New developments in Material and Standard EM

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16th Geant4 Workshop
19-23 September 2011
SLAC, Stanford, CA, USA

Outline

- Overview of activity
- Based material approach
- Unification of EM sub-packages
- Urban95 msc model
- Recent validation results
- Biasing options for EM physics
- Summary

Overview of activity

- Several upgrades of software infrastructure:
  - Base material approach (variable density) is introduced
  - Completed migration to new design of atomic de-excitation
  - Extended applicability range for standard models down in energy and for lower cuts
  - Improved algorithm for smoothing transition of high and low energy models
  - Introduced prototype of biasing options
- New models:
  - Photo-electric effect
  - Compton scattering
  - Rayleigh scattering (in progress)
  - Bremsstrahlung (in progress)
  - Urban95 msc
  - Ion single scattering
- Extended validation
  - New benchmark are added
  - Regular run of CPU benchmark

Overview of activity

- A significant part of work was performed in the framework of ESA funded project ELSHIELD (Contract 22839/10/NL/AT)
  - J.Allison, V.M.Grichine, A.Howard, V.N.Ivanchenko, M.Maire and L.Urban
- Close collaboration with low-energy working group

Material category

Base material approach

- Material may be constructed using existing ("based") material
  - Allowing reuse all corrections and data tables of any NIST material for many materials defined by users with different by name and density
- Reducing initialisation time and size of data tables
- Feasible applications
  - Needed for DNA where density of a voxel may be function of geometry definition
  - Medical applications (DICOM)
  - Definition of atmosphere
  - May be useful for HEP and any other complex simulation

Base material approach

- New constructor of G4Material:

  G4Material(newName, density, baseMaterialPointer)
- New method in G4NistManager:

  BuildMaterialWithNewDensity(newName,baseName, density)
- In the case when a base material is not used in geometry an extra G4MaterialCutCouple is created at initialisation
  - Increased number of these couples
  - G4PhysicsVector is created and filled only for base materials so overall size of tables should be smaller

Base material approach

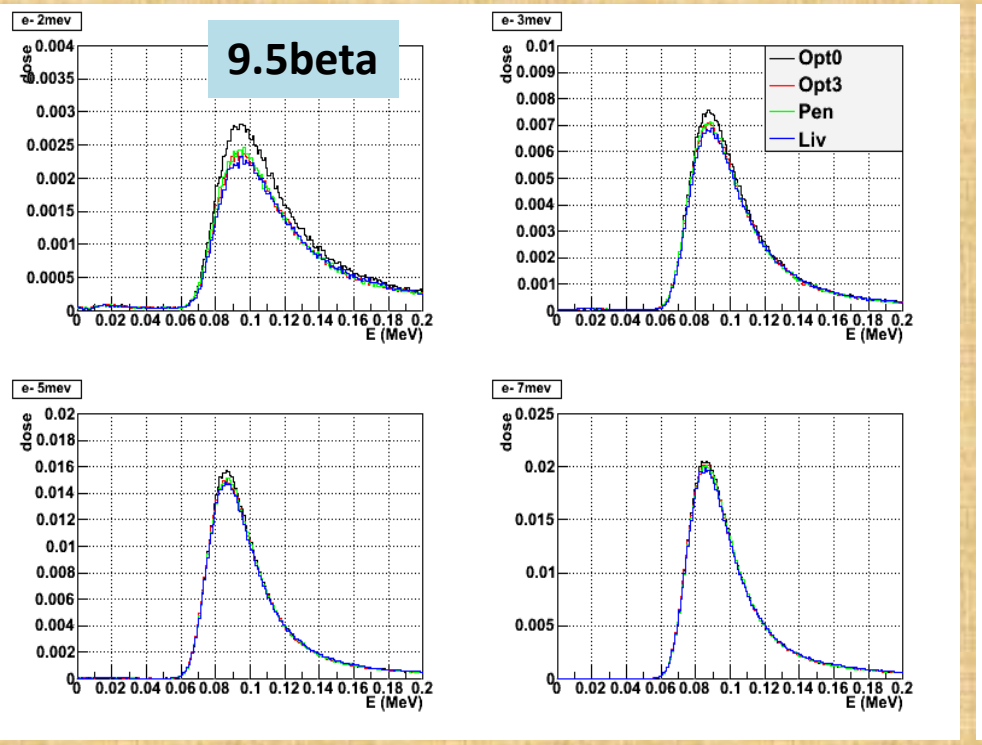
- Available since 9.5beta
- Improved in recent reference tags
- Validated in DNA example
- Validation in DICOM and other medical oriented examples is hardly required!

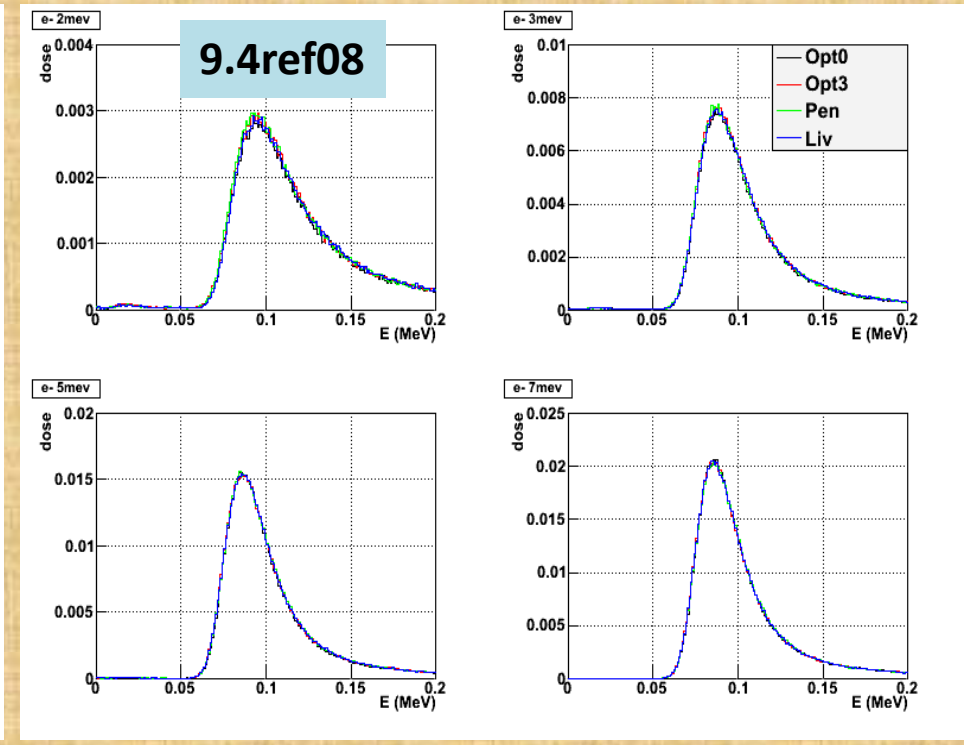
Unification of EM sub-packages

Unification of physics

- In Geant4 9.4 common interface for de-excitation module was introduced
- For 9.5 we plan to complete migration and remove old interface
  - Penelope shell ionisation cross section is not yet ready
- Number of issues were discovered in Physics Lists where we combine low-energy and standard models
  - We need not only technically allow to work models together but also provide physics compatible

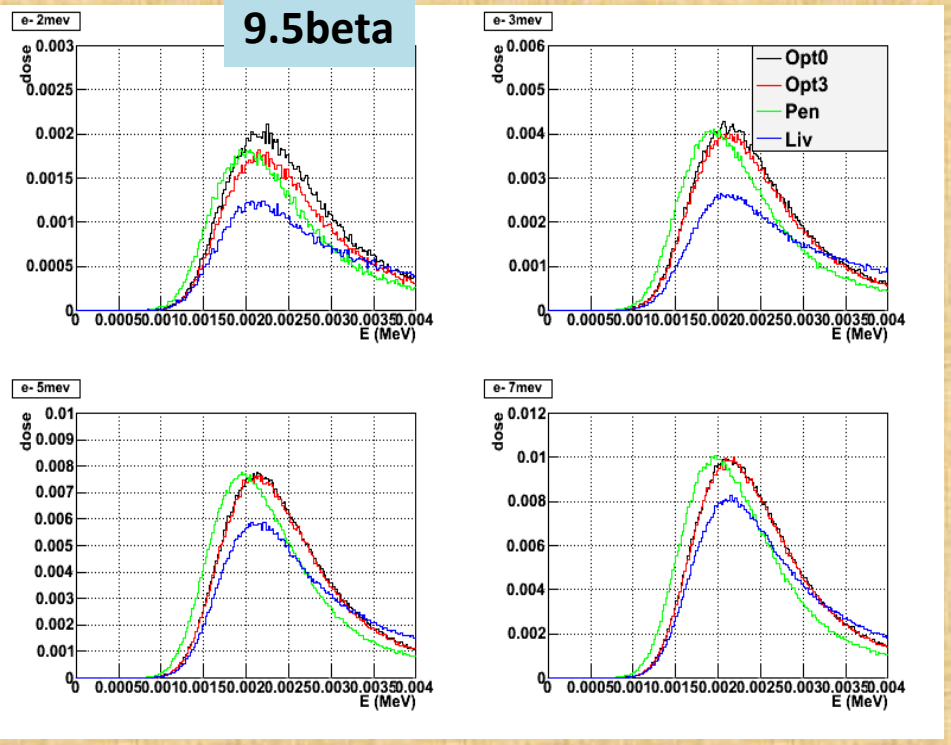
Dose deposition in 300 um Si layer from high energy electron beams and 2 mm Al shielding

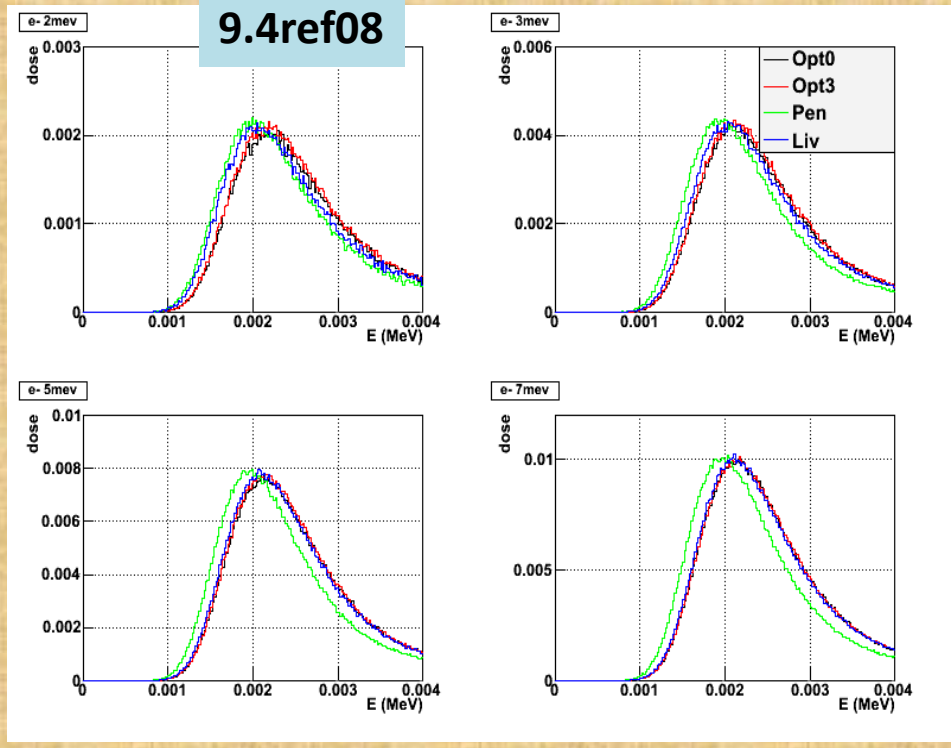




- All Physics Lists well agree, Opt0 is narrower for Aluminum at 2 MeV for 9.5beta, now is fixed
- ELSHIELD 1-D benchmark

Dose deposition in 10 um Si layer from high energy electron beams and 2 mm Al shielding



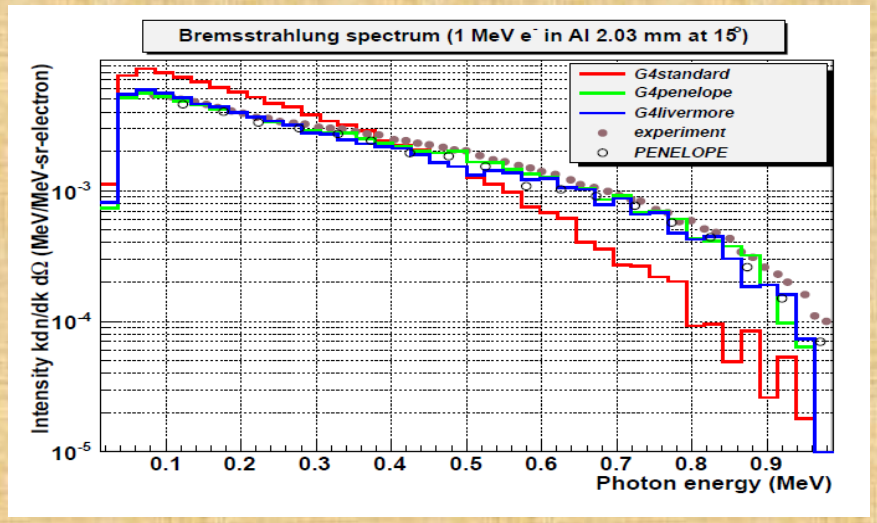


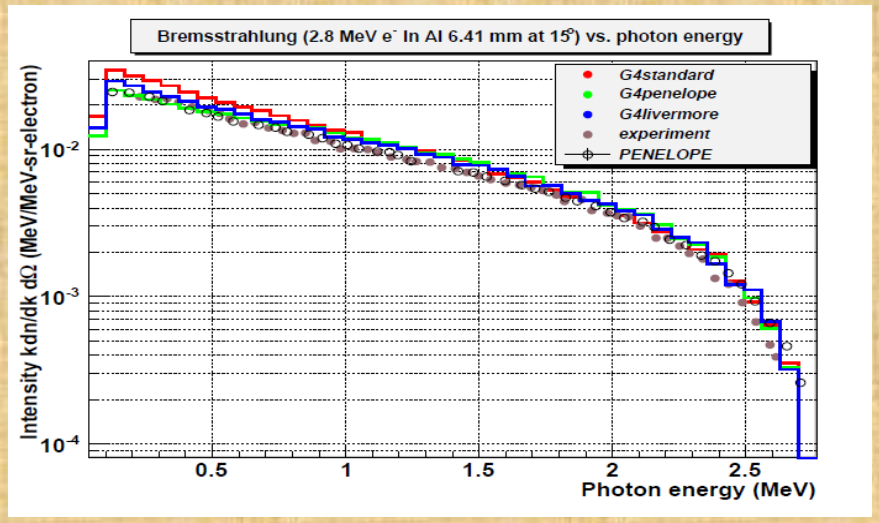
- Livermore predicts significantly wider dose with the same peak position in 9.5beta – now is fixed
- Penelope predicts a bit lower peak position
- ELSHIELD 1-D benchmark

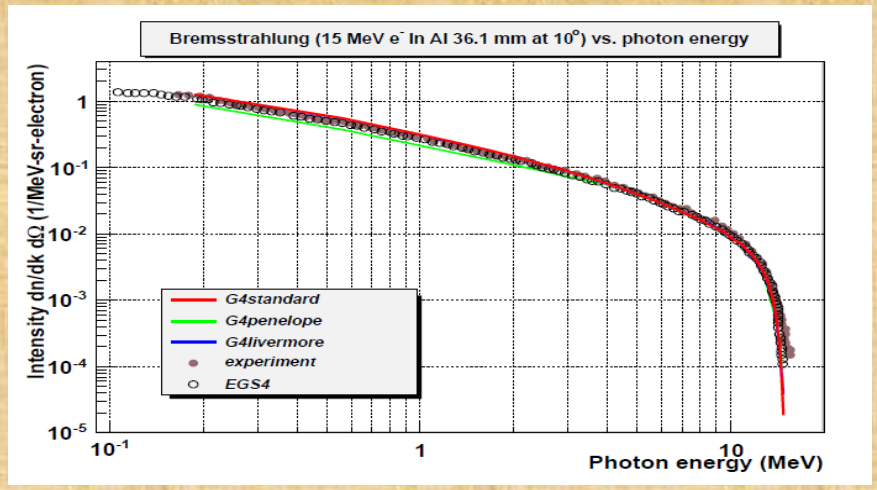
List of updated standard models

	Model	Status	Phys List
1	G4PEEffectFluoModel	Added deexcitation	All standard
2	G4KleinNishinaModel	Added de-excitation and Doppler broading	Opt2, Opt3
3	G4MollerBhabhaModel	Reduced low-limit	All standard
4	G4eBremParameterizedModel	In progress	
5	G4XrayRayleighModel	In progress	
6	G4PAIModel	Reduced low-limit	
7	G4eCoulombScatteringModel	Reduced low-limit	All for muons
8	G4WenttelVIModel	Reduced low-limit	All for muons, Opt1, Opt2 for hadrons

Bremsstrahlung energy spectra (ELSHIELD benchmark of V.Grichine)

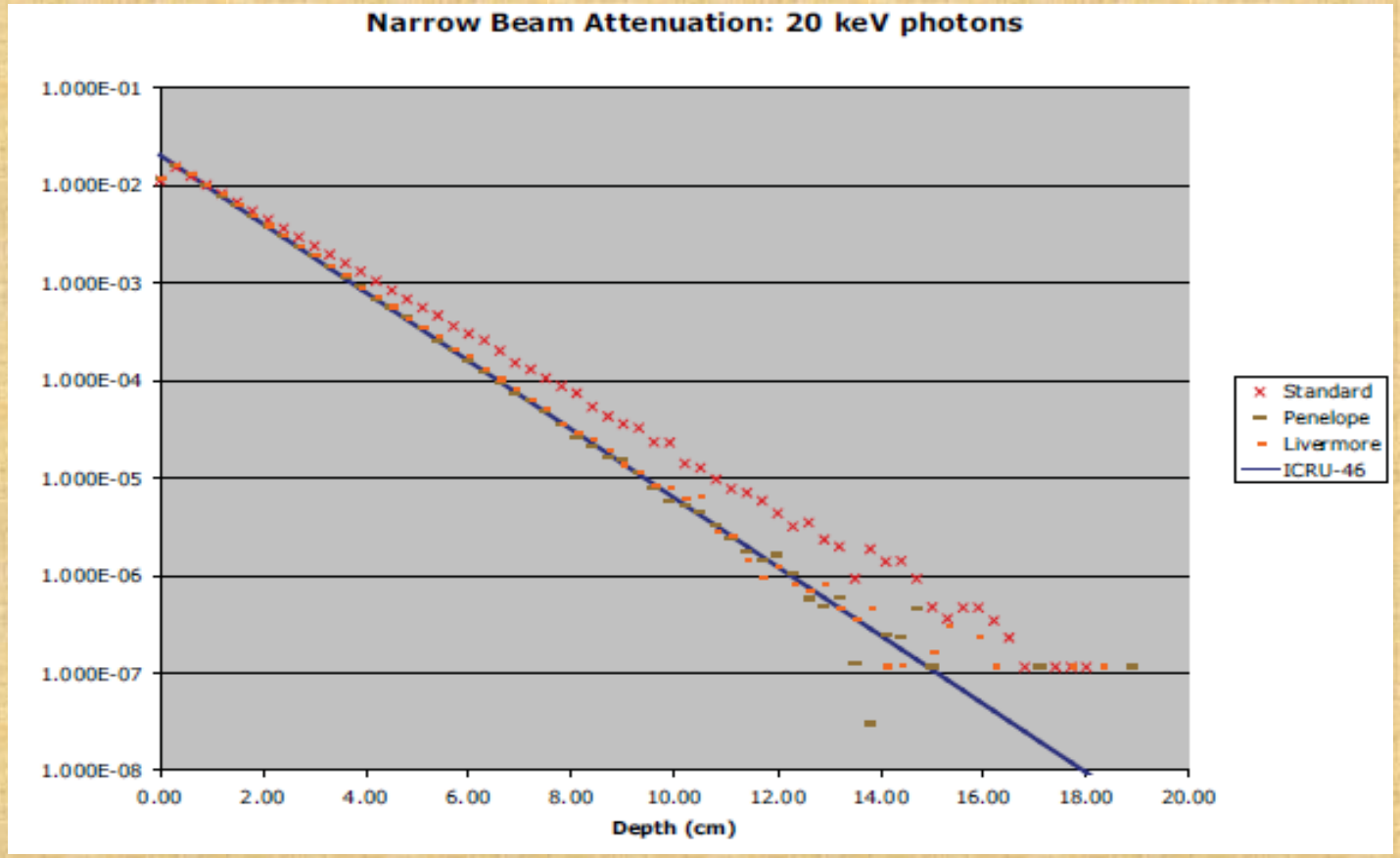






- Statistics 10^8 per run
- At 15 MeV Geant4, EGS and data agree each other
- At 1 MeV Standard model far from the data and Penelope predictions
- **Below 10 MeV Standard model should be substituted!**

Gamma Absorption Geant4/EGSnrc 1st Australian Geant4 Workshop



- Rayleigh scattering must be taken into account for keV energy gamma transport – Opt3 standard Physics List

Urban95 multiple scattering model

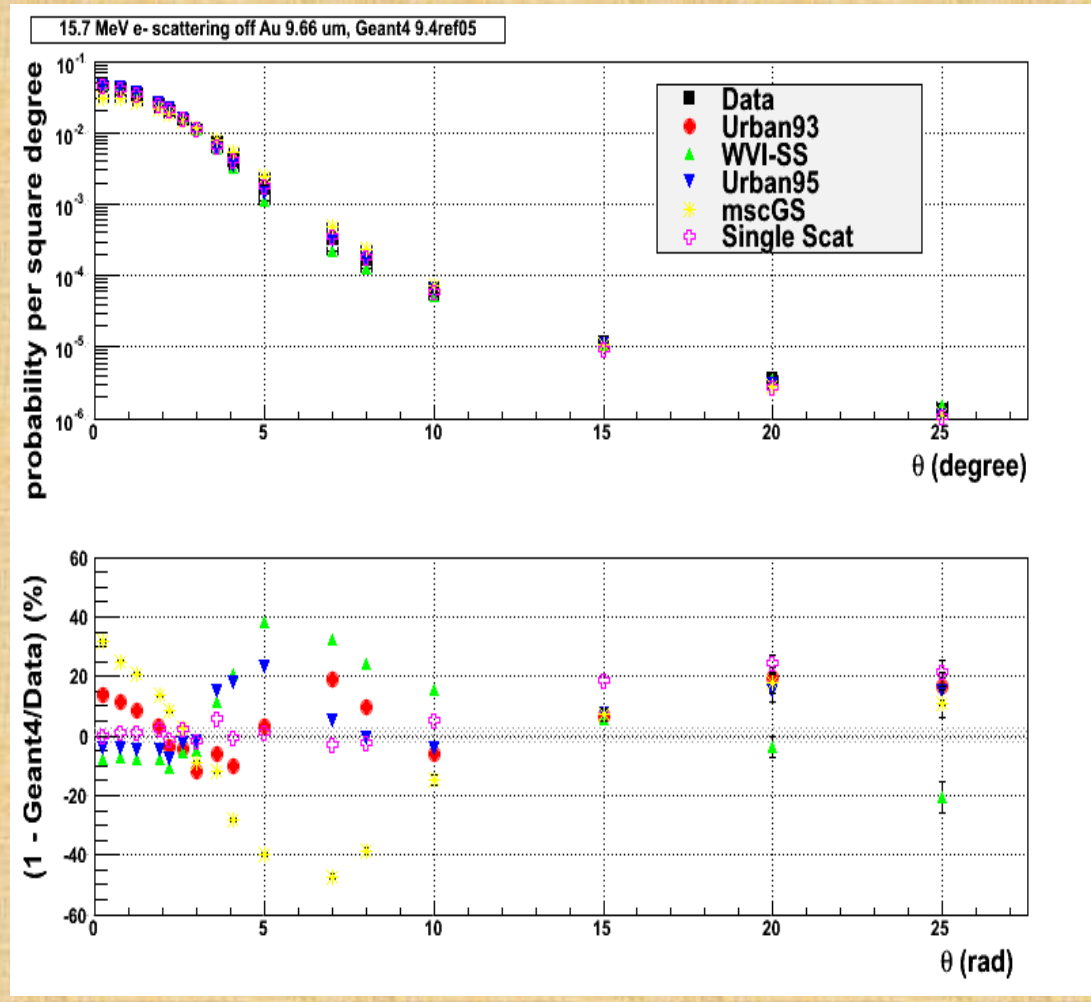
see also presentations at parallel session 2B and plenary 3

Upgrade of multiple scattering (L.Urban)

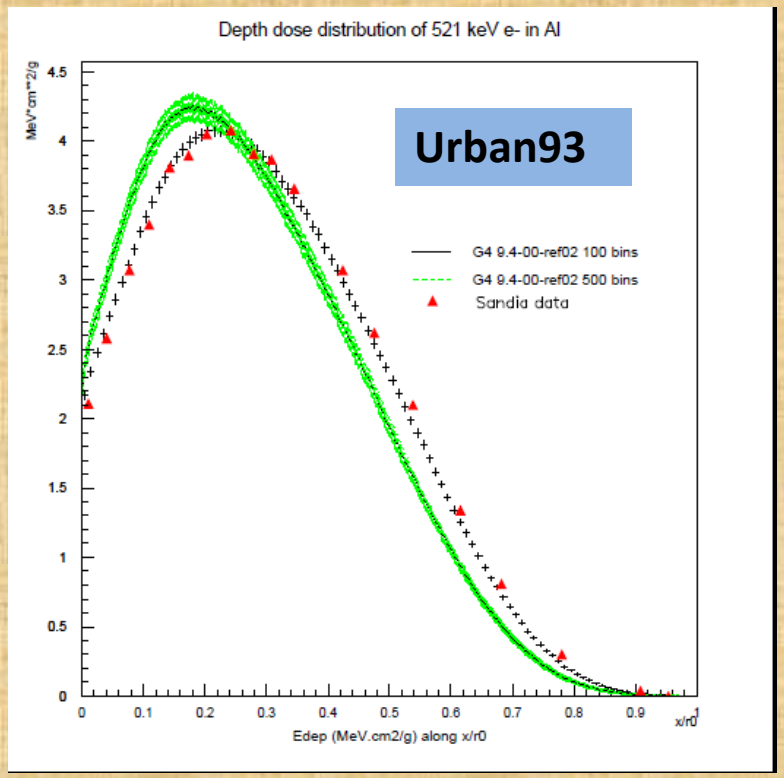
- New G4UrbanMscModel95 become default since 9.4ref08
  - Improved lateral displacement sampling
  - Added sampling along Z-axis
  - Improved tail sampling
  - Validation tests show similar or improved results with the new model
- Old default G4UrbanMscModel93 will be kept for backward compatibility
- Fixes are made also for alternative models
  - G4GoudsmithSaundersonMscModel
  - G4WentzelVIModel

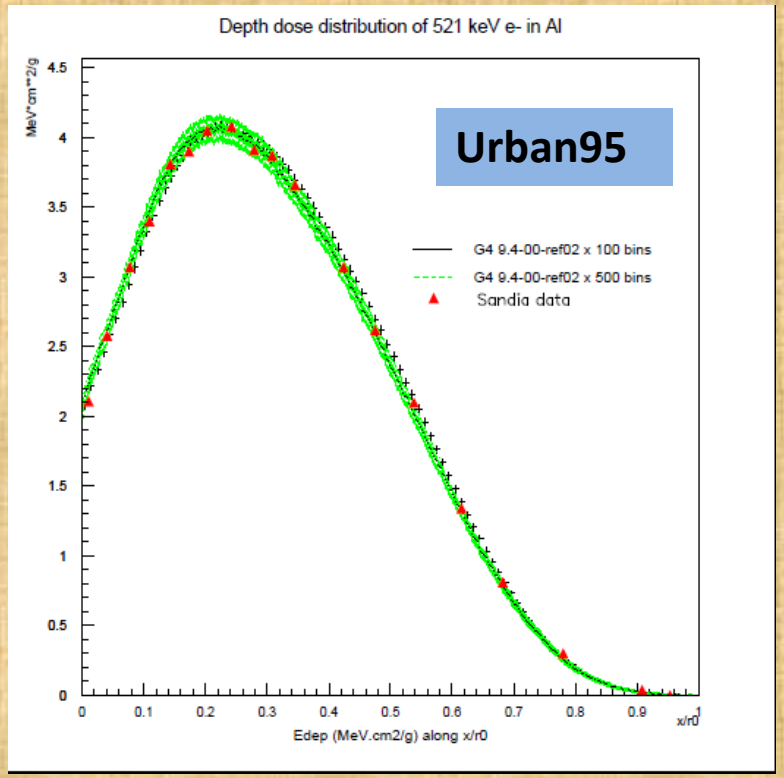
New electron scattering test for the Hanson data
Monte Carlo over data plot is added

- Single scattering model is the most precise
- Urban95 is better for central part and tail than other msc models
- Goudsmith-Saunderson model has lower precision than Urban
- A significant argument to use Urban95



SANDIA data for 0.521 MeV electron transport in Aluminum media without geometry boundaries but with step limitation (L.Urban)

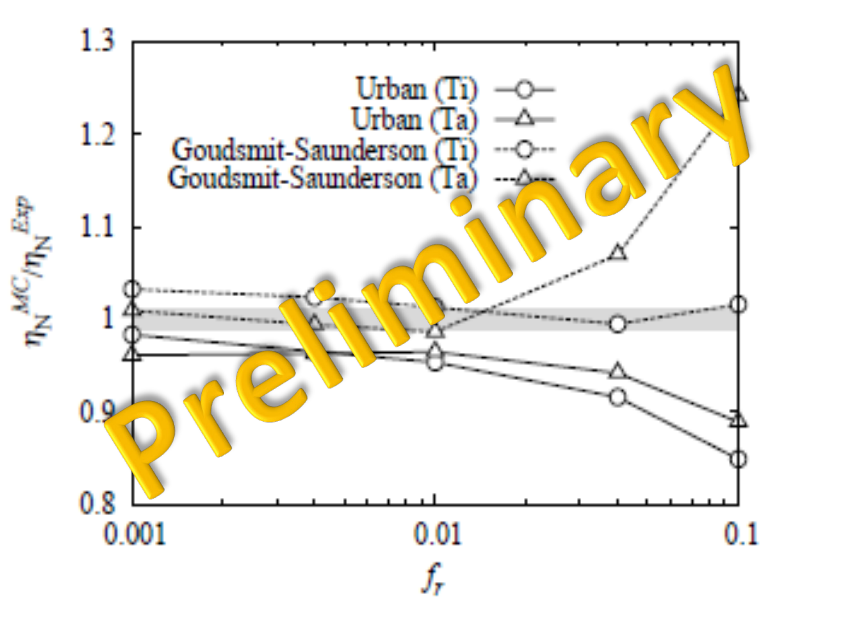




Urban95 is more stable than Urban93

Recent validation results

New benchmark on electron backscattering using Sandia data (A.Lechner)

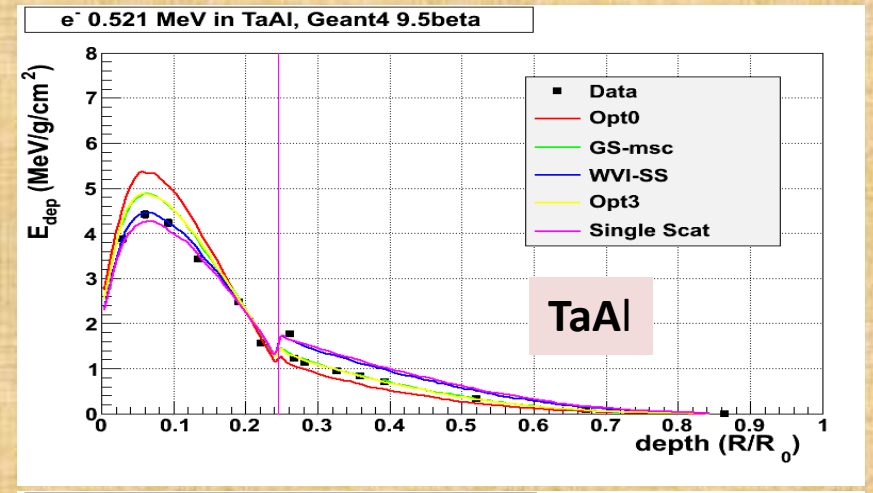


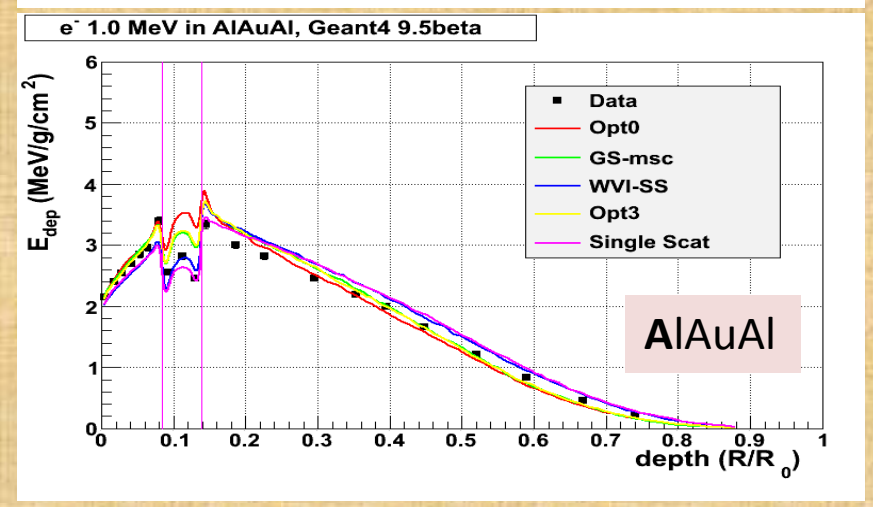
Optimization of f_r (FactorRange) parameter: default value 0.04 should be reduced to 0.01 to provide stable simulation at low energy

- New benchmark have been developed using Sandia data on backscattering and energy deposition in semi-infinite media
- Electron energy 0.1 – 1 MeV
- Beam angles from 0 and 75 degrees
- Be, C, Al, Ti, Cu, Mo, Ag, Ta, Au, U

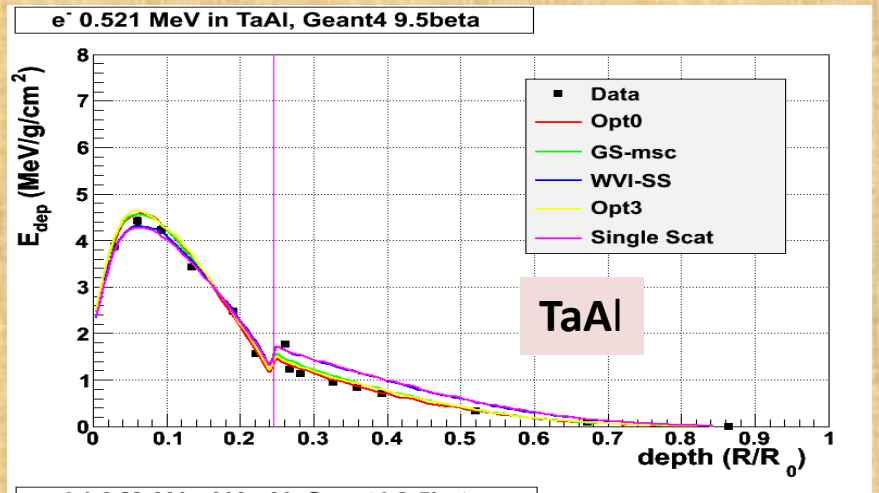
Factor-Range and energy profiles for Sandia data (test37)

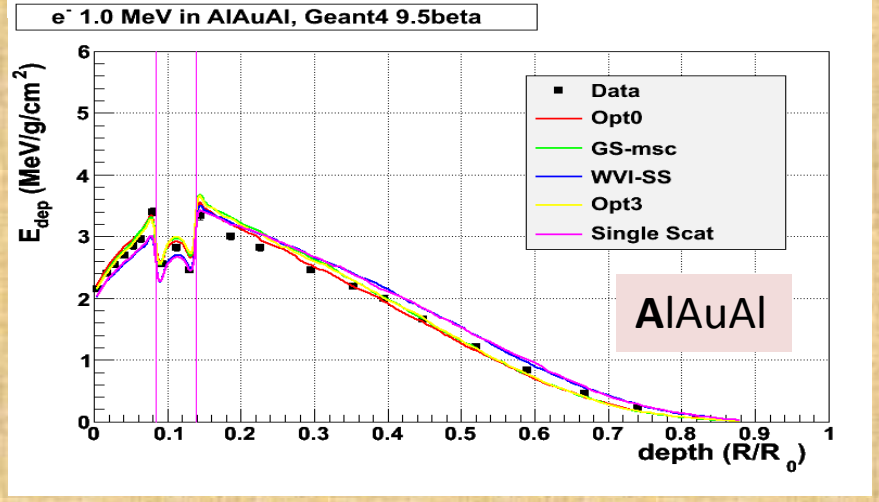
F_R = 0.04 (default)





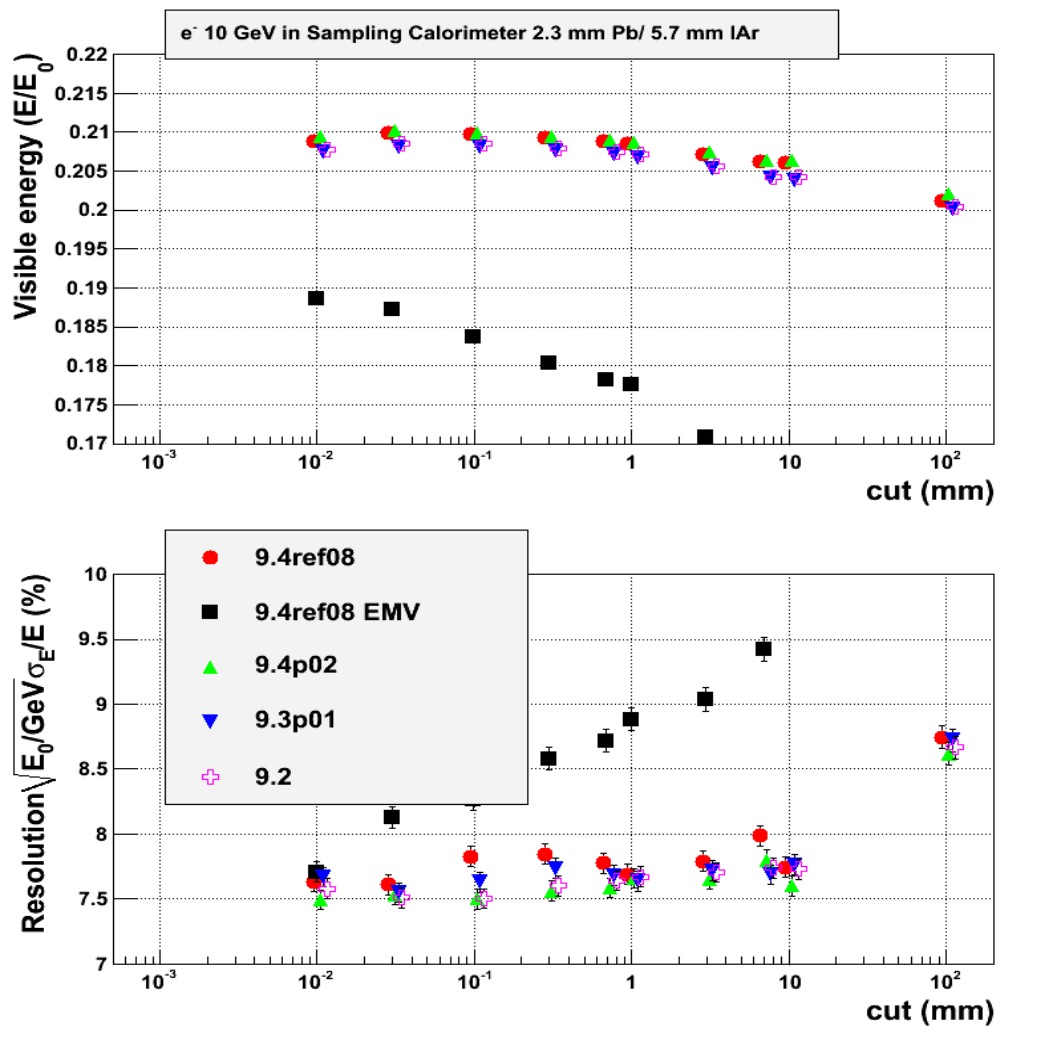
F_R = 0.01



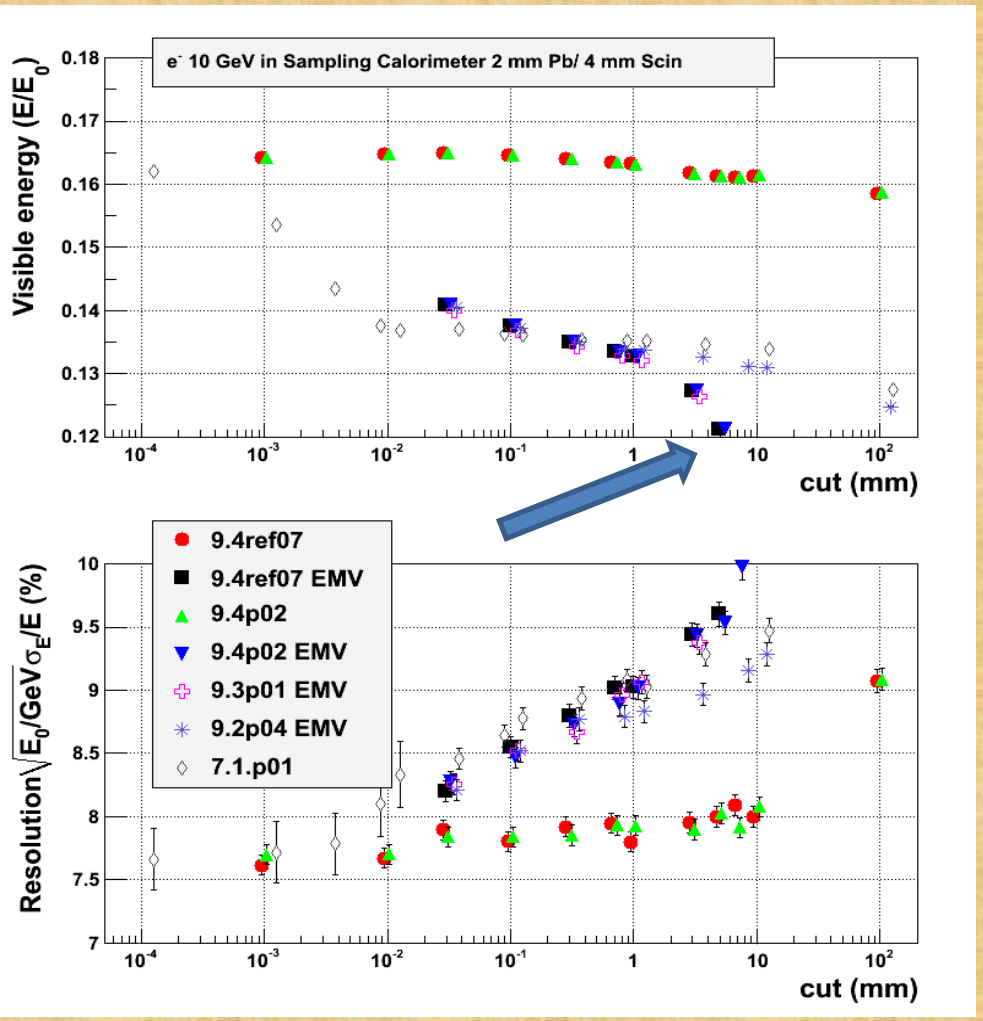


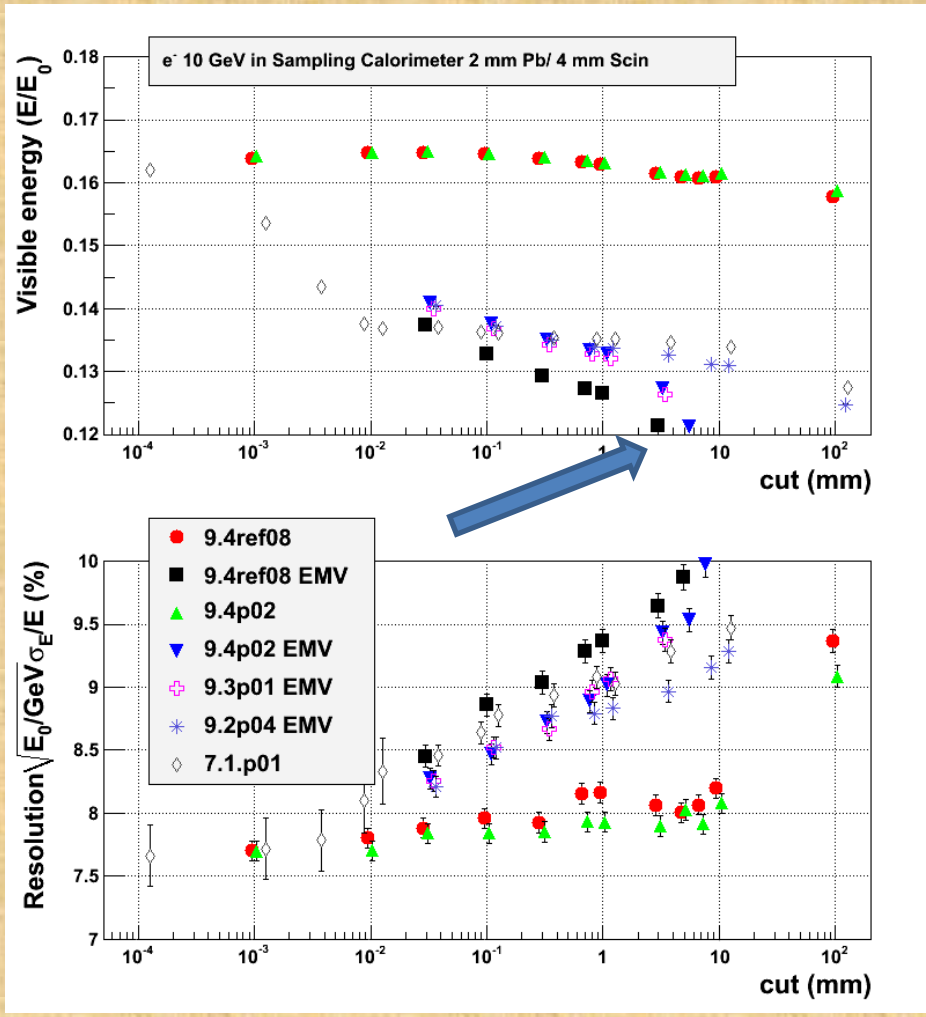
ATLAS barrel simplified calorimeter

- No change of visible energy or resolution between 9.4p02 and 9.4ref08
  - msc95 become default
- About 1% increase of visible energy was in 9.4p02

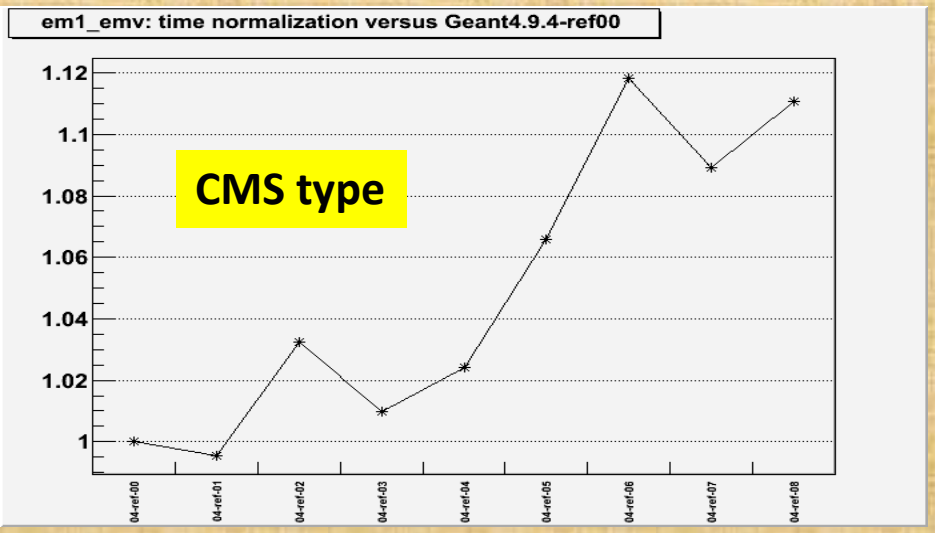


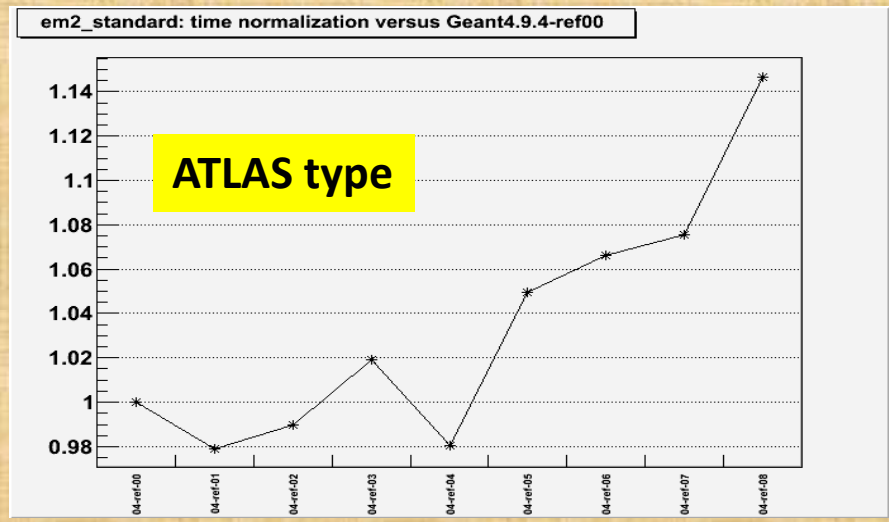
LHCB problem – visible energy changed for 9.4ref08





CPU benchmark for EM physics (J. Jacquemier, LAPP)





- CPU measurement is more complicate than it was in past due to improvements in hardware
- I personally do not see similar increase in my laptop
- These results needs confirmation from simplified calorimeter tests and other CPU analysis

Profiling with igprof – there is no one method which may be responsible

Each sample counts as 0.01 seconds.

% time	cumulative seconds	self seconds	calls	self s/call	total s/call	name
9.01	5.04	5.04	4138303	0.00	0.00	G4UniversalFluctuation::SampleFluctuations
6.46	8.65	3.61	68024498	0.00	0.00	G4PhysicsVector::Value(double)
4.50	11.17	2.52	9130431	0.00	0.00	G4SteppingManager::Stepping()
3.59	13.17	2.01	9080006	0.00	0.00	G4Navigator::ComputeStep(CLHEP::Hep3Vector const&, CLHEP::Hep3Vector const&, double, double&)
3.42	15.09	1.92	9080006	0.00	0.00	G4SteppingManager::DefinePhysicalStepLength()
3.24	16.90	1.81	4847049	0.00	0.00	G4Navigator::LocateGlobalPointAndSetup(CLHEP::Hep3Vector const&, CLHEP::Hep3Vector const*, bool, bool)
3.17	18.67	1.77	19775136	0.00	0.00	G4PhysicsVector::Interpolation(int)

Biasing options for EM physics

(very new development within ELSHEILD project)

Why not wrapper process?

- Wrapper process approach was in Geant4 for long time and there are a lot of examples of implementation of user applications
- Advantages:
  - Biasing is independent from main EM development
  - Default simulation is not affected
- Disadvantages:
  - Biasing is independent from main EM development
  - EM group is not involved in validation and in usage of biasing options
  - Wrapper process implemented for one version of Geant4 may not work for other version

Physics based biasing options

- New options are added to EM infrastructure:
  - Cross section biasing
  - Forced interaction of primary
  - Secondary splitting
  - Russian roulette for secondary
- Simple UI commands activate/deactivate biasing options for any EM Physics Lists per process and G4Region

New UI commands

/process/em/setBiasingFactor procName factor

/process/em/setForcedInteraction procName regionName length

/process/em/setSecBiasing procName regionName factor

New class G4EmBiasingManager is added to a process selected by these commands. Main EM interfaces are practically unchanged, run time CPU penalty is minimal

These features are available with ref-08 for the first time

Validation and discuss are hardly required

Summary

- Based material approach is ready
- We are working on unification not only interfaces by also model capabilities
- We are working on extension of the testing suite
- Problems to be resolved for 9.5 :
  - We need to understand CPU benchmark results
  - We need to understand a shift in response for LHCb type calorimeters
  - Standard bremsstrahlung model for low-energy
  - There are requirements from LHC and other HEP (SLAC) to improve multiple scattering for GeV particles
  - We can try to reduce time of initialisation of muon/hadron bremsstrahlung and e+e- pair production
  - Validation of EM physics should be first priority