# IX SEMINAR ON SOFTWARE FOR NUCLEAR, SUBNUCLEAR AND APPLIED PHISICS

Porto Conte, Alghero, Italy
28th May - 1th June 2012

# Detector description: materials and geometry


Geant 4 tutorial course

# Part I: Materials

## Materials:

- The System of units & constants
- Definition of elements
- Materials and mixtures
- Some examples …
- The NIST Data Base

# Units

- Geant4 has no default unit.
- To introduce the input data, unit **must** be “multiplied” to the number.
  - for example :

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

  - Almost all commonly used units are available.
  - The user can define new units.
  - Refer to CLHEP: `SystemOfUnits.h`
- To output the data you can **divide** a variable by a unit you want to get.

```
G4cout << dE / MeV << “ (MeV)” << G4endl;
```

# System of Units

- System of units are defined in CLHEP, based on:
  - millimetre (**`mm`**), nanosecond (**`ns`**), Mega eV (**`MeV`**), positron charge (**`eplus`**) degree Kelvin (**`kelvin`**), the amount of substance (**`mole`**), luminous intensity (**`candela`**), radian (**`radian`**), steradian (**`steradian`**)
- All other units are computed from the basic ones
- Alternative way to outpup data: Geant4 can choose the most appropriate unit to use. Just 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

# Defining new Units

- New units can be defined directly as constants, or (suggested way) via **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**
- To print the list of units:
  - From the code

    **G4UnitDefinition::PrintUnitsTable();**
  - At run-time, as UI command:

    **Idle> /units/list**

# Definition of 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, cross-sections per atoms, etc…
- **`G4Material`** describes the *macroscopic* properties of the matter:
  - temperature, pressure, state, density
  - Radiation length, absorption length, etc…
- **`G4Material`** is the only class used and visible to the toolkit: it is used by tracking, geometry and physics

# Elements and isotopes

- Isotopes can be assembled into elements

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

# 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("liquidArgon", z=18, a, density);
```

- A molecule is made of several elements (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);
```

# Compound and mixture

- Mixture: 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 compound materials

```
G4Element* elC  = …;    // define "carbon" element
G4Material* SiO2 = …;   // define "quartz" material
G4Material* H2O = …;    // define "water" material
density = 0.200*g/cm3;
G4Material* Aerog = new G4Material("Aerogel",density,ncomponents=3);
Aerog->AddMaterial(SiO2,fractionmass=62.5*perCent);
Aerog->AddMaterial(H2O ,fractionmass=37.4*perCent);
Aerog->AddElement (elC ,fractionmass= 0.1*perCent);
```

# Example: gas

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

```
G4double density = 27.*mg/cm3;
G4double temperature = 325.*kelvin;
G4double pressure = 50.*atmosphere;
G4Material* CO2 = new G4Material("CarbonicGas", 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 density !
  - Cannot define materials composed of multiple elements through **Z** or **A**, or with $\rho$=0

```
G4double atomicNumber = 1.;
G4double massOfMole = 1.008*g/mole;
G4double density = 1.e-25*g/cm3;
G4double temperature = 2.73*kelvin;
G4double pressure = 3.e-18*pascal;
G4Material* Vacuum = new G4Material("interGalactic",
 atomicNumber,massOfMole, density, kStateGas,temperature, pressure);
```

# NIST Material Data-Base in Geant4

- NIST database for materials is imported inside Geant4

  http://physics.nist.gov/PhysRefData
- Additional interfaces defined
- 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*

# NIST materials in Geant4

```
=====================================
###  Elementary Materials from the NIST Data Base
=====================================
 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
12  G4_Mg                    1.74            156
13  G4_Al                    2.6989          166
14  G4_Si                    2.33            173
```

```
=====================================
###  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
```

- 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**
- It is possible to build mixtures of NIST and user-defined materials

# How to use the NIST DB

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

```
G4NistManager* manager = G4NistManager::Instance();

G4Material* H2O = manager->FindOrBuildMaterial("G4_WATER");
```

- Some UI commands …

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

# Part II: Geometry

## Geometry:

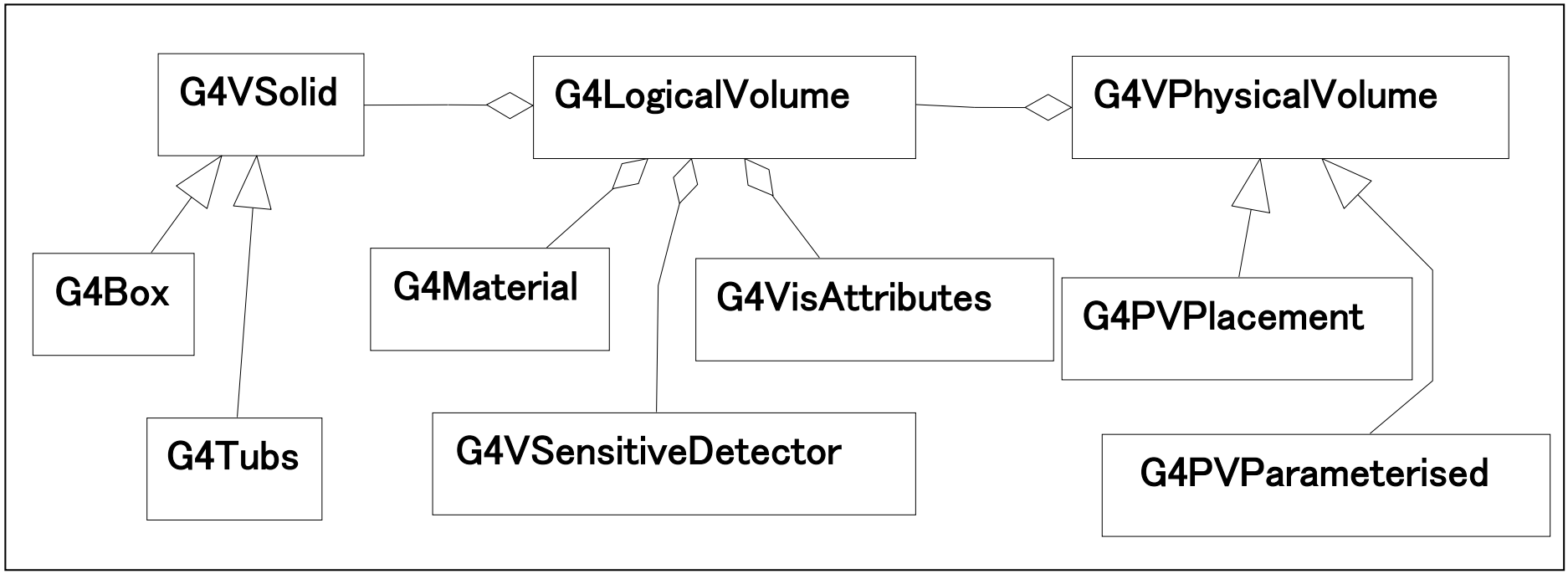
- Detector description: the basic
  - Detector geometry components
  - Define detector geometry
- Describing a detector
  - Solids
  - Logical volumes
  - Physical volumes
- Tools for geometry check

# Describe your detector

- Derive your own concrete class from `G4VUserDetectorConstruction` abstract base class.
- Implementing the method `Construct()`:
  - Modularize it according to each detector component or sub-detector:
    - Construct all necessary materials
    - Define shapes/solids required to describe the geometry
    - Construct and place volumes of your detector geometry
    - ➢ Define sensitive detectors and identify detector volumes which to associate them
    - ➢ Associate magnetic field to detector regions
    - ➢ Define visualization attributes for the detector elements

# Detector geometry components

- Three conceptual layers
  - G4VSolid -- *shape, size*
  - G4LogicalVolume -- *daughter physical volumes,*
    *material, sensitivity, magnetic field, etc.*
  - G4VPhysicalVolume -- *position, rotation*

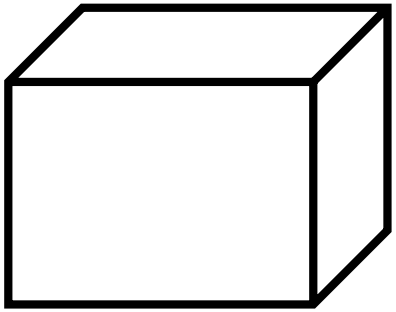


# Define detector geometry

- Basic strategy

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

Solid : shape and size



**Step 1**
Create the geom. object : box

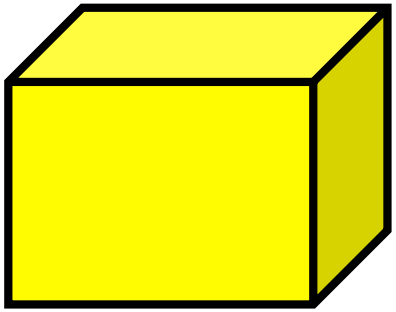
# Define detector geometry

- 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

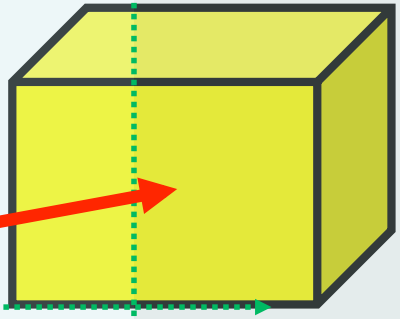
- Basic strategy

```
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

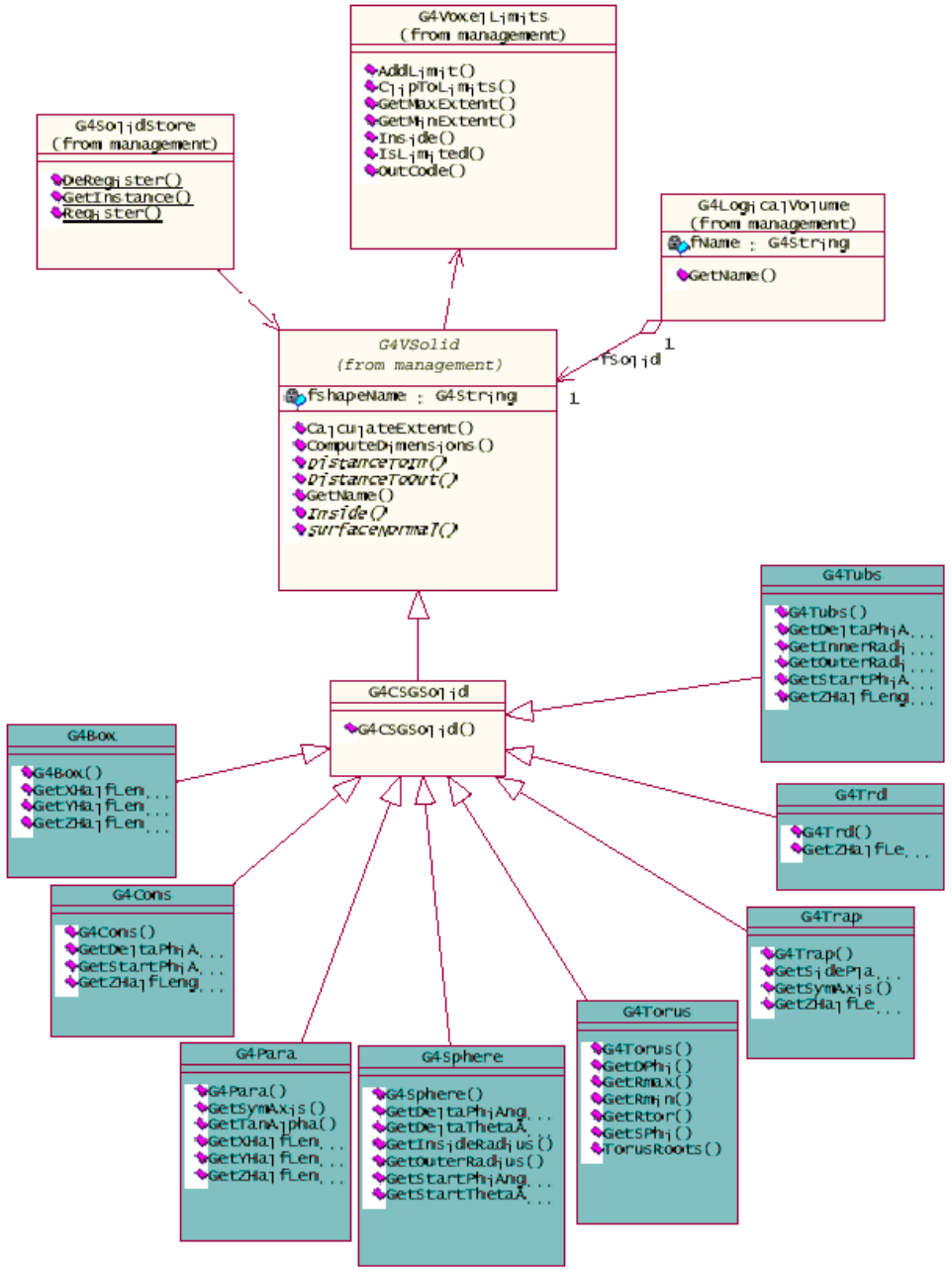
**Step 2**
Assign properties to object : material

**Step 3**
Place it in the coordinate system of mother volume

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

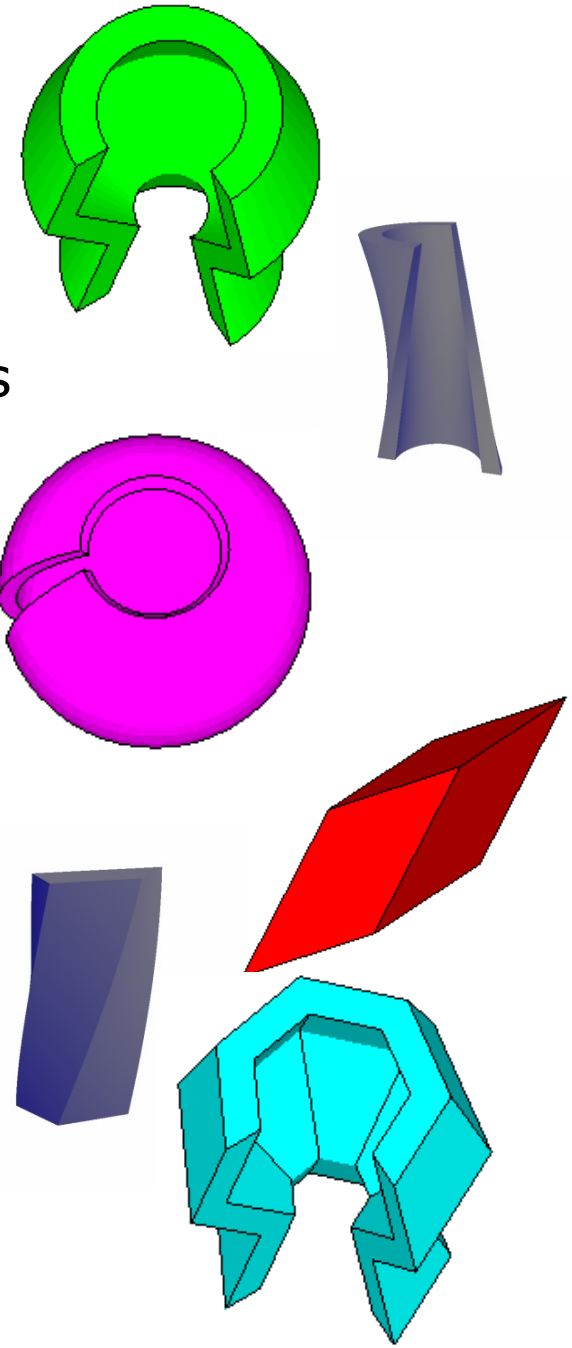
# G4VSolid

- Abstract class. All solids in Geant4 derive from it
  - Defines but does not implement all functions required to:
    - compute distances to/from the shape
    - check whether a point is inside the shape
    - compute the extent of the shape
    - compute the surface normal to the shape at a given point
- Once constructed, each solid is automatically registered in a specific solid store



# Solids

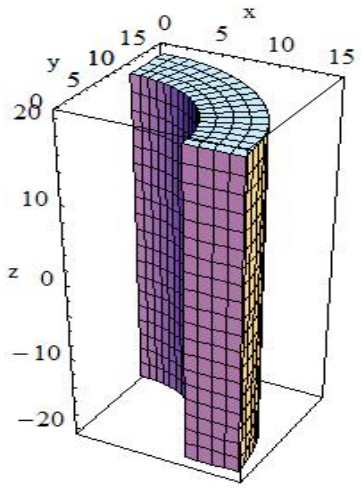
- Solids defined in Geant4:
  - CSG (Constructed Solid Geometry) solids
    - G4Box, G4Tubs, G4Cons, G4Trd, …
    - Analogous to simple GEANT3 CSG solids
  - Specific solids (CSG like)
    - G4Polycone, G4Polyhedra, G4Hype, ..
    - G4TwistedTubs, G4TwistedTrap, …
  - BREP (Boundary REPresented) solids
    - G4BREPSolidPolycone, G4BSplineSurface, …
    - Any order surface
  - Boolean solids
    - G4UnionSolid, G4SubtractionSolid, …

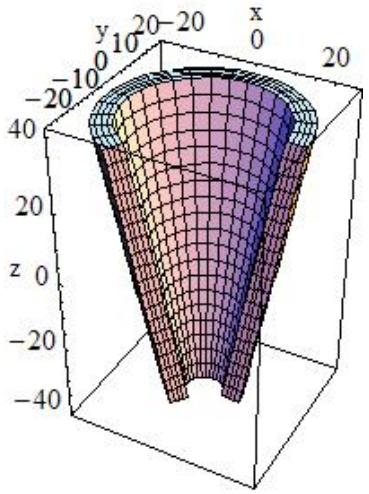


# CSG: G4Tubs, G4Cons

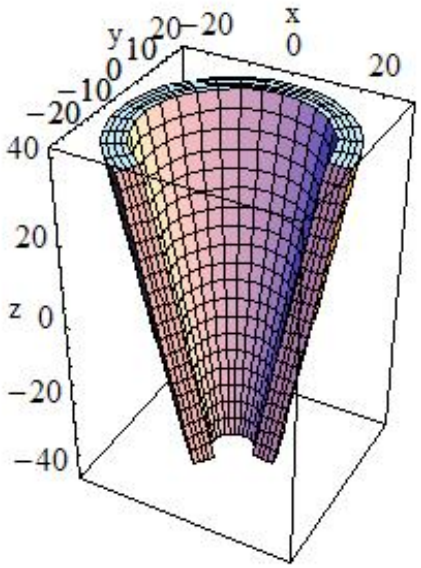
```
G4Tubs(const G4String& pname,   // name
               G4double  pRmin,   // inner radius
               G4double  pRmax,   // outer radius
               G4double  pDz,     // Z half length
               G4double  pSphi,   // starting Phi
               G4double  pDphi); // segment angle

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
               G4double  pSphi,   // starting Phi
               G4double  pDphi); // segment angle
```

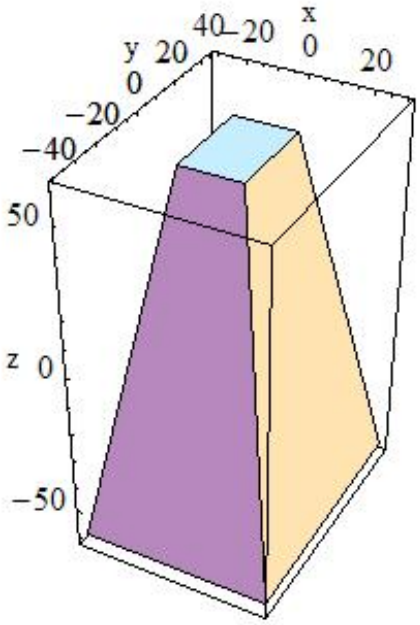


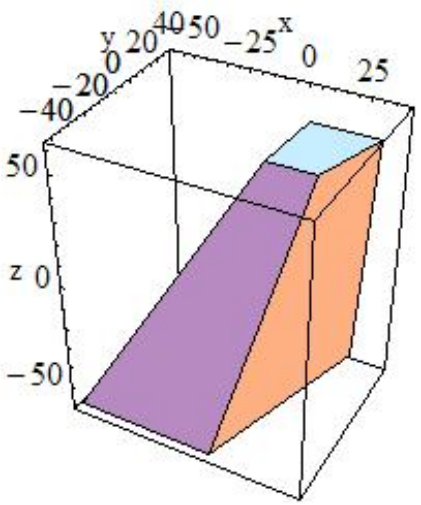
# Other CSG solids



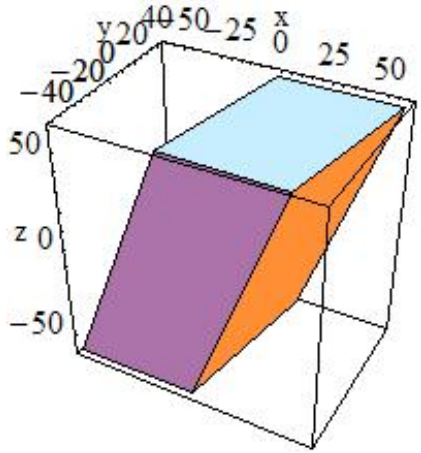
G4Cons



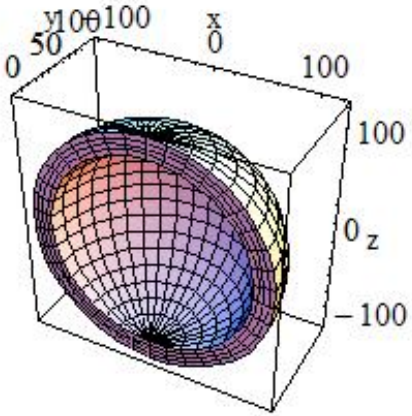
G4Trd



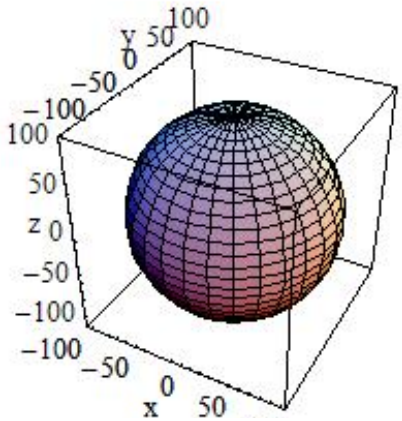
G4Trap



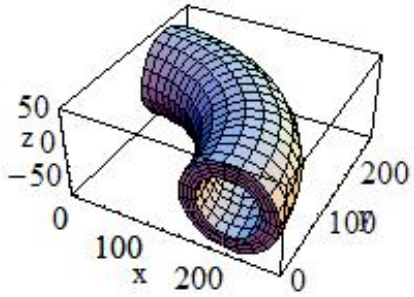
G4Para
(parallelepiped)



G4Sphere



G4Orb
(full solid sphere)

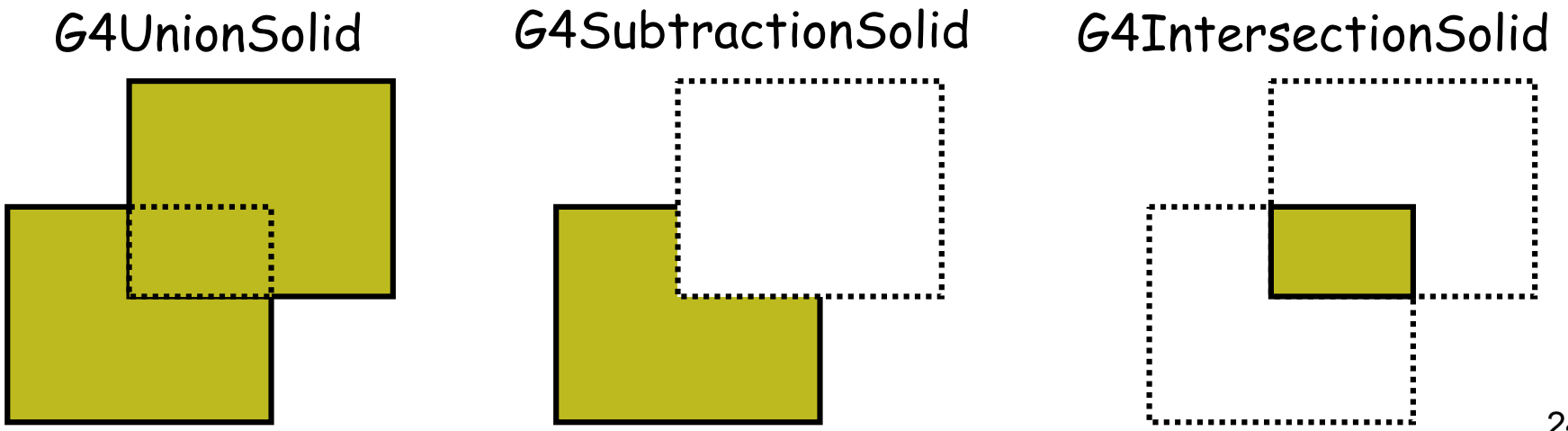


G4Torus

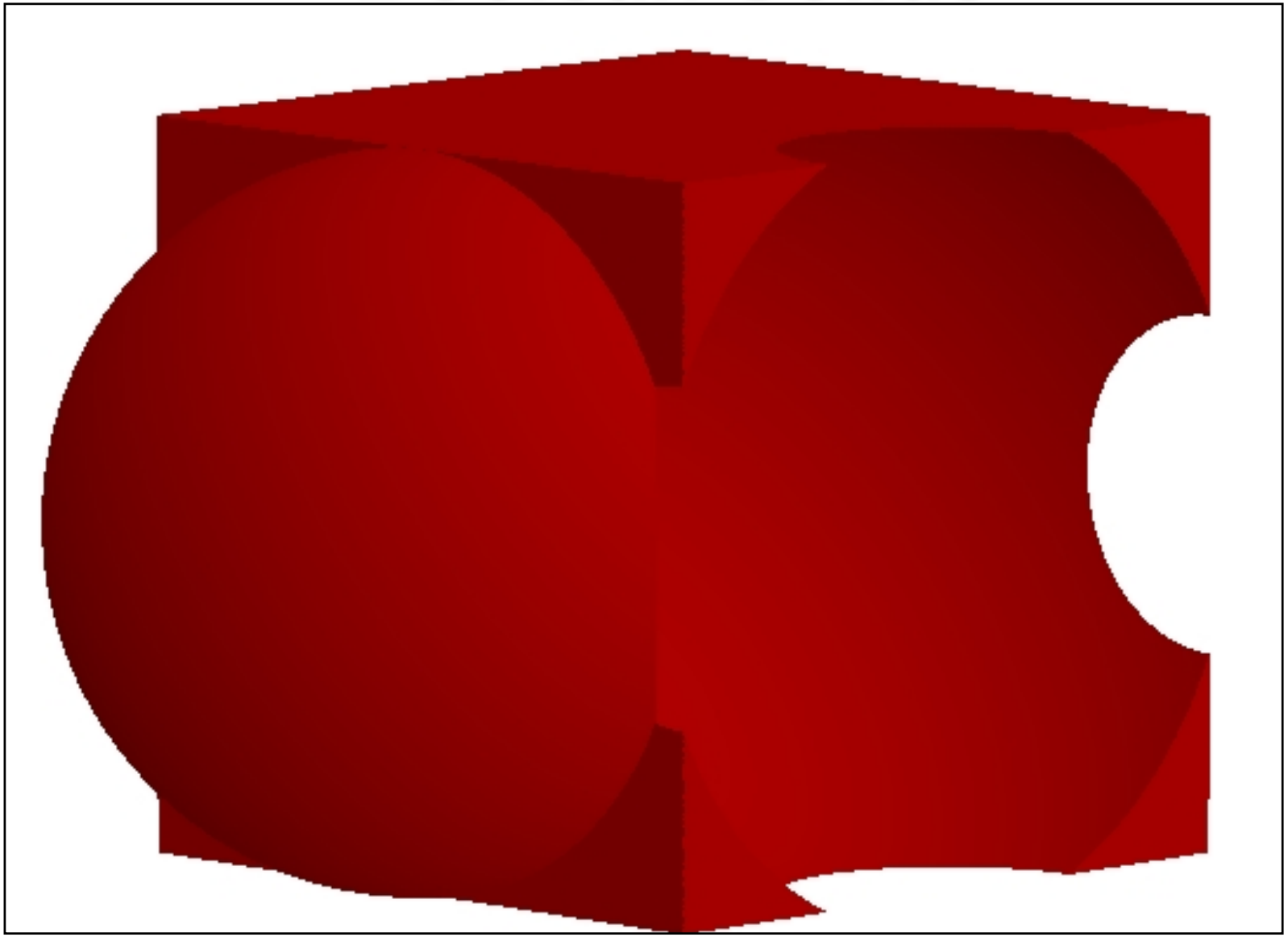
Consult to
[Section 4.1.2 of Geant4 Application Developers Guide ] for all available shapes.

# 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. Thus the third solid can be combined to the resulting solid of first 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



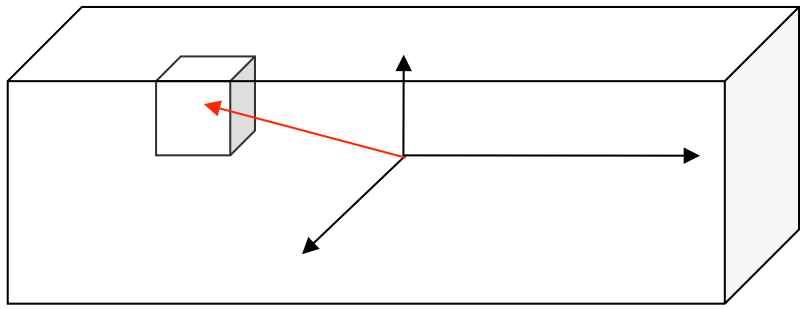
# G4LogicalVolume

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

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

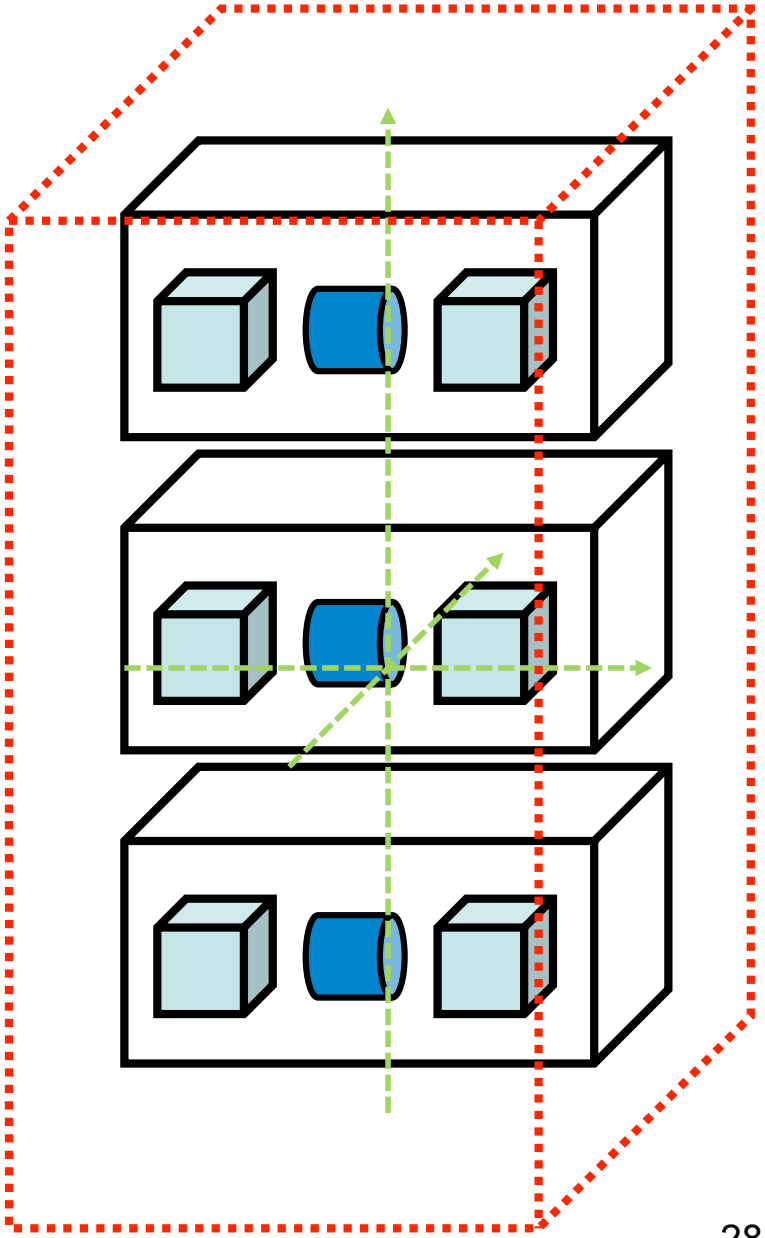
# Geometrical hierarchy

- Mother and daughter volumes
  - 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



# Geometrical hierarchy

- One logical volume can be placed more than once. One or more volumes can be placed in a mother volume
- Note that 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 with some margin all the 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

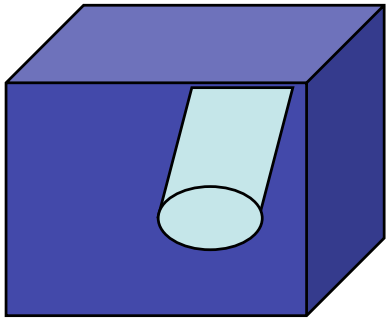


# Region

- 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.
    - You can set user limits directly to logical volume as well. If both logical volume and associated region have user limits, those of logical volume wins.
  - 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.

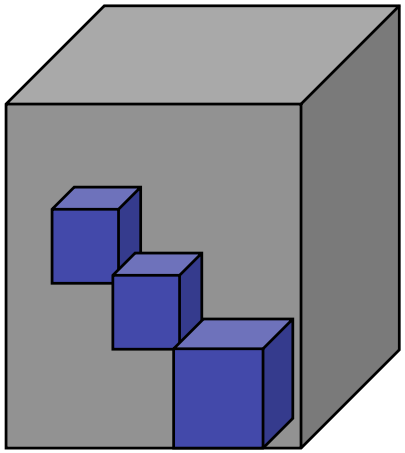
# Physical Volumes

- Placement: it is one positioned volume



*placement*

- Repeated: a volume placed many times
  - can represent any number of volumes
  - reduces  use of memory.
  - Replica
    - simple repetition, similar to G3 divisions
  - Parameterised



*repeated*

# G4PVPlacement

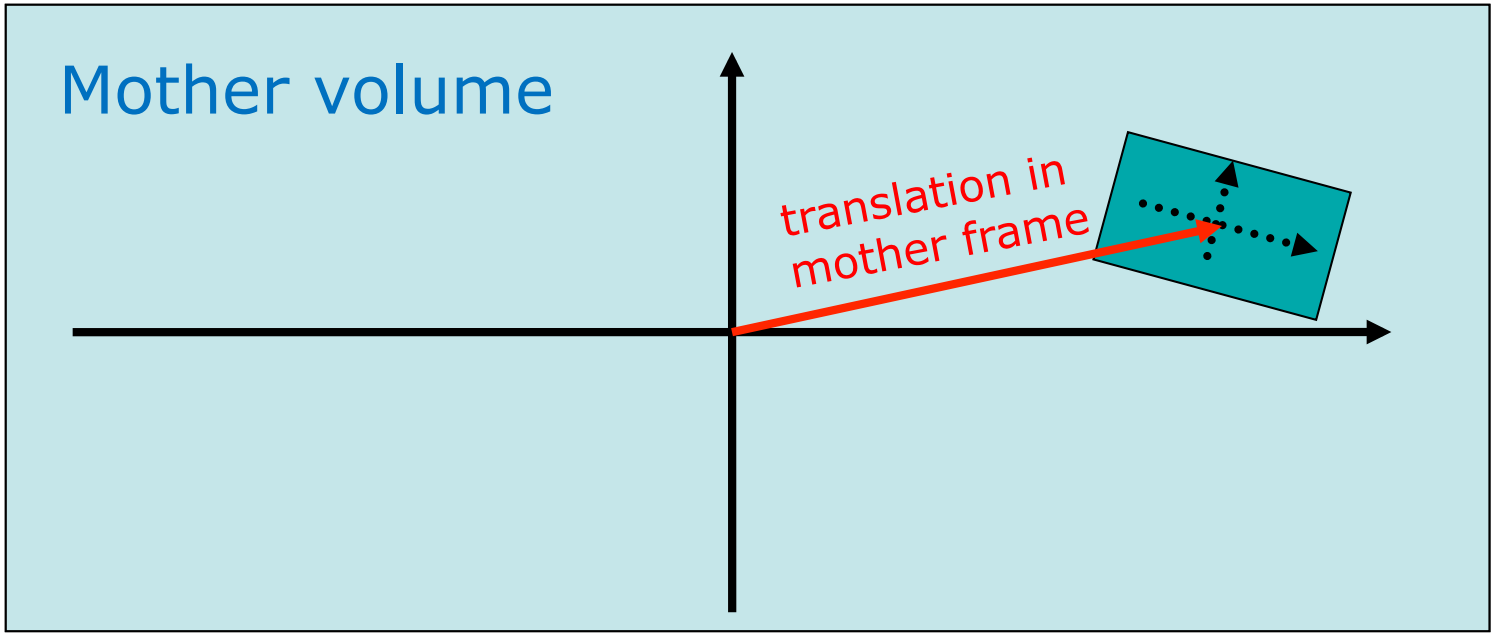
```
G4PVPlacement(G4RotationMatrix* pRot,     // rotation of mother frame
              const G4ThreeVector& tlate, // position in rotated frame
              G4LogicalVolume* pCurrentLogical,
              const G4String& pName,
              G4LogicalVolume* pMotherLogical,
              G4bool pMany,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

- Single volume positioned relatively to the mother volume
  - In a frame rotated and translated relative to the coordinate system of the mother volume
- Three additional constructors:
  - A simple variation: specifying the mother volume as a pointer to its physical volume instead of its logical volume.
  - Using `G4Transform3D` to represent the direct rotation and translation of the solid instead of the frame (*alternative constructor*)
  - The combination of the two variants above

# G4PVPlacement
## Rotation of mother frame …

```
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
```

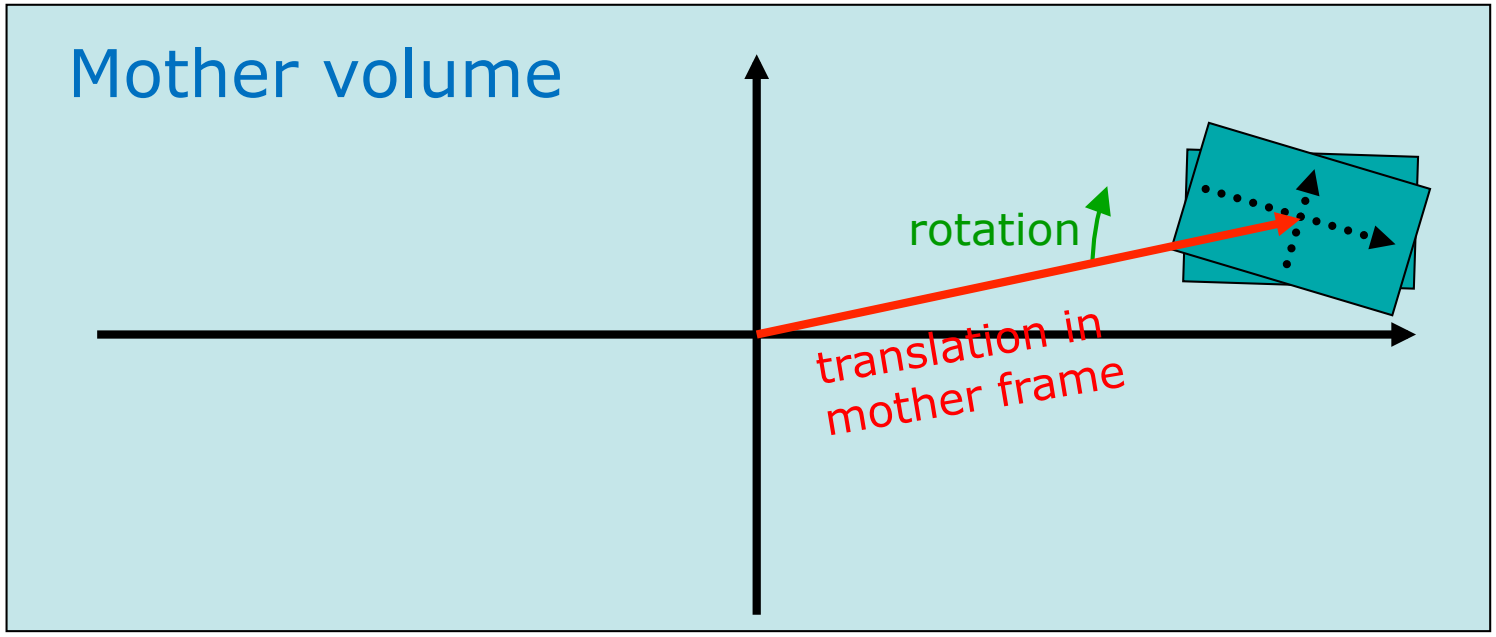
- Single volume positioned relatively to the mother volume



# G4PVPlacement

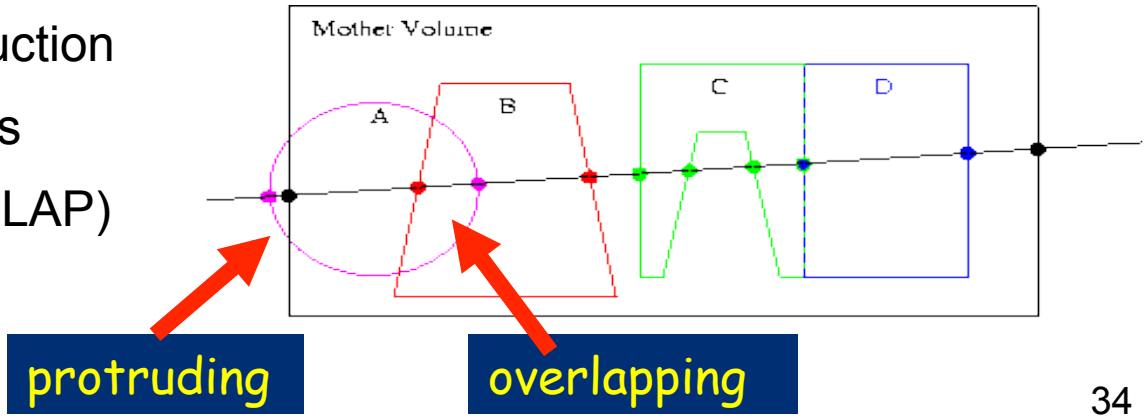
## Rotation in mother frame …

```
G4PVPlacement( G4Transform3D( G4RotationMatrix &pRot,      // rotation of 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
```



# Tools for geometry check

- A protruding volume is a contained daughter volume which actually protrudes from its mother volume.
- Volumes are also often positioned in a same volume with the intent of not provoking intersections between themselves. When volumes in a common mother actually intersect themselves are defined as overlapping.
- Geant4 does not allow for malformed geometries, neither protruding nor overlapping.
  - 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, OLAP)



# 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`**
    *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 lots of CPU time!)*
  - **`geometry/test/line_test`**
    *to shoot a line along a specified direction and position*
  - *...*

# Thanks for your attention