Geant4 CERN Group Meeting

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Status of a energy loss simulation for negatively charged particles in Geant4

G4QAOLowEnergyLoss

History:

In Geant4 there is a class to simulate stopping power of low energy negatively charged hadrons: processes/electromagnetic/lowenergy/G4QAOLowEnergyLoss

S. Chauvie, P. Nieminen, M.G. Pia. Geant 4 Model for the Stopping Power of Low Energy Negatively Charged Hadrons. IEEE Trans. Nucl. Sci. 54 (2007) 578

A model for a calculation of the stopping power by regarding the target atom as an ansemble of quantum harmonic oscillators is implemented

Motivation:

The class doesn't work in the context of current EM design

Plan:

1) Migration of anti-proton energy-loss at low energies to current EM design
2) Modification and development of the class
3) Application to other negatively charged particles
4) Tests

The Barkas Correction

Stopping power can be calculated from Bohr-Bethe-Bloch theory with the expression

$$S = -\frac{dE}{dx} = N Z_2 \frac{4\pi e^4}{mv^2} Z_1^2 L$$

The dimensionless stopping number *L* can be expanded in powers of Z_1

$$L = \left(Z_1^2 L_0 + Z_1^3 L_1 + Z_1^4 L_2 + \ldots \right)$$

1st term – well-known Bethe formula, 2nd – the Barkas correction (of Z^3).

The presence of terms with odd powers in *Z* leads to a different stopping behaiviour of positevely and negatively charged particles.

For antiprotons (Z_1 = -1)

$$L = L_0 - L_1 + L_2$$

The Quantal Harmonic Oscillator Model

• Bohr suggested the model of atoms as a collection harmonic oscillators for the description of inelastic collisions of charged particles

• Sigmund and co-workers considered a harmonic oscillator target treated within the framework of quantum mechanics

They suggested for a stopping number of an atom

$$L_{atom} = \sum_{n}^{shells} f_n L\left(\frac{2mv^2}{\hbar\omega_n}\right),$$

where ω_n, f_n − resonance frequencies (excitation energies) and the optical oscillator strengths

The excitation energies and oscillator strengths must satisfy the sum rules

$$\sum_n f_n = Z_2, \quad \sum_n f_n \ln(\hbar\omega_n) = Z_2 \ln(I)$$

The Quantal Harmonic Oscillator Model - Implementation

G4QAOLowEnergyLoss:

- there are tabulated data sets $\boldsymbol{\omega_n}, \boldsymbol{f_n}$ only for 6 materials

Aluminum, Silicon, Copper, Tantalum, Gold, Platinum

- for other materials

1) the oscillator strength is set equal to the number of electrons in the *n*-th atomic shell

$$f_n = Z_n / Z_2$$

2) the resonance frequencies can be obtained from

$$\hbar\omega_n = \sqrt{(a U_n)^2 + \frac{2}{3}\frac{f_n}{Z_2}(\hbar\omega_p)^2}, \quad \hbar\omega_p = \sqrt{\frac{4\pi\hbar^2 e^2 N Z_2}{m}},$$

where U_n is the ionization energy of the n-th shell, $\hbar\omega_p$ – the nominal plasma energy,

$a \sim \exp(1/2) \approx 1.65$

processes/electromagnetic/standard/G4ICRU73QOModel

Old implementation (G4QAOLowEnergyLoss):

Tabulated data - "Aluminum", "Silicon", "Copper", "Tantalum", "Gold", "Platinum"

TABLE I. Oscillator strengths w and energies E used in the harmonic-oscillator model calculations.

	Al	Si	Cu	Ta	Pt	Au
w_K	0.1349	0.1222	0.0505	0.0126	0.0129	0.0139
E_K (keV)	2.795	3.179	16.931	88.926	95.017	96.235
w_L	0.6387	0.5972	0.2561	0.0896	0.0745	0.0803
E_L (keV)	0.202	0.249	1.930	18.012	25.590	25.918
w_M	0.2264	0.2806	0.4913	0.2599	0.2295	0.2473
E_M (keV)	0.0169	0.0203	0.199	3.210	4.063	4.116
w_N			0.2021	0.3413	0.4627	0.423
E_N (keV)			0.0396	0.575	0.576	0.599
w_O				0.2057	0.1324	0.1124
E_O (keV)				0.1087	0.0819	0.0873
w_P				0.0908	0.0879	0.1231
E_P (keV)				0.0308	0.0314	0.0369
I (keV)	0.164	0.168	0.322	0.709	0.764	0.800

ICRU73 Report:

Tabulated data – for 25 elements plus "Ta" from old data

- Total: data for 26 elements

processes/electromagnetic/standard/G4ICRU73QOModel – structure and methods of the new class corresponding to the current EM design

class G4BraggPbarModel : public G4VEmModel
public:
- G4BraggPbarModel
- virtual ~G4BraggPbarModel
- virtual void Initialise
- virtual G4double ComputeCrossSectionPerElectron
- virtual G4double CrossSectionPerVolume
- virtual void SampleSecondaries
- virtual G4double MinEnergyCut
- virtual G4double ComputeCrossSectionPerAtom
- virtual G4double ComputeDEDXPerVolume
- virtual void CorrectionsAlongStep

protected:
- virtual G4double MaxSecondaryEnergy

private:
- inline void SetParticle
- G4double DEDX
- G4double DEDXPerElement

Methods from G4QAOLowEnergyLoss:
- G4int GetNumberOfShells
- G4double GetShellEnergy
- G4double GetOscillatorEnergy
- G4double GetShellStrength
- G4double GetL0 // terms in Z^2
- G4double GetL1 // terms in Z^3
- G4double GetL2 // terms in Z^4

processes/electromagnetic/standard/G4ICRU73QOModel – data

```
// Z of element at now avaliable for the model
  const G4int NQOELEM  = 26;
  static const G4int ZElement[NQOELEM];

  // number, energy and oscillator strenghts  for an harmonic oscillator model of material
  static const G4int startElemIndex[NQOELEM];
  static const G4int nbofShellsForElement[NQOELEM];
  static const G4int ShellEnergy[130];
  static const G4int SubShellOccupation[130];  // Z * ShellStrength

//  variable for calculation of stopping number of L's term
  static const G4double L0[67][2];
  static const G4double L1[22][2];
  static const G4double L2[14][2];

  static const G4int nbOfElectronPerSubShell[1540] → G4AtomicShells::fNumberOfElectrons[1540]
  static const G4int fNumberOfShells[101]           → G4AtomicShells::fNumberOfShells[101]

  G4int sizeL0;
  G4int sizeL1;
  G4int sizeL2;
```

$L_i\left(\frac{2mv^2}{\hbar\omega_n}\right)$ is evaluated by means of linear interpolation in the tables of L

G4ICRU73QOModel

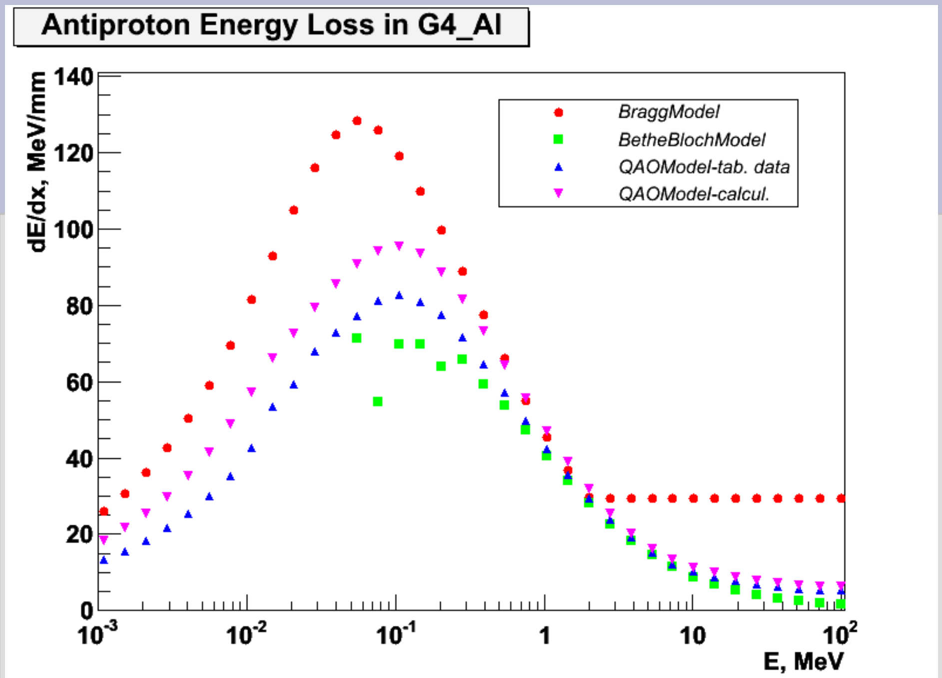
Implementation:

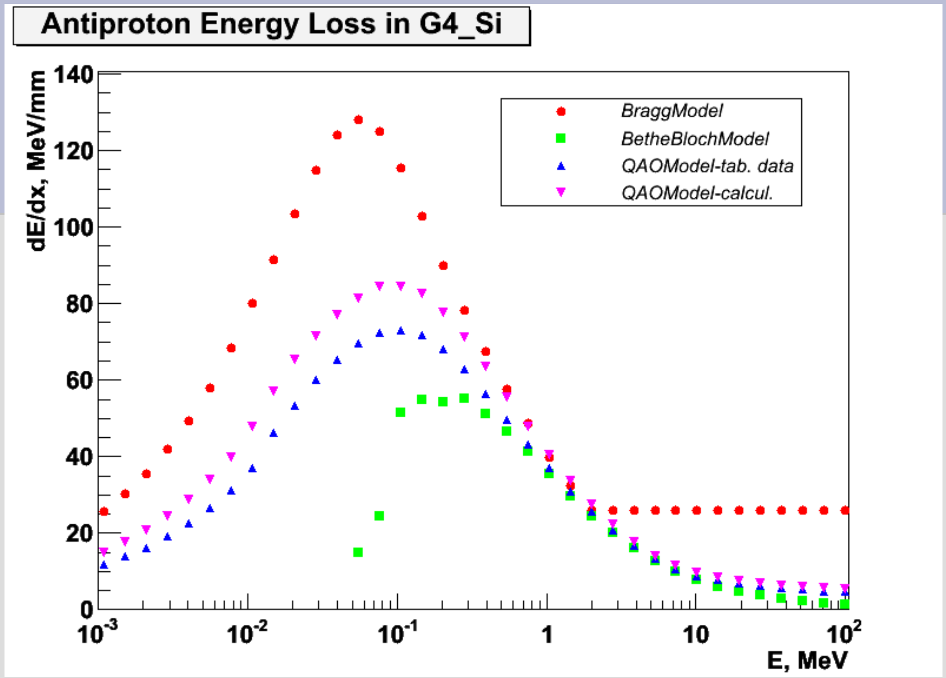
- introduce delta-electron poduction threshold (cut) above cut
- simulation of energy loss for compound materials by using of Bragg's rule
- set spline interpolation under calculation of L_i in the tables instead of linear intepolation
- plasma energy is supposed to take from G4DensityEffectData::GetPlasmaEnergy() instead of to calculate by formula
- values of nbOfElectronPerSubShell[1540] and NumberOfShells[101] is supposed to take from G4AtomicShells::GetNumberOfElectrons(Z,nbOfTheShell), G4AtomicShells::GetNumberOfShells(Z) instead of to contain inside the class the same arrays

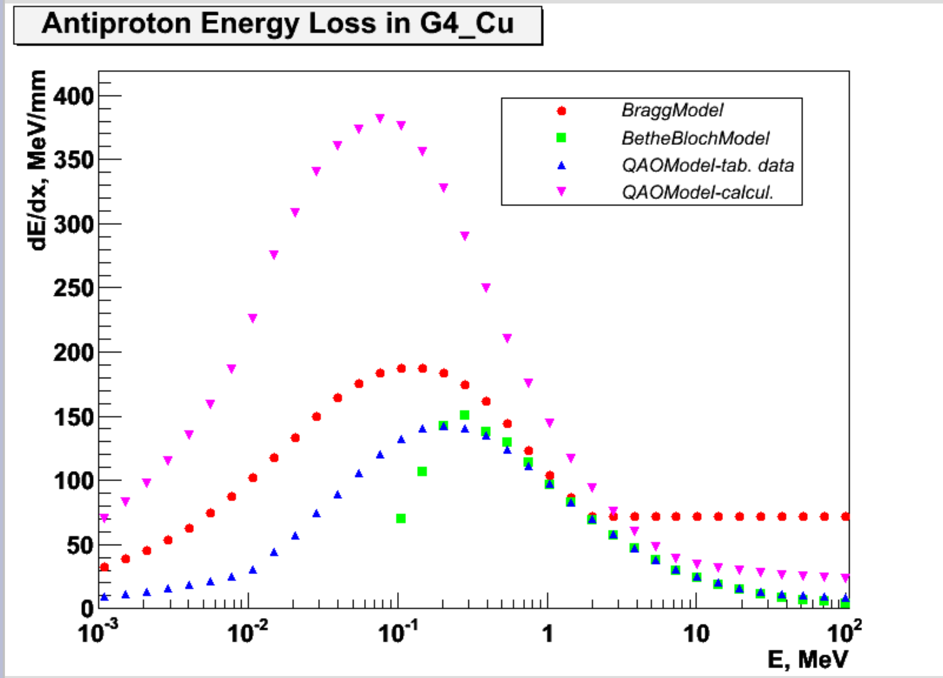
Tests:

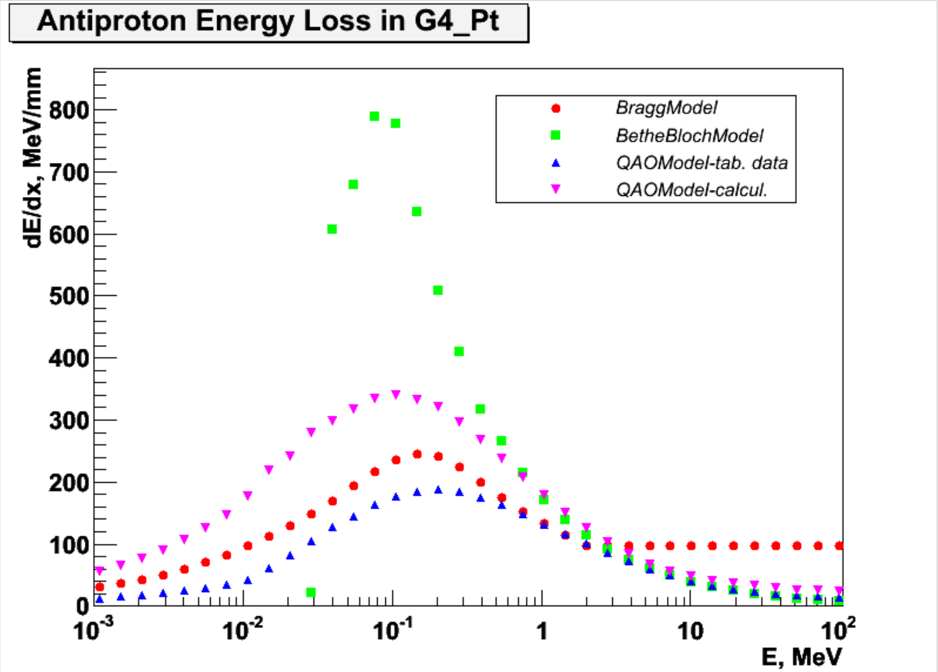
- comparison of energy loss simulation by harmonic oscillator model for 6 materials: shell energies and shell strengths from tables and from formulas
- comparison of energy loss simulation by oscillator model and by Bethe-Bloch formula for different particles and different materials especially for energy region 2 – 10 MeV
- study of alternative publications concerning stopping number calculation

G4ICRU73QOModel – Tests (The model is used in tests with energy limits: 1 keV – 100 MeV)









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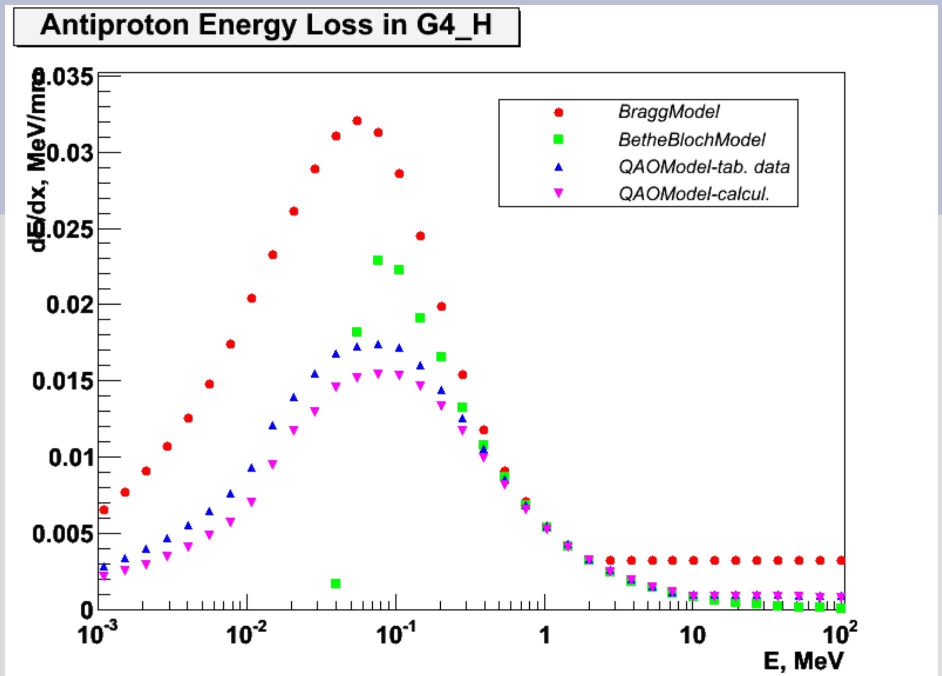
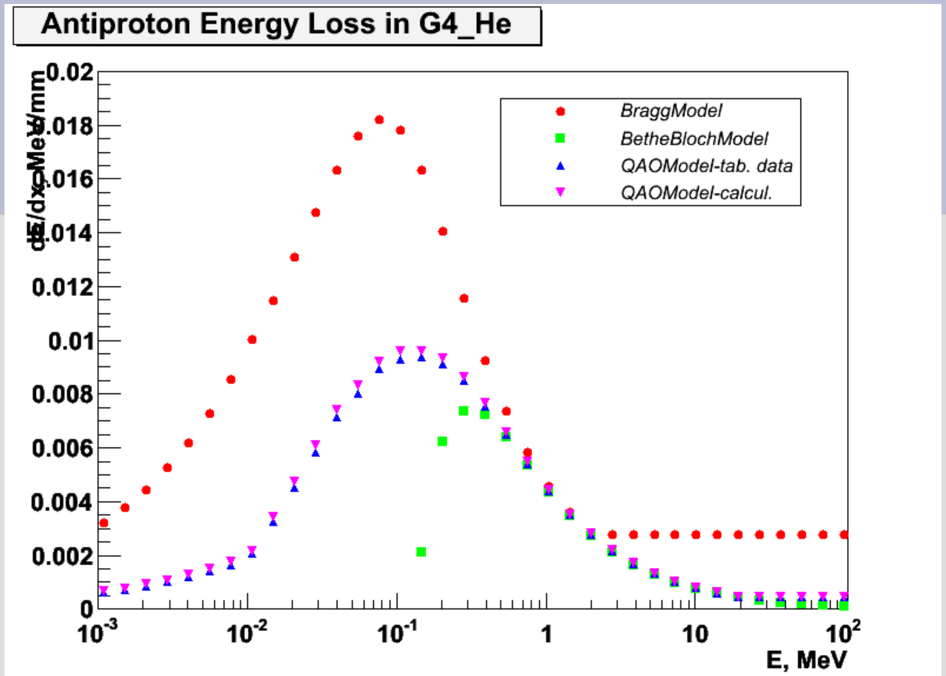
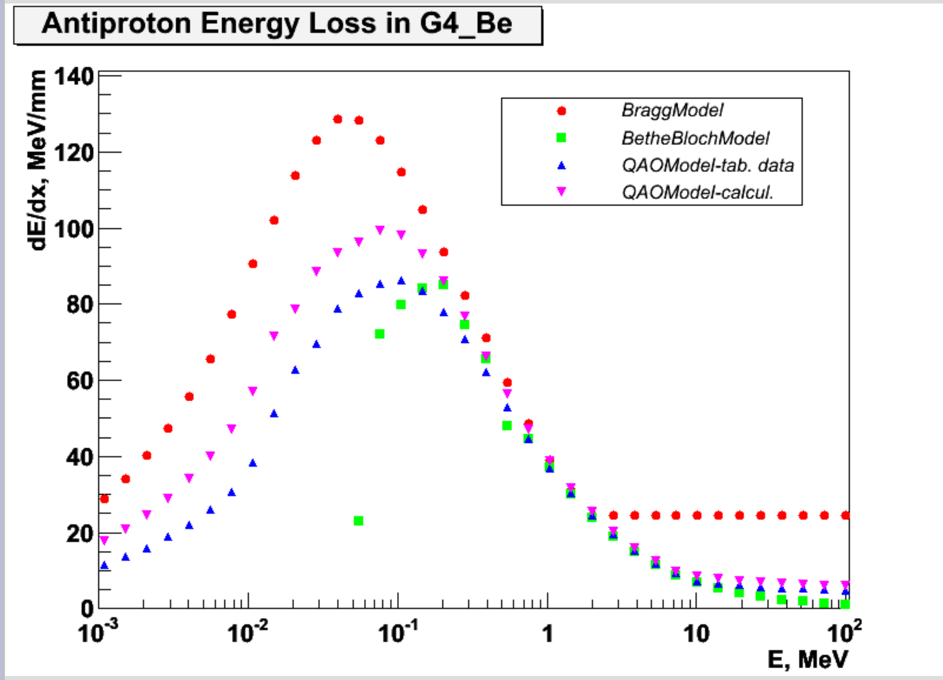
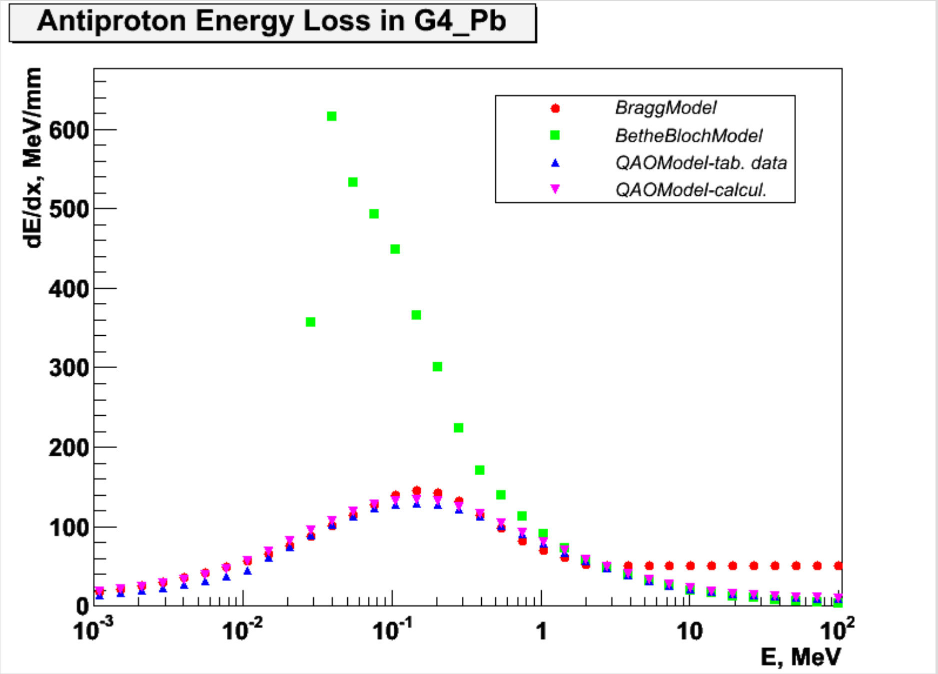


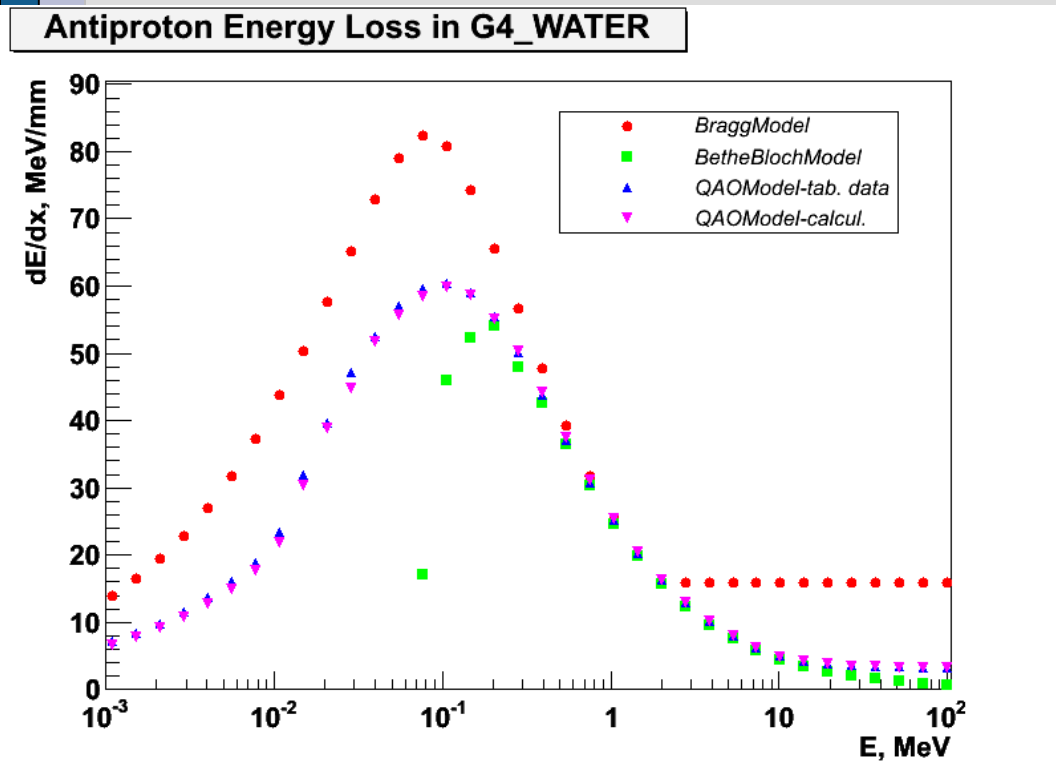


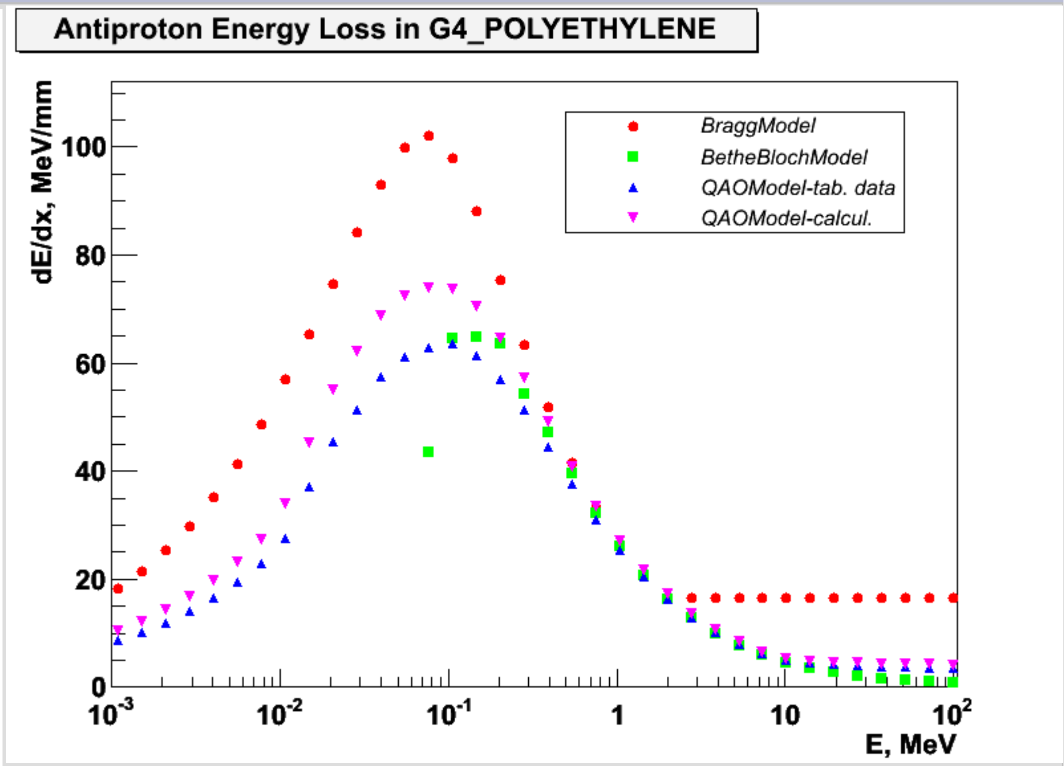




G4ICRU73QOModel – Tests

dE/dx for compound materials





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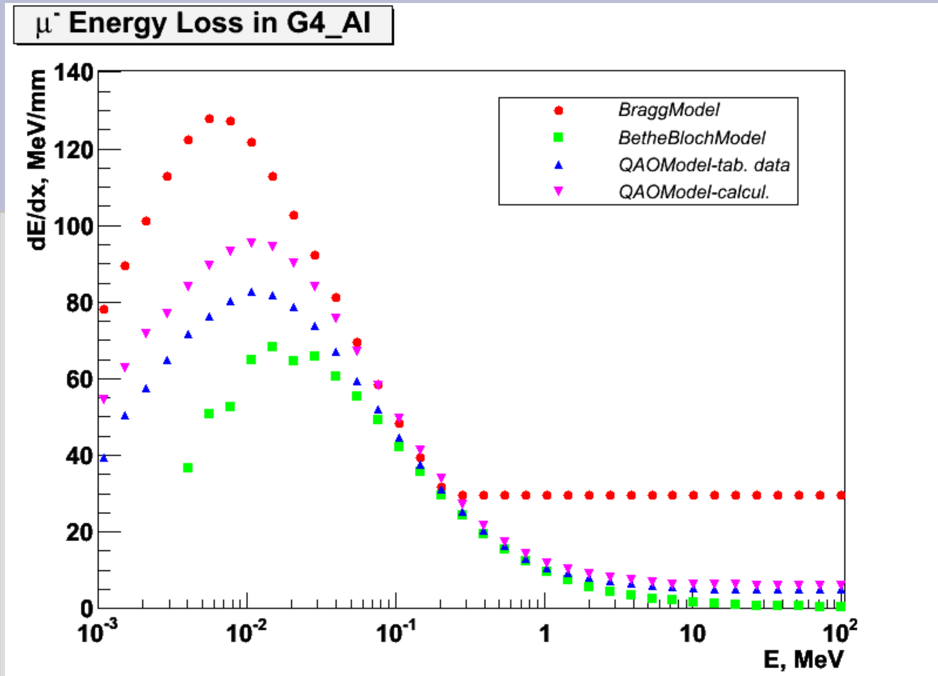

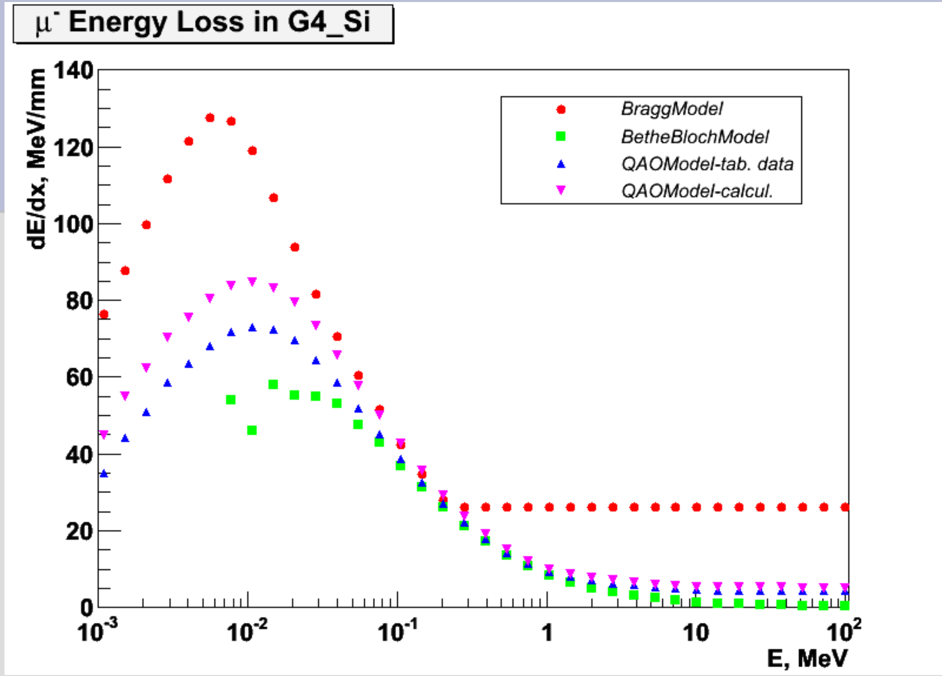

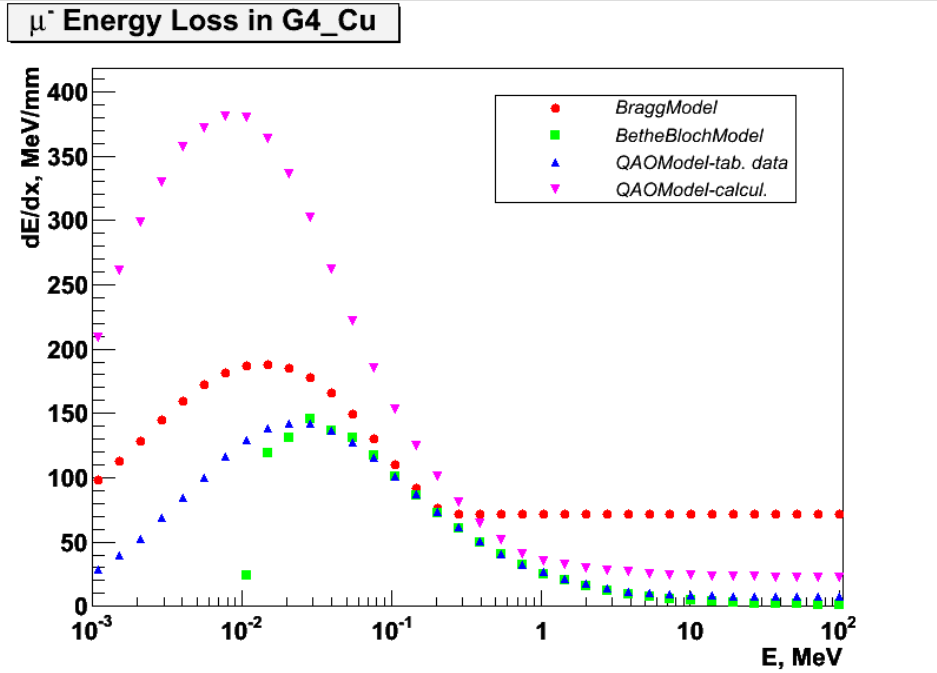

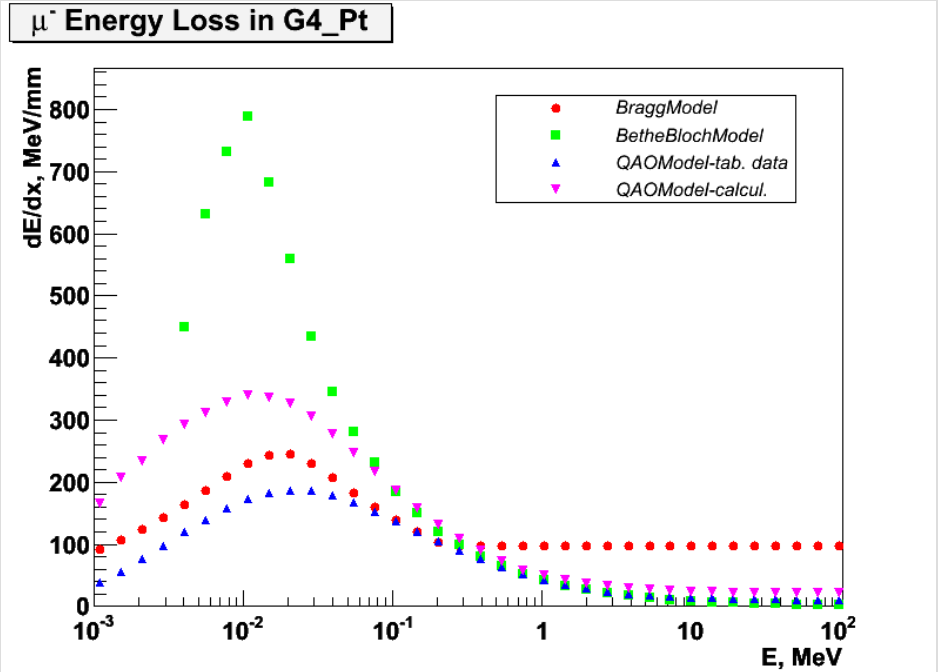

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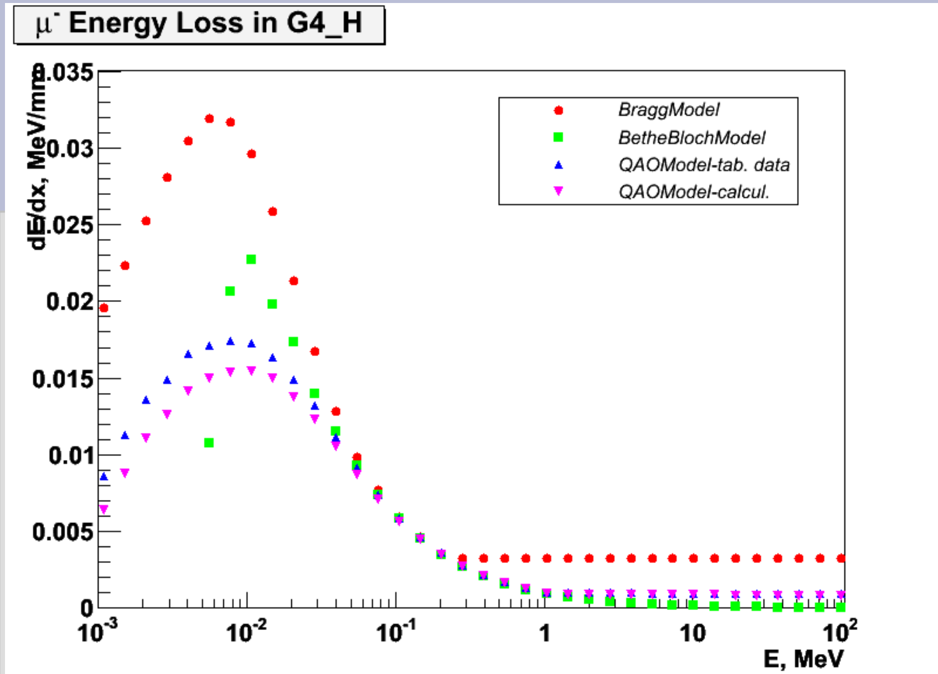
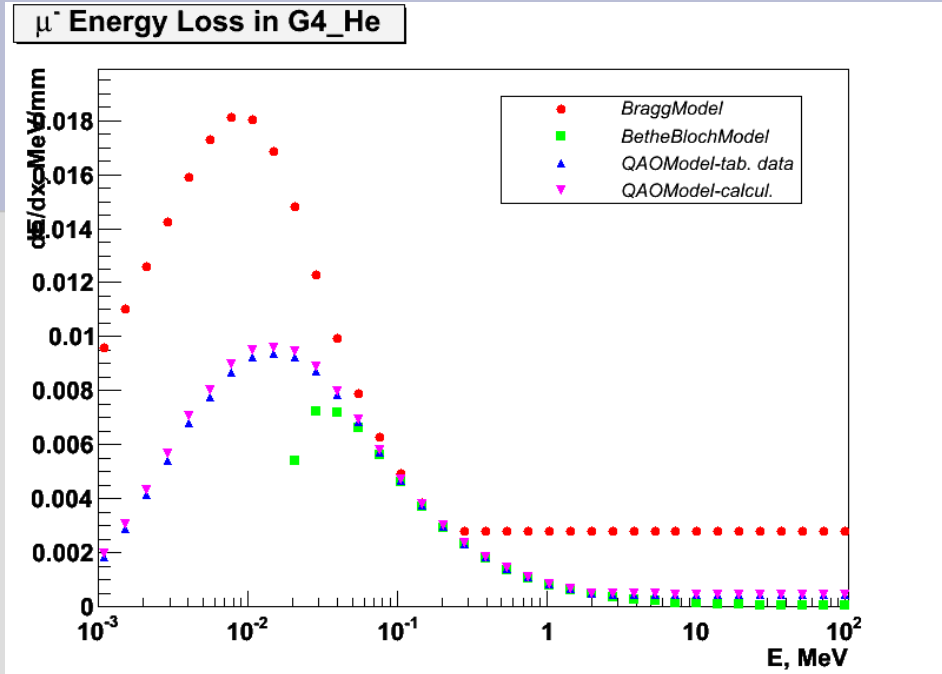
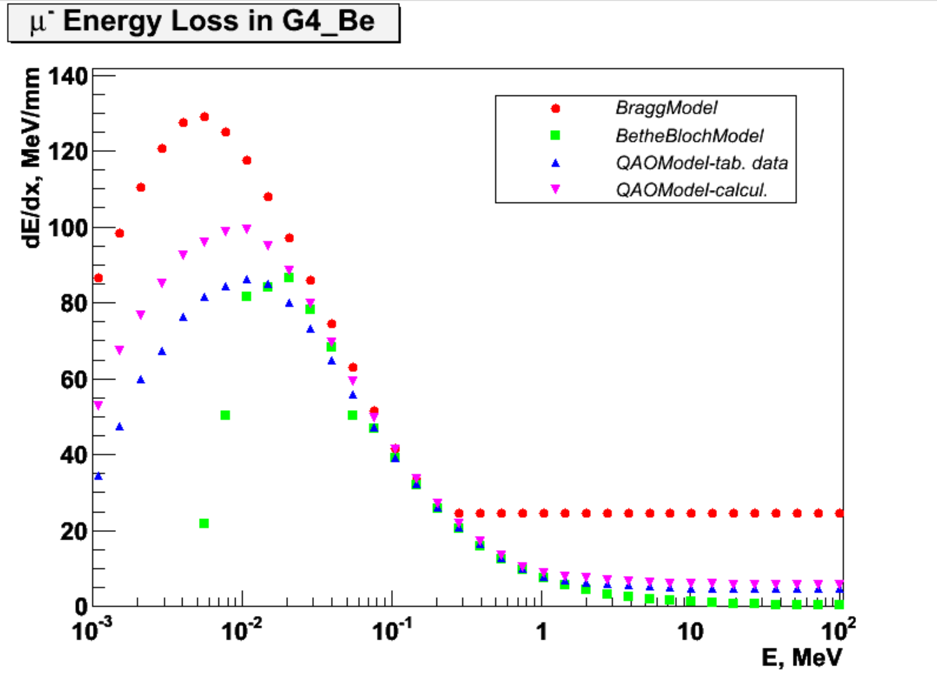
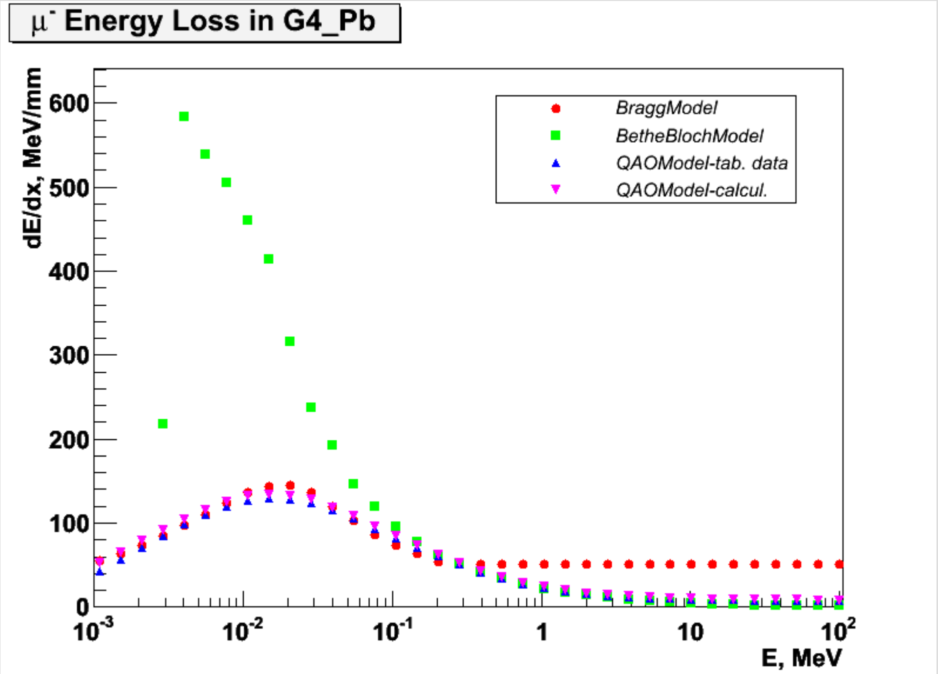


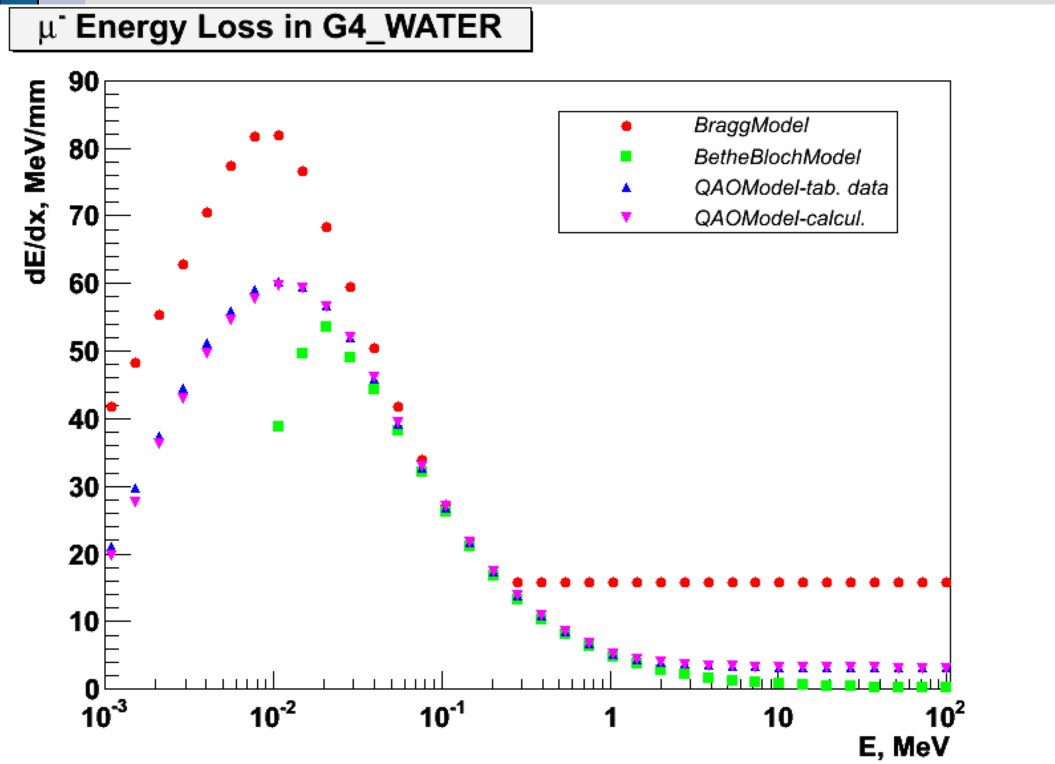


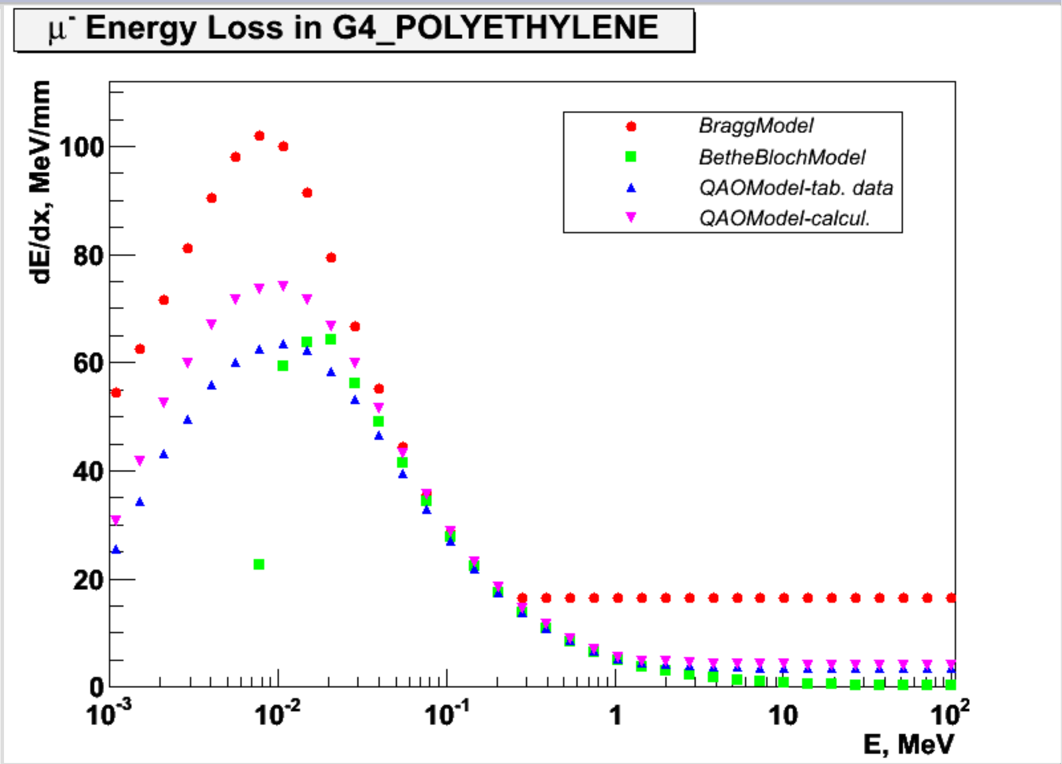




G4ICRU73QOModel – Tests

dE/dx for compound materials





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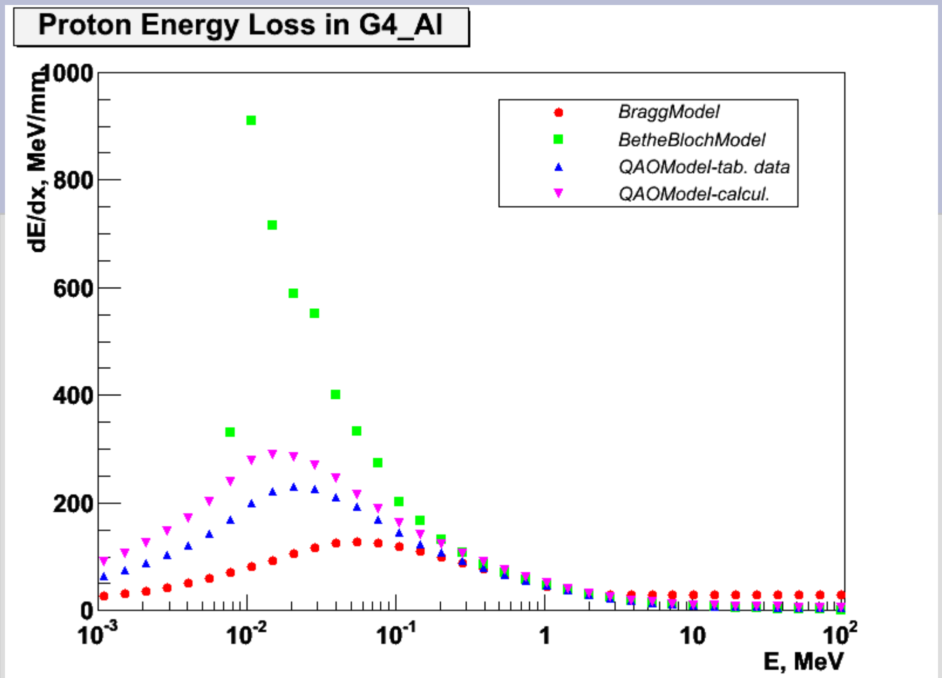

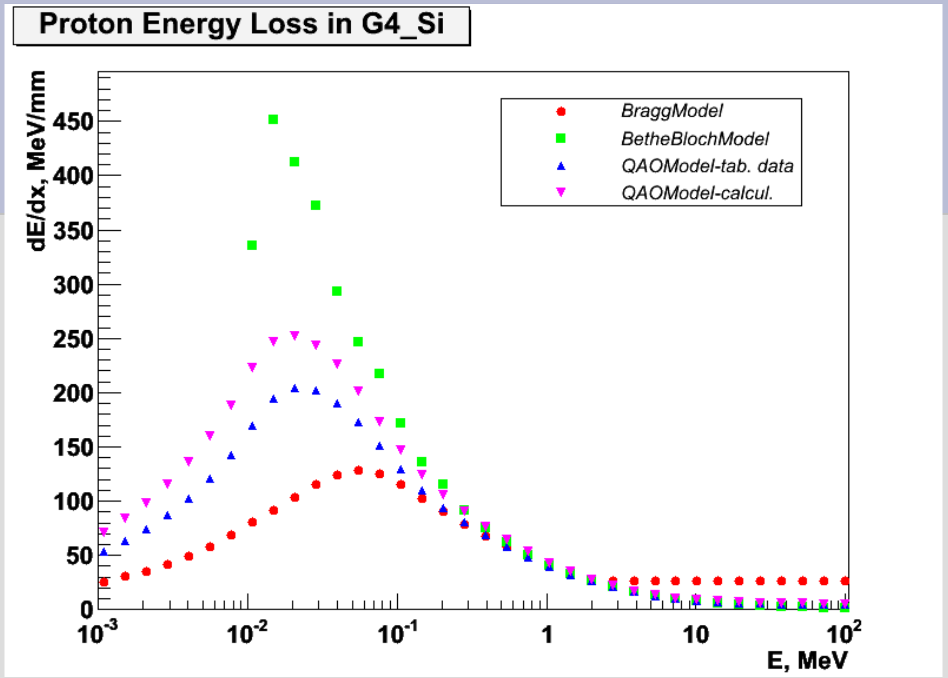

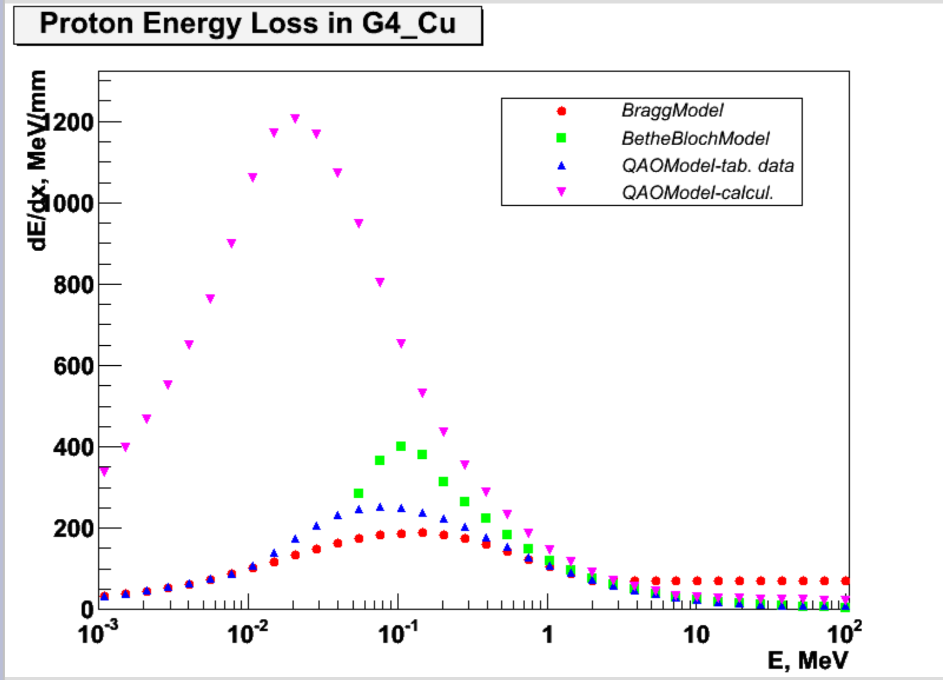

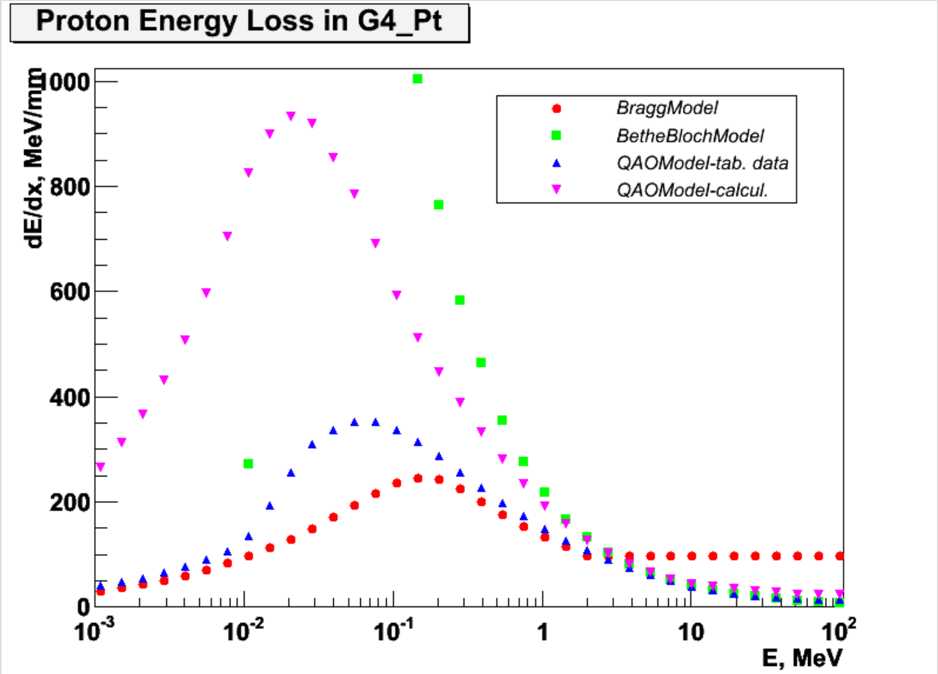

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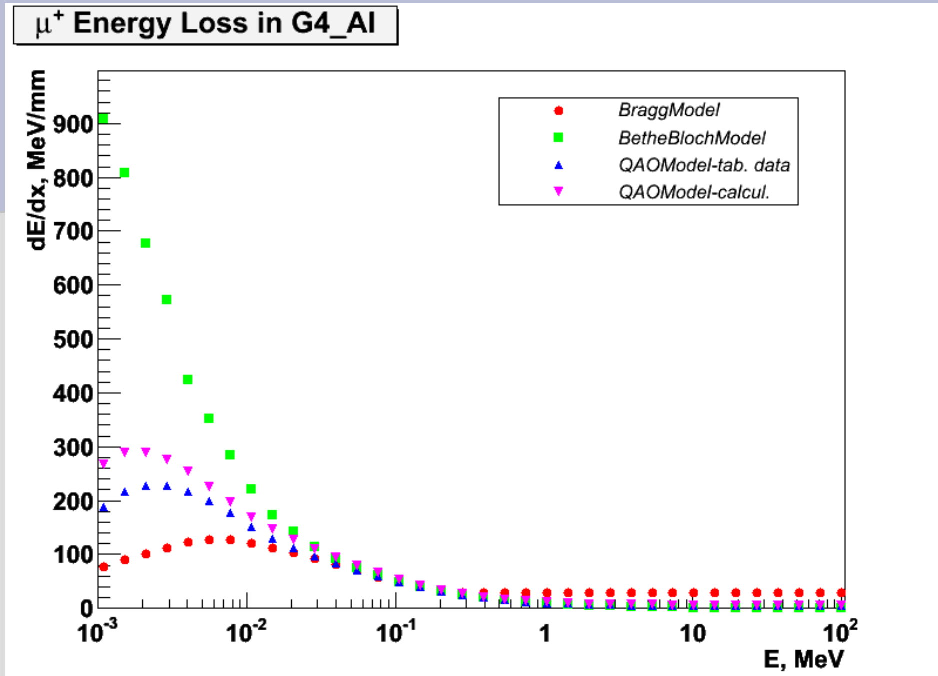

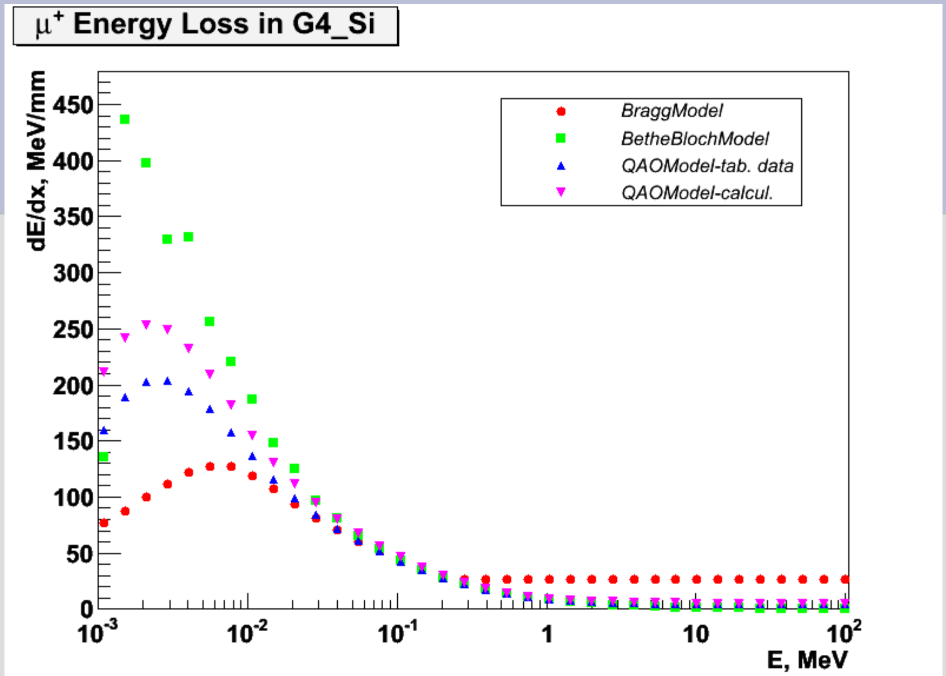

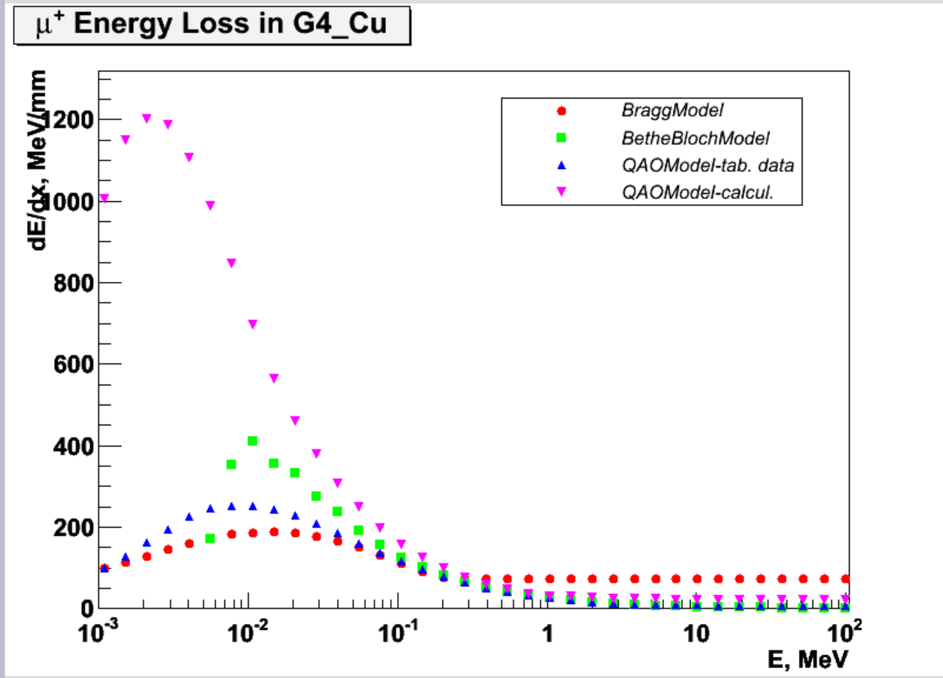

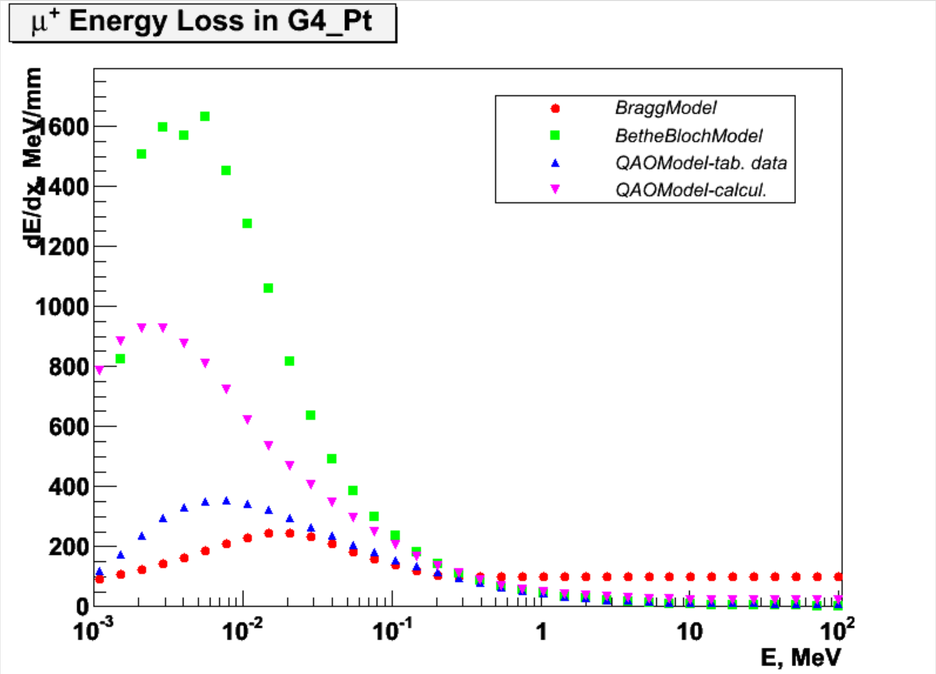

G4ICRU73QOModel – Results

- G4ICRU73QOModel for energy loss simulation of negatively charged particles has been implemented
- Files have been committed
- Comparison with experimental data