Generic Processes & Materials : latest updates and plans

ESA/ESTEC G4 meeting, october 2010

Plenary Session VI :

“Plenary Session VIII : Status/progress reports of developments (1)”

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For “*Generic Processes & Materials*” WG

layout

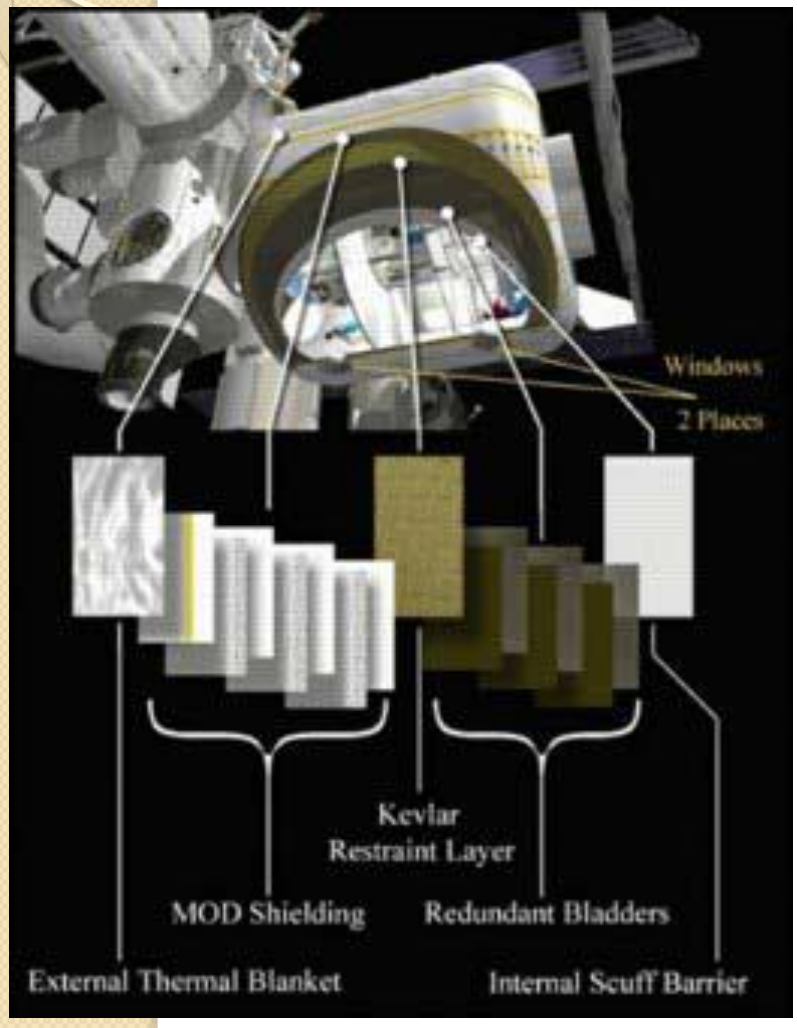
- Materials
- Differential cross-section
- Biasing
- Reverse MC

Material developments

Materials sub-library [updates]

- Mean ionisation energy of atoms now is taken directly from NIST data (3-digit values) and not anymore from ICRU'37 (2-digit values)
- Parameterization of density effect for simple materials is taken from new class G4DensityEffectData via atomic number and state (NIST name is not needed)
- ASTAR and PSTAR data have been rechecked (T.Koi report on Oxygen)
  - May be moved to material category (in standard for now)
  - Data for 6 materials were fixed
  - G4PhysicsVector with spline instead of old interpolation
- G4AtomicShell class was updated (optimized computation of binding energy by introduction of extra array)

New materials



New method added to G4NistMaterialBuilder class:
G4SpaceMaterials()

New space materials added, frequently asked for (put in "space materials" in NIST DB):
G4_KEVLAR, G4_NEOPREN, G4_DACRON

And extra metallic materials:
G4_BRASS, G4_HIGHGRADESTEEL

Proposal for variable density

Motivation for medical applications

- There are many medical applications in which many voxels with materials slightly different from each other
  - DICOM interface
- Optimisation of EM packages performance for applications with many voxels
  - CPU performance for initialisation and run time
  - Size of the application

Motivation for other applications

- In general the name of a material may be defined by geometry description which may not coincide with the NIST name
- Is it possible to reduce size of EM tables for LHC simulation without modification of geometry description?
- Cosmic rays in atmosphere
- DNA project – materials are scaled from water in many cases

Involved Geant4 categories

- source/materials
- source/processes/cuts
- source/processes/electromagnetic/utils

- Others modifications are not mandatory and necessary modifications should be identified

Proposed changing for materials

- G4Material:
  - Add **fBaseMaterial** pointer and access method
    - Const G4Material* GetBaseMaterial();
    - By default return 0;
  - Add extra constructor which will build new material from existing material
    - G4Material(const G4String& newname, const G4Material* oldmaterial, G4double newdensity);
- G4NistManager:
  - Add extra method to build material with given density from NIST material
    - BulidNewMaterialWithDensity(const G4String& newname, const G4String& NISTname, G4double newdensity);
- These modifications are easy
- Potential change and benefit if the project will be approved: analysis of user define material and identification of identical description, so concept of base material can be applied automatically reducing size of tables in user application

DIFFERENTIAL CROSS-SECTION PROPOSAL

Differential cross-section [1/2]

- There is not today a well identified concept of differential cross-section (DCS) in Geant4 which is
  - Shared among the physics packages
  - And would provide DCS objects to which you can talk to
  - Asking in particular

$$value = \sigma(\vec{f} \rightarrow \vec{f}')$$

  - Today, each physics package implements part of the DCS functionality, but limited to the DCS sampling needs
  - And DCS are mixed in processes or models that sample them
- We have proposed to introduce such a concept in Geant4
  - To have DCS objects providing the above deterministic computation

$$value = \sigma(\vec{f} \rightarrow \vec{f}')$$

  - And that have the possibility to be sampled or to sample themselves

Differential cross-section [2/2]

- Use cases / initial motivations:
  - Reverse MC
    - Having a DCS functionality would allow to “invert” the cross-section “easily”
    - This would ensure that the reverse MC is “the reverse of the forward”
  - Biasing
    - Having DCS would allow easy DCS-biasing, in which the natural DCS is substituted with a biased one, recording the weight to be propagated as ratio of the two:

$$w = \sigma\left(i \to \vec{f}\right) / \sigma_{biased}\left(i \to \vec{f}\right)$$

    - This would ensure that the biased MC is “the biased of the unbiased”
  - Ie : in both cases, the usual physics would be the reference physics : it would be “just” processed in different ways
- Early prototype should be available by the end of this year, but will not likely goes into 9.4

UPDATE ON BIASING

Reviving the biasing activity

- Yesterday's session shown quite enthusiasm in reviving the biasing activity in Geant4
- Medium/long term plans to be discussed
- First decisions:
  - Write down theoretical aspects of biasing in physics reference manual
    - For reference and for our own understanding
    - Write the mathematics of biasing
    - Push for the related statistics
    - Validate with toy Monte Carlo
  - Promote G4ConvergenceTester –re-implementation of MCNP statistical convergence criteria- from dark-lost example to a noble directory under the source one
    - After revisiting and refreshing this class
  - Refresh memory and documentation about use-cases

REVERSE MC

Updates and plans

- No significant updates in the toolkit this year
  - FYI : GRAS code updated to use reverse MC
- Plans:
  - Introduce point-like detector functionality
    - Dose will be computed either by response function (prepared/precomputed dose) or dE/dx
  - Address bremsstrahlung issue
    - Too many high energy gammas generated for now
  - Participate to biasing plans :
    - Documentation
    - And differential cross-section