Defining Materials

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Geant 4

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Contents

- Why / Where materials ?
- Material definition
- Guidelines for C++ and GDML implementation of material definitions
- NIST material database in Geant4

Why / Where materials ?

- Physics process behaviour during tracking in Geant4 depend on the materials used for the volumes in the geometry

```
G4eIonisation → G4VEnergyLossProcess::BuildDEDXTable( … )
```

- To make this possible, at geometry definition users are requested to associate materials to logical volumes

```
G4LogicalVolume::G4LogicalVolume ( G4VSolid* solid,
G4Material* material, const G4String name, … )
```

Material definition

Materials in Geant4

- In nature,
  materials (chemical compounds, mixtures) are made of elements and elements are made of isotopes

  → Three main classes in the Geant4 design

– Isotopes	←→	G4Isotope
– Elements	←→	G4Element
– Molecules, compounds, mixtures	←→	G4Material

- G4Isotope and G4Element describe the 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 class
  - The only one visible to the rest of the toolkit:
    Used by tracking, geometry, physics
  - Contains all the information relative to the eventual elements and isotopes of which it is made
    (at the same time hiding implementation details)

“Simple” materials

- Single element material
  - Defined by name, density, mass per mole, and atomic number

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

- Avoid “effective” average A, Z with hadronic physics !
  - Cross-section are not a function of material properties, but a function of nuclear properties.

    → At least correct set of elements are needed
  - Using effective numbers, the element composition cannot be automatically recovered.

    → Cross-section will be approximative, final states will have wrong properties.

Material: molecule

- Material built from its elements
  - Defined by number of atoms per each element in the molecule (chemical formula)

```
a = 1.01*g/mole;
G4Element* ele_H = new G4Element("Hydrogen",symbol="H",z=1.,a);
a = 16.00*g/mole;
G4Element* ele_O = new G4Element("Oxygen",symbol="O",z=8.,a);

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

- Note
  - CH_2 is equivalent to C_4H_8, etc

Material: compound

- Material built from its elements
  - Defined by fraction of mass of each element in the material

```
a = 14.01*g/mole;
G4Element* ele_N = new G4Element(name="Nitrogen",symbol="N",z= 7.,a);
a = 16.00*g/mole;
G4Element* ele_O = new G4Element(name="Oxygen",symbol="O",z= 8.,a);


density = 1.290*mg/cm3;
G4Material* Air = new G4Material(name="Air",density,ncomponents=2);
G4double fracMass;
Air->AddElement(ele_N, fracMass=70.0*perCent);
Air->AddElement(ele_O, fracMass=30.0*perCent);
```

Material: mixture

- Material built from pre-defined materials or elements
  - Defined by fraction of mass of each component

```
G4Element* ele_C  = …;    // 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 (ele_C ,fractionmass= 0.1*perCent);
```

Element with user defined abundance

- When necessary, elements can be built from pre-defined isotopes
  - Defined by abundance of each isotope

- Ex. enriched Uranium for nuclear power generation

```
G4Isotope* iso_U235 = new G4Isotope(“U235", iz=92, ia=235, a=235.0439242*g/mole);
G4Isotope* iso_U238 = new G4Isotope(“U238", iz=92, ia=238, a=238.0507847 *g/mole);

G4Element* ele_enrichedU = new G4Element(“enriched U", symbol=“U" ,
   ncomponents=2);

ele_enrichedU->AddIsotope(iso_U235, abundance=80.*perCent);
ele_enrichedU->AddIsotope(iso_U235, abundance=20.*perCent);

G4Material* mat_enrichedU =
   new G4Material(“U for nuclear  power generation" , density= 19.050*g/cm3 ,
                 ncomponents = 1 , kStateSolid );
mat_enrichedU->AddElement( ele_enrichedU , fractionmass = 1 );
```

- Now user defined abundances are used also by hadronic processes

G4Material attributes

- Attributes associated to G4Material
  - Temperature, Pressure, State, Density
  - All can affect physics process parameters

- 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(ele_C,natoms = 1);
CO2->AddElement(ele_O,natoms = 2);
```

Materials in GDML

- GDML
  Geometry Description Markup Language
  - Application independent geometry description format
  - Geometry data exchange
  - GDML Schema: a set of XML schema definition (.xsd) files specifying the GDML syntax
  - Looks similar to HTML, with specific tags for materials, shapes, positions, rotations, …
  - External ASCII file: easy to create, read, debug, modify,…
- http://cern.ch/gdml

GDML
Some details

Define elements and materials*

Define shapes

Define volume tree

```
<materials>
    <element name="Oxygen"    formula="O"  Z="8.">
          <atom value="16.0"/>   </element>
    <element name="Silicon"  formula="Si" Z="14.">
          <atom value="28.09"/>  </element>
    <material name="SiO2"> <D value="2.200"/>
          <composite n="1" ref="Silicon"/>
          <composite n="2" ref="Oxygen"/> </material>
...

<solids>
  <box name="solid_World" x="50.0" y="50.0" z="50.0"/>
...

<volume name="World">
    <materialref ref="Vacuum"/>
    <solidref ref="solid_World"/>
    <physvol> <volumeref ref=“Satellite"/>
          <positionrefref="center"/> <rotationref ref="identity"/>
          </physvol>
    <physvol> <volumeref ref="support"/> <positionref ref="center"/>
          <rotationref ref="identity"/> </physvol>
    <physvol> <volumeref ref="b1"/> <positionref ref="p1"/>
          <rotationref ref="identity"/> </physvol>
...
```

GDML: simple materials

- Single element

```
<material name="Al" Z="13.0" >
     <D value="2.70" />
     <atom value="26.98" />
</material>
```

GDML: materials by number of atoms

- Material by number of atoms (chemical formula)

```
<element Z=“1” formula=“H” name=“Hydrogen” >
     <atom value="1.00794" />
</element>
<element Z="8" formula="O" name="Oxygen" >
     <atom value="15.9994" />
</element>

<material name="Water" formula="H2O">
     <D value="1.0" />
     <composite n="2" ref="Hydrogen" />
     <composite n="1" ref="Oxygen" />
</material>
```

GDML: materials by fraction of mass

- Built from elements

```
<material formula="air" name="Air" >
     <D value="0.00128999999999999" />
     <fraction n="0.7" ref=“ele_Nitrogen" />
     <fraction n="0.3" ref=“ele_Oxygen" />
</material>
```

- Built as mixture of materials and elements

```
<material formula=“aerogel" name="Aerogel" >
     <D value="0.2" />
     <fraction n=“0.625" ref=“SiO2" />
     <fraction n="0.374" ref=“H2O" />
     <fraction n="0.001" ref=“ele_Carbon" />
</material>
```

GDML: elements by isotope abundances

- Isotopes

```
<isotope name="U235" Z="92" N="235">
     <atom type="A" value="235.01">
</isotope>
<isotope name="U238" Z="92" N="238">
     <atom type="A" value="235.03">
</isotope>
```

- Element

```
<element name="enriched_uranium" >
     <fraction ref="U235" n="0.9" />
     <fraction ref="U238" n="0.1" />
</element>
```

NIST material database in Geant4

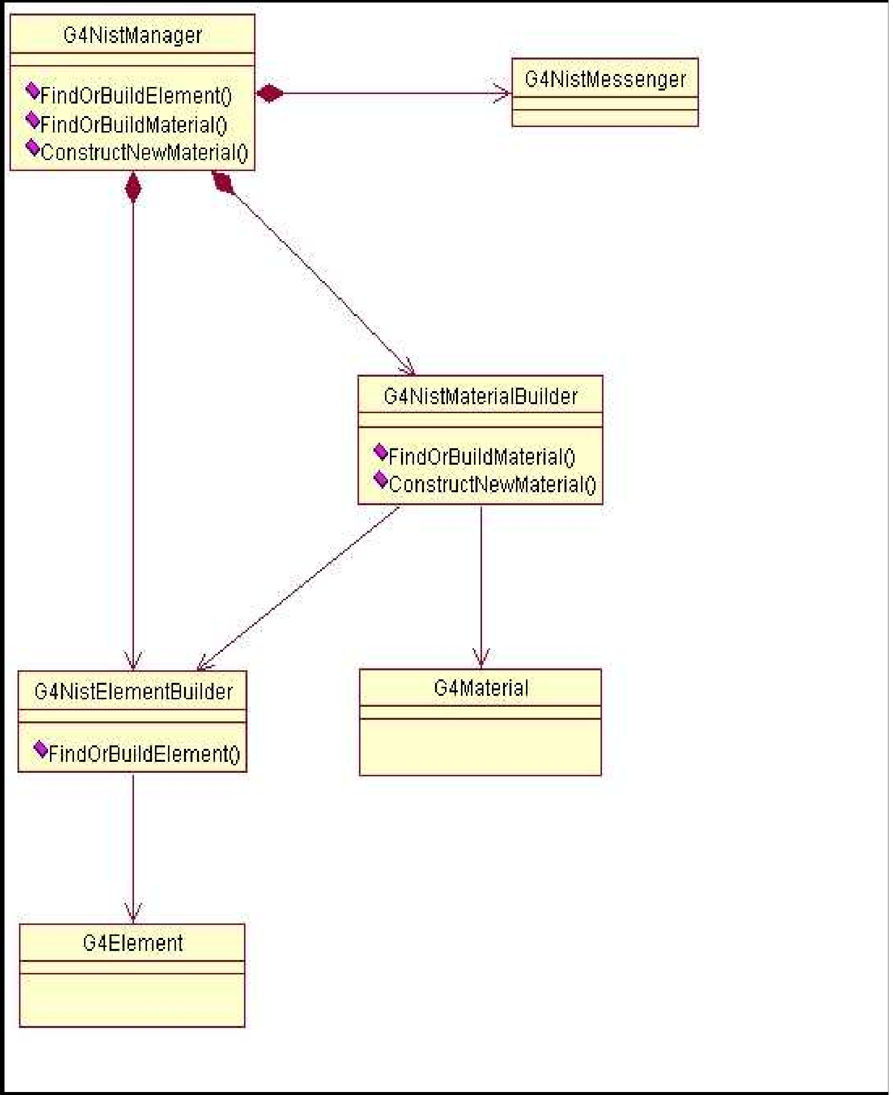
Material category upgrade

- Goal:
  Guarantee accuracy in major parameters
  - Density
  - Mean excitation potential
  - Chemical bounds
  - Element composition
  - Isotope composition

- NIST database for materials is imported inside Geant4 (http://physics.nist.gov/PhysRefData)

- Introduced in release 7.1

- New interfaces are added, old are kept



NIST Elements from Isotopes

Z	A	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	26.98670476	(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 3000 isotope masses are used for definition

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       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
```

- NIST Elementary Materials
  - H → Cf (Z=1→98)
- NIST compounds
  - E.g. “G4_ADIPOSE_TISSUE_ICRP”
- HEP and Nuclear Materials
  - E.g. liquid Ar, $PbWO_4$

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

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

NIST: How to use

- Do not need anymore to predefine elements and materials

- Main new user interfaces:

```
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);

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);
```

- UI commands

```
/material/nist/printElement    ← print defined elements
/material/nist/listMaterials   ← print defined materials
```

NIST database in GDML

- GDML is a specialized XML-based language
  - Only references to materials already defined in the GDML model are allowed (in principle)
- The GDML-Geant4 binding (C++ module) lets you break this rule
  - Make direct use of all NIST elements and materials available in Geant4
  - By enabling the NIST option at GDML setup phase (GDMLSetup script)

```
Would you like to enable NIST support? Default:NO  [y/n]   y
```