GEANT4

A SIMULATION TOOLKIT

Version 10.7

Material definition

Vladimir Ivanchenko (CERN, EP-SFT & Tomsk State University, Russia)
based on materials provided by: M. Asai (SLAC) and M. Novak (CERN)

Geant4 beginners course at CERN, Geneva (Switzerland), 25-31 May 2021

Outline

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

Material definition

THE GEANT4 MATERIAL MODEL

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 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`. Base material or number of components is defined. Components may be G4Element or G4Material. Material description may be Extended with extra properties
- ***Unique indexes***: a pointer to the created object is automatically stored in a global table (isotope, element and material tables)

The Geant4 material model

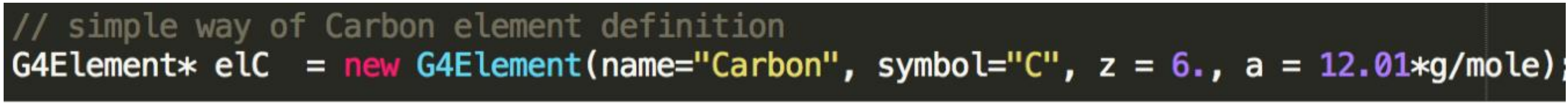
- The material density must be set (> zero) by the user at definition
- The material temperature and pressure can optionally be set:
  - default: Normal Temperature and Pressure(NTP) 293.15 [k], 1 [atm] = 101.325 [kPascal]
- The material state can be solid, liquid or gas:
  - default is either solid or gas depending on the density (`kGasThreshold` = 10 [mg/cm^3])
  - 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

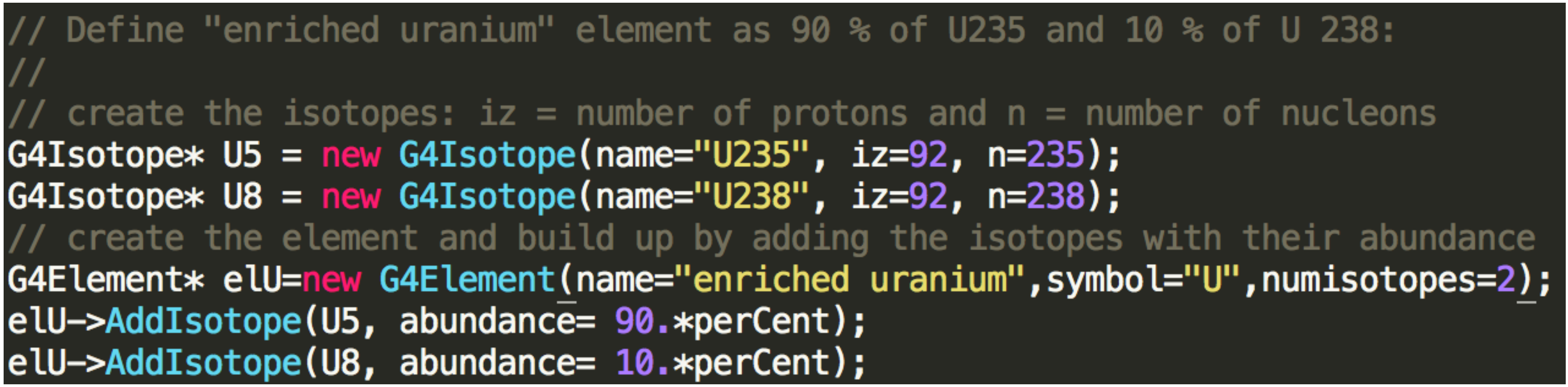
Material definition: elements and isotopes

- 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` will be overritten)
  - ***G4Element*** object by specific (non-natural) isotope composition:

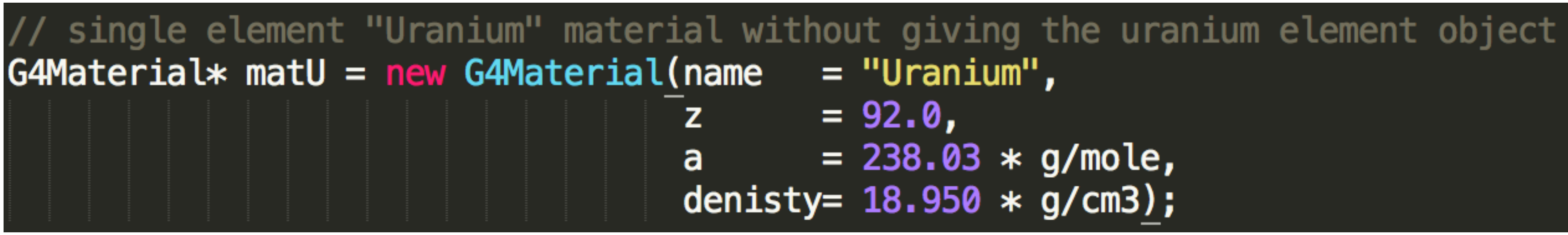


```
// Define "enriched uranium" element as 90 % of U235 and 10 % of U 238:
//
// create the isotopes: iz = number of protons and n = number of nucleons
G4Isotope* U5 = new G4Isotope(name="U235", iz=92, n=235);
G4Isotope* U8 = new G4Isotope(name="U238", iz=92, n=238);
// create the element and build 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

Material definition: simple material definition

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

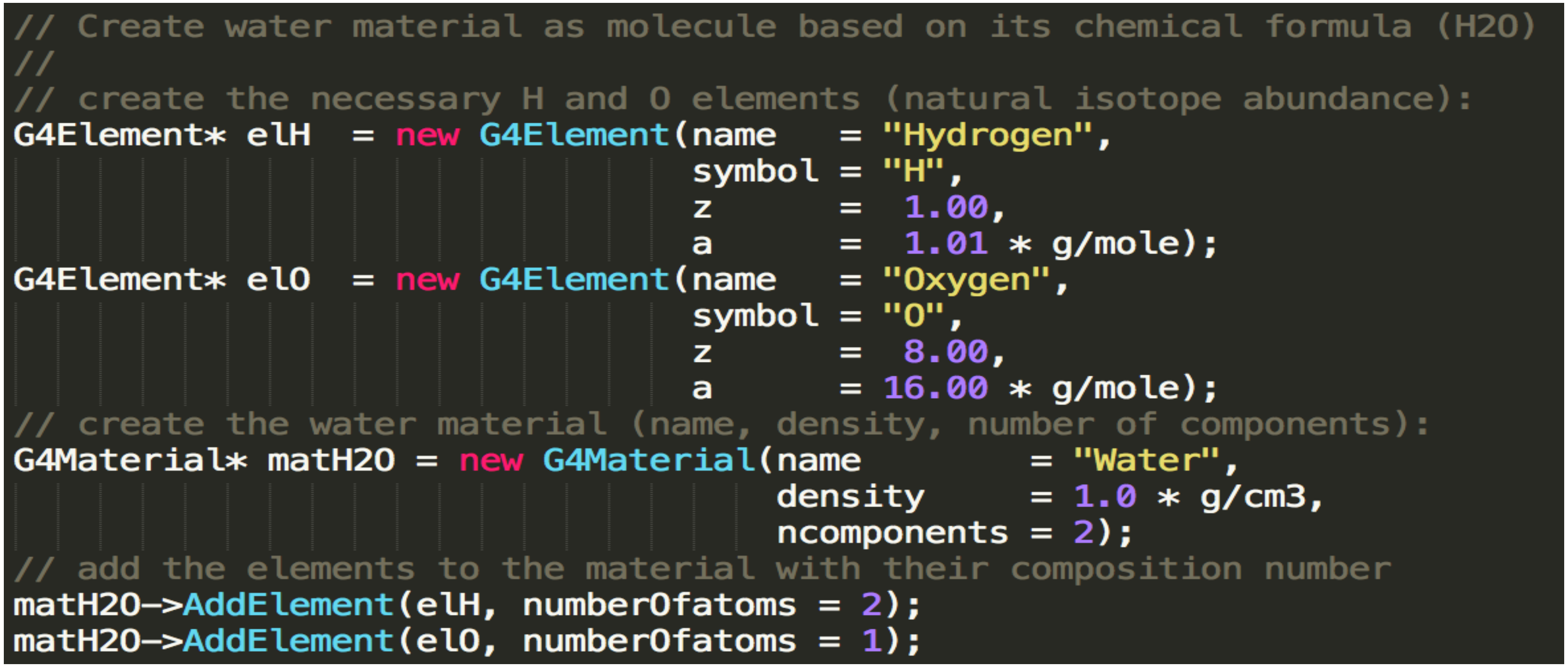


```
// single element "Uranium" material without giving the uranium element object
G4Material* matU = new G4Material(name   = "Uranium",
                                  z      = 92.0,
                                  a      = 238.03 * g/mole,
                                  denisty= 18.950 * g/cm3);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

- the corresponding ***G4Element*** object will be automatically created (with 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 isottopes

Material definition: chemical molecule

- *G4Material* object definition as chemical molecule:
  - molecules build up from (several) elements with composition specified by the number of element (e.g. water = H_2O)
  - 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, numberOfatoms = 2);
matH2O->AddElement(elO, numberOfatoms = 1);
```

Material definition: mixture

- ***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 number of atoms

```
 // C3H8, 20 C, 2 atm
G4double  density = 3.758*mg/cm3;
G4Material* C3H8 = new G4Material("C3H8", density, 2, kStateGas,
                                                  293.15*kelvin,2.*atmosphere);
C3H8->AddElementByNumberOfAtoms(elC, 3);
C3H8->AddElementByNUmberOfAtoms(elH, 8);
```

Material definition: mixture

- ***G4Material*** object definition as mixture:
  - mixture of elements (*G4Element*), mixture of other materials (*G4Material*) or even mixture of elements and materials using fraction of mass:

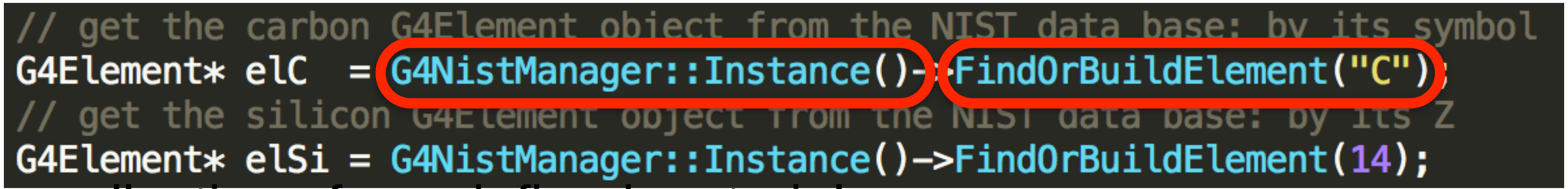
```
// ALICE mixture TPC_Ne-CO2-2
G4double density = 0.939*mg/cm3 ;
G4Material* NeCO2 =
   new G4Material("TPC_Ne-CO2-2", density, 2, kStateGas,
                              NTP_Temperature, 1.*atmosphere);
NeCO2->AddElementByMassFraction ( elNe, 0.8039 ) ;
NeCO2->AddMaterial( carbon_dioxide,  0.1961 ) ;
```

Material definition

THE NIST MATERIAL DATA BASE

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);
```

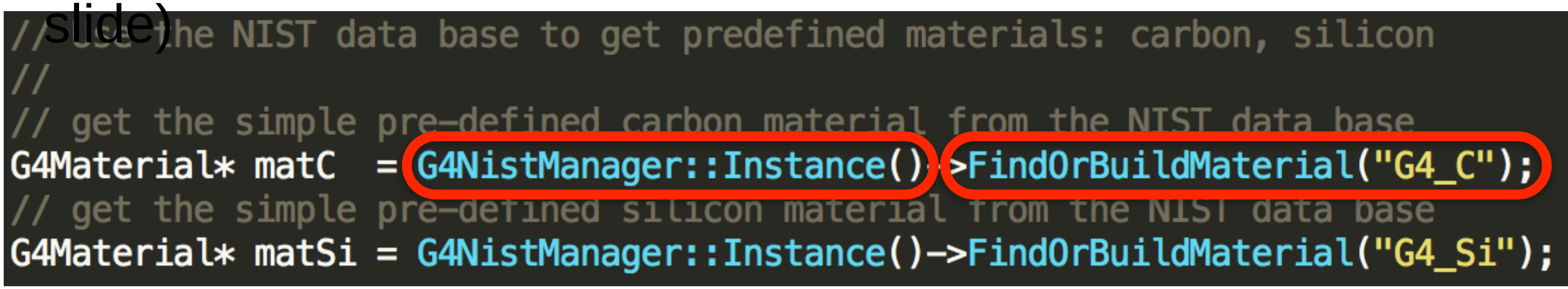
- Large collection of pre-defined materials:
  - pre-defined: density, elemental composition (with the pre-defined natural isotopic composition), mean ionization energy, density effect parameters, etc.

The NIST material data base

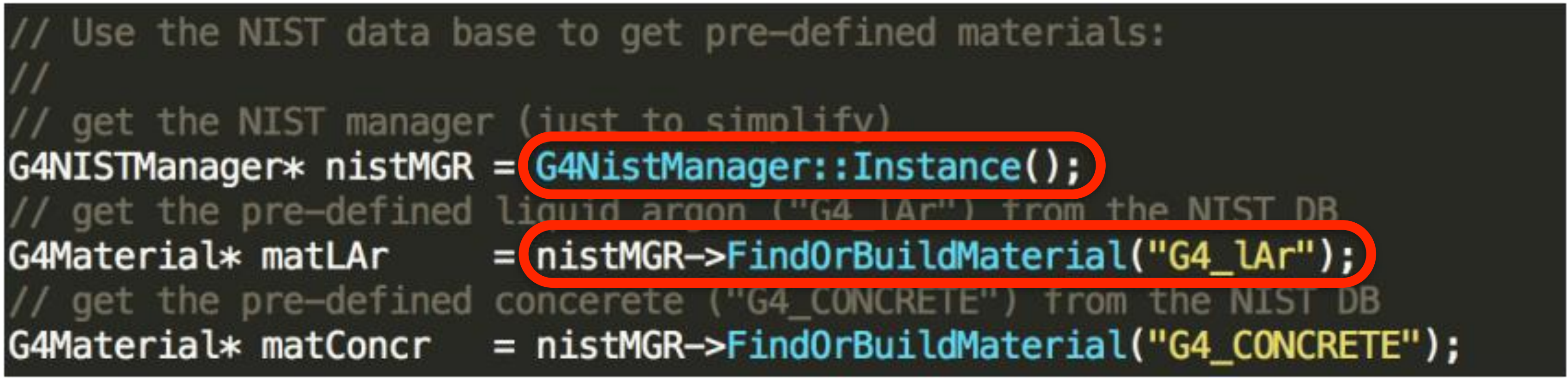
- Use these pre-defined materials whenever possible:
  - guaranties high accuracy for many derived parameters (consistency)
- NIST and more pre-defined materials (318 at the moment):
  - single element NIST materials with Z = [1-98] and named after the atomic symbol:
    - aluminum (“`G4_Al`”), silicon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

The NIST material data base

- 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 slide)



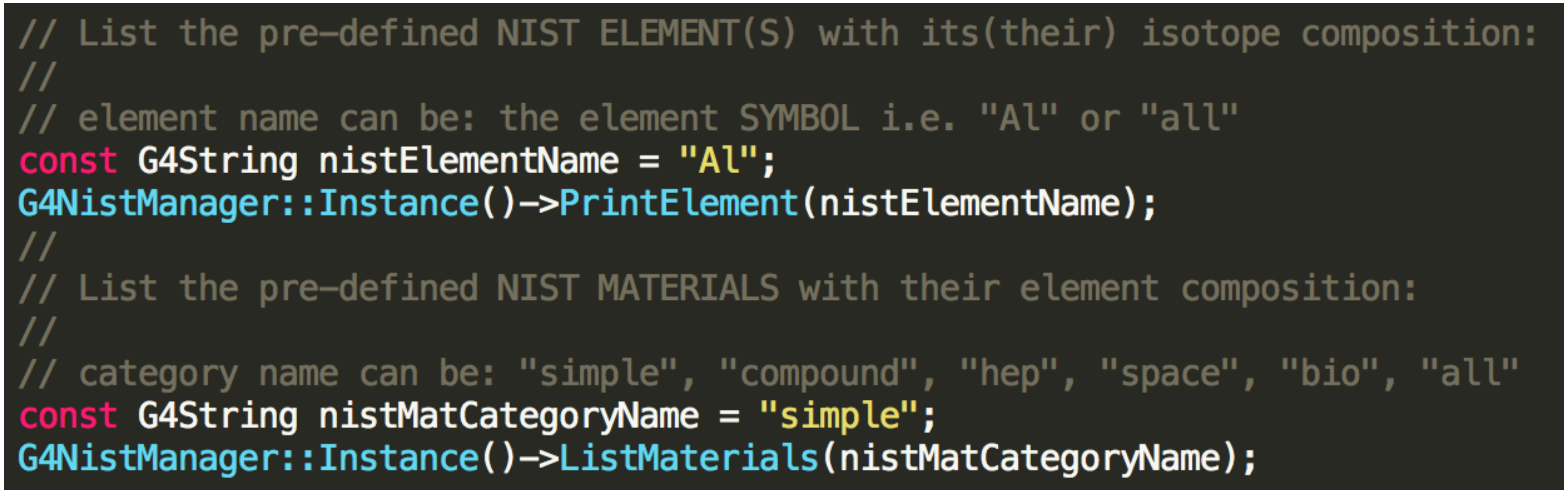
```
// Use the NIST data base to get predefined materials: carbon, silicon
//
// get the simple pre-defined carbon material from the NIST data base
G4Material* matC  = G4NistManager::Instance()->FindOrBuildMaterial("G4_C");
// get the simple pre-defined silicon material from the NIST data base
G4Material* 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 concerete ("G4_CONCRETE") from the NIST DB
G4Material* matConcr   = nistMGR->FindOrBuildMaterial("G4_CONCRETE");
```

The NIST material data base

- 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