Simulation of elastic scattering with mixed approach

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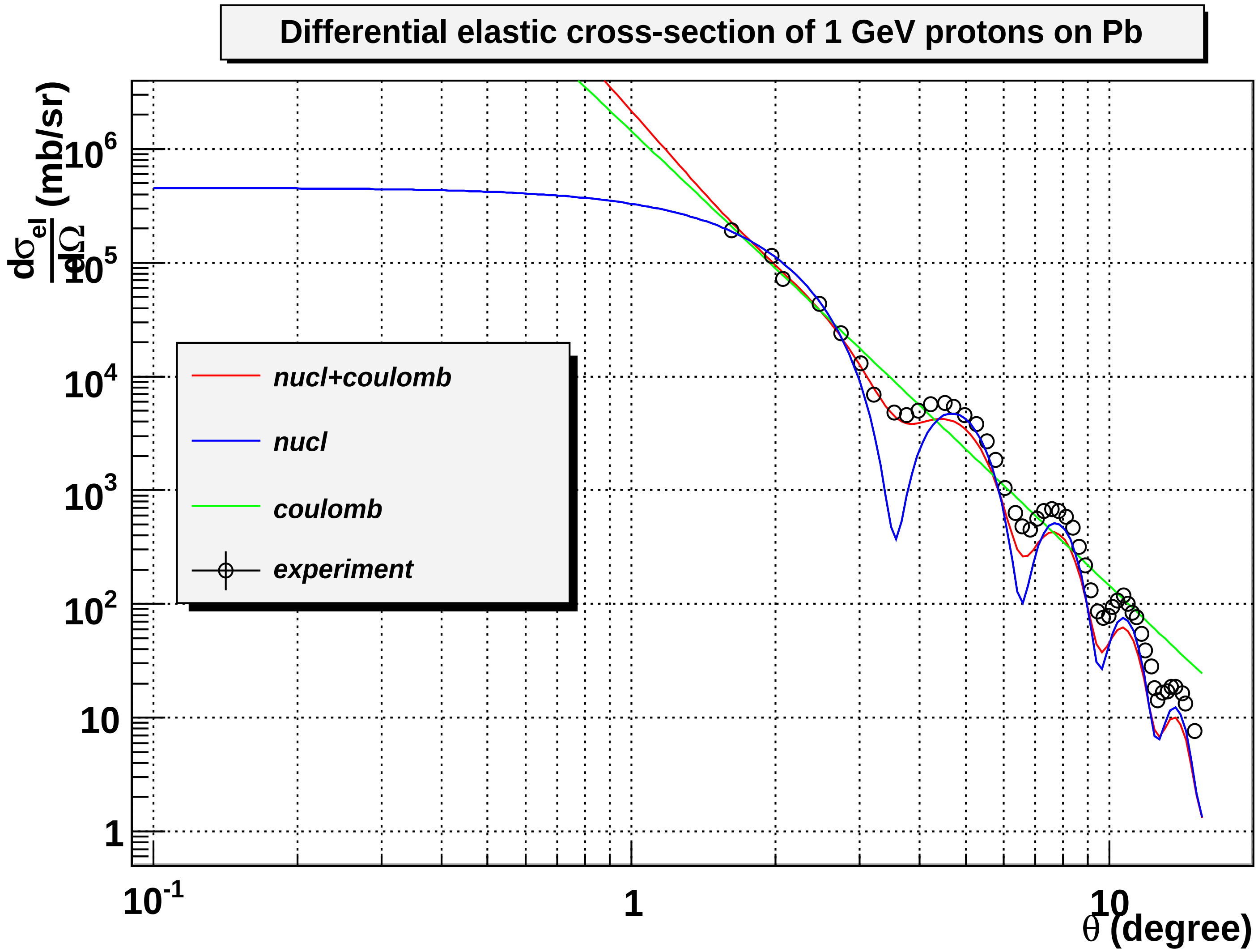
Abstract

Lewis theory of the Coulomb multiple scattering is considered in the Gauss approximation for small scattering angles. The model is similar to the Yang theory expressed in terms of the true path length. A mixed algorithm of the Coulomb elastic scattering simulation based on condensed along step consideration of small angles and single post step scattering for the rest of angular spectrum is proposed for the GEANT4 LHC applications

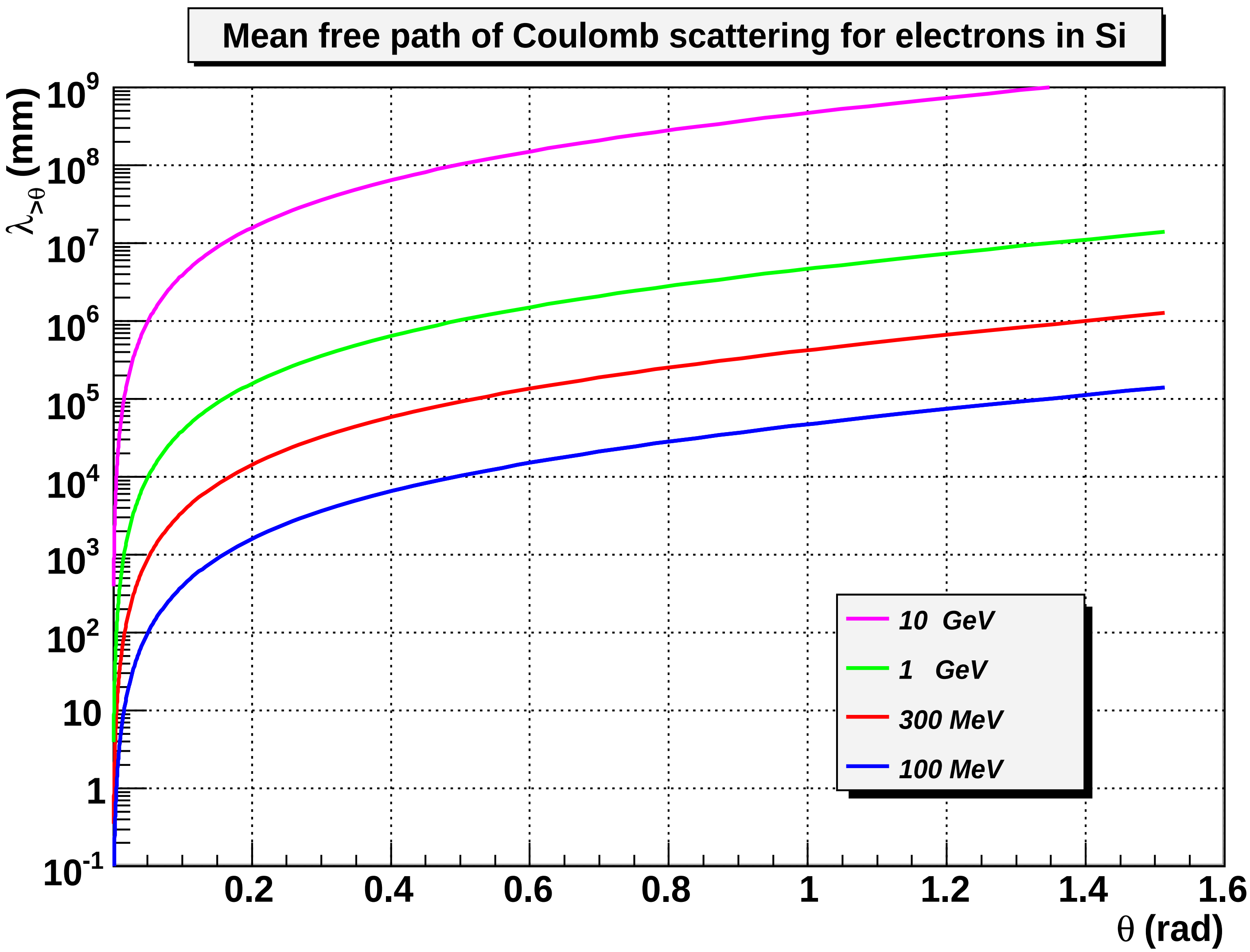
1 Outline

1. Single elastic scattering, mixed elastic scattering, multiple scattering.
2. Motivation of mixed elastic scattering for high energy hadrons and muons
3. The model description.
4. Monte-Carlo algorithms and some parameter fitting.
5. Comparison with experimental data and performance.
6. Design issues and to do.

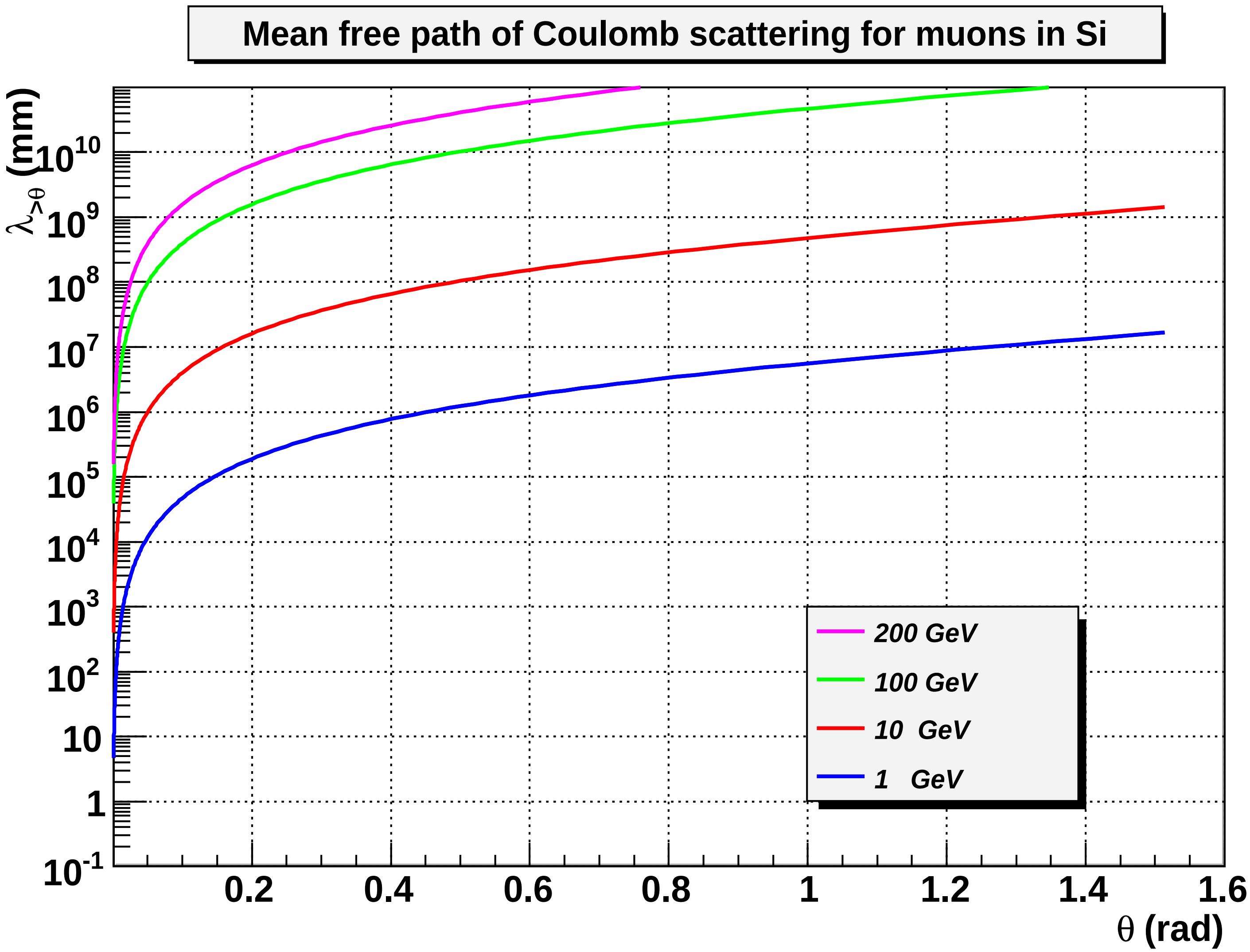


$$\sigma_{el}^{cw}(0, 2^o) \sim \sigma_{el}^{cw} = 2.36423 \cdot 10^9 \text{ mb, with } \lambda = 0.12 \text{ micron, } (10^{-4} \text{ mm!})$$

$$\sigma_{el}^{cw}(2^0, 16^o) = 642.65 \text{ mb, with } \lambda = 47 \text{ cm.}$$



One can see that λ is small for very small scattering angles $\theta \ll 1$ only.



Mixed approach: msc for $\chi < \chi_s \ll 1$ and single scattering for $\chi_s < \chi < \chi_{max}$

2 Motivation

GEANT4 has different models for multiple scattering. The current GEANT4 statement is that the multiple scattering does not limit step [1]. It is not completely true, since steps are limited near the interface between volumes and user step limitation provides better simulation in some important for LHC applications.

Mixed algorithm of multiple scattering

(multiple scattering for $\chi < \chi_s \ll 1$ and single scattering for $\chi_s < \chi < \chi_{max}$)

was proposed many years ago, probably initially for the simulation of muon cooling for neutrino factory. Then it was discussed by PENELOPE team. GEANT4 recently started a development in this direction [2] by implementation of the PENELOPE approach [3] with few modifications.

Here we consider another model for the mixed algorithm of multiple scattering based on small angle (Gaussian) approximation of the Lewis theory resulting in the Yang model-like approach expressed in terms of the true path length. The approach is considered for GEANT4 LHC applications.

3 The model description

Lewis developed an integro-differential equation describing the particle transport due to elastic scattering [4]. The equation can be transformed to the pure differential form for the small angle or Gaussian (taking in to account terms up to θ^2, where θ is the scattering angle) approximation:

$$\frac{\partial f}{\partial t} = \frac{1}{W^2}\left(\frac{\partial^2 f}{\partial \theta_x^2} + \frac{\partial^2 f}{\partial \theta_y^2}\right) - \theta_x \frac{\partial f}{\partial x} - \theta_y \frac{\partial f}{\partial y} + \frac{\theta_x^2}{2}\frac{\partial f}{\partial \Delta_x} + \frac{\theta_y^2}{2}\frac{\partial f}{\partial \Delta_y},$$

where $f(t; x, \theta_x, \Delta_x; x, \theta_y, \Delta_y)$ is the probability distribution function, t is the true path length (free variable), x, y and z are the particle coordinates. θ_x and θ_y are the projections of the scattering angle on x and y axes, respectively. It is assumed that at the start (Geant4 pre-step) point the particle is moving along z axis. Then $\Delta = \Delta_x + \Delta_y = t - z \geq 0$ is the difference between t and z. It is convenient to factorize the distribution function:

$$f(t; x, \theta_x, \Delta_x; y, \theta_y, \Delta_y) = F(t; x, \theta_x, \Delta_x) \cdot F(t; y, \theta_y, \Delta_y).$$

Then the equation for $F(t; x, \theta_x, \Delta_x)$ (the same for y) reads:

$$\frac{\partial F}{\partial t} = \frac{1}{W^2}\frac{\partial^2 F}{\partial \theta_x^2} - \theta_x \frac{\partial F}{\partial x} + \frac{\theta_x^2}{2}\frac{\partial F}{\partial \Delta_x},$$

which is similar to the Yang equation [5] expressed in terms of the true path length t rather than z ($z \to t$ and $\Delta_x \to -\Delta_x$). This equation provides us the description of typical Monte-Carlo process: for given t find the distributions of the particle final (GEANT4 post-step) point (x, y, z) and the direction (θ_x, θ_y).

The parameter W depends on the mean square scattering angle per unit path length. It reads for the Moliere-Wentzel scattering model [3]:

$$\frac{1}{W^2} = \frac{1}{4}\frac{d\langle\theta_s^2\rangle}{dt} \simeq \pi N \left(\frac{Z_1 Z_2 e^2}{pc\beta}\right)^2 \left[\ln\frac{\mu_s + A_m}{A_m} - \frac{\mu_s}{\mu_s + A_m}\right]$$

where N is the number of atoms per unit volume, and:

$$\mu_s = \frac{1 - \cos\chi_s}{2} \simeq \frac{\chi_s^2}{4} \ll 1,$$

is proportional to the maximum scattering angle squared χ_s^2 limiting the multiple scattering consideration.

The parameter A_m reflects the Coulomb atomic shell screening and can be estimated as:

$$A_m = \frac{1.13 + 3.76n^2}{(1.77ka_oZ^{-1/3})^2}, \quad n = \frac{\alpha Z_1 Z_2}{\beta},$$

where a_o is the Bohr radius, and Z is the atomic number.

This relation corresponds to the Moliere-Wentzel elastic scattering model described by the PENELOPE team [3]:

$$\frac{d\sigma_{el}^{mw}}{d\Omega} = \frac{n^2}{4k^2}\left[\sin^2(\frac{\theta}{2}) + A_m\right]^{-2}, \quad V(r) = \frac{e^2 Z_1 Z_2}{r^2}\exp(-r/R), \quad A_m = (2kR)^{-2}.$$

The Moliere-Wentzel cross-sections read:

$$\sigma_{el}^{mw} = \frac{n^2}{k^2}\frac{\pi}{A_m(1+A_m)}, \quad \sigma_{el}^{mw}(\theta_1, \theta_2) = 2\pi\frac{n^2}{k^2}\frac{\cos\theta_1 - \cos\theta_2}{(1-\cos\theta_1 + 2A_m)(1-\cos\theta_2+2A_m)}.$$

4 Monte-Carlo algorithm

We start with the distribution of $\Delta \geq 0$ which is expressed in the dimensionless variable v, $v_x = 2W^2\Delta_x/t^2$. According to the Yang theory the variable v is distributed as the Yang $B-$function. The latter can be approximated by the $\Gamma-$function:

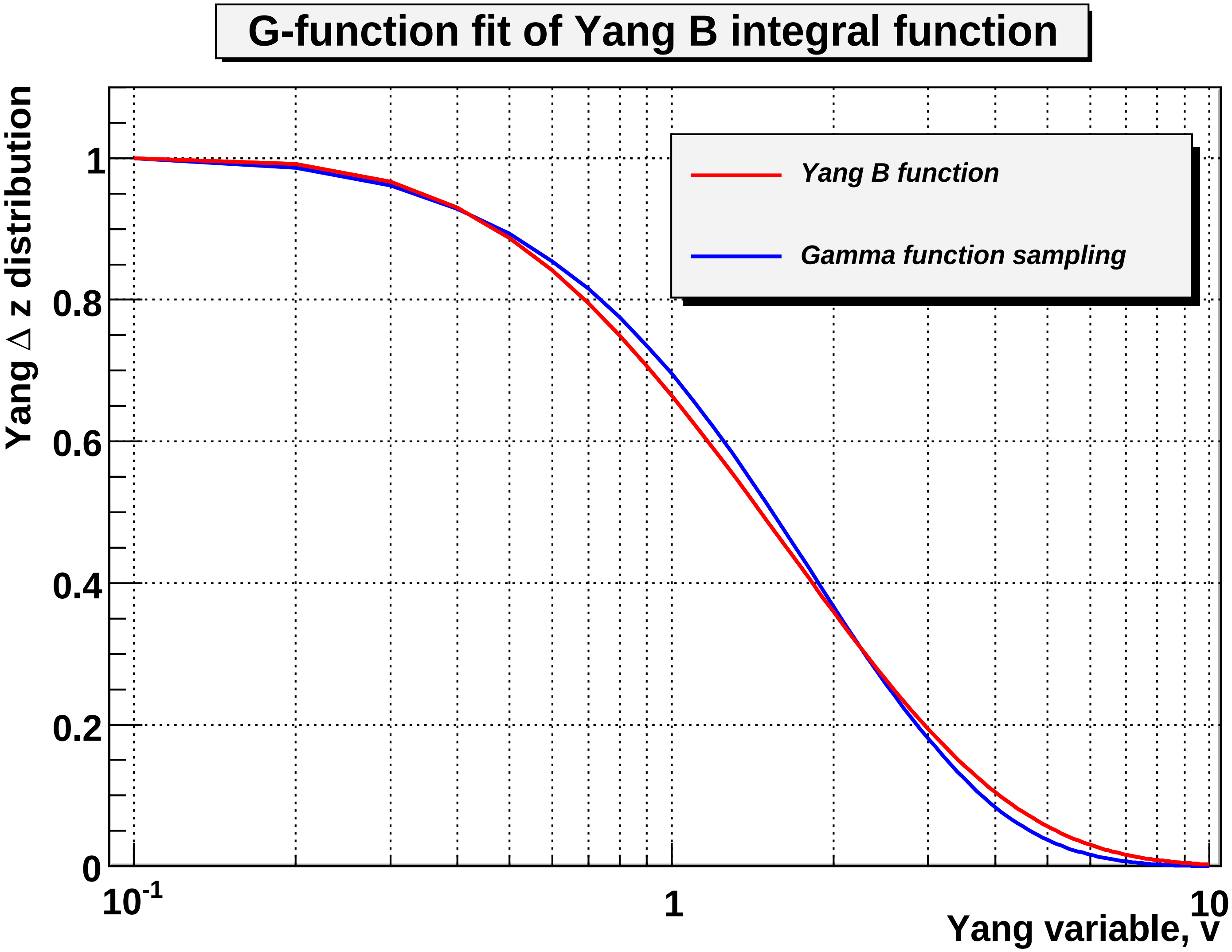
$$p(v) = \left(\frac{a}{\bar{v}}\right)^a \frac{v^{a-1}}{\Gamma(a)} \exp\left\{-a\frac{v}{\bar{v}}\right\},$$

where Γ is the Euler gamma function, $a \sim 16/\pi^2$ and $\bar{v} \sim 1.8$.

Other variables can be approximately sampled according to the Fermi distribution [6] for the thickness $\bar{z} = t - \bar{\Delta}$, ($\bar{\Delta} = \bar{v}t^2/W^2$):

$$F(\bar{z}; x, \theta_x) = \frac{W^2\sqrt{3}}{2\pi\bar{z}^2} \exp\left\{-W^2\left(\frac{\theta_x^2}{\bar{z}} - \frac{3x\theta_x}{\bar{z}^2} + \frac{3x^2}{\bar{z}^3}\right)\right\}.$$

Transverse displacement $\mathbf{r}_\perp(x, y)$ is the subject of general GEANT4 treatment for the possible interface crossing. Hard collisions with scattering angles $\chi > \chi_s$ are sampled according to the Moliere-Wentzel model with nuclear form-factor.


G-function fit of Yang B integral function
Yang B function
Gamma function sampling
Yang Δ z distribution
Yang variable, v
0
0.2
0.4
0.6
0.8
1
10^{-1}
1
10

5 Critical angle

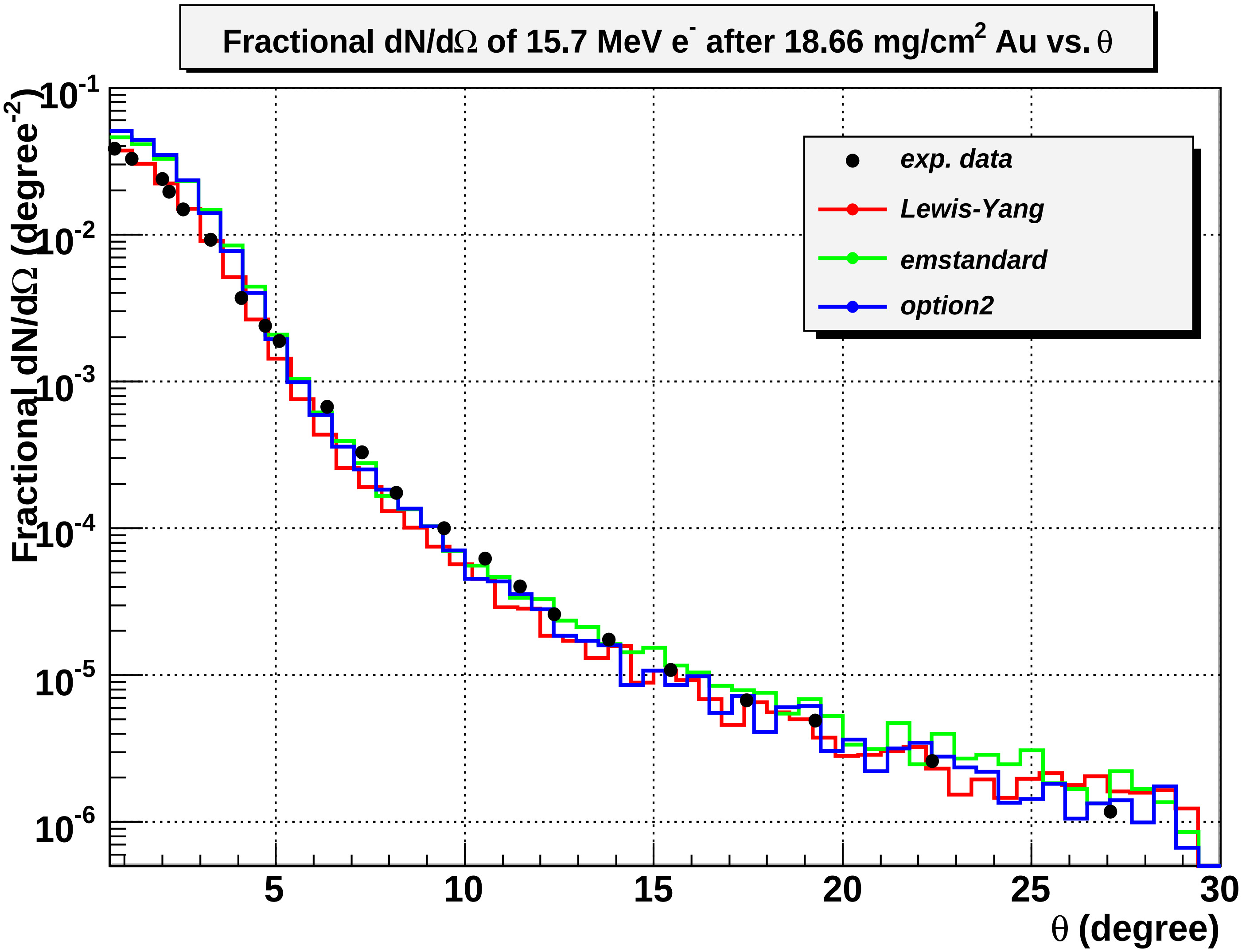
In the first implementation $\chi_s = 0.2$. Starting from geant4-09-02-ref-10, the value of angle between multiple and single modes of elastic scattering is defined based on the momentum transfered during the elastic collision:

$$\mu_s = \frac{1 - \cos\chi_s}{2} = A^{-2/3}\left(\frac{a\hbar c}{pcr_o}\right)^2 \leq 0.1,$$

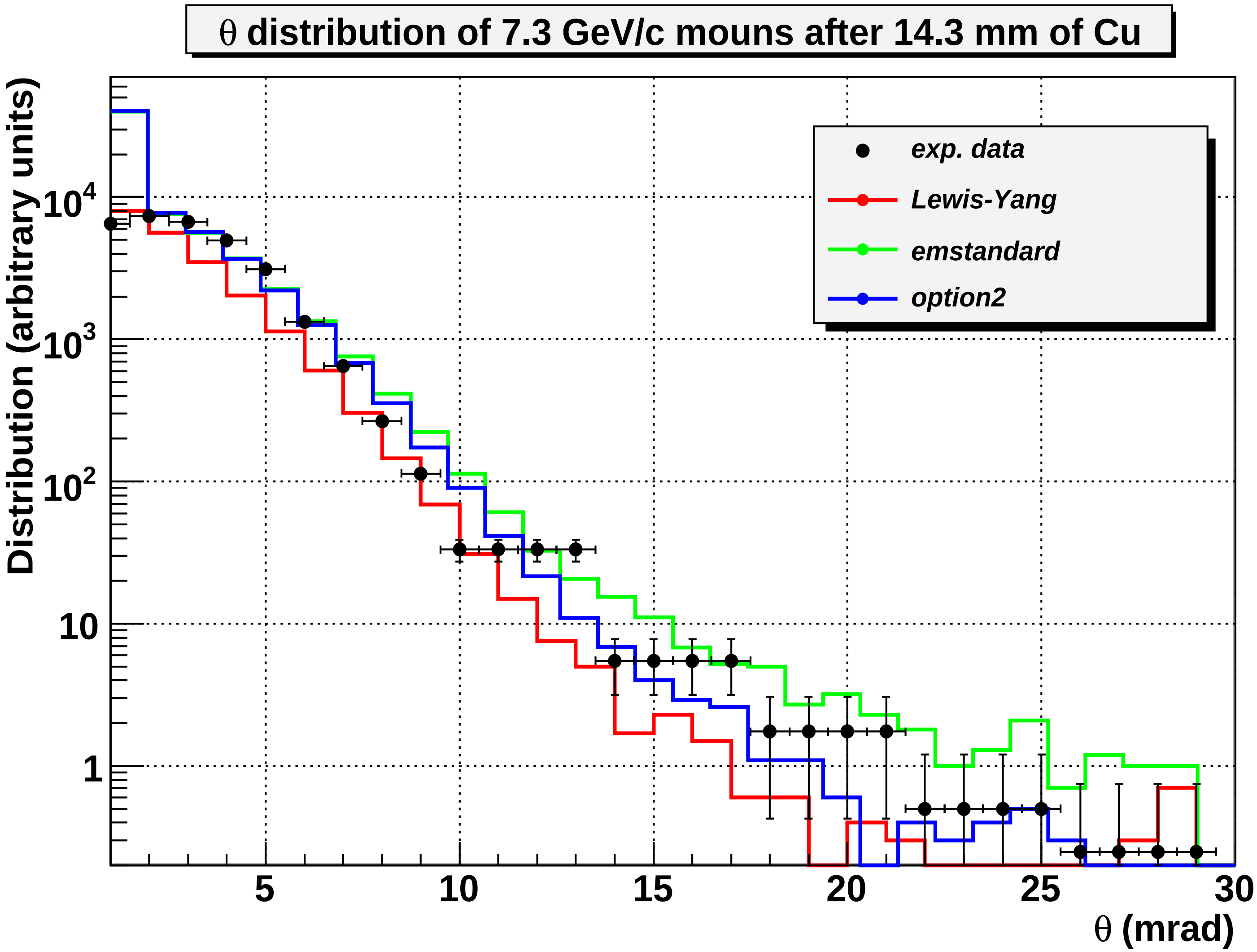
where A is the atomic weight, $r_o \sim 1$ fm, and $a \leq 0.5$ is the parameter, which can be modified by a user.

6 Comparison with experiments

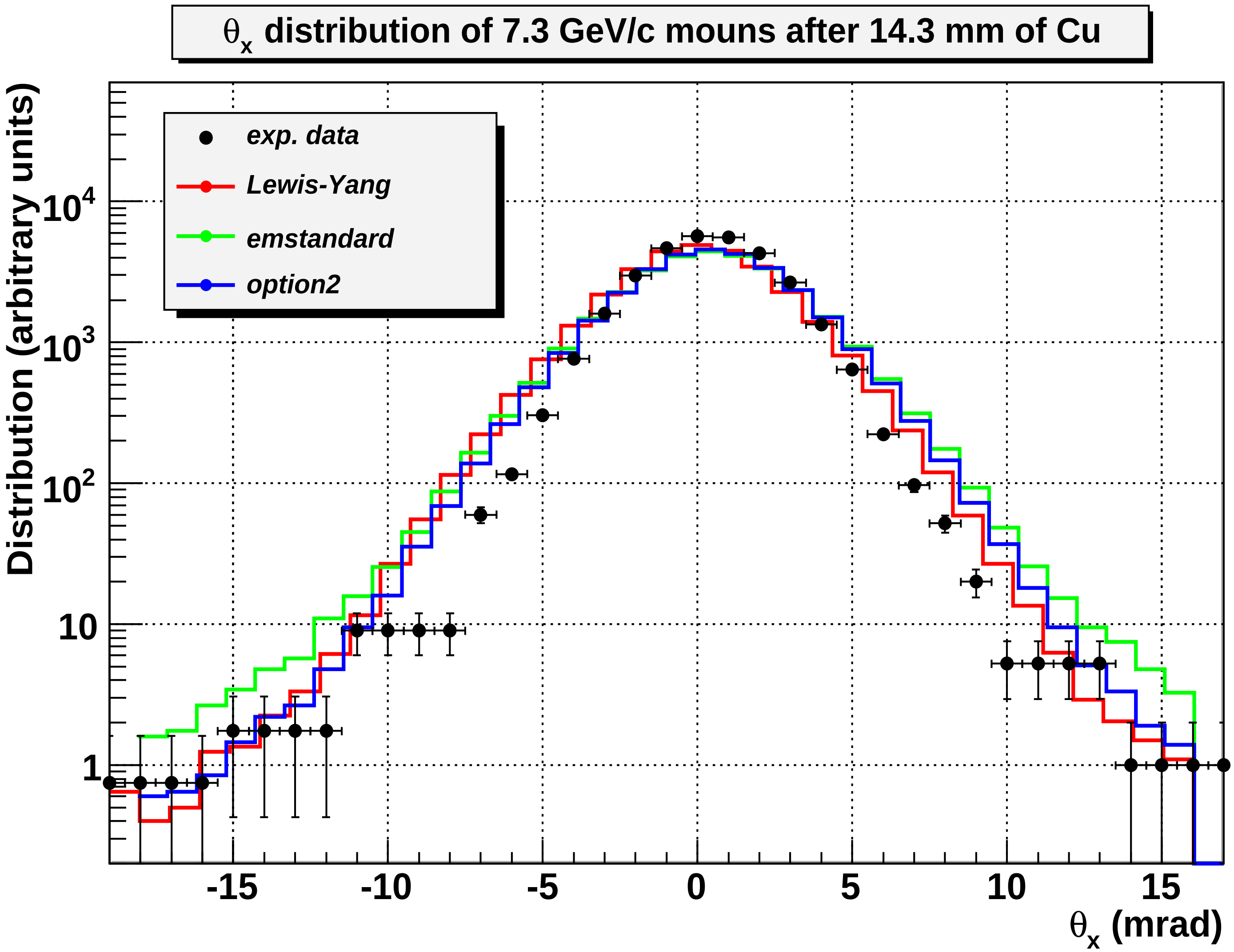
Lewis-Yang model was compared with experiments for electrons, muons and protons as well with other GEANT4 models, option 2 [2] and em-standard [1].



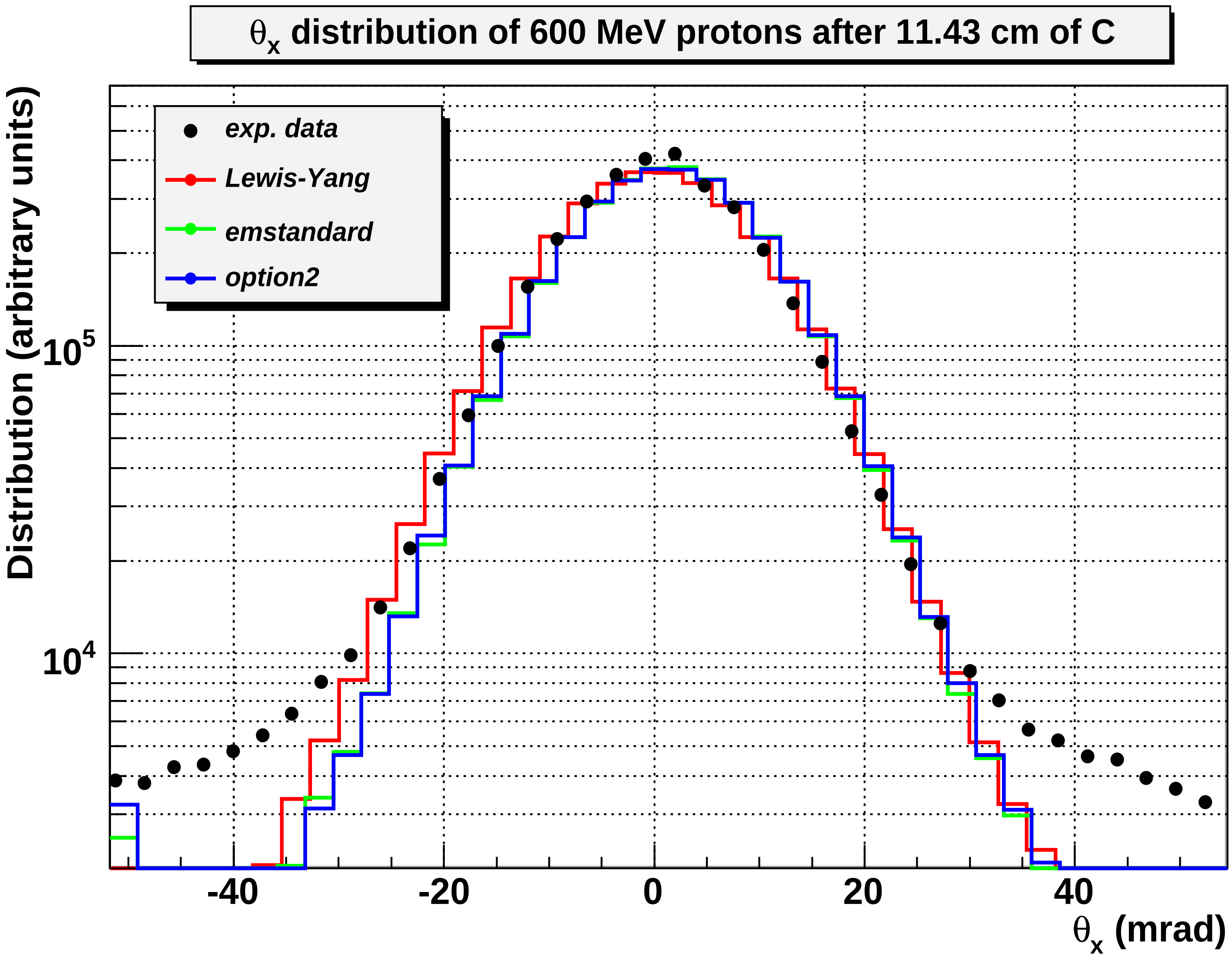
Experimental data from [7].



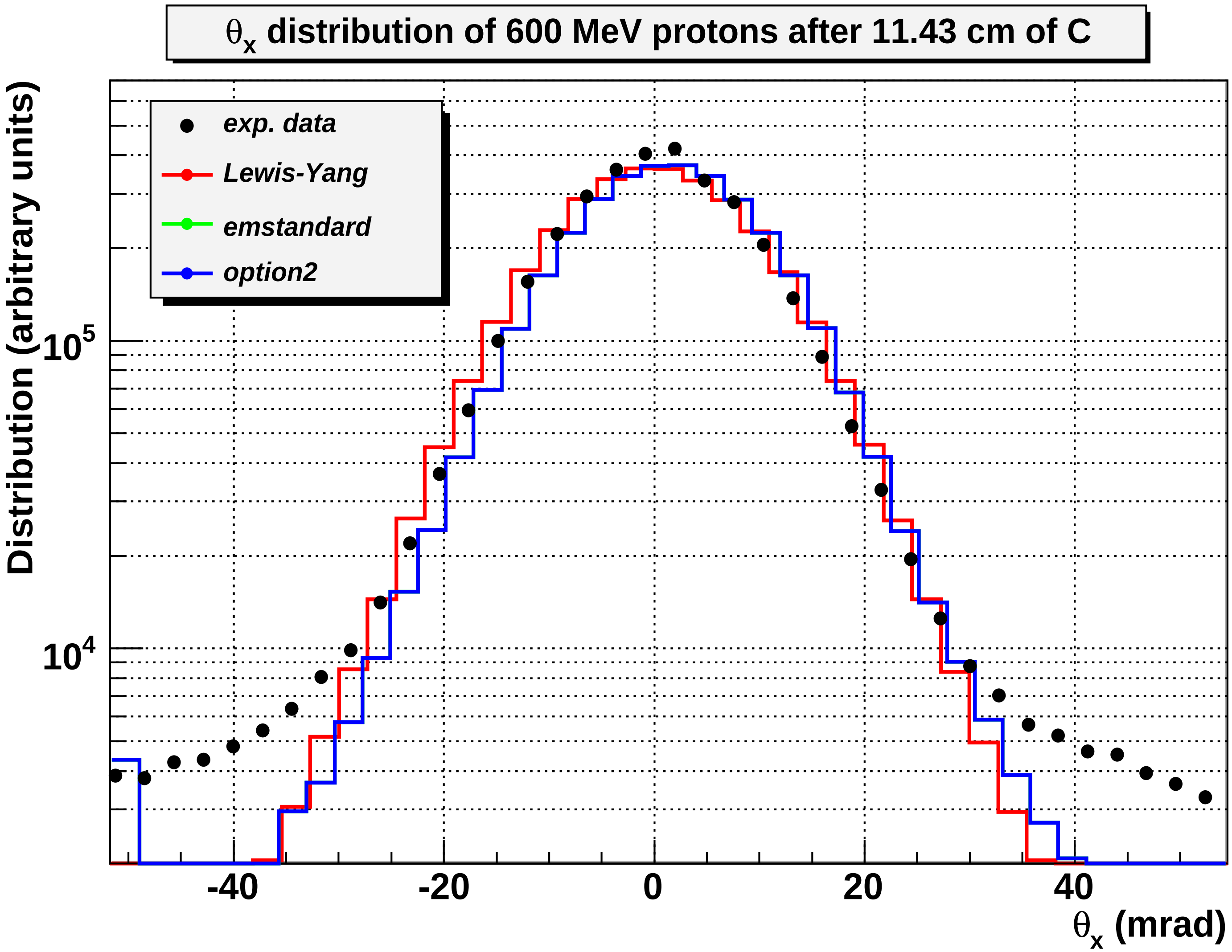
Experimental data from [8].



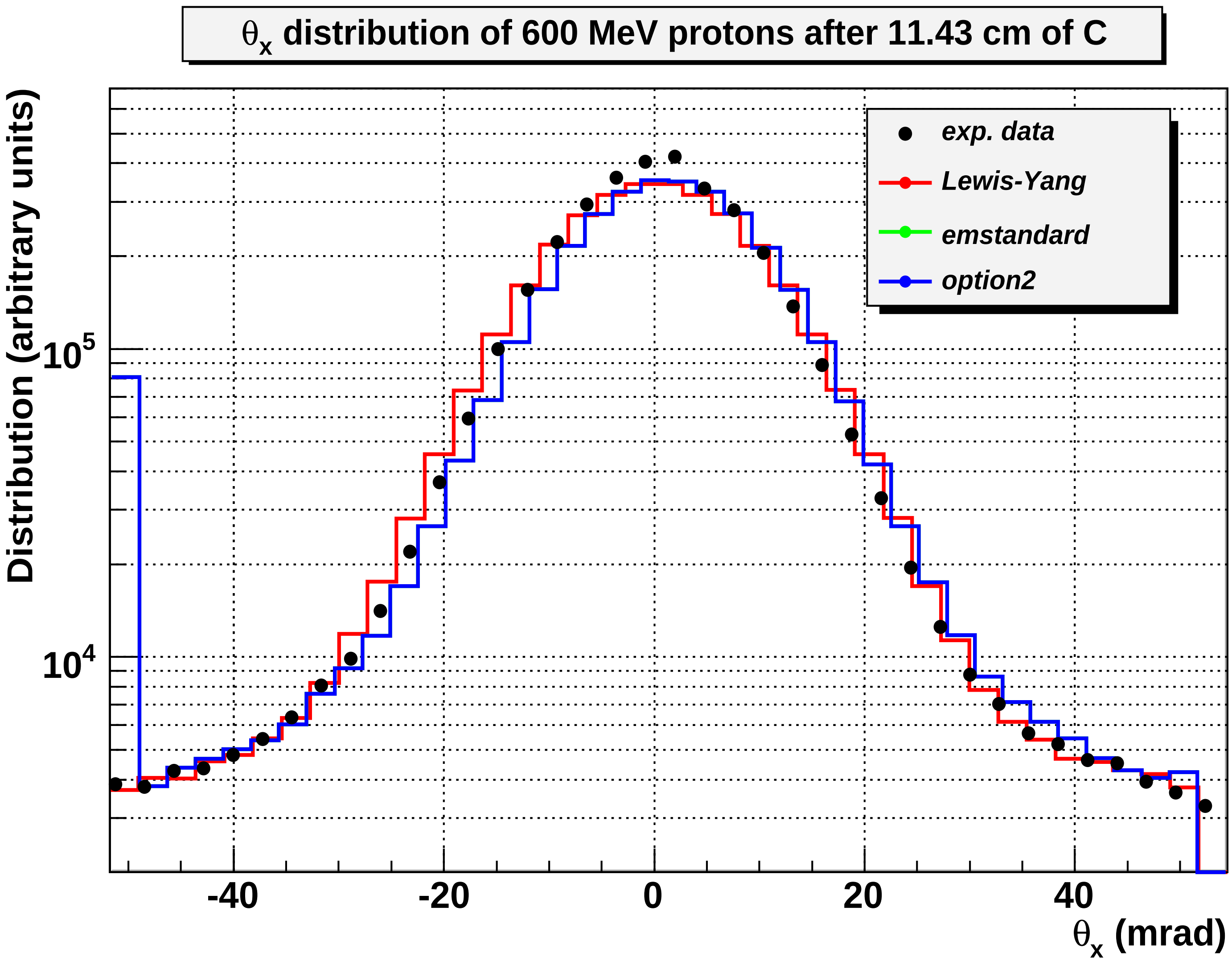
Experimental data from [8].



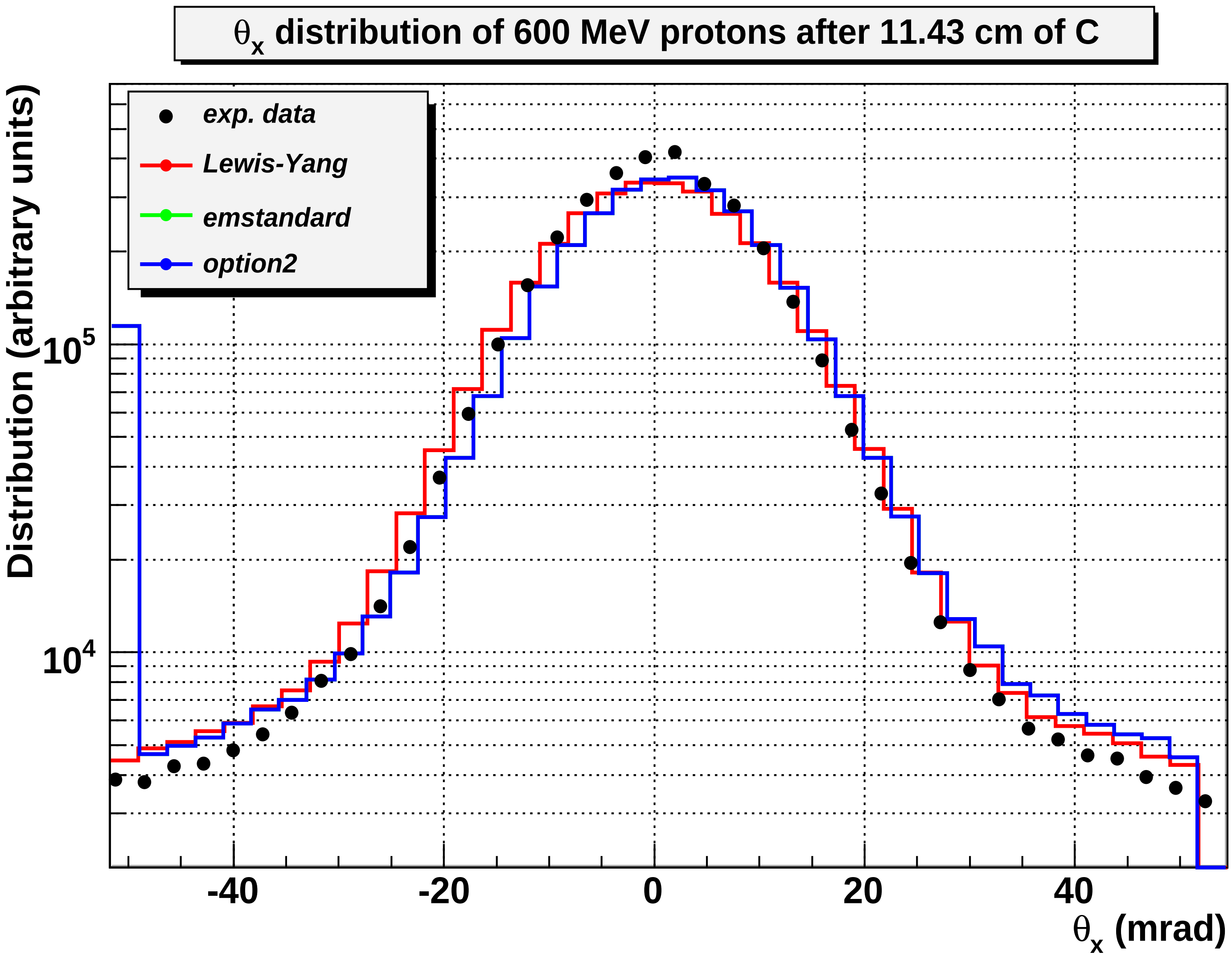
Data [9]. Default $\chi_s = 0.2$ was used. Is it too much? Is carbon too light for Tomas-Fermi screening?



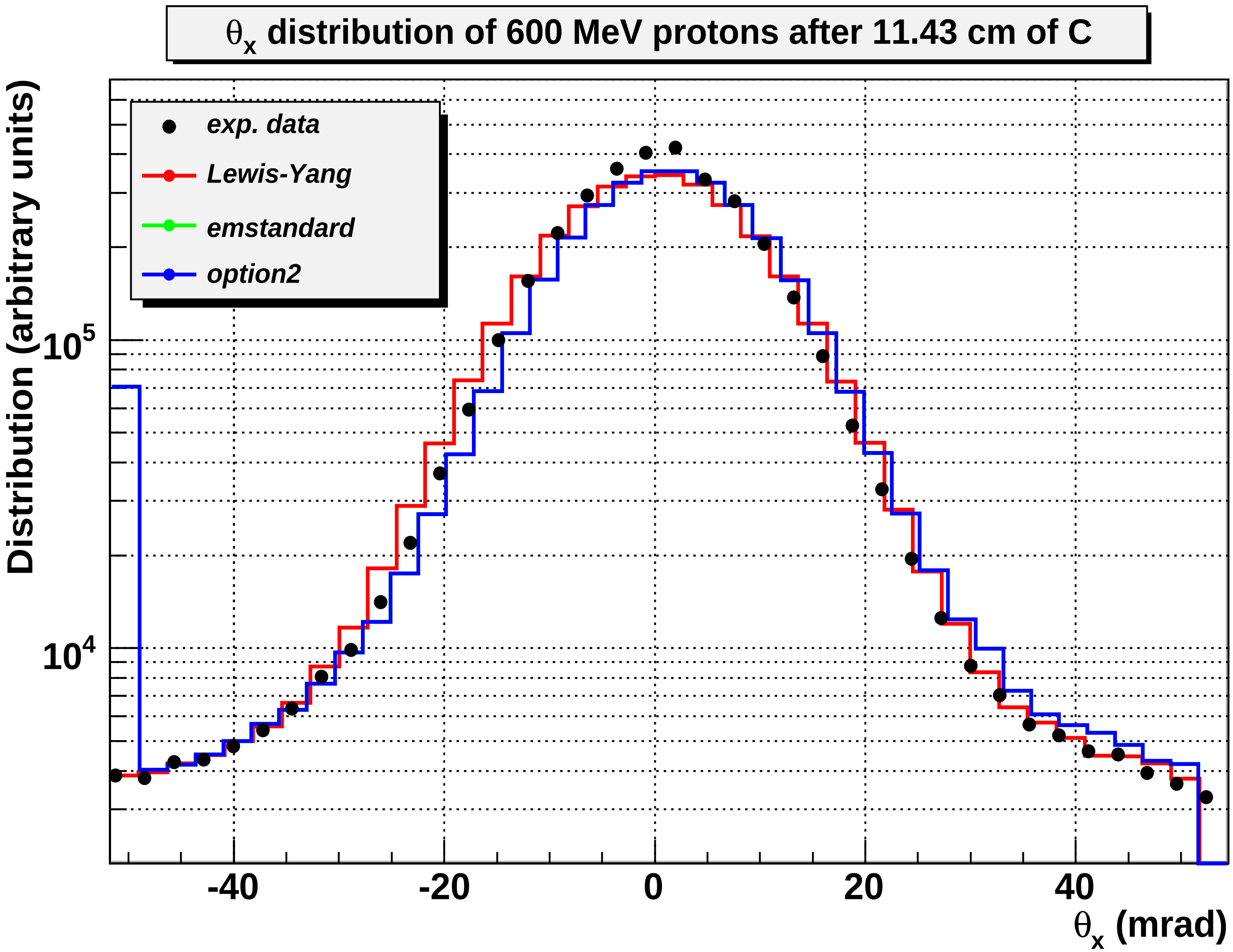
$\chi_s = 0.01$ for the Lewis-Yang model was used. Option2 $\equiv$ emstandard (for ref10)?



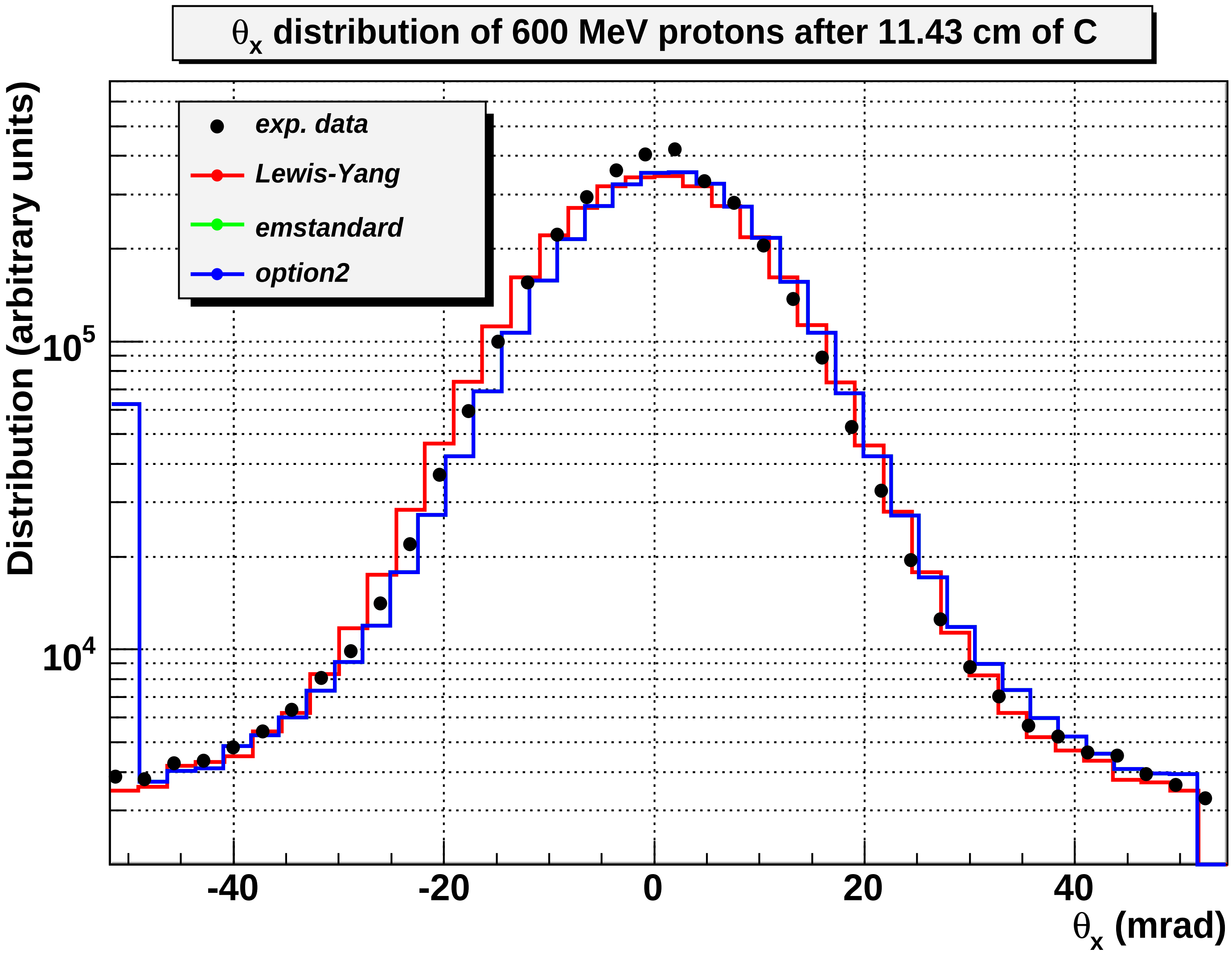
However, just activation of hadronic builder with diffuse elastic hadron scattering restores the tails.



The same but with G4HadronElasticPhysics builder



The same but with G4HadronHElasticPhysics builder



The same but with G4HadronQElasticPhysics builder

7 Performance

The first version of the Lewis-Yang model is a bit slower that emstandard ($\sim$30 %) or ($\sim$3-5 %) opt2 for muons, but faster than opt2 for protons in heaver materials. This implementation issue is under study.

8 Design

From tracking point of view the multiple scattering looks like the propagation in (random Coulomb) field combined with either electro-magnetic or hadron single scattering. Can the multiple scattering base classes be implemented in process management (future design review)?

9 Conclusions and ToDo

1. The Lewis theory of multiple scattering is considered in the Gauss approximation for small angles. The model is similar to the Fermi-Yang theory expressed in terms of true path length.
2. The model shows satisfactory agreement with experimental data and other Geant4 models even without parameter fitting. It can be applied for all heavy charged particles as well fast electrons. Tails are an issue?
3. The model testing and parameter tuning together with performance optimization are current activities

References

[1] L. Urban, CERN-OPEN-2006-077, 18p.

[2] V.N. Ivantchenko, O. Kadri, M. Maire, and L. Urban, accepted for publication in J. of Physics (2009).

[3] J.M. Fernandez-Varea et al., Nucl. Instr. and Meth., **B73** (1993) 447.

[4] H.W. Lewis, Phys. Rev., **78** (1950) 526.

[5] C.N. Yang, Phys. Rev., **84** (1951) 599.

[6] B. Rossi and K. Greisen, Rev. Mod. Phys., **13** (1941) 240.

[7] A.O. Hanson et al., Phys. Rev., **84** (1951) 634.

[8] S.A. Akimenko et al., Nucl. Instr. and Meth., **A243** (1986) 518.

[9] E.V. Hungerford et al., Nuclear Phys., **A197** (1972) 515.