




# Material Definition

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Geant4 ED PHENIICS Tutorial,
13 - 17 May 2019, Orsay

# Outline

- The System of units & constants
- NIST Database
- Definition of elements
- Materials and mixtures

# The System of Units

- Geant4 has no default unit. To give a number, unit must be “multiplied” to the number, for example :
  - `G4double width = 12.5*m;`
  - `G4double density = 2.7*g/cm3;`
- If no unit is specified, the internal G4 unit will be used, but this is discouraged !
- Almost all commonly used units are available.
- Refer to CLHEP: SystemOfUnits.h
- To get a value in a given unit divide a variable by this unit:
  - `G4cout << dE / MeV << " (MeV)" << G4endl;`
- Users can define their own units using G4UnitDefinition class

# The System of Units (2)

- Geant4 uses system of units defined in CLHEP and based on:
  - millimeter (**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.
- In output, Geant4 users 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 value

# Definition of Materials

- Geant4 models materials mimicking what happens in nature
- With different kind of materials
  - Isotopes, elements, molecules, compounds and mixtures => G4Isotope, G4Element, G4Material
- Attributes associated:
  - Temperature, pressure, state, density

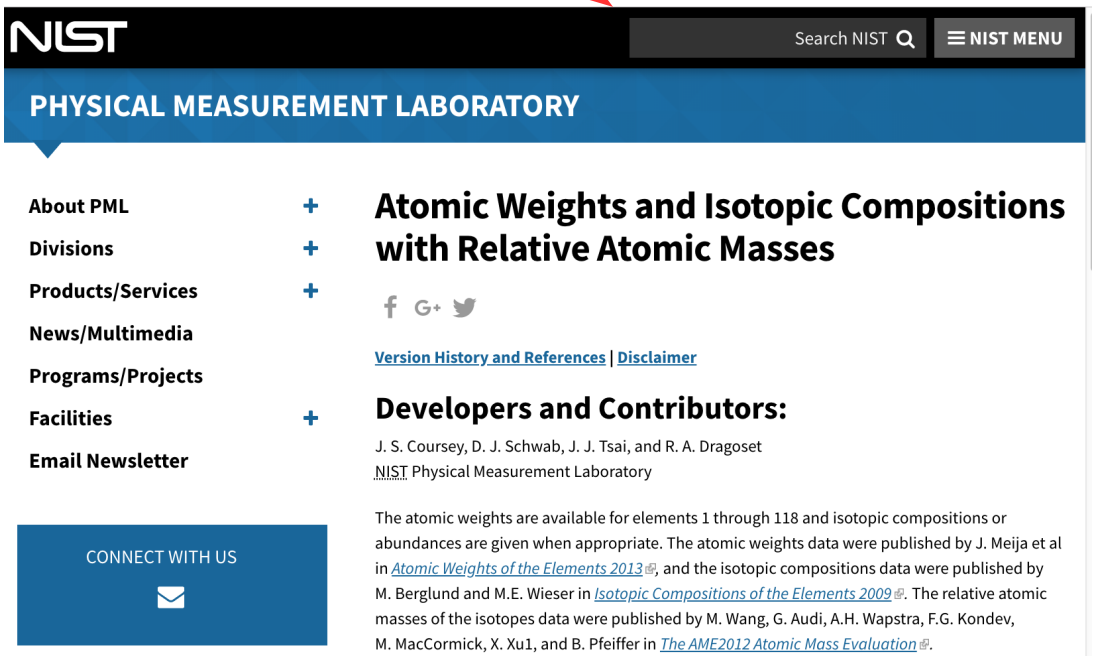
- Note that modeling is in most of the cases limited to “High Energy Physics” approximation:
  - Ie : molecular or crystal structure do not count at high energy
- But with notable exceptions:
  - Very low energy DNA simulation does take into account DNA structure
  - New developments regarding channeling effects are ongoing…

# Isotopes, Elements and Materials

- 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…

# NIST Database

- NIST database:
  - https://www.nist.gov/pml/atomic-weights-and-isotopic-compositions-relative-atomic-masses
- Imported inside Geant4
- Simplifies definition of materials in users applications as it is sufficient just to choose a material or an element by its name
- Guarantees accuracy in major parameters:
  - Density, mean excitation potential, elemental composition, isotopic composition, ...



# Predefined materials in NIST

- Elementary materials
  - Up to Californium (Cf, Z=98)
- 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

# Getting Material from NIST

- Element/Material is retrieved from Geant4 material database by its name:

```
#include “G4NistManager.hh”

// Get NIST manager
G4NistManager* manager = G4NistManager::Instance();

// Get/build elements, materials
G4Element* elC = manager->FindOrBuildElement("G4_C");
G4Material* water = manager->FindOrBuildMaterial("G4_WATER");
```

- The list of currently available material names can be found in the Geant4 User's Guide for Application Developers
  - Appendix 6: Geant4 Material Database
  - The list is permanently being extended

# More about NIST

- Scaling the density of a defined material in NIST:

```
G4double density = 1.03*mg/cm3;
G4Material* water2
  = G4NistManager::Instance()
    ->BuildMaterialWithNewDensity("Water_1.03","G4_WATER",density);
```

- A compound can be built by specifying a vector of atomic numbers and weights using

```
G4NistManager::ConstructNewMaterial(
                const G4String& name,
                const std::vector<G4int>& Z,
                const std::vector<G4double>& weight,
                G4double density, G4bool iso);
```

- Isotope masses are accessible using

```
G4NistManager::GetMass(G4int Z, G4int N);
```

# NIST materials in Geant4

## Elements

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

## Compounds

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

# Explicit Material Definition

# Elements

- Elements are defined by name, symbol, atomic number and mass of mole:

```
G4double a, z;
G4String symbol;

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);
```

# Elements & Isotopes

- If necessary, elements can be built from pre-defined isotopes:

```
G4int iz, n, nComponents;
G4double abundance;

// isotopes
G4Isotope* u235
  = new G4Isotope("U235", iz=92, n=235, a=235.01*g/mole);
G4Isotope* u238
  = new G4Isotope("U238", iz=92, n=238, a=238.03*g/mole);

// element composed of isotopes
G4Element* uranium
  = new G4Element("Enriched Uranium", "U", nComponents=2);
uranium->AddIsotope(u235, abundance= 90.*perCent);
uranium->AddIsotope(u238, abundance= 10.*perCent);
```

# Material of One Element

- Single element material:

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

- Do not try to use the single element capability as a replacement of a mixture, by making an “effective” average A, Z : *it will crash with hadronic physics !*
  - Remember : cross-sections are not a function of material properties, but a function of nuclear properties.
  - Provide the correct set of elements instead.

# Material: Molecule

- Material as a composition by number of atoms (molecule):

```
G4double a, z, density;
G4int nComponents, nAtoms;
G4String symbol;

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* water
  = new G4Material("Water", density, nComponents=2);
water->AddElement(elH, nAtoms=2);
water->AddElement(elO, nAtoms=1);
```

*To repeat: in most of the cases, the molecular structure is not taken into account in Geant4 : this a high energy approximation*

# Material: Compound

- Compound: a composition of elements by fraction of mass

```
G4double a, z, density;
G4int nComponents;
G4String name, symbol;

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);
```

# Material: Mixture

- Composition of compound materials and elements by mass fraction

```
G4double density, fractionMass;
G4int nComponents;

G4Element* elC = …;      // define “carbon” element
G4Material* siO2  = …;   // define “quartz” material
G4Material* water = …;   // define “water” material

density = 0.200*g/cm3;
G4Material* aerogel
  = new G4Material("Aerogel", density, nComponents=3);
aerogel->AddMaterial(siO2, fractionMass=62.5*perCent);
aerogel->AddMaterial(water,fractionMass=37.4*perCent);
aerogel->AddElement (elC , fractionMass= 0.1*perCent);
```

# Example of Gas

- It may be necessary to specify temperature and pressure
  - As dE/dx computation is affected

```
G4double density = 27.*mg/cm3;
G4double temperature = 325.*kelvin;
G4double pressure = 50.*atmosphere;
G4int nComponents, nAtoms;

G4Material* carbonicGas
  = new G4Material("CarbonicGas", density, nComponents=2,
                   kStateGas, temperature, pressure);
carbonicGas->AddElement(elC, nAtoms = 1);
carbonicGas->AddElement(elO, nAtoms = 2);
```

# Example of Vacuum

- Absolute vacuum does not exist: it is a gas at very low density !
  - Cannot define materials composed of multiple elements through Z or A, with density = 0 !

```
G4double atomicNumber = 1.;
G4double massOfMole = 1.008*g/mole;
G4double density = 1.e-25.*mg/cm3;
G4double temperature = 2.73*kelvin;
G4double pressure = 3.e-18*pascal;

G4Material* vacuum
  = new G4Material(“interGalactic",
                   atomicNumber, massOfMole, density,
                   kStateGas, temperature, pressure);
```

# Summary

- Materials in Geant4 describe the macroscopic properties
- You may use the NIST database
  - Includes many isotopes, elements and materials
  - As well as “advanced” materials (organic tissues, etc.)
- You may also create new materials for the NIST database scaling material densities

- When needed, the materials, elements and isotopes can be defined from scratch, using Geant4 classes