Defining Materials in Geant4

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Tutorial based on Geant4 v9.5-p01
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  o Isotopes
  o Compounds
  o Mixtures

• The NIST material database and Geant4
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  o How to access it from Geant4
Single Element Materials

Need G4Material* in order to instantiate G4LogicalVolume

```cpp
G4Material(name, atomic_number, atomic_weight, density);
G4Material(name, density, number_of_components);
```

Defining a simple material:

```cpp
G4double atomic_weight = 39.95*g/mole;
G4double density = 1.390*g/cm3;
G4Material* lAr =
    new G4Material(“liquidArgon”, Z=18, atomic_weight, density);
```
Molecules

Molecules are defined from instances of the G4Element class.

Defining the components of H2O:

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

G4Element* oxygen =
    new G4Element("Oxygen", symbol="O", z=8, a=16.00*g/mole);
```

Assemble elements into H2O molecule:

```cpp
G4Material* H2O =
    new G4Material("Water", density=1.000*g/cm3,n_comps=2);

G4int number_of_atoms;
H2O->AddElement(hydrogen, number_of_atoms=2);
H2O->AddElement(oxygen, number_of_atoms=1);
```
Isotopes

Elements can comprise different components, just like molecules

G4Isotope* isoU235 =
    new G4Isotope("U235", Z=92, A=235, a=235.044*g/mole);

G4Isotope* isoU238 =
    new G4Isotope("U238", Z=92, A=238, a=238.051*g/mole);

G4Element* enrichedU =
    new G4Element("enriched U", symbol="U", n_comp=2);

enrichedU->AddIsotope(isoU235, abundance=80.*perCent);
enrichedU->AddIsotope(isoU238, abundance=20.*perCent);

The element is then added to a single-component material:

G4Material* mat_enrichedU=
    new G4Material("enr. U", density, ncomp = 1);

mat_enrichedU
    ->AddElement( enrichedU, fraction_mass = 1 );
Compounds

Compounds are mixtures of elements not bound into molecules and can be specified by fraction of mass:

```c++
G4Element* nitrogen = new G4Element("Nitrogen", symbol="N", z= 7., a=14.01*g/mole);
G4Element* oxygen = new G4Element("Oxygen", symbol="O", z=8., a=16.00*g/mole);

G4Material* Air = new G4Material("Air", density=1.290*mg/cm3, ncomp=2);
Air->AddElement(nitrogen, fracMass=70.0*perCent);
Air->AddElement(oxygen, fracMass=30.0*perCent);
```
Mixtures

Mixtures allow the combination of G4Materials and G4Elements into a single G4Material instance, allowing the combination of molecules, isotopes and elements:

```cpp
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);
```
The NIST Material Database

- The National Institute of Standards (NIST) provides a detailed database of material properties, particularly:
  - Density
  - Excitation potential
  - Element composition
  - Isotope composition

- More than 3000 isotopes and their properties are being tracked

- A version of this database is part of the Geant4 distribution
The NIST Material Database - Si

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<th>Z</th>
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<th>m</th>
<th>error</th>
<th>(%)</th>
<th>( A_{\text{eff}} )</th>
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• The table to the right shows the physical properties of 20 known Si isotopes

• The table also provides natural isotope abundances and a single „average isotope“

• Various molecules and compounds are also provided
Using NIST Materials - I

Database access is managed by a singleton manager class:

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

G4Element and G4Material can both be loaded straight from the database:

```cpp
G4Element* elm = manager->FindOrBuildElement(symbol="H", G4bool iso);
G4Element* elm = manager->FindOrBuildElement(G4int Z, G4bool iso);
G4Material* mat = manager->FindOrBuildMaterial(name="G4_Air", G4bool iso);
```
Using NIST Materials - II

A compound can be built by specifying a vector of atomic numbers and weights to retrieve NIST elements:

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

The database can also be queried for isotope masses:

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

Finally, the UI commands to list defined elements/materials are:

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

• Simple materials can be defined directly by using the `G4Material()` constructor

• Molecules are defined by declaring multi-component materials and using `AddElement(...)` method to add `G4Element` instances

• Mixtures are arbitrary combinations of elements and `G4Material` objects

• The NIST database can be used to obtain precise physical data for elements and their isotopic composition as well as molecules