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

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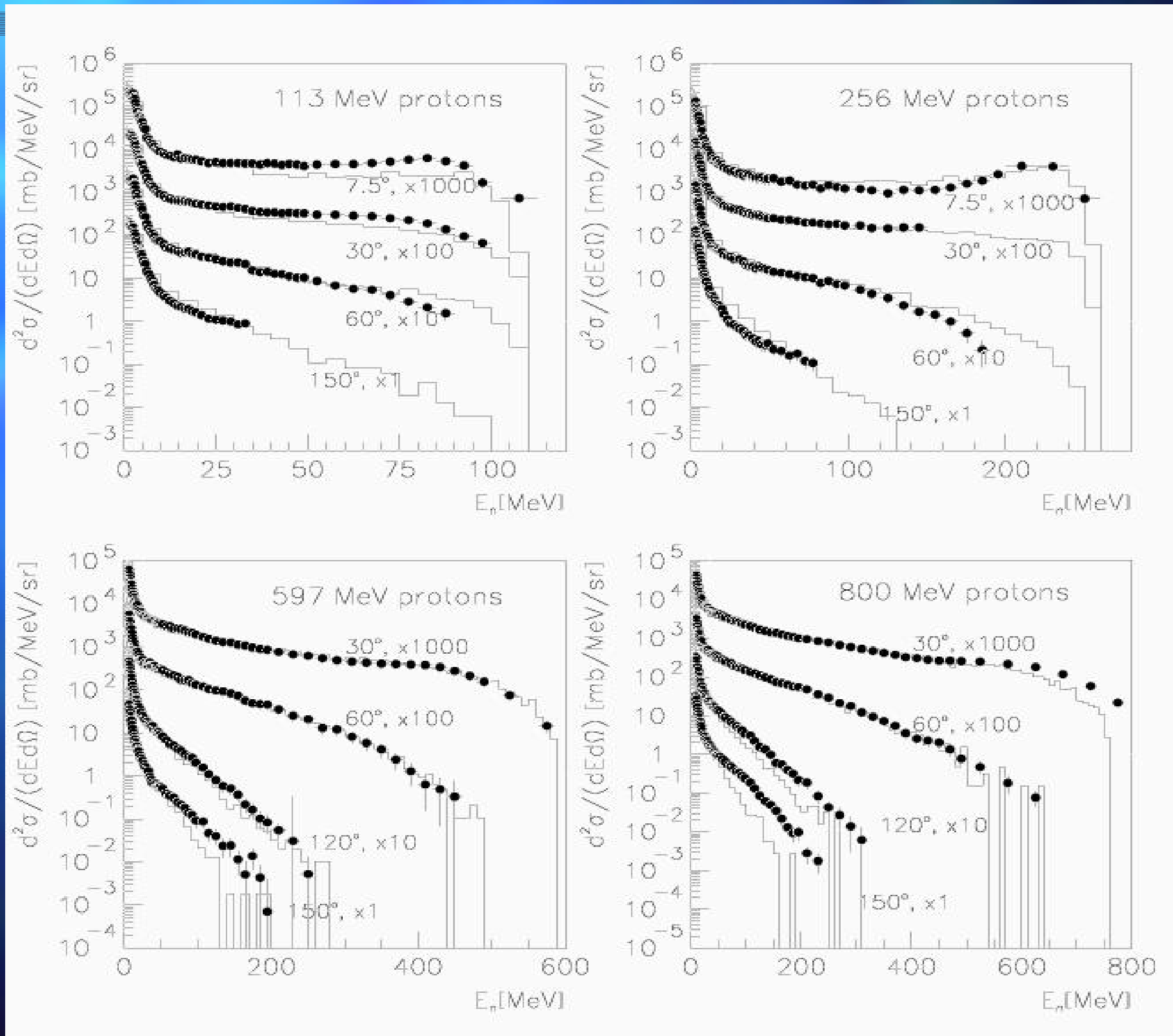
The Monte Carlo Roadmap

- 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.
  - Examples of electromagnetic showers.
  - Selected topics on electromagnetic shower physics.

Pre-equilibrium decay

- Example: Griffin's Exciton model
  - Phys.Rev.Lett. 17, 9 (1966)

Scattering off lead at various angles and energies



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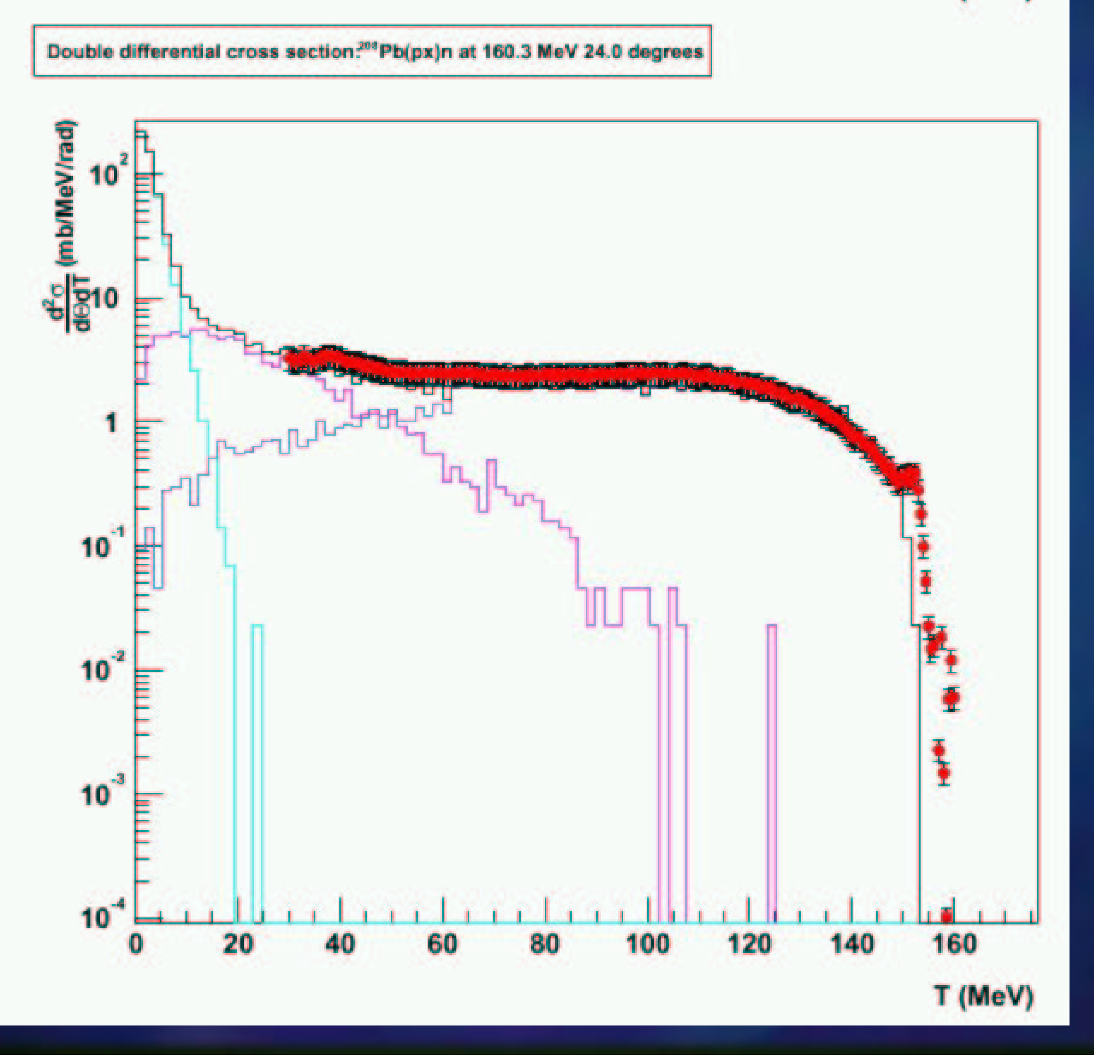
Contributions of the model components to the neutron spectrum



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Exciton pre-compound model

- In this model, the pre-compound nucleus is viewed as falling apart onto two parts.
  - A system of excitons that carry the excitation energy and the momentum of the excited system
  - A nucleus, that itself is otherwise undisturbed (Bogolubov's transformation diagonal, excitons as quasi-particles)

- The initial state of pre-equilibrium decay consists of
  - A, Z of the pre-compound nucleus,
  - The number pf excitons (n)
  - The number of holes (h)
  - The number of charged excitons (c)
  - The momentum and mass of the exciton system

- This system is allowed to evolve, and collisions between excitons ($\Delta n=0,-2$), as well as collisions of excitons with nucleons ($\Delta n=2$) are put into competition with particle or fragment emission.
- The pre-compound transitions and emissions are iterated, until the residual system corresponds to an equilibrated nucleus.

Transition probabilities

- The probability of changing the exciton number by Δn is defined by the matrix element of the allowed transitions, and the density of accessible final states

$$\omega_{\Delta n}(n,U) = \frac{2\pi}{h}\left\langle |M|^2 \right\rangle \rho_{\Delta n}(n,U)$$

Level densities

- For further calculation, assumptions have to be made about the level densities.
- If we assume an equidistant scheme of single particle levels with level density $g \approx 0.595aA$ where *a* is the level density parameter, we can derive the density of states for n excitons as a function of the excitation energy as

$$\rho_n(U) = \frac{g(gU)^{n-1}}{p!h!(n-1)!}$$

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- Where the densities of the accessible final states can be written as (Nucl.Phys.A205, 545 (1973))

$$\rho_{\Delta n=+2}(n,U)=\frac{1}{2}g\frac{\left[gU-F(p+1,h+1)\right]^2}{n+1}\left[\frac{gU-F(p+1,h+1)}{gU-F(p,h)}\right]^{n-1}$$

$$\rho_{\Delta n=0}(n,U)=\frac{1}{2}g\frac{\left[gU-F(p,h)\right]}{n}\left[p(p+1)+4ph+h(h+1)\right]$$

$$\rho_{\Delta n=-2}(n,U)=\frac{1}{2}gph(n-2)$$

- With

$$F(p,h)=(p^2+h^2+p-h)/4-h/2$$

- To estimate the matrix element, we assume that the creation probability for 2 excitons is the scattering probability of nucleon-nucleon scattering

$$\omega_{\Delta n=+2}(n,U)=\frac{<\sigma(v)v>}{V_{scat.}}$$

- Where we can estimate

$$V_{scat.}=\frac{3}{4}\pi\left(2r_c+\lambda/_{2\pi}\right)^3$$

- with λ being the De Broglie wave length, corresponding to a relative velocity $<v>=\sqrt{2T_{rel}/m}$
- Here m is the nucleon mass, and $r_c=0.6\,fm$.

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- Assuming the the averaging of velocity and cross-section factorizes, and taking the cross-section as

$$\sigma(v) = 0.5 * \left[\sigma_{pp}(v) + \sigma_{np}(v)\right] Pauli(T_F / T_{rel})$$

- We have all informartion to calculate the transition probabilities.

$$\omega_{\Delta n=0}(n,U) = \frac{<\sigma v>}{V_{scat.}} \frac{n+1}{n} \left[\frac{gU - F(p,h)}{gU - F(p+1,h+1)}\right]^{n+1} \frac{p(p-1)+4ph+h(h-1)}{gU - F(p,h)}$$

$$\omega_{\Delta n=-2}(n,U) = \frac{<\sigma v>}{V_{scat.}} \left[\frac{gU - F(p,h)}{gU - F(p+1,h+1)}\right]^{n+1} \frac{ph(n+1)(n-2)}{(gU - F(p,h))^2}$$

Emission probabilities

- In geant4, these are similar to the emission probabilities of the Weisskopf evaporation model.
- We calculate the probability to emit a nucleon in the energy interval $[T, T+dT[$

$$W_N(n,U,T) = \sigma_{N,inverse}(T)\frac{(2s_N+1)\mu_N}{\pi^2 h^3} R_N(p,h)\frac{\rho_{n-N}(E^*)}{\rho_n(U)}T$$

Fragment emission

- To justify fragment production, we need to assume that the nucleons in the nucleus condense into fragments with a certain probability γ. We write for the probability to find a fragment with nucleon contents N in the nucleus as

$$\gamma_N \propto N_N^3 (V_N / V_A)^{N-1} \approx N_N^3 (N_N / A)^{N-1}$$

Emission probabilities

- The emission probabilities are identical in structure to the nucleon emission probabilities, except for the condensation probability and a level density factor for the fragment

$$W_N(n,U,T) = \gamma_N \frac{\rho(N,0,T+Q)}{g(T)} \sigma_{N,inverse}(T) \frac{(2s_N+1)\mu_N}{\pi^2 h^3} R_N(p,h) \frac{\rho_{n-N}(E^*)}{\rho_n(U)} T$$

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Thermalization

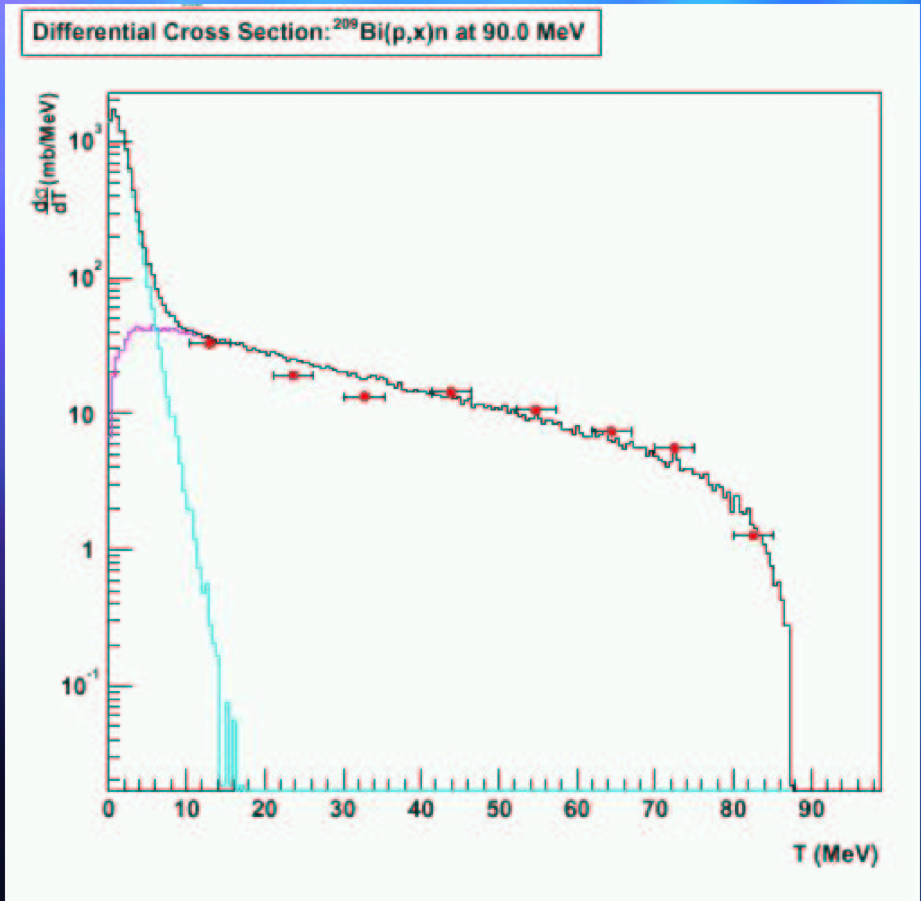
- In statistical equilibrium, the transition probabilities (ω) for creating ($\Delta n=+2$) or destroying ($\Delta n=-2$) excitons are equal.
- Hence the equilibrium number of excitons can be found from

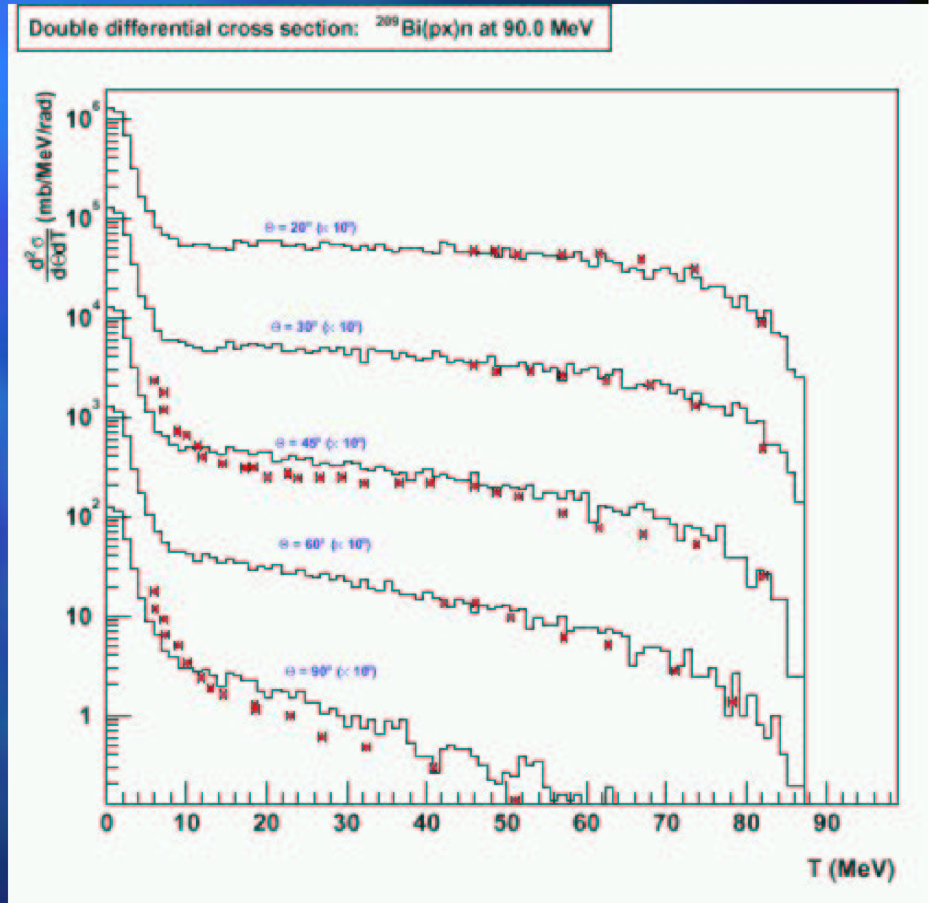
$$\omega_{+2}(n_{equ.},U) = \omega_{-2}(n_{equ.},U)$$

- To be

$$n_{eq} = \sqrt{2gU}$$

90 MeV protons scattering off Bismuth





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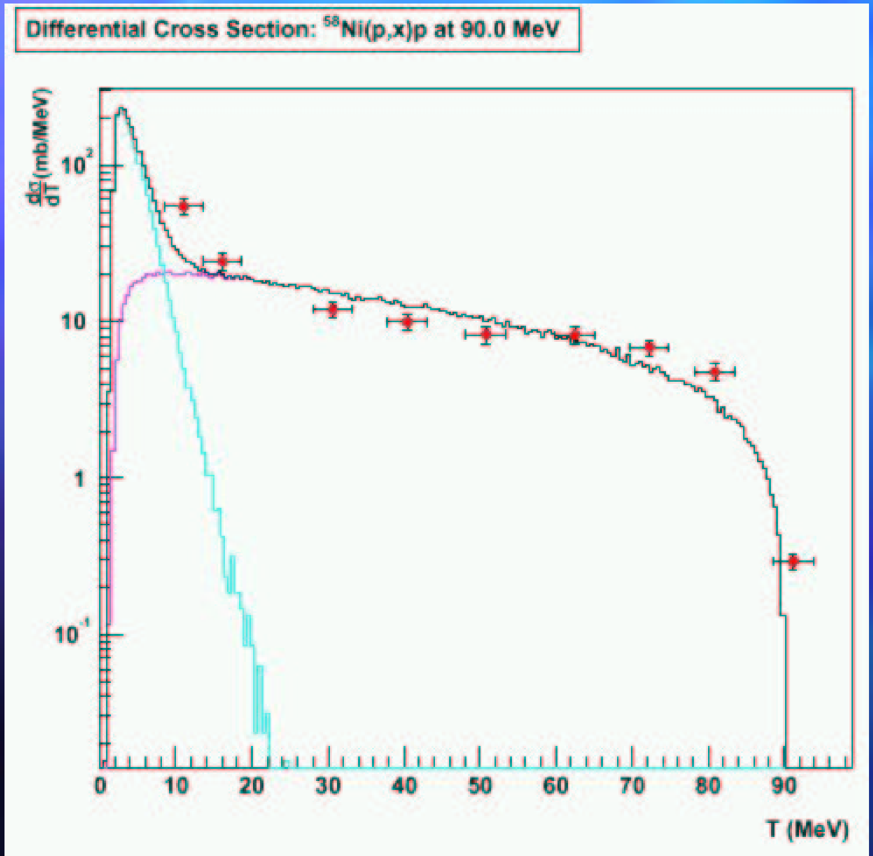
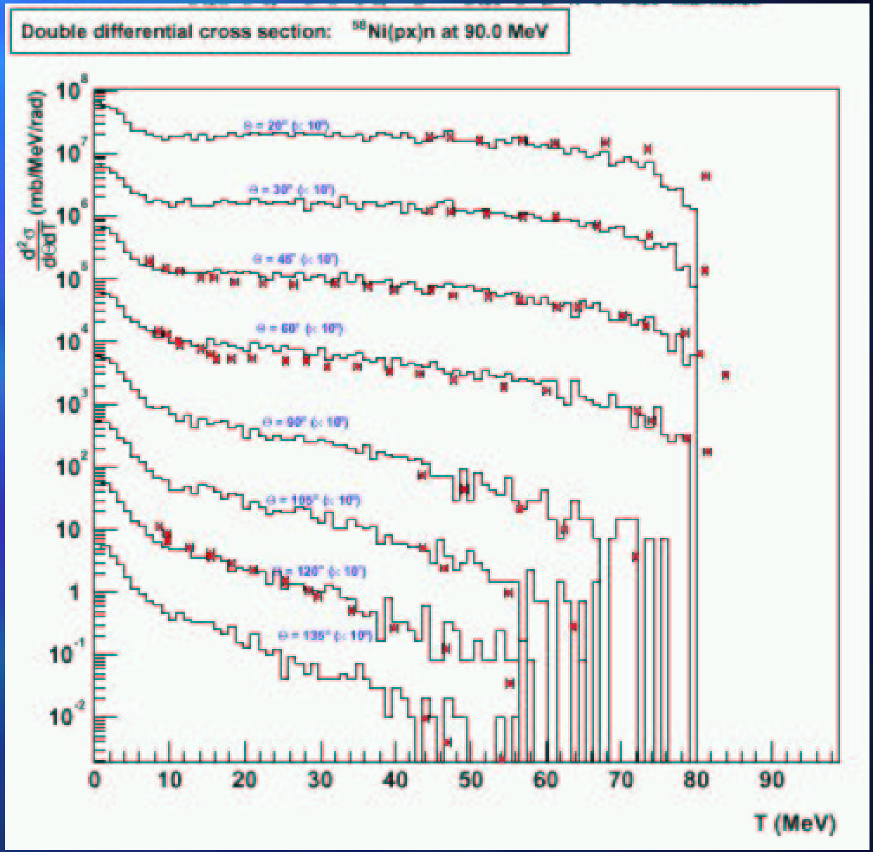
90 MeV protons scattering off Nickel





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Statistical evaporation models.

- Weisskopf-Ewing evaporation
- Furihata's generalized evaporation model
- Fission
- Photon evaporation
- Fermi-breakup
- Multifragmentation

- Notes on evaporation
  - Treats excited nuclear system in equilibrium
  - Evaporation produces most of the neutrons in a hadronic shower
  - It defines to a large extent the isotope that is left after the reaction, and may activate the detector material

The Weisskopf Ewing model

- Weisskopf's treatment is based on the principle of detailed balance

$$\rho(i)P_{i\to f} = \rho(f)P_{f\to i}$$

- Since the probability $P_{f\to i}$, is proportional to the cross-section of the inverse reactions, we can write the probability of a nucleus with excitation energy U to emit a particle j with kinetic energy T in its ground state as

$$P_j(T)dT = \frac{(2s_j+1)m}{(\pi\hbar)^2}\sigma_{scat.}\frac{\rho_f(E_{\max}-T)}{\rho(U)}TdT$$

- In general, we take Dostrovsky’s cross-section for the inverse reactions

$$\sigma_{scat.}(T) = \pi R^2 \alpha \left(1 + \frac{\beta}{T}\right)$$

- With

$$\alpha = 0.76 + 2.2 A^{-1/3},$$

$$\beta = (2.12 A^{-2/3} - 0.05) / \alpha$$

- For neutrons, and use Shapiro’s tabulation (PhysRev 90, 171 (1953)) for α and β=-’coulomb barrier’ for charged particles

- The coulomb barrier calculated from electrostatics is not directly applicable, but needs correction for various effects, for example for tunneling through the barrier.
- To keep the probability distributions in an integrable form, a tabulated coefficient (also from Shapiro) can be used

$$V_j = k_j \frac{Z_j Z_f e^2}{R_c}$$

- For the contact radius, please see A.S.Iljinov, et. al Intermediate Energy Nuclear Physics, CRC press, 1994

- The simplest and widely used level densities are based on those of Weisskopf, based on a completely degenerate Fermi gas.

$$\rho(E) \propto \exp\left(2\sqrt{a(E-\delta)}\right)$$

- We use this with a level density parameter of

$$a(E,A,Z) = a'(A)\left\{1+\frac{\delta}{E}\left(1-\exp(-\gamma E)\right)\right\}$$

- With parameters taken from Ilijof at al (NPA 543, 517 (1992)), and nuclear shell corrections from Truran, Cameron, and Hilf.

It can be more sophisticated…

- Furihata's general evaporation model (NIM,B171,251(2000)
  - with parameters from Matuse, et al (Phys.Rev.C26,2338)
  - Based on the Fermi gas model, the level density functions can be written as

$$\rho(E) = \begin{cases} \dfrac{\sqrt{\pi}}{12} \dfrac{e^{2\sqrt{a(E-\delta)}}}{a^{1/4}(E-\delta)^{5/4}}, & E \geq E_x \\ \dfrac{1}{T} e^{(E-E_0)/T}, & E < E_x \end{cases}$$

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- With $E_x = U_x + \delta, \;\; U_x = 15 - / M_d - 2.5$
- the nuclear temperature

$$\frac{1}{T} = \sqrt{\frac{a}{U_x} - 1.5 U_x}$$

- and

$$E_0 = E_x - T\left(\log(T) - \log(a/4) - (5/4)\log(U_x) + 2\sqrt{aU_x}\right)$$

$$P_j(\varepsilon)dT = \frac{(2s_j+1)m}{(\pi\hbar)^2}\sigma_{scat.}\frac{\rho_f(E_{\max}-\varepsilon)}{\rho(U)}\varepsilon d\varepsilon$$

- Substituting this into the formula for the emission probabilities, we get the width for fragment emission

$$\Gamma_j = \frac{\sqrt{\pi} g_j \pi R_d^2 \alpha}{12\rho E^*} \bullet \begin{cases} \{I_1(t,t_x) + (\beta - V)I_0(t)\}, \varepsilon_j^{\max} - V_j < E_x \\ \left\{ \begin{matrix} I_1(t,t_x) + I_3(s,s_x)e^s + \\ (\beta + V)(I_0(t_x) + I_2(s,s_x)e^s) \end{matrix} \right\}, \varepsilon_j^{\max} - V_j \geq E_x \end{cases}$$

- here $t = (\varepsilon_j^{\max} - V_j)/T, t_x = E_x/T, s = 2\sqrt{a(\varepsilon_j^{\max} - V_j - \delta_j)}, s_x = 2\sqrt{a(E_x - \delta)}.$

$$I_0(t) = e^{-E_0/T}(e^t - 1),$$

$$I_1(t,t_x) = e^{-E_0/T}T[(t - t_x + 1)e^{t_x} - t - 1]$$

$$I_2(s,s_x) = \sqrt{8}\{(s^{-3/2} + 1.5s^{-5/2} + 3.75s^{-7/2}) - (s_x^{-3/2} + 1.5s_x^{-5/2} + 3.75s_x^{-7/2})\}$$

$$I_3(s,s_x) = \frac{1}{\sqrt{8}}\{2s^{-1/2} + 4s^{-3/2} + 13.5s^{-5/2} + 60.0s^{-7/2} + 325.125s^{-9/2} -$$
$$[(s^2 - s_x^2)s^{-3/2} + (1.5s^2 + 0.5s_x^2)s_x^{-9/2} + (3.75s^2 + 0.25s_x^2)s_x^{-7/2} +$$
$$(12.875s^2 + 0.625s_x^2)s_x^{-9/2} + (59.0625s^2 + 0.9375s_x^2)s^{-11/2} + (324.8s^2 + 3.28s_x^2)s_x^{-13/2}]\}$$

- 60 nuclids up to Mg(28) are considered, including their quasi-stable excited states with half-lives

$$T_{1/2} / \ln(2) > \hbar / \Gamma_j^*$$

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Summary

- We have looked at inelastic hadron nuclear reactions and some of the modeling possibilities realized in geant4.
- In doing so, we covered about 20% of the geant4 hadronic models (8 of 37 packages).
- For the remaining majority, please refer to the physics reference manual.

Part 3

Trying to answer the question:

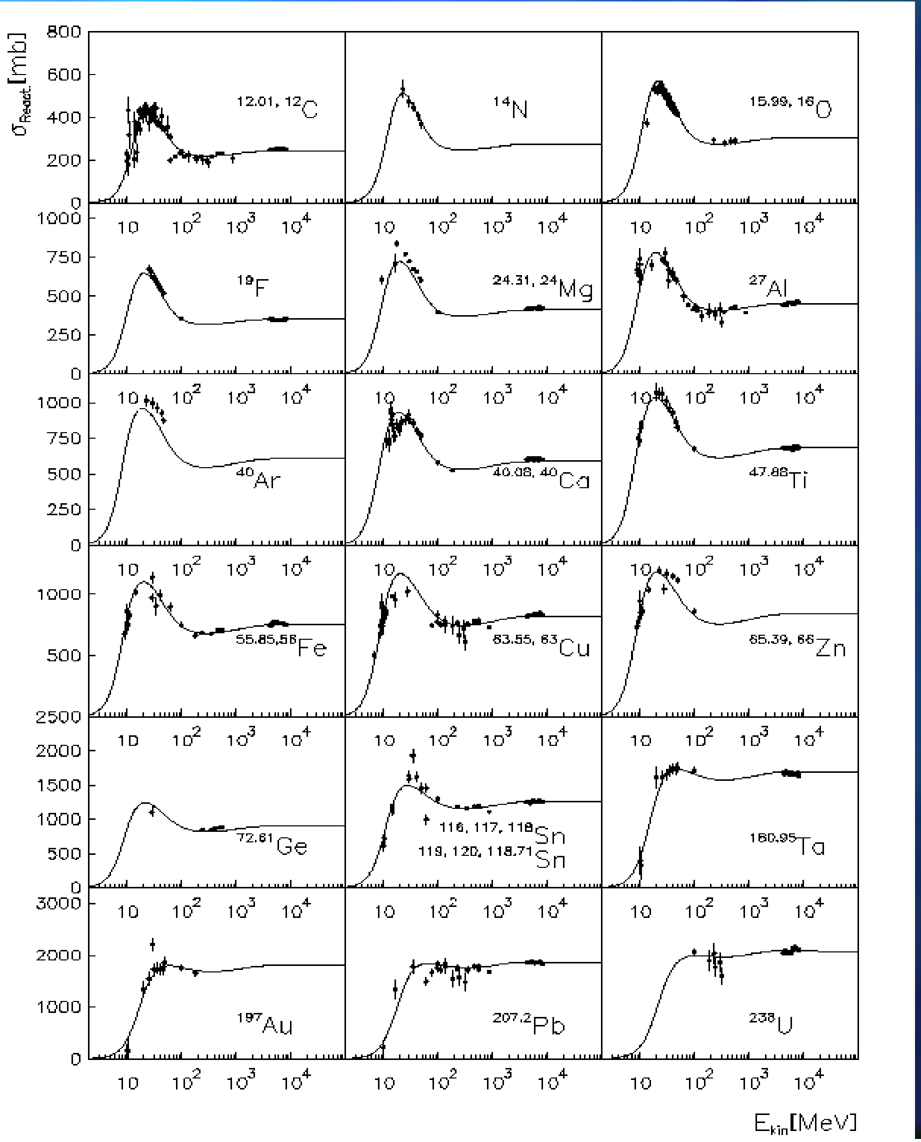
How good is it really?

Verification – grouped into sections

- The verification effort of the geant4 hadronic working group is grouped into several sections:
  - Inclusive cross-sections
  - Thin target comparisons
  - Verification of model components
  - Code comparisons (least effective)
  - Complete application tests
  - Robustness.
- I give a few examples of each in the following slides.

A few total cross-section examples

Proton reaction cross-section:



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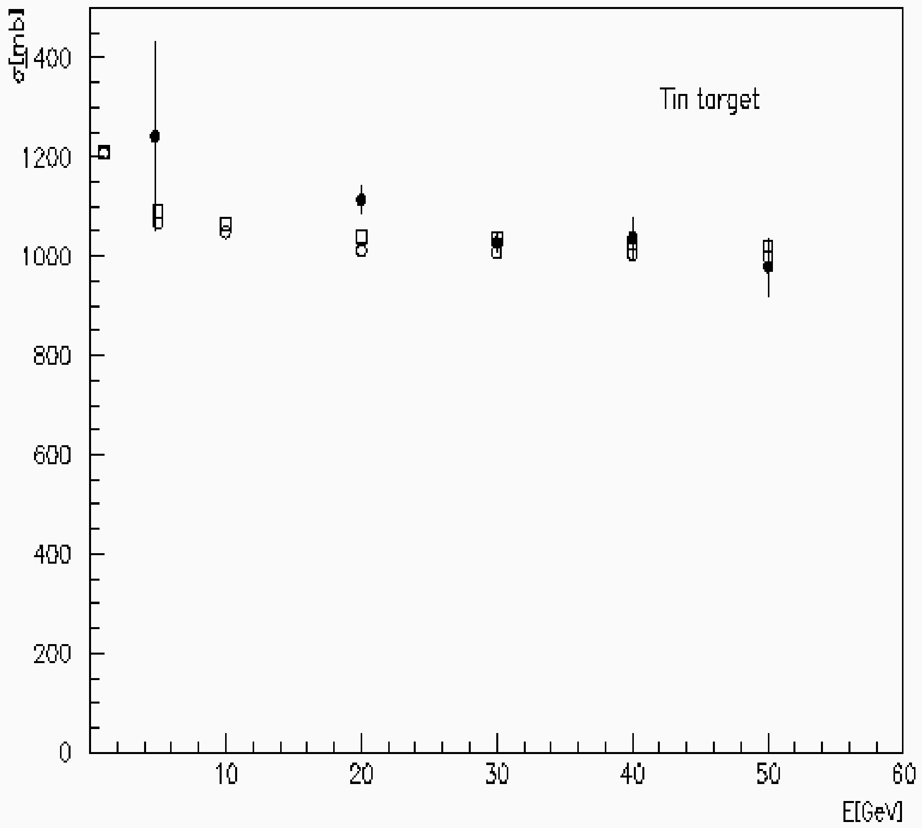
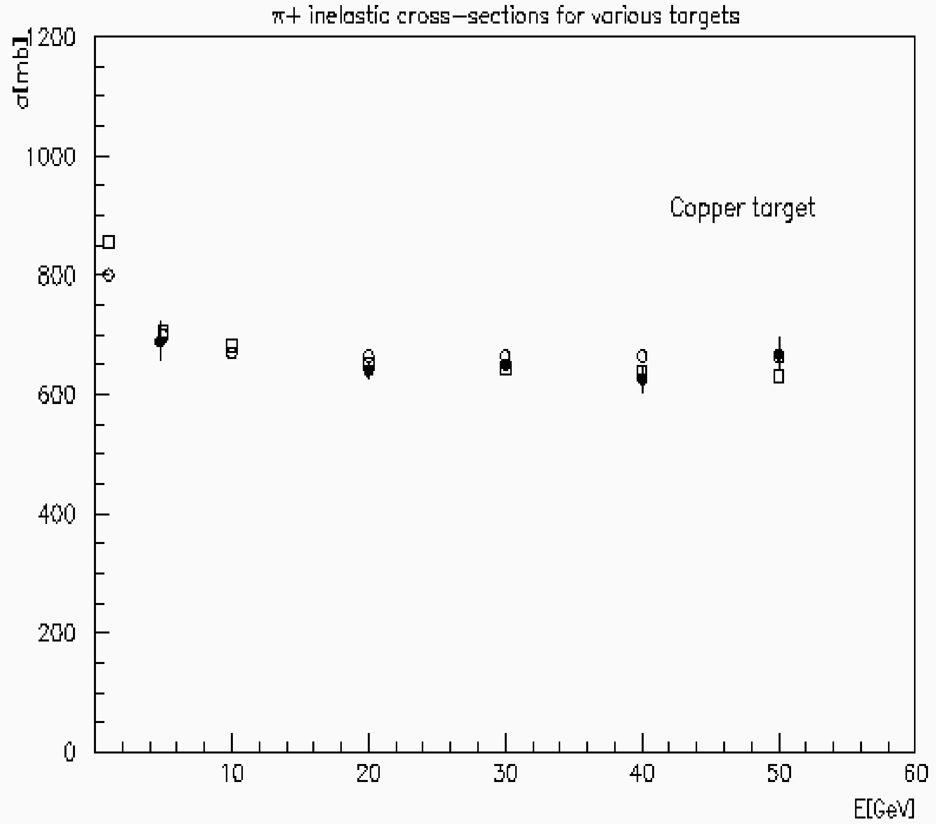
Pi+ reaction cross-sections: dots: data, open symbols: two different parametrization





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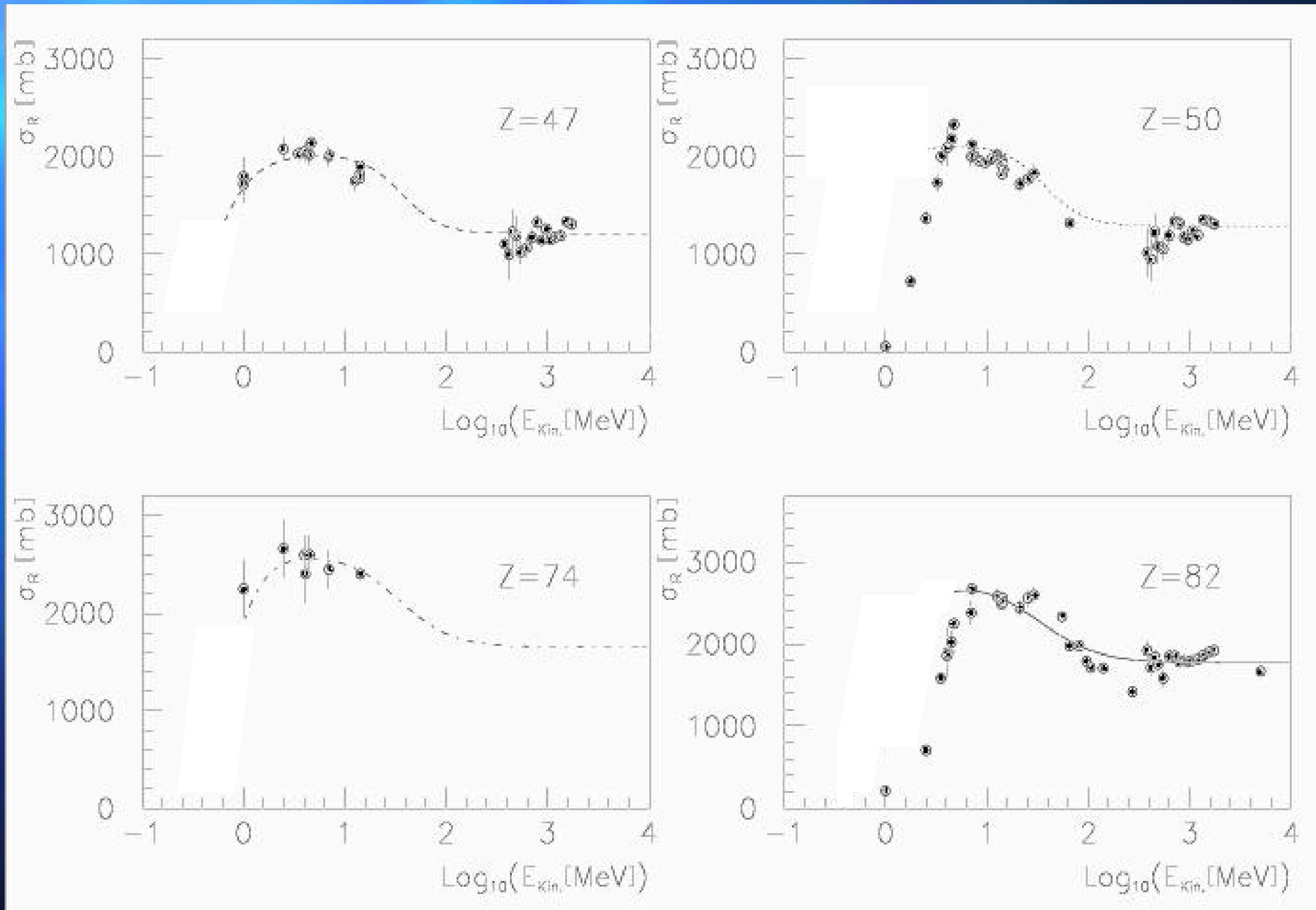
neutron-nuclear reaction cross-sections at high energies



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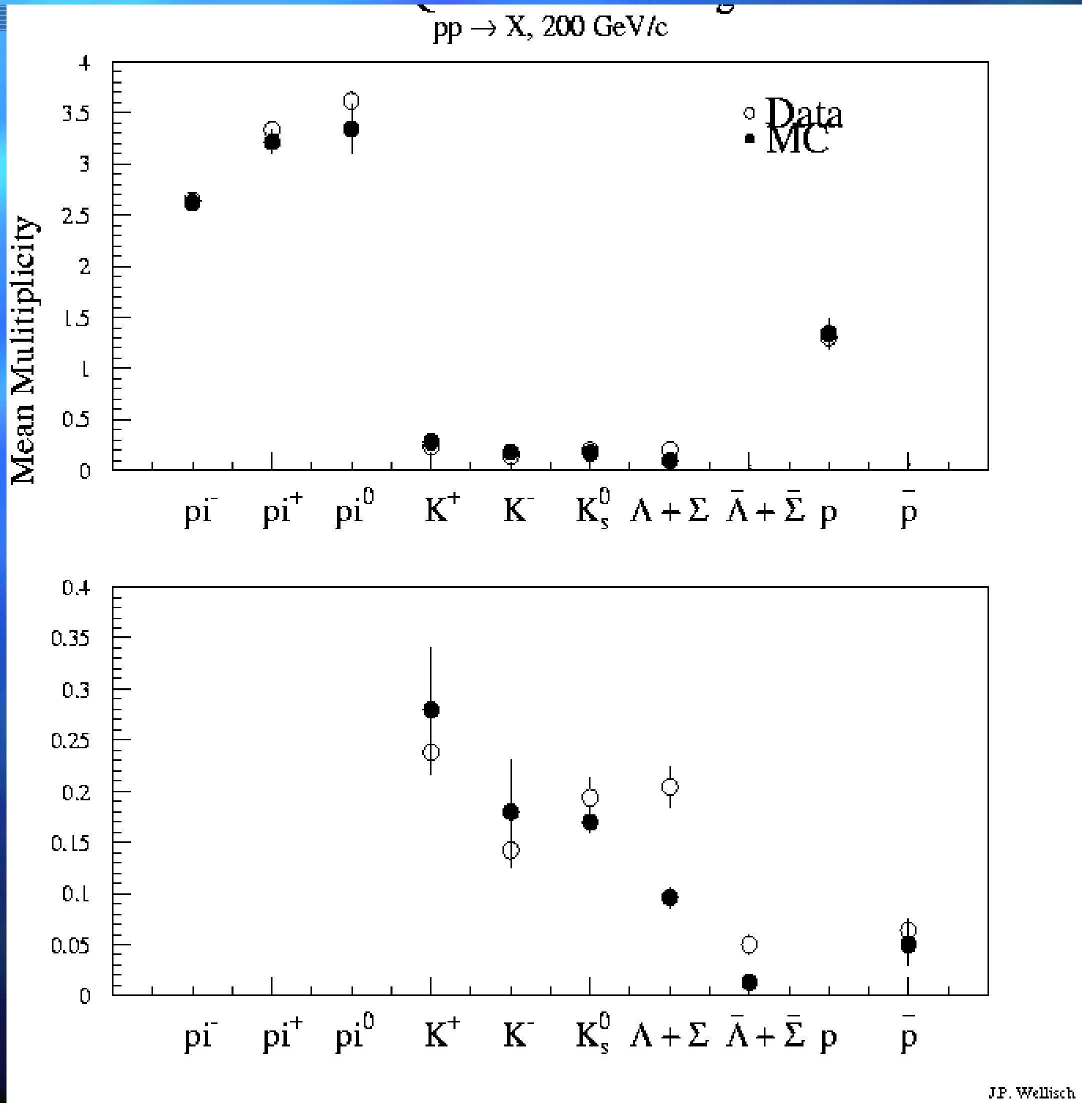
A few examples of thin target comparisons

Particle multiplicities, QGS model

(dots are data, circles are MC)



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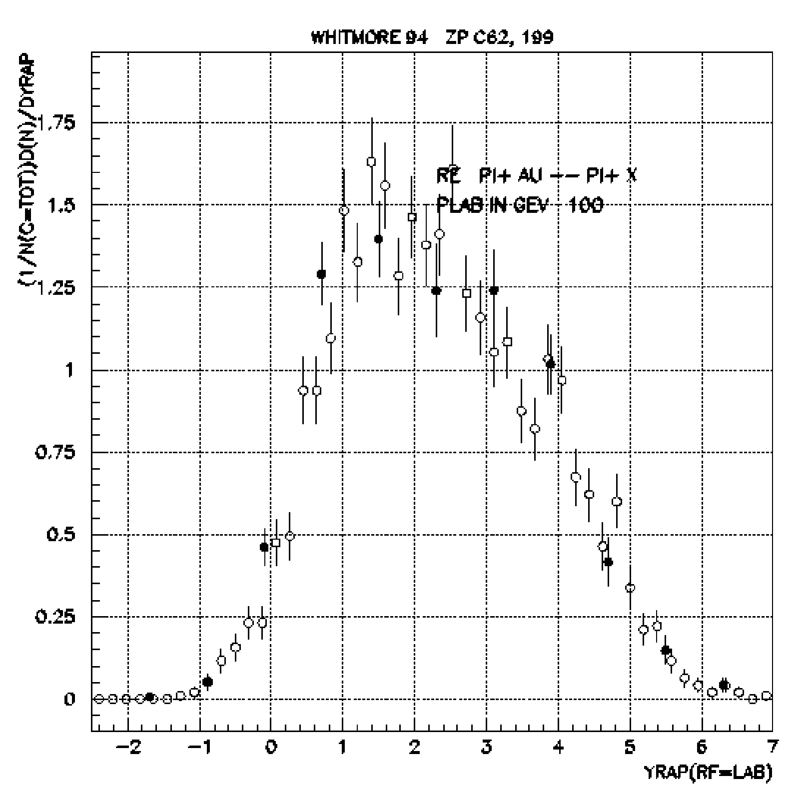
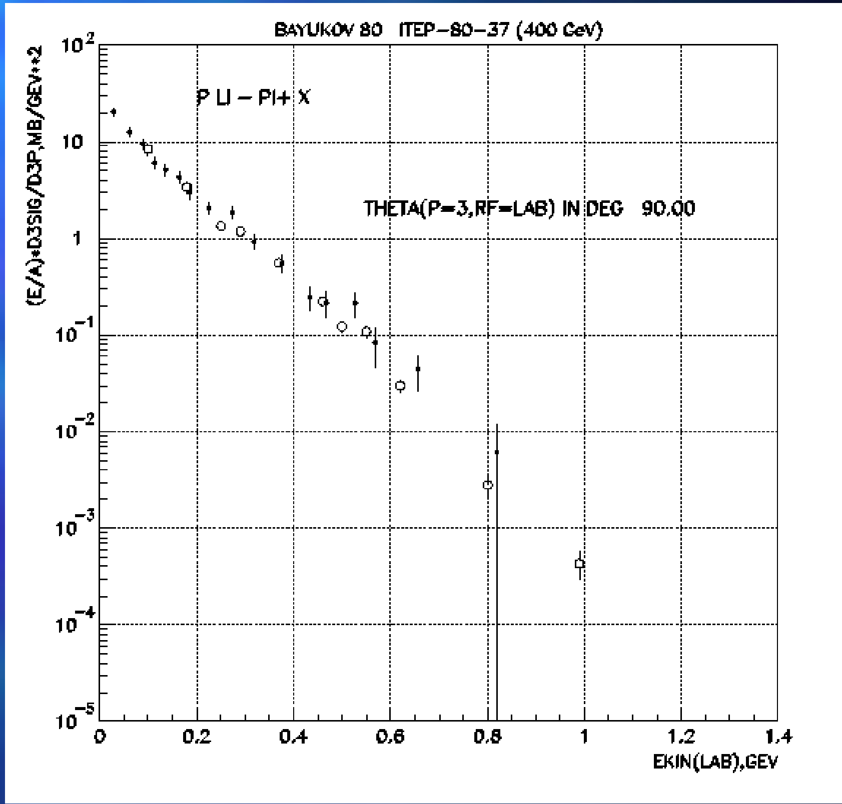
Pion production examples, QGS:

Rapidity distributions and invariant cross-section predictions in quark gluon string model



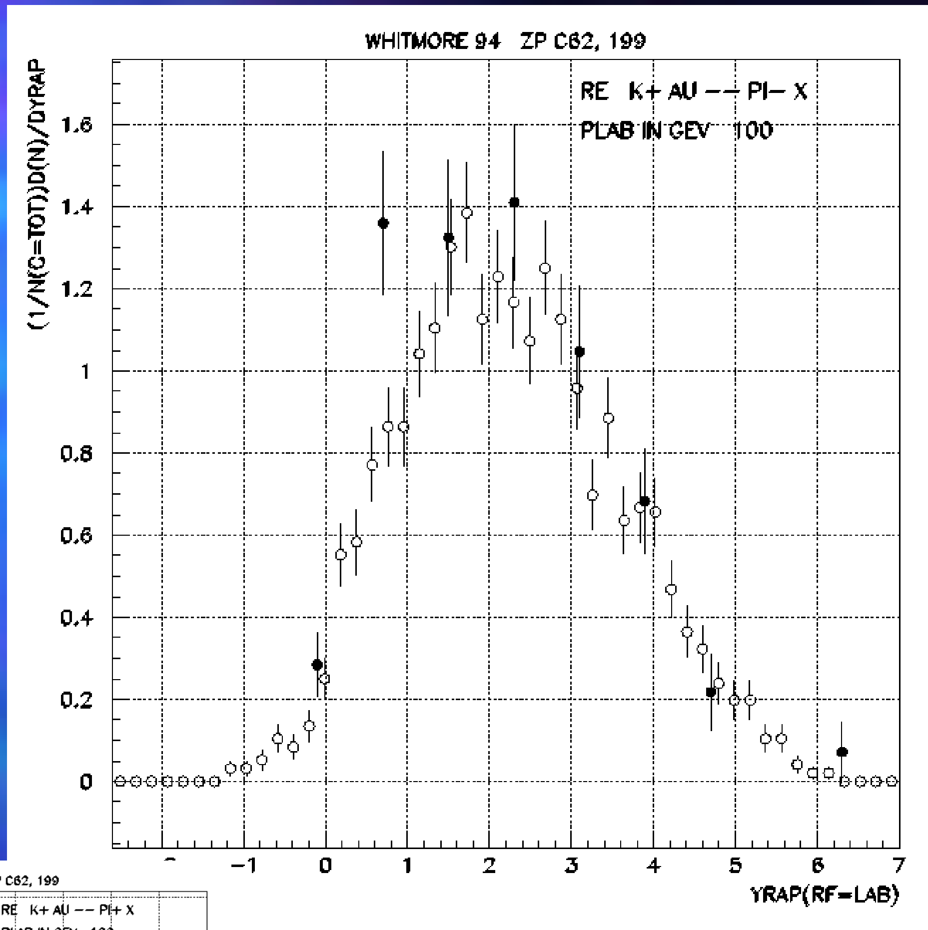
100 GeV pi+ on Gold

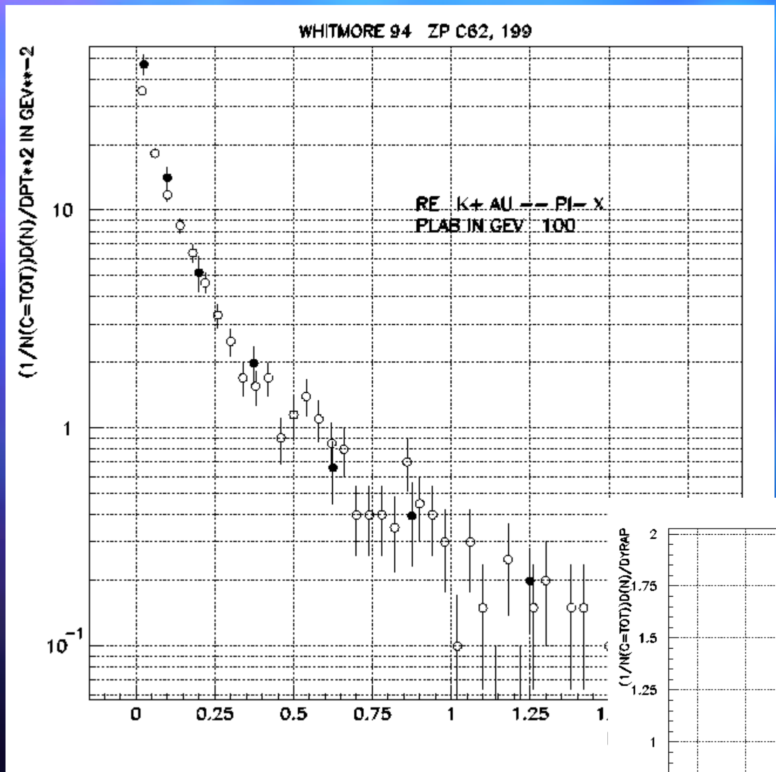


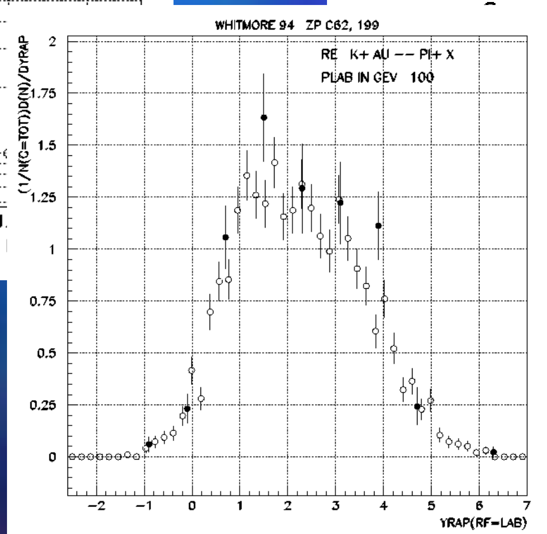
400GeV protons on Lithium

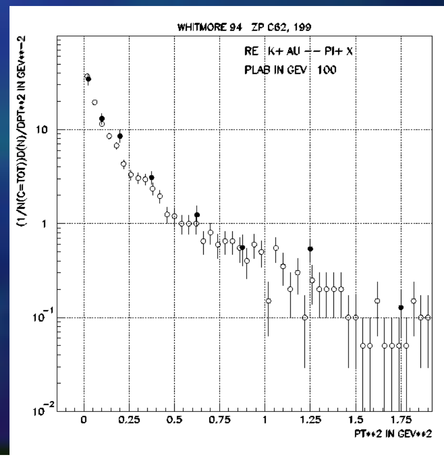
QGS Model

K+ scattering off Gold









Distributions of eta

And transverse momentum.

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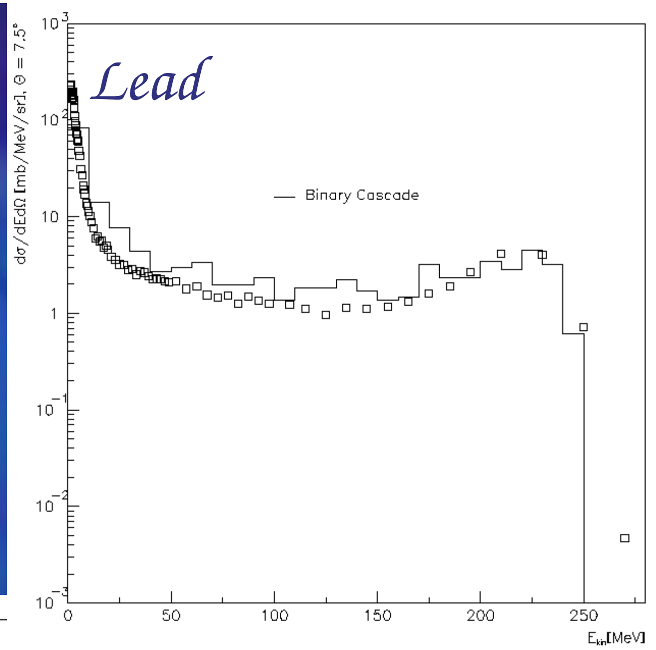
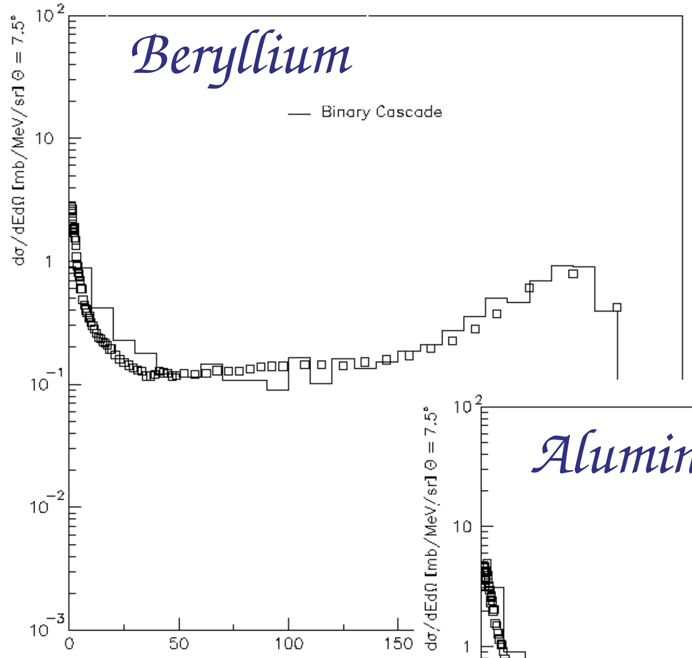
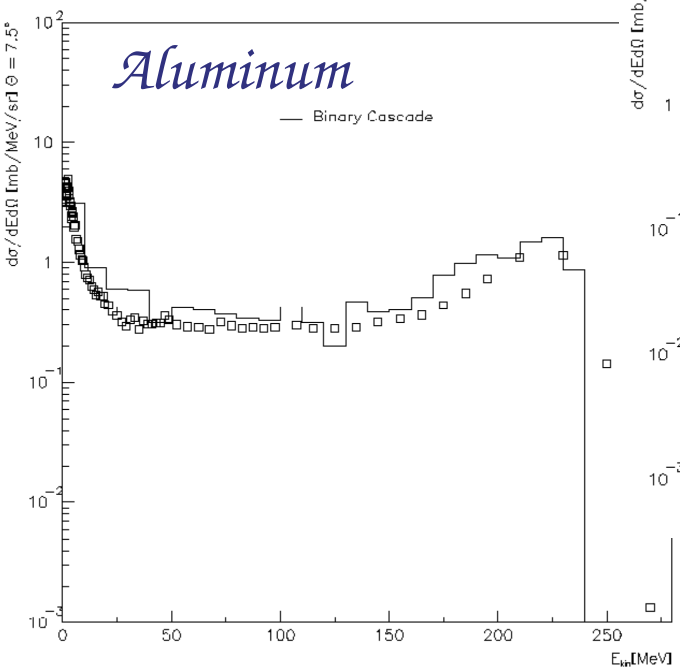
Forward peaks in proton induced neutron production

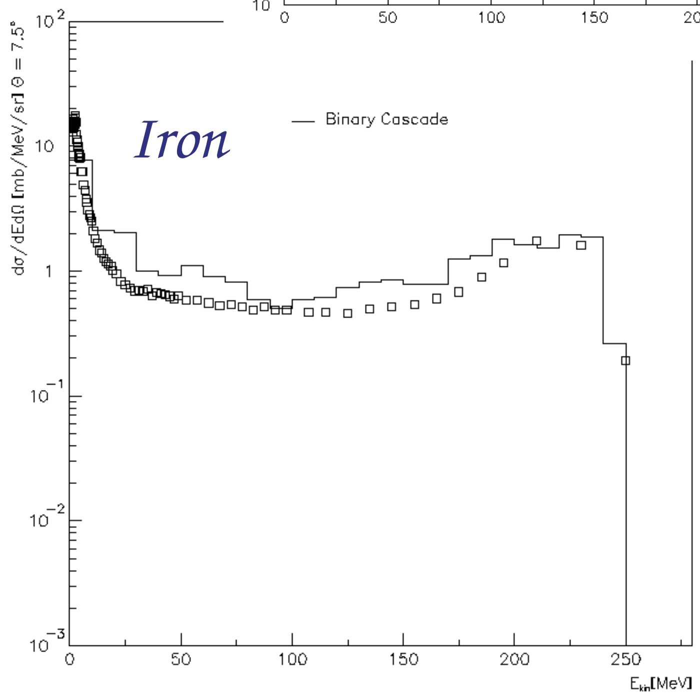
256 MeV data

Neutrons at 7.5deg.









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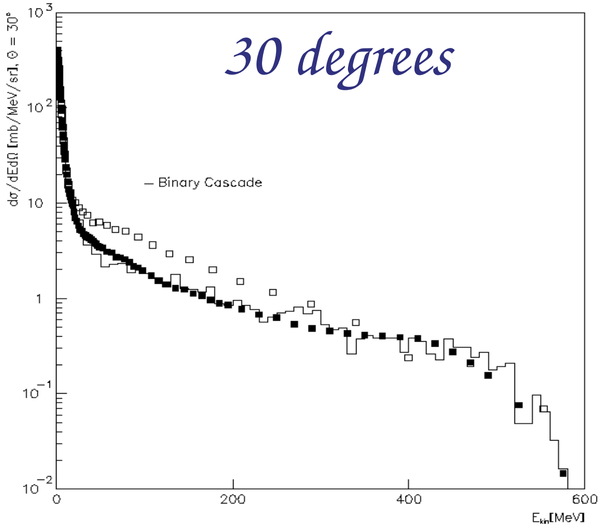
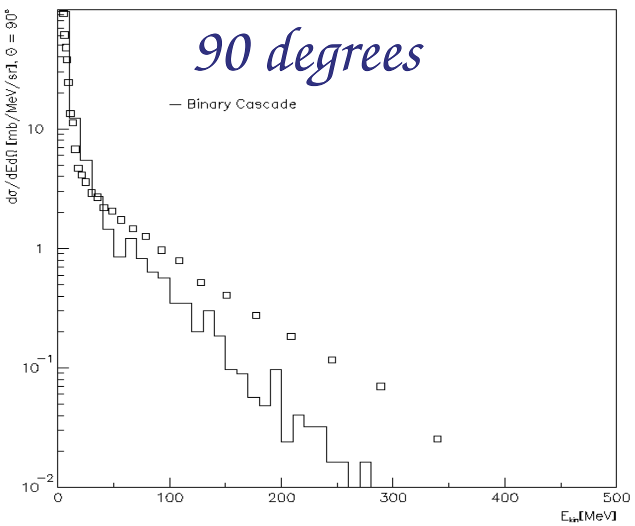
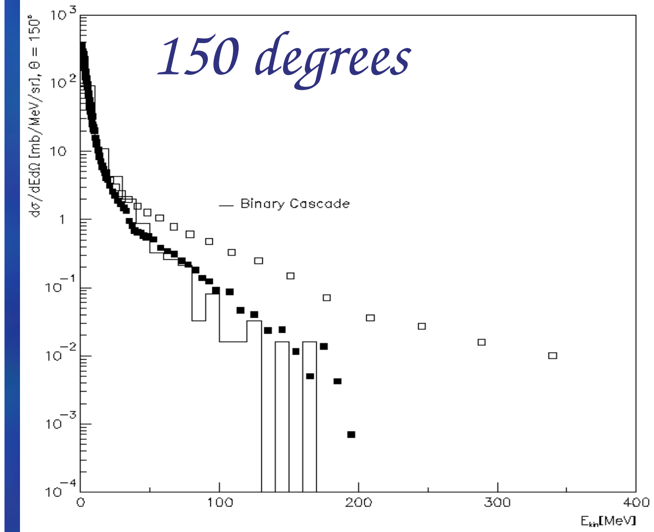
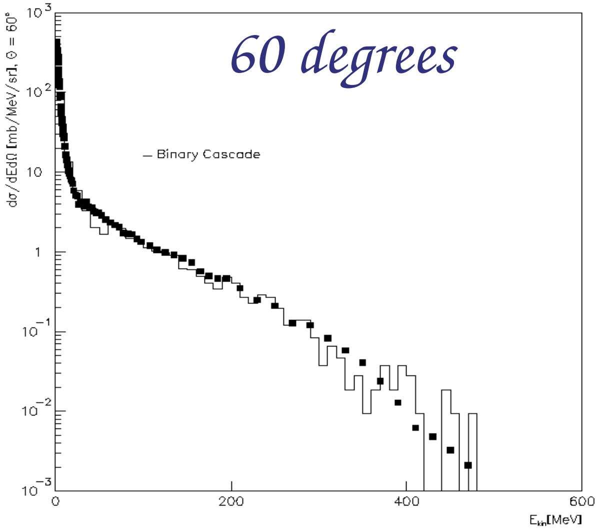
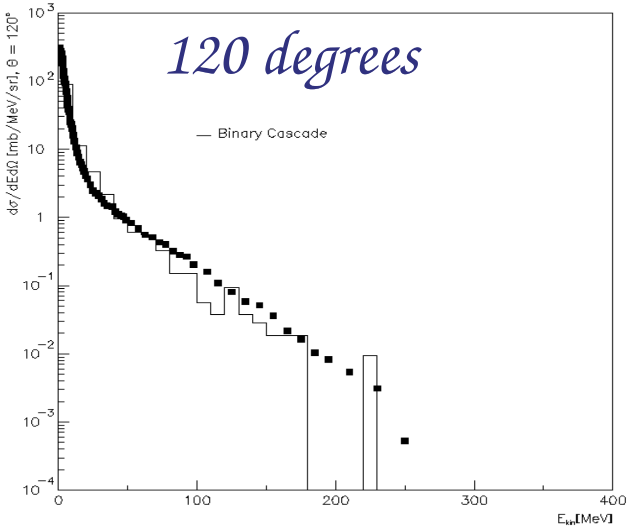
Binary cascade: Neutrons from 597 MeV p on Pb (PRC 22, p1184)











Neutron production
At 30, 60, 90, 120
And 150 degrees

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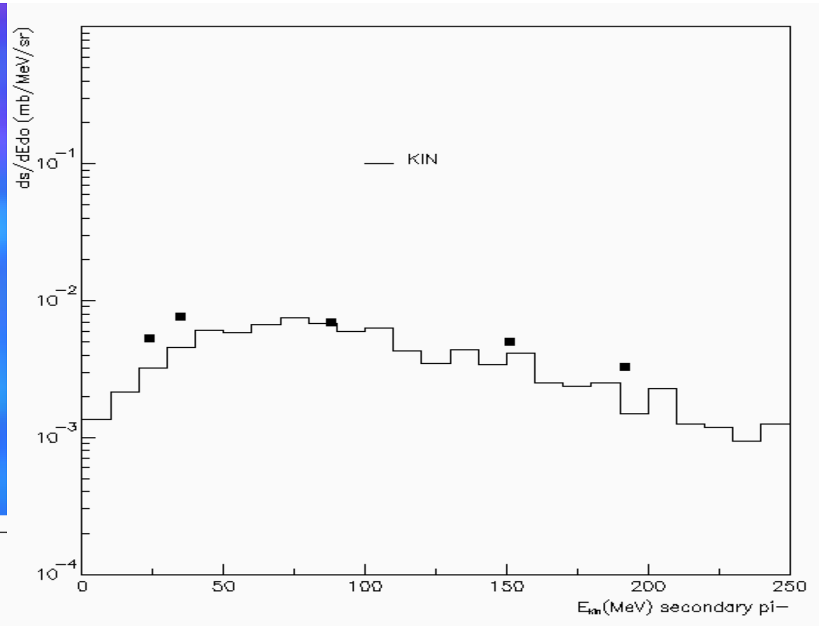
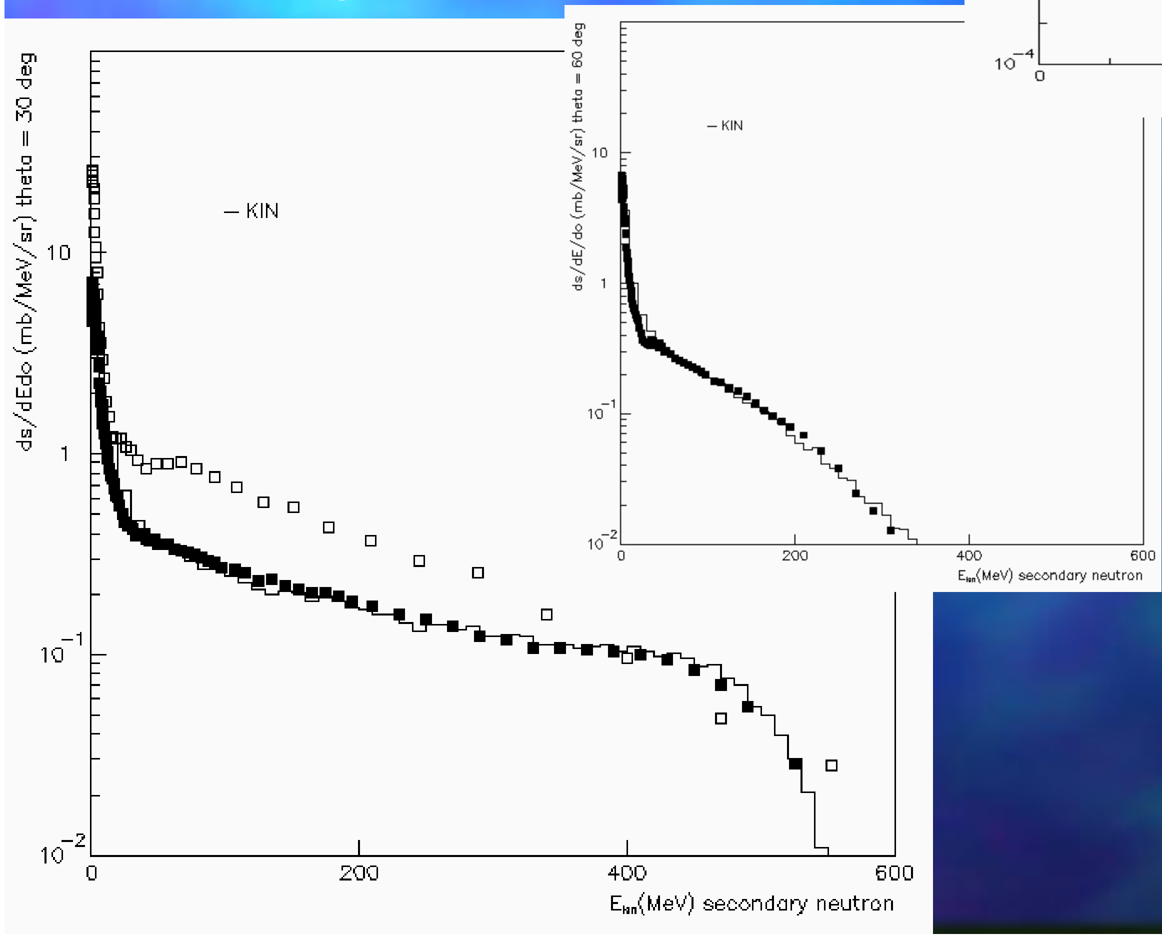
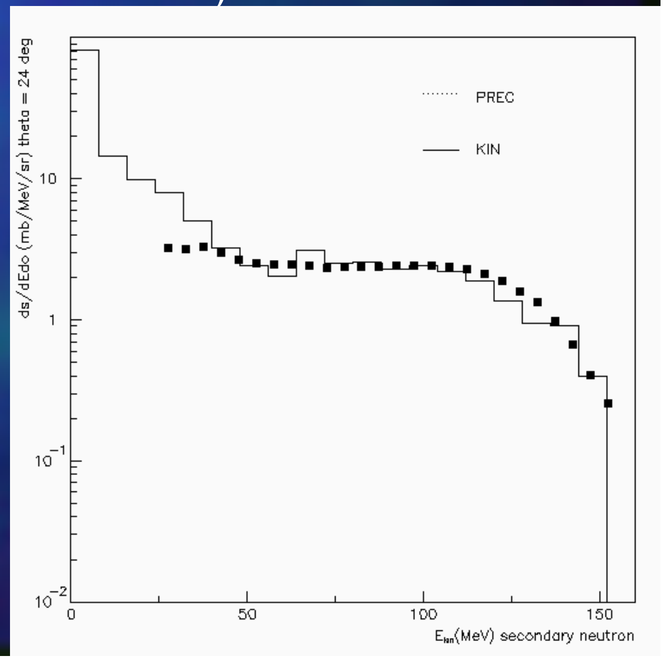
Binary cascade

585MeV p on Al, forward
And backward n and π

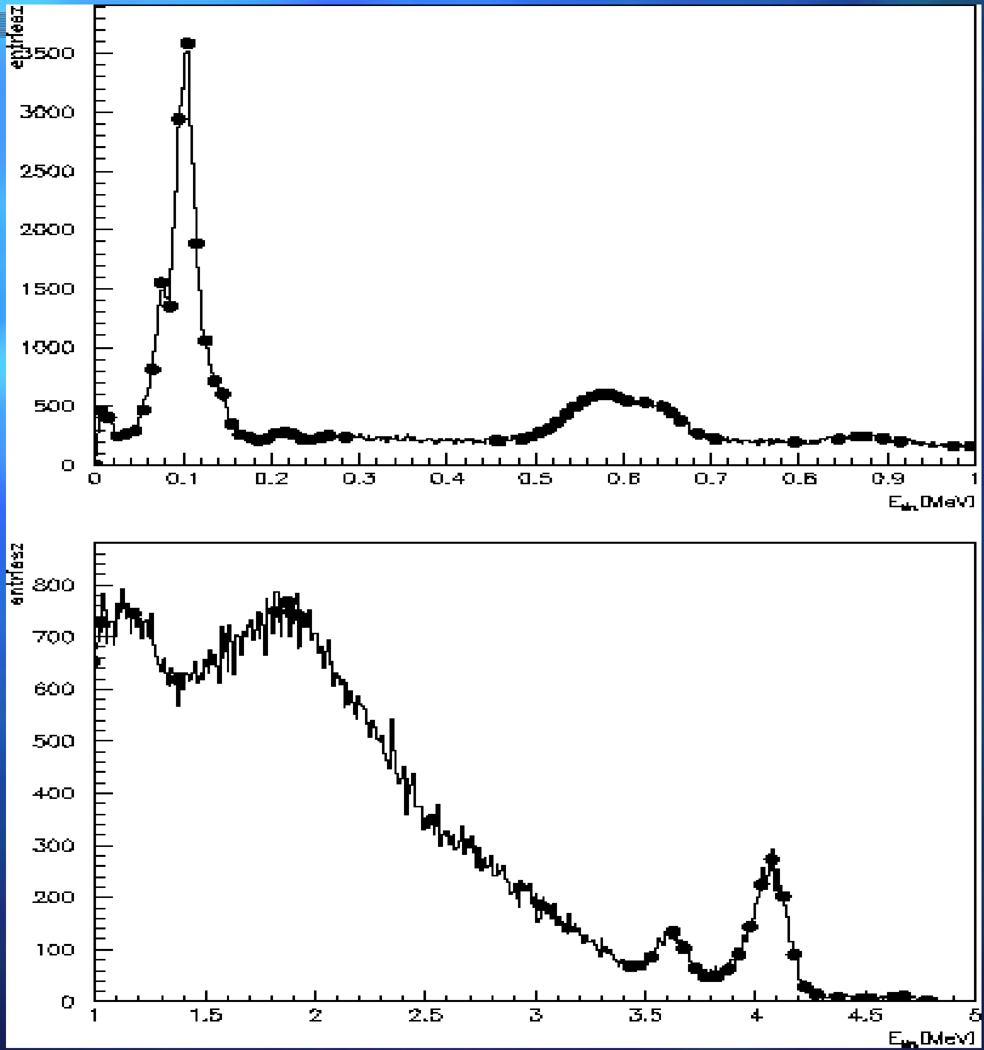




160 MeV p on Pb,
forward neutrons



Low energy neutron capture:
gammas from 14 MeV capture on Uranium



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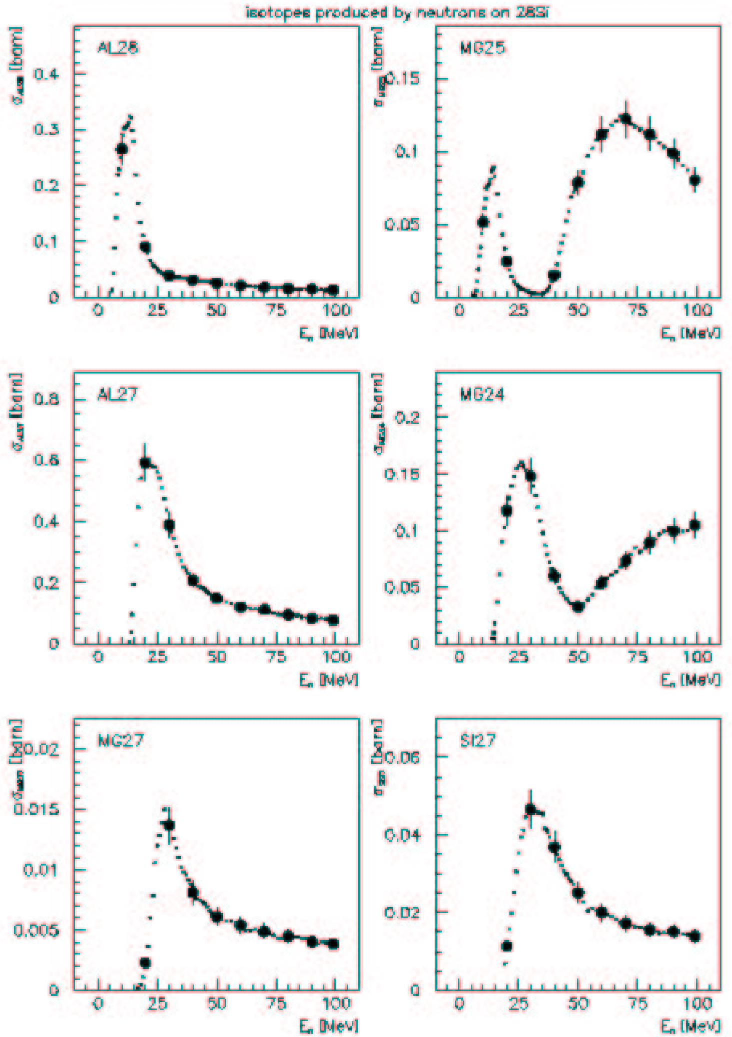
Neutron induced isotope production



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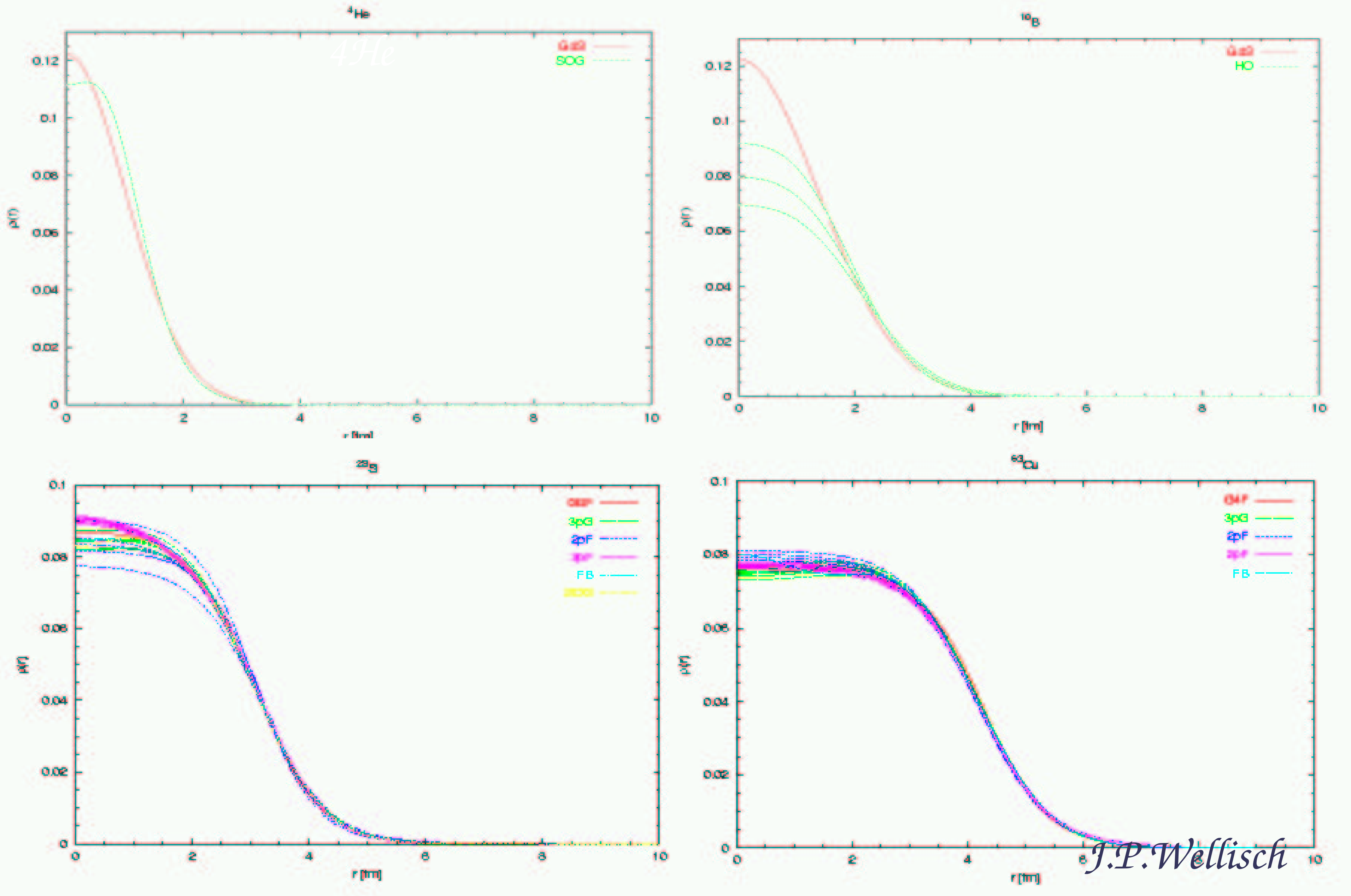
A few verification plots for model components

Nuclear densities: Ex. 4He, 10B, 28Si, and 63Cu



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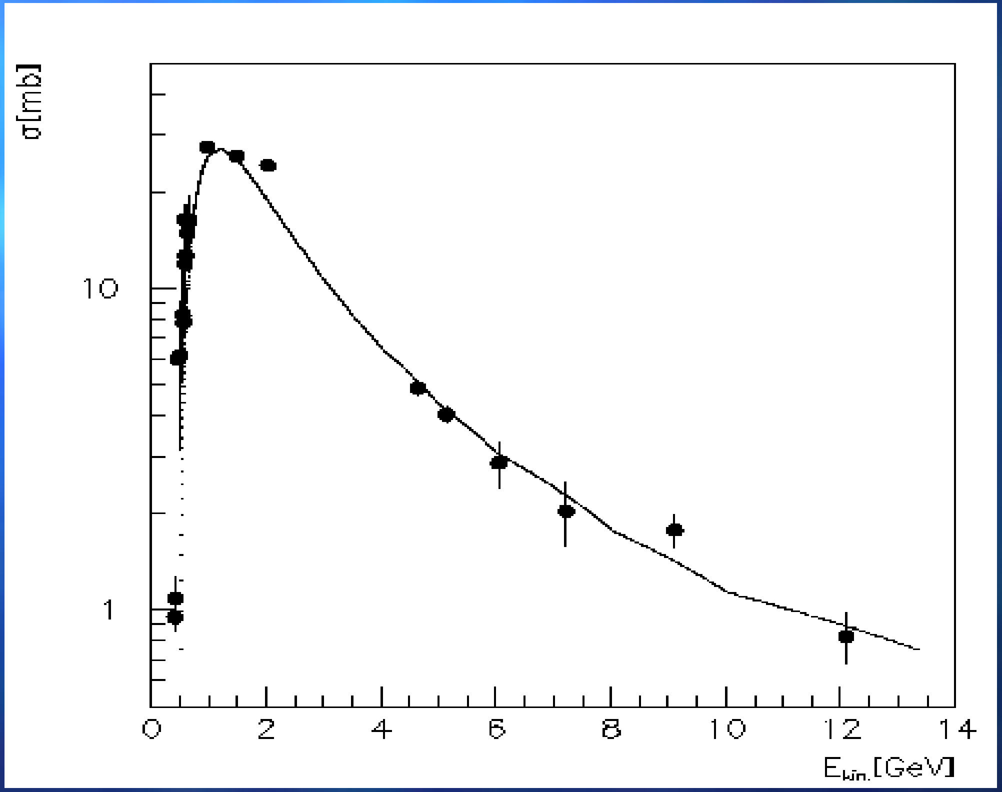
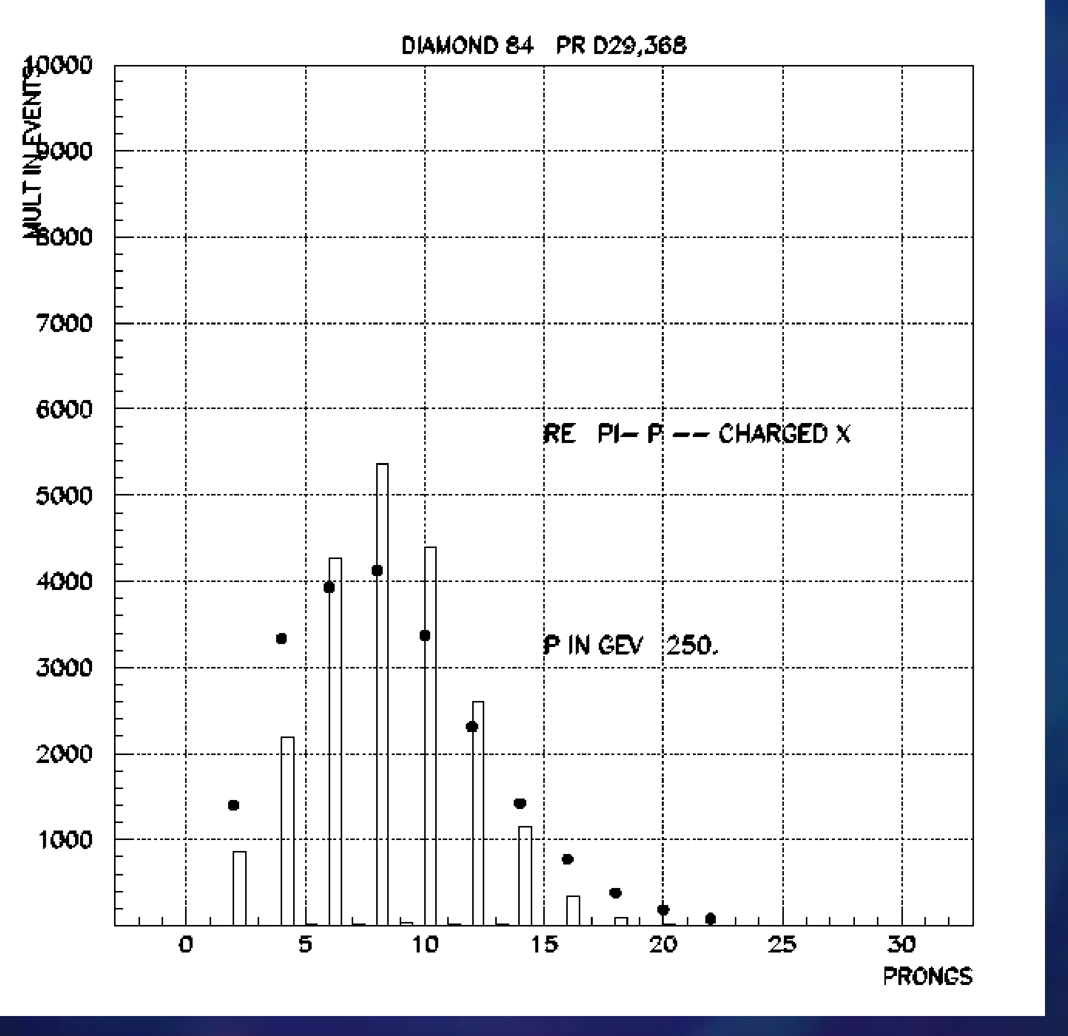
Predicting the Delta production cross-section in pp scattering by binary casacde



prongs prediction in QGS model , single pomeron exchange approximation.



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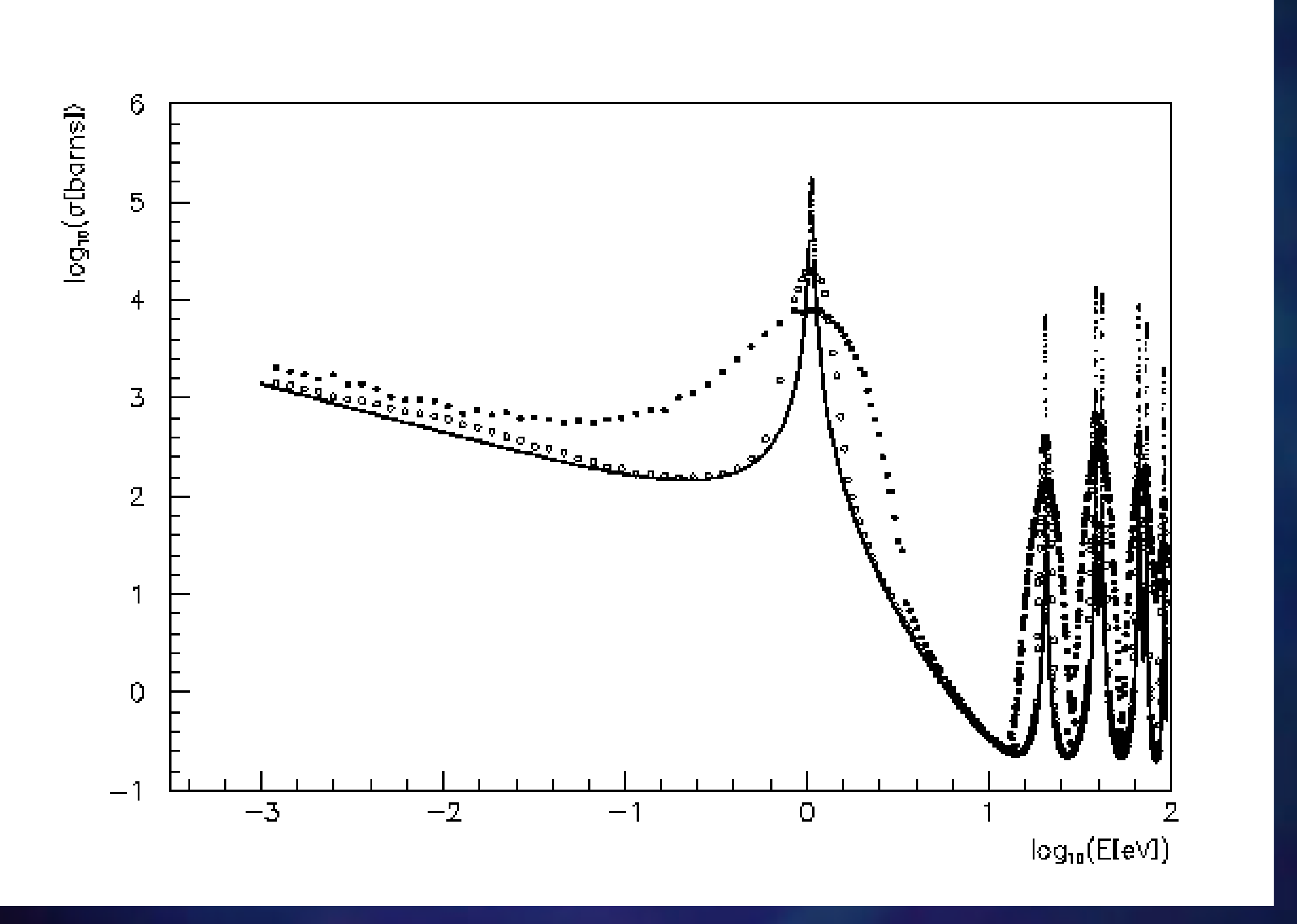
Doppler broadening (low energy neutrons)



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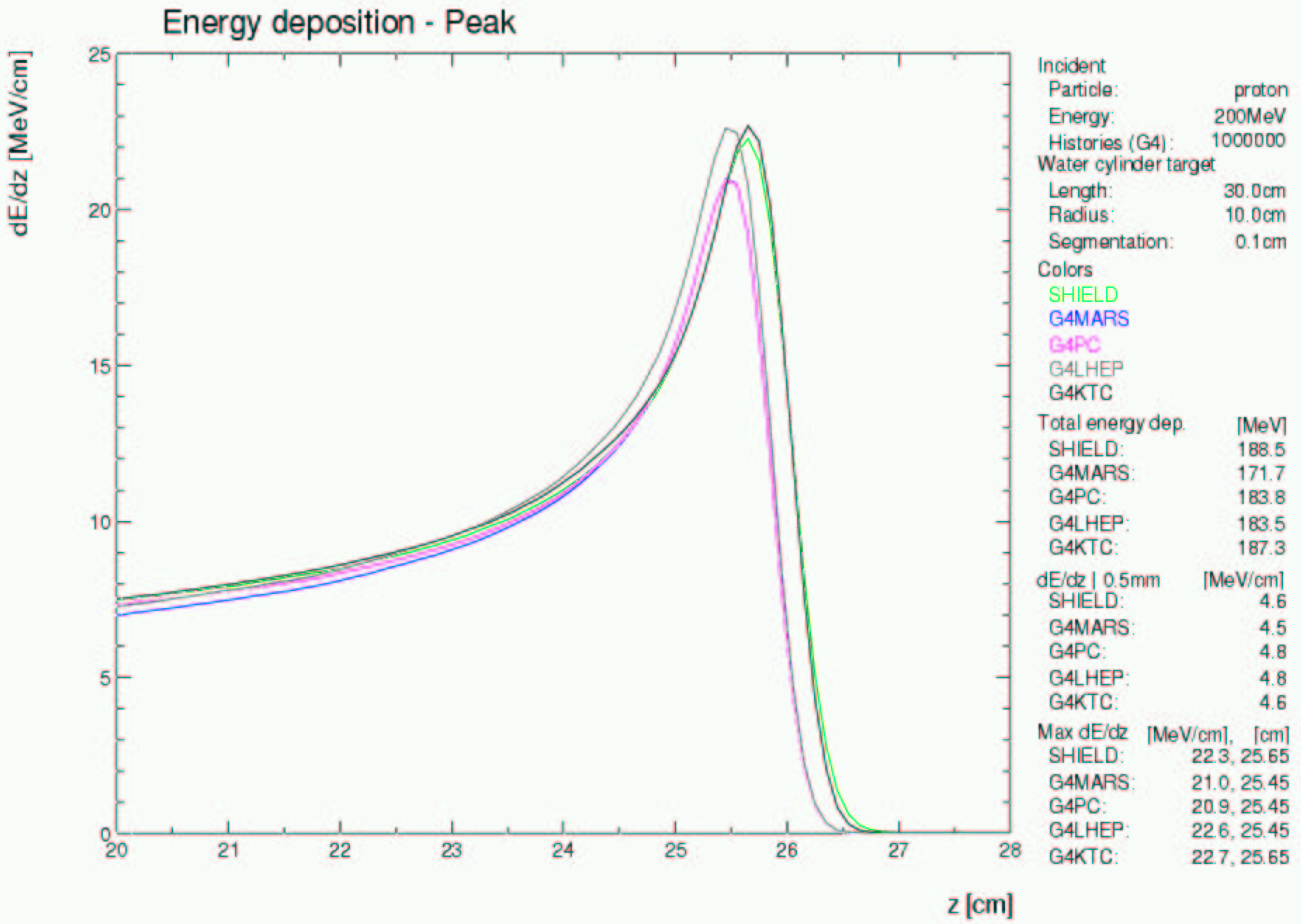
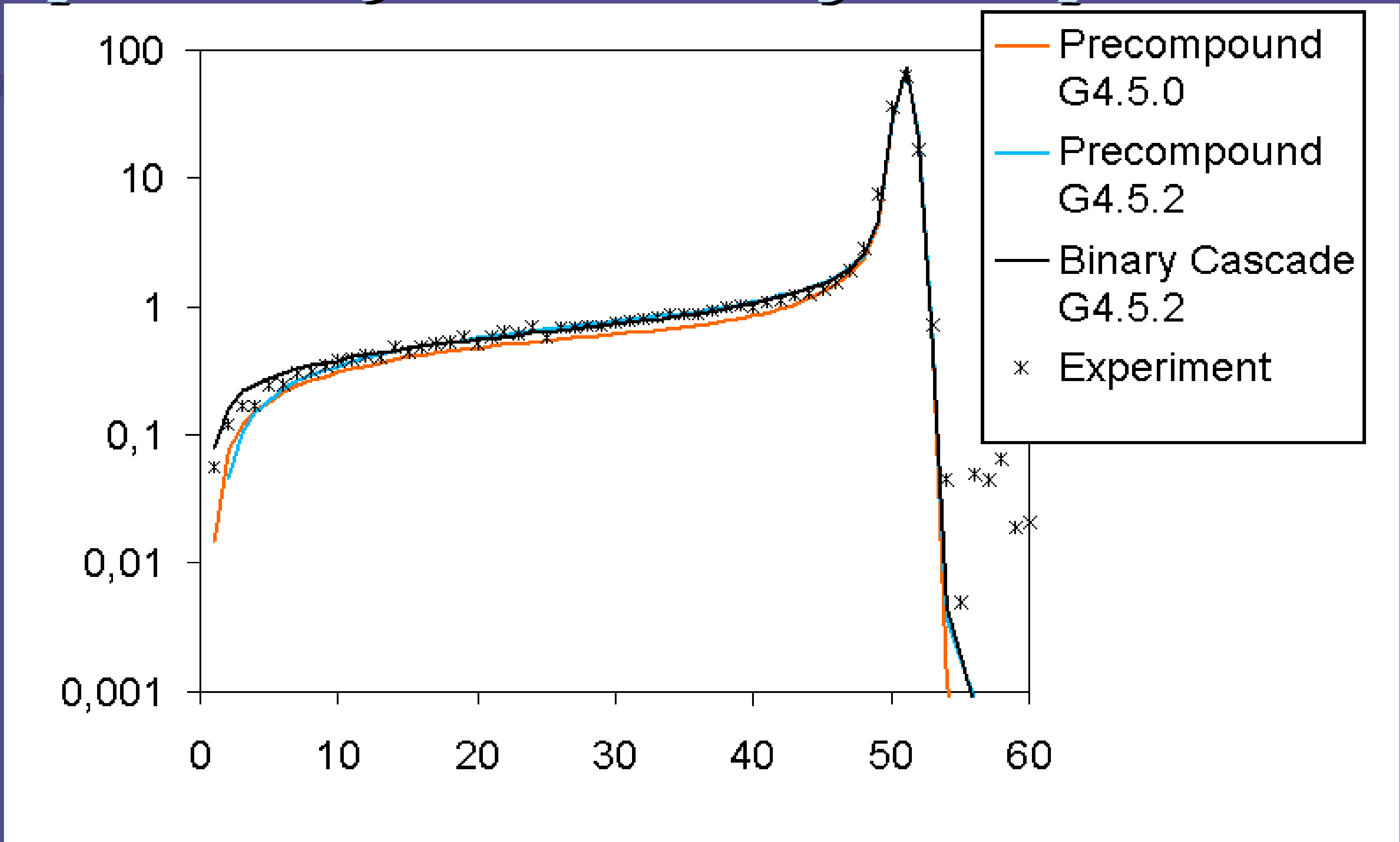
A few code comparisons

Gammas and conversion electrons in ^{57}Co: geant4 vs. RADLIST

	RADLIST (BNL)		Geant4	
Radiation	Energy (keV)	Intensity (100dks)	Energy (keV)	Intensity (100dks)
CE K	7.301	71.00 (6.0)	7.301	70.55 (1.88)
CE			12.899	10.00 (0.70)
CE L	13.567	7.40 (0.6)	13.562	5.95 (0.54)
CE			13.687	0.35 (0.13)
CE			14.315	0.85 (0.21)
CE			14.405	0.45 (0.19)
CE K	114.949	1.83 (0.14)	114.949	1.95 (0.31)
CE			120.497	5.70 (0.53)
CE L	121.215	0.19 (0.020)		
CE M+	121.968	0.03 (0.005)		
CE K	129.361	1.30 (0.16)	129.362	1.25 (0.25)
CE			134.910	0.25 (0.11)
γ	14.413	9.16 (0.15)	14.413	10.05 (0.71)
γ	122.061	85.60 (0.17)	122.061	86.05 (2.07)
γ	136.474	10.68 (0.08)	136.474	10.05 (0.71)
γ	692.410	0.15 (0.01)	692.030	0.15 (0.09)

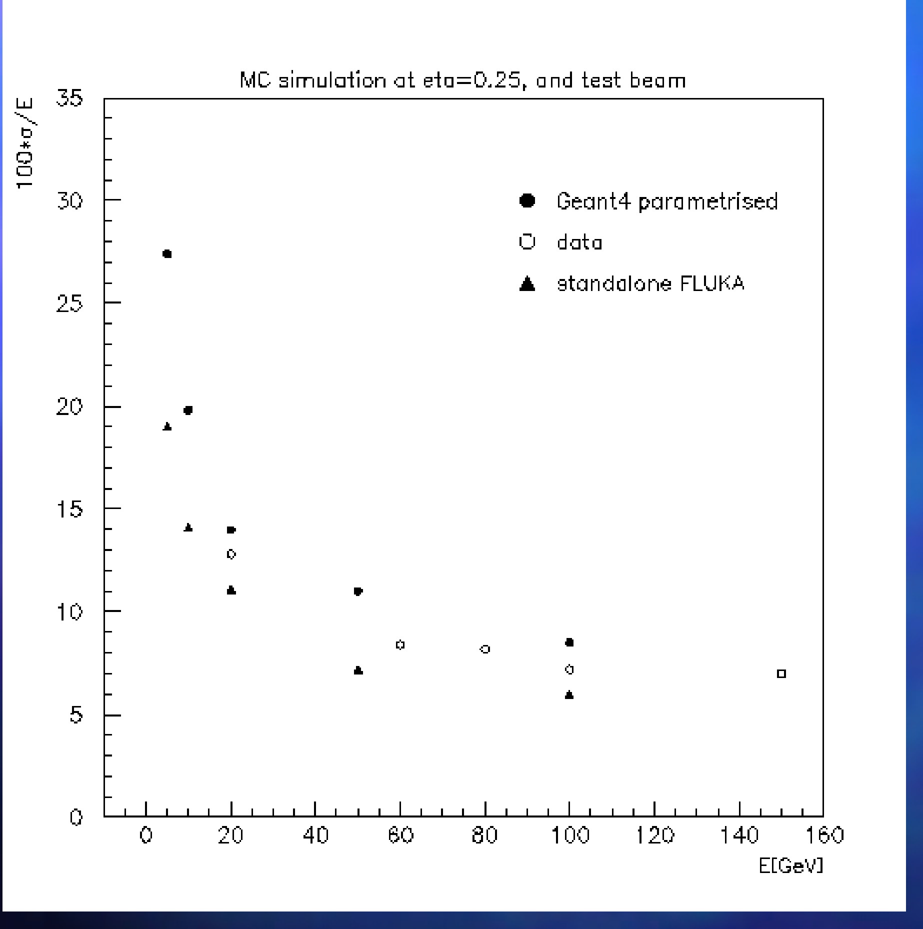

Energy deposition - Peak
dE/dz [MeV/cm]
z [cm]
Incident
Particle: proton
Energy: 200MeV
Histories (G4): 1000000
Water cylinder target
Length: 30.0cm
Radius: 10.0cm
Segmentation: 0.1cm
Colors
SHIELD
G4MARS
G4PC
G4LHEP
G4KTC
Total energy dep. [MeV]
SHIELD: 188.5
G4MARS: 171.7
G4PC: 183.8
G4LHEP: 183.5
G4KTC: 187.3
dE/dz | 0.5mm [MeV/cm]
SHIELD: 4.6
G4MARS: 4.5
G4PC: 4.8
G4LHEP: 4.8
G4KTC: 4.6
Max dE/dz [MeV/cm], [cm]
SHIELD: 22.3, 25.65
G4MARS: 21.0, 25.45
G4PC: 20.9, 25.45
G4LHEP: 22.6, 25.45
G4KTC: 22.7, 25.65

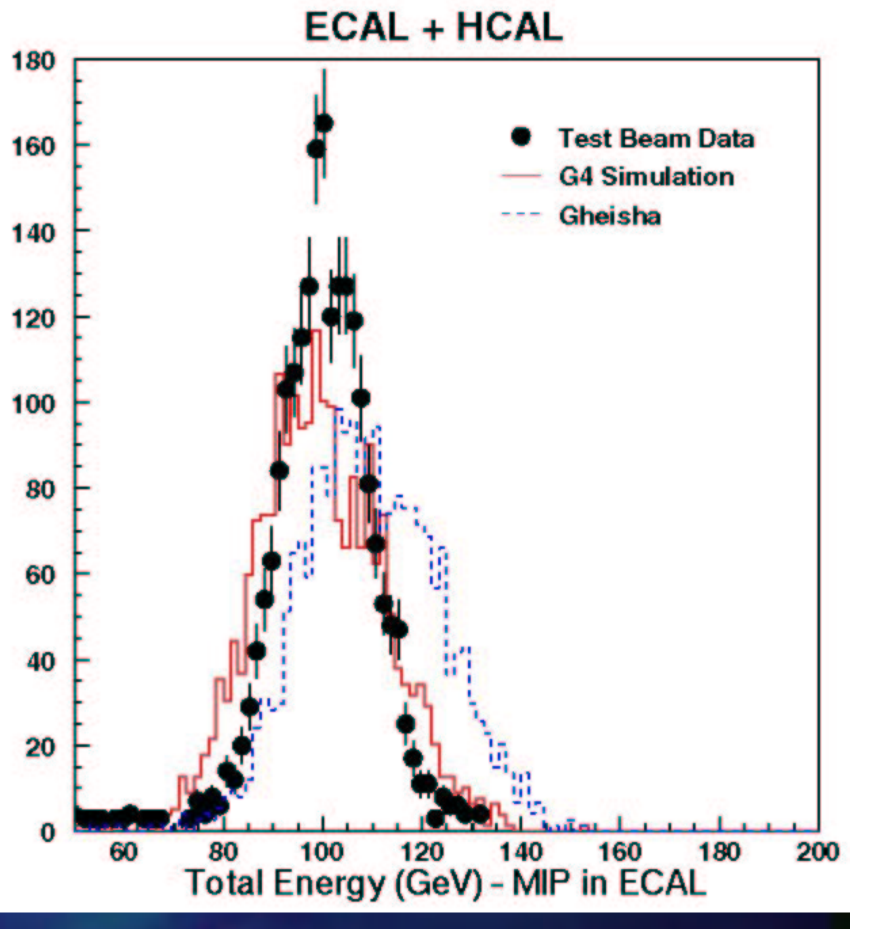
Nuclear interactions with Geant4 versus experiment (G4 5.2 results by Soukup, et al.)



Phantom and experimental results from *H.Paganetti, B.Gottschalk, Medical physics Vol. 30, No.7, 2003*

Test-beam sample result,
(a courtesy of the ATLAS and CMS detector groups)





ATLAS TILE prelim.

CMS combined prelim.

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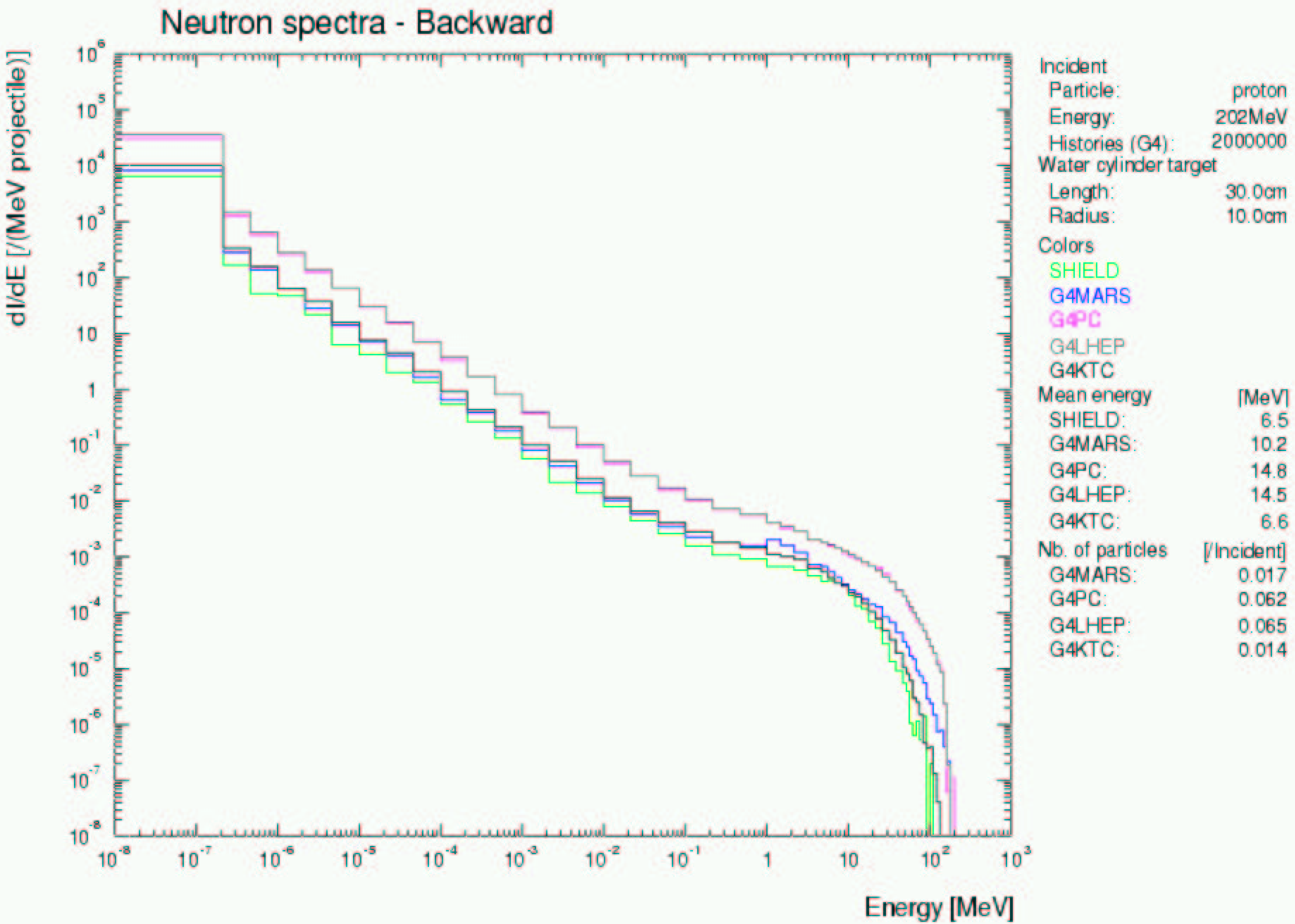
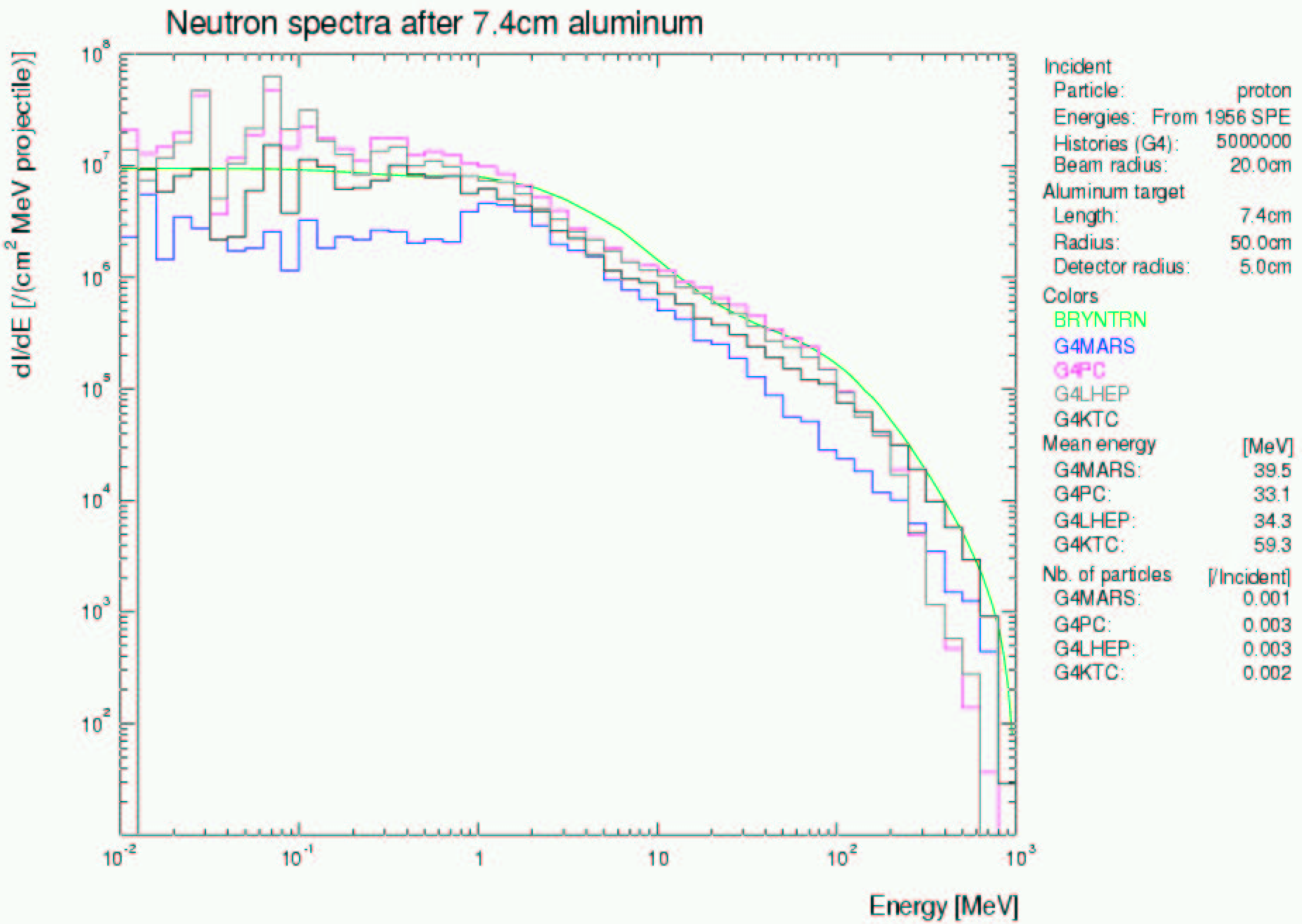
CERN/PH

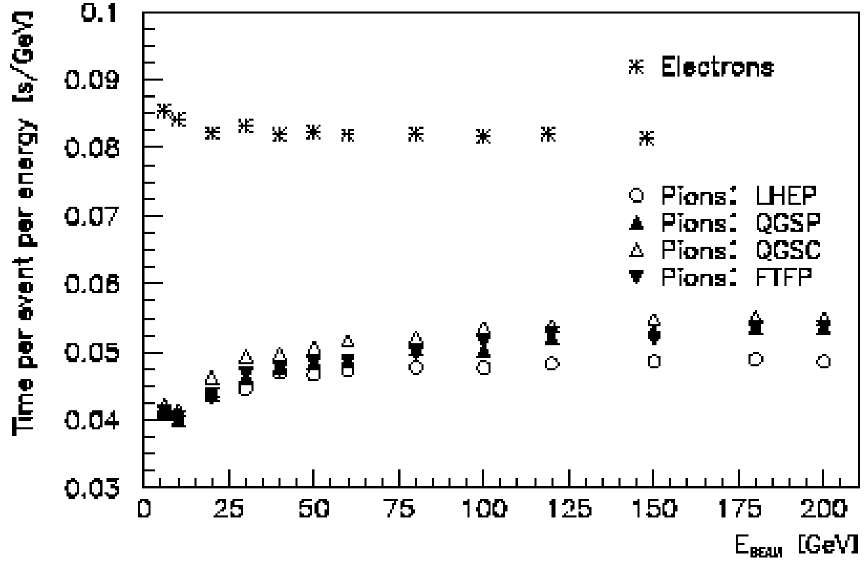


Neutron spectra - Backward
dI/dE [/(MeV projectile)]
Energy [MeV]
Incident
Particle: proton
Energy: 202MeV
Histories (G4): 2000000
Water cylinder target
Length: 30.0cm
Radius: 10.0cm
Colors
SHIELD
G4MARS
G4PC
G4LHEP
G4KTC
Mean energy [MeV]
SHIELD: 6.5
G4MARS: 10.2
G4PC: 14.8
G4LHEP: 14.5
G4KTC: 6.6
Nb. of particles [/Incident]
G4MARS: 0.017
G4PC: 0.062
G4LHEP: 0.065
G4KTC: 0.014

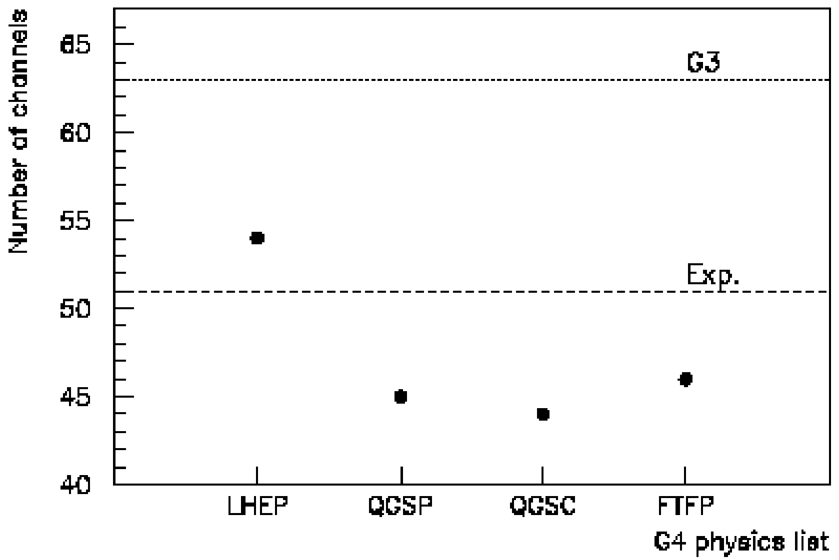


Neutron spectra after 7.4cm aluminum
dI/dE [/(cm² MeV projectile)]
Energy [MeV]
Incident
Particle: proton
Energies: From 1956 SPE
Histories (G4): 5000000
Beam radius: 20.0cm
Aluminum target
Length: 7.4cm
Radius: 50.0cm
Detector radius: 5.0cm
Colors
BRYNTRN
G4MARS
G4PC
G4LHEP
G4KTC
Mean energy [MeV]
G4MARS: 39.5
G4PC: 33.1
G4LHEP: 34.3
G4KTC: 59.3
Nb. of particles [/Incident]
G4MARS: 0.001
G4PC: 0.003
G4LHEP: 0.003
G4KTC: 0.002

A few calorimeter simulation comparisons

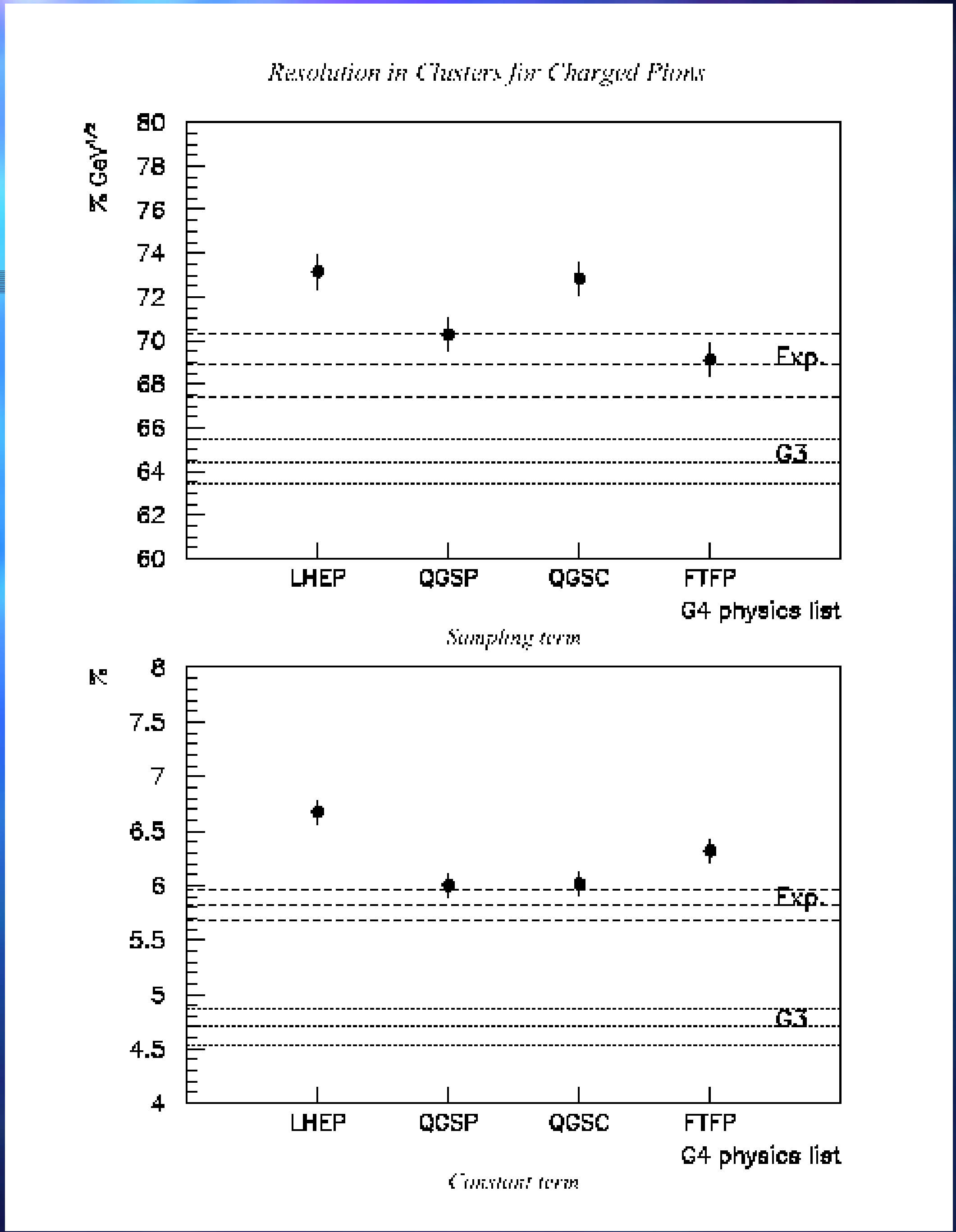


Time of different G4 simulations



Size of a pion cluster

Courtesy of The ATLAS HEC community

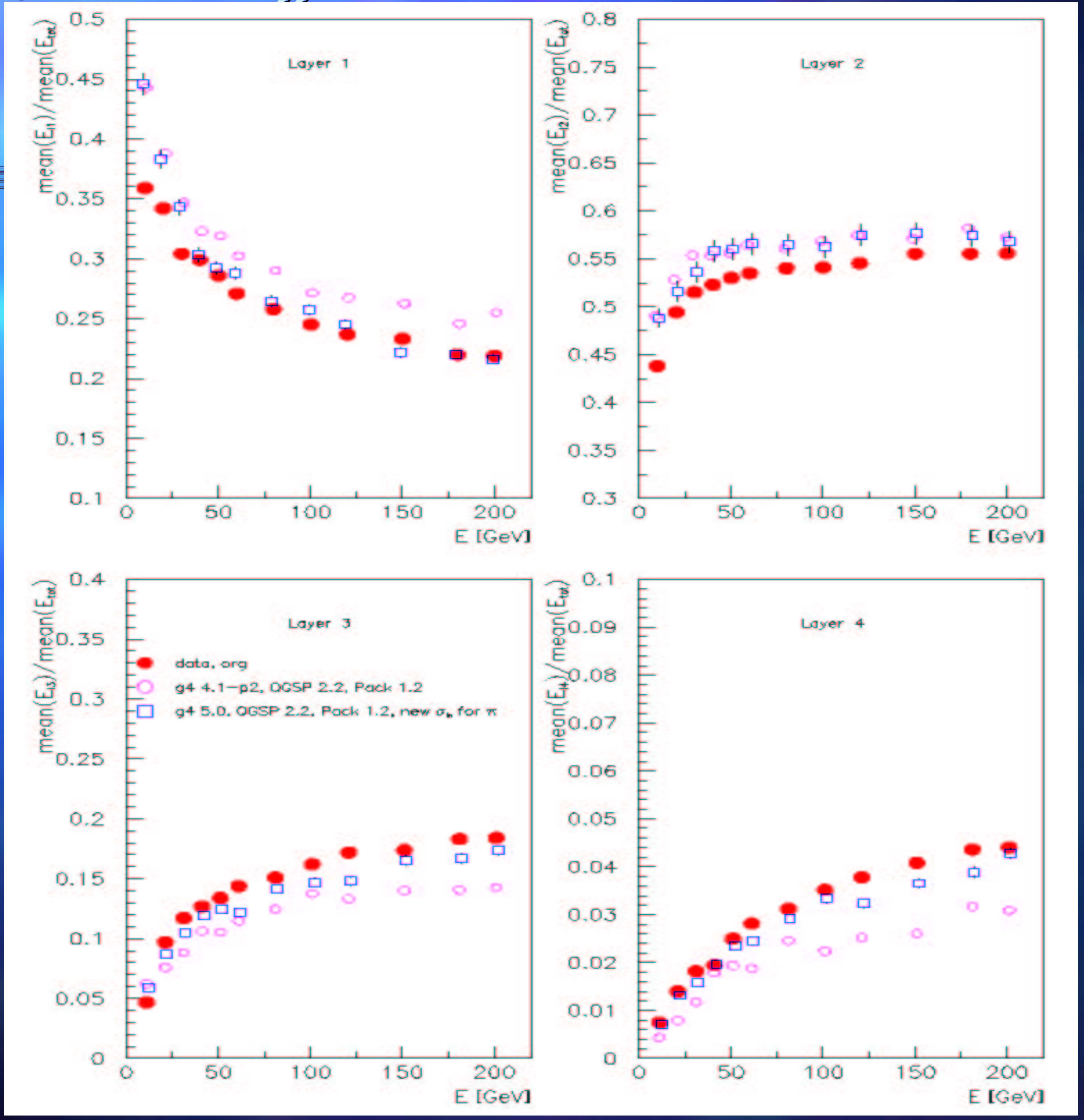


Courtesy of
The ATLAS
HEC community

J.P. Wellisch,
CERN/PH

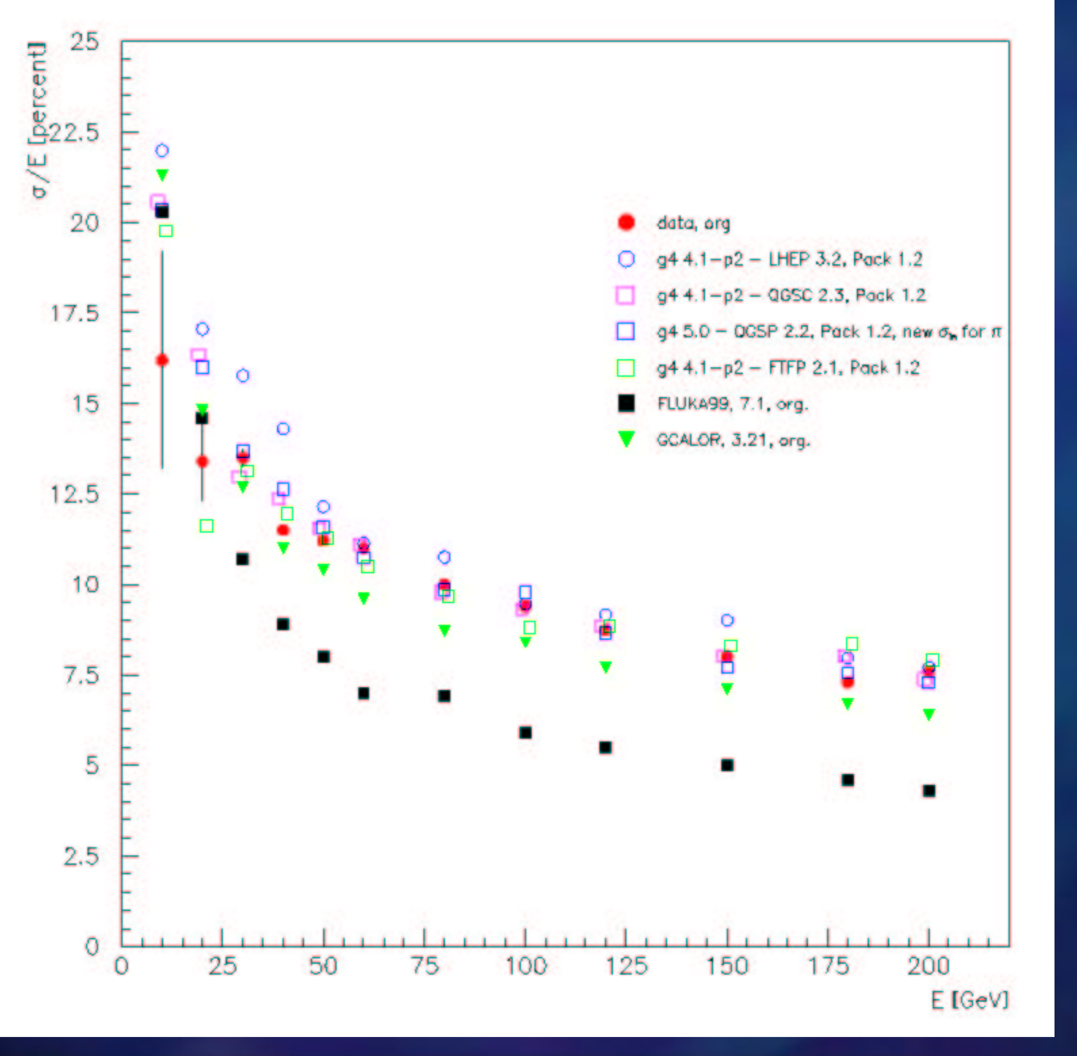
HEC shower shapes G4 5.0 (true geometry, my toy analysis)

data from NIM, A482,94ff.



J.P. Wellisch,
CERN/PH

HEC G4 5.0 (true geometry, my toy analysis) data from NIM, A482,94ff.



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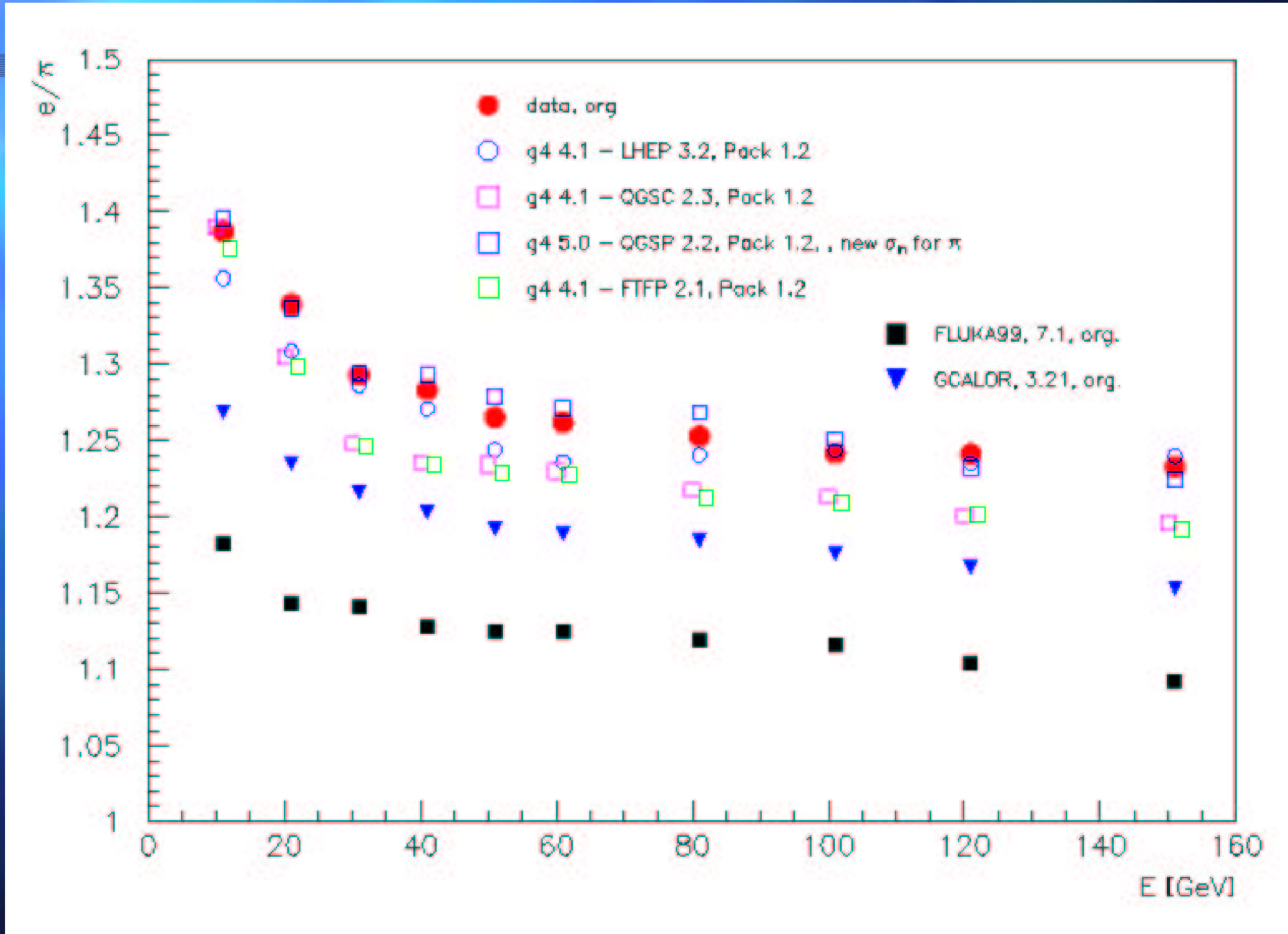
CERN/PH

ATLAS HEC G4 5.0 (true geometry, my toy analysis) data from NIM, A482,94ff.



J.P. Wellisch, CERN/PH

The END?

Tomorrow

- Selected topics of electromagnetic physics
- Some complete calorimeter simulations
  - A courtesy of the validation project, and the detector groups

The END.