Geant 4

Detector Description: Materials

http://cern.ch/geant4

PART I

Materials

- *The System of units & constants*
- *Definition of elements*
- *Materials and mixtures*
- *Some examples …*
- *The NIST Data Base*

Unit system

- 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.
  - The user can define new units.
  - Refer to CLHEP: `SystemOfUnits.h`
- Divide a variable by a unit you want to get.

  ```
  G4cout << dE / MeV << “ (MeV)” << G4endl;
  ```

System of Units

- System of units are defined in CLHEP, based on:
  - millimetre (**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 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

Defining new units

- New units can be defined directly as constants, or (suggested way) via `G4UnitDefinition`.
  - `G4UnitDefinition ( name, symbol, category, value )`
- Example (mass thickness):

  -
    ```
    G4UnitDefinition (“grammpercm2”, “g/cm2”,
                       “MassThickness”, g/cm2);
    ```
  - The new category “`MassThickness`” will be registered in the kernel in **`G4UnitsTable`**
- To print the list of units:
  - From the code

    ```
    G4UnitDefinition::PrintUnitsTable();
    ```
  - At run-time, as UI command:

    ```
    Idle> /units/list
    ```

Definition of Materials

- Different kinds of materials can be defined:
  - isotopes <> G4Isotope
  - elements <> G4Element
  - molecules <> G4Material
  - compounds and mixtures <> G4Material
- Attributes associated:
  - temperature, pressure, state, density

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…

Elements & Isotopes

- Isotopes can be assembled into elements

```
G4Isotope (const G4String& name,
                 G4int     z,    // atomic number
                 G4int     n,    // number of nucleons
                 G4double  a );  // mass of mole
```

- … building elements as follows:

```
G4Element (const G4String& name,
           const G4String& symbol, // element symbol
                 G4int     nIso ); // # of isotopes
G4Element::AddIsotope(G4Isotope* iso,  // isotope
                      G4double relAbund); // fraction of atoms
                                          // per volume
```

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);
```

- Prefer low-density material to vacuum

Material: molecule

- A Molecule is made of several elements (composition by number of atoms):

```
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* H2O =
   new G4Material("Water",density,ncomp=2);
H2O->AddElement(elH, natoms=2);
H2O->AddElement(elO, natoms=1);
```

Material: compound

- Compound: composition by fraction of mass

```
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

```
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);
```

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(C,natoms = 1);
CO2->AddElement(O,natoms = 2);
```

Example: 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, or with $\rho = 0$.

```
G4double atomicNumber = 1.;
G4double massOfMole = 1.008*g/mole;
G4double density = 1.e-25*g/cm3;
G4double temperature = 2.73*kelvin;
G4double pressure = 3.e-18*pascal;
G4Material* Vacuum =
   new G4Material(“interGalactic", atomicNumber,
                  massOfMole, density, kStateGas,
                  temperature, pressure);
```

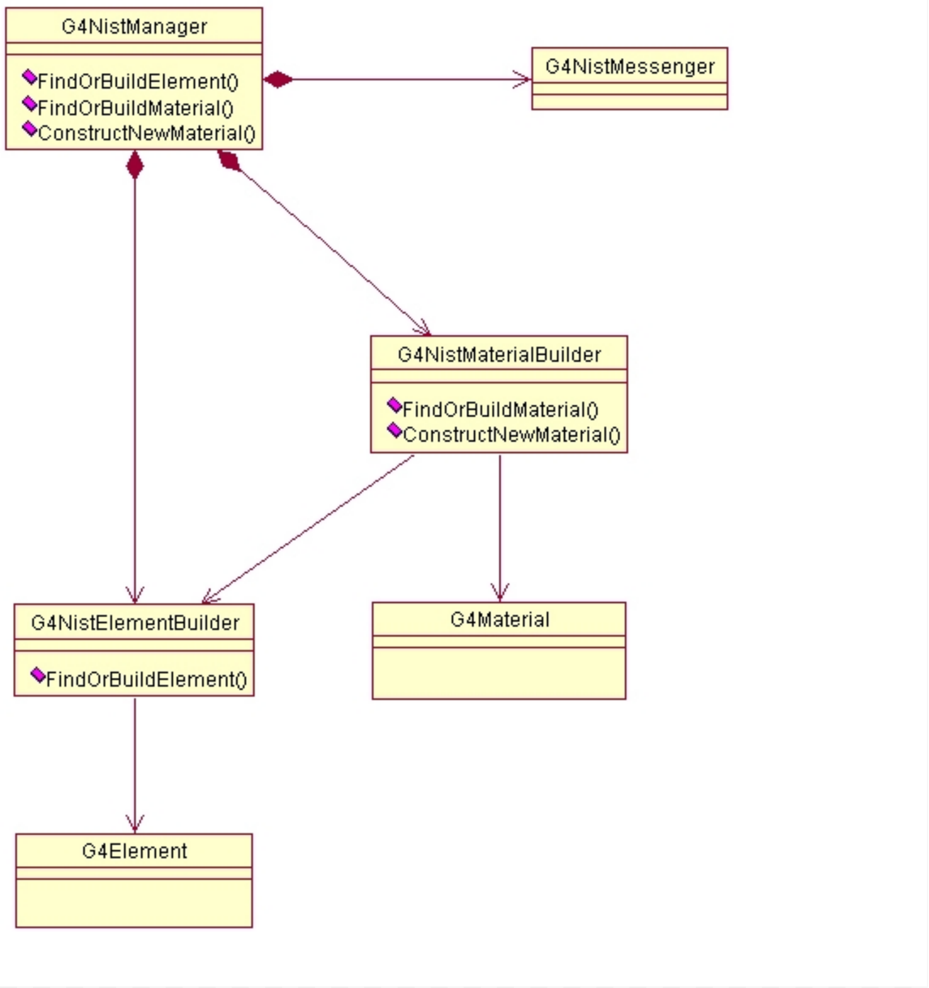
PART I

NIST Material Data-Base in Geant4

- *Class structure*
- *NIST Isotopes, Elements and Materials*
- *How to use it …*

NIST Manager & Messenger

- NIST database for materials is imported inside Geant4 (http://physics.nist.gov/PhysRefData)
- Additional interfaces defined
- UI commands specific for handling materials
- The best accuracy for the most relevant parameters guaranteed:
  - Density
  - Mean excitation potential
  - Chemical bounds
  - Element composition
  - Isotope composition
  - Various corrections



NIST Element and Isotopes

```
Z     A      m       error     (%)        Aeff
============================
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

NIST materials

```
======================================
###   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
- NIST Compounds
- Nuclear Materials …
- 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
```

How to use the NIST DB

- No need to predefine elements and materials
- Retrieve materials from NIST manager:

```
G4NistManager* manager = G4NistManager::Instance();

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<G4String>& elements,
                           const std::vector<G4int>& numberAtoms,
                           G4double density, G4bool iso);
G4double isotopeMass = manager->GetIsotopeMass(G4int Z, G4int N);
```

- Some UI commands …

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

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

Availability…

- NIST database for isotopes/elements/materials available since Geant4 release 7.1
  - UI messenger with predefined commands
- Driven by needs of EM physics
  - Increase precision of elements/material definition
  - Open door for better interface to EM corrections
  - Any physics model can have specific setup associated with predefined materials
- Natural isotope compositions
- More 3000 isotope masses

Material Scanner

- Tool to measure material thickness in units of geometrical length, radiation length and interaction length
  - Region sensitive: you can measure the thickness of one particular region
- **`/control/matScan`**
  - **`scan`** - *Start material scanning*
  - **`theta`** - *Define theta range*
  - **`phi`** - *Define phi range*
  - **`singleMeasure`** - *Measure thickness for one particular direction*
  - **`eyePosition`** - *Define the eye position*
  - **`regionSensitive`** - *Set region sensitivity*
  - **`region`** - *Define region name to be scanned*