Material Definition

I. Hrivnacova, IJCLab Orsay

Credits:
V. Ivantchenko, T. Nikitina, J.Apostolakis, G.Cosmo, A. Lechner, (CERN), S.Incerti (CENBG), Tatsumi Koi (SLAC), M. Verderi (LLR) and others

Outline

- The System of units & constants

- G4 material model

  - Definition of elements and materials from scratch

- NIST Material Database

  - Getting predefined elements and materials from a database

The System of Units

- Geant4 has no default unit. To give a number, a 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 the 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

Geant4 Material Model

- Geant4 models materials mimicking what happens in nature: materials are made of elements and elements are made of isotopes

- The 3 main classes to describe these objects are

  - G4Isotope: describes the properties of atoms

    - Z - atomic number, N - number of nucleons and A - molar mass with unique name and Isomer level (optimal)

  - G4Element: describes the properties of elements

    - Z - atomic number, number of isotopes, and the list of isotopes

  - G4Material: describes the macroscopic properties of matter

    - density, state, temperature, pressure, etc. with unique name.

- Unique indexes: a pointer to the created object is automatically stored in a global table (isotope, element and material tables)

Geant4 Material Model - 2

- The material **density** must be set (> zero) by the user at definition

- The material **temperature** and **pressure** can be se optionally:
  - Default is Normal Temperature and Pressure(NTP):
    `293.15 [k], 1 [atm] = 101.325 [kPascal]`

- The material **state** can be solid, liquid or gas:
  - Default is either solid or gas depending on the density
    `kGasThreshold = 10 [mg/cm3]`
  - non-crystalline (i.e. amorphous) solid by default (special extension for incorporating some information on the crystal structure)

- Special set of pre-defined materials: **NIST material** composition data base with some frequently used HEP materials

- Geant4 material documentation: Material Documentation

Elements

- Elements can be defined without specifying the isotope composition

  - Need to give: name, symbol, Z and A (effective atomic number and molar mass)

  - Isotopes will be automatically added with natural abundances (A will be overwritten

```
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

- Elements can be also built with specific (non-natural) from pre-defined isotopes:

  - Isotopes need to be added by their relative abundance

```cpp
G4int z, n, nComponents;
G4double abundance;

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

// 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);
```

Simple Material

- "simple": the material contains only one element and the corresponding G4Element object is not provided:

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

- The G4Element object will be automatically created (with the natural isotope abundance)

- Name, density of the material, Z are user defined, a closest pure NIST Material will be used for element with natural abundances of isotopes

Material: Chemical Molecule

- Molecules build up from (several) elements with composition specified by the number of element (e.g. water = H2O) accordingly

- G4Material object can be created by adding G4Element objects to it together with their composition number:

```
G4double density;
G4int nComponents;

// G4Element* elH = ...
// G4Element* elO = ...

density = 1.000*g/cm3;
G4Material* water
  = new G4Material("Water", density, nComponents=2);
water->AddElement(elH, nAtoms=2);
water->AddElement(elO, nAtoms=1);
```

Material: Mixture

- Mixture of elements (G4Element), mixture of other materials (G4Material) or even mixture of elements and materials

- Similar to molecules with the differences:

  - Components can be other materials not only elements

  - The ratio of the components must be given as "fractional mass" not as "number of atoms"

- Example of a mixture of elements (G4Element) and other material (G4Material) using fraction of mass:

```
// ALICE mixture TPC_Ne-CO2-2
G4double density = 0.939*mg/cm3;
// G4Element* elNe = …
// G4Material* carbonDioxide = ...

G4Material* NeCO2 =
  new G4Material("TPC_Ne-CO2-2", density, 2, kStateGas,
                 NTP_Temperature, 1.*atmosphere);
NeCO2->AddElementByMassFraction (elNe, 0.8039);
NeCO2->AddMaterial(carbon_dioxide, 0.1961);
```
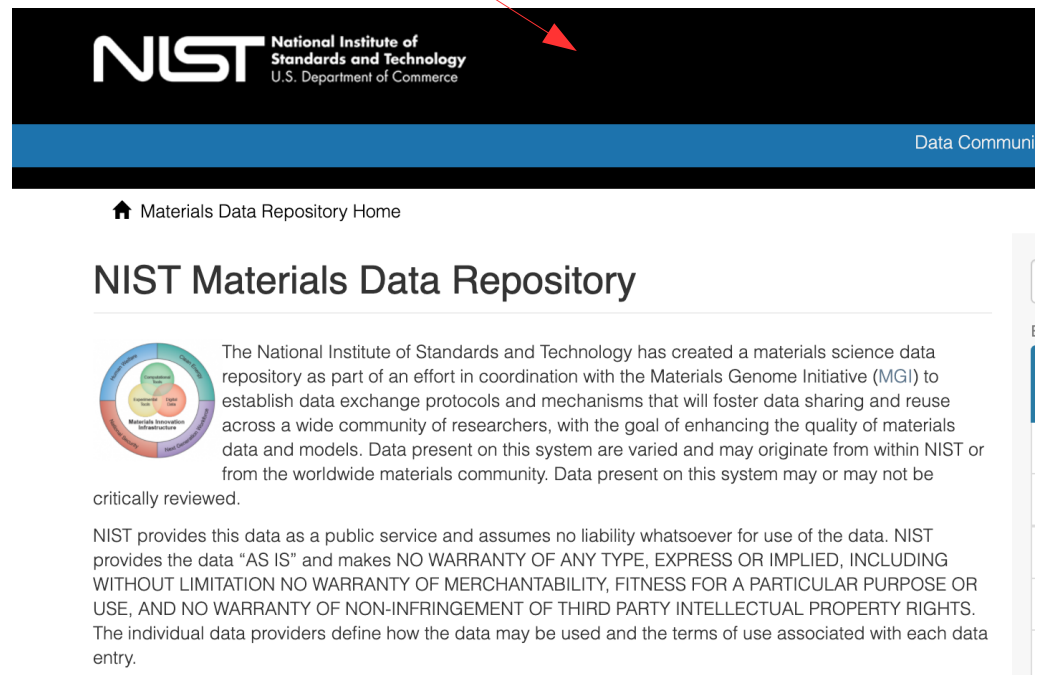
Material: Mixture - 2

- Example of a mixture of elements using number of atoms:

```
// C3H8, 20 C, 2 atm
G4double density = 3.758*mg/cm3;
// G4Element* elC = …
// G4Element* elH = …

G4Material* C3H8 =
  new G4Material("C3H8", density, 2,
                 kStateGas, 293.15*kelvin, 2.*atmosphere);
C3H8->AddElementByNumberOfAtoms(elC, 3);
C3H8->AddElementByNUmberOfAtoms(elH, 8);
```

NIST Database

- NIST database:
  - https://materialsdata.nist.gov/
- 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, ...
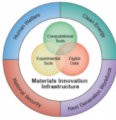

NIST National Institute of Standards and Technology
U.S. Department of Commerce

Data Communi

🏠 Materials Data Repository Home

NIST Materials Data Repository

The National Institute of Standards and Technology has created a materials science data repository as part of an effort in coordination with the Materials Genome Initiative (MGI) to establish data exchange protocols and mechanisms that will foster data sharing and reuse across a wide community of researchers, with the goal of enhancing the quality of materials data and models. Data present on this system are varied and may originate from within NIST or from the worldwide materials community. Data present on this system may or may not be critically reviewed.

NIST provides this data as a public service and assumes no liability whatsoever for use of the data. NIST provides the data "AS IS" and makes NO WARRANTY OF ANY TYPE, EXPRESS OR IMPLIED, INCLUDING WITHOUT LIMITATION NO WARRANTY OF MERCHANTABILITY, FITNESS FOR A PARTICULAR PURPOSE OR USE, AND NO WARRANTY OF NON-INFRINGEMENT OF THIRD PARTY INTELLECTUAL PROPERTY RIGHTS. The individual data providers define how the data may be used and the terms of use associated with each data entry.

NIST Database - 2

- The data base includes *more than 3000 isotopes*

- Isotopic composition of elements (Z = [1-108]) with their natural isotopic abundance: using the NIST Atomic Weights and Isotopic Compositions data base [link]

- Large collection of pre-defined materials *(318 at the moment)*:

  - pre-defined: density, elemental composition (with the pre-defined natural isotopic composition), mean ionization energy, density effect parameters, etc.

Predefined materials in NIST

- Elementary (single element) materials with Z = [1-98] and named after the atomic symbol
  - Aluminum ("G4_Al"), silicon ("G4_Si"), gold ("G4_Au"), etc.

- Compounds and mixtures
  - "G4_AIR", "G4_ALUMINUM_OXIDE", "G4_MUSCLE_SKELETAL_ICRP", etc.

- HEP and Nuclear Materials
  - liquid argon "G4_lAr", lead tungstate "G4_PbWO4", "G4_STAINLESS-STEEL", etc.

- Space Materials
  - "G4_KEVLAR", "G4_NEOPRENE", etc.

- Bio Chemical Materials
  - the DNA bases "G4_ADENINE", "G4_GUANINE", "G4_CYTOSINE", "G4_THYMINE", etc.

Getting Material from NIST

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

  - can be obtained from the Geant4 NIST data base by using their name; the names start with the "G4_" prefix

```cpp
#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: GEANT4 Material Database

Getting Material from NIST - 2

Elements

Simple Materials (Elements)

Z	Name	density(g/cm^3)	I(eV)
1	G4_H	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

Compounds

NIST Compounds

```
========================================================================
Ncomp              Name        density(g/cm^3)  I(eV) ChFormula
========================================================================
6              G4_A-150_TISSUE      1.127        65.1
    1             0.101327
    6             0.7755
    7             0.035057
    8            0.0523159
    9             0.017422
   20             0.018378
3                G4_ACETONE      0.7899         64.2
    6                3
    1                6
    8                1
2                G4_ACETYLENE   0.0010967       58.2
    6                2
    1                2
3                G4_ADENINE        1.6           71.4
    6                5
    1                5
    7                5
7       G4_ADIPOSE_TISSUE_ICRP    0.95          63.2
    1             0.114
    6             0.598
    7             0.007
    8             0.278
   11             0.001
   16             0.001
   17             0.001
```

Getting Material from NIST - 3

List available pre-define NIST elements, materials from the data base with their composition:

- User interface command:

  ```
  /material/nist/printElement symbol
  /material/nist/listMaterials category
  ```

- Directly from C++ code:

```cpp
// Print element - name can be symbol (i.e. "Al") or "all"
G4String elementName = "Al";
G4NistManager::Instance()->PrintElement(elementName);

// List predefined materials with their element composition
// categoryName can be: "simple", "hep", "space", "bio", "all"
G4String categoryName = "simple";
G4NistManager::Instance()->ListMaterials(categoryName);
```

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.)

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