Material Definition

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Contents

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A volume in simulation geometry must have information that describes its material

How to define a material by hand

How to use predefined material database of Geant4

G4Material

G4Material contains material properties

- elemental, isotope composition
- density
- temperature, pressure and state(Solid, Liquid, Gas and Undefined) of the material
  - Several physics model use these information
- chemical formula
- ionization parameters
- MaterialPropertiesTable
  - For extension

G4Material can be created from

- Single G4Element
- Multiple G4Elements
- Other G4Materials

Various examples will be shown in later slides

Pointer of G4Material object will be registered into G4LogicalVolume

G4Element

G4Element contains element properties

- Z as atomic number
- A as mass

G4Element be created from

- Z and A
  - Assuming natural abundance of isotope

```
G4Element* elH  =
    new G4Element("Hydrogen", symbol="H", z=1., a=1.01*g/mole);
```

- G4Isotope(s)
  - User can define isotope composition of an element
  - An example will be shown in slide #8

G4Isotope

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contains isotope properties

- Z as atomic number
- N as number of nucleon
- m as isomer level
  - Excitation energy for isomer level is not automatically defined

be created from

- Z and N

```
G4Isotope* isoU235 =
      new G4Isotope("U235", iz=92, in=235);
```

- Z, N, A and m

```
G4Isotope* isoAm242m1 =
      new G4Isotope("Am242m1", iz=95, in=242,
                    mass=massAm242 + 48.63*keV, im=1);
```

Examples of defining material #1

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Single element material

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

Molecule is made of several elements

- composition by number of atoms

```
G4Element* elH  =
  new G4Element("Hydrogen",symbol="H",z=1.,a=1.01*g/mole);
G4Element* elO  =
  new G4Element("Oxygen",symbol="O",z=8., a = 16.00*g/mole);
G4Material* H2O =
  new G4Material("Water",density=1.000*g/cm3,ncomp=2);
H2O->AddElement(elH, natoms=2);
H2O->AddElement(elO, natoms=1);
```

Examples of defining material #2

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Compound: composition by fraction of mass

```
G4Element* elN  =
  new G4Element(name="Nitrogen",symbol="N",z= 7.,a = 14.01*g/mole);
G4Element* elO  =
  new G4Element(name="Oxygen",symbol="O",z=8.,a=16.00*g/mole);
G4Material* Air =
  new G4Material(name="Air",density=1.290*mg/cm3,ncomponents=2);
Air->AddElement(elN, fracMass=70.0*perCent);
Air->AddElement(elO, fracMass=30.0*perCent);
```

Composition of compound materials (and elements)

```
G4Element* elC  = …;   // define “carbon” element
G4Material* SiO2 = …;  // define “quartz” material
G4Material* H2O = …;   // define “water” material

G4Material* Aerog =
    new G4Material("Aerogel",density 0.200*g/cm3,ncomponents=3);
Aerog->AddMaterial(SiO2,fractionmass=62.5*perCent);
Aerog->AddMaterial(H2O ,fractionmass=37.4*perCent);
Aerog->AddElement(elC ,fractionmass= 0.1*perCent);
```

Examples of defining material #3

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A material from user defined abundance element

```
G4Isotope* isoU235 =
   new G4Isotope("U235", iz=92, ia=235, a=235.043*g/mole);
G4Isotope* isoU238 =
   new G4Isotope("U238", iz=92, ia=238, a=238.050*g/mole);

G4Element* elenrichedU =
   new G4Element("enriched U", symbol="U" , ncomponents=2);
elenrichedU->AddIsotope(isoU235, abundance=80.*perCent);
elenrichedU->AddIsotope(isoU238, abundance=20.*perCent);

G4Material* matenrichedU=
   new G4Material("U for nuclear power generation" , density= 19.050*g/
cm3, ncomponents = 1, kStateSolid );
matenrichedU>AddElement( elenrichedU, fractionmass = 1.00);
```

Predefined material database in Geant4

NIST database for material is imported inside Geant4

- http://physics.nist.gov/PhysRefData

Guarantee the best accuracy for major parameters

- Density
- Mean excitation potential
- Chemical bounds
- Element composition
- Isotope composition

Easy access through G4NistManager and UI commands

What materials are in the predefined database

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NIST elementary materials

- Up to Californium (Cf, Z=98)

NIST compounds and mixtures

- A-150 Tissue-Equivalent Plastic, Air Dry (near sea level) and many others

HEP and Nuclear Materials

- liquid Ar, PbWO4, CR39 and so on

Space Materials

- Kevlar, Dacron and so on

Bio Chemical Materials

- Cytosine, thymine and so on

Total number of predefined material in the database is 315

How to use predefined material data base

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Get Manager

G4NistManager manager = G4NistManager::GetPointer();*

Get Element

G4Element elm = manager->FindOrBuildElement("C");*
G4Element elm = manager->FindOrBuildElement(Z=6);*

Get predefined material

G4Material mat = manager->FindOrBuildMaterial("G4_C");*
G4Material mat = manager->FindOrBuildMaterial("G4_Galactic");*
G4Material mat = manager->FindOrBuildMaterial("G4_WATER");*

Get full list of predefined material

manager->ListMaterials("all");

UI commands

/material/nist/printElement --- print defined elements
/material/nist/listMaterials --- print defined materials

- equivalent to *manager->ListMaterials("all");*

Tips for material implementation

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- Geant4 does not allow pure vacuum (material has a density of zero).
  - Make an ultra-low density material.
  - G4_Galactic (density = 1.0^{-25} [g/cm^3]) in predefined database is one of such examples.
- Use the predefined material database as much as possible
  - Easy and acute
- Cast a density of material
  - Create new material from the material with a target density
  - predefined database has a method "BuildMaterialWithNewDensity" for converting density