X SEMINAR ON SOFTWARE FOR NUCLEAR, SUBNUCLEAR AND APPLIED PHISICS

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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");</pre>
```

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):

 - 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, <u>density</u>
- 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 ${\bf Z}$ or ${\bf A}$, 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);10
```

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

```
(\%)
           m
                    error
Si 22 22.03453
                     (22)
                                           28.0855(3)
  23 23.02552
                    (21)
      24.011546
                    (21)
      25.004107
                    (11)
  26 25.992330
                    (3)
      26.98670476
                    (17)
  28 27.9769265327 (20)
                              92.2297 (7)
  29 28.97649472
                               4.6832 (5)
                     (5)
                               3.0872 (5)
      29.97377022
      30.97536327
                     (7)
  32 31.9741481
                    (23)
                    (17)
  33 32.978001
      33.978576
                    (15)
  35 34.984580
                    (40)
      35.98669
                    (11)
      36.99300
                    (13)
  38 37,99598
                    (29)
      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			
2 G4_He 3 G4_Li	0.000166322 0.534	41.8 40		
4 G4_Be 5 G4 B	1.848 2.37	63.7 76		
6 G4_C	2	81		
7 G4_N N_2 8 G4 O O 2	0.0011652 0.00133151	82 95		
9 G4_F 10 G4 Ne	0.00158029 0.000838505	115 137		
10 G4_Ne 11 G4_Na	0.971	149		
12 G4_Mg 13 G4 Al	1.74 2.6989	156 166		
14 G4_Si	2.33	173		

- 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

======================================				
N Name	ChFormula	density(g/cm^3	===) I(eV)	
13 G4 Adi	======== pose_Tissue	0.92	=== 63.2	
_ 1	0.119477			
6	0.63724			
7	0.00797			
8				
	0.0005			
12				
15				
16				
17				
19				
20				
	2e-05			
30	2e-05	0.00400470	05.7	
4 G4_Air	0.000104	0.00120479	85.7	
6 7	0.000124			
8	0.755268 0.231781			
18	0.231781			
2 G4 Csl	0.012027	4.51	553.1	
53	0.47692	4.01	JJJ. I	
55				
55	0.02300			

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:

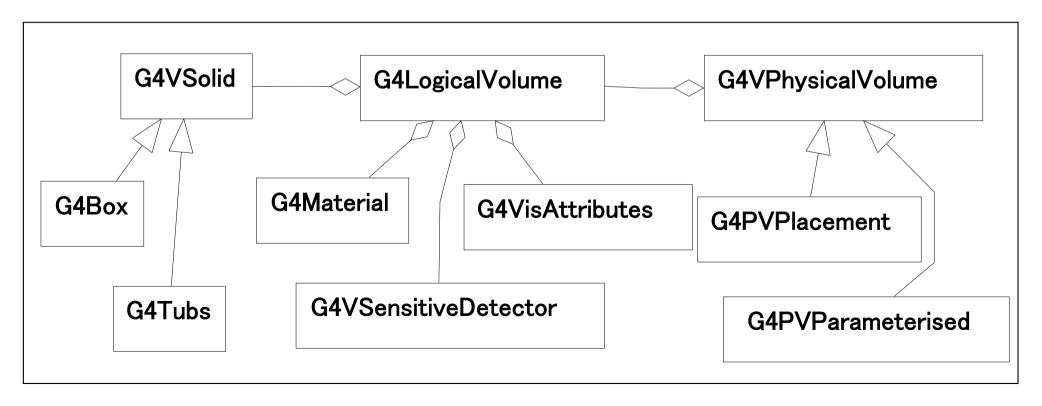
- Detector description: the basic
 - Detector geometry components
 - Define detector geometry
- Describing a detector
 - Solids
 - Logical volumes
 - Physical volumes
- Tools for geometry check

Describe your detector

- 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 method construct():
 - Modularize it according to each detector component or subdetector:
 - Define shapes/solids required to describe the geometry
 - Construct all necessary materials
 - 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

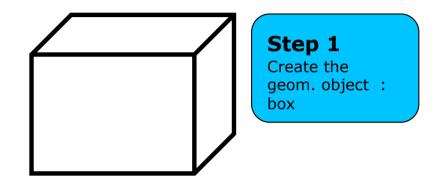
- Three conceptual layers
 - G4VSolid -- shape, size
 - G4LogicalVolume -- <u>daughter physical volumes</u>,
 material, sensitivity, magnetic field, etc.
 - G4VPhysicalVolume -- position, rotation



Define detector geometry

Basic strategy

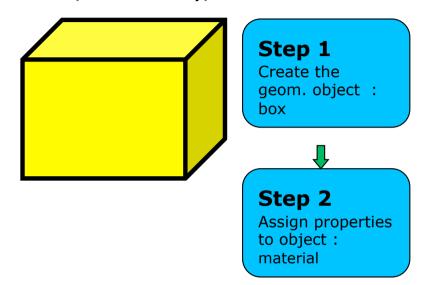
Solid: shape and size



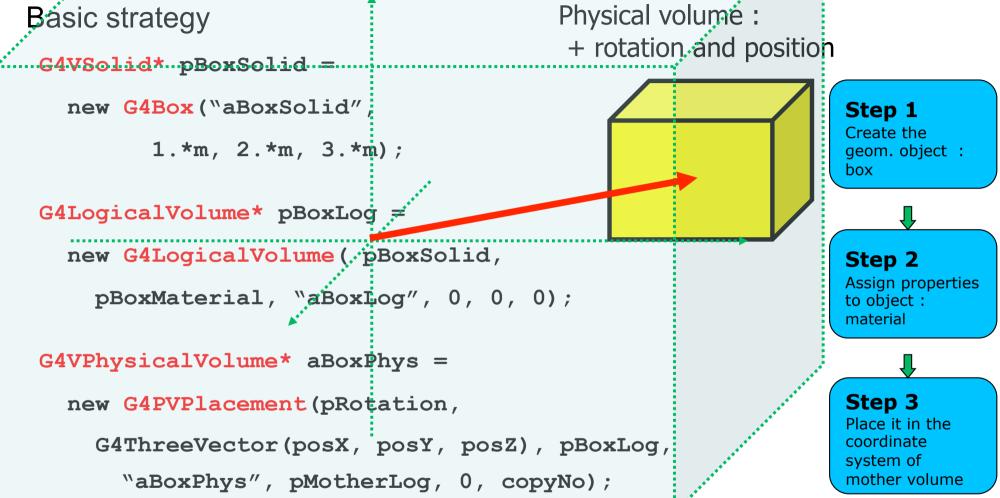
Define detector geometry

Basic strategy

Logical volume : + material, sensitivity, etc.



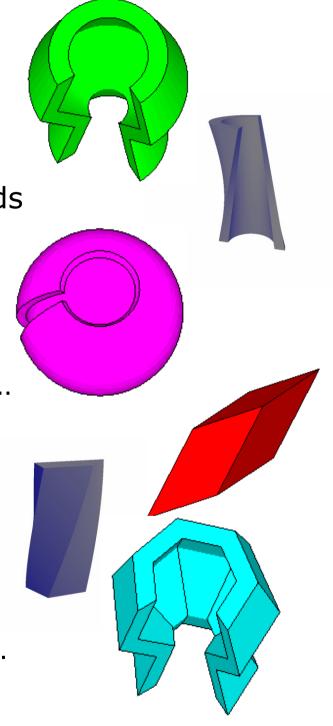
Define detector geometry Physical volume:



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

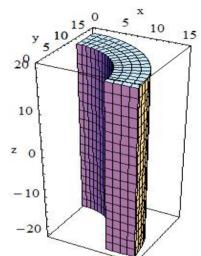
Solids

- 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, ...

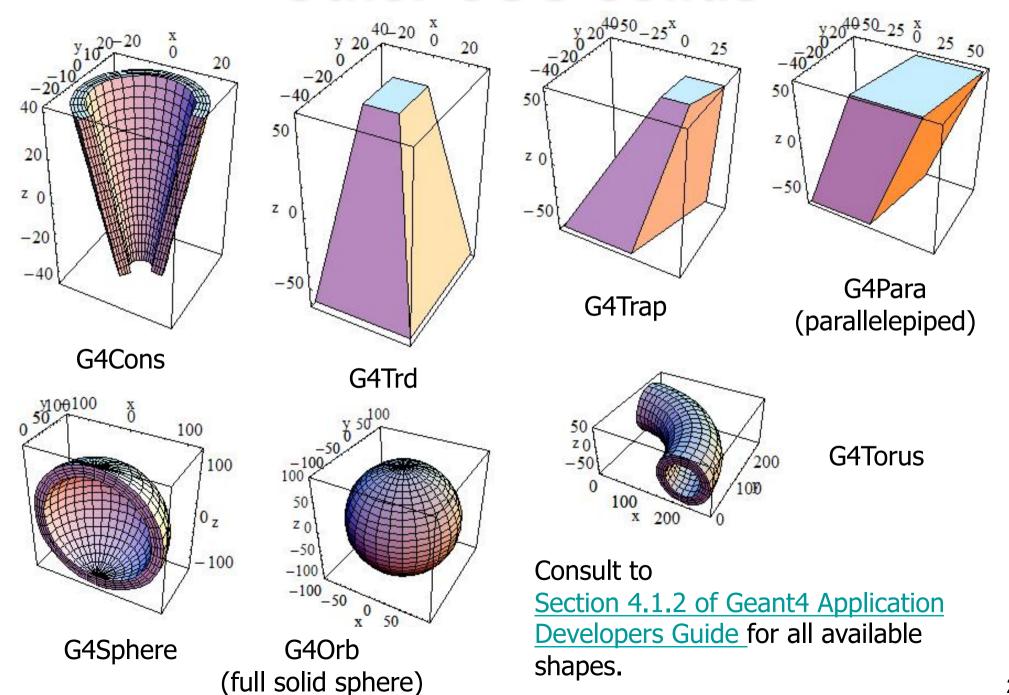


CSG: G4Tubs, G4Cons

```
G4Tubs (const G4String& pname, // name
             G4double pRmin, // inner radius
             G4double pRmax, // outer radius
                                                    z 0
             G4double pDz, // Z half length
             G4double pSphi, // starting Phi
                                                     -10
             G4double pDphi); // segment angle
G4Cons (const G4String& pname, // name
             G4double pRmin1, // inner radius -pDz
             G4double pRmax1, // outer radius -pDz
             G4double pRmin2, // inner radius +pDz
                                                     20
             G4double pRmax2, // outer radius +pDz
                                                    z 0
             G4double pDz, // Z half length
                                                     -20
             G4double pSphi, // starting Phi
             G4double pDphi); // segment angle
```

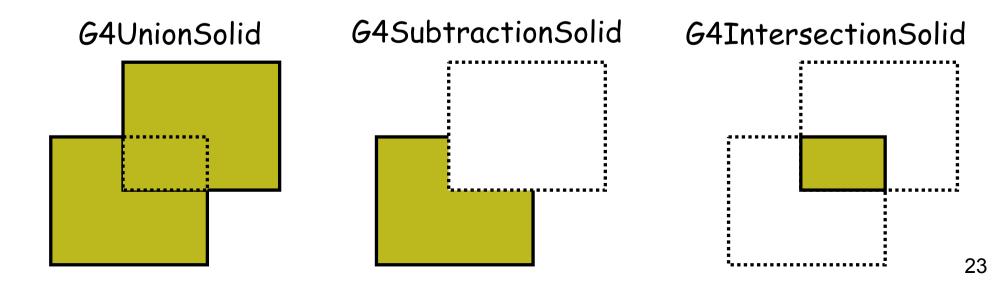


Other CSG solids

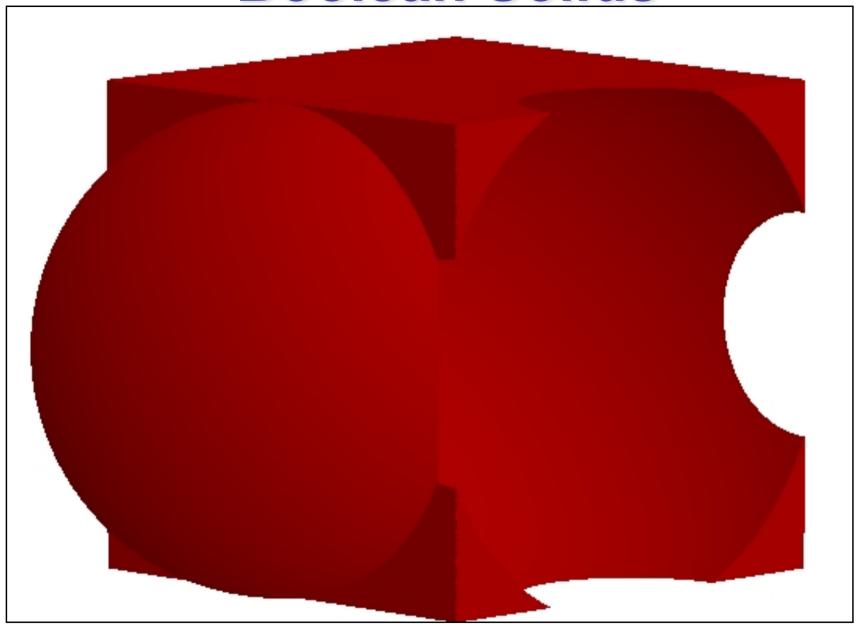


Boolean Solids

- 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. 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



Boolean Solids - example

```
G4VSolid* box = new G4Box("Box", 50*cm, 60*cm, 40*cm);
G4VSolid* cylinder
 = new G4Tubs("Cylinder", 0., 50.*cm, 50.*cm, 0., 2*M PI*rad);
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.));
```

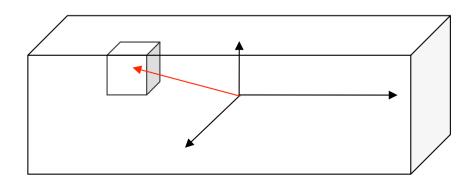
G4LogicalVolume

```
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
- Physical volumes of same type can share a logical volume.
- The pointers to solid and material must be NOT null

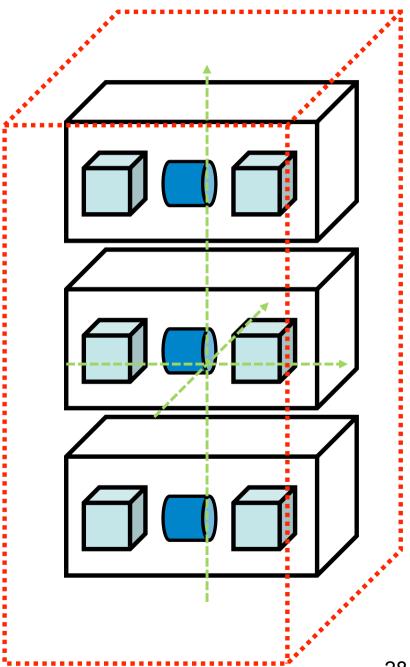
Geometrical hierarchy

- 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 <u>fully contains with some margin</u> 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

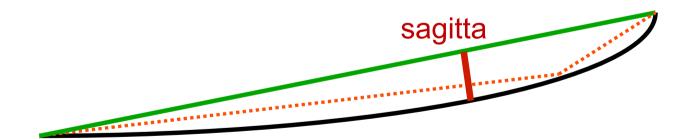


Region

- 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.

Fields

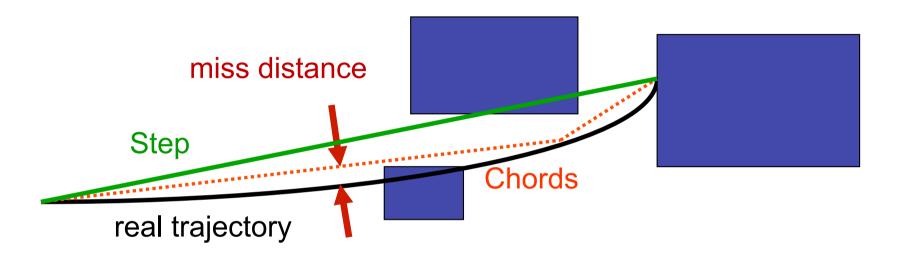
- In order to propagate a particle inside a field (e.g. magnetic, electric or both), we integrate the equation of motion of the particle in the field
- In general this is best done using a Runge-Kutta (RK) method for the integration of ordinary differential equations
 - Several RK methods are available
- In specific cases other solvers can also be used
- Once a method is chosen for calculating the track's motion in a field,
 Geant4 breaks up this curved path into linear chord segments



- The chord segments are determined so that they closely approximate the curved path; they're chosen so that their sagitta is small enough
 - The sagitta is the maximum distance between the curved path and the straight line

Fields

- Chords are used to interrogate the Navigator
 - to see whether the track has crossed a volume boundary



- The accuracy of the volume intersection can be tuned
 - by setting a parameter called the "miss distance":
 - Upper bound for the value of the sagitta
 - It provide a measure of the error resolution
 - Setting small miss distance may be highly CPU consuming
- One step can consist of more than one chord
 - In some cases, one step consists of several turns

Create a Magnetic Field

- How to create Uniform field?
 - Use the constructor of G4UniformMagField

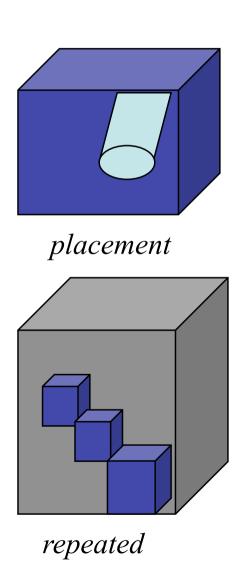
```
    G4ThreeVector fieldV ( 0.1 * Tesla, 1.0*Gauss, 0.0 );
```

- G4MagneticField *myField = new G4UniformField(fieldV);
- Non-uniform field
 - Concrete class derived from G4MagneticField
- A field is packaged together with properties and accuracy parameters into a field manager:
 - G4FieldManager* localFieldMgr = new G4FieldManager(myField);
- One field manager is associated with the 'world'
- Other volumes/regions in the geometry can override this
 - An alternative field manager can be associated with any logical volume:
 G4FieldManager* localFieldMgr = new G4FieldManager (myField);
 logVolume->setFieldManager (localFieldMgr, true);
 - The field is propagated to all the daughter volumes.

Physical Volumes

Placement: it is one positioned volume

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



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...

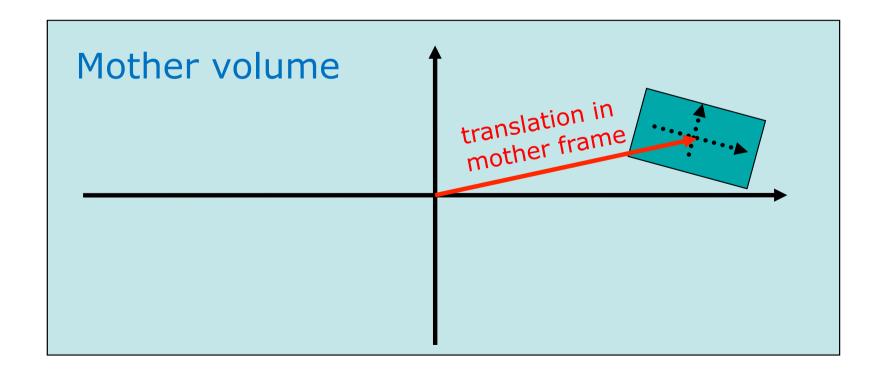
G4int pCopyNo, // unique arbitrary index G4bool pSurfChk=false); // optional overlap check
```

- 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
```

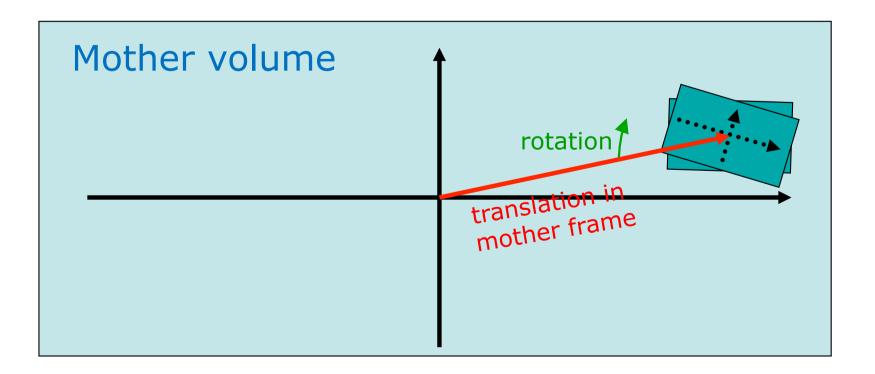
Single volume positioned relatively to the mother volume



G4PVPlacement Rotation in mother frame ...

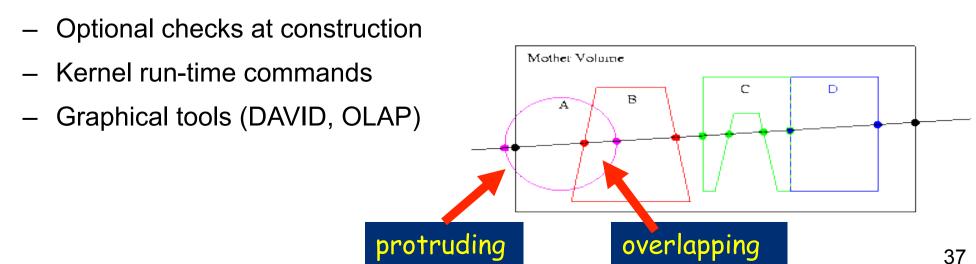
```
G4PVPlacement( G4Transform3D( G4RotationMatrix &pRot, // rotation of daughter frame const G4ThreeVector &tlate), // position in mother frame G4LogicalVolume *pDaughterLogical, const G4String &pName, G4LogicalVolume *pMotherLogical, G4bool pMany, // not used, set it to false...

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.
- 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



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

- ...

Tools for geometry check

```
void MGManagerDetectorConstruction::CheckOverlaps()
 G4PhysicalVolumeStore* thePVStore =
G4PhysicalVolumeStore::GetInstance();
 G4cout << thePVStore->size() << " physical volumes are
defined" << G4endl:
 G4bool overlapFlag = false;
 G4int res=1000:
 G4double tol=0.: //tolerance
 for (size t i=0;i<thePVStore->size();i++)
   overlapFlag = (*thePVStore)[i]->CheckOverlaps
(res,tol,fCheckOverlapsVerbosity) | overlapFlag;
 if (overlapFlag)
  G4cout << "Check: there are overlapping volumes" <<
G4endl:
```

Output example:

```
136 physical volumes are defined
 Checking overlaps for volume BeamLineSupport ... OK!
  Checking overlaps for volume BeamLineCover ... OK!
 Checking overlaps for volume BeamLineCover2 ... OK!
   Checking overlaps for volume VacuumZone ... OK!
 Checking overlaps for volume FirstScatteringFoil ... OK!
----- WWWW ----- G4Exception-START ----- WWWW -
      *** G4Exception : GeomVol1002 issued by :
           G4PVPlacement::CheckOverlaps()
          Overlap with volume already placed!
          Overlap is detected for volume BrassTube2
              with HoleNozzleSupport volume's
    local point (12.6381,12.8171,-25.1867), overlapping by
                    at least: 3.5 mm
         *** This is just a warning message. ***
----- WWWW ----- G4Exception-END ----- WWWW -
```

This method can be called at any point after run->Initialize();

Thanks for your attention