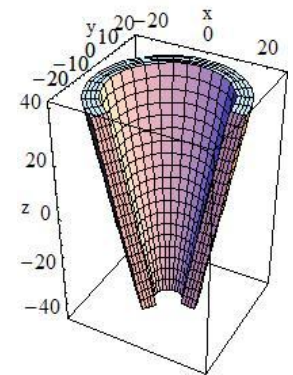


CSG: G4Tubs & G4Cons

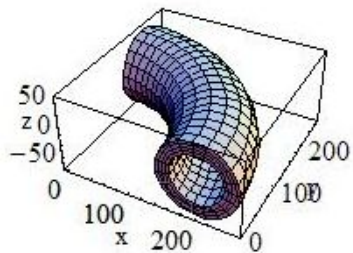
```
G4Tubs (const G4String& pname, // name
        G4double pRmin, // inner radius (0)
        G4double pRmax, // outer radius
        G4double pDz, // Z half! length
        G4double pSphi, // starting Phi (0)
        G4double pDphi); // segment angle (twopi)
```



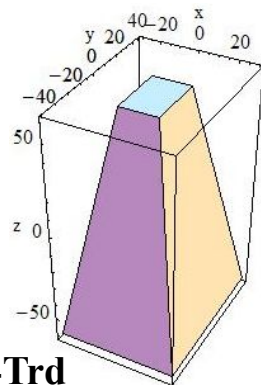
```
G4Cons (const G4String& pname, // name
        G4double pRmin1, // inner radius -pDz
        G4double pRmax1, // outer radius -pDz
        G4double pRmin2, // inner radius +pDz
        G4double pRmax2, // outer radius +pDz
        G4double pDz, // Z half length
        G4double pSphi, // starting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



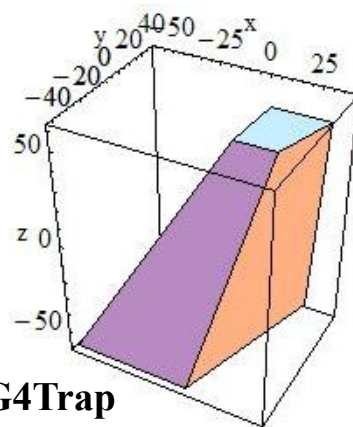
Other CSG Solids



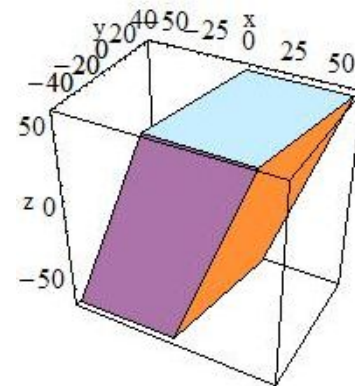
G4Torus



G4Trd

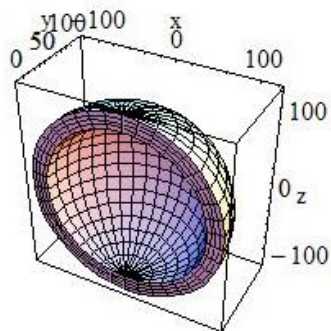


G4Trap

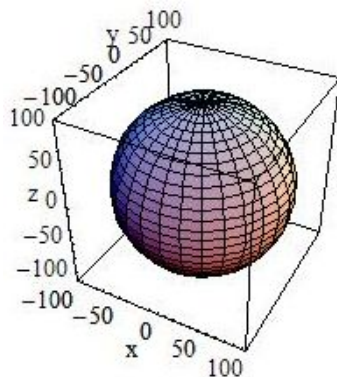


G4Para
(parallelepiped)

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

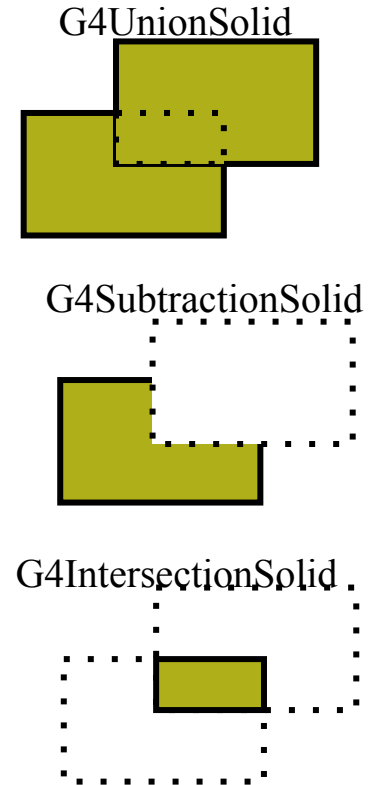
Requires: 2 solids, 1 boolean operation, and an (optional) transformation for the 2nd solid

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

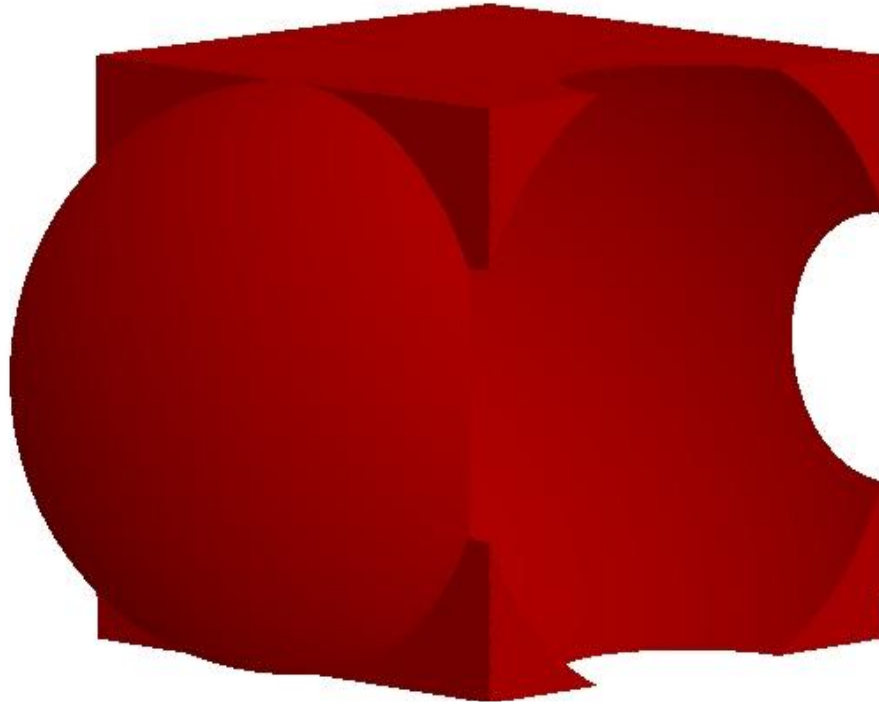
```
G4VSolid* box = new G4Box("Box",50*cm,60*cm,40*cm);
G4VSolid* cylinder =
    new G4Tubs("Cylinder",0.,50.*cm,50.*cm,0.,twopi);

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

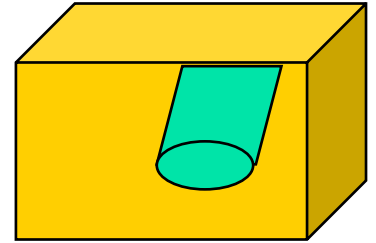
can represent any number of volumes

reduces use of **memory**

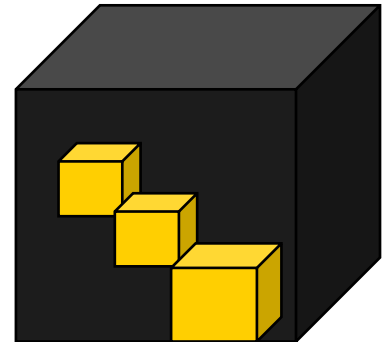
G4PVReplica (= simple repetition)

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

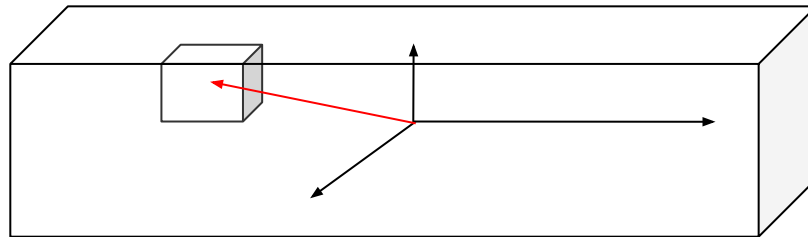
The **origin** of the mother's local coordinate system is at the **center** of the mother volume

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

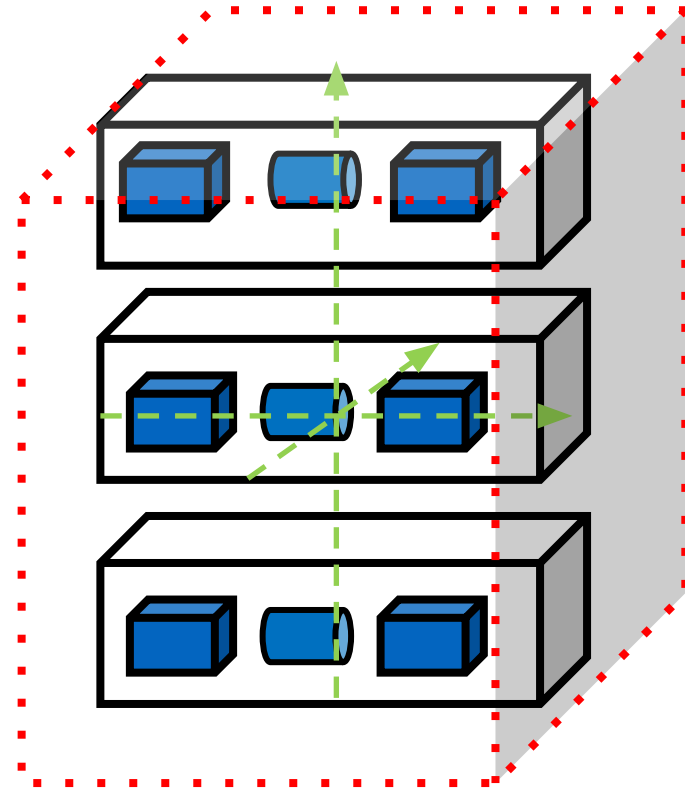
The **mother-daughter relationship** is an information of **G4LogicalVolume**

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

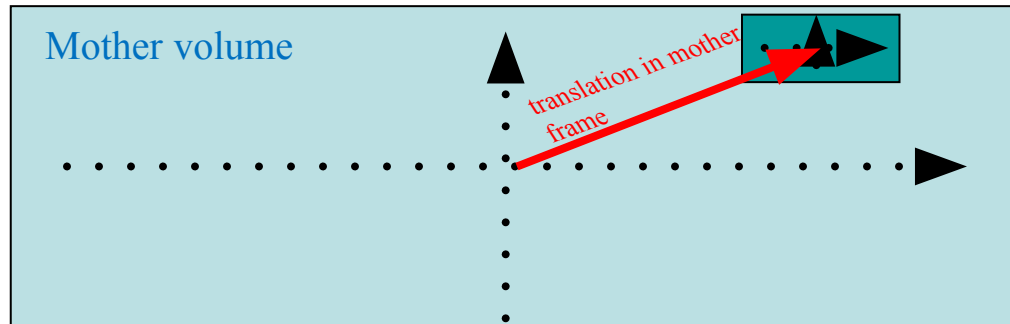
logical OR physical volume as mother

active OR passive transformation of the coordinate system

G4PVPlacement: Rotation **of** mother frame ...

Single volume positioned relatively to the mother volume ([passive transformation](#))

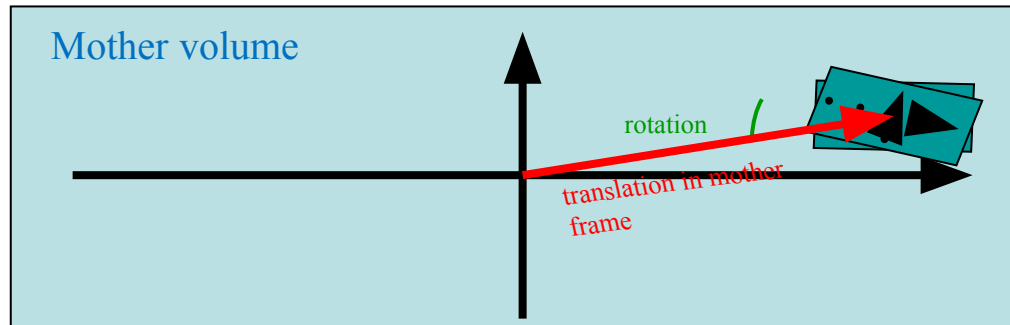
```
G4PVPlacement(G4RotationMatrix* pRot,          // rotation of mother frame
              const G4ThreeVector& tlate,      // position in mother frame
              G4LogicalVolume* pCurrentLogical,
              const G4String& pName,
              G4LogicalVolume* pMotherLogical,
              G4bool 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

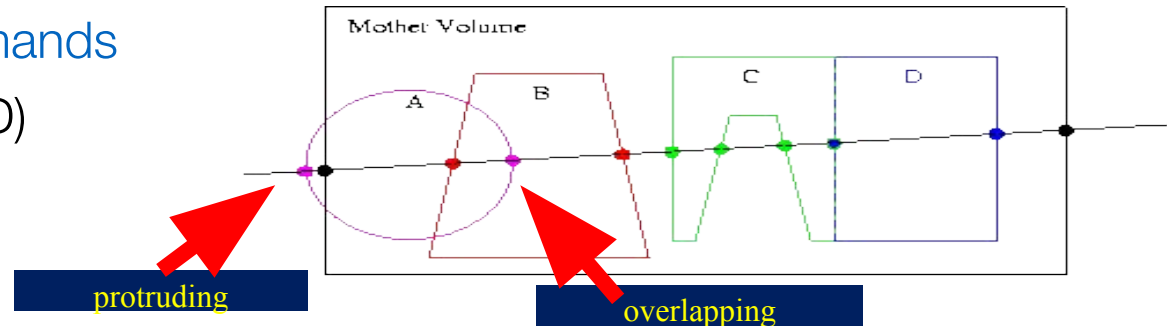
The problem of **detecting overlaps** between volumes is bounded by the complexity of the solid models description

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 intensive!)
```

Tools for Geometry Check

```
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;  
}
```

Source

```
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!
```

Output

```
.....  
----- WWWWW ----- G4Exception-START ----- WWWWW -  
*** 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 ***  
----- WWWWW -----
```

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

Task 1

Link to the Tasks:

<http://geant4.lns.infn.it/alghero2023/task1>

Task 1 - Geant4 geometry

Exercises

- **Task 1a Geant4 Materials**
- **Task 1b Geant4 Geometry: solids and placements**