

Simulation of Multiple and Single Scattering in GEANT4

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- Geant4 history and status
- Configuration of EM physics
- Multiple and single scattering
 - List of Geant4 models and options
 - Specifics in models for electrons, muons, hadrons
 - Recent validation results
 - Recent TOTEM data
- Summary



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CERN AC - HE267 - 04-07-199

Geant4 History

Layout of the LEP tunnel including future LHC infrastructures.

- Dec 1994 Project start ٠
- Dec 1998 First Geant4 public release version 1.0 •
- ...
- Dec 2010 Geant4 version 9.4 RUN 1 LHC •
- ٠ . . .
- Dec 2012 Geant4 version 9.6 consolidation of 9.X •
- Dec 2013 Geant4 version 10.0 multi-threading ٠
-
- Dec 2017 Geant4 10.4 •
- Geant4 developments were strongly supported by HEP community •
 - LHC experiments always were the goal •
 - Space and medical user communities also contribute significantly to Geant4 developments
- Geant4 approach to collect alternative models and approaches applicable for different use cases •



Geant4 general references

- Recent Developments in Geant4. J. Allison et al., by the Geant4 Collaboration., <u>Nucl. Instrum. Meth. A 835, 186-225, 2016.</u>
- Recent Improvements in Geant4 Electromagnetic Physics Models and Interfaces. V. Ivanchenko et al., Progress in NUCLEAR SCIENCE and TECHNOLOGY, Vol. 2, pp.898-903, 2011.
- Geometry and physics of the Geant4 toolkit for high and medium energy applications. J. Apostolakis et al., Radiation Physics and Chemistry 78: 859-873, 2009.
- Geant4 developments and applications. J. Allison et al., IEEE Trans. Nucl. Sci. 53 (1): 270-278, 2006.
- Geant4: A Simulation toolkit. By GEANT4 (S. Agostinelli et al.), Nucl. Instrum. Meth. A506 (3): 250-303, 2003.
 - ~10000 citations

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Consolidation of Physics with Geant4 9.6

- Standard EM development was concentrated on HEP
 - Important physics sub-package for LHC experiments
- For many years EM low-energy sub-package was developed separately
 - Focused on medical and space science requirements
- For Geant4 9.6 unification of EM processes and models was completed
 - Low and High energy models can work inside the same run
 - Angular generators for sampling of final states interchangible
 - Atomic de-excitation module is common
- Full set of hadronic models covering interactions
 - p, n, π , K⁺, K⁻, K⁰_L, K⁰_S, Λ , Σ^+ , Σ^- , Ξ^- , Ξ^0 , Ω^- , γ , e-, d, t, He3, He4, ions and their anti-particles
 - Energy up to 100 TeV
 - Stopping of negatively charged particles
 - Elastic scattering
 - Low-energy neutron transport based on recent ENDF data

Memory usage in multithreaded mode – Geant4 10.X seria



First of all, we are making it faster!



ATLAS : "The 10% CPU improvement we gain from the move from G4 9.6 to 10.1 is invaluable to the collaboration."

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General trend in Geant4 physics developments

- Geant4 9.6 complete set of physics models
- Geant4 10.4 and beyond
 - More attention to physics than to technical aspects of the code
 - migration to the MT mode is done
 - Geant4 code is C++11 compatible
 - More attention to next to leading order effects in EM physics
 - Requirements from dark matter search experiments
 - Rare processes are responsible for background
 - FCC project preparation
 - Hadronic physics developments
 - Extended set of low-energy data for gamma, protons and light ions
 - Several projects to improve ion-ion interaction models

Recent EM physics developments

- Implementation of LPM suppression in e<u>+</u> bremsstrahlung and in gamma conversion process is revised
 - Better agreement with CERN and SLAC experimental data
- Upper energy limit of EM physics is extended from 10 TeV to 100 TeV.
 - Essential for FCC R&D
- Goudsmit-Saunderson multiple-scattering model is fully revised.
 - Angular distribution is improved, as well as computing performance
 - Details will be discussed below
- New direct e+e- pair production process by electrons and positrons
- Added optional variants of EM form factor parameterization



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CONFIGURATION OF EM PHYSICS



Reference Physics Lists and EM constructors

- Geant4 provide set of reference Physics Lists
 - Geant4 main recommendation is to use reference physics lists
 - These physics configuration are validated by Geant4 team
 - Allowed cross experiments validations
 - Current default is FTFP_BERT
- In practice, to get optimal CPU/accuray balance EM and hadronic physics requires extra configuration on top
 - ATLAS uses FTFP_BERT_ATL
 - Specific transition between cascade and string hadronic model
 - CMS uses FTFP_BERT_EMM
 - Custom configuration of EM physics in different calorimeters
 - LHCb uses custom configuration similar to FTFP_BERT_EMY
 - Simplified simulation of the calorimeter
- It is natural to optimase Geant4 model configuration per experiment

EM Physics builders for HEP

- Urban multipe scattering for e⁺⁻ below 100 MeV only
 - WentzelVI + Single scattering above 100 MeV
- WentzelVI + single scattering for muons and hadrons
- Urban multiple scattering model for ions

Constructor	Components	Comments	
G4EmStandardPhysics	Default (QGSP_BERT, FTFP_BERT)	ATLAS, and other HEP productions, other applications	
G4EmStandardPhysics_option1	Fast due to simple step limitation, cuts used by photon processes (FTFP_BERT_EMV)	Similar to one used by CMS, good for crystals, not good for sampling calorimeters	
G4EmStandardPhysics_option2	Fast due to simple step limitation, updated photon models and bremsstrahlung angular generator	Similar to one used by LHCb	

EM Physics for Accurate Simulations

- Focus on accuracy instead of maximum simulation speed
- Ion stopping model based on the ICRU'73 data
 - Step limitation for multiple scattering using UseDistanceToBoundary option
- Strong step limitation by the ionisation process defined per particle type
- Recommended for hadron/ion therapy, space applications

Constructor	Components	Comments
G4EmStandardPhysics_option3	Urban MSC model for all particles	Proton/ion therapy
G4EmStandardPhysics_option4	The best combination of models per particle type and energy range, Goudsmit-Saunderson multiple scattering model for e+- below 100 MeV with error free stepping approach	Goal to have the most accurate EM physics
G4EmLivermorePhysics	Livermore models for γ , e ⁻ below 1 GeV, Standard models above 1 GeV	Livermore low- energy electron and gamma transport
G4EmPenelopePhysics	Penelope models for γ,e^{\pm} below 1 GeV, Standard models above 1 GeV	Penelope low- energy e [±] and gamma transport

Special EM Physics List Constructors

Constructor	Components	Comments
G4EmStandardPhysicsGS	Goudsmit-Saunderson multiple scattering model for e+- below 100 MeV	May be considered as an alternative to standard Opt0
G4EmStandardPhysicsWVI	WVI + SS combination	Is good for high energy interactions
G4EmStandardPhysicsSS	Single elastic scattering for all charged particles	Mainly for validation and verification
G4EmLowEPPhysics	Monarsh University Compton scattering model, WVI-LE model, potentially GS model	Used new low- energy models
G4EmLivermorePolarized	Polarized gamma models	An extention of Livermore physics

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Electromagnetic parameters



- First of all, one of EM constructors should be chosen
 - Optimization accuracy versus CPU speed
- Cut in range should be optimized
 - It is possible to define G4Regions groups of logical volumes corresponding to a sub-detector
 - Cut in range may be defined per G4Region
 - Recommendation to have cut to be less than thickness of a sensitive layer inside G4Region
- Additional step limitation may be added on top of any physics list
 - In gaseous detectors it is recommended to have 2 steps within a cell
- With Geant4 10.2 a new class G4EmParameters class was introduced
 - In 10.4 this is the main method for fine tuning of EM parameters
 - There is a new dump method
 - Each parameter may be changed via c++ interface and via UI command
 - Parameters may be changed only at initialization and only from the master thread

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EM physics configuration

- Until Geant4 10.2 we had a limitation Geant4 EM physics should be customized by a user for any special needs:
 - Different models for G4Region
 - Different model options for G4Region
 - Standard/DNA models
- This customization can be done properly only by an expert user and make problems even for top experts
- For 10.2 we provide new UI commands:
 - /process/em/AddPAIRegion all myregion PAI
 - /process/em/AddMicroElecRegion myregion
 - /process/em/AddDNARegion myregion DNA_Opt0
- Since 10.3 we provide new UI command:
 - /process/em/AddEmRegion myregion PhysListName
- It is possible to configure single scattering model per G4Region



GEANT4 MULTIPLE AND SINGLE SCATTERING MODELS



MSC and Single Scattering Models

Model	Particle type	Energy limit	Specifics and applicability
G4UrbanMscModel (L. Urban 2006)	Any	-	Default model for electrons and positrons below 100 MeV, (Lewis 1950) approach, tuned to data, <u>used for LHC</u> <u>production</u> .
G4ScreenedNuclearRecoil (M.H.Mendenhall and R.AWeller 2005) TestEm5	p, ions	< 100 MeV/A	Theory based process, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space applications
G4GoudsmitSaundersonMscModel (O. Kadri 2009, fully revised by M.Novak for Geant4 10.2 and 10.4)	e ⁺ , e ⁻	< 1 GeV	Theory based cross sections (Goudsmit and Saunderson 1950). EPSEPA code developed by Penelope group, final state using EGSnrc method (Kawrakov et al. 1998), precise electron transport
G4eCoulombScatteringModel G4hCoulombScatteringModel (V. Ivanchenko 2008)	Any	-	Theory based (Wentzel 1927) single scattering model, uses nuclear form-factors (Butkevich et al. 2002), focused on muons and hadrons (full Mott correction is not added yet)
G4WentzelVIMscModel (2009) G4LowEnergyWentzelVI (2014) (V. Ivanchenko)	Any	-	MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons; low-energy model is applicable for low-energy e-
G4IonCoulombScatteringModel (2010) G4eSingleCoulombScatteringModel (2016) P. G. Rancoita, C. Consolandi and M.Tacconi.	lons e⁺, e⁻	-	Model based on Wentzel formula + relativistic effects + screening effects for projectile & target + Mott corrections implemented

Geant4 default: combination of G4WentzelVIModel + G4eCoulombScatteringModel for e+- (E > 100 MeV), muons, hadrons; G4UrbanMscModel for e+- (E < 100 MeV), ions

Electron/positron multiple scattering models



- Multiple scattering model should be able to sample deflection angle, displacement of the end point and true step length for any step of a charged particle and for any primary energy
 - And correlations between these values
- Calorimeter results directly depend on choice of multiple scattering parameters for electrons
 - Energy deposition of low-energy electron component of EM and hadronic showers is substantial
- The Urban model was initially proposed as a universal solution
 - It was starting from Lewis theory but includes many phenomenological formulas and many parameters tuned to the available data
 - Including Highland formula
 - Now we know that the model has limitations and is valid not in all circumstances
 - Several parameters were introduced allowing increasing of CPU speed or accuracy
- Until now, the Urban model for low-energy electron transport is the optimal choice for large HEP experiments simulation
 - However, limitations of the Urban model approach are well known and alternatives were developed.



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Goudsmit-Saunderson multiple scattering model

- Was proposed as an alternative model fully based on theory
 - O. Kadri et al., NIM B 267 (2009) 3624
 - It turned out, that the 1st implementation was not competitive versus the Urban model
- M.Novak did a review and practically rewrite the code
 - A.Bagulya et al. J. Phys: Conf. Ser. 898: 042032, 2017
 - Still the Urban model was competitive
- For Geant4 10.4 M.Noval added Mott corrections and "error free stepping" algorithm to the model
 - CHEF 2017 Conference, Lyon, France, accepted by JINST
 - Now it is the variant of e+- multiple scattering in Opt4 EM physics

Geant4 Goudsmit-Saunderson model is the

Kawrakow-Bielajew model for elastic scattering

[I.Kawrakow, A.F.Bielajew, NIMB 134(1998)325-336]

- based on Goudsmit-Saunderson theory of multiple elastic scattering [S.Goudsmit, J.L.Saunderson, PR 57(1940)24-29]
- hybrid model for (no, single) and multiple elastic scattering of e⁻/e⁺
 [A.F.Bielajew, NIMB 111(1996)195-208]
- the screened Rutherford DCS is used for elastic scattering

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M. Novak evaluation

Goudsmit-Saunderson angular distribution after travelling a path s:

$$F(s;\theta)_{GS} = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \exp(-s/\lambda_{\ell}) P_{\ell}(\cos(\theta))$$

dσ/dΩ-elastic DCS; σ = ∫ dσ/dΩ dΩ-elastic cross section; λ⁻¹ = Nσ-elastic mean free path
f₁(θ) = 1/σ dσ/dΩ is single elastic scattering distribution (note that 2πf₁(θ) = 2π 1/σ dσ/dΩ = p(cos(θ)))
f₁(θ) is expressed in terms of orthogonal polynomials (Legendre series)
f₁(θ) = ∑_{ℓ=0}[∞] 2ℓ+1/4π F_ℓP_ℓ(cos(θ))
F_ℓ = 2π ∫¹_{-1} f₁(θ)P_ℓ(cos(θ))d(cos(θ)) = ⟨P_ℓ(cos(θ)))
G_ℓ are the ℓ-th transport coefficients G_ℓ ≡ 1 - F_ℓ = 1 - ⟨P_ℓ(cos(θ)))
λ_ℓ⁻¹ ≡ G_ℓ/λ = 1-⟨P_ℓ(cos(θ)))/λ
then F(s; θ) = ∑_{n=0}[∞] f_n(θ)W_n(s)
f_n(θ) the angular distribution after n elastic interactions f_n(θ) = ∑_{ℓ=0}[∞] 2ℓ+1/4π (F_ℓ)ⁿP_ℓ(cos(θ))
W_n(s) = exp(-s/λ) (s/λ)ⁿ/n! is the probability of having exactly n elastic interaction along a path s (i.e. Poisson)

[[]S.Goudsmit, J.L.Saunderson, PR 57(1940)24-29; J.M.Fernández-Varea, R.Mayol, J.Baró, F.Salvat NIMB 73(1993)447-473]

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M. Novak evaluation

Using a simple exponentially screened Coulomb potential as the scattering potential in the computation of the scattering amplitudes under the first Born approximation(Wentzel model):

- $\frac{d\sigma}{d\Omega} = |f|^2$ where $f \equiv f(\theta, \phi)$ is the scattering amplitude
- which $f_{B1}(\theta, \phi) = -\frac{2m}{4\pi\hbar^2} \int e^{i(\bar{k}_f \bar{k}_i)\bar{r}'} V(\bar{r}') d^3r'$ in the first Born approximation [where: \bar{k}_i , \bar{k}_f and $V(\bar{r}')$ are the wave vectors of the incident plane, the outgoing(scattered) spherical spherical wave and the scattering potential respectively. Note that: (i) in case of elastic scattering $k_i = k_f \equiv k$; (ii) $\hbar \bar{q} = \hbar(\bar{k}_f - \bar{k}_i)$ is the momentum transfer and $q^2 = |\bar{k}_f - \bar{k}_i|^2 = 2k^2(1 - \cos(\theta)) = 2k^2(2\sin^2(\theta/2))$ where $\theta \equiv \angle(\bar{k}_i, \bar{k}_f)$ is the scattering angle]
- assuming $V(\bar{r}) \equiv V(r)$ i.e. spherically symmetric scattering potential, substituting $\bar{q} = \bar{k}_f \bar{k}_i$ and choosing the coordinate system for the integration such that $\bar{q} = q\hat{\bar{z}}$ $f_{B1}(\theta) = -\frac{2m}{q\hbar^2} \int_0^\infty \sin(qr')r'V(r')dr'$

M. Novak evaluation

So DCS for elastic scattering within the Wentzel model is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{(W)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{1}{(1-\cos(\theta)+2A)^2}$$

$$\mathbf{Key angular distribution for all Geant4 scattering models}$$

$$\sigma^{(W)} = \left(\frac{ZZ'e^2}{pc\beta}\right)^2 \frac{\pi}{A(1+A)}$$

$$\mathbf{f}_1^{(W)}(\theta) = \frac{1}{\pi} \frac{A(1+A)}{(1-\cos(\theta)+2A)^2}$$

$$\mathbf{G}_{\ell}^{(W)}(A) = 1 - F_{\ell} = 1 - \ell[Q_{\ell-1}(1+2A) - (1+2A)Q_{\ell}(1+2A)] [Q_{\ell}(x) \text{ are Legendre functions of the second kind]}$$

$$\mathbf{G}_{\ell=1}^{(W)}(A) = 2A \left[\ln\left(\frac{1+A}{A}\right)(A+1) - 1\right]$$

$$\mathbf{P} \text{ note that } \frac{1}{\lambda_1} = \frac{\mathbf{G}_{\ell=1}^{(W)}(A)}{\lambda} \text{ gives the possibility set the screening parameter } A \text{ such that the corresponding DCS } \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{(W)} \text{ will give back } \lambda_1 \text{ [therefore e.g. } \langle \cos(\theta) \rangle = \exp(-s/\lambda_1) \text{ will be correct]}$$

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Energy deposition in semi-infinite media SANDIA REPORT SAND79-0414.UC-34a





- Recent GS (Geant4 10.4) model describes now data for both lowdensity and high density data as WVI and SS models
 - This test directly couples with the problem of accurate simulation of electron transport in sampling calorimeters

Hanson data for electron scattering off Gold target (Phys. Rev. 84, 634-637, 1951)



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Backscattering validation results



- Simulation of electron backscattering from AI (left) and Au (right) targets versus data from different experiments.
- Opt4 EM configuration is with the Urban model (yellow) and the GS model with "error-free" stepping (blue)

P.G. Rancoita and M. Tacconi developments on electron single scattering model

Electron Cross Section $d\sigma(\theta)$ $(1-\cos\theta)^2$ $d\sigma(\theta)$ (q $(2A_s+1-\cos\theta)^2$ $d\Omega$ $d\Omega$ Ruth(c.m.) Mott+Scrr.+NFF Molier's Screening Rutherford in the center of mass: Nuclear Form Factor Coefficient: Ze^2 $d\sigma(\theta)$ High Z 1.13 + 3.76 $d\Omega$ computation 0.88534a Ratio of Mott cross section over Rutherford $d\sigma(\theta)$ Mott Cross Section fit: $R = \sum a_i (1 - \cos \theta)$ $d\Omega$ $R \equiv$ Mott $d\sigma(\theta)$ $d\Omega$ Ruth

References:

P.G. Rancoita C. Leroy, "Silicon solid state devices and radiation detection", Singapore, World Scientific, 2012. Sec. 1.3.1, 1.3.3

M.J. Boschini et al."Nuclear and Non-Ionizing Energy-Loss of Electrons with low and Relativistic Energies in Materials and Space Environment" Proc. Of the 13th ICATPP (13th ICATPP, Como 3-7/10/2011).

M.J. Boschini et al "An Expression for the Mott cross section of electrons and positrons on nuclei with Z up to 118" Radiat. Phys. Chem. (2013), http://dx.doi.org/10.1016/j.radphyschem.2013.04.020

Nuclear Form Factor

It takes into account the effect of the finite nuclear size of the target nucleus and depends on the **trasferred momentum q** and **atomic weight A** of the target nucleus



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P.G. Rancoita and M. Tacconi simulations

183 MeV Electrons

Experimental Data From B.Hahn et al. Phys. Rev. 101 (1956) 1131



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250-500 MeV Electrons in Si (z=14)

Experimental Data From G.C. Li and M.R. Yearian, Phys. Rev. C, Vol.9 N.5 (1974)



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 $E_{d} = 21 \, eV$

375-750 MeV Electrons in C (z=6)

Experimental Data From I. Sick and J.S. McCarthy, Nucl. Phys. A150 (1970) 631-654



 $E_{d} = 35 \, eV$

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Uniform charge form factor better describe Si and C data

Why we need WentzelVI and SS models?

- Currently, GS model of M.Novak and SS model of P.G.Rancoita are the best Geant4 models full theory based
 - Both models includes internal tables precomputed using ELSEPA code and uploaded at initialization of Geant4
 - Both models provide the same results if GS is used in single scattering mode
 - Both models have upper limits of applicability and can be applied only for e+-
- G4WentzelVIModel and G4eCoulombScatteringModel
 - V. N. Ivanchenko et el., J. Phys: Conf. Ser. 219 (2010) 032045
 - Applicable for any particle type
 - Based on Wentzel formula with options
 - to choose nuclear form factor type (Exponential is the default)
 - to tune screening parameter A
 - Dynamically select a boundary between single and multiple scattering
 - Legendre expansion is not needed because single scattering regime is used
 - Dynamically switch to single scattering mode for small steps
 - Excluded direct delta-electron production from scattering
 - Is Geant4 default for muons and hadrons
 - Applied for electrons and positrons above 100 MeV

L3 muon scattering benchmark



CERN Summer student project (M.Schenk) – implemented simplified L3 detector geometry and use Z->µµ events WentzelVI better agree with the data compared to the Urban model

MuScat benchmark Nucl. Instr. Meth. B 251 (2006) 41



Single scattering and WentzelVI models are closer to the data than the Urban model.

Thick target proton scattering benchmark (B. Gottschalk et al., NIM B 74 (1993) 467)



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Thick target proton scattering benchmark (B. Gottschalk et al., NIM B 74 (1993) 467)



For hadrons the interference between strong and electromagnetic amplitudes should be taken into account. There is an attempt to Implement this in G4DiffuseElasticModel (V.Grichine)



G4hCoulombScatteringModel K.Mashtakov (CERN summer student)



Relativistic single scattering model with scattering in center of mass of projectile and target

- In the default single scattering model sampling is in Lab system
- Update proposed by P.G.Rancoita

The model has been restored and validated

 In 10.4 is used in SS EM PhysList for muons, pions, kaons, protons, antiprotons as an experiment

Comparison with the default demonstarte that the difference is seen near central part of distribution

- This means that WVI model may be corrected for mass effects
 - not yet done



Ratio plot for the space angle





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MuScat benchmark Nucl. Instr. Meth. B 251 (2006) 41

Single scattering with mass corrections shows a slight degradation and WentzelVI models are closer to the data

New TOTEM Results on pp Cross Sections (CERN-EP-2017-321)

- Overview of elastic (σ^{el}), inelastic (σ^{inel}), total (σ^{tot}) cross section for pp and pp⁻ collisions
- The continuous black lines the best fits of the total cross section data
- The dashed line results from a fit of the elastic scattering data
- The dash-dotted lines refer to the inelastic cross section and are obtained as the difference between the continuous and dashed fits

New measurement of the interference of the strong and EM amplitudes in pp elastic scattering (CERN-EP-2017-335)

- Fit results provides $\rho = 0.09 \pm 0.01$ or $\rho = 0.10 \pm 0.01$ depending on a model
- Possible interpretation of such small value Odderon state contribution to elastic scattering

Summary

- Geant4 10.4 offers several improvements
 - New options for EM model configuration
 - New GS model for e+-, improved Opt4 EM physics
 - Several form factor parameterisations
 - Electron single scattering model
 - Mass corrections to single scattering of muons and hadron
- There are several problems to be understood and/or implemented
 - GS model to be configured in a way that keep accuracy but provide competitive speed versus the Urban model
 - Upper energy limits for GS and SS models
 - WentzelVI for e+- needs Mott corrections and tune of screening parameter
 - Some degradation of results for the MuScat benchmark to be understood
 - Strong/EM interference terms for hadrons to be evaluated
 - Second order EM processes under development

