

NIST Material Data Base and Geant4

Geant4 Workshop

9 November 2005, Bordeaux, France

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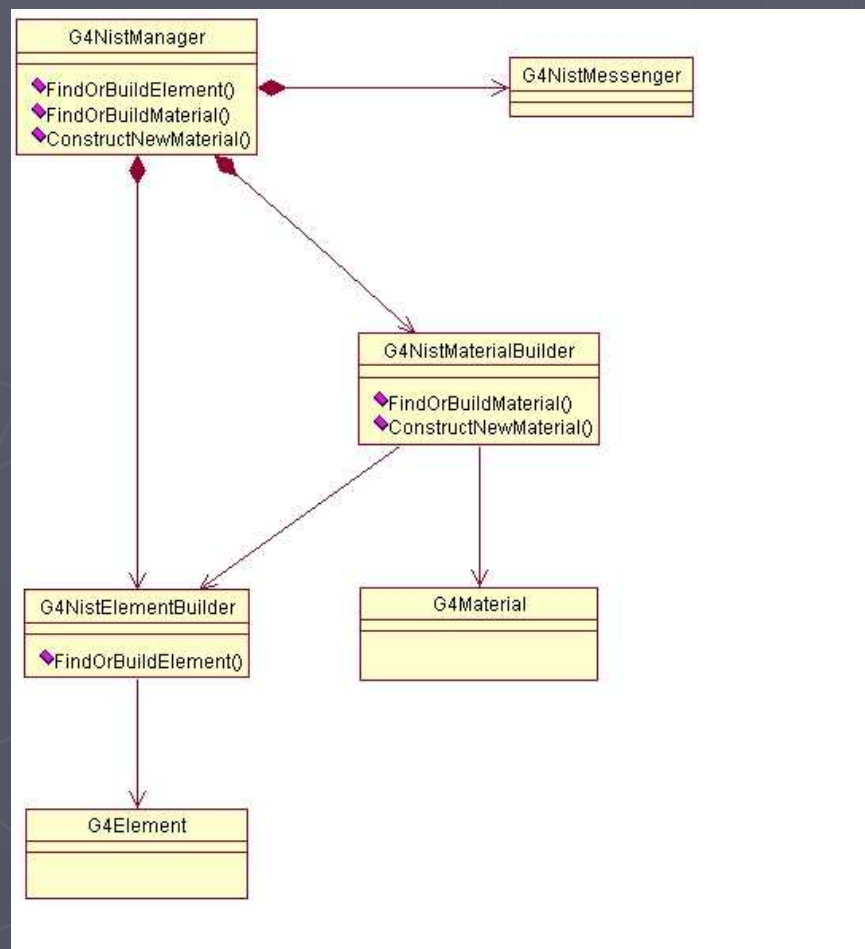
Thanks to M.Maire

Motivation

- ▶ There hundreds (?) Geant4 users
- ▶ There are only ~ 100 elements, which in case of the natural isotope composition are the same for any user
- ▶ There are many common materials for different applications
- ▶ Geant4 is working on precise validation against NIST
- ▶ **Why not to take NIST DB on elements and materials?**

Material category upgrade

- ▶ NIST database for materials is imported inside Geant4
(<http://physics.nist.gov/PhysRefData>)
- ▶ New interfaces are added, old are kept
- ▶ UI commands for material category
- ▶ **Guarantee the best accuracy for major parameters:**
 - ▶ Density
 - ▶ Mean excitation potential
 - ▶ Chemical bounds
 - ▶ Element composition
 - ▶ Isotope composition
 - ▶ Various corrections



NIST Element and Isotopes

Z	A	m	error (%)	A_{eff}	
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)	

NIST materials in Geant4

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 ### 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

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 ### 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		

- ▶ NIST Elementary Materials
- ▶ NIST Compounds
- ▶ Nuclear Materials
- ▶ Space Materials?

How to use

- ▶ Do not need anymore to predefine elements and materials
- ▶ Main new user interfaces:

```
G4NistManager* manager = G4NistManager::GetPointer();
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<G4int>& Z,
    const std::vector<G4double>& weight,
    G4double density, G4bool iso);
G4double isotopeMass = manager->GetMass(G4int Z, G4int N);
```

Conclusion

- ▶ NIST database for isotopes/elements/materials is available from G4 7.1
- ▶ Old constructors are kept
- ▶ UI messenger is added to material category
- ▶ Was 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 associated with predefined materials
- ▶ **Natural isotope compositions**
- ▶ **More 3000 isotope masses**