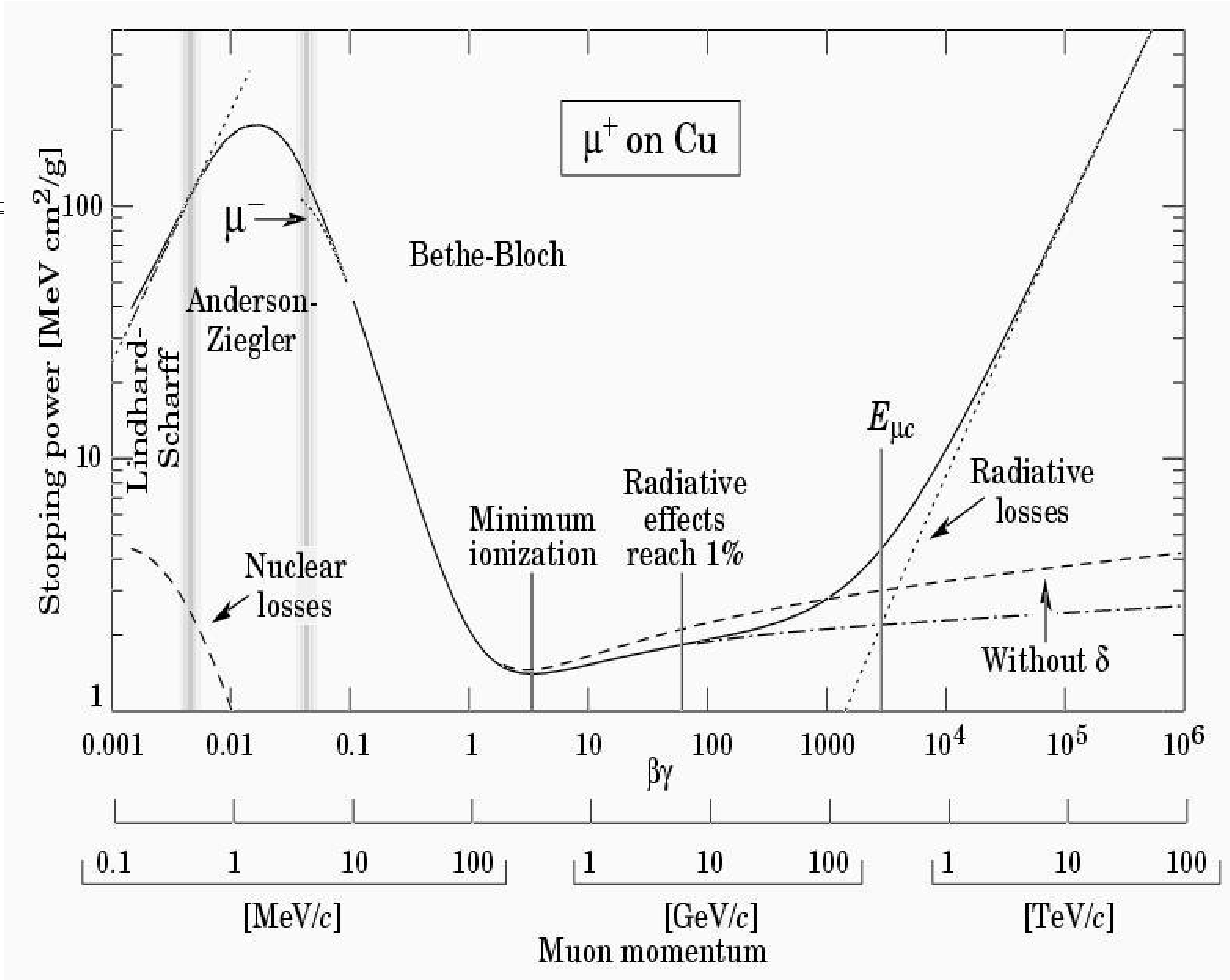
Physics of shower simulation at LHC, at the example of GEANT4.

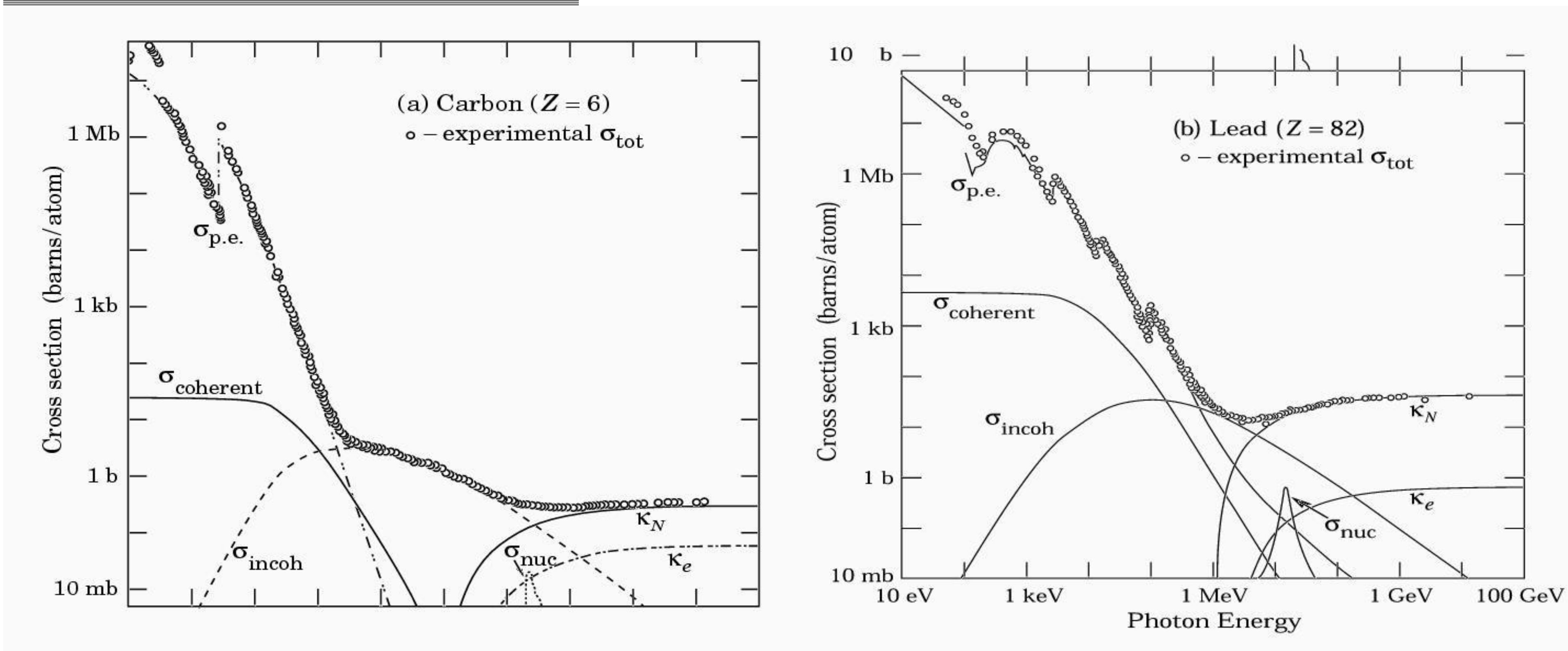
J.P. Wellisch
CERN/PH

The Monte Carlo Roadmap

- Part 1: Introduction
  - LHC related use cases - LCG.
  - Analyzing showers and their development in matter.
  - Brief overview of hadronic models in geant4
- Part 2: Hadronic showers in bulk matter.
  - Selected topics on hadronic shower simulation:
    - Theory driven modeling of inelastic reactions.
- Part 3: ghad – how good is it really?
- Part 4: Modeling electromagnetic showers.
  - Selected topics on electromagnetic shower physics.
- Part 5: Test-beam comparisons from the validation project



J.P. Wellisch,
CERN/PH



J.P. Wellisch,
CERN/PH

Modeling electromagnetic showers

- Physics processes involved:
  - Photo effect
  - Compton scattering
  - Pair production (*)
  - Ionization (*)
  - Annihilation
  - Bremsstrahlung (*)
  - Multiple coulomb scattering

- For more detail, please see the complete lecture notes by Michel Maire (LAPP) on the geant4 WWW site, or the geant4 physics reference manual.

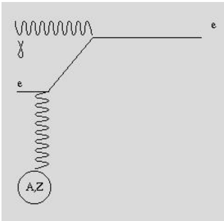


Photo effect

- An electron in the material is acquiring the energy of a gamma completely, while an atom in the medium is taking the momentum balance:

  - The electron acquires a kinetic energy that equals the gamma energy minus the binding energy of the electron in the atom.

Photo effect

- The cross-section for each shell can be parametrized as (F.Briggs, R.Lighthill, Sandia Laboratory, SAND-87-0070)

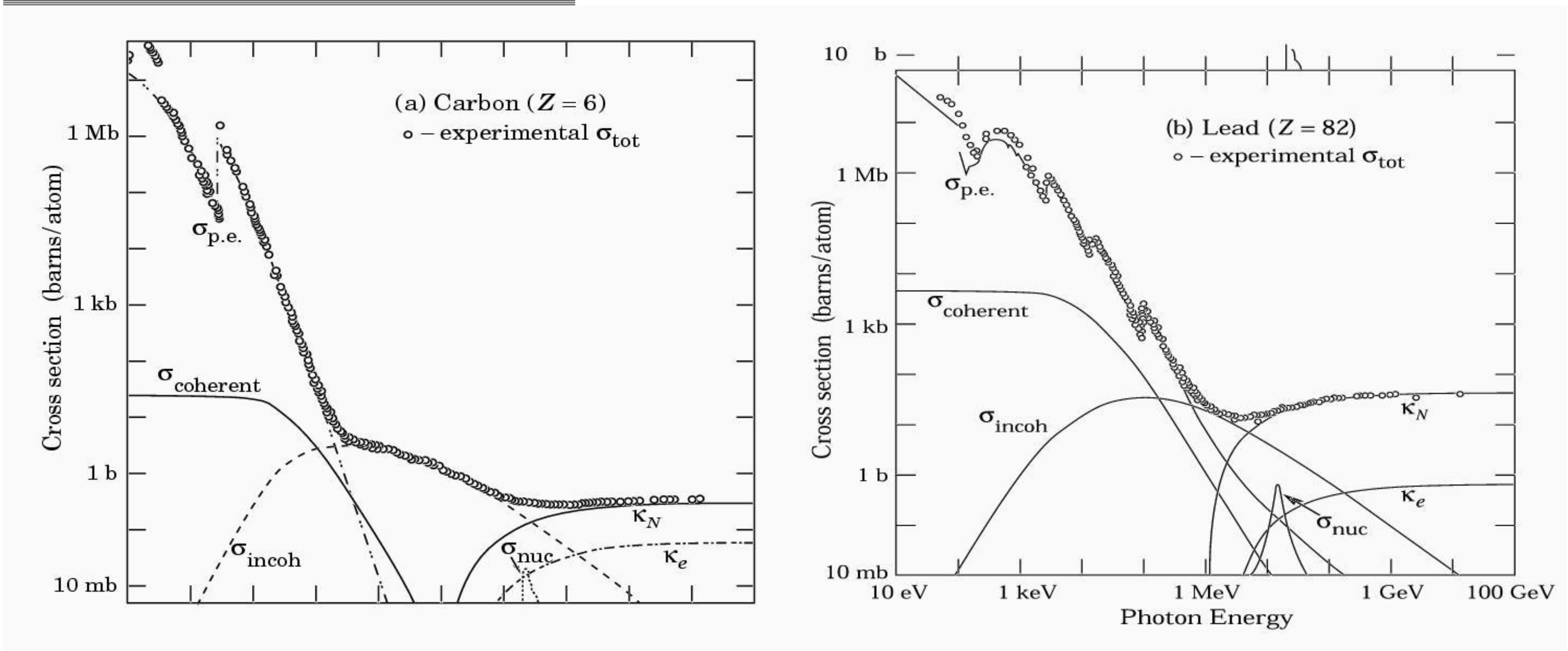
- Here f is a non-trivial function, and the exponent a lies between 1 and 4.

Gamma energies above 50 keV.

- Here geant4 uses the same functional form as geant3 for the K shell:
- with
- Similar formulas are used for L1 and L2 shells.
- The accuracy is 25% near the absorption edges, and 10% elsewhere.

Gamma energies below 50 keV.

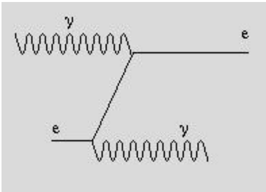
- Here a formula proposed by Biggs is used, where the parameters were fitted to experimental data separately for each energy interval defined by a pair of adjacent absorption edges:



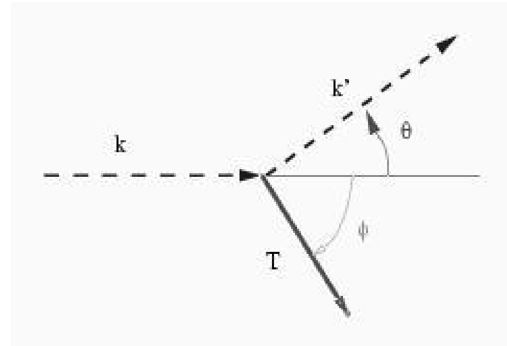
J.P. Wellisch,
CERN/PH

Notes on photo effect

- The total cross-section exhibits edges where the gamma energy reaches the absorption edges the individual shells.
- After photo-effect, characteristic X-ray or Auger electron emission occurs.
- In geant4, the electron is parallel to the incident gamma. Note that in the real world the electron is emitted in forward direction for high energy gammas, and perpendicular to the gamma direction for low gamma energies.



Compton effect

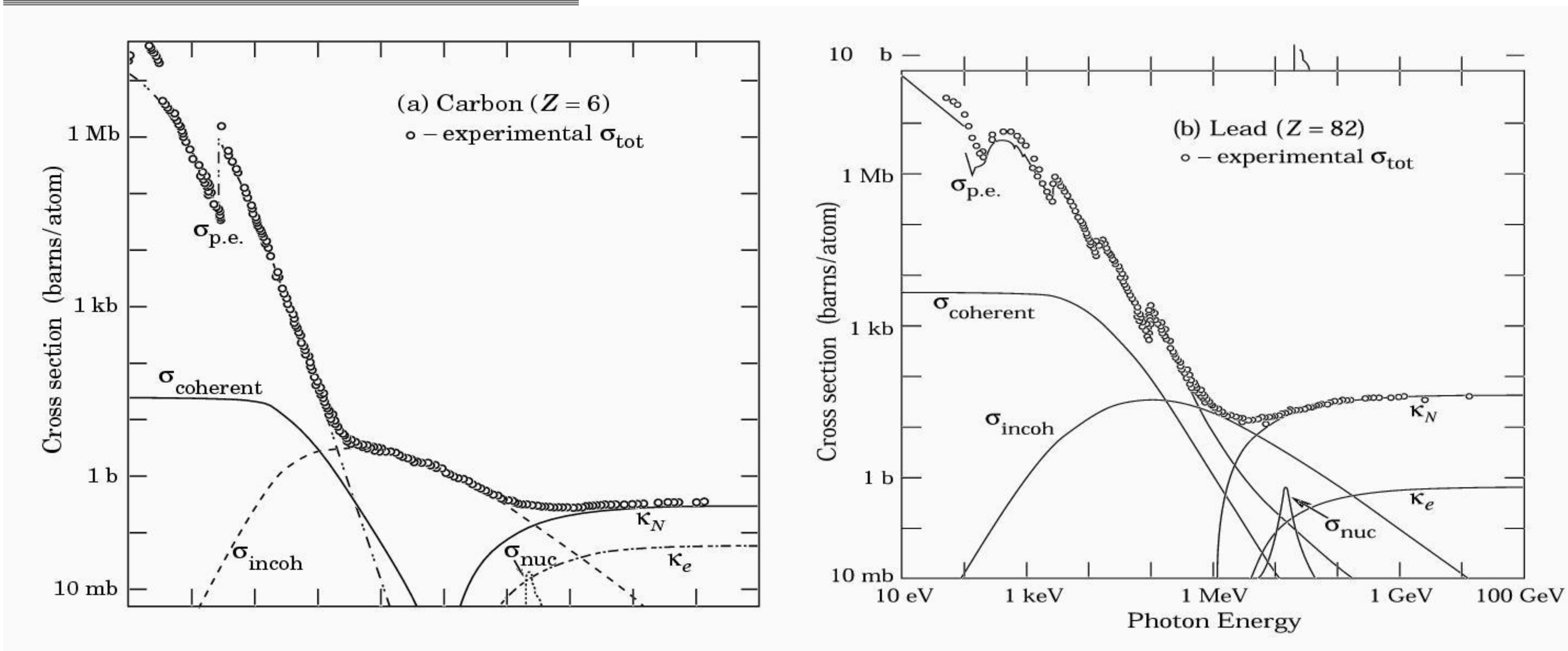


- The compton effect is scattering of quasi-free electrons, and the kinematics is that of free 2-particle scattering.
- Assuming the electron unbound, in the Breit frame we can write:

Gamma energy spectrum

- The energy spectrum, assuming unbound electrons, is given by the Klein-Nishima formula

- And hence the total cross-section per atom is given by:



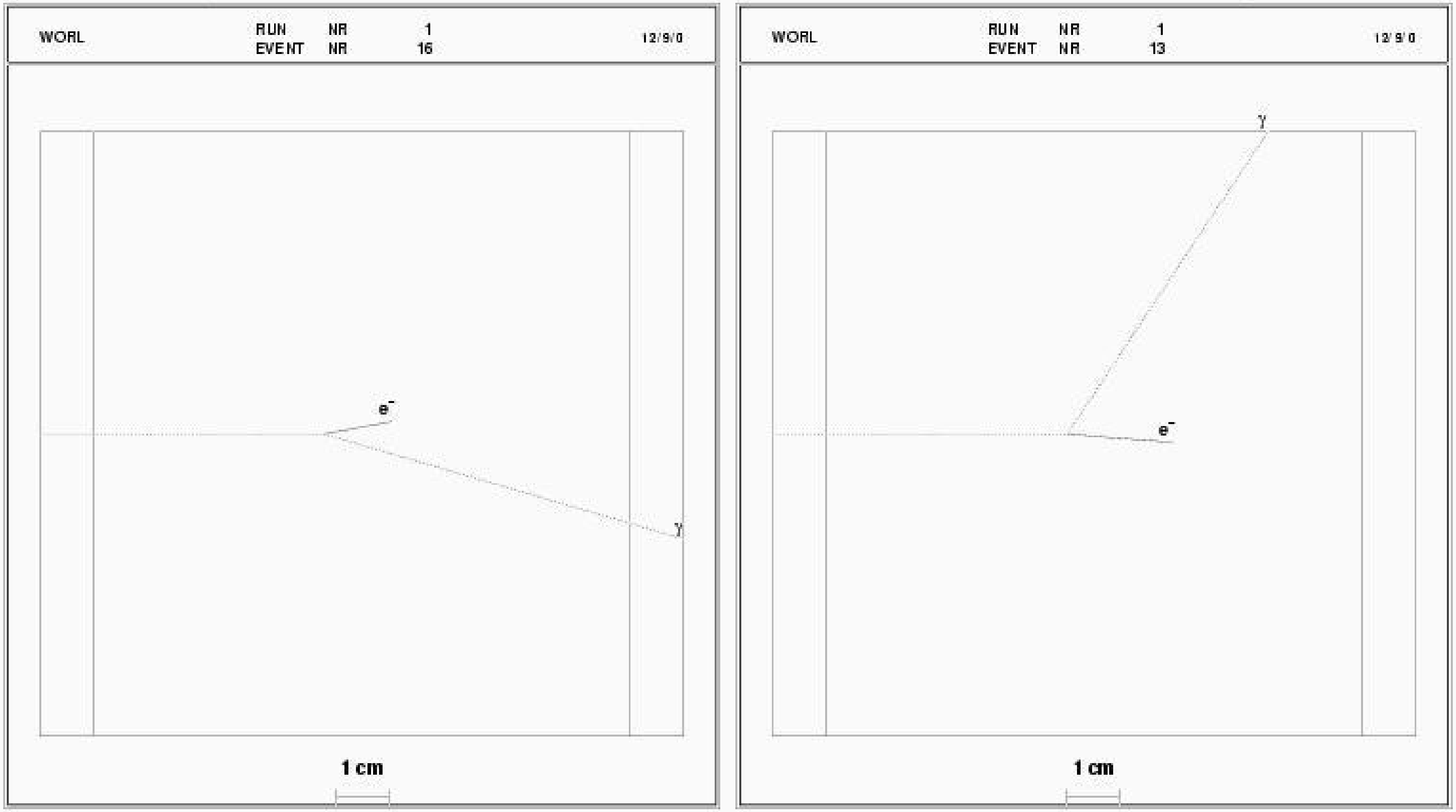
J.P. Wellisch,
CERN/PH

Cross-section per atom in geant4

- Geant4 uses the geant3 parameterization:

- With
- The parameters were fitted on 511 data points for Z between 1 and 100 and k between 10 keV and 100 GeV.
- The accuracy is estimated to be 10% below 20 keV, and better than 6% for higher energies.

γ 10 MeV in 10 cm Aluminium: Compton scattering

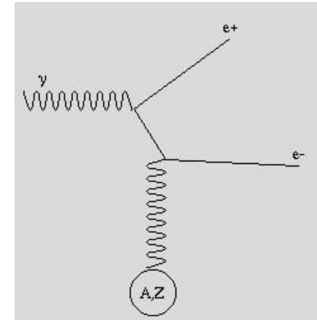


J.P. Wellisch,
CERN/PH

Notes on Compton effect

- The cross-section per atom is Z times the cross-section per electron.
- Inverse Compton scattering exists and has been seen in experiments.
- For kà 0, we find the classical Thomson cross-section.

Pair production



- Pair production is the creation of an electron positron pair from a gamma in the presence of a nucleus.
- It can be described by the Bethe-Heitler cross-section, which will be corrected for various effects.

Bethe Heiter including corrections

- Gives the cross-section for producing an electron of energy $\varepsilon * E_\gamma$ in a material with nuclear charge Z.
- Φ_1, Φ_2, F, and ξ leave us to wonder where they come from.

$Z(Z+\xi(Z))$, *or the triplet correction*

- The gamma does not only feel the charge of the nucleus (with Ze in one vertex, hence proportional to Z*Z), it also sees the charge of the atomic electrons.
- Since the cross-section, and not the amplitudes sum (incoherent), this gives a correction that is proportional to the number of electrons, Z.

F(Z), *or the coulomb correction*

- Corrects for the fact that the formula is calculated with plane waves (should be Coulomb waves, Phys.Rev.96,p76ff,1954, Phys.Rev.97,p542ff,1955).
- Two function are used for low and high energies respectively.
  - Below 50 MeV: $F(Z)=8/3\ln(Z)$
  - Above 50 MeV: $F(Z)=8/3\ln(Z)+f_c(Z)$
- With

Φ, *the screening corrections*

- Depending on the gamma energy, the coulomb field of the nucleus can be more or less screened by the electron cloud.
- A screening variable is defined to describe the impact parameter of the gamma:

- It is worth noting that this keeps also the screening corrections fully symmetric in ε.

- The screening functions are then defined as

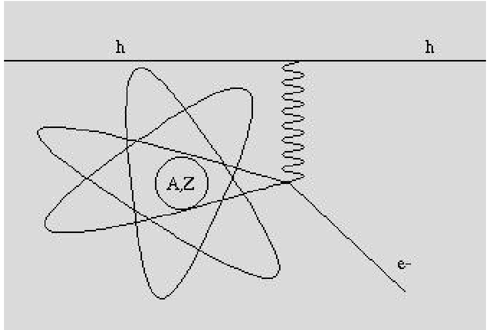
Final states

- Electron and positron and assumed to be coplanar with the incident gamma.
- The polar angle is sampled from Urbans density function, which is an approximation to Tsai's distribution function:

Notes on pair production

- Pair production is a crossed channel of Bremsstrahlung
- Pair production has a threshold of 2m(1+m/M)
- Above a few MeV gamma energy, it is the dominant process in all materials.
- Recoil electrons associated with the correction ξ are not explicitly simulated in geant4
- The formalism is symmetric with respect to, hence any sampling algorithm can be restricted to the interval
- While not explicitly discussed here, the pair production suppression due to LPM effect is also included

Ionization



- The basic ionization mechanism is the collision of a charged particle, p, with an atomic electron.

- In each individual collision, the transferred energy is small, but the total number of collisions is very large.
- The definition of average energy loss per (macroscopic) unit path length imposes itself, also for practical reasons.

Continuous energy loss and explicit delta ray production

- In a shower, modeling as average energy loss is appropriate only for knock-out electron energies that are reasonably small.
- For high energy transfers, the approximation cannot be made. These electrons need to be explicitly generated as delta rays.

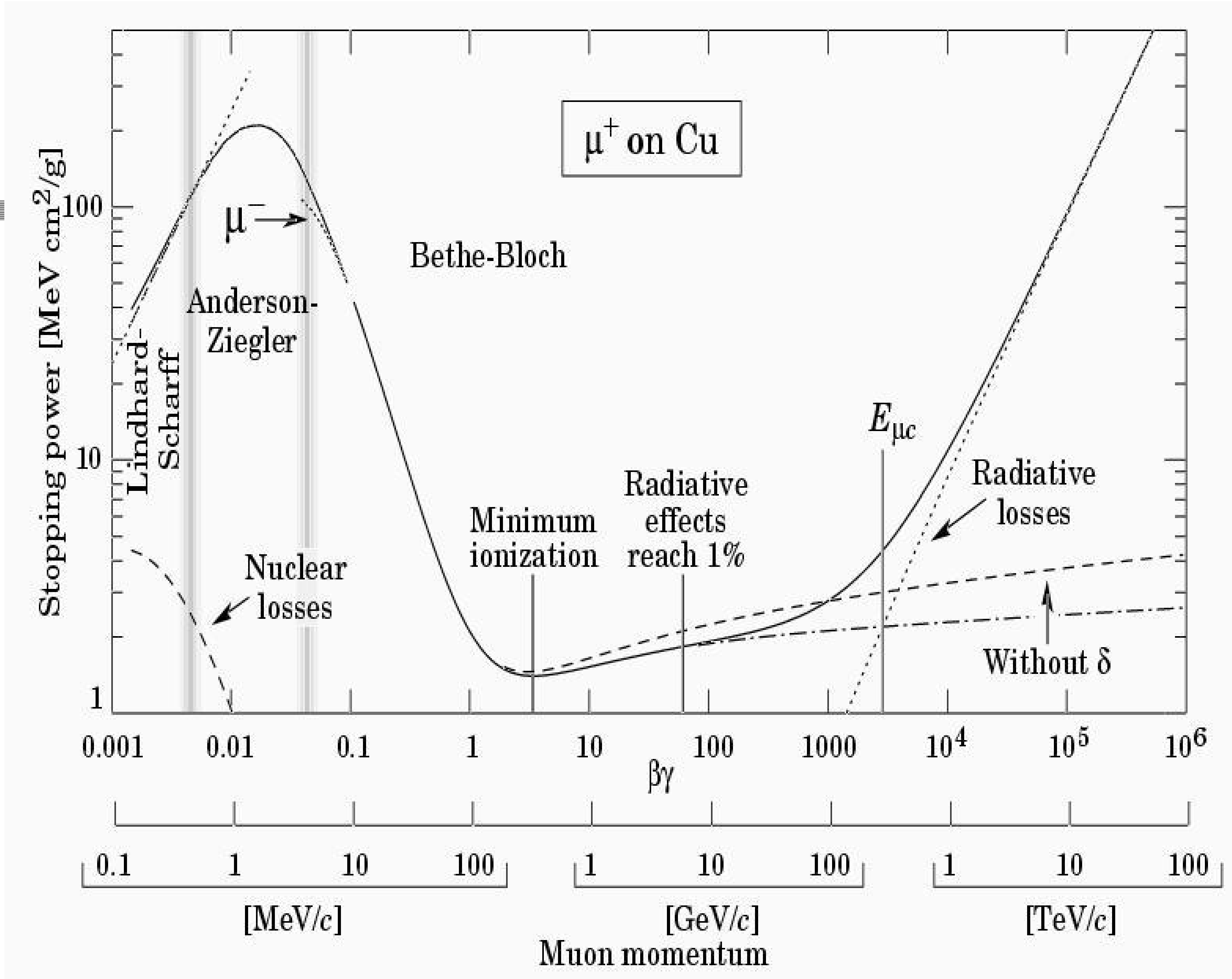
Reduced energy loss and delta cross-section

- This leads to the concept of reduced energy loss.
- If is the cross-section for producing an electron with energy T by an incident particle with energy E, in a material with atom density density ρ, the reduced energy loss is
- While the cross-section for ejecting a ‘hard’ delta ray is

Energy loss by heavy particles

- The truncated energy loss formula (truncated Bethe-Bloch)

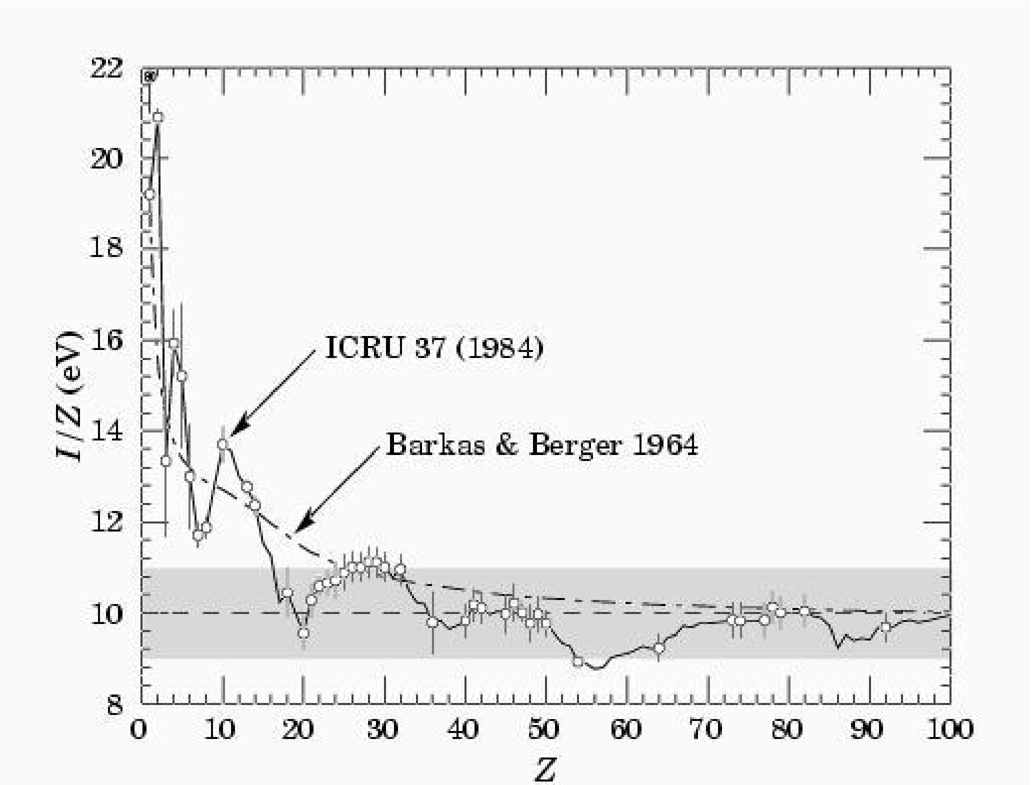
- With the classical electron radius, the mass of the electron, the electron density in the material, the charge of the incident particle,
I the mean ionization potential, δ the density effect function, and the shell correction function, with



J.P. Wellisch,
CERN/PH

Ionization potential

- Many approximation of I are available, the simplest being I=10eV*Z.
- In geant4, we use the ICRU recommended values.



Density effect correction

- The density effect correction would be better named as polarization function. It corrects for a reduction of the energy loss (at high energies), due to polarization of the medium. For details, see

  M.R. Sternheimer et al, Phys. Rev. B, 3681 (1971).

Shell corrections

- is the shell correction term. Under certain conditions, the probability of collisions with inner shells is much reduced. This term takes this into account.
- Geant4 uses the semi-empirical formula of Barkas:

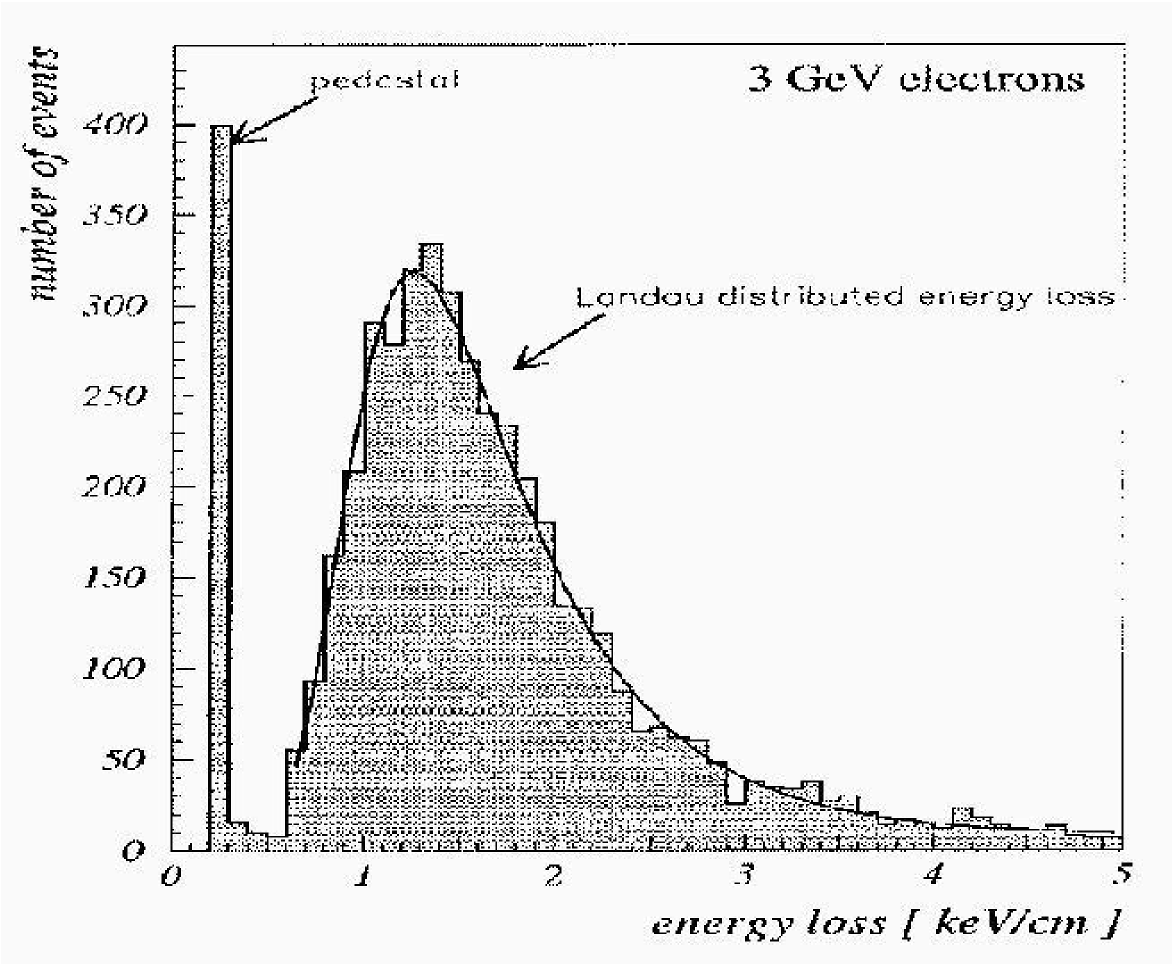
Velocities below orbital electron velocities

- ICRU Report 49 discusses low energy corrections in detail.
  - Bethe-Bloch is no longer applicable, and other formalisms need to be used.
  - Ex. Anderson and Zielger for $0.01<\beta<0.05$ (Stopping power and ranges in all elements, Pergamon Press, 1977)
  - Ex. Lindhard, Scharff, Schiott for $\beta<0.01$ (Kgl.Danske Videnskab.Selskab,Mat.-Fys.Medd., 33 V14, 1963)
- In the geant4 standard package, a simple functional form is used to parameterize the energy loss for very small particle energies

Fluctuations

- Depending on the amount of material considered, there can be large fluctuations in the continuous energy loss
- These can be strongly asymmetric, leading to a Landau distribution.
- The large fluctuations are due to a small number of collisions with relatively large energy transfer.

Energy loss fluctuations (thin gas layer).



J.P. Wellisch,
CERN/PH

Fluctuations

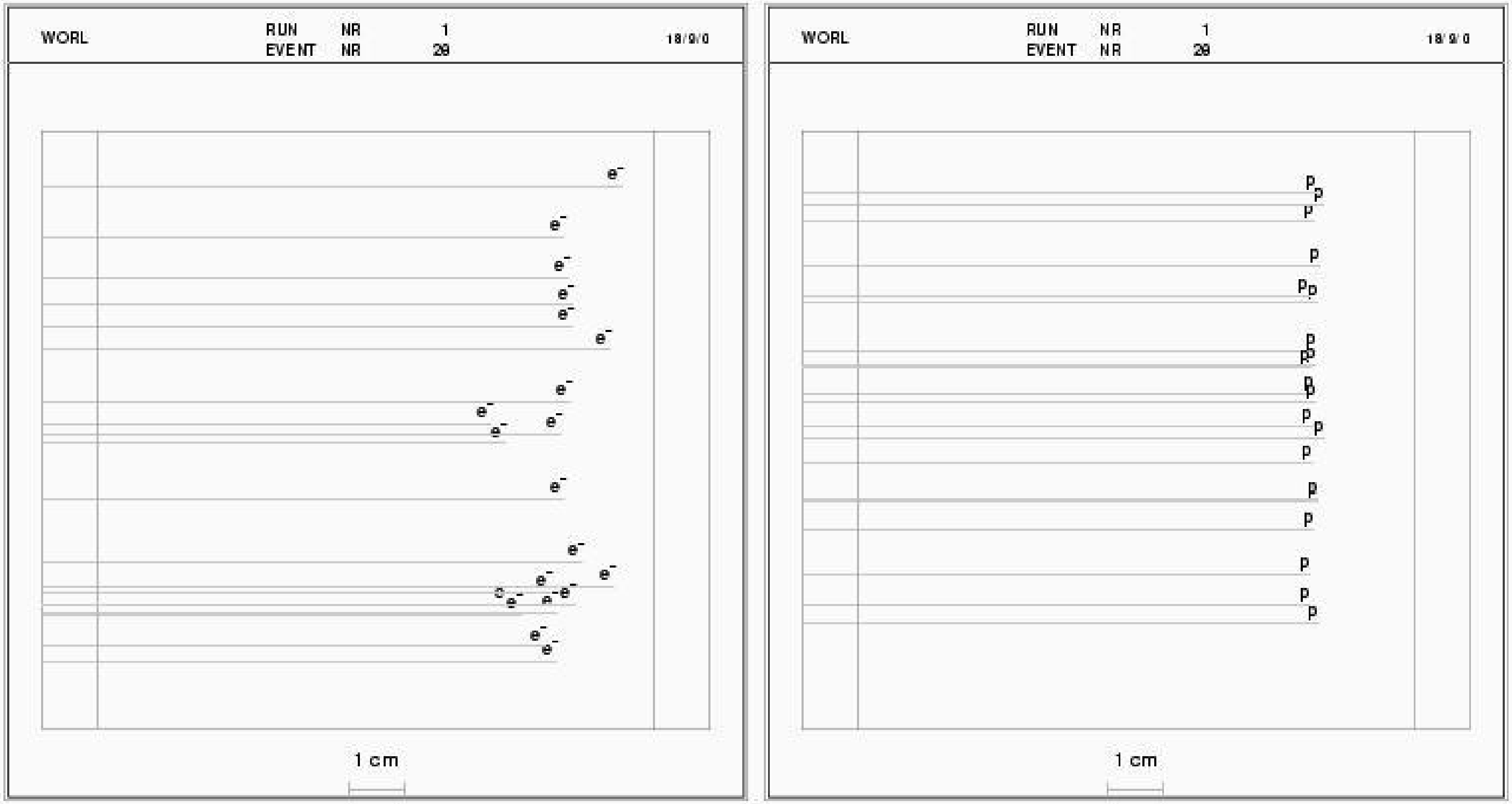
- To model fluctuations, geant4 uses a very simple particle-atom interactions model:
  - We use only two energy levels per atom
  - We consider an excitation of the energy levels, and the ionization with energy loss distribution function (g) proportional to

- Is Σ the macroscopic cross-section, then, in a path on length Δx, the number of collisions for each type of interactions (excitation, ionization) follows a Poisson distribution:

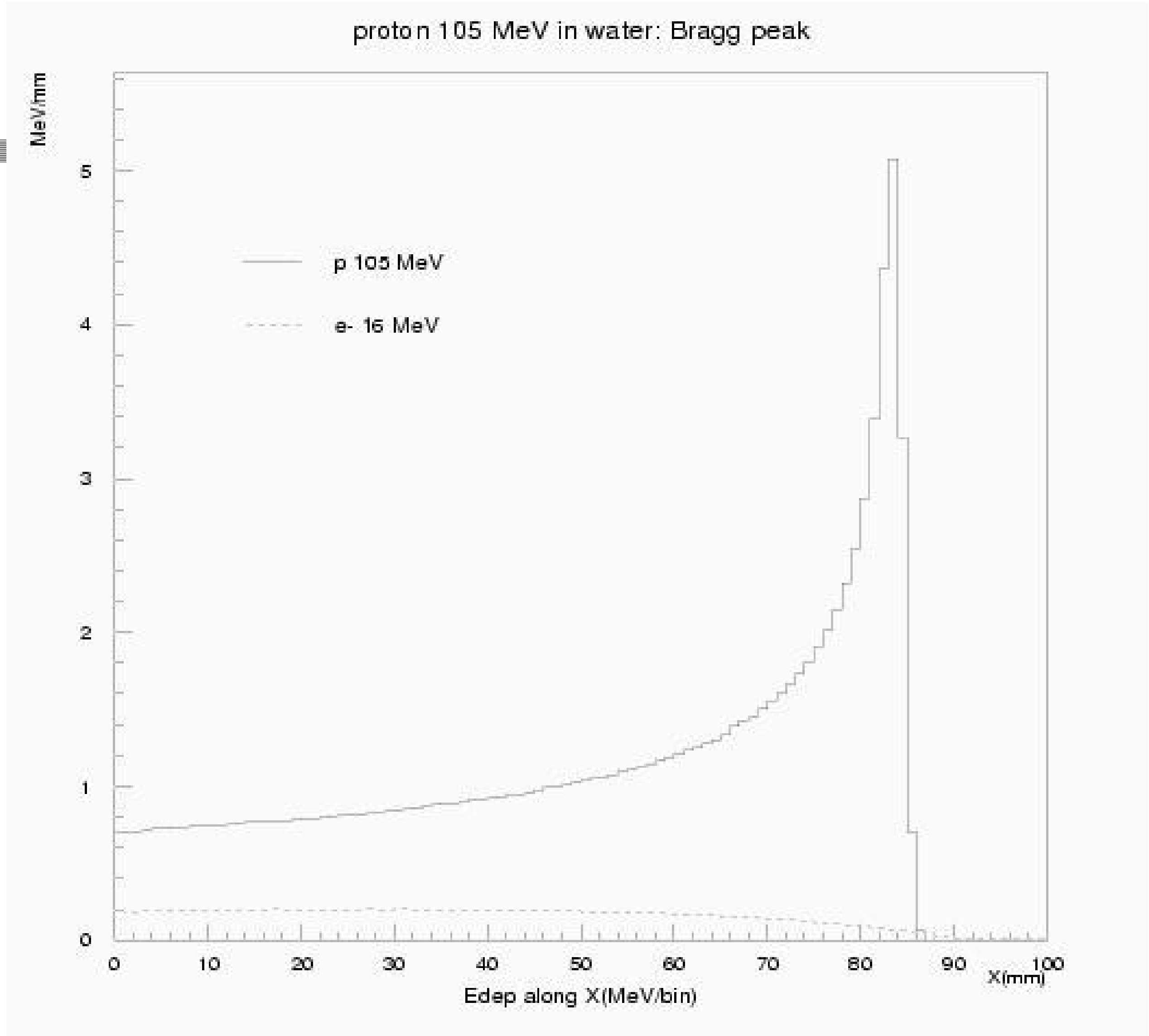
- The energy loss in a thickness is the the sum over all collisions:

- And the introduction of fluctuations becomes straightforward.

penetration of e^- (16 MeV) and proton (105 MeV) in 10 cm of water.

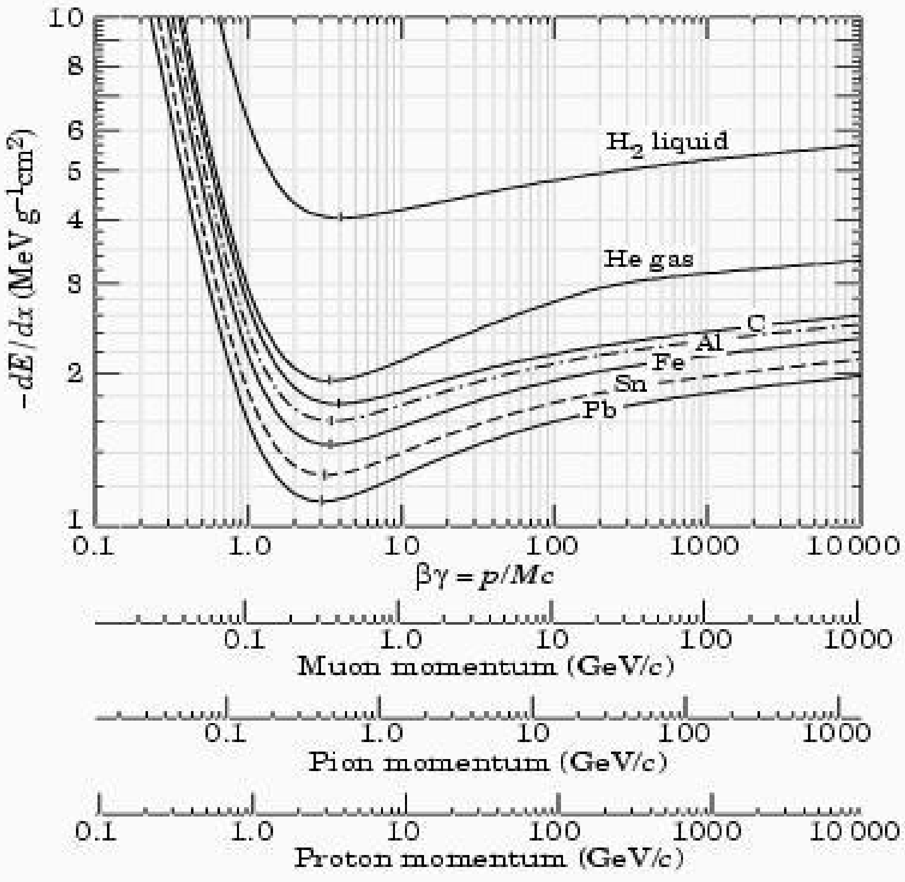


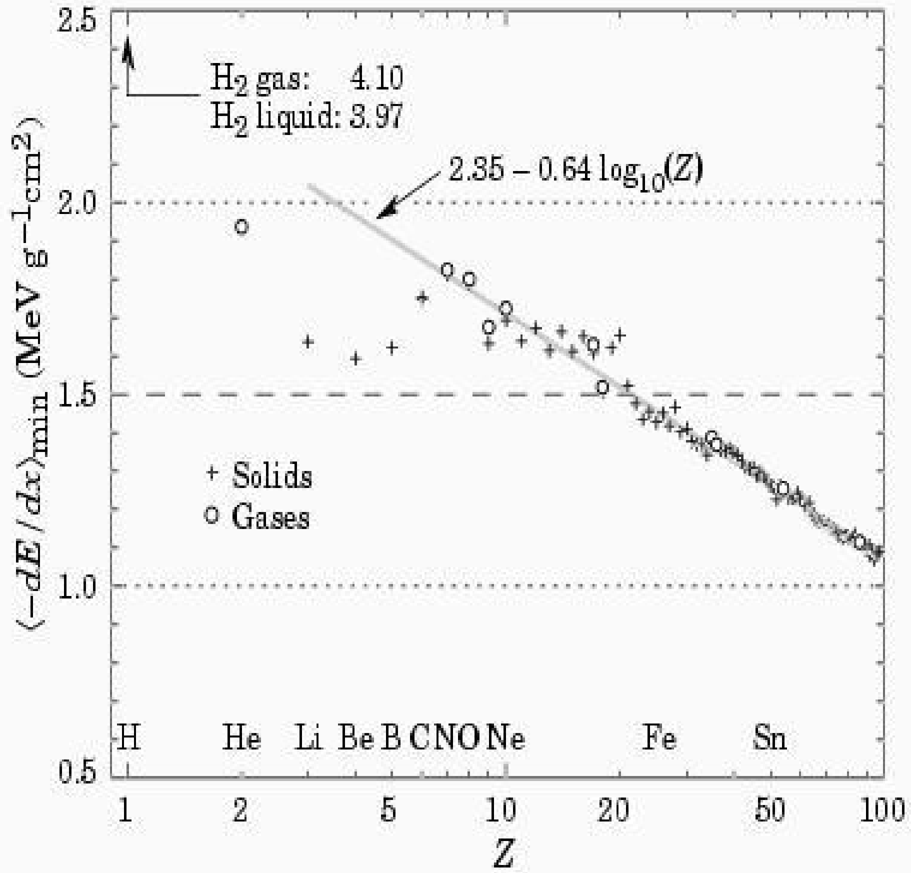
J.P. Wellisch,
CERN/PH



J.P. Wellisch,
CERN/PH

Minimum ionizing particles





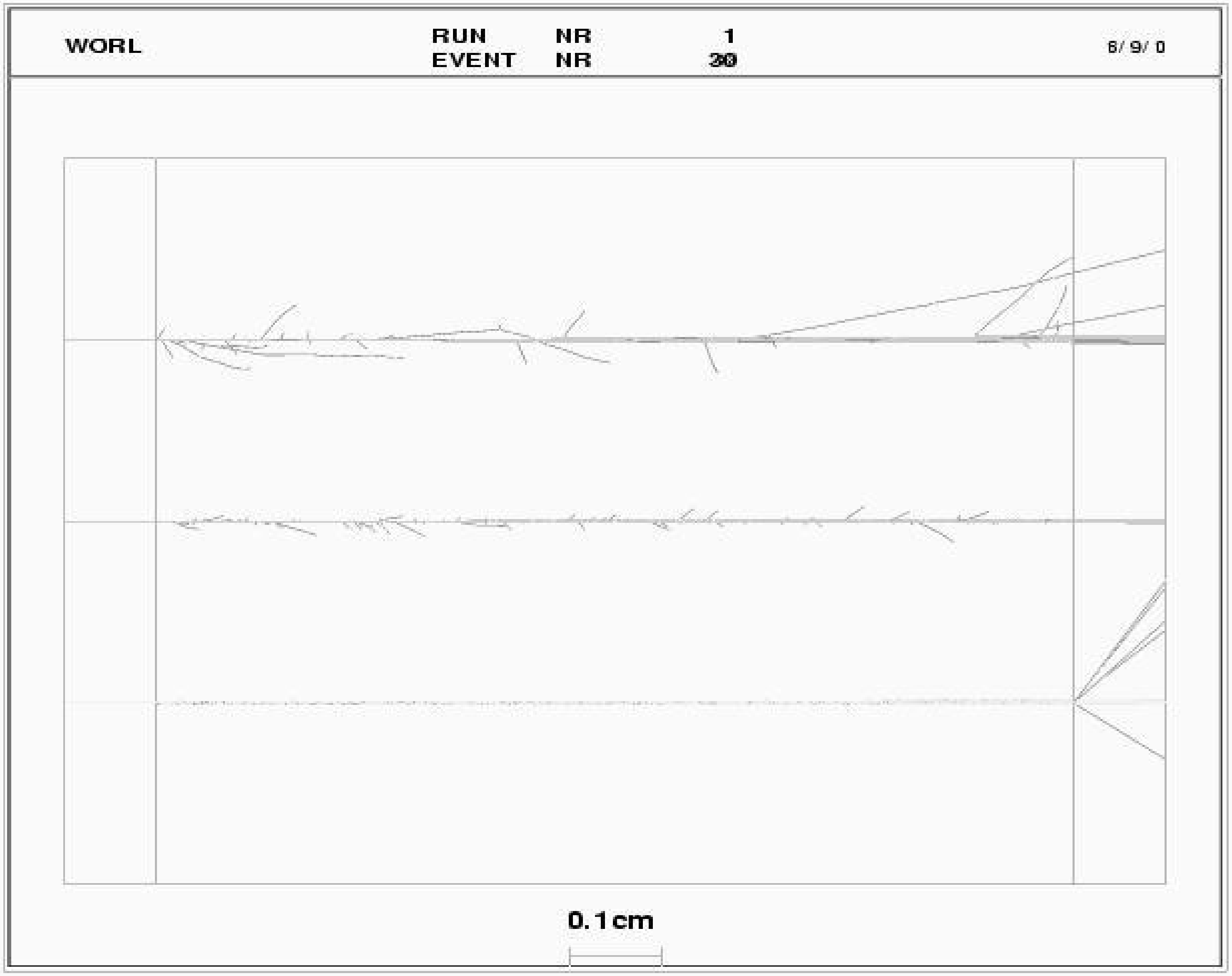
J.P. Wellisch,
CERN/PH

Delta ray emission

- The differencial cross-section can be written as:

- And the integration gives us for the total, cut dependent cross-sections

200 MeV electrons, protons, alphas in 1 cm of Aluminium



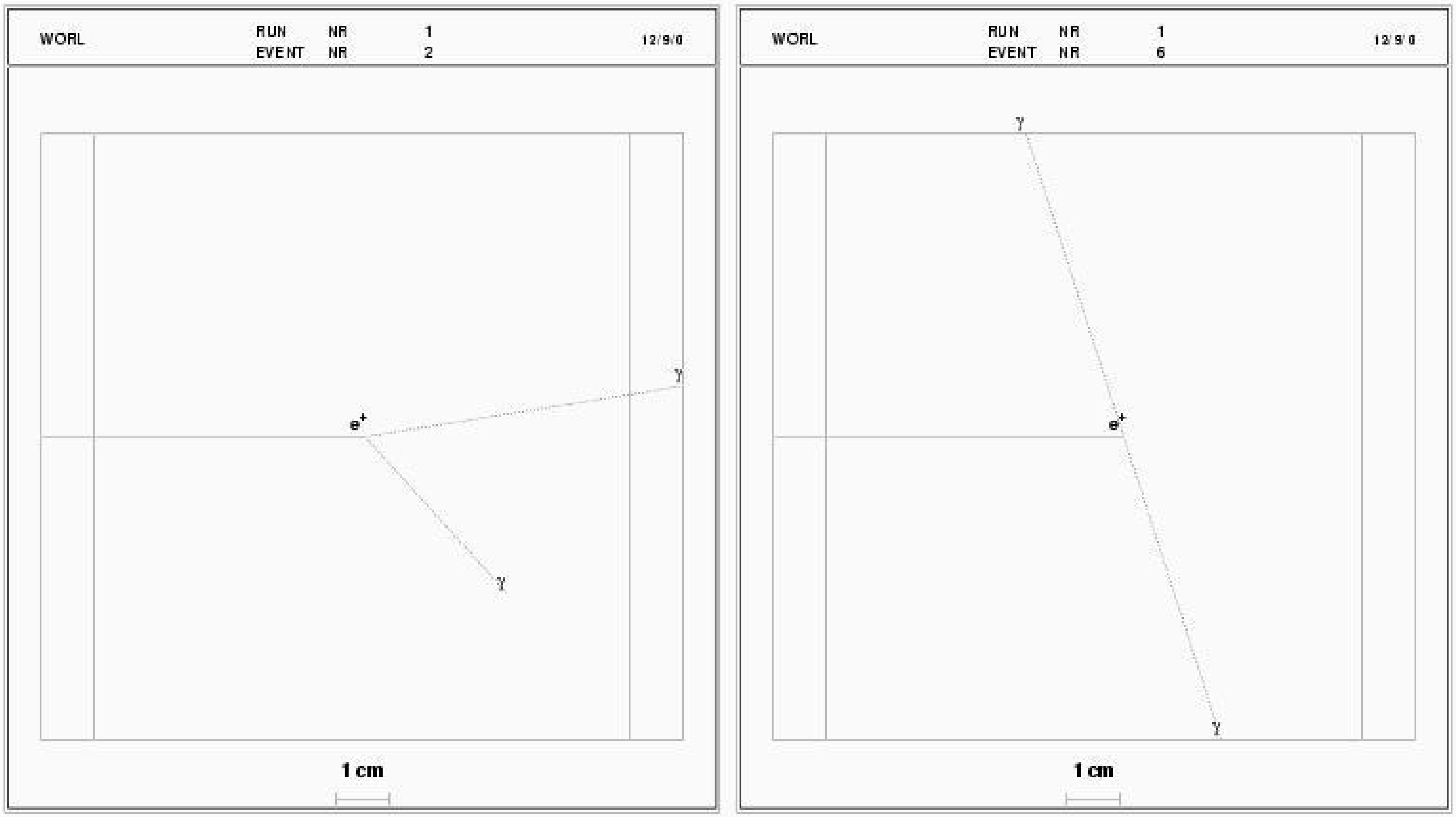
J.P. Wellisch,
CERN/PH

Special cases: electrons and positrons

- They are special, due to the low mass, and, for the electron, the fact that the scattering partners are identical particles.
- We get Moller or Bhabha scattering, and can use the Berger and Seltzer energy loss formulas.
- For more details see
  - H. Messel, D.F.Crawford, Pergamon Press, Oxford 1970
  - S.M.Seltzer, M.J.Berger, Int. J. of App. Rad. 35,665,1984

Also special: e+e- annihilation

- e^+ 30 MeV in 10 cm Aluminium. Annihilation in fly (left), at rest (right).

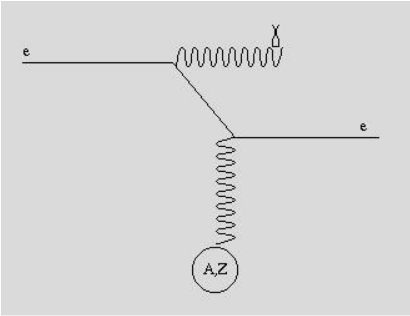


e+e- annihilation

- The cross-section of the process
can be described by Heitler's cross-section formula

- And the differential cross-section can be written as

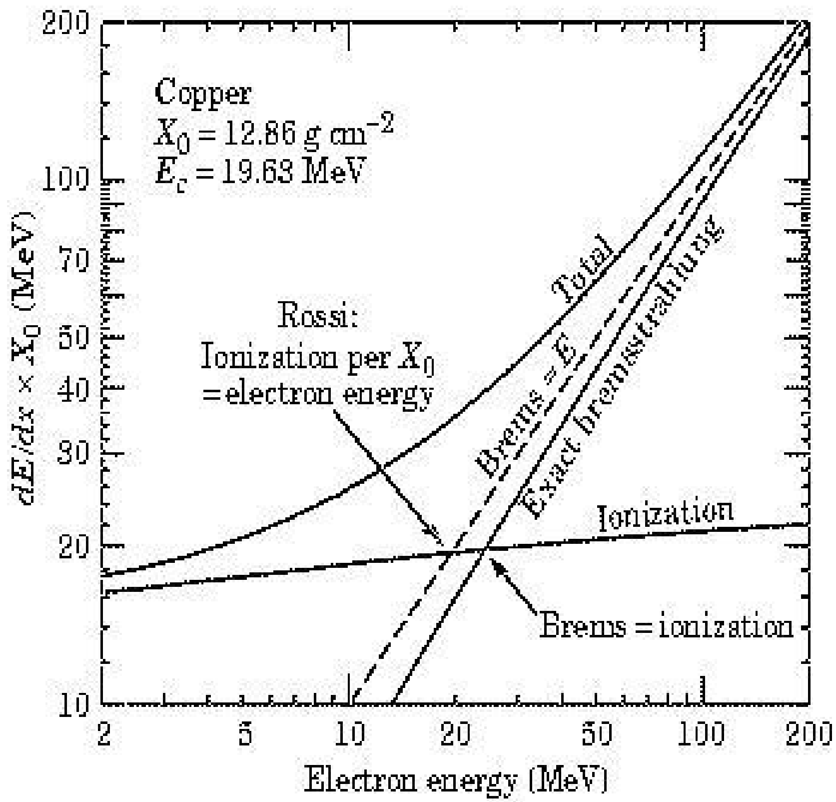
Bremsstrahlung

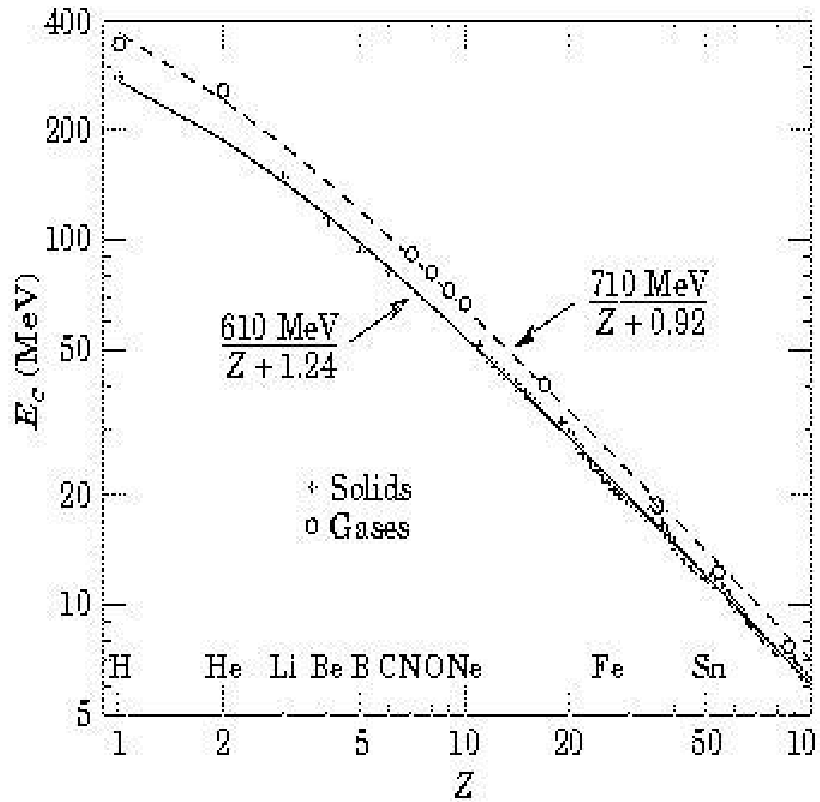


- A fast charged particle is decelerated in the Coulomb field of an atom, and emits part of its energy in form of a gamma.
- Notes:
  - Above a few 10 MeV, this is the dominant energy loss mechanism for electrons and positrons
  - For heavier particles (ex. pions) it becomes significant only above a few 100 GeV.
  - It is very closely related to pair production

Critical energy E_c

- The critical energy is defined as the energy at which energy loss by ionization and bremsstrahlung are equal.





J.P. Wellisch,
CERN/PH

Correction to the Bethe Heitler cross-section

- Screening crorrections
- Bremsstrahlung on atomic electrons
- Correction to the Born approximation
- Matter polarization (dielectric suppression)
- Landau Pomerantchuk Migdal effect
- ...
  - See the discussion of pair production, or S.M. Seltzer, M.J. Berger, NIM B12, 95 (1985) , Atomic Data and Nuclear Data Tables 35, p345ff, (1986)

Note that for high particle energies, the cross-section becomes simple (Y.-S. Tsai, Rev.Mod.Phys.46,p815ff,1974)

- For electrons, above a few GeV, we an write

- Here α is the fine structure constant, k the photon energy (   ), r the classical electron radius, f a Coulomb correction function, and

Radiation length, X_0

- The radiation length is defined by

- Which, given the integration of Tsai's formula

- Results in

A few corrections for in-medium effects:

- Formation length of the gamma
  - In bremsstrahlung, the longitudinal momentum transfer from the nucleus to the electron can be very small. For E>m and E>k, we have
  - Hence Heisenberg's uncertainty principle implies that the coherence length of emission (formation length) is substantial
  - If anything happens during this length, the emission is disrupted.

Two medium effects can take place

- The photon can, during creation, interact with the electrons in the material (dielectric suppression mechanism).
- The electron can, during the creation of the photon, interact (multiple scatter) with the atoms in the material (LPM effect).

Dielectric suppression

- It can be shown, that in medium the formation length is shortened by this effect, to read

- Where the additional term is related to the dielectricity of the medium by

and

Dielectric suppression

- To take the effect into account in the cross-section, we write
- With
- It is worth noting, that for small k, this corrections becomes which cancels the infra-red divergence in the Bethe Heitler formula.

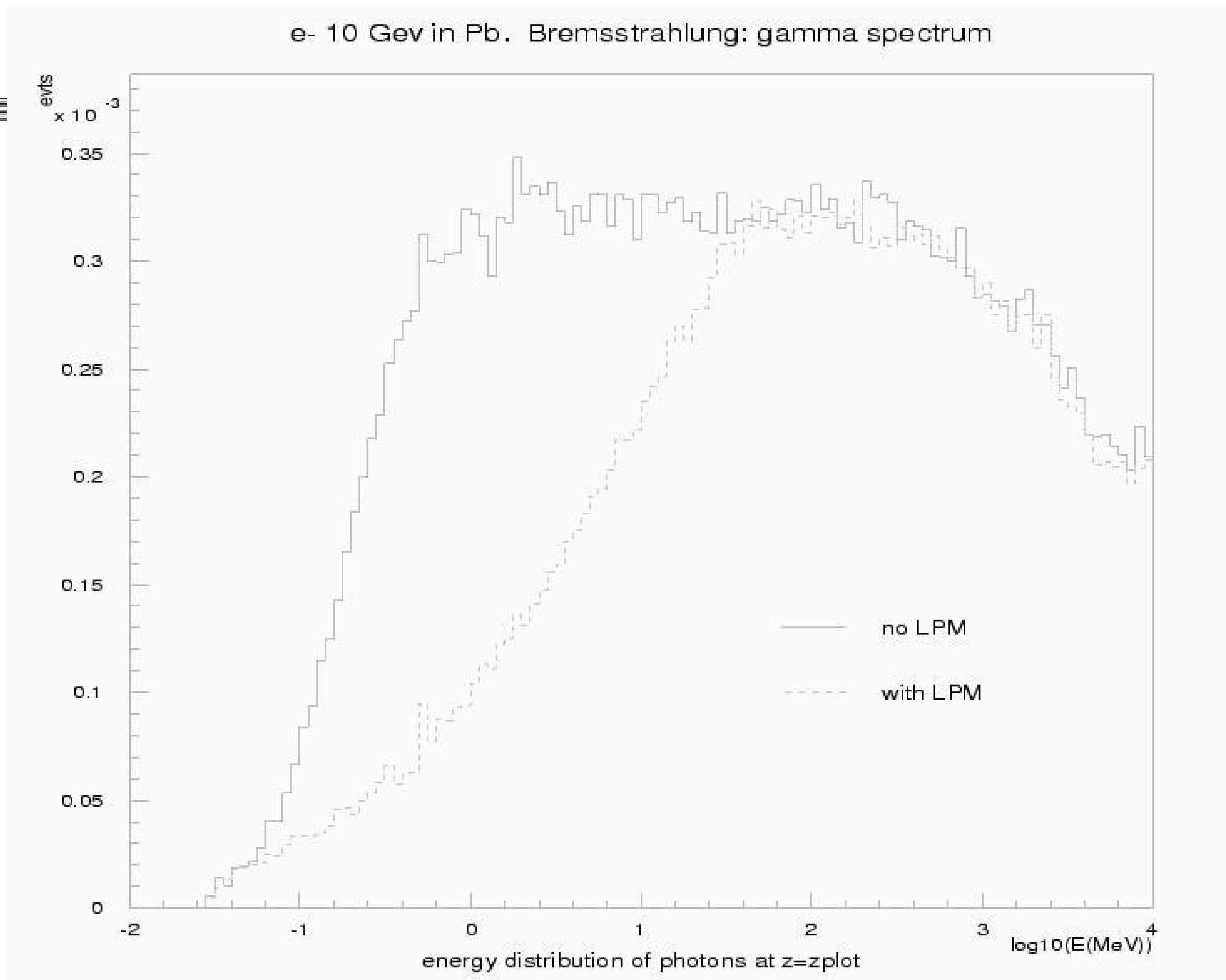
LPM suppression mechanism

(Docl.Acad.Nauk.SSSR 92,(1953),535,735; Phys.Rev.103(1956)p1811ff)

- Where does it matter?
  - We can argue, that the effect matters, when the angle due to multiple scattering becomes comparable or greater than a typical emission angle ( ) of the photon.
  - From we can show that the effect is relevant for photon energies below the characteristic energy of the effect where
  - We obtain

LPM correction

- Multiple scattering increases the longitudinal momentum transfer from the nucleus to the electron, to read
- Since the uncertainty principle reads we can calculate the formation length if
- And obtain the suppression function



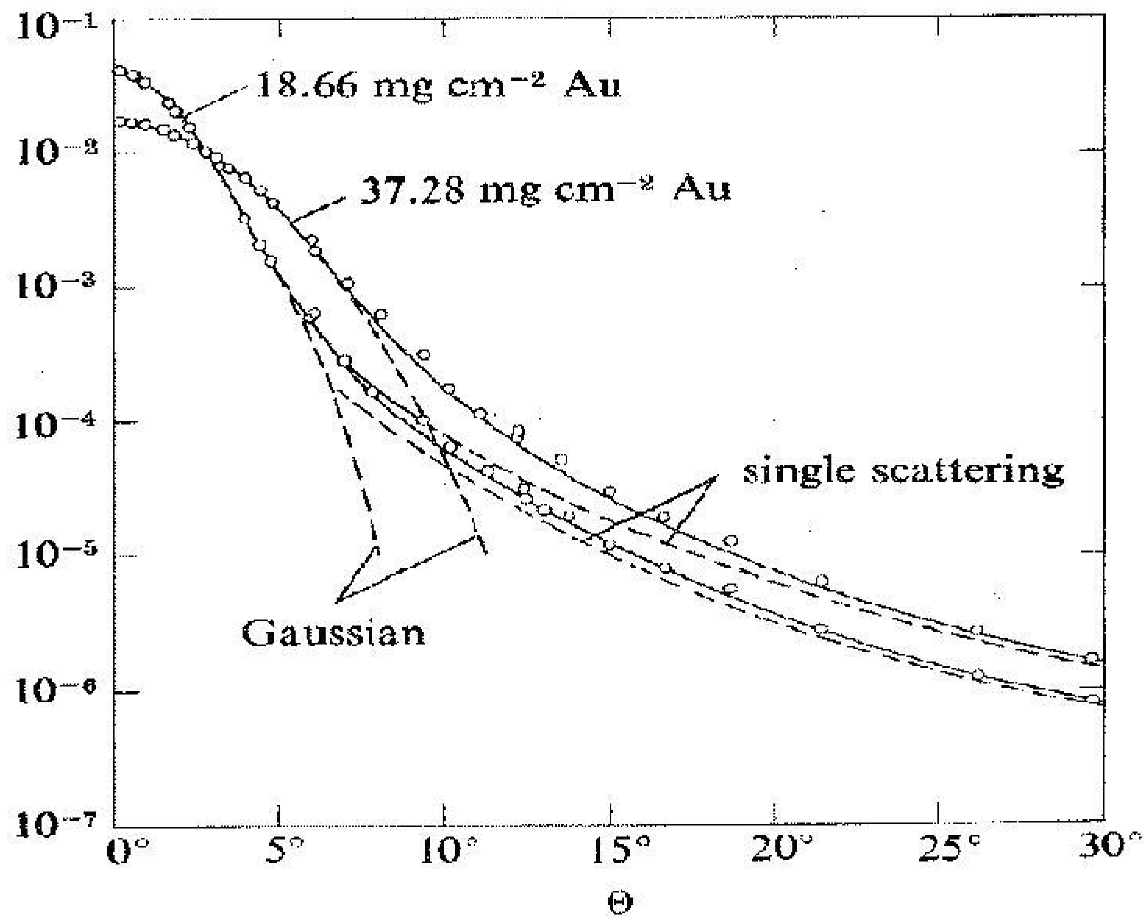
J.P. Wellisch,
CERN/PH

Combined suppression

- It is worth noting that both LPM and dielectric mechanisms operate on the same quantity. The correction hence do not factorize. Instead we have

Multiple Coulomb scattering

- As a charged particle passes through matter, it suffers small angle elastic Coulomb scattering.
- The cummulative effect of these will result in a deflection and displacement of the particle with respect to the otherwise expected path.
- If the number of individual collision is large, the angular distribution is Gaussian. Otherwise, it is quite similar to Rutherford scattering.
- Moliere theory reproduces this distribution quite well.



10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
18.66 mg cm^{-2} Au
37.28 mg cm^{-2} Au
single scattering
Gaussian
0°
5°
10°
15°
20°
25°
30°
Θ

The Gaussian part

- One parameterization that can be used for the Gaussian part is

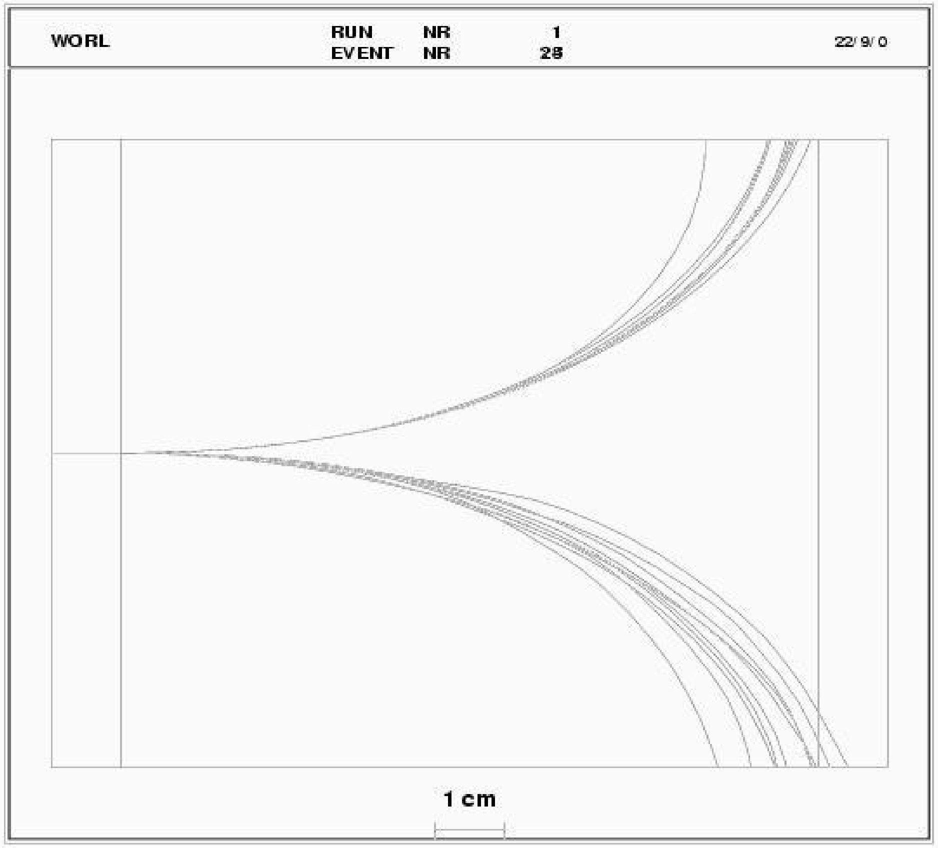
- Where

- This comes from a fit to the Moliere distributions, and is good better than 10% for

10 cm of Aluminium. Field 5 tesla.

top: 10 e^- (300 MeV): energy loss fluctuations only (no muls)

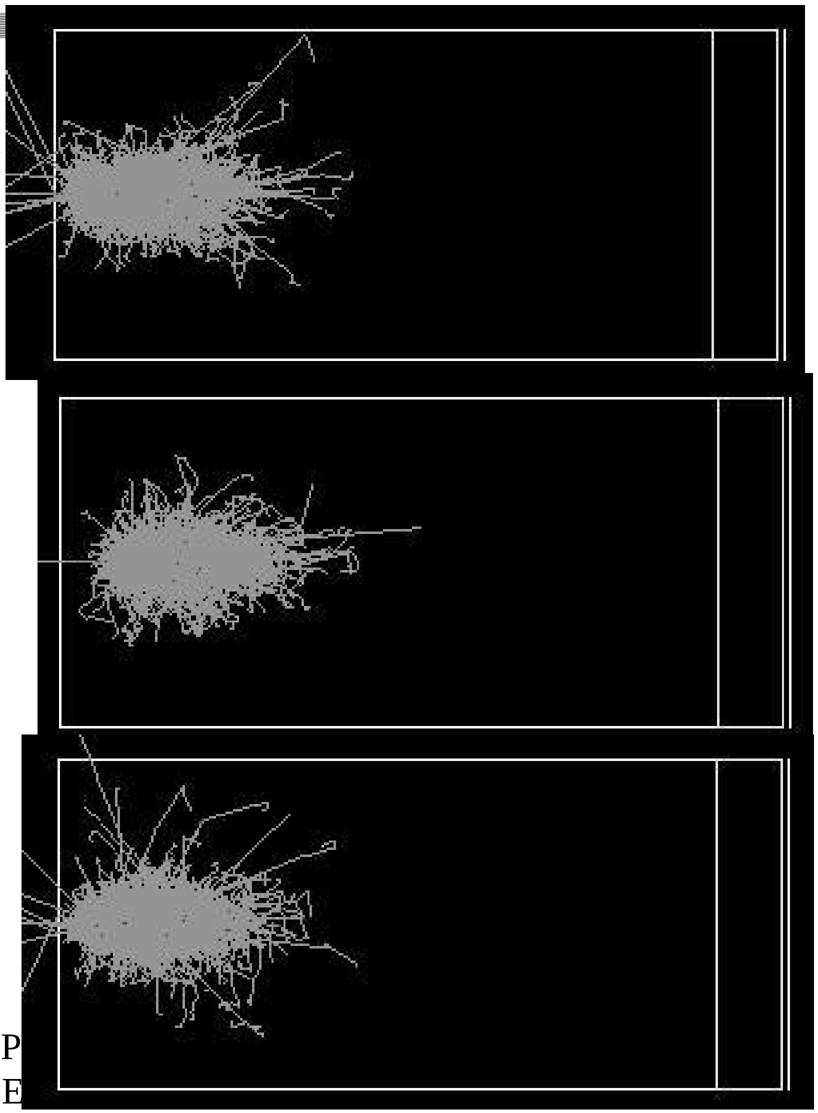
bottom: 10 e^+ (300 MeV): multiple scattering only (no eloss fluct)

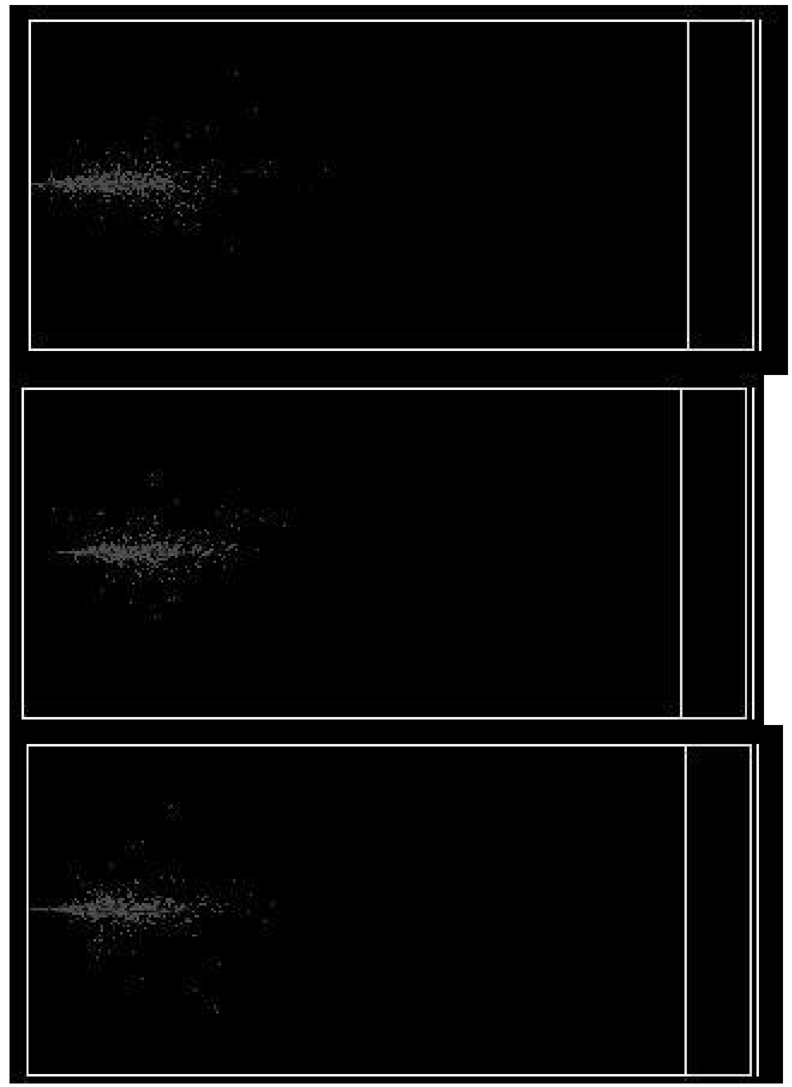


Multiple scattering in geant4

- Uses a model proposed by L.Urban, based on Lewis theory.

20 GeV gammas in copper (right, charged particles only, left complete





Test beams experiments studied in the context of the LCG validation project

- CMS 1996 HCAL
- CMS 1996 combined
- CMS 2000 HCAL
- ATLAS TILE standalone
- ATLAS end-cap hadronic

- Many thanks to F. Gianotti, for permission to use this material here

Validation of G4 hadronic physics lists with ATLAS Tilecal

C. Alexa, S. Diță, Ş. Constantinescu

Pions and protons: TB data, Geant3 and Geant4

- Geant4.5.2 (FADS/Goofy):
  - § **QGSP** 2.7: theory driven modeling
  - § **LHEP** 3.6: LEP and HEP parameterized models
- Geant3: G-Calor
- 2002 and 2003 test beam data

§ 2002 test beam data:
(π is normalized to e response for each energy and rapidity)

- E_{beam}: 50(e), 100(π), 180(π) GeV
- η: 0.25, 0.35, 0.45, 0.55, 0.65

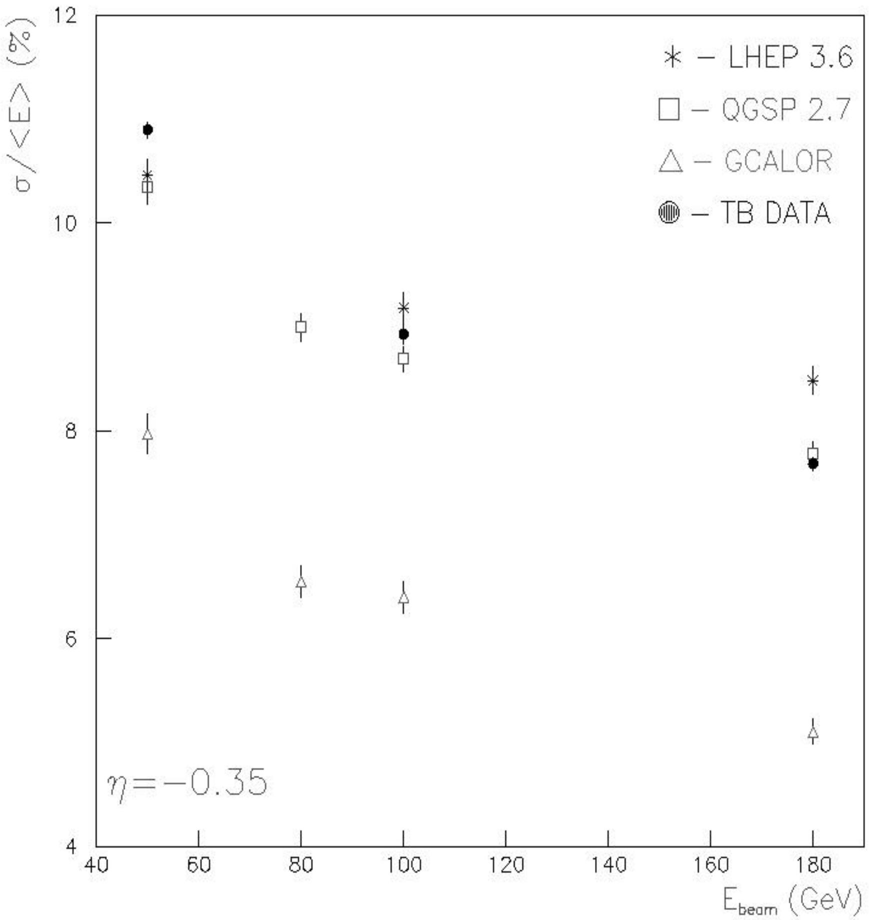
§ 2003 test beam data:
(π is normalized to e response for each energy and rapidity)

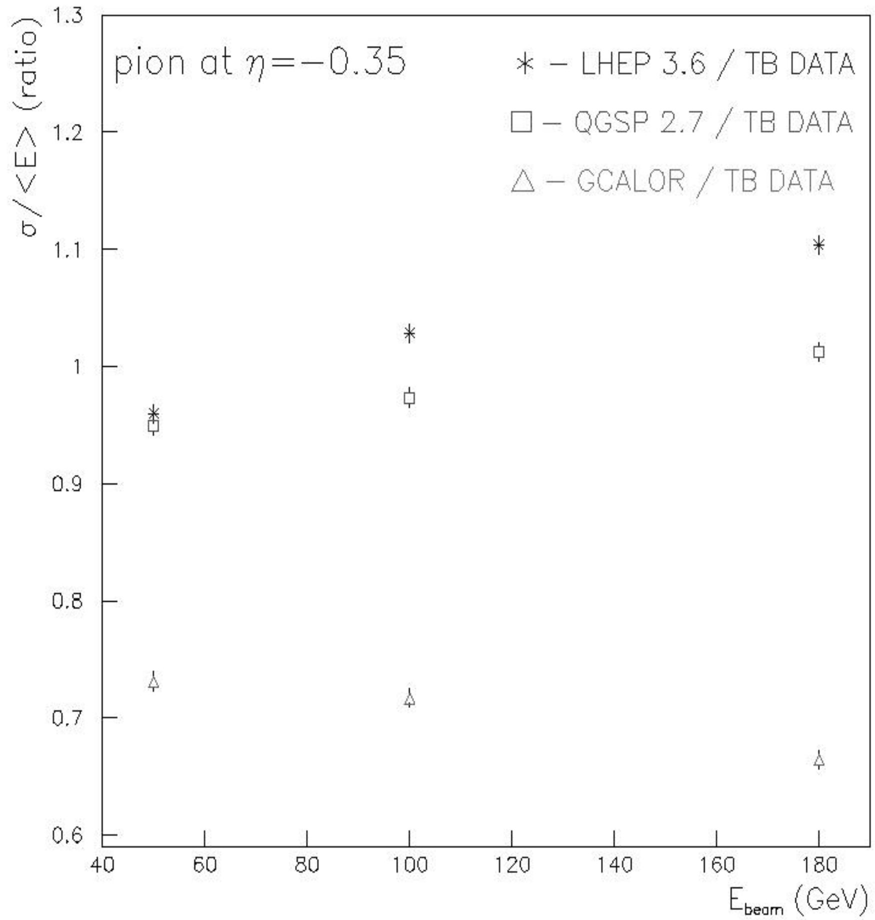
- E_{beam}: 1, 2, 3, 5 and 9 GeV (π)
- η: 0.25, 0.35, 0.45, 0.55, 0.65

§ Geant4.5.2: QGSP 2.7 and LHEP 3.6

- E_{beam}: 50, 80, 100, 180 GeV
- η: 0.25, 0.35, 0.45, 0.55, 0.65

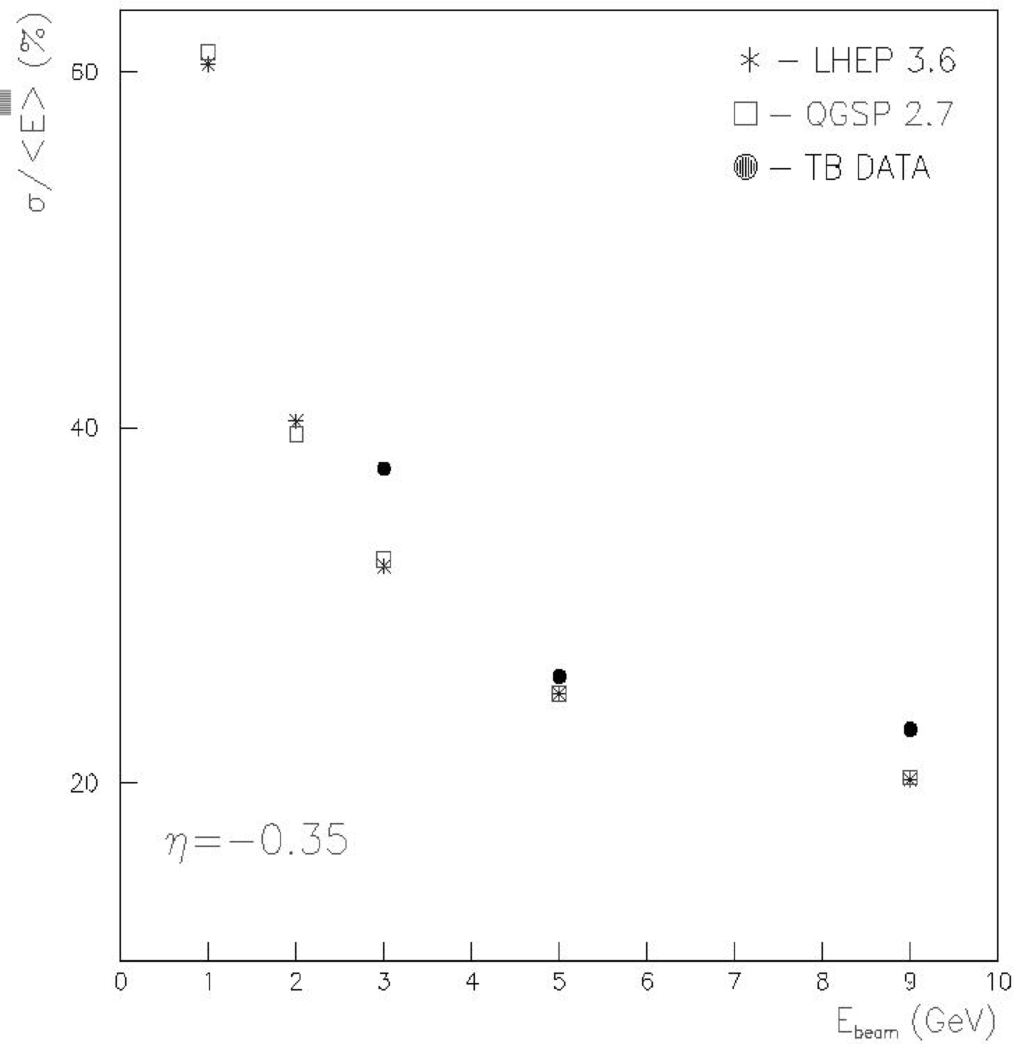
pion resolution





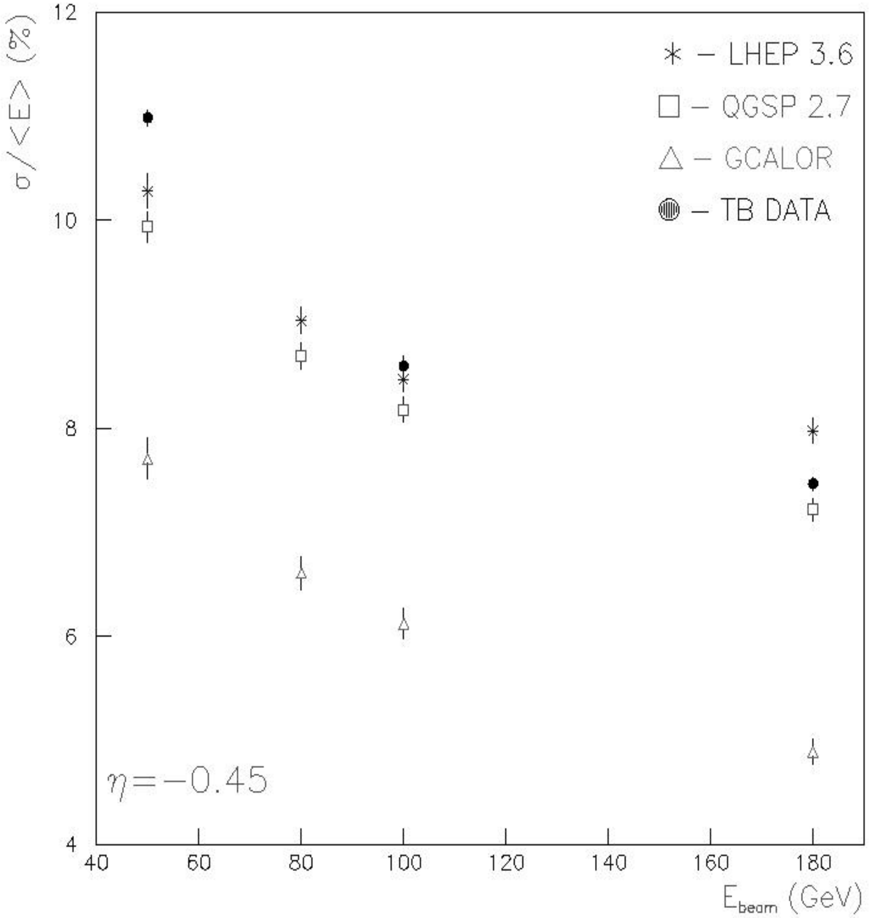
J.P. Wellisch,
CERN/PH

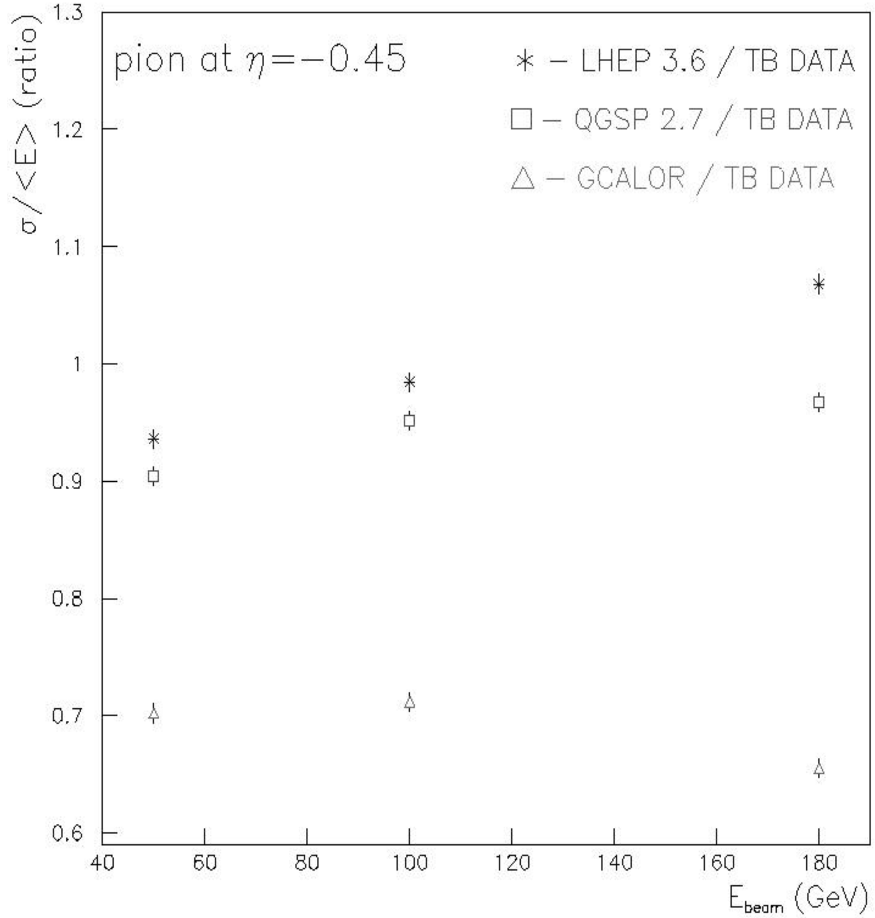
pion resolution



J.P. Wellisch,
CERN/PH

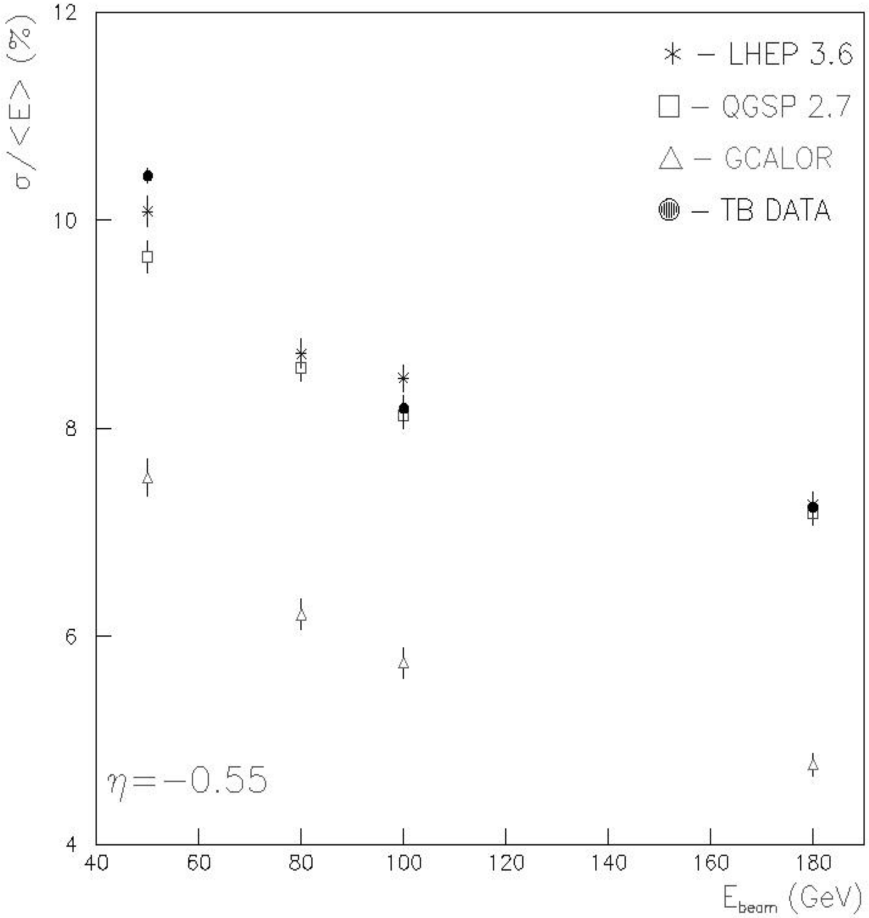
pion resolution

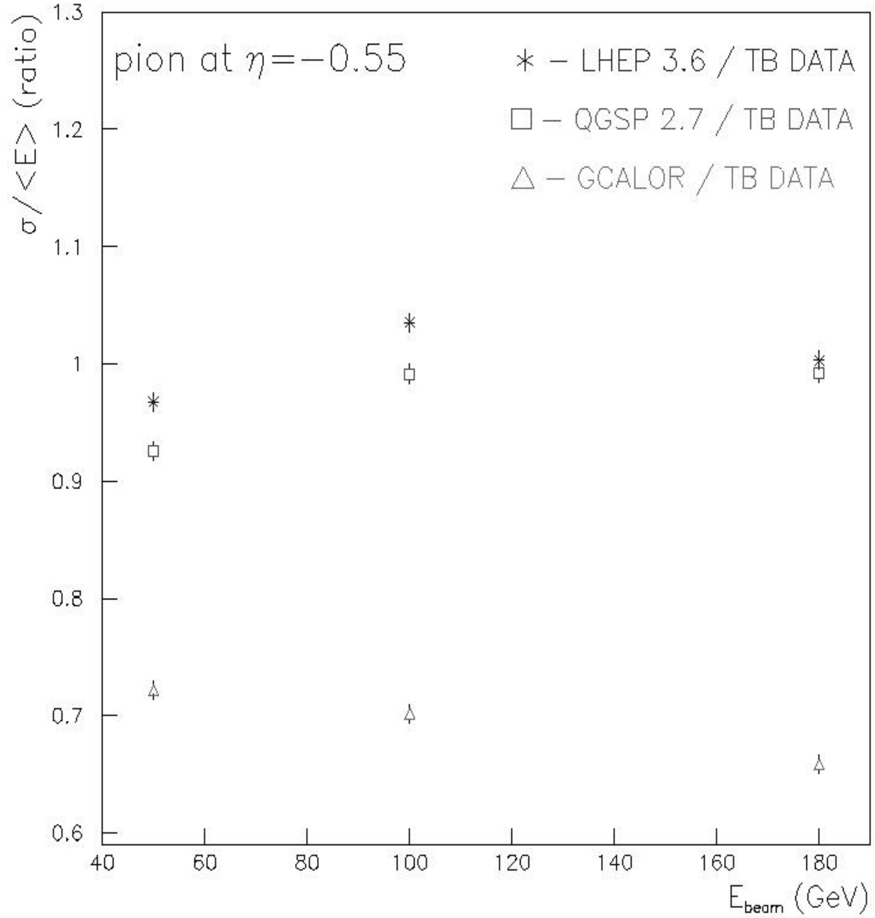




J.P. Wellisch,
CERN/PH

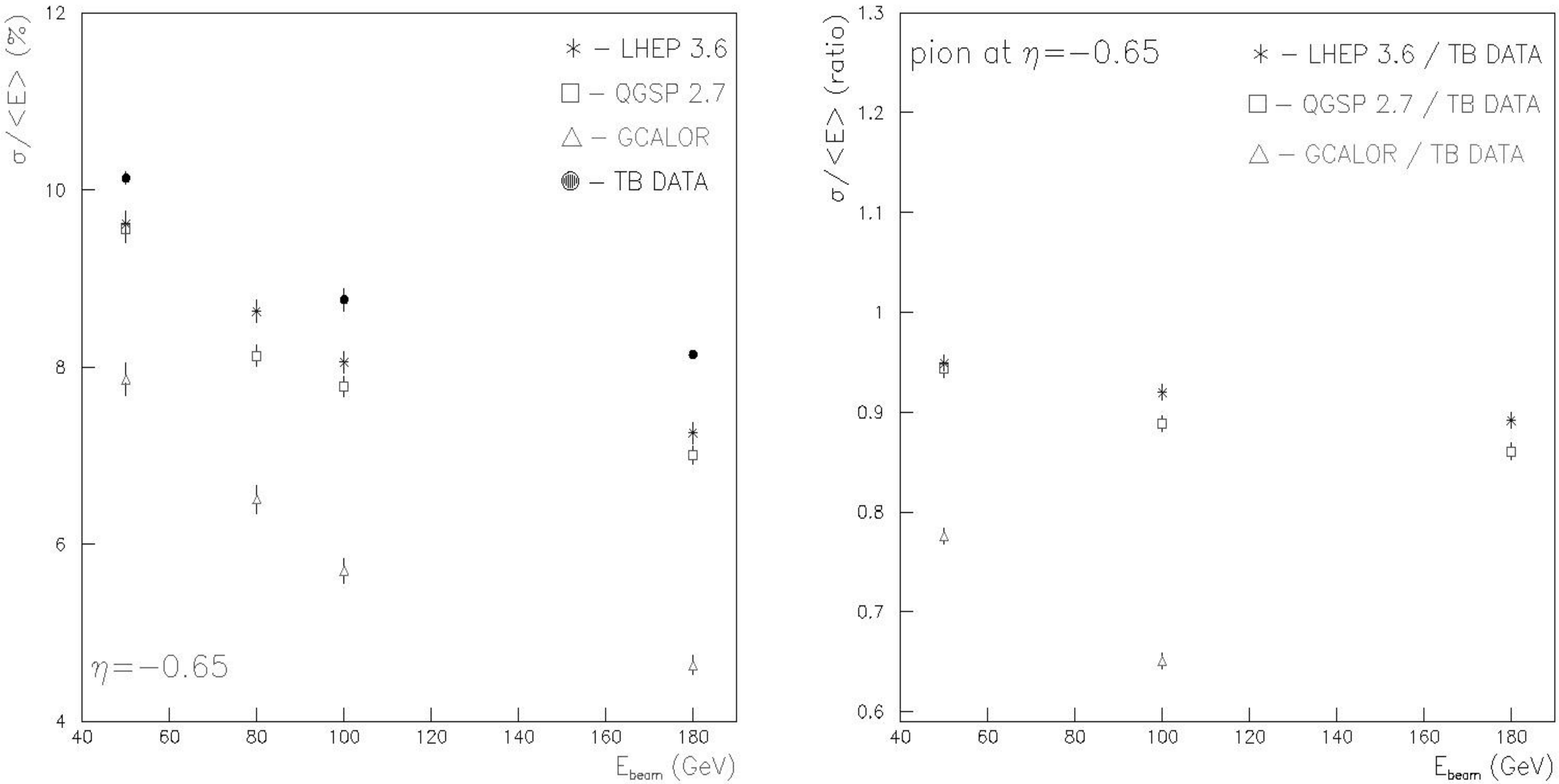
pion resolution





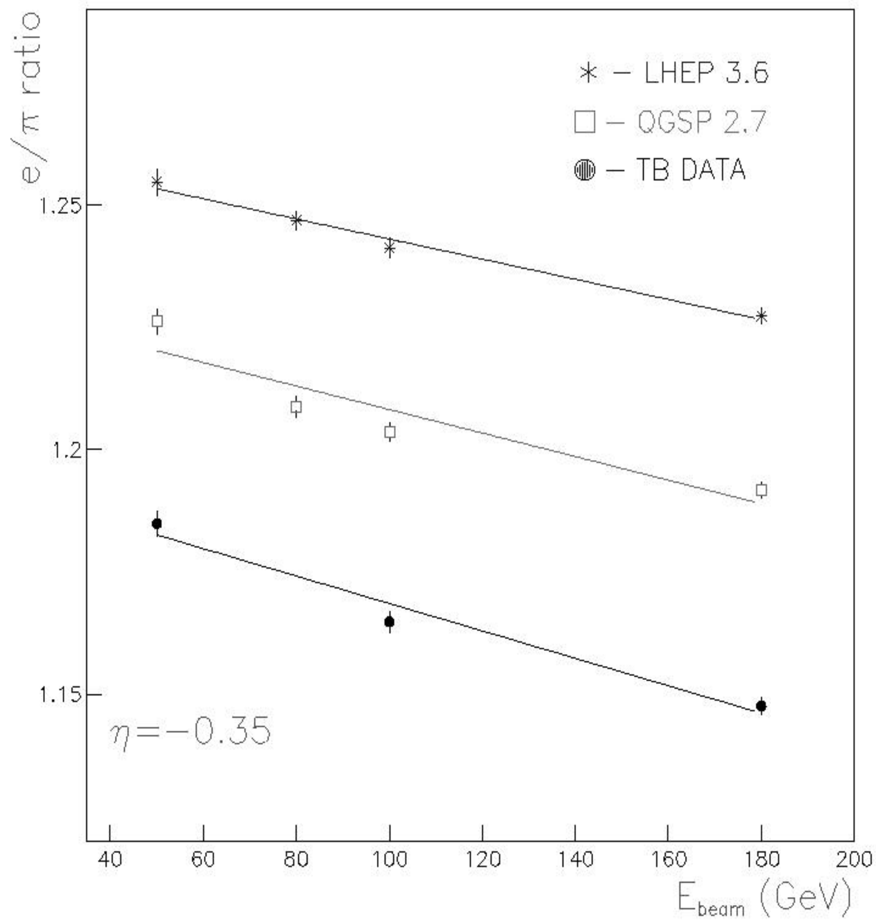
J.P. Wellisch,
CERN/PH

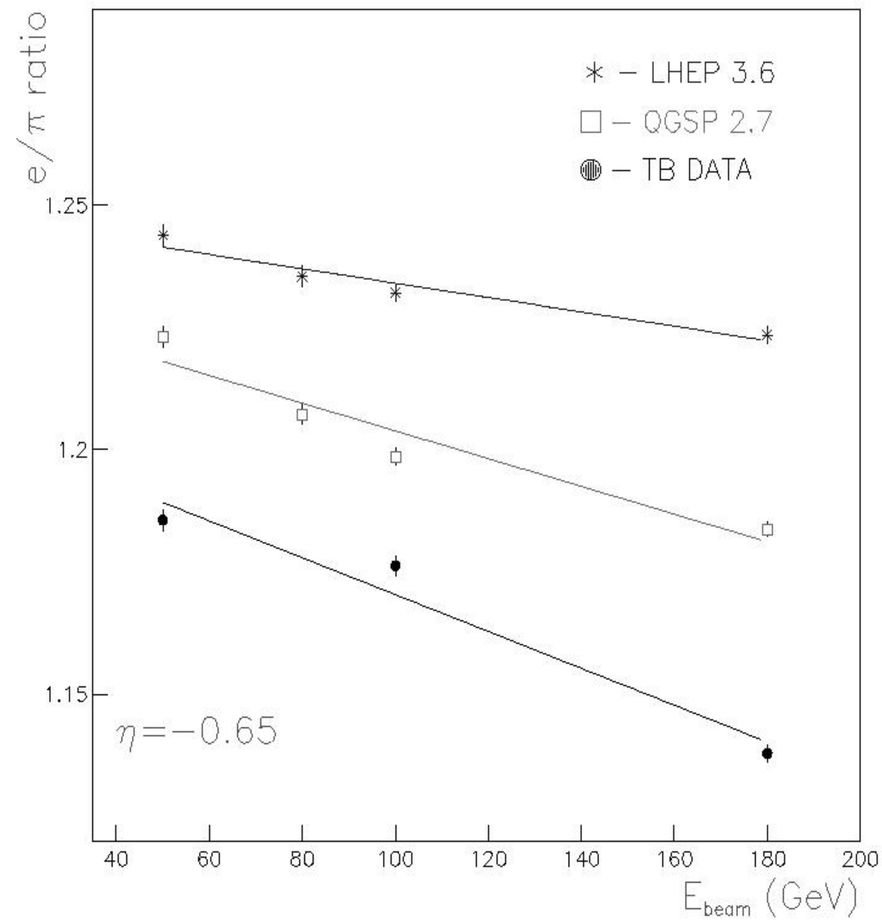
pion resolution



J.P. Wellisch,
CERN/PH

E_{beam} dependence of the e/π ratio





J.P. Wellisch,
CERN/PH

G4 Validation using CMS HCAL Test Beam

V. Daniel Elvira

LCG validation meeting

Fermilab
Discovering the Nature of Nature

Motivation

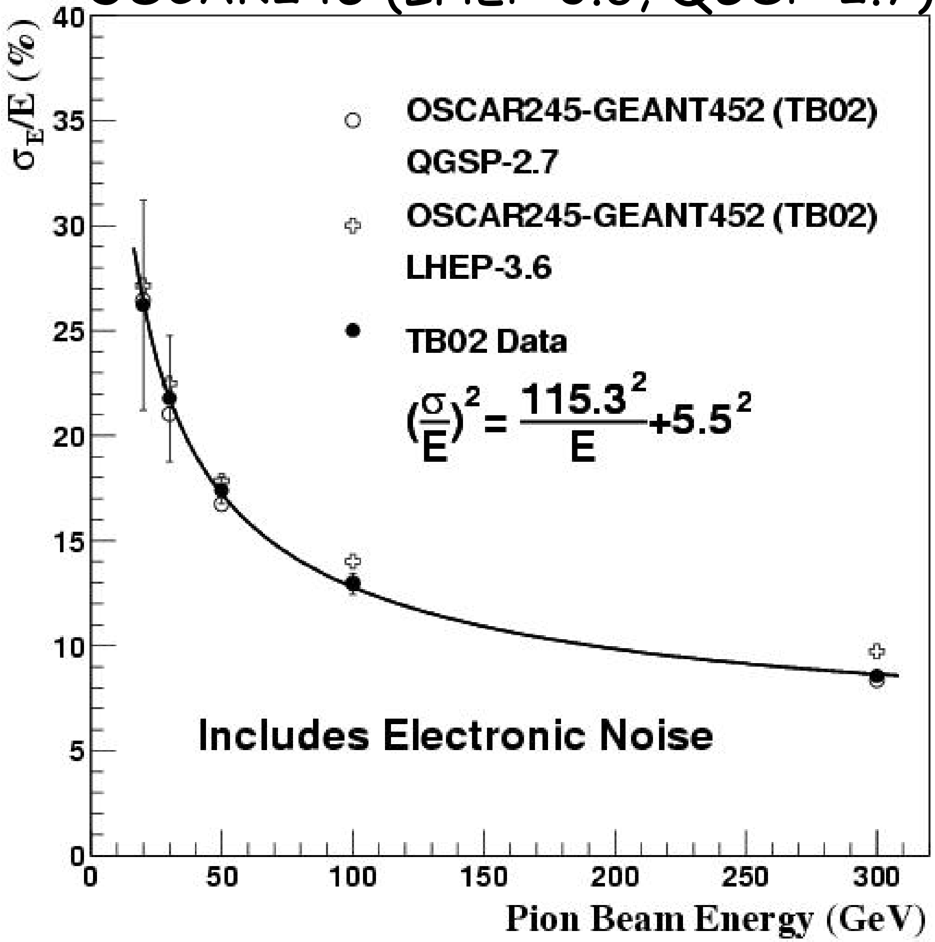
- Validation of GEANT4-OSCAR
- Understanding of the successive Hcal test beam experiments (02,03,04)

Use OSCAR_2_4_5 (G4.5.2), LHEP-3.6, QGSP-2.7
(HcalTB02 has been released as an OSCAR2 example)

- Beam Line System (trigger tiles & wire chambers)
- ECAL box (Crystal Matrix sub-system)
- HCAL Barrel
- HO
- Allow translation & rotation of both BL & ECAL box
- Root analysis package

Pion Energy Resolution

OSCAR245 (LHEP-3.6, QGSP-2.7)



Syst.

Data

E	$\sigma_E/E(\%)$	stat	bkgnd	calib
20.	26.22	0.15	5.00	0.1
30.	21.76	0.12	3.00	0.2
50.	17.40	0.10	0.60	0.2
100.	12.95	0.07	0.40	0.3
300.	8.55	0.05	0.00	0.3

Syst. Errors 100% correlated in Energy, uncorrelated with each other (added in quadrature)

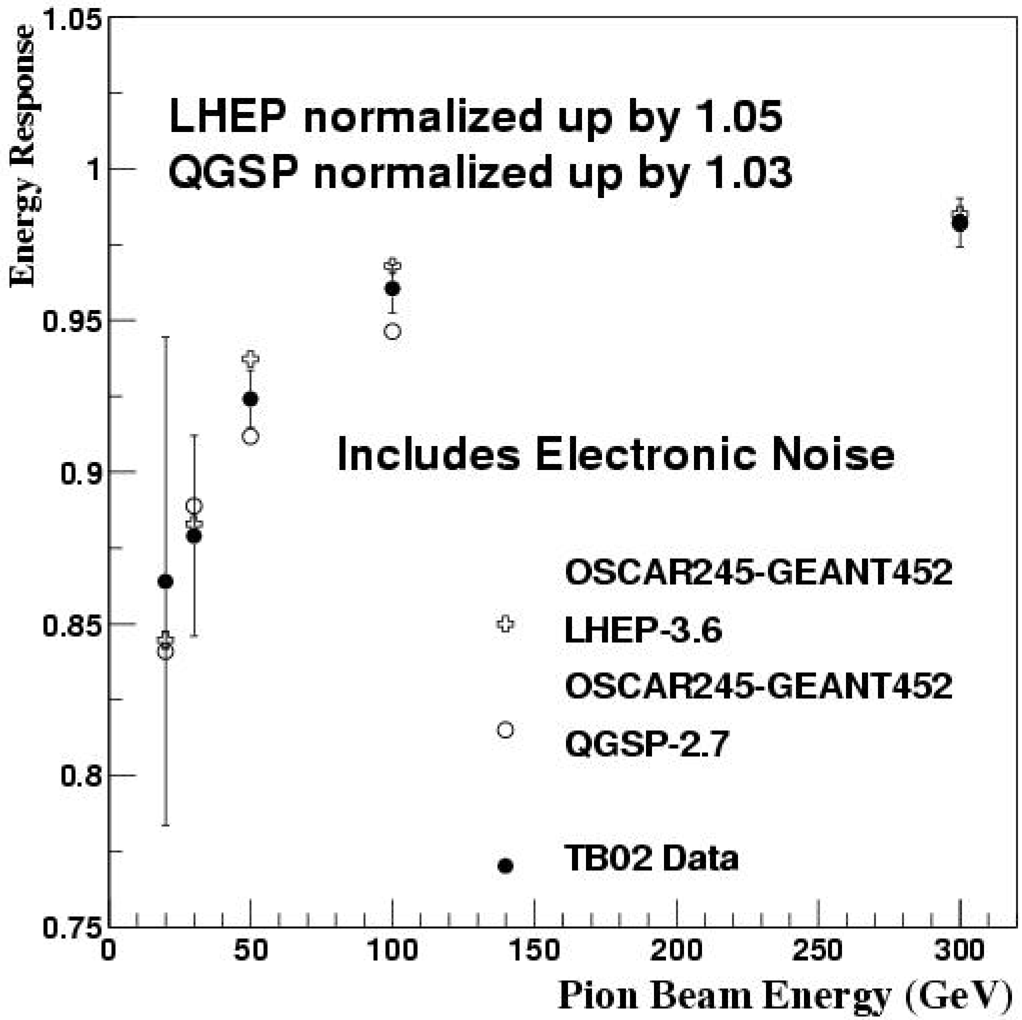
Excellent agreement in resolution

(LHEP a little higher than QGSP)

J.P. Wellisch,
CERN/PH

Pion Energy Linearity

OSCAR245 (LHEP-3.6, QGSP-2.7)



Syst.

Data

E	σ_E/E	stat	bkgnd	calib
20.	0.8640	0.0015	0.0800	0.008
30.	0.8790	0.0010	0.0320	0.008
50.	0.9240	0.0010	0.0050	0.008
100.	0.9604	0.0007	0.0003	0.008
300.	0.9823	0.0004	0.0003	0.008

Syst. Errors 100% correlated in Energy, uncorrelated with each other (added in quadrature)

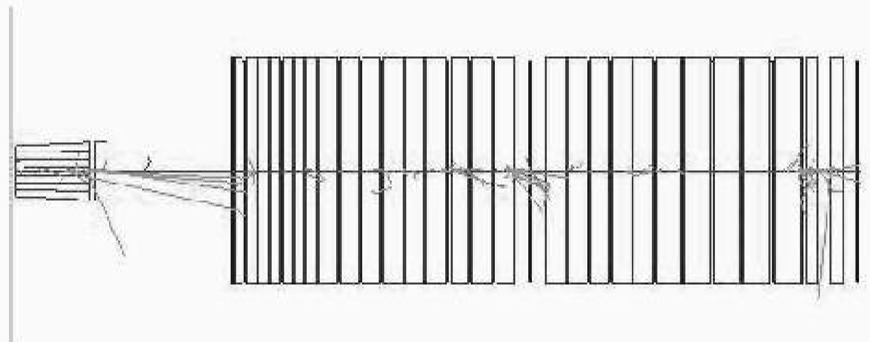
Excellent agreement in linearity

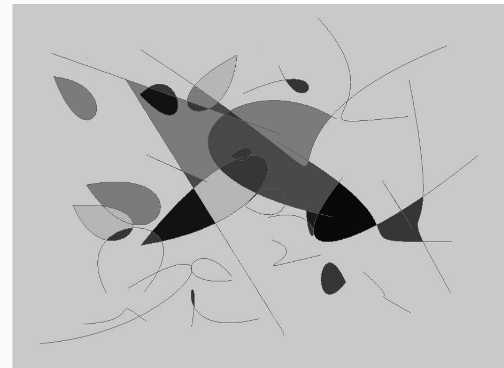
(LHEP/QGSP grows a little faster/slower than data)

J.P. Wellisch,
CERN/PH

Simulation

- Use GEANT 4.5.2.p02 with the Test Beam description given as one of the advance examples

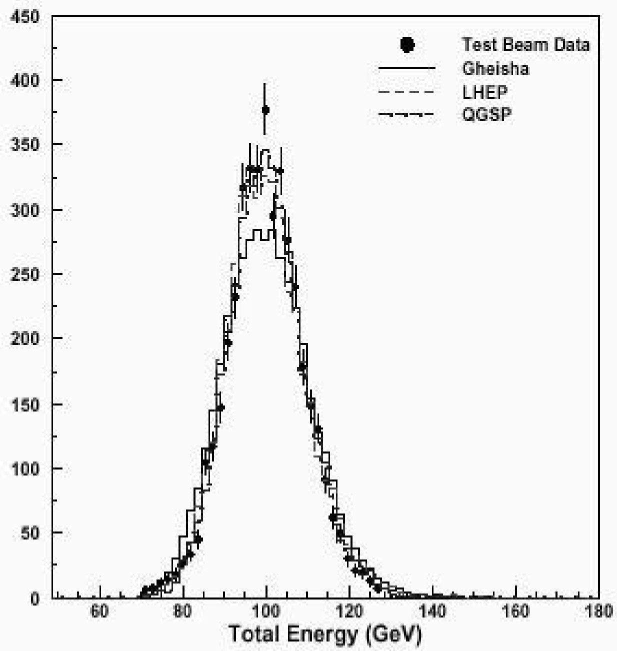




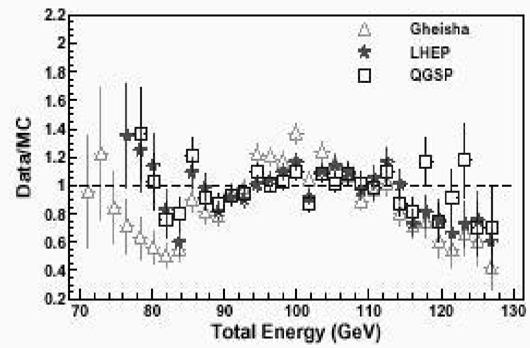
- ❒ The absorber layers are made of a special type of Brass (not Copper) of substantial lower density (interaction length)
- ❒ All Monte Carlo event samples are regenerated with the new setup definition and using the physics list of version PACK 2.3:
  - ❖ LHEP version 3.6
  - ❖ QGSP version 2.7
  - ❖ QGSC version 2.8
  - ❖ FTFP version 2.7

HCal alone data

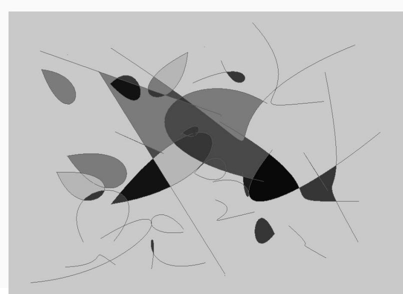
100 GeV π sample has been used to obtain the energy scale factor

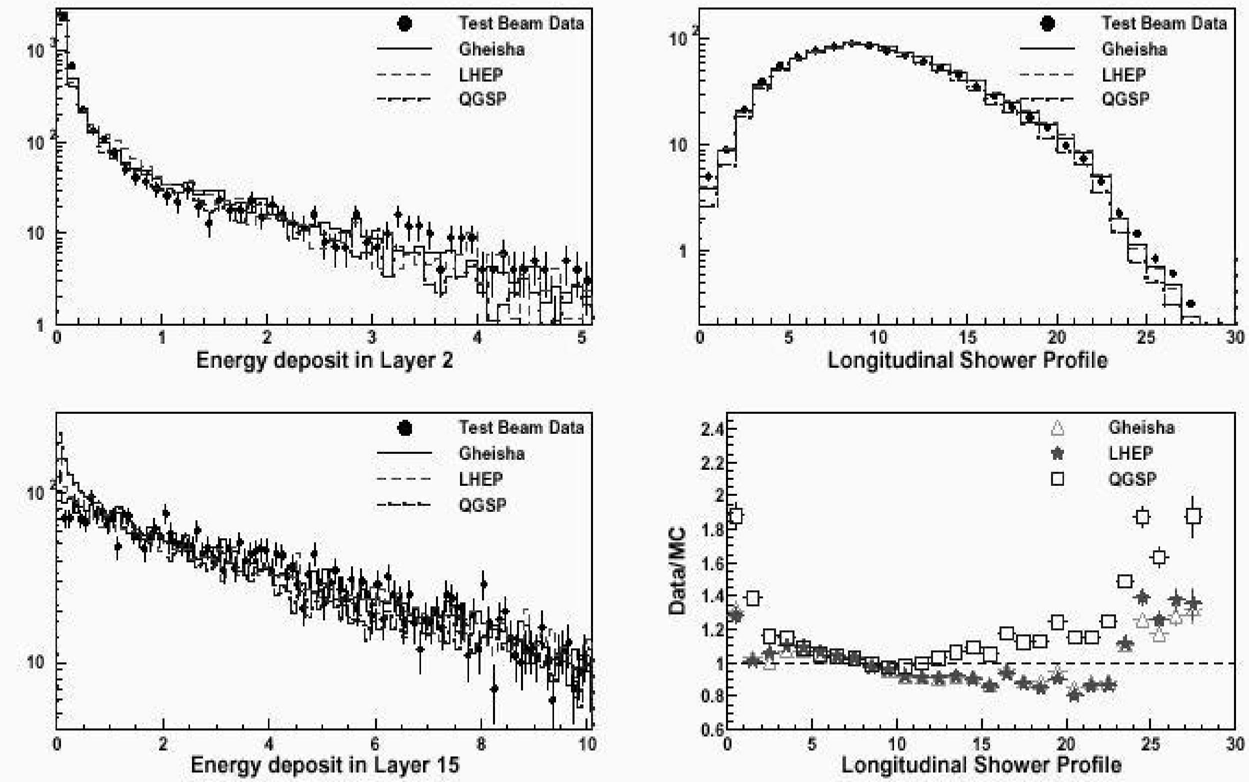


	σ (GeV)	RMS (GeV)
Data	9.2±0.1	9.4±0.1
LHEP	9.8±0.1	10.3±0.1
QGSP	9.2±0.1	9.5±0.1
Gheisha	10.2±0.1	11.0±0.1

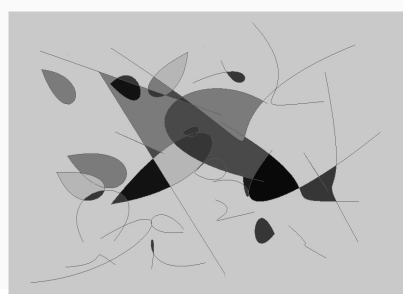


Geant4 models (particularly QGSP) provide good description of energy resolution

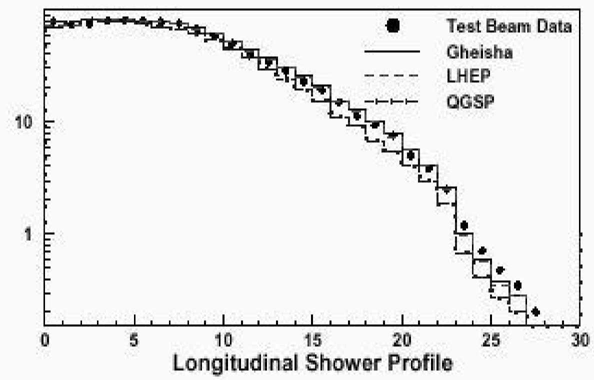


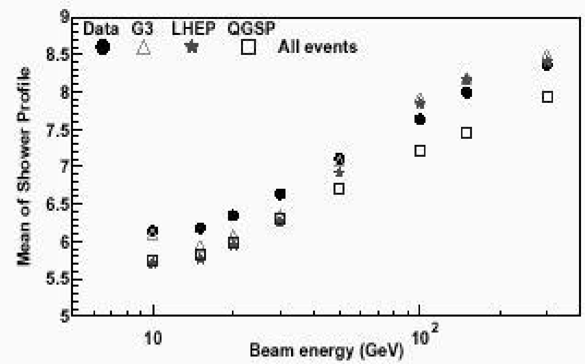


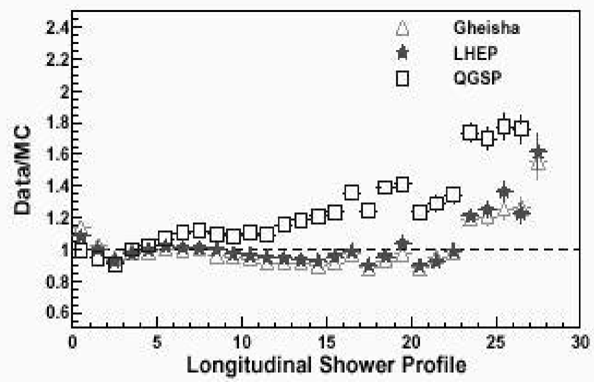
For longitudinal shower profile, data lie between predictions from LHEP and QGSP

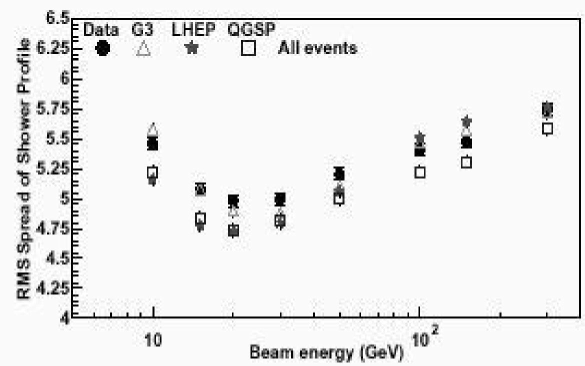


Longitudinal shower profile:

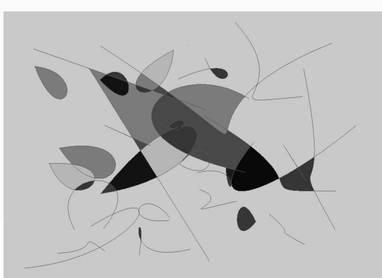








- Difference between data and Monte Carlo reduces at higher energies
- Parametrised models are in better agreement



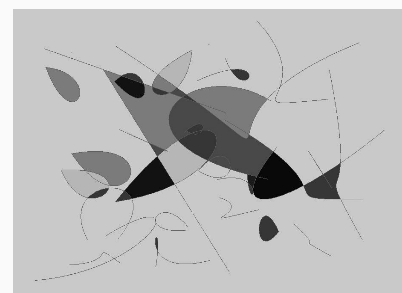
J.P. Wellisch,
CERN/PH

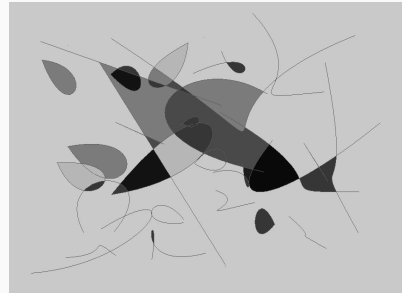
Pion Simulations for the ATLAS HEC Testbeam

A. Kiryunin, D. Salihagić, P. Strizenec

presented by P. Schacht

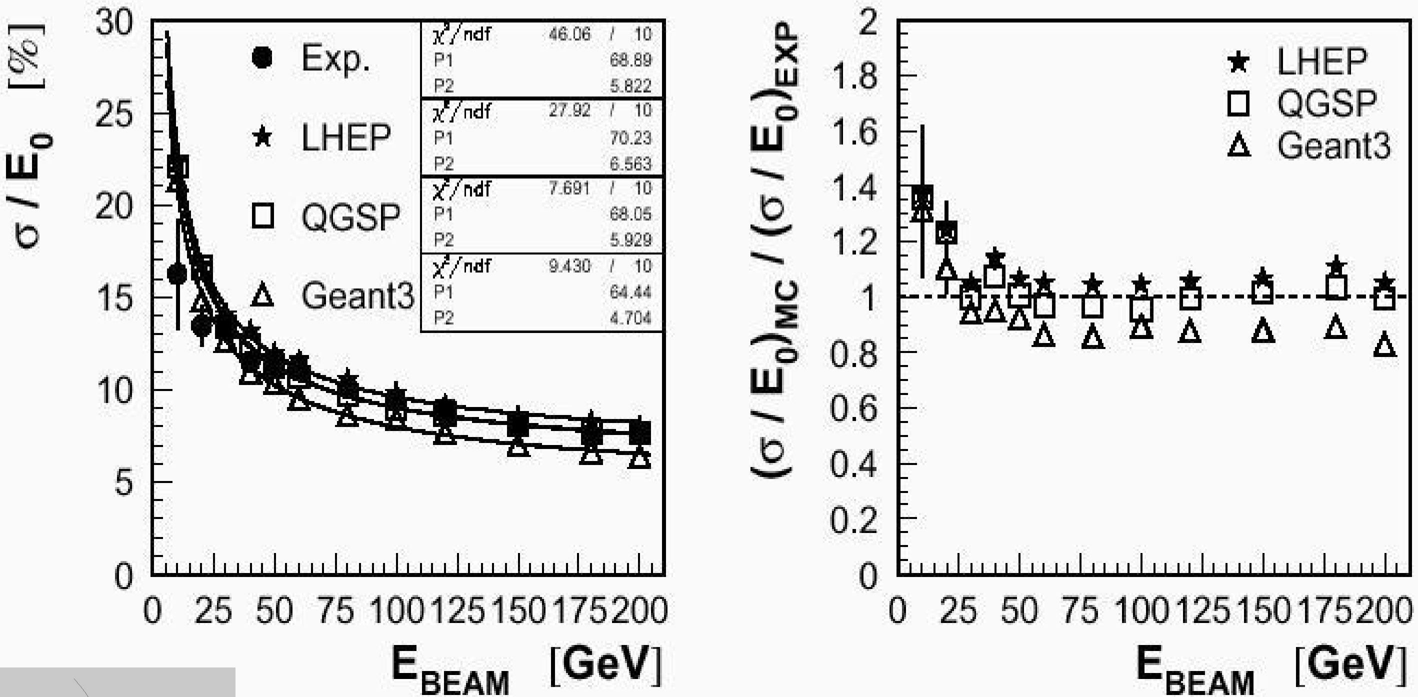
- No new results since December 2003 meeting *(http://agenda.cern.ch/age?a036494)*



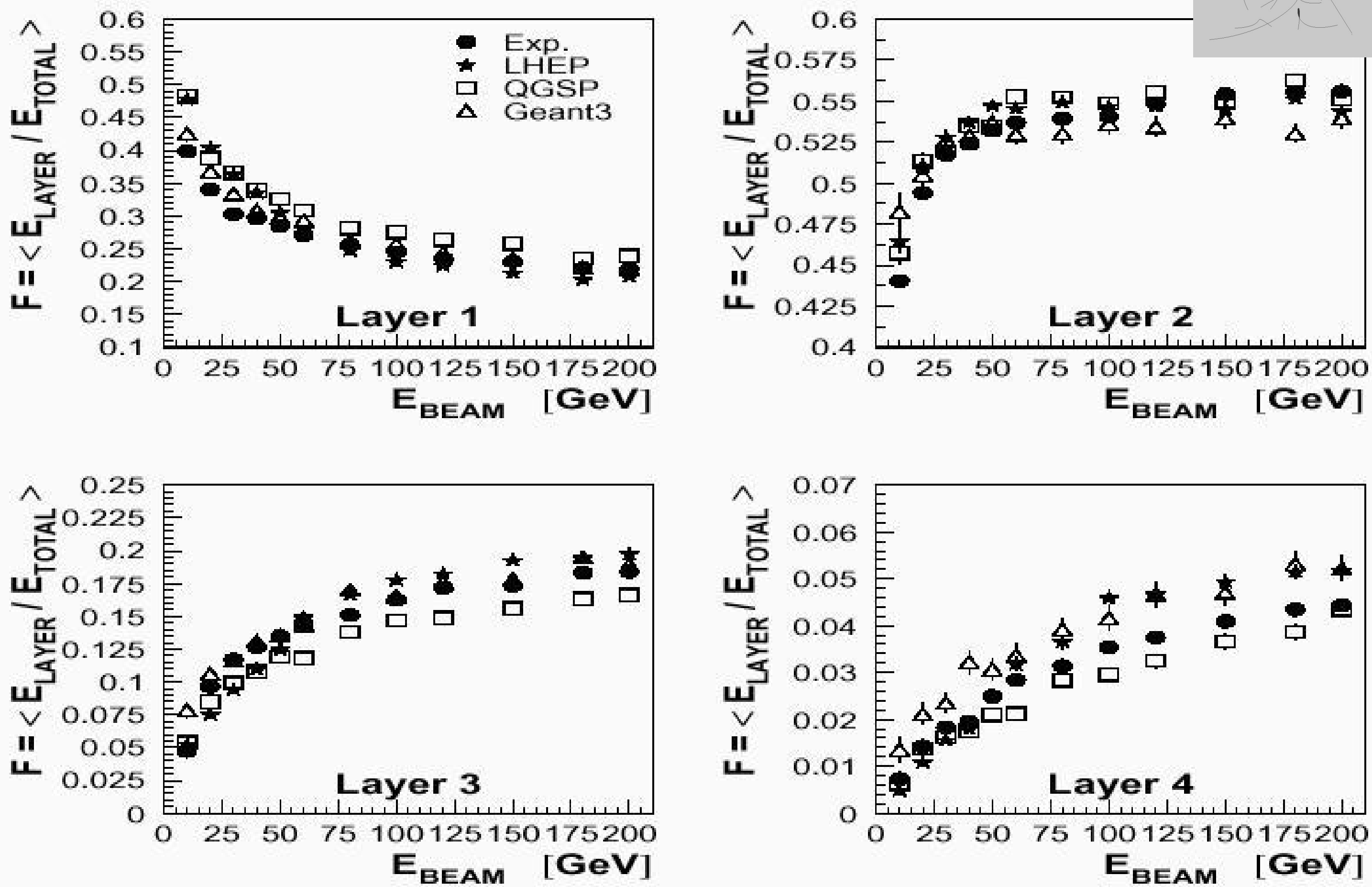


- HEC stand-alone testbeam
- Geant4
  - Version 5.0p01
  - Hadronic physics lists for calorimetry
    - ∗ LHEP 3.3
    - ∗ QGSP 2.3
  - 20 μm range cut
- Geant3
  - Version 3.21
  - G-CALOR (hadronic shower code)
  - 100 keV transport cuts and 1 MeV process cuts

Pion energy resolution

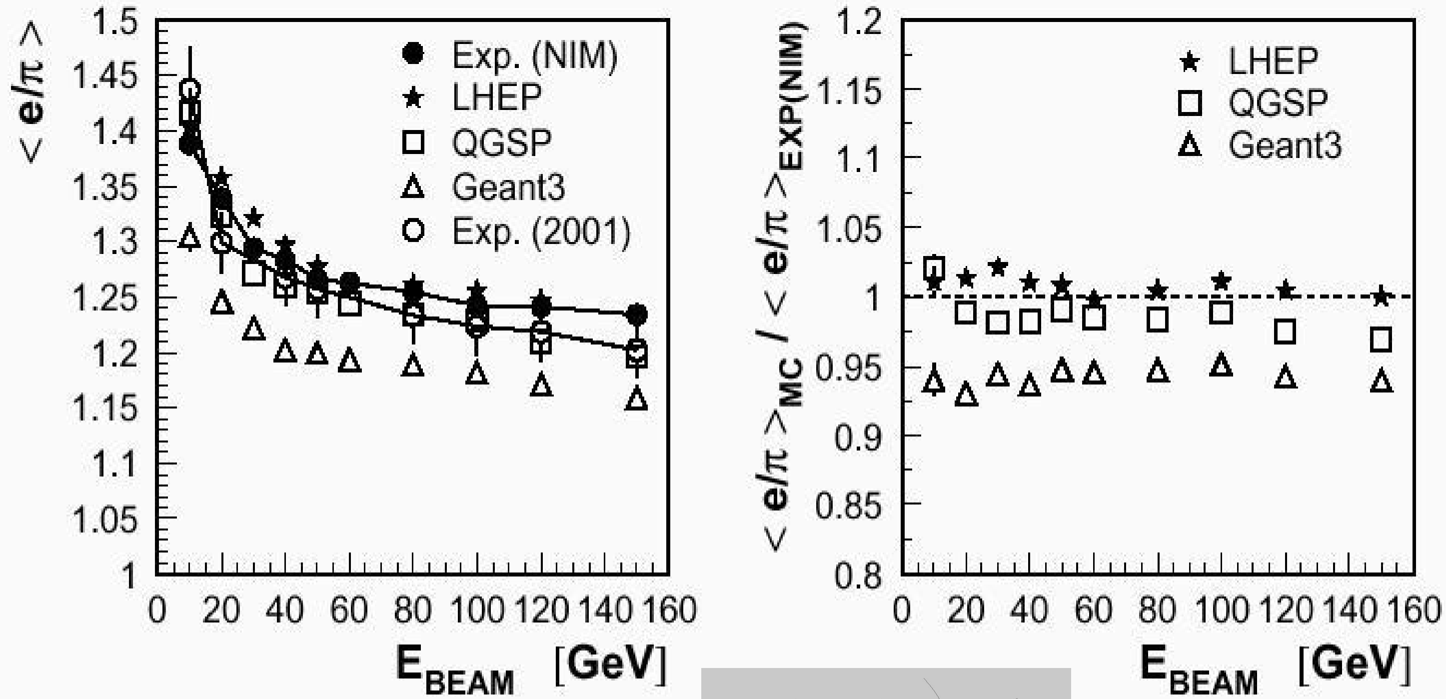


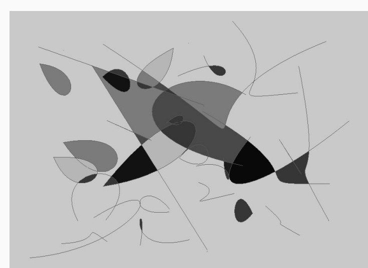
Fraction of energy in HEC layers



J.P. W
CERN/PH

Ratio e/π


< e/π >
Exp. (NIM)
LHEP
QGSP
Geant3
Exp. (2001)
E_BEAM [GeV]
< e/π >_MC / < e/π >_EXP(NIM)
LHEP
QGSP
Geant3
E_BEAM [GeV]



The END?

Additional reading:

- The GHAD WWW pages.
  - http://cmsdoc.cern.ch/~hpw/GHAD/HomePage/
- The LCG physics list pages.
  - http://cmsdoc.cern.ch/~hpw/GHAD/LCGPage
- The geant4 physics reference manual.
  - http://geant4.web.cern.ch/geant4/G4UsersDocuments/Overview/html/index.html
- References given throughout these lectures.
  - Slides available from the CERN main page, and the corresponding entries in the agenda system.

The END.