Material Definition

Geant4 Tutorial 2011 in Seoul
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MATERIAL DEFINITION

Materials in Geant4

Material is defined as molecules, compounds, or mixtures.

1) Molecules or compounds are consists of Elements
2) Mixtures are consists of Materials and/or Elements

Elements have a list of isotopes

3 classes are provided.

- Isotope ←→ G4Isotope
- Elements ←→ G4Element
- molecules, compounds and mixtures ←→ G4Material

G4Isotope and G4Element define characteristics in atomic level.

- atomic number (Z), number of nucleons(N), molecular mass(A), shell structure, etc.
- used for material definition

G4Material

- defines element constitution
- specify macroscopic properties: temperature, pressure, state, density
  - ✓ Do not use materials with zero density (Even for vacuum, it should have non-zero density.)
- used for geometry definition

Material definition for single element material

Single element material is defined by name, density, Z, A.

e.g., Liquid argon

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

(You do not have to define G4Element in this case.)

Material definition for molecule

Molecule is defined by stoichiometry, i.e. number of atoms (Elements)
Step1) Define elements by name, symbol, atomic number(Z) and atomic weight(A).
Step2) Define material using elements by name, density and number of components.

Step1) Define Elements e.g. H and O

```
G4String symbol;
G4double z;
G4double 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);
```

Step2) Define Material e.g. H2O

```
G4int ncomp;
G4double density = 1.000 * g/cm3;
G4Material* H2O = new G4Material("Water", density, ncomp=2);
G4int natoms;
H2O-> AddElement(elH, natoms=2);
H2O-> AddElement(elO, natoms=1);
```

Material definition of compound

Compound is defined by mass fraction of Elements.
Step1) Define elements by name, symbol, atomic number(Z) and atomic weight(A).
Step2) Define material using elements by name, density and mass fractions.

Step1) Define Elements e.g. H and O

```
G4String symbol;
G4double z;
G4double 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);
```

Step2) Define Material e.g. Vapor

```
G4int ncomp;
G4ouble density = 1.290 * mg/cm3;
G4Material* Air = new G4Material("Air", density, ncomp=2);
G4double fracMass;
Air-> AddElement(elN, fracMass=70.0*perCent);
Air-> AddElement(elO, fracMass=30.0*perCent);
```

Tips:
If second argument is given in double, it means fraction mass.
If second argument is given in integer, it means number of atoms.
(Overload of methods)

Material definition of mixture

Mixture is defined by mass fraction of
Elements and/or materials (single element material, compounds, molecules).
Step1) Define elements/materials to be used for the mixture materials.
Step2) Define material using materials by name, density and mass fractions.

Step1) Define Elements/Materials to be used.

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

Step2) Define Material by mass fractions.

```
G4int ncomp;
G4double fractionmass;
G4double density = 0.200 * g/cm3;
G4Material* Aerog = new G4Material("Aerogel", density, ncomp=3);
Aerog-> AddMaterial(SiO2, fractionmass=62.5*perCent);
Aerog-> AddMaterial(H2O , fractionmass=37.4*perCent);
Aerog-> AddElement (elC , fractionmass= 0.1*perCent);
```

Isotopes and abundances

If you define an element, it is treated by default as if it has the natural isotope abundance
 - even if the A (g/mole) value you enter is quite different from the natural abundance.
You can define an element with non-natural abundance by assigning to G4Element a list of G4Isotope instances

Ex. Create an enriched Uranium for nuclear power generation.

```
G4Isotope* isoU235 = new G4Isotope(“U235", iz=92, ia=235, a=235.0439242*g/mole);
G4Isotope* isoU238 = new G4Isotope(“U238", iz=92, ia=238, a=238.0507847*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, 640*kelvin, 1.5e7*pascal);
matenrichedU-> AddElement(elenrichedU, fractionmass=1.);
```

Notes on material definition

Prefer low-density material to vacuum

- use "*universe_mean_density* (=1.e-25*g/cm^3)"

For hadronic processes, a correct set of elements is crucial for cross sections and interactions.

- You should NOT use "*averaged material*".

Once you create materials, these materials are retrieved by

```
G4Material*  mat =
        G4Material::GetMaterial(G4String name, G4bool warning=true)
```

NIST MATERIAL DATABASE

NIST database in Geant4

NIST database for materials is imported inside Geant4.

- http://www.nist.gov/pml/data/index.cfm
  - ✓ All elements with natural isotopic abundance
  - ✓ Stable and unstable isotopes are included (3000 up to Cf)

Guarantee the best accuracy for major parameters :

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

UI commands are provided in material category

NIST elements and isotopes

Example of Elemental composition in Si

Z	A	m	error	(%)	Aeff
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 3,000 isotopes are available.

NIST materials

```
=====================================
###   Elementary Materials from the NIST Data Base
=====================================
 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
12   G4_Mg                    1.74             156
13   G4_Al                    2.6989           166
14   G4_Si                    2.33             173
```

UI commands :

Print defined elements
/material/nist/printElement

Print defined materials
/material/nist/listMaterials

```
=====================================
###    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
```

How to use NIST materials

G4NistManager manage all of NIST materials/elements.

```
G4NistManager* manager = G4NistManager::GetPointer();

G4Element* elm = manager-> FindOrBuildElement("symb", G4bool iso);

G4Element* elm = manager-> FindOrBuildElement(G4int Z, G4bool iso);

G4Material* mat = manager-> FindOrBuildMaterial("name", G4bool iso);
// iso is omitable (true by default, i.e. create isotopes)
// If iso is false, isotopes are not explicitly build.
```

```
G4Material* mat = manager-> ConstructNewMaterial("name",
                            const std::vector<G4int>& Z,
                            const std::vector<G4double>& weight,
                            G4double density, G4bool iso);

G4double isotopeMass = manager-> GetMass(G4int Z, G4int N);
```

Summary

Users have to define materials used for simulation.

- G4Element, G4Isotope, G4Material classes provided.
- Material conditions are set by
  - ✓ Density, state, temperature, pressure
- Materials are used for geometry definition.

Predefined materials in NIST database are also available.

- Guarantee the best accuracy for major parameters :