GSSI, L'Aquila (Italy) 12nd May 2014

Detector description: materials and geometry



Geant 4 tutorial course

Introduction

Mandatory user classes in a Geant4:

- G4VUserPrimaryGeneratorAction
- G4VUserDetectorConstruction
- G4VUserPhysicsList

Materials, Volumes, SD and Fields to be used in the simulation must be defined in the G4VUserDetectorConstruction class

Part I: Materials

Materials:

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

Units

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

G4double width = 12.5 *m;

G4double density = $2.7 \times g/cm3$;

- 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 output 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,
 - static const G4double inch = 2.54*cm;
- Or via G4UnitDefinition (suggested way)
 - new G4UnitDefinition (name, symbol, category, value)
- Example (speed):
 - new 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 atomic properties:
 - 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, refractive index, etc... → linking a G4MaterialPropertyTable
- 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 material (composition by chemical formula):

 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 = 0.3*mg/cm3;
G4double temperature = 500.*kelvin;
G4double pressure = 2.*atmosphere;
G4Material* steam = new G4Material("Water steam", density,
ncomponents=1, kStateGas, temperature, pressure);
steam->AddMaterial(H2O, fractionmass = 1.);
```

<u>Absolute vacuum does not exist</u>: gas at very low density !

- Materials must have $\rho > 0$

```
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, <u>kStateGas</u>,temperature, pressure);
```

NIST Material Data-Base in Geant4

- NIST database for materials is imported inside Geant4 <u>http://physics.nist.gov/PhysRefData</u>
- 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

Ζ	A	m	error	(%)	A _{eff}
Z == 14	Si 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38	22.03453 23.02552 24.011546 25.004107 25.992330 26.98670476 27.976926532 28.97649472 29.97377022 30.97536327 31.9741481 32.978001 33.978576 34.984580 35.98669 36.99300 37.99598	(22) (21) (21) (11) (3) (17) (7) (20) (3) (5) (7) (23) (17) (15) (40) (11) (13) (29)	(%) 92.2297 (7) 4.6832 (5) 3.0872 (5)	A _{eff} 28.0855(3)
	39 40 41 42	39.00230 40.00580 41.01270 42.01610	(43) (54) (64) (75)		

- Natural isotope compositions
- More than 3000 isotope masses

NIST materials in Geant4

### Elementary Materials from the NIST Data Base							
Z Name ChFormula	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	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 AI	2.6989	166					
14 G4_Si	2.33	173					

- NIST Elementary materials:
 - H -> Cf (Z = 1 -> 98)
- NIST compounds:
 - e.g. "G4_ADIPOSE_TISSUE_ICRP"
- HEP and Nuclear materials:

• e.g. Liquid Ar, PbWO

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

======== ### Comp	ound Materia	ls from the NIST	=== Data Base 					
N Name ChFormula density(g/cm^3) I(eV)								
======================================	======================================		=== 63.2					
1	0.119477							
6	0.63724							
7	0.00797							
8	0.232333							
	0.0005							
. –	2e-05							
	0.00016							
	0.00073							
	0.00119							
19	0.00032							
	2e-05							
26 30	2e-05							
4 G4 Air	2e-05	0.00120479	85.7					
_	0.000124	0.00120479	00.7					
7	0.755268							
8	0.231781							
18	0.012827							
2 G4 Csl		4.51	553.1					
53	0.47692							
55	0.52308							

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

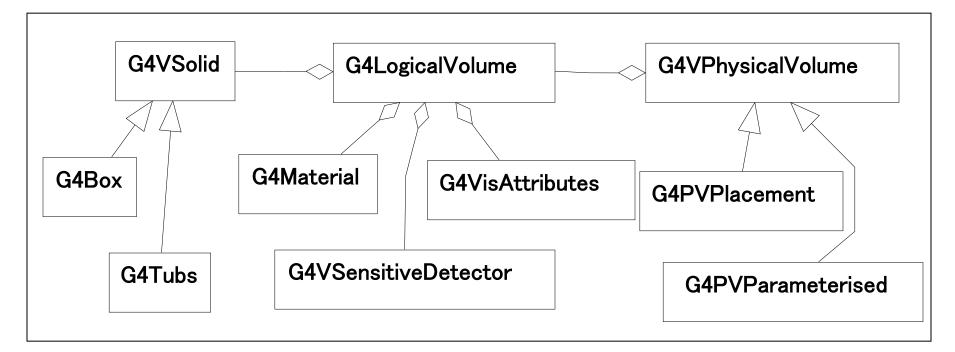
- A detector geometry is made of a number of volumes
- The largest volume is called **World** volume
 - It must contain all other volumes
- Derive your own concrete class from G4VUserDetectorConstruction abstract base class.
- Implementing the method **construct**():
 - Modularize it according to each detector component:
 - Define shapes/solids
 - Construct all materials
 - Construct and place volumes
 - 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, user limits, etc.

- G4VPhysicalVolume -- position, rotation



Define detector geometry

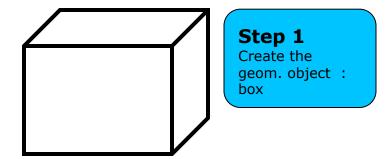
Basic strategy

G4VSolid* pBoxSolid =

new G4Box("aBoxSolid",

1.*m, 2.*m, 3.*m);

Solid : shape and size



Define detector geometry

Basic strategy

G4VSolid* pBoxSolid =

new G4Box("aBoxSolid",

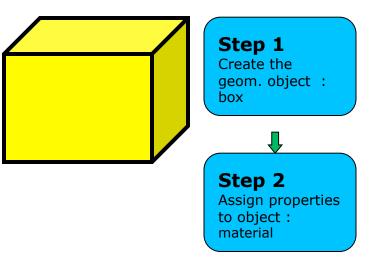
1.*m, 2.*m, 3.*m);

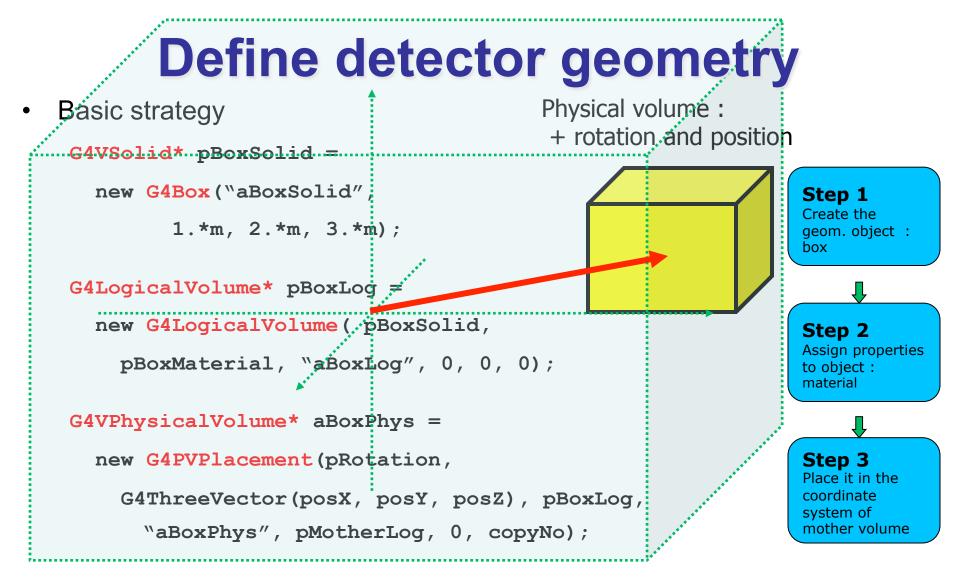
G4LogicalVolume* pBoxLog =

new G4LogicalVolume(pBoxSolid,

```
pBoxMaterial, "aBoxLog", 0, 0, 0);
```

Logical volume : + material, sensitivity, etc.





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

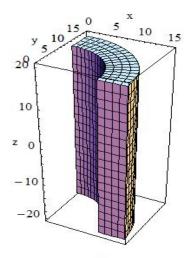
Solids

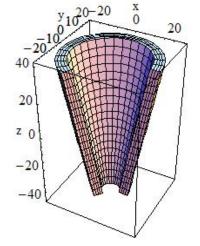
- Solids defined in Geant4:
 - CSG (Constructed Solid Geometry) solids
 - G4Box, G4Tubs, G4Cons, G4Trd, ...
 - Analogous to simple GEANT3 CSG solids
 - Specific solids (CSG like)
 - G4Polycone, G4Polyhedra, G4Hype, ...
 - G4TwistedTubs, G4TwistedTrap, ...
 - Boolean solids
 - G4UnionSolid, G4SubtractionSolid, G4IntersectionSolid
 - Tessellated Solids (made of facets)
 - G4TessellatedSolid

CSG: G4Tubs, G4Cons

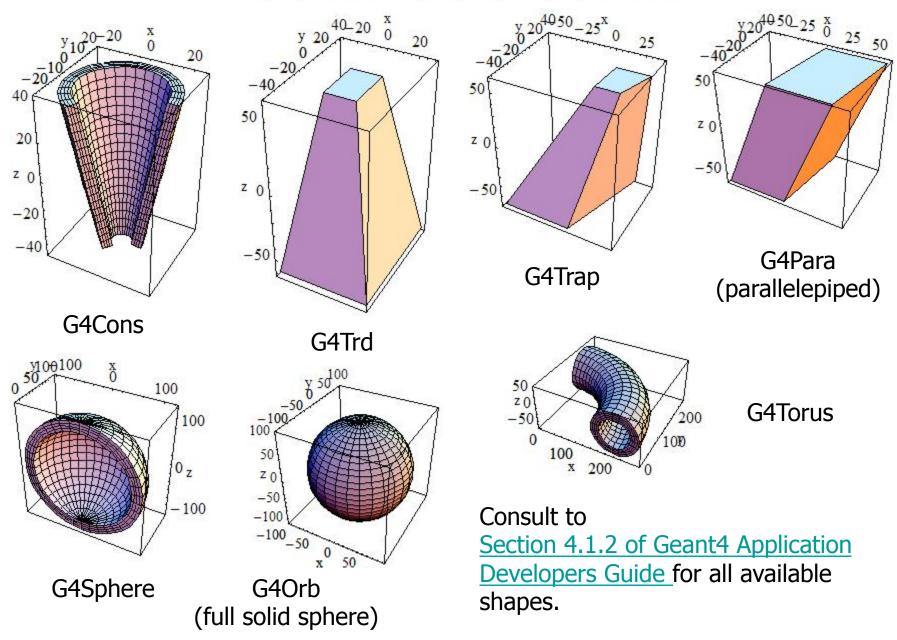
G4Tubs (const	G4String&	pname,	//	name
	G4double	pRmin,	//	inner radius
	G4double	pRmax,	//	outer radius
	G4double	pDz,	//	Z half length
	G4double	pSphi,	//	starting Phi
	G4double	pDphi);	//	segment angle

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





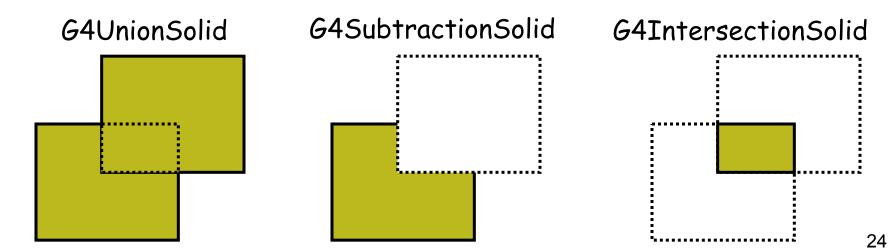
Other CSG solids



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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 is a solid which coordinate system is the same as the 1st solid
- 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



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);
```

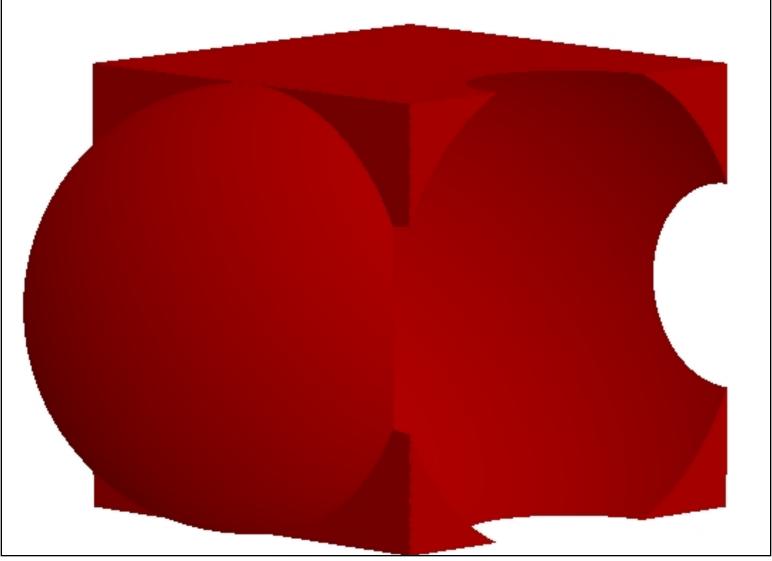
```
G4VSolid* subtract
```

= 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.));
```

Boolean Solids



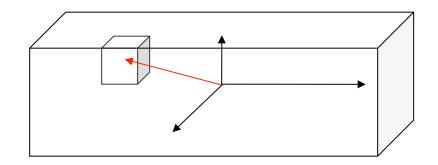
G4LogicalVolume

G4LogicalVolume(G4VSolid* pSolid, G4Material* pMaterial, const G4String& name, G4FieldManager* pFieldMgr=0, G4VSensitiveDetector* pSDetector=0, G4UserLimits* pULimits=0, G4bool tracking 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

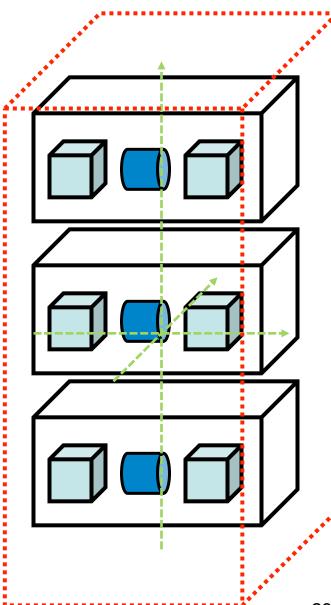
Geometrical hierarchy

- 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 <u>cannot protrude</u> from the mother volume
 - Daughter volumes <u>cannot overlap</u> with each other
 - The logical volume of mother knows the daughter volumes it contains
 - It is uniquely defined to be their mother volume



Geometrical hierarchy

- One or more volumes can be placed in a mother volume. One logical volume can be placed more than once.
- Note: mother-daughter relationship is an information of G4LogicalVolume
 - If the mother volume is placed more than once, all daughters appear in each placed physical volume
- World volume must be a unique physical volume which fully contains all volumes
 - 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

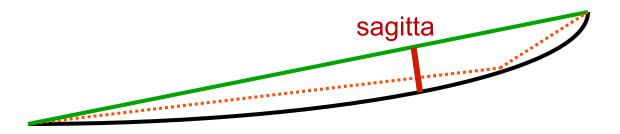


Region

- A **region** is an Envelope of Logical Volumes which may have common characteristics
- A region may have its unique
 - Production thresholds (cuts)
 - If a region 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 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
- Notice :
 - World logical volume is recognized as the default region. User is not allowed to define a region to the world logical volume.

Fields

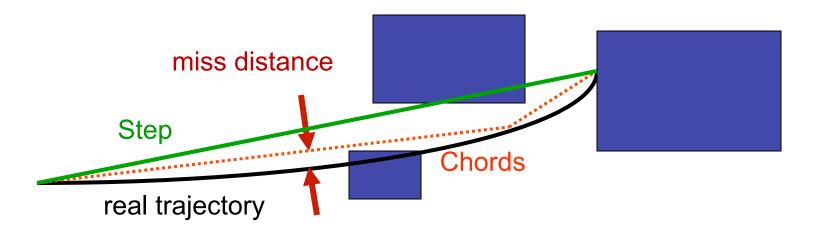
- In order to propagate a particle inside a field (e.g. magnetic, electric or both), we integrate the equation of motion of the particle in the field
- In general this is best done using a Runge-Kutta (RK) method for the integration of ordinary differential equations
 - Several RK methods are available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



• The chord segments are determined to closely approximate the curved path; approximation level is set through an upper bound to the sagitta (maximum distance between the curved path and the straight line)

Fields

- Chords are used to interrogate the Navigator
 - to check 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
 - 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

Example: Create a Magnetic Field

- ♦ Uniform field :
 - Create the field

```
G4MagneticField* magField =
new G4UniformMagField(G4ThreeVector(1.*Tesla,0.,0.);
```

• Set it as default field

G4FieldManager* globalFieldMgr =
G4TransportationManager::GetTransportationManager()
->GetFieldManager();

globalFieldMgr->SetDetectorField(magField);

- Create the chord finder
 globalFieldMgr->CreateChordFinder(magField);

Associate a Field to a logical volume

- ♦ It is possible to describe a field inside a logical volume and all its daughters.
- This can be done creating a local G4FieldManager and attaching it to a logical volume:

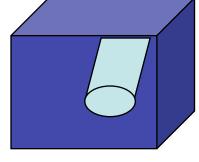
```
G4FieldManager* localFieldMgr =
    new G4FieldManager(magField);
G4bool allLocal = true;
logicVolWithField->SetFieldManager(localFieldMgr,allLocal);
```

If true, field assigned to all daughters If false, field assigned only to daughters w/o their own field manager

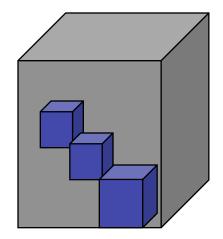
Physical Volumes

A physical volume represent the spatial positioning of the volumes describing your detector

- Placement: it is one positioned volume <u>Note</u> that a Placement Volume <u>can still represent</u> <u>multiple detector elements</u>, if several copies exist of the mother logical volume
- Repeated Volumes: a single Physical Volume represents multiple copies of a volume within its mother volume
 - reduces use of memory
 - <u>Replicas</u>
 - simple repetition, similar to G3 divisions
 - Parameterised Volumes
 - Divided Volumes



placement



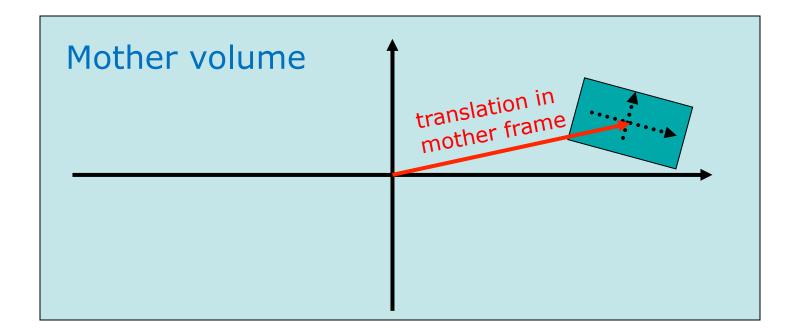
repeated

G4PVPlacement

- 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

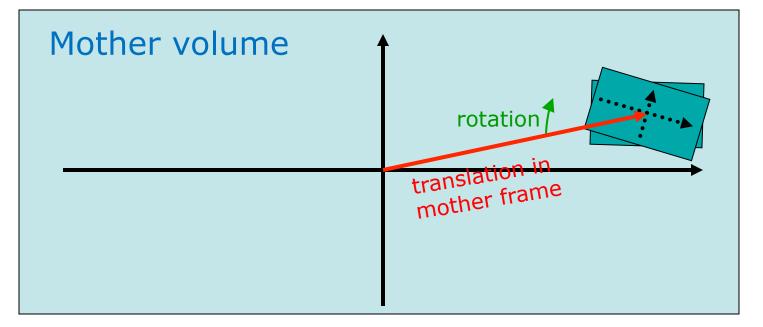
G4PVPlacement Rotation <u>of</u> mother frame ...

• Single volume positioned relatively to the mother volume



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

G4PVPlacement(G4Transform3D(G4Rotation	Matrix	&pRot,	,	// :	rotation	of	daughte	er frame
		const G4Th	reeVecto	or &tl	ate),	// r	position	in	mother	frame
	G4LogicalVolume	*pDaughte	rLogica	l,						
	const G4String &pName,									
	G4LogicalVolume *pMotherLogical,									
	G4bool pMany,		// not	used,	set it	to	false			
	G4int pCopyNo,		// <u>uniq</u>	<u>ue</u> arb	oitrary	in	teger			
	G4bool pSurfChk	=false);	// opti	onal c	overlap	che	eck			



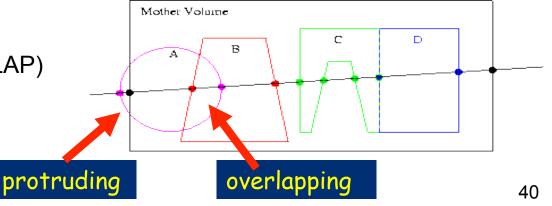
Volume Stores

- All volumes must be allocated using new in the user's application
- At construction, they get registered to a proper Volume Store
- At the end of the job, they will also be automatically deallocated
- Stores:
 - G4SolidStore
 - G4LogicalVolumeStore
 - G4PhysicalVolumeStore
 - G4RegionStore
- Volumes can be retrieved at any convenience, for instance:
 - by index

```
G4LogicalVolume* logicVol =
G4LogicalVolumeStore::GetInstance()->GetVolume("logicLAr");
```

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 in 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, G4PVParameterised and G4PVDivision 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 and configure verification tests for the user geometry:
 - /geometry/test/run to start verification of geometry for overlapping regions based on a standard grid setup, limited to the first depth level
 - /geometry/test/recursion_depth
 Set the depth in the geometry tree for recursion
 - /geometry/test/tolerance Define tolerance (in mm) by which overlaps reports

Thanks for your attention

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();