Geant4 materials & geometry

A lot of material by J. Pipek

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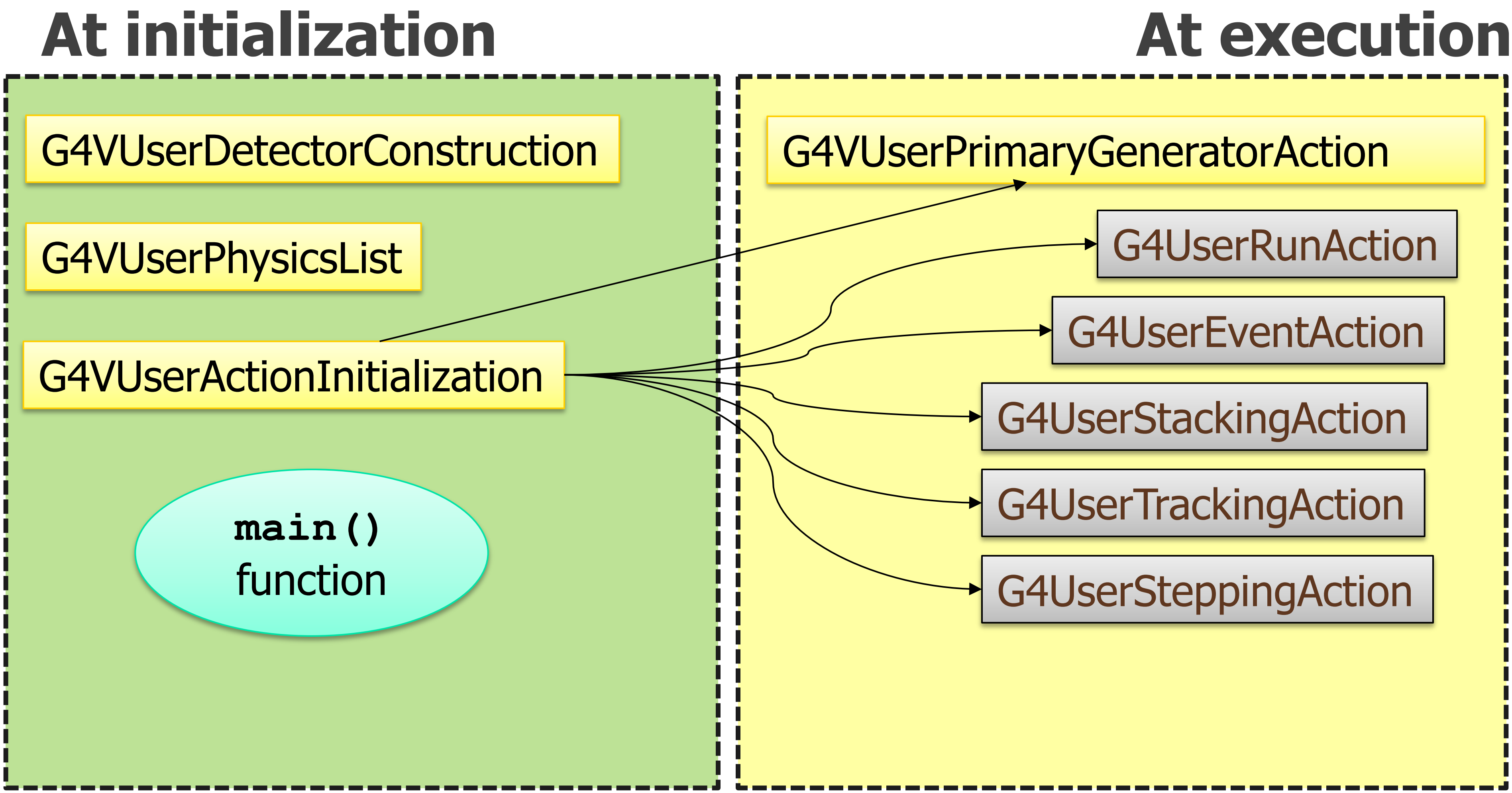
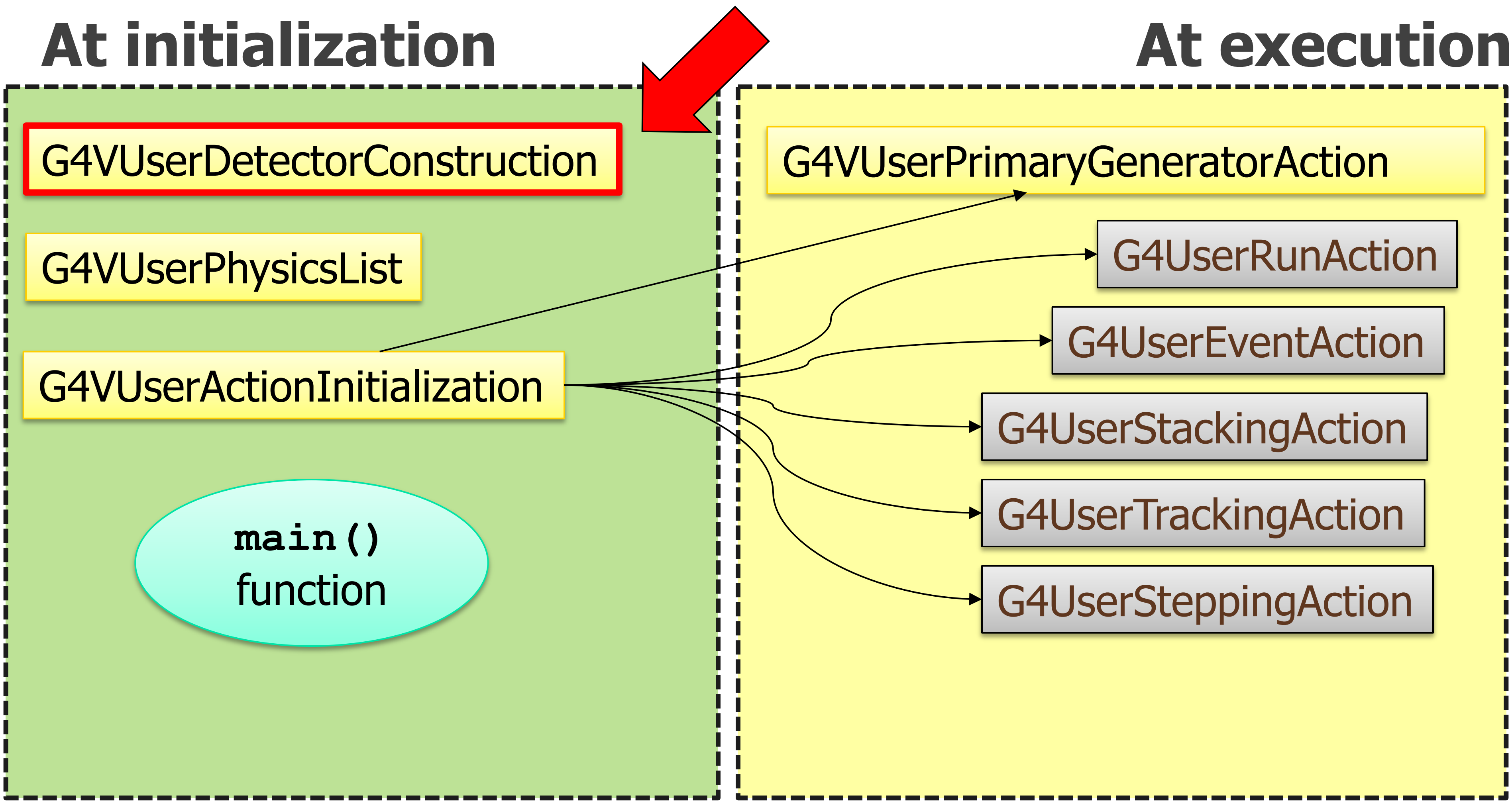
Geant4 Course
at the XXI Seminar on software for nuclear, subnuclear and applied physics
Alghero, June 9th- 14th, 2024

Mandatory (and optional) user classes



Mandatory (and optional) user classes



The Detector Construction

- User class which describes the geometry must inherit from **G4VUserDetectorConstruction** and registered in the Run Manager

- Define the geometry of your model
  - All materials
  - All volumes & placements
- (Optionally) add fields
- (Optionally) define volumes for read-out (sensitive detectors)

```
// ...
class G4VUserDetectorConstruction
{
  public:
    G4VUserDetectorConstruction();
    virtual ~G4VUserDetectorConstruction();

  public:
    virtual G4VPhysicalVolume* Construct() = 0;
    virtual void ConstructSDandField();
    // ...
}
```

Part I: Units

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 (examples 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.)

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):

► G4SystemOfUnits.hh

► CLHEP/SystemOfUnits.hh

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

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

System of units in Geant4

nanosecond (ns)

unit charge (eplus)

megaelectronvolt (MeV)

radian

kelvin

millimeter (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

Defining new units

- **New units** can be defined directly as constants, or (suggested way) via `G4UnitDefinition`
  - `G4UnitDefinition ( "name", "symbol", "category", value )`
- Example (mass thickness):
  - `G4UnitDefinition ("grammpercm2", "g/cm2", "MassThickness", g/cm2);`
  - The new category "MassThickness" 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`

Part II: Materials

Materials

- Different levels of material description:
  - isotopes → **`G4Isotope`**
  - elements → **`G4Element`**
  - molecules → **`G4Material`**
  - compounds and mixtures → **`G4Material`**
- Attributes associated:
  - **Density** (mandatory)
  - Temperature, Pressure, State (gas, liquid, …)

Materials

- **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 in Geant4
  - Material properties computed from elemental properties → assuption of linear combination

Elements and isotopes

- If you need an element made by a non-natural isotopic composition (e.g. ^{enr}Ge)
- Build isotopes

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

- … and assemble into elements

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

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

… for instance

- Build ^{enr}U

Do not forget unit (g/mole)

```
G4Isotope* U5 = new G4Isotope(name="U235", iz=92, n=235,
       a=235.01*g/mole);
G4Isotope* U8 = new G4Isotope(name="U238", iz=92, n=238,
       a=238.03*g/mole);
G4Element* elU = new G4Element(name="enriched Uranium", symbol="U",
       ncomponents=2);
elU->AddIsotope(U5, abundance= 90.*perCent);
elU->AddIsotope(U8, abundance= 10.*perCent);
```

- For element with *natural isotopic composition*, definition is easier

Do not forget unit (g/mole)

```
a = 16.00*g/mole;
G4Element* elO = new G4Element("Oxygen", symbol="O", z=8., a);
G4cout << elO << G4endl; //printout of element info
```

Elements and molecules

- Single-element materials

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

- Molecule (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);
```

Materials: compounds

- 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);
```

Materials: mixtures

- 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);
```

Example: a 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("CO2Gas", density,
    ncomponents=2, kStateGas, temperature, pressure);
CO2->AddElement(C, natoms = 1);
CO2->AddElement(O, natoms = 2);
```

"Vacuum"

- Absolute vacuum does not exist:
  - Model it as a gas at **very low density**!
  - Cannot define materials composed of multiple elements through Z or A, or with ρ=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);
```

The NIST database

- All elements and many commonly-used materials available in Geant4 through the NIST database
- No need to predefine elements and materials
- Retrieve materials from NIST manager:

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

- UI commands

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

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

The NIST database: elements

- NIST database for elements and materials is imported in 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
  - 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

http://geant4.cern.ch/UserDocumentation/UsersGuides/ForApplicationDeveloper/html/apas08.html

NIST 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		

- NIST Elements:
  - 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

Part III: Geometry

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 virtual methods **`Construct()`** **(pure virtual)** and **`ConstructSDandFields()`**:
  - 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)
- Note2: you should not delete the **MyDetector** instance! Run manager does that automatically.

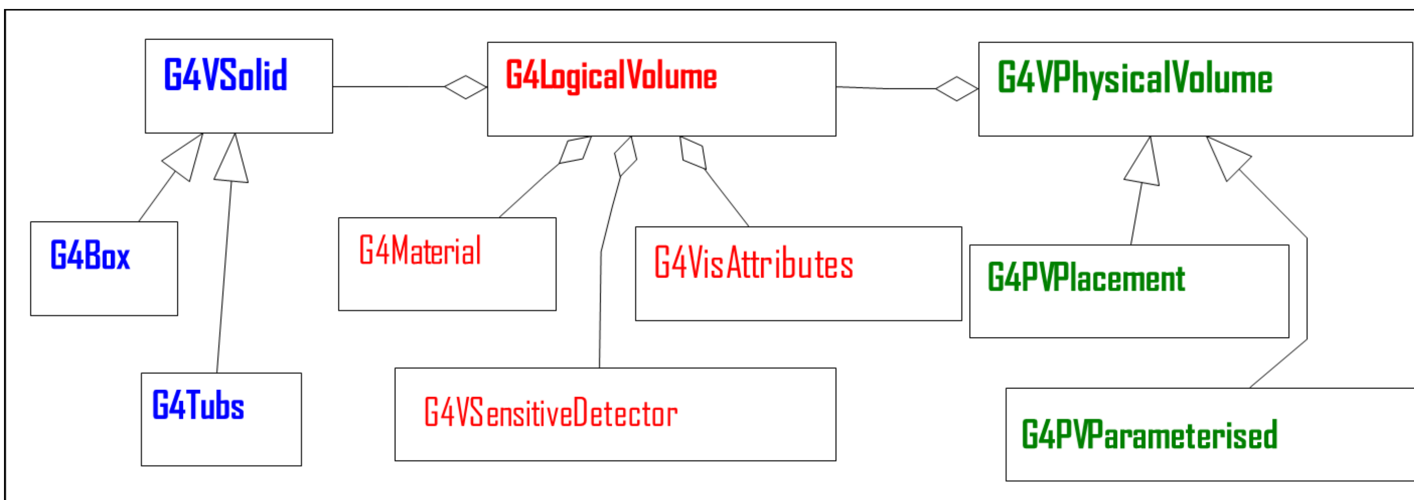
G4VUserDetectorConstruction

- 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()`** MT
  - 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)

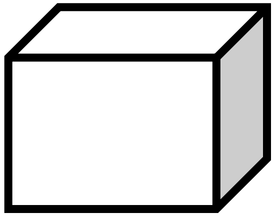


Define detector geometry

- Basic strategy

```
G4VSolid* pBoxSolid =
  new G4Box("aBoxSolid",
        1.*m, 2.*m, 3.*m);
G4LogicalVolume* pBoxLog =
   new G4LogicalVolume( pBoxSolid,
   pBoxMaterial, "aBoxLog", 0, 0, 0);
G4VPhysicalVolume* aBoxPhys =
    new G4PVPlacement(pRotation,
    G4ThreeVector(posX, posY, posZ),
     pBoxLog,"aBoxPhys", pMotherLog, 0, copyNo);
```

Solid: shape and size.



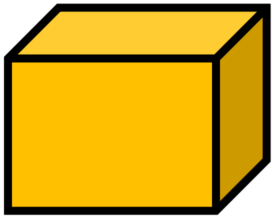
Step 1
Create the geom. object: box

Define detector geometry

Logical volume : + material, sensitivity, etc.

- 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);
```



Step 1
Create the geom. object: box

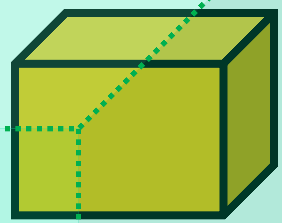
Step 2
Assign properties to object : material

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



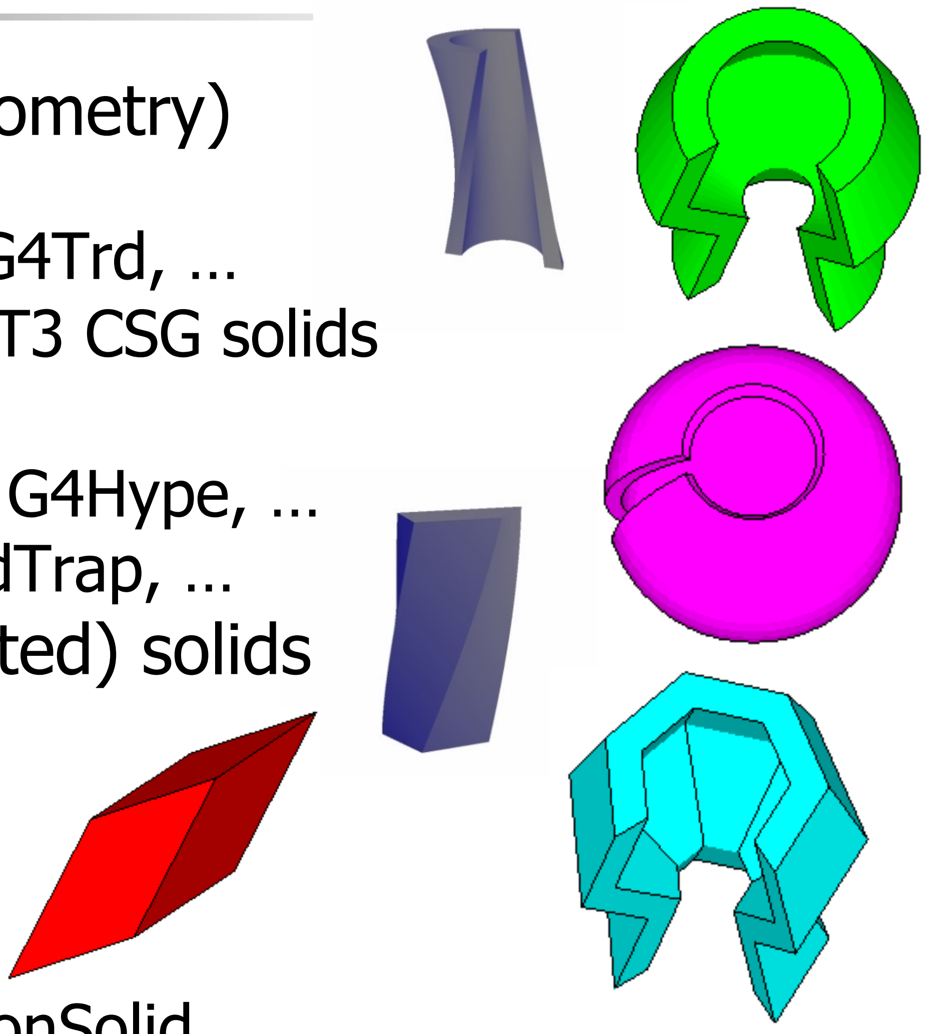
Step 1
Create the geom. object: box

Step 2
Assign properties to object : material

Step 3
Place it in the coordinate system of mother volume

Solids

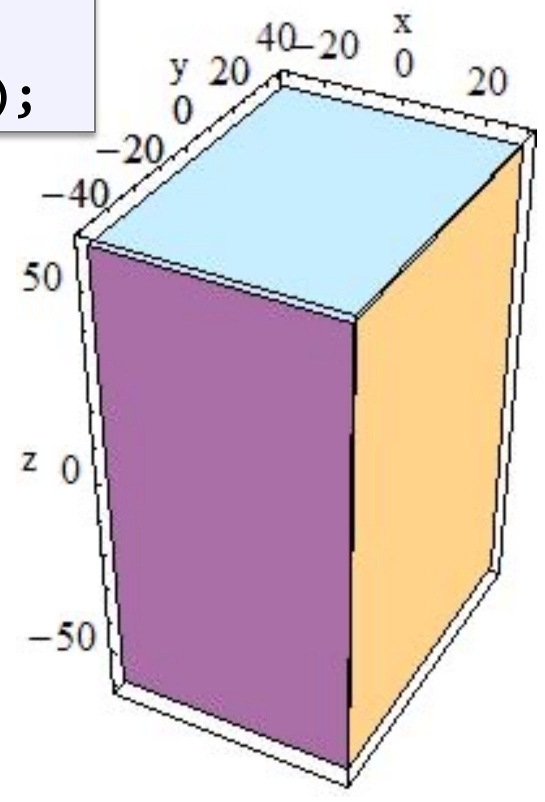
- **CSG** (Constructed Solid Geometry) solids
  - G4Box, G4Tubs, G4Cons, G4Trd, …
  - Analogous to simple GEANT3 CSG solids
- **Specific** solids (CSG like)
  - G4Polycone, G4Polyhedra, G4Hype, …
  - G4TwistedTubs, G4TwistedTrap, …
- **BREP** (Boundary REPresented) solids
  - G4BREPSolidPolycone, G4BSplineSurface,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



CGS: G4Box

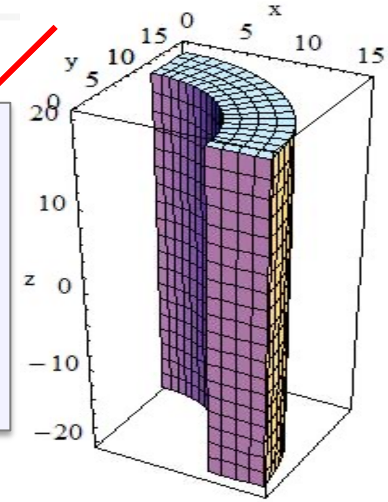
```
G4Box(const G4String& pname,  // name
             G4double  pX, // half-length in X
             G4double  pY, // half-length in Y
             G4double  pZ, // half-length in Z);
```

Note the half-length!

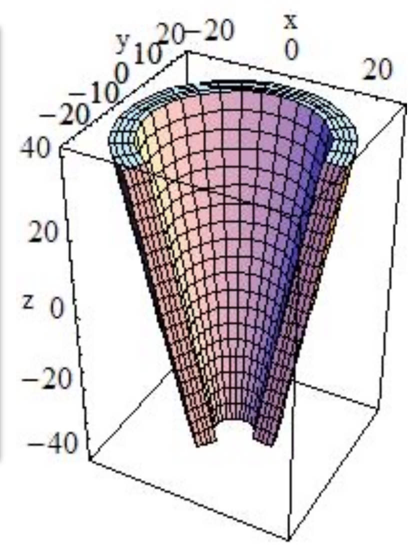


CGS: G4Tubs & G4Cons

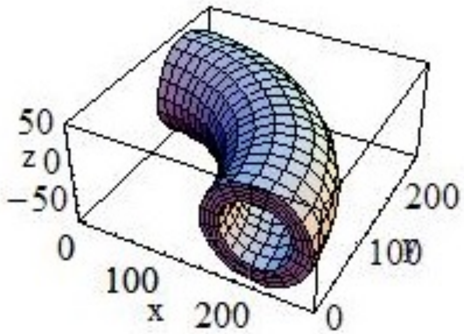
```
G4Tubs(const G4String& pname,   // name
             G4double  pRmin,   // inner radius (0)
             G4double  pRmax,   // outer radius
             G4double  pDz,     // Z half! length
             G4double  pSphi,   // starting Phi (0)
             G4double  pDphi);  // segment angle (twopi)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



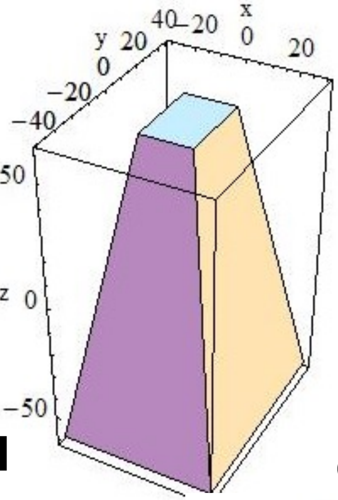

```
G4Cons(const G4String& pname,   // name
             G4double  pRmin1,  // inner radius -pDz
             G4double  pRmax1,  // outer radius -pDz
             G4double  pRmin2,  // inner radius +pDz
             G4double  pRmax2,  // outer radius +pDz
             G4double  pDz,     // Z half length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



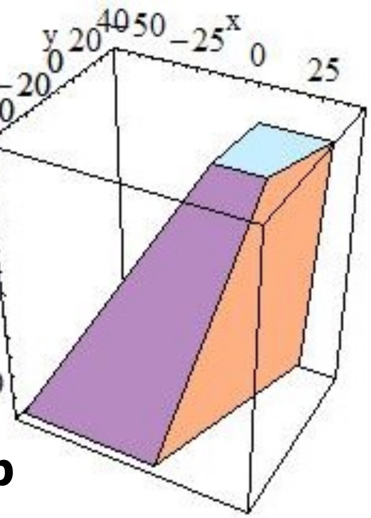
Other CGS solids



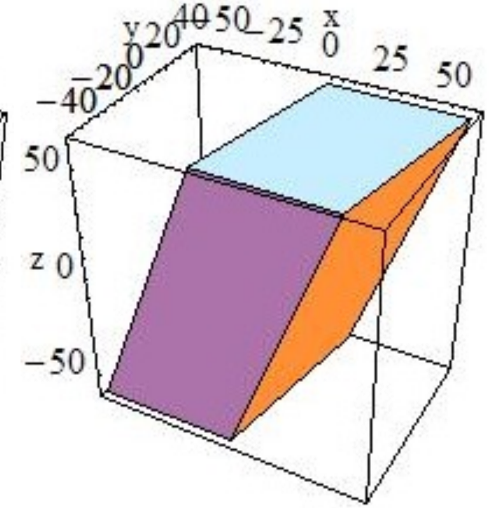
G4Torus



G4Trd

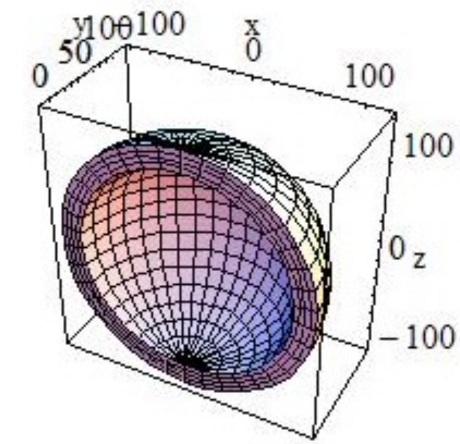


G4Trap

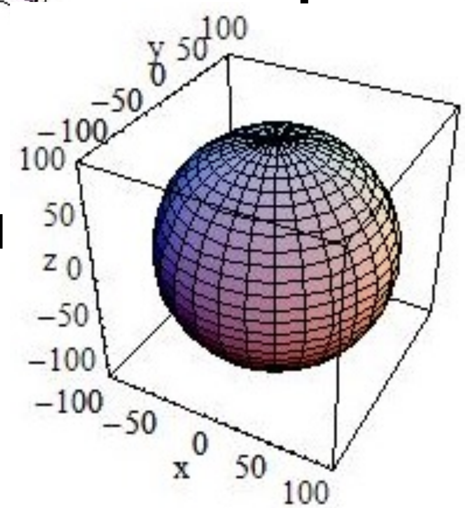


G4Para
(parallelepiped)

G4Sphere



G4Orb
(full solid sphere)

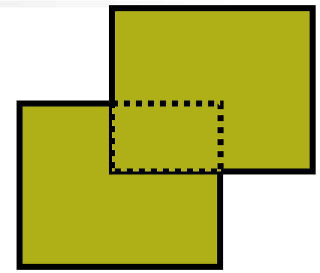


Check Section 4.1.2 of Geant4 Application Developers Guide for all available shapes

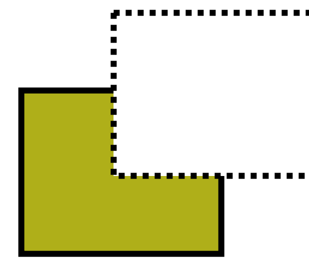
Boolean solids

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

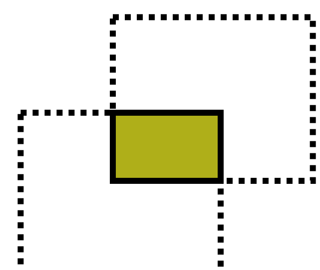
G4UnionSolid



G4SubtractionSolid



G4IntersectionSolid



Boolean solids – an example

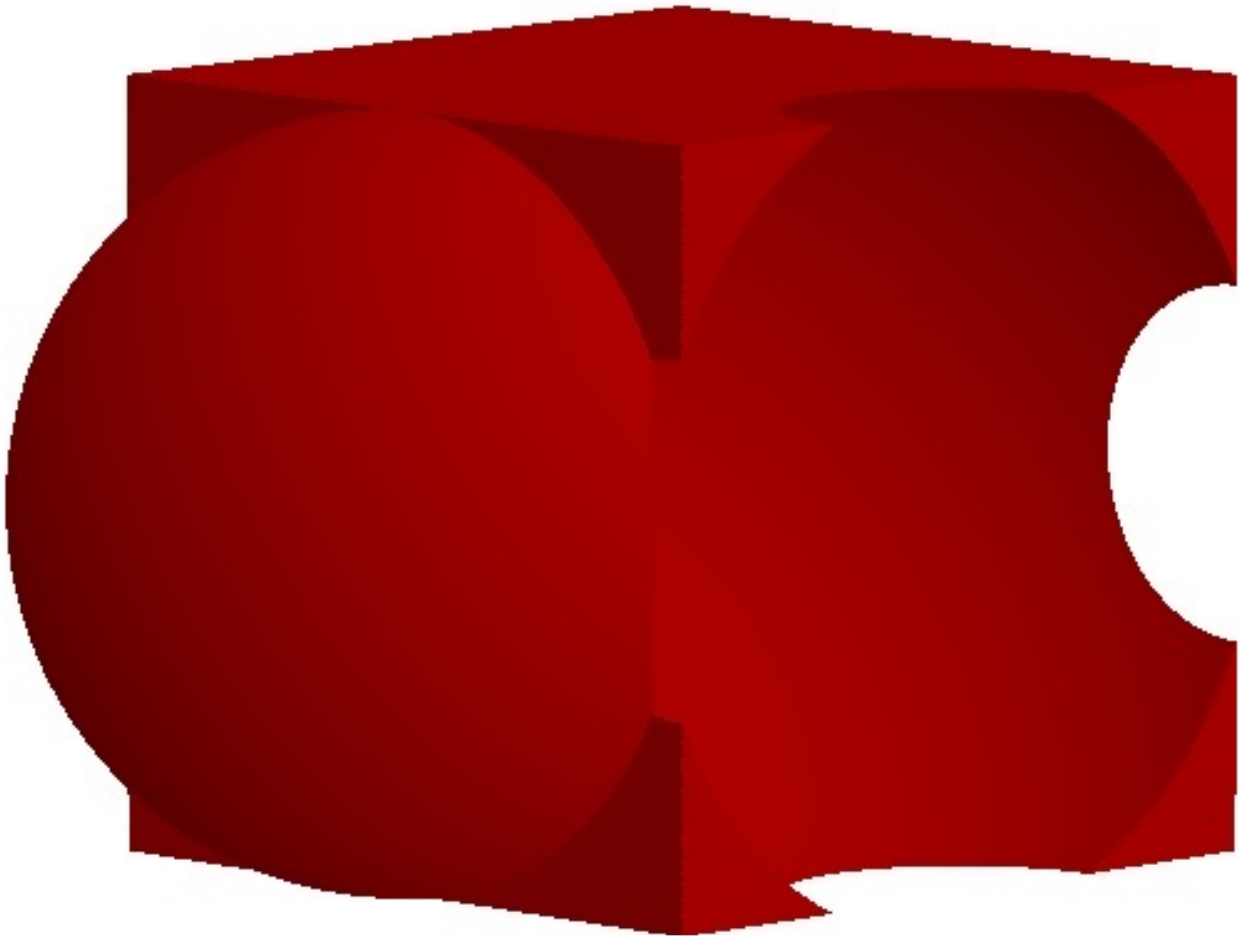
```
G4VSolid* box = new G4Box("Box",50*cm,60*cm,40*cm);
G4VSolid* cylinder =
    new G4Tubs("Cylinder",0.,50.*cm,50.*cm,0.,twopi);

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

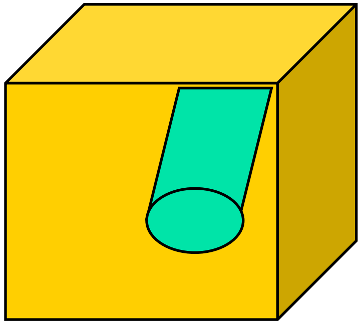
- Contains all information of volume **except position**:
  - Shape and dimension (`G4VSolid`)
  - Material, sensitivity, visualization attributes
  - Hierarchy of daughter volumes
  - Magnetic field, User limits
- Physical volumes of same type **can share** a logical volume.
- The pointers to solid 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);
```

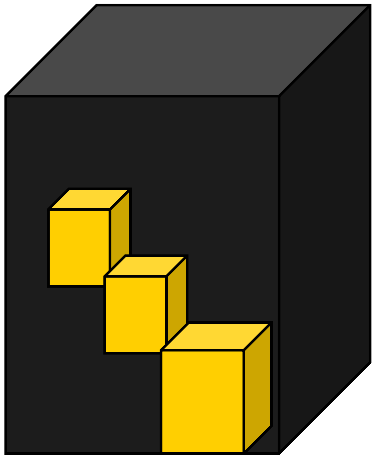
optional

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`**



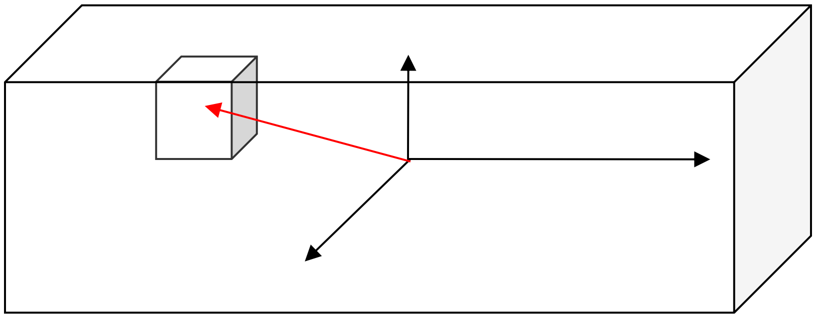
placement



repeated

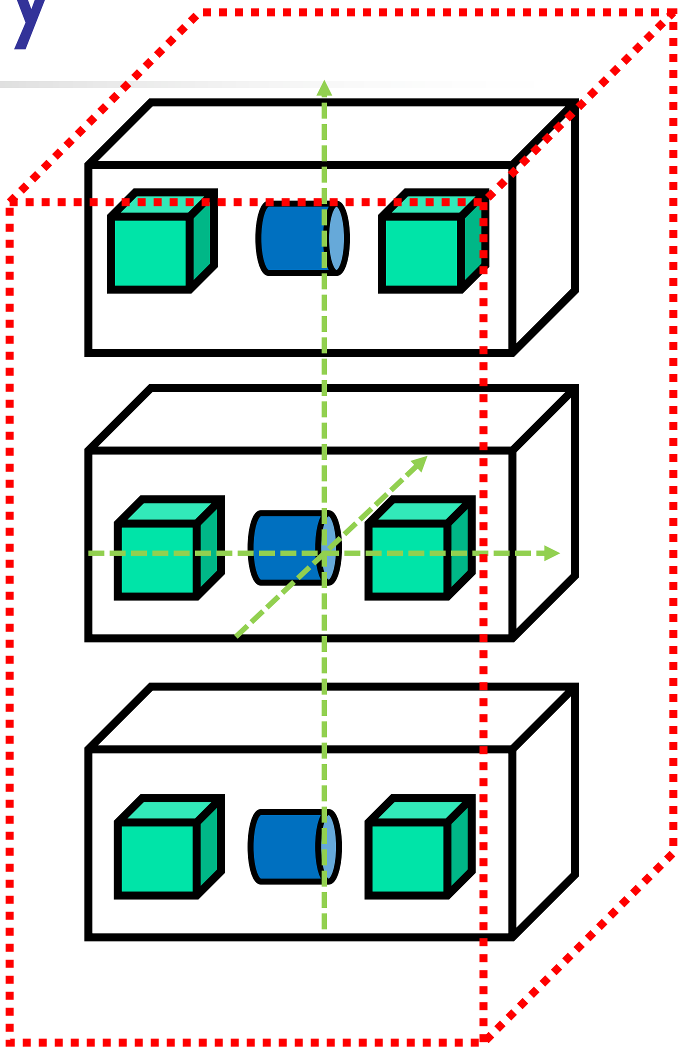
Geometry hierarchy

- 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



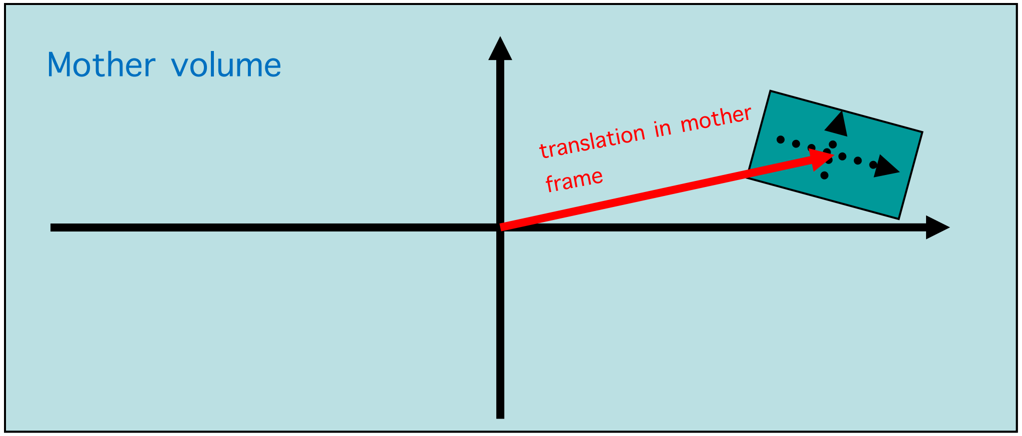
G4PVPlacement

- 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)

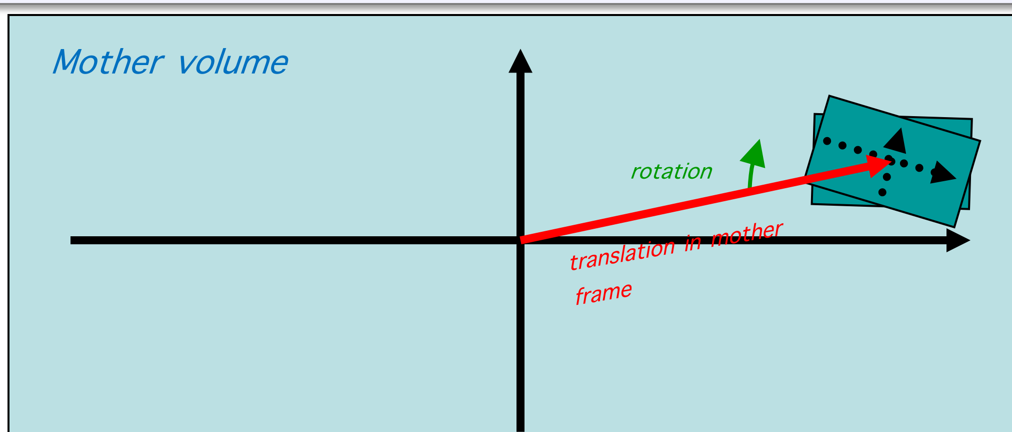
```
G4PVPlacement(G4RotationMatrix* pRot,          // rotation of mother frame
              const G4ThreeVector& tlate,      // position in mother frame
              G4LogicalVolume* pCurrentLogical,
              const G4String& pName,
              G4LogicalVolume* pMotherLogical,
              G4bool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



G4PVPlacement Rotation in mother frame …

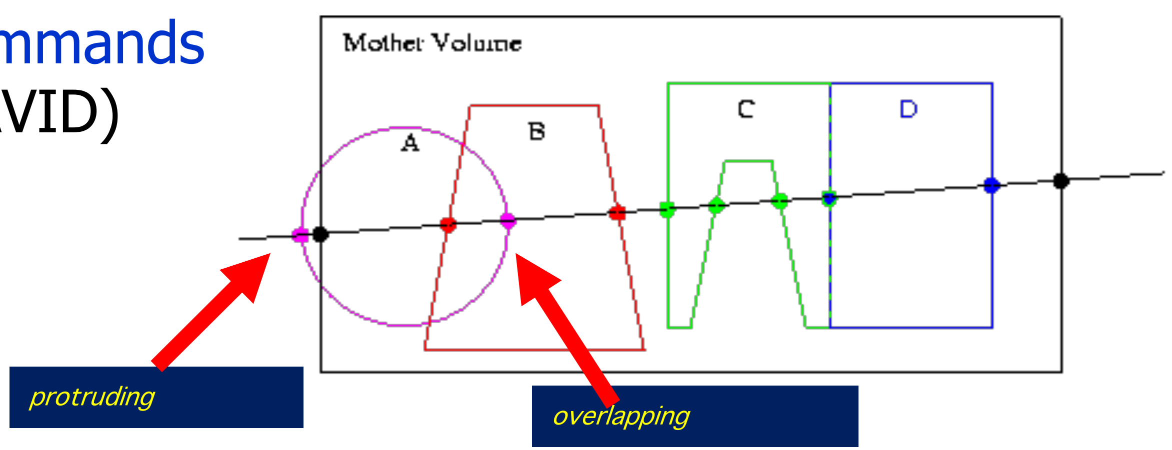
Single volume positioned relatively to the mother volume (active transformation)

```
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
```



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!)

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

Hands on....