



GEANT 4 materials & geometry

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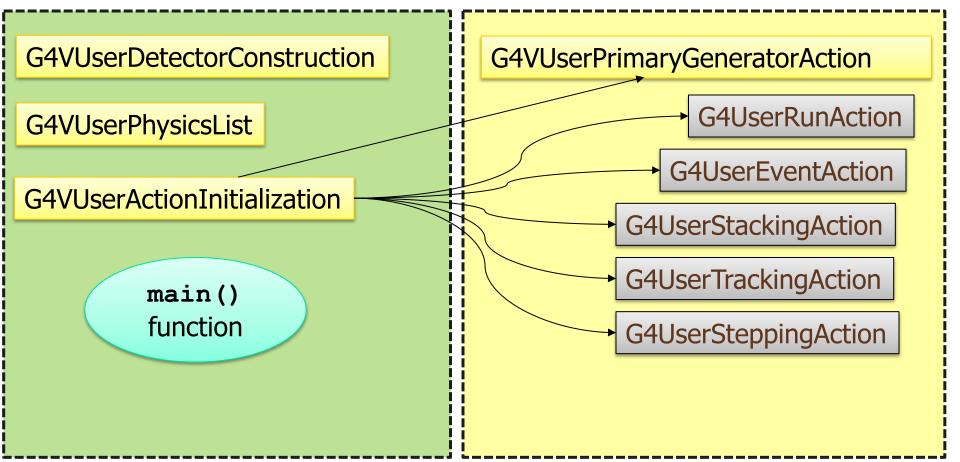
A lot of material by J. Pipek

Geant4 Course, Vienna (A), April 2024

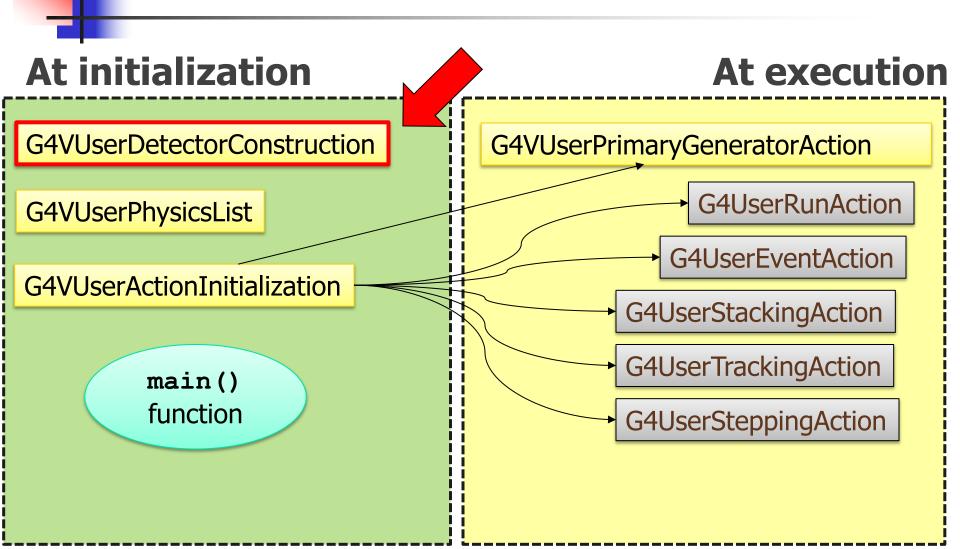
Mandatory (and optional) user classes

At initialization

At execution



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();
    // ...
}
Remember
```

Part I: Units

4

Note: Geant4 basic types

- Aliases for the **primitive data types** to provide crossplatform 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:

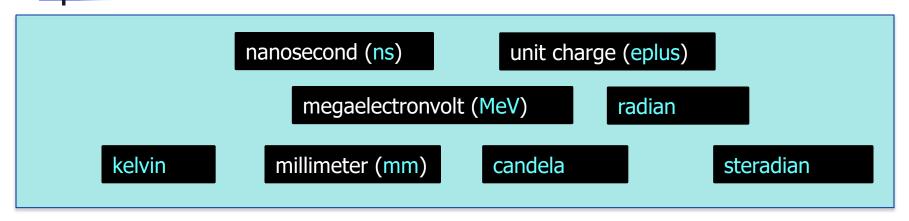
```
G4double width = 12.5 * m;
G4double density = 2.7 * g/cm3;
```

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



- 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. enrGe)
- 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
```

... for instance

Build enrU

Do not forget unit (g/mole)

 For element with natural isotopic composition, definition is easier

Do not forget unit (g/mole)

```
a = 16.00*g/mole;
G4Element* el0 = new G4Element("Oxygen", symbol="0", z=8., a);
G4cout << el0 << G4endl; //printout of element info</pre>
```

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* el0 = new G4Element(name="0xygen",symbol="0", z= 8., a);
density = 1.290*mg/cm3;
G4Material* Air = new G4Material(name="Air", density, ncomponents=2);
Air->AddElement(elN, 70.0*perCent);
Air->AddElement(elO, 30.0*perCent);
```

Materials: mixtures

Composition of mixtures

Example: a gas

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

"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 $\rho=0$

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/Phys RefData
- 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	Α	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	26.9867047	76 (17)		
		27.976926	· · · · · · · · · · · · · · · · · · ·	92.2297 (7)
		28.9764947	\ /	4.6832 (5	6)
	30	29.9737702	\ /	3.0872 (5	6)
		30.9753632	(-)		
		31.9741481	1 (23)		
		32.978001	(17)		
		33.978576	(15)		
		34.984580	(40)		
		35.98669	(11)		
	37	36.99300	(13)		
	38	37.99598	(29)		
		39.00230	(43)		
		40.00580	(54)		
		41.01270	(64)		
	42	42.01610	(75)		

- Natural isotope compositions
- More than 3000 isotope masses

NIST materials

Z Name ChFormula	density(g/cm^3)
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

- NIST Elements:
 - $H \rightarrow Cf (Z = 1 \rightarrow 98)$
- 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

```
density(g/cm^3) I(eV)
13 G4 Adipose Tissue
                                       63.2
           0.119477
           0.63724
           0.00797
           0 232333
       11 0 0005
            2e-05
            0.00016
            0.00073
            0.00119
            0.00032
            2e-05
            2e-05
       30 2e-05
4 G4 Air
                         0.00120479 85.7
           0.000124
           0.755268
           0.231781
           0.012827
2 G4 Csl
                         4.51
                                     553.1
            0.47692
            0.52308
```

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

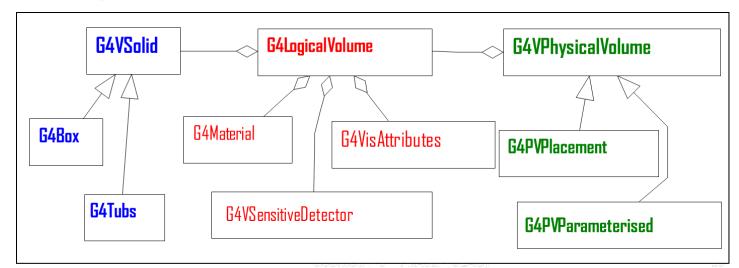
- Method Construct()
 - Define materials
 - Define solids and volumes of the geometry
 - Build the tree hierarchy of volumes
 - Define visualization attributes
 - Return the world physical volume!



- Method ConstructSDAndField() MT
 - Assign magnetic field to volumes / regions
 - Define sensitive detectors and assign them to volumes

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)



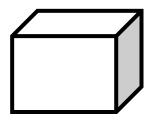


Define detector geometry

Basic strategy

```
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.



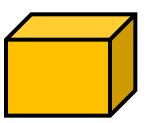
Step 1
Create the geom. object: box



Define detector geometry

Logical volume: + material, sensitivity, etc.

Basic strategy



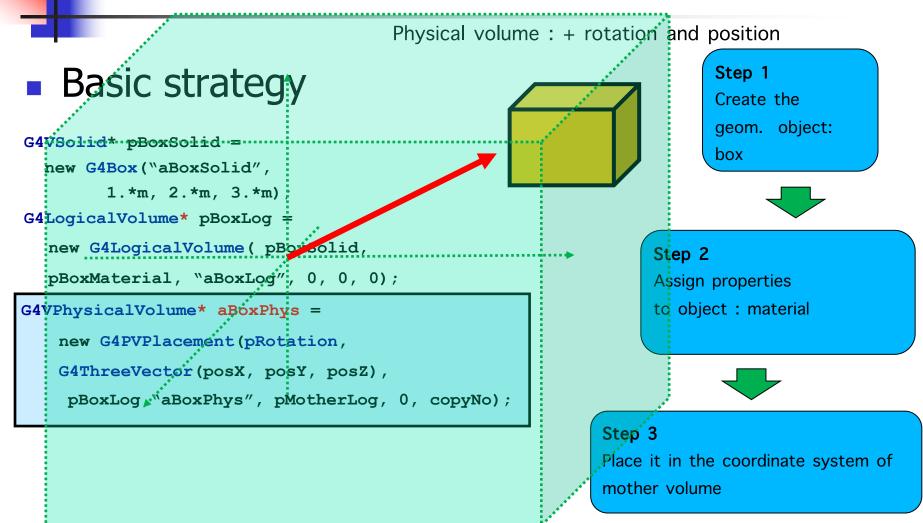
Step 1
Create the
geom. object:
box



Step 2

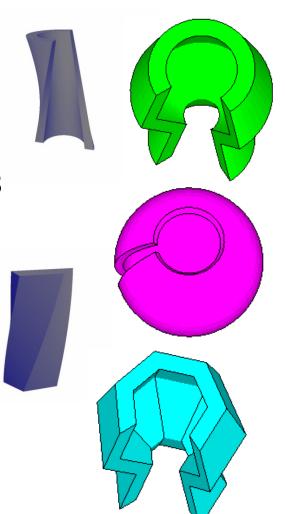
Assign properties to object : material

Define detector geometry



Solids

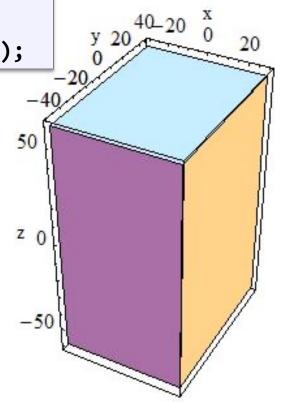
- CSG (Constructed Solid Geometry) solids
 - G4Box, G4Tubs, G4Cons, G4Trd, ...
 - Analogous to simple GEANT3 CSG solids
- Specific solids (CSG like)
 - G4Polycone, G4Polyhedra, G4Hype, ...
 - G4TwistedTubs, G4TwistedTrap, ...
- BREP (Boundary REPresented) solids
 - G4BREPSolidPolycone, G4BSplineSurface, ...
 - 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);
```

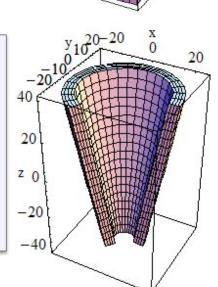
Note the half-length!



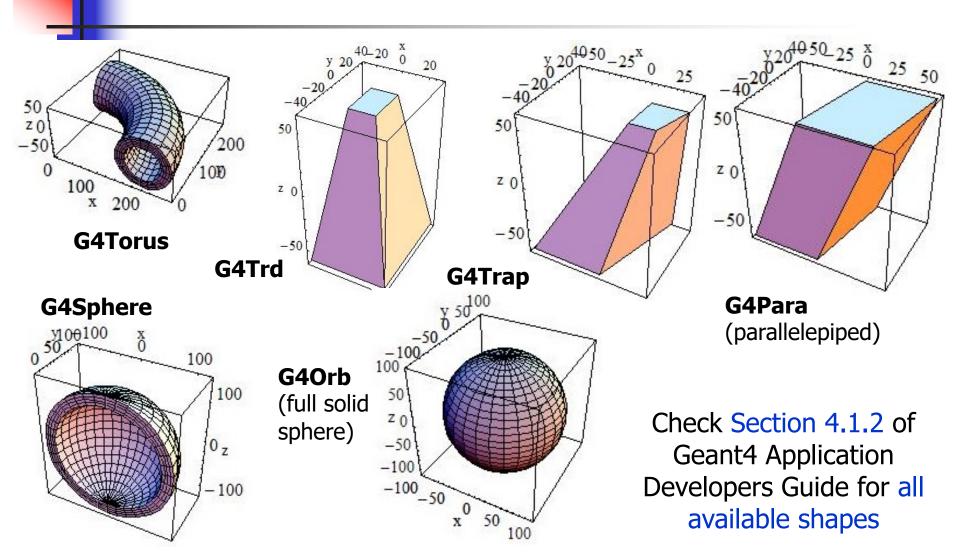
CGS: G4Tubs & G4Cons

```
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
```

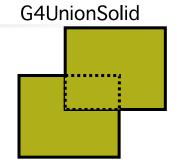


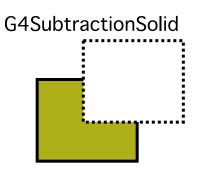
Other CGS solids

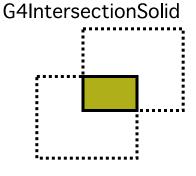


Boolean solids

- 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



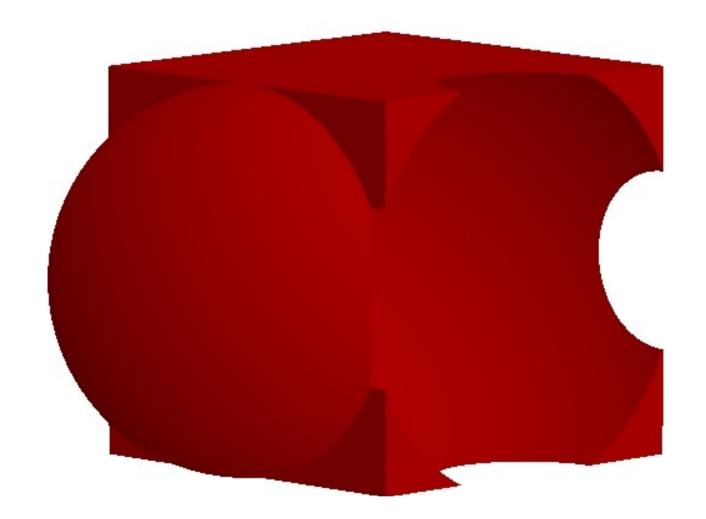




Boolean solids – an example

```
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

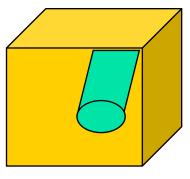
- Contains all information of volume except position:
 - Shape and dimension (G4VSolid)
 - Material, sensitivity, visualization attributes
 - Hierarchy of daughter volumes
 - Magnetic field, User limits
- Physical volumes of same type can share a logical volume.
- The pointers to solid and material must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

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

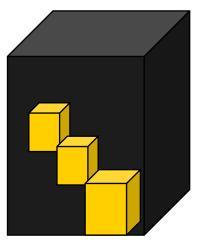
Optional
```

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



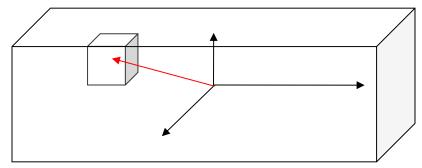
placement



repeated

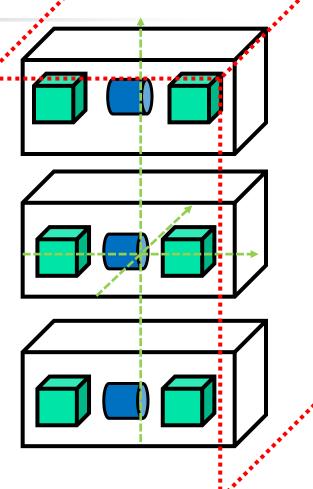
Geometry hierarchy

- 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

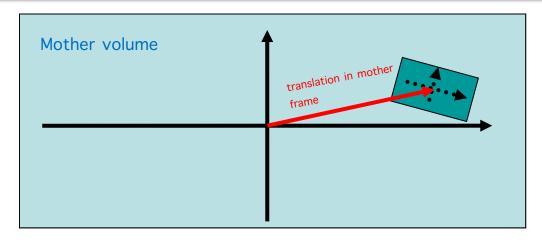
- Single volume positioned relatively to the mother volume
 - In a frame rotated and translated relative to the coordinate system of the mother volume
- A few variants available:
 - Using G4Transform3D to represent the direct rotation and translation of the solid instead of the frame (alternative constructor)
 - 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
```

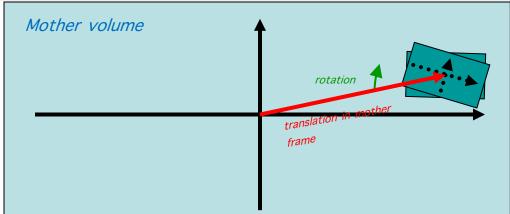




G4PVPlacement Rotation <u>in</u> mother frame ...

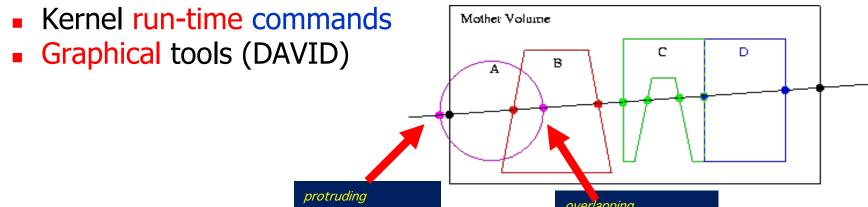
Single volume positioned relatively to the mother volume (active transformation)

```
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
```





- 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



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....