

Material definition

Mihaly Novak (CERN, EP-SFT)

Geant4 beginners course at CERN, Geneva (Switzerland), 22-23

January 2019

- The Geant4 material model
- Material definition
- The NIST material data base
- Questions

Material definition

THE GEANT4 MATERIAL MODEL

- The Geant4 **material** model follows the natural one: 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 `index`
 - ***G4Element***: describes the properties of elements (Z - effective atomic number, N - effective number of nucleons and A - effective molar mass, number of isotopes, etc.) with unique `name`, `symbol` and `index`
 - ***G4Material***: describes the macroscopic properties of matter (**density, state, temperature, pressure**, etc.) with unique `name` and `index`
- Unique index: a pointer to the created object is automatically stored in global table (isotope, element and material tables)

- The **material density** must be set ($> \text{zero}$) by the user at definition (except NIST materials) !
- The **material temperature** and **pressure** can optionally be set:
 - default: 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](#)

Material definition

MATERIAL DEFINITION

- Elements and isotopes:

- *G4Element* object without specifying the isotope composition:

```
// simple way of Carbon element definition
G4Element* elC = new G4Element(name="Carbon", symbol="C", z = 6., a = 12.01*g/mole);
```

- need to give: name, symbol, Z and A (effective atomic number and molar mass)
- isotopes will be automatically added with natural abundances (A won't be updated)

- *G4Element* object by specific (non-natural) isotope composition:

```
// Define "enriched uranium" element as 90 % of U235 and 10 % of U 238:
//
// create the isotopes: iz = number of protons and n = number of nucleons
G4Isotope* U5 = new G4Isotope(name="U235", iz=92, n=235);
G4Isotope* U8 = new G4Isotope(name="U238", iz=92, n=238);
// create the element and build up by adding the isotopes with their abundance
G4Element* elU=new G4Element(name="enriched uranium",symbol="U",numisotopes=2);
elU->AddIsotope(U5, abundance= 90.*perCent);
elU->AddIsotope(U8, abundance= 10.*perCent);
```

- element object must be created: name, symbol, number of isotopes
- isotope objects must be created: name, number of protons and nucleons
- isotopes need to be added by their relative abundance

- Simple *G4Material* object definition:
 - “simple”: the material contains only one element and the corresponding *G4Element* object is not provided:

```
// single element "Uranium" material without giving the uranium element object
G4Material* matU = new G4Material(name    = "Uranium",
                                   z       = 92.0,
                                   a       = 238.03 * g/mole,
                                   density= 18.950 * g/cm3);
```

- the corresponding *G4Element* object will be automatically created (with natural isotope abundance)
- need to give: `name`, `density` of the material, `Z` and `A` (effective atomic number and molar mass) of the single *G4Element*
- what happens if we want the single element to have non-natural isotope abundance e.g. the previously created `enriched uranium` (see later)

- *G4Material* object definition as 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:

```
// Create water material as molecule based on its chemical formula (H2O)
//
// create the necessary H and O elements (natural isotope abundance):
G4Element* elH = new G4Element(name = "Hydrogen",
                                symbol = "H",
                                z = 1.00,
                                a = 1.01 * g/mole);
G4Element* elO = new G4Element(name = "Oxygen",
                                symbol = "O",
                                z = 8.00,
                                a = 16.00 * g/mole);
// create the water material (name, density, number of components):
G4Material* matH2O = new G4Material(name = "Water",
                                    density = 1.0 * g/cm3,
                                    ncomponents = 2);
// add the elements to the material with their composition number
matH2O->AddElement(elH, number0fatoms = 2);
matH2O->AddElement(elO, number0fatoms = 1);
```

- *G4Material* object definition as 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”
 - **mixture of elements** example: using the `AddElement` method

```
// Create air material as 70-30 % mixture of N and O elements
// (assuming that N and O Geant4 elements have already been created as
//  elN and elO)
//
// create the air material (name, density, number of components):
G4Material* matAir = new G4Material(name      = "Air",
                                   density    = 1.290 * mg/cm2,
                                   ncomponents = 2);
// add the elements to the material with their fractional mass
matAir->AddElement(elN, fractionmass = 0.7);
matAir->AddElement(elO, fractionmass = 0.3);
```

- *G4Material* object definition as mixture:
 - **mixture of element(s) and material(s)** example: using the `AddElement` and `AddMaterial` methods

```
// Create aerogel material as 62.5 % silicon dioxide (SiO2), 37.4 % water (H2O)
// materials and 0.1 % carbon element. Assuming that the materials (matSiO2 and
// matH2O) as well as the carbon element (elC) have already been created.
//
// create the aerogel material (name, density, number of components):
G4Material* matAerog = new G4Material(name      = "Aerogel",
                                     density     = 0.2 * g/cm3,
                                     ncomponents = 3);
// add the elements to the material with their fractional mass
matAerog->AddMaterial(matSiO2, fractionmass = 62.5 * perCent);
matAerog->AddMaterial(matH2O , fractionmass = 37.4 * perCent);
matAerog->AddElement (elC      , fractionmass = 0.1 * perCent);
```

Material definition

THE NIST MATERIAL DATA BASE

- 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
- **NIST elements** can be obtained easily from the Geant4 NIST data base **by** using **their** `symbol` or `Z - atomic number`:

- the corresponding *G4Isotope* objects will be automatically built
- “find or build” i.e. avoids duplication of element objects

```
// get the carbon G4Element object from the NIST data base: by its symbol
G4Element* elC = G4NistManager::Instance()->FindOrBuildElement("C");
// get the silicon G4Element object from the NIST data base: by its Z
G4Element* elSi = G4NistManager::Instance()->FindOrBuildElement(14);
```

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

- **Use these pre-defined materials whenever possible:**
 - guarantees high accuracy for many derived parameters (consistency)
- **NIST** and more pre-defined **materials** (318 at the moment):
 - **single element NIST** materials with $Z = [1-98]$ and named after the atomic symbol:
 - aluminum (“G4_Al”), silicon (“G4_Si”), gold (“G4_Au”), etc.
 - **compound NIST** materials:
 - “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.

- How to access these pre-define materials:
 - can be obtained from the Geant4 NIST data base **by** using **their name**
 - their name starts with the “**G4_**” **prefix** (see in the previous

```
// Use the NIST data base to get predefined materials: carbon, silicon
//
// get the simple pre-defined carbon material from the NIST data base
G4Material* matC = G4NistManager::Instance()->FindOrBuildMaterial("G4_C");
// get the simple pre-defined silicon material from the NIST data base
G4Material* matSi = G4NistManager::Instance()->FindOrBuildMaterial("G4_Si");
```

```
// Use the NIST data base to get pre-defined materials:
//
// get the NIST manager (just to simplify)
G4NISTManager* nistMGR = G4NistManager::Instance();
// get the pre-defined liquid argon ("G4_LAr") from the NIST DB
G4Material* matLAr = nistMGR->FindOrBuildMaterial("G4_LAr");
// get the pre-defined concrete ("G4_CONCRETE") from the NIST DB
G4Material* matConcr = nistMGR->FindOrBuildMaterial("G4_CONCRETE");
```

- 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:

```
// List the pre-defined NIST ELEMENT(S) with its(their) isotope composition:
//
// element name can be: the element SYMBOL i.e. "Al" or "all"
const G4String nistElementName = "Al";
G4NistManager::Instance()->PrintElement(nistElementName);
//
// List the pre-defined NIST MATERIALS with their element composition:
//
// category name can be: "simple", "compound", "hep", "space", "bio", "all"
const G4String nistMatCategoryName = "simple";
G4NistManager::Instance()->ListMaterials(nistMatCategoryName);
```


Material definition

QUESTIONS