The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

**1930-10**

# Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions

***4 - 8 February 2008***

## The Description of Nuclear Collision within the Quantum Molecular Dynamics Model

Christoph Hartnack

*SUBATECH*
*Nantes Cedex 3*
*France*

# Description of heavy ion collisions within the Isopin Quantum Molecular Dynamics model (IQMD)

*Christoph Hartnack, SUBATECH, Nantes*

- **What is IQMD?**
- **What ingredients do we use? Why?**
- **What are their influences on observables?**

# What is IQMD?

Not MCNP!

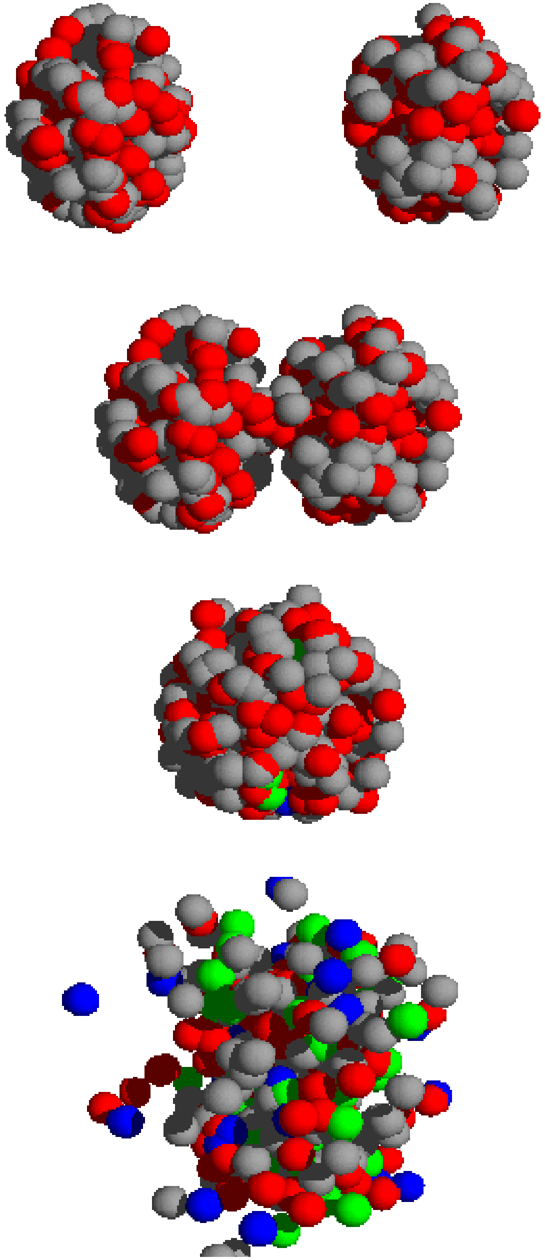
- semiclassical model with quantum features

- microscopic N-body description

- calculation of heavy ion collisions on an event-by-event-basis

- includes N, Δ, π with isospin d.o.f.

- potentials of Skyrme type for describing nuclear eos



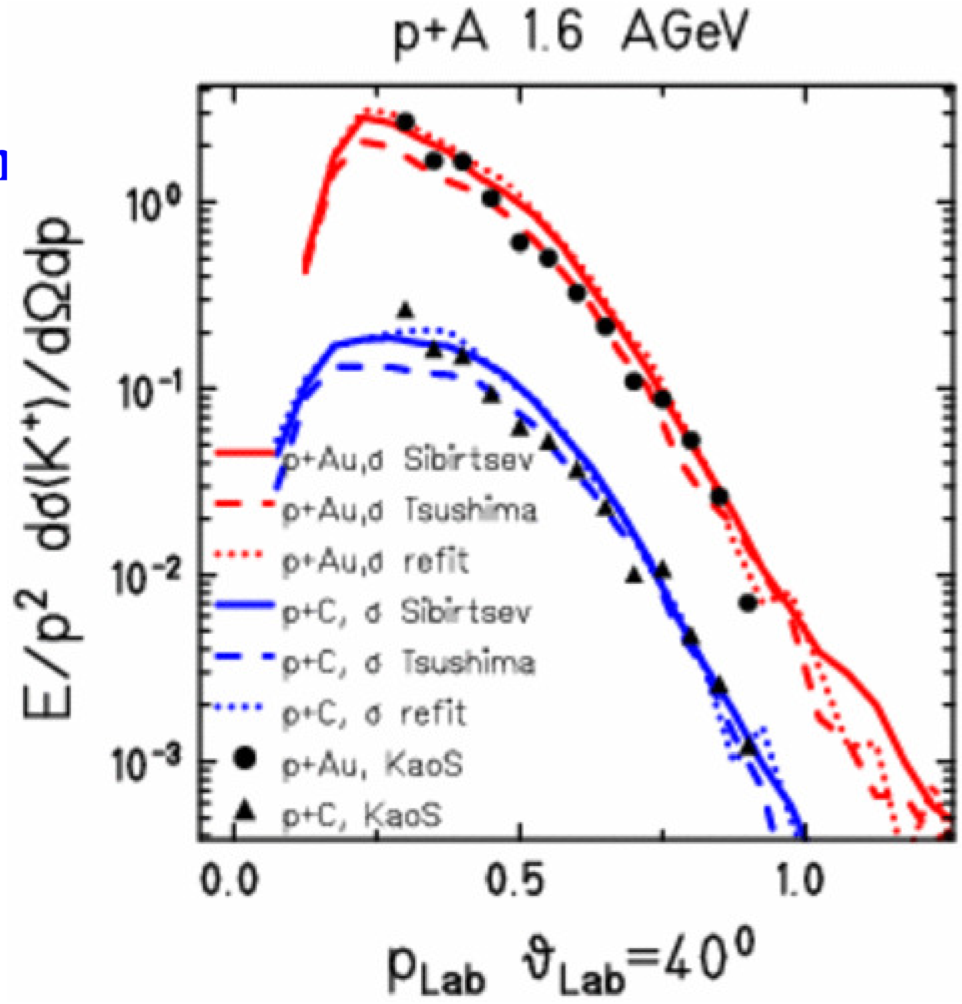
# Basic application

- Simulation of heavy ion collisions (symmetric/asymmetric)
- Energy range of few hundred MeV (about 100 MeV-2GeV)
- Basically issued to the study of particle production and dynamical observables (flow, squeeze, …) at SIS energies
- Used in part for simulating detectors at GSI
- Multifragmentation is not an issue of priority
- A big interest is giving to the tracing of particles in order to understand the reaction mechanisms
- A playground of parameters to vary in order to understand the origin of the effects

# Applications in p+A

• Limiting case of A+A
• Systematics for production of secondary particles,
  e.g Kaon production near threshold

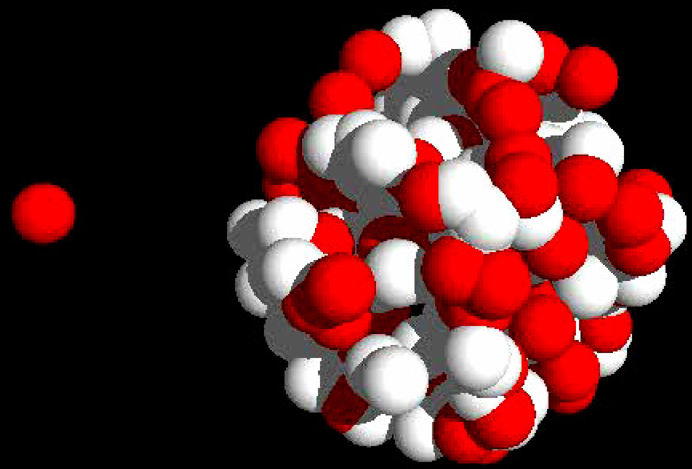
•Basic problem:collisional chaos might not really be assumed in p+A



# And why collisional chaos?

- No-go-theorem: a relativistic covariant treatment of the dynamics of an interacting N-body system is not possible
- Problems with the causality and the time-ordering of collisions
- When assuming a huge number of collisions (collisional chaos) the time-ordering might be no more relevant.
- Reactions of p+A type may be a limiting case…

# Collision of p+A  at 1 GeV b=1fm



# The ruling equation

**for the Wigner distribution function *f***

$$\begin{aligned}\frac{\partial f}{\partial t} + \vec{v}\cdot\nabla_r f - \nabla_r U\cdot\nabla_p f \quad &= \quad -\frac{4\pi^3(\hbar c)^4}{\hbar(mc^2)^2}\int \frac{\mathrm{d}^3p_1'}{(2\pi\hbar)^3}\,\frac{\mathrm{d}^3p_2'}{(2\pi\hbar)^3}\,\mathrm{d}^3p_2\,\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\\ &\times [f f_2(1-f_1')(1-f_2') - f_1' f_2'(1-f)(1-f_2)]\\ &\times \delta^4(p+p_2-p_1'-p_2').\end{aligned}$$

**VUU/BUU type equation**
**(one body level):**

**Boltzmann-eq.+Pauli blocking**
**(Uehling-Uhlenbeck factors)**

**But on a N-body level: dH/dp , dH/dq**

# Definition of *f* and *H*

$$f_i(\vec{r},\vec{p},t) = \frac{1}{\pi^3\hbar^3}\mathrm{e}^{-(\vec{r}-\vec{r}_i(t))^2\frac{2}{L}}\mathrm{e}^{-(\vec{p}-\vec{p}_i(t))^2\frac{L}{2\hbar^2}}$$

**Distribution function obeying Heisenbergs uncertainty principle**

$$\begin{aligned}\langle H\rangle &= \langle T\rangle + \langle V\rangle \\ &= \sum_i \frac{p_i^2}{2m_i} + \sum_i \sum_{j>i} \int f_i(\vec{r},\vec{p},t)\, V^{ij} f_j(\vec{r}\,',\vec{p}\,',t)\, d\vec{r}\, d\vec{r}\,' d\vec{p}\, d\vec{p}\,'\end{aligned}$$

**Hamiltonian containing two and three-body interactions**

# Definition of the potential

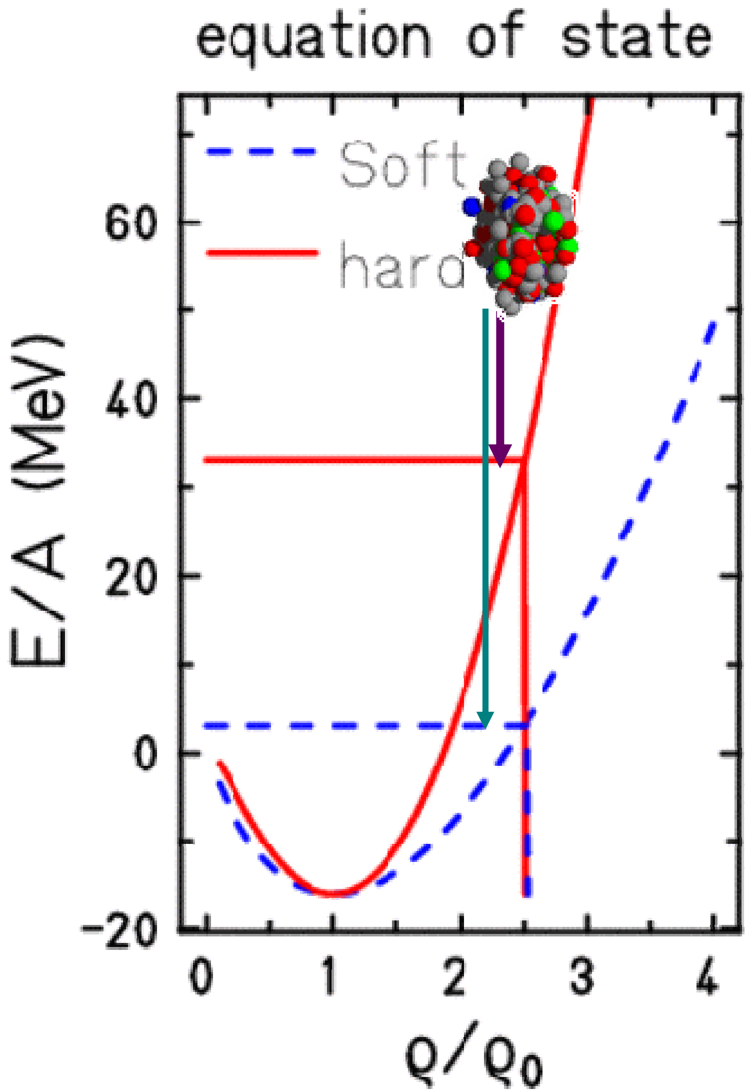
$$
\begin{aligned}
V^{ij} &= G^{ij} + V^{ij}_{\mathrm{Coul}} \\
&= V^{ij}_{\mathrm{Skyrme}} + V^{ij}_{\mathrm{Yuk}} + V^{ij}_{\mathrm{mdi}} + V^{ij}_{\mathrm{Coul}} + V^{ij}_{sym} \\
&= t_1 \delta(\vec{x}_i - \vec{x}_j) + t_2 \delta(\vec{x}_i - \vec{x}_j) \rho^{\gamma-1}(\vec{x}_i) + t_3 \frac{\exp\{-|\vec{x}_i - \vec{x}_j|/\mu\}}{|\vec{x}_i - \vec{x}_j|/\mu} + \\
&\quad t_4 \ln^2(1 + t_5(\vec{p}_i - \vec{p}_j)^2)\delta(\vec{x}_i - \vec{x}_j) + \frac{Z_i Z_j e^2}{|\vec{x}_i - \vec{x}_j|} + \\
&\quad t_6 \frac{1}{\varrho_0} T_3^i T_3^j \delta(\vec{r}_i - \vec{r}_j)
\end{aligned}
$$

**Bethe Weizsaecker –mass formula:**

**Volume term +Surface term +Coulomb term +symmetry term**

**(+pairing term not included)**

# The nuclear equation of state




- **Eos describes the energy needed to compress nuclear matter**
- **A hard eos requires more energy for a given density than a soft one**
- **For a given density and a given available energy a soft eos leaves more thermal energy to the system than a hard eos**
- **The eos can be obtained from our potentials by integration of the volume part of our interactions**

# Volume term integrated:

$$U = \alpha \cdot \left(\frac{\rho_{int}}{\rho_0}\right) + \beta \cdot \left(\frac{\rho_{int}}{\rho_0}\right)^{\gamma} + \delta \cdot \ln^2\left(\varepsilon \cdot (\Delta\vec{p})^2 + 1\right) \cdot \left(\frac{\rho_{int}}{\rho_0}\right)$$

**Skyrme type potential**
**(density dependent)**

**Momentum dependent**
**Interactions (mdi)**

$$U_{mdi} = \delta \cdot \ln^2\left(\varepsilon \cdot (\Delta\vec{p})^2 + 1\right) \cdot \left(\frac{\rho_{int}}{\rho_0}\right)$$

**« optical pot. »**
**linear in density**

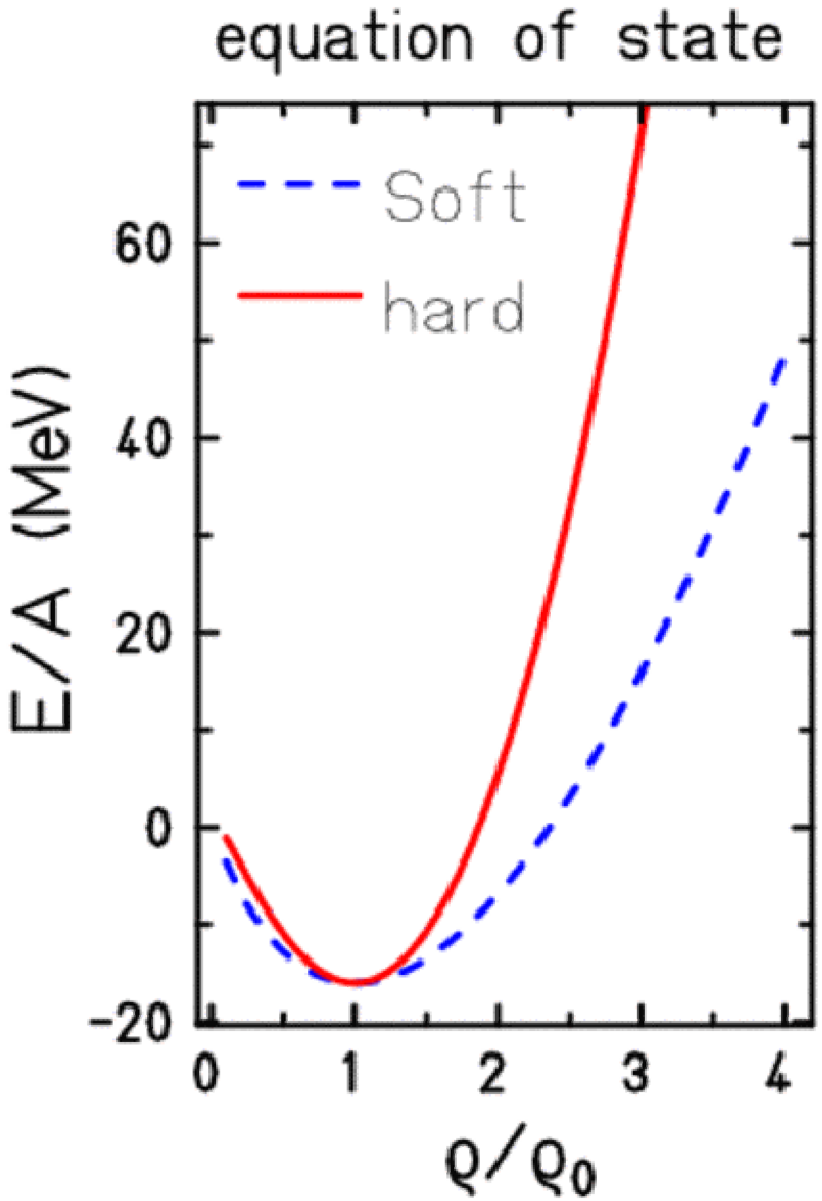
# Parameters of the potential

| | $\alpha$ (MeV) | $\beta$ (MeV) | $\gamma$ | $\delta$ (MeV) | $\varepsilon\left(\frac{c^2}{\mathrm{GeV}^2}\right)$ | $\kappa$ (MeV) |
|---|---|---|---|---|---|---|
| S | -356 | 303 | 1.17 | — | — | 200 |
| SM | -390 | 320 | 1.14 | 1.57 | 500 | 200 |
| H | -124 | 71 | 2.00 | — | — | 376 |
| HM | -130 | 59 | 2.09 | 1.57 | 500 | 376 |
| INT | -157 | 103 | 1.58 | — | — | 284 |
| VH | -110 | 56 | 2.40 | — | — | 456 |

**Sets of the nuclear equation of state: hard, soft, etc**

**Parameters of the potential related to the interactions.**

# « Our nuclear eos »



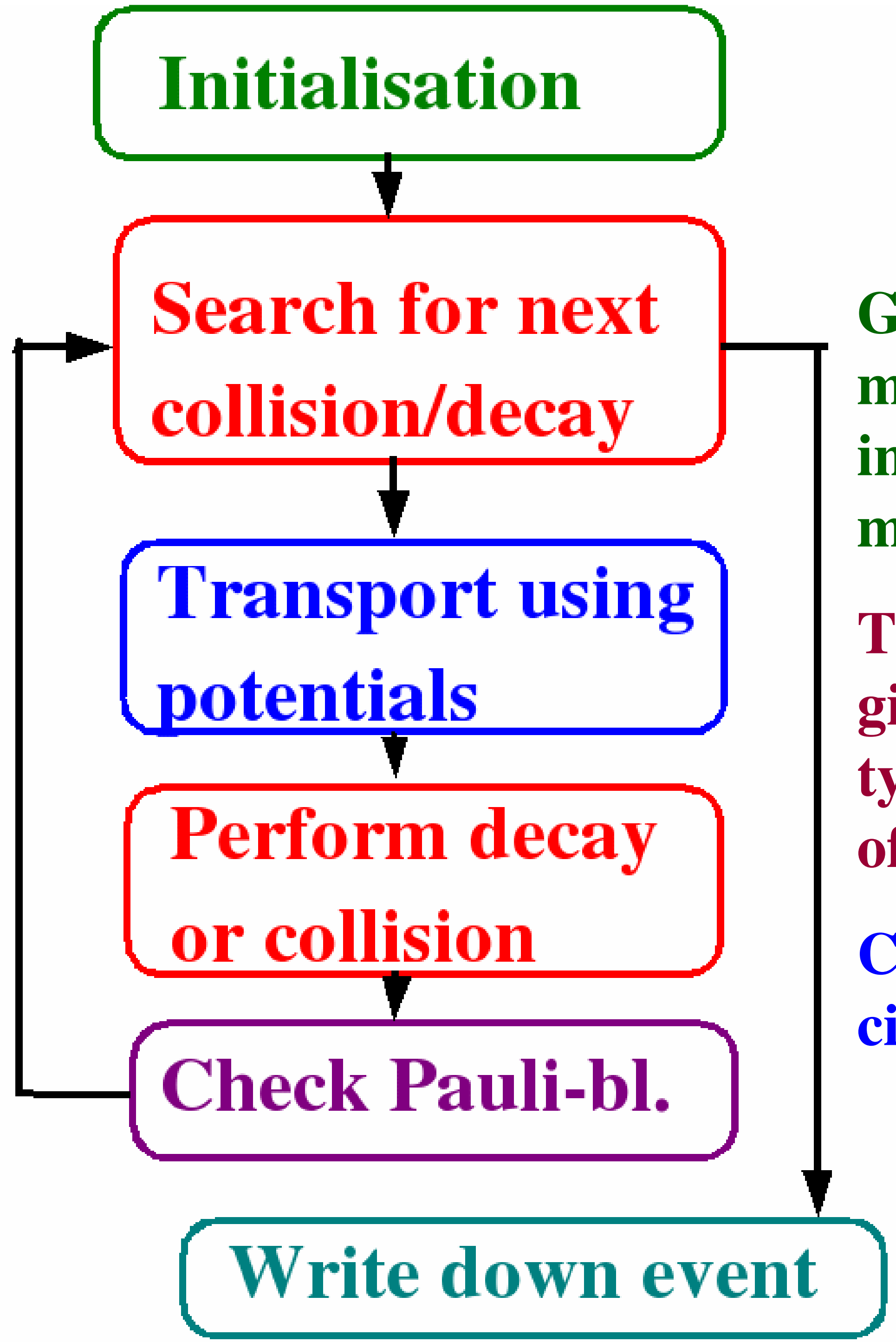

A hard eos (H) yield higher compressional energy at high denities than a soft eos.

A soft eos with mdi (SM) shows the same density dependence for T=0 than a soft eos without mdi (S).

Our interactions work also far off from equilibrium, the eos is only the infinite matter limit of our interactions.

High energy limit of several GeV (5-7 $\rho_0$) for causality reasons.

# Scheme of a calculation




General scheme similar for most models but the ingredients of the modules may differ

The collision is followed for a given number of timesteps, typically several hundred steps of 0.2-0.5 fm/c

Calculations using relativistic cinematics

Fragments are extracted afterwards using MST or simulated annealing (SACA)

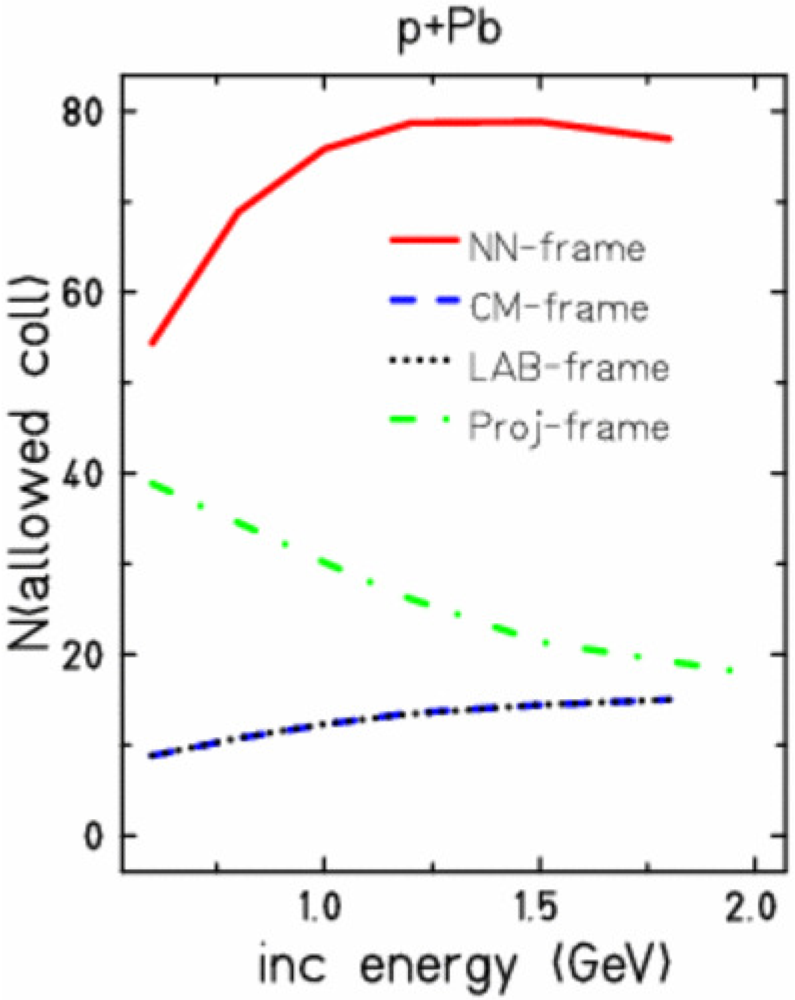
# Relativistic cinematics does not mean covariant

- We have to define a reference frame, where our clock is synchronized.
  Time-ordering is done with respect to this frame.
- The choice of the reference frame may depend on the observable we are interested in:

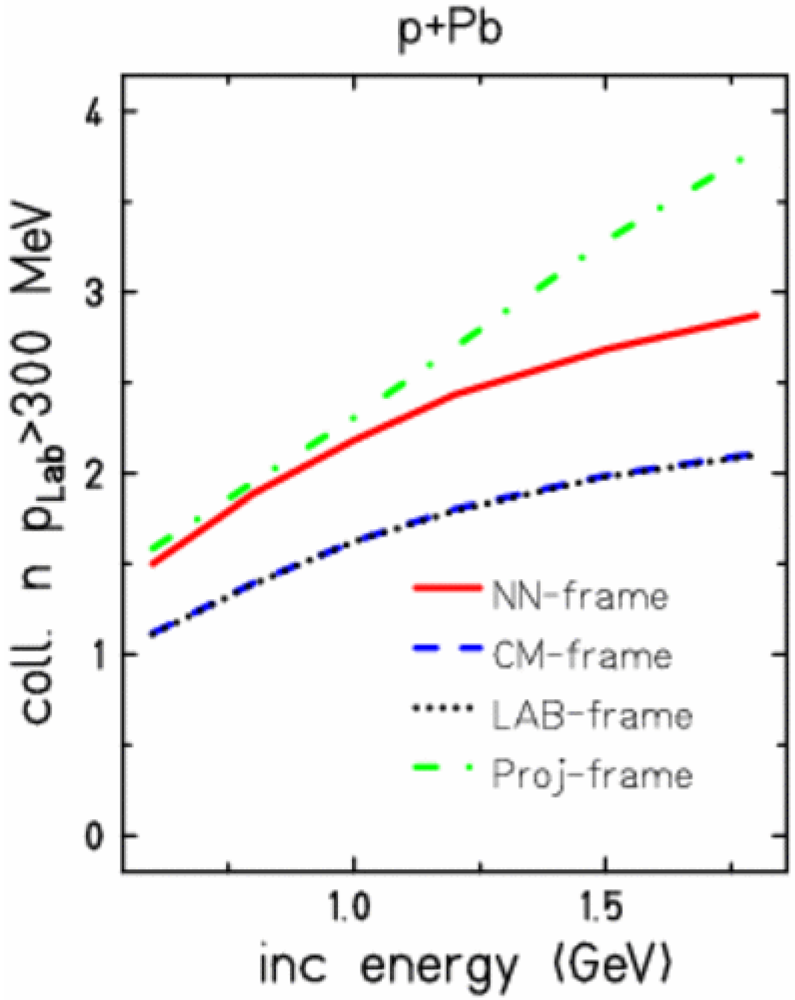
| | |
|---|---|
| laboratory frame: | target fragmentation |
| nucleus-nucleus-cm: | nuclear equilibration |
| N-N –cm (equal speed): | secondary particles (π,K) |

- The result of our calculation may depend on this choice (see Kodama et al.)

# Collision numbers and low energy yields may be effected

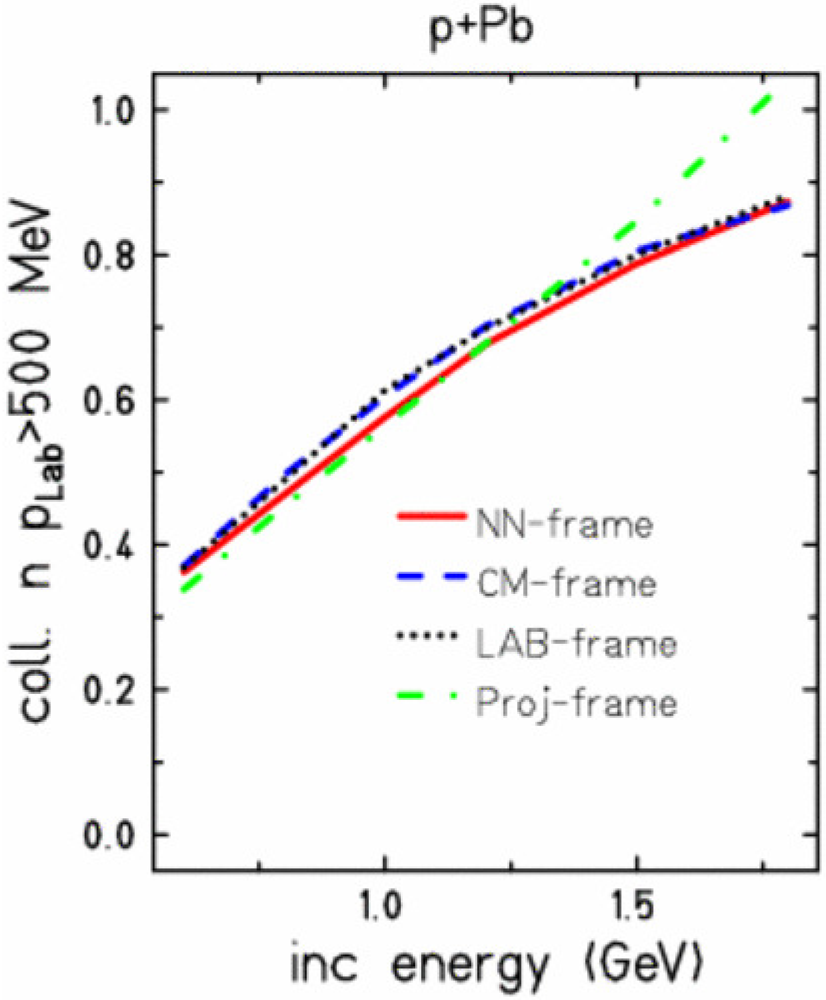


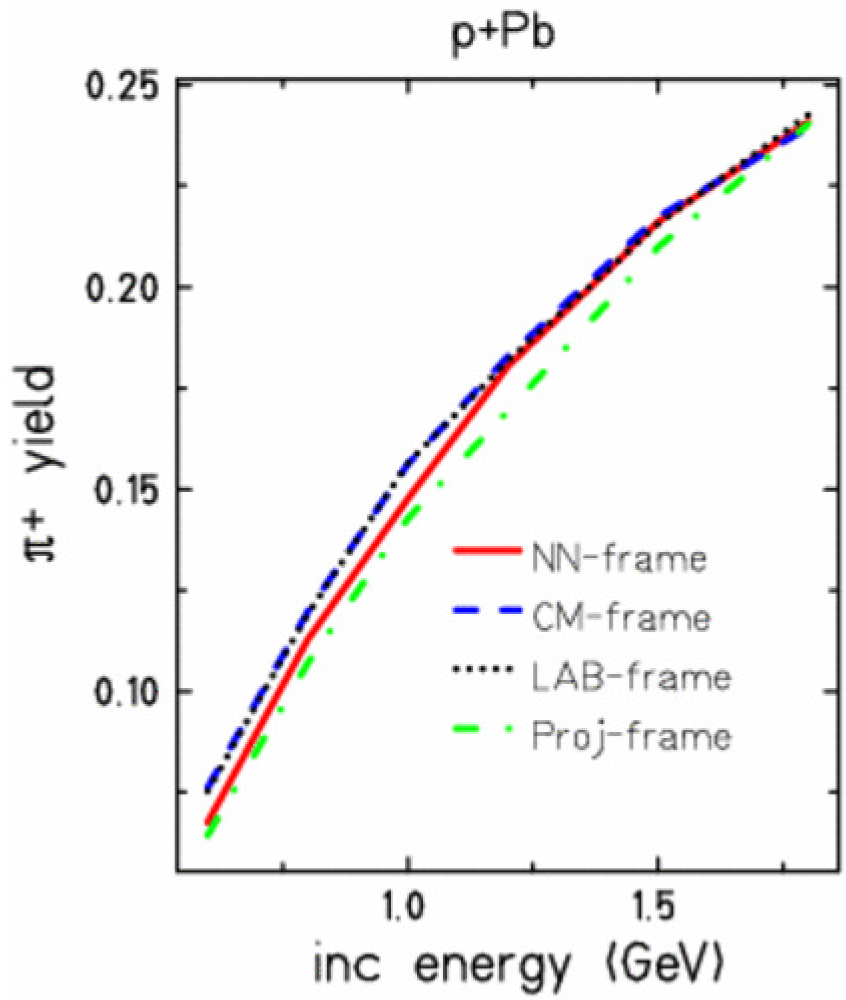

Allowed collisions out of about 1000 attempted coll.



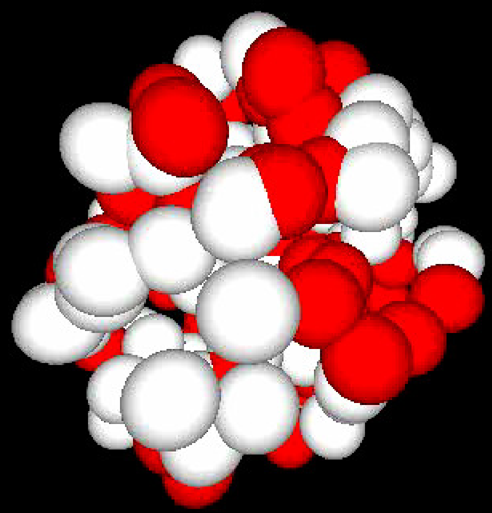

Initialisation momenta p<270 MeV

# …but not so much high energy particles and secondary probes



# Let's go into the details of matter



# Collision term

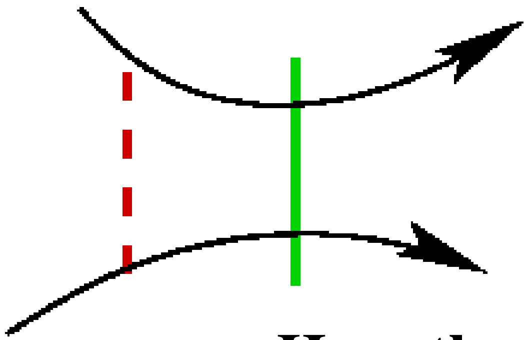
**The collission of two particles is treated in in their own centre-of-mass frame (invariant description).**

**Two particles collide if their minimum distance fulfills:**

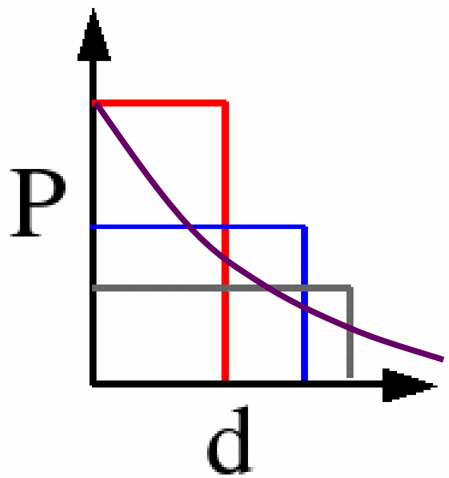
$$d \leq d_0 = \sqrt{\frac{\sigma_{\rm tot}}{\pi}}, \qquad \sigma_{\rm tot} = \sigma(\sqrt{s},\ \text{type}).$$

**(like INC, BUU, VUU, …)** **particles: N, Δ, π**

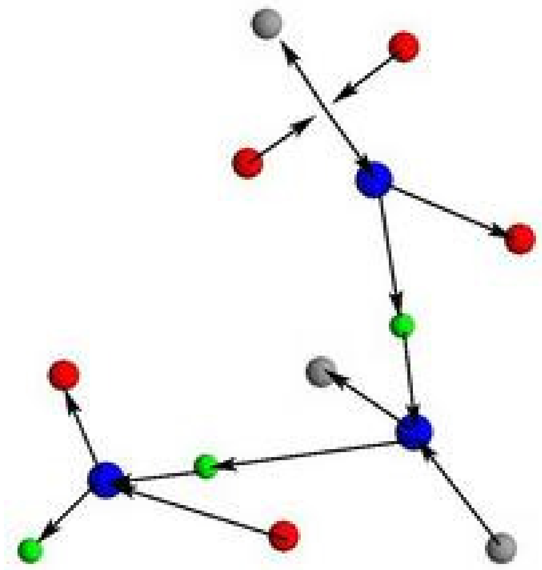
**default: black disk, but weighted P(d) possible**



**Here the coll. happens**



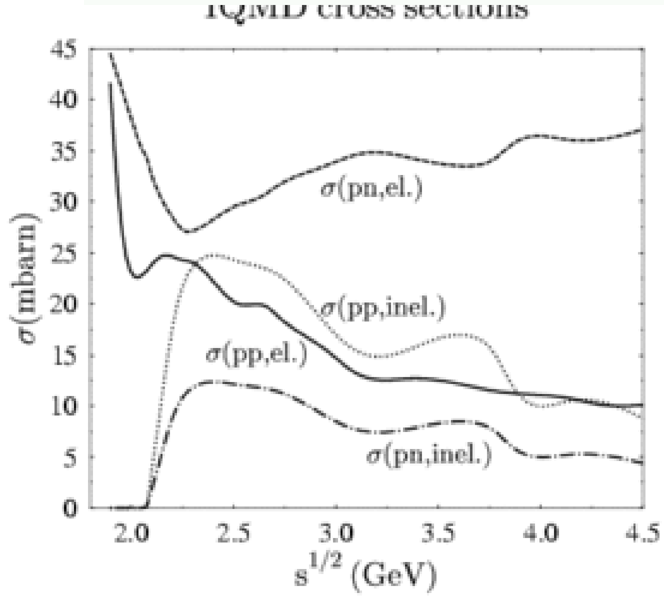
# Pion production



- Pions are produced via the Δ (1232)
  NN ↔ NΔ Δ ↔N π
- Frequent rescattering in the nucleus
- Use of Clebsch Gordon coeeficients and detailed balance with spectra function corrections (Danielewicz and Bertsch)
- Decay of the D with mass-dependence width (Kitazoe, Randrup or phaseshift)
- Effects of lifetime parametrization and det.bal spectral function corrections in the order of 10% for pion yields

# Cross section parametrization

$$\sigma_{\text{tot}} = \sigma_{\text{el}} + \sigma_{\text{inel}} = \sigma_{\text{el}} + \sum_{\text{channels}} \sigma_i$$



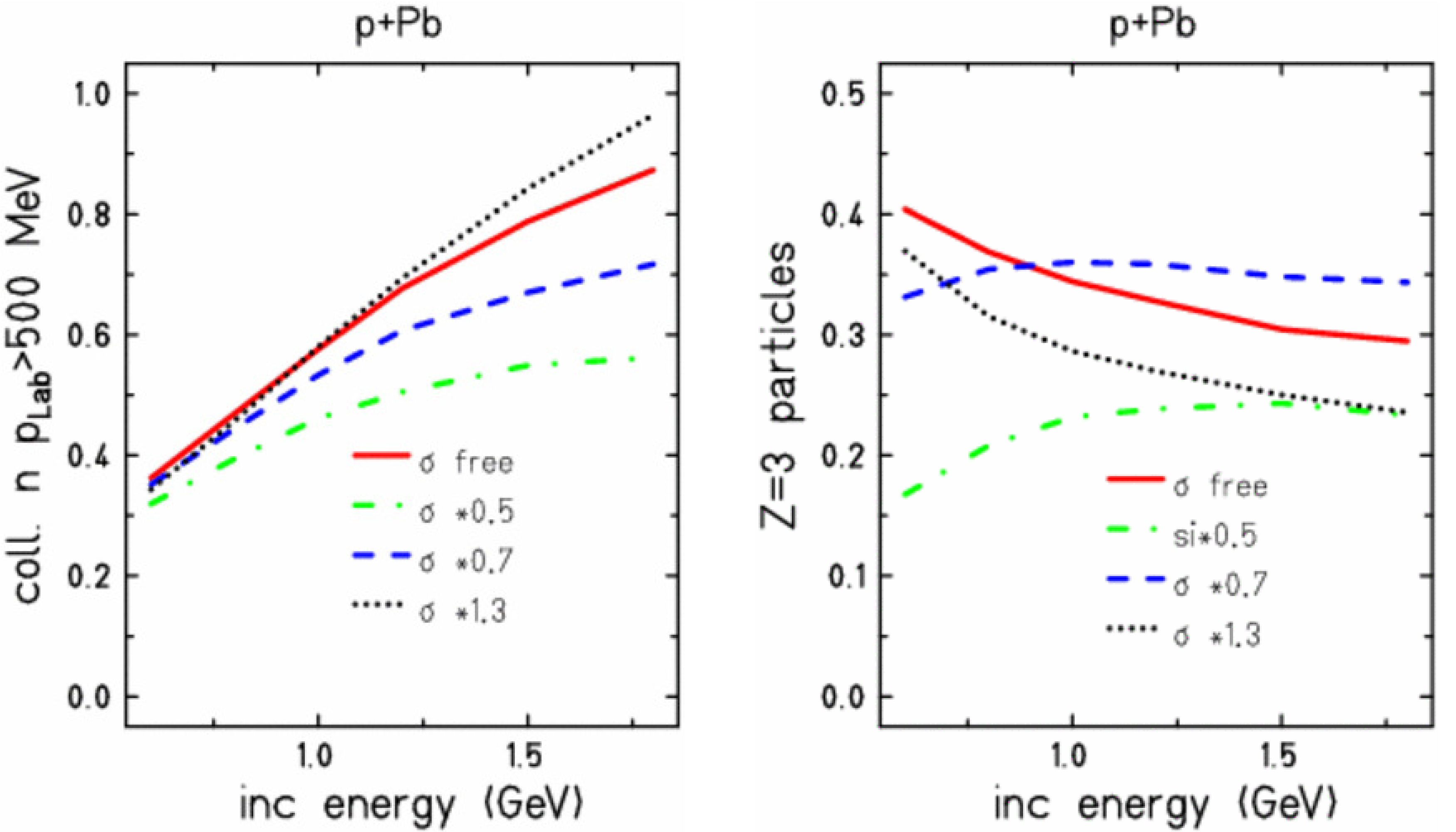

**Parametrized according to experimental data (table)**

**Use of Clebsch-Gordon coefficients and detailed balance for reactions with unknown cross sections.**

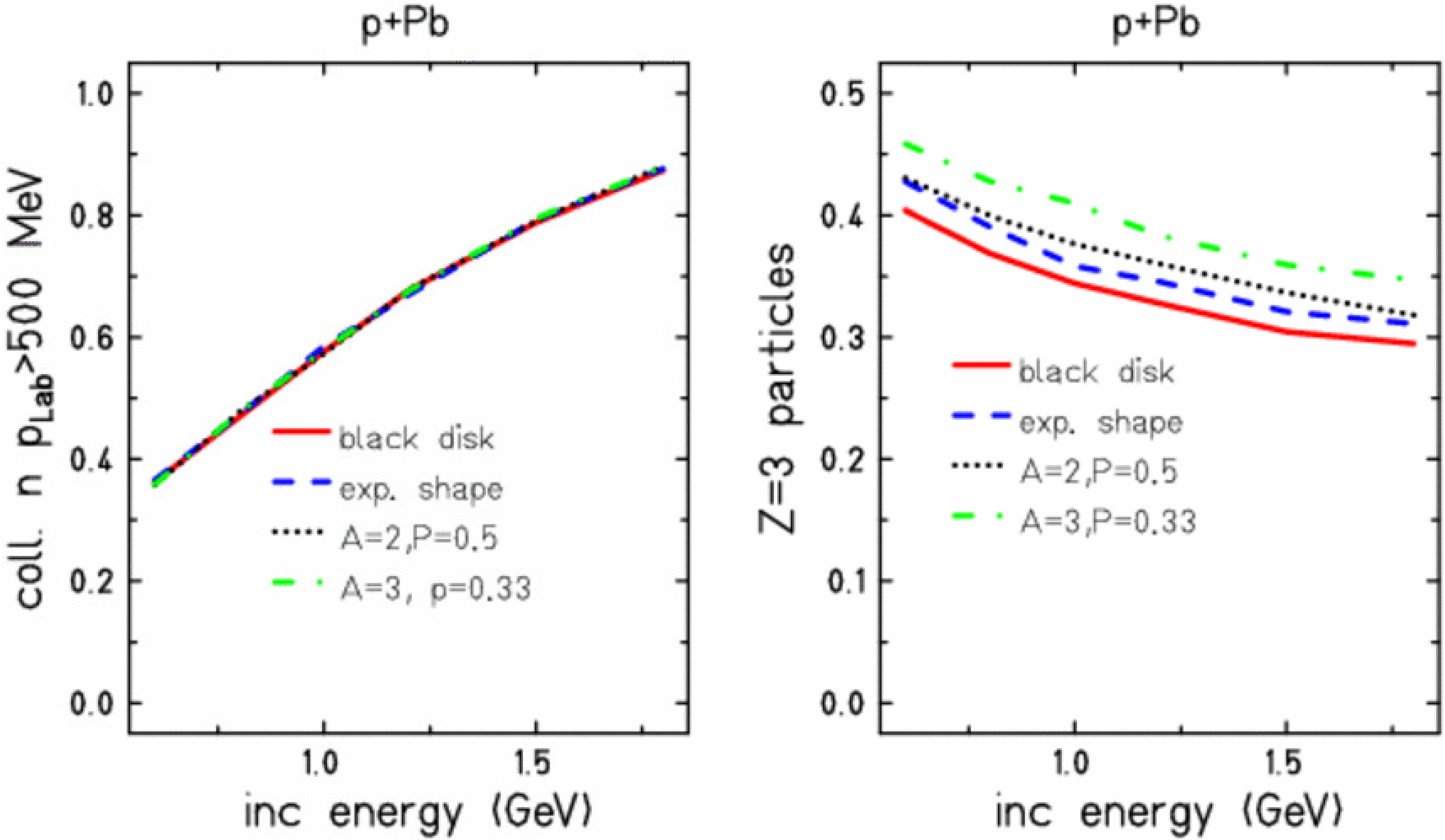
**Use of free cross sections, but scaling factors possible.**

**Optional: use of density dependent scaling, formation time …**

# The absolute scale of the cross sections influences collision rates, energy spectra, fragmentation …



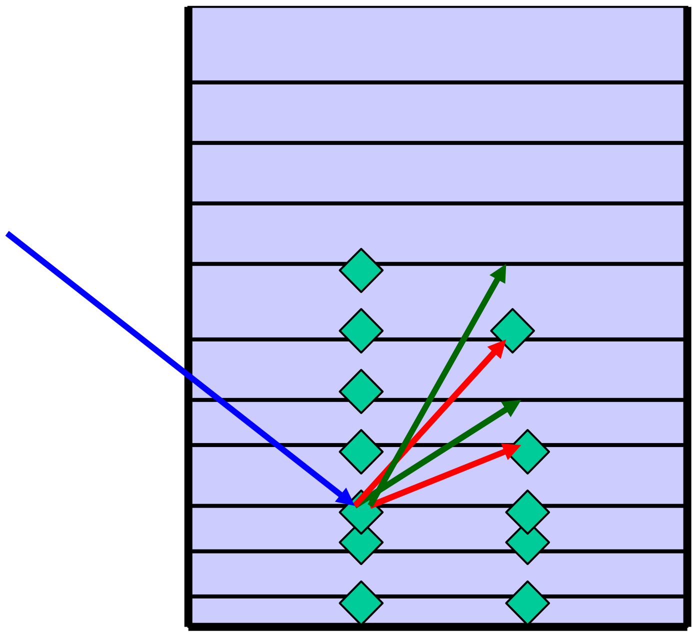
## The definition of the cross section shape does not influence coll. Numbers, pion prod, high E spectra

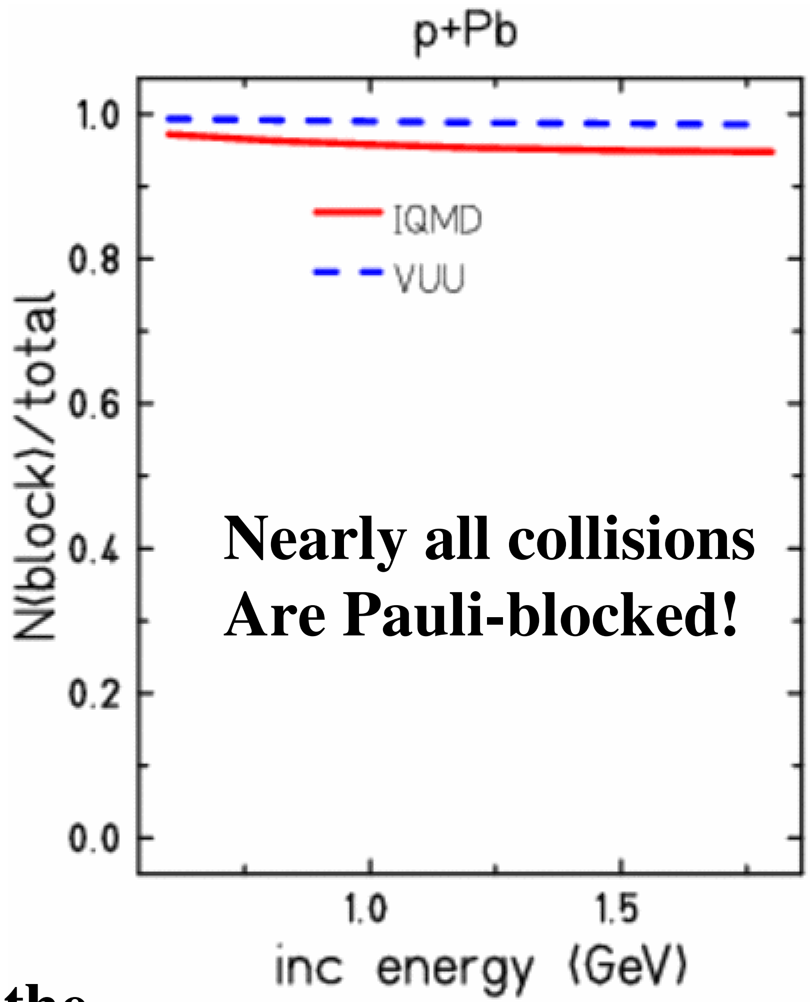



## But different granularities may affect the fragmentation

# Pauli blocking of the final states

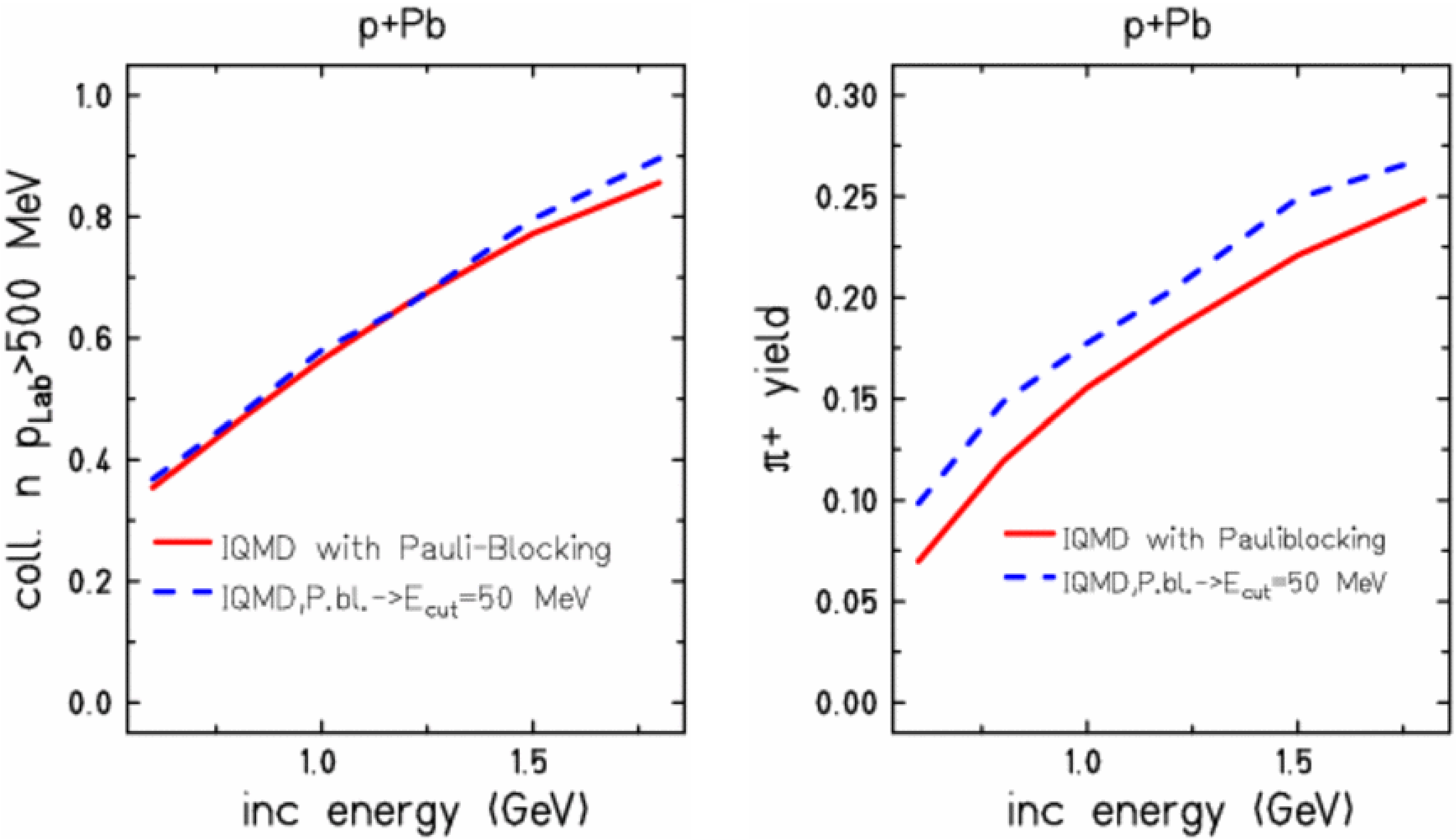
**A collision is only allowed if the final states are not occupied by other nucleons**





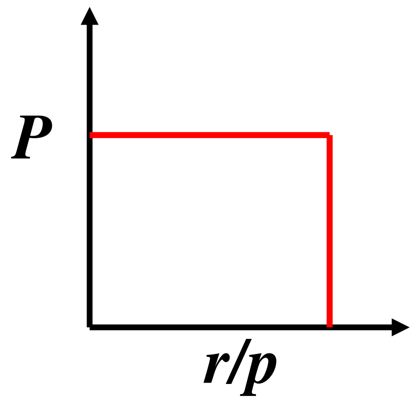

**Pauli blocking tested by analysing the phase space density of the final state**

# Pauli blocking replaced by E-cut



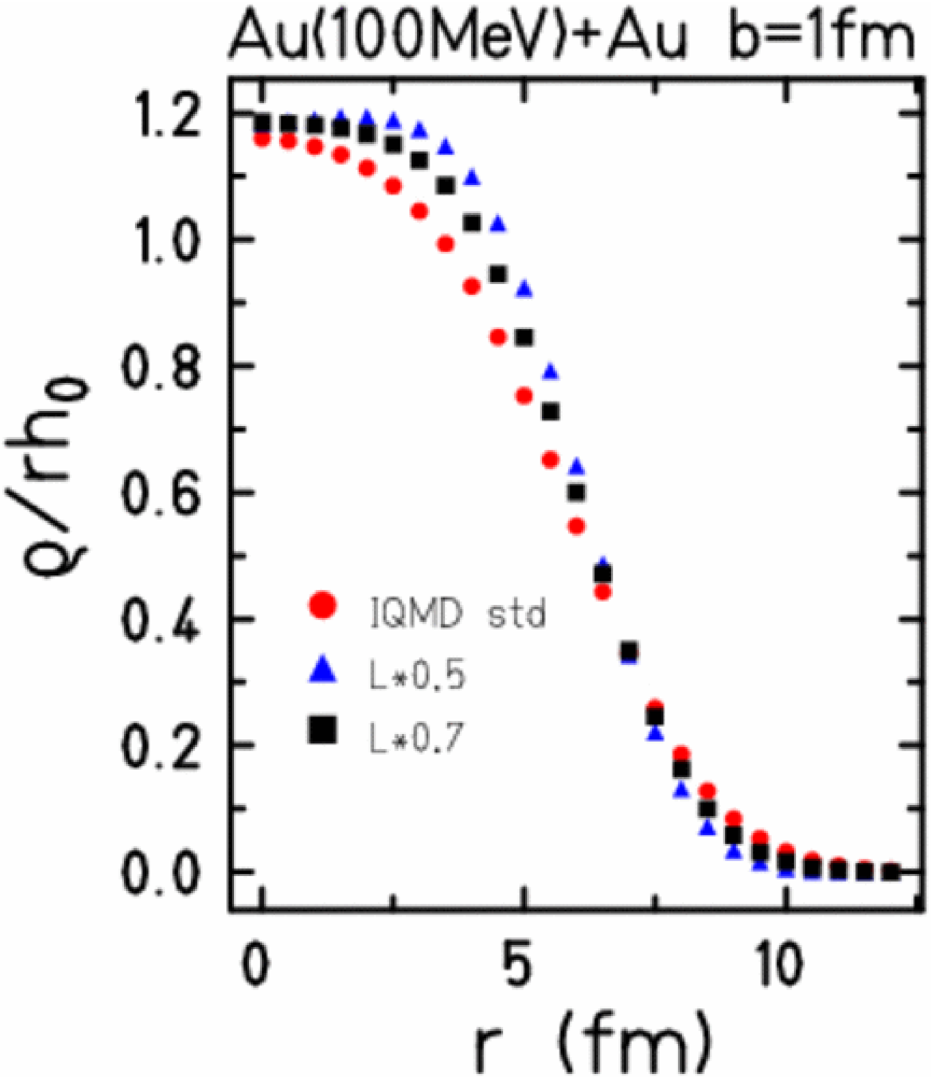
# Choices for initialisation

- Thomas Fermi for infinite matter
- Ground state density of 0.17 $fm^2$




This results in an initialisation of

- a hard sphere in coordinate space with
  $R_{max} = R_0 A^{1/3}$   $R_0 = 1.12$ fm
- a hard sphere in momentum space with $P_F = 268$ MeV
- Optional Wood-Saxon , deformation (not in std. Vers.)
  spectral function (only cascade, not standard)



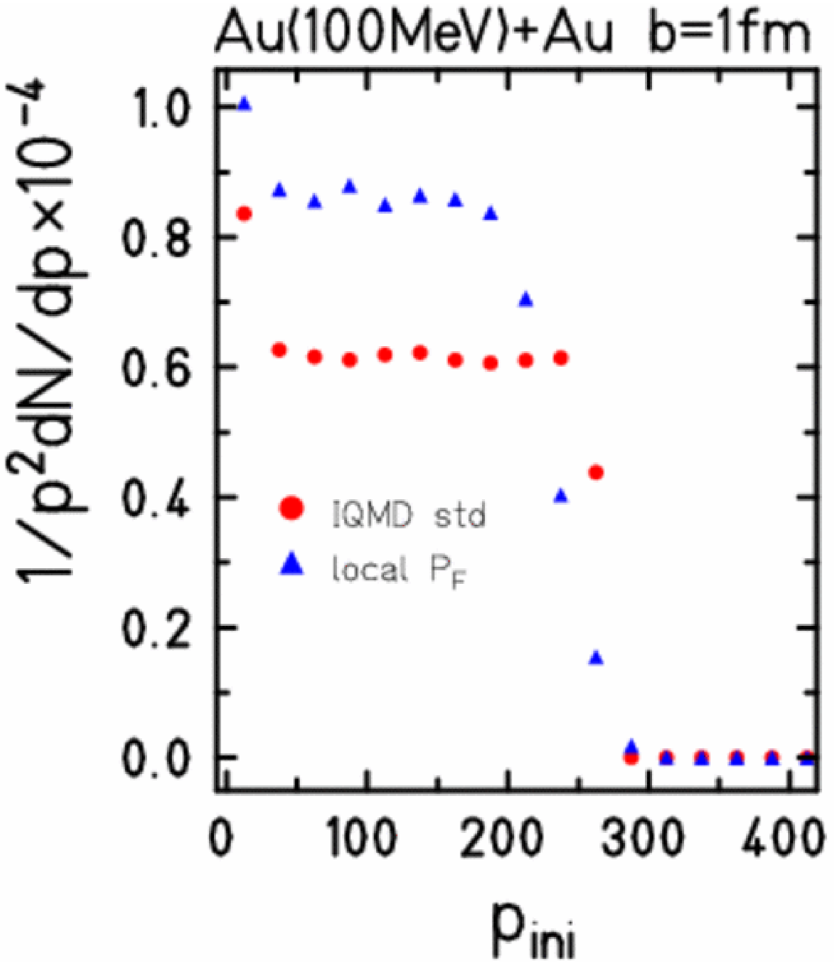

# Density profile

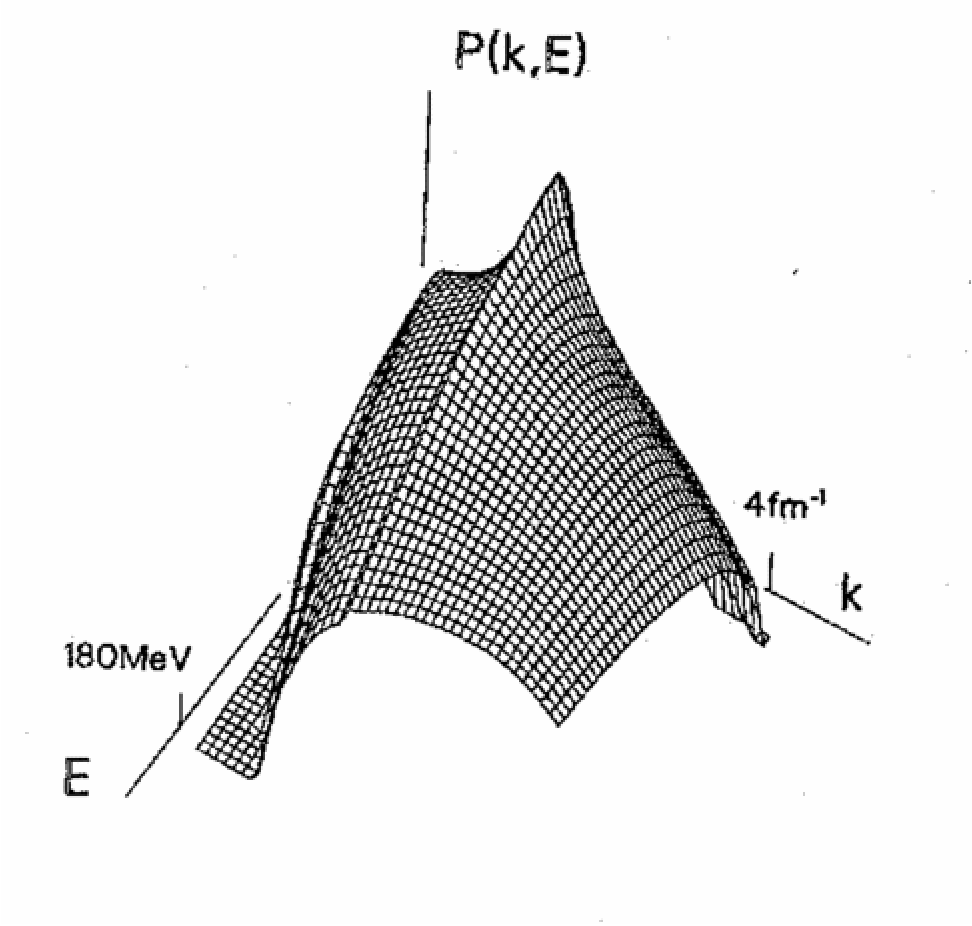
**Smooth profile caused by Gaussian width L**

**free parameter, but enters also into the range of the potentials**

$$f_i(\vec{r},\vec{p},t) = \frac{1}{\pi^3\hbar^3} e^{-(\vec{r}-\vec{r}_i(t))^2 \frac{2}{L}} e^{-(\vec{p}-\vec{p}_i(t))^2 \frac{L}{2\hbar^2}}$$

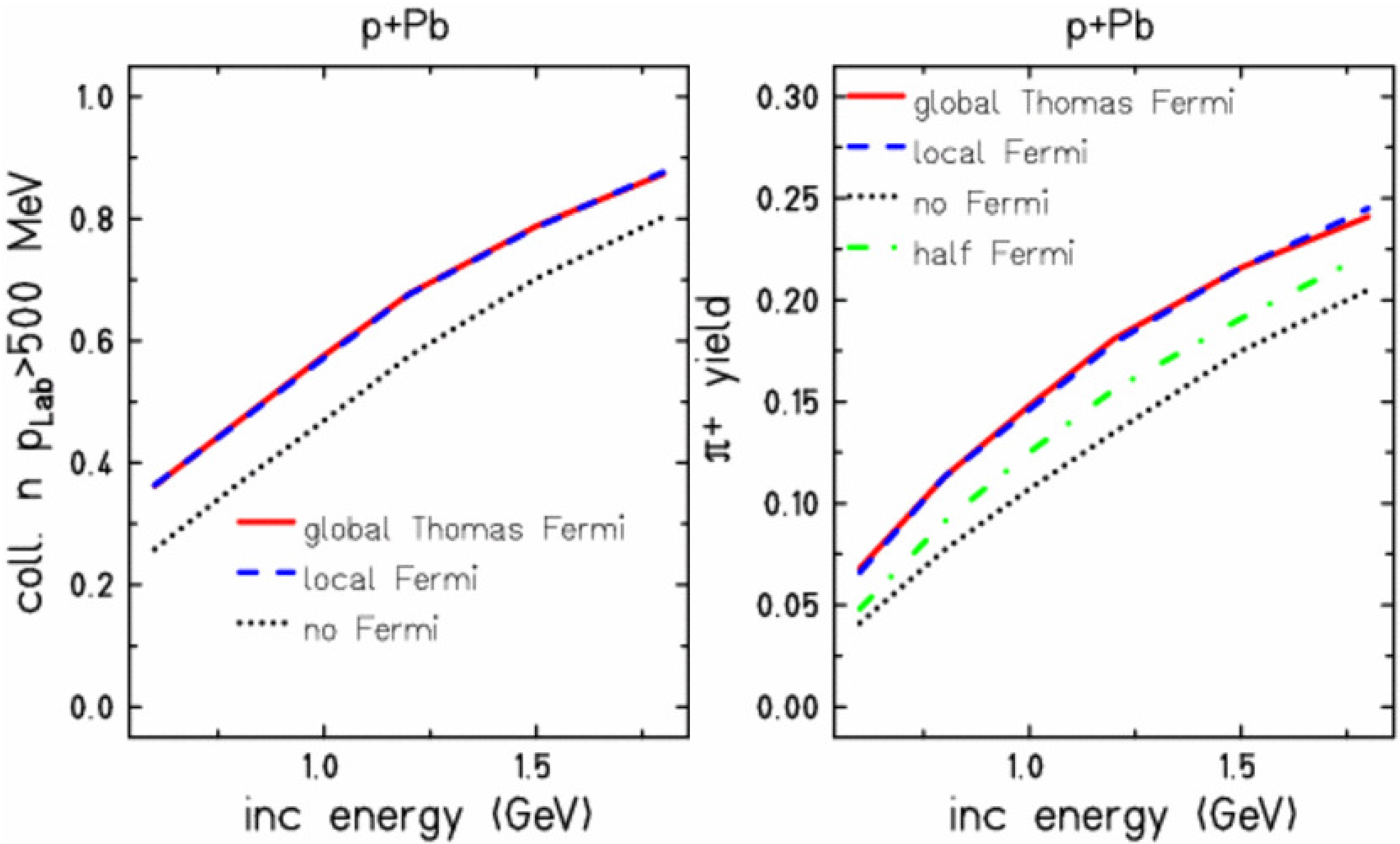
# Optional: local Thomas Fermi



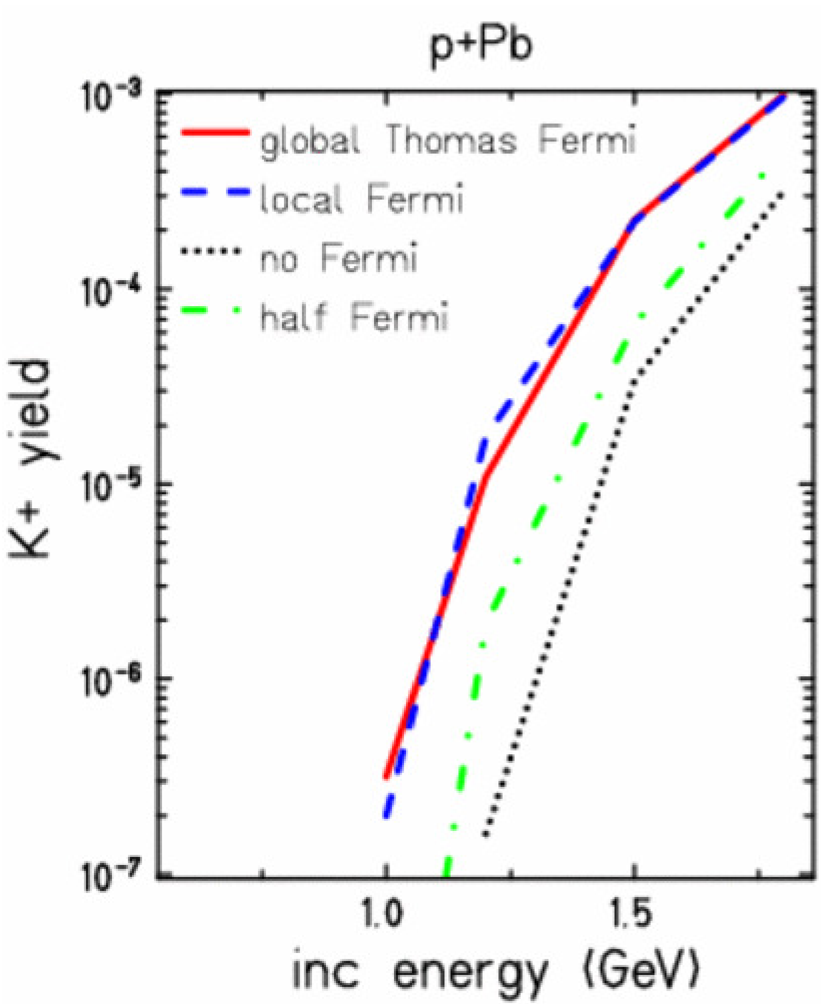



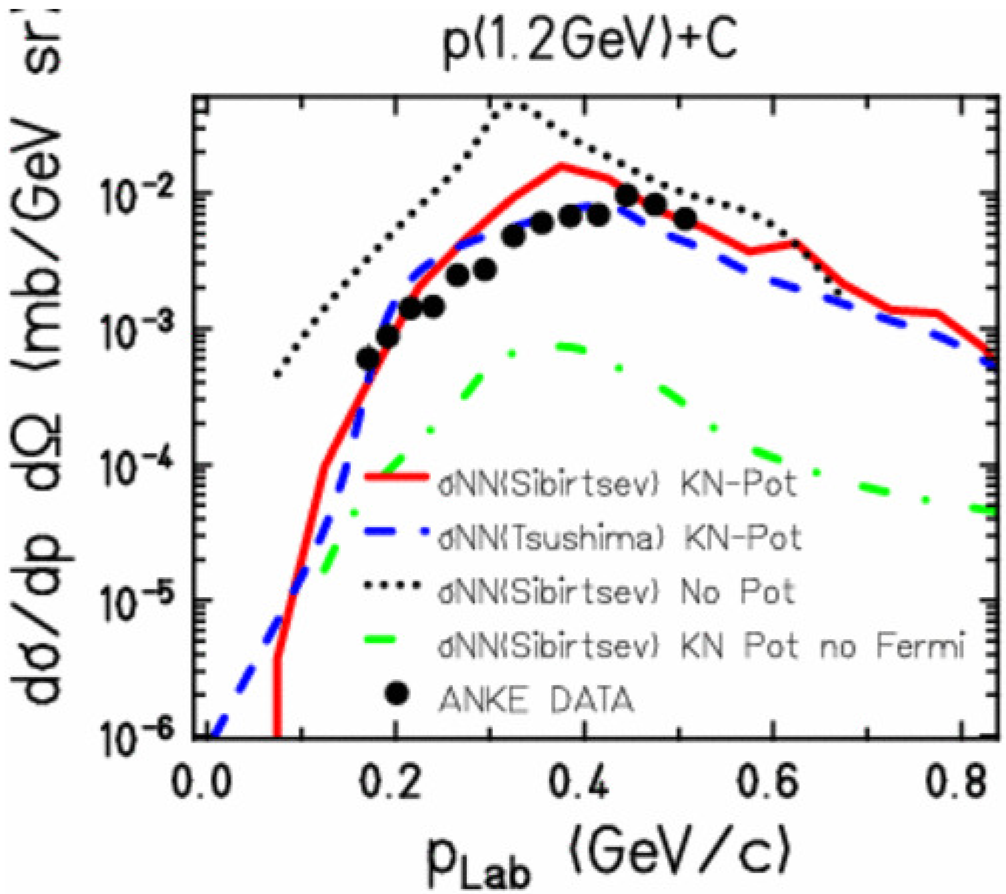

For p+A cascade: spectral function (not in std.version)

# Fermi momentum influences pion number and high energy spectra

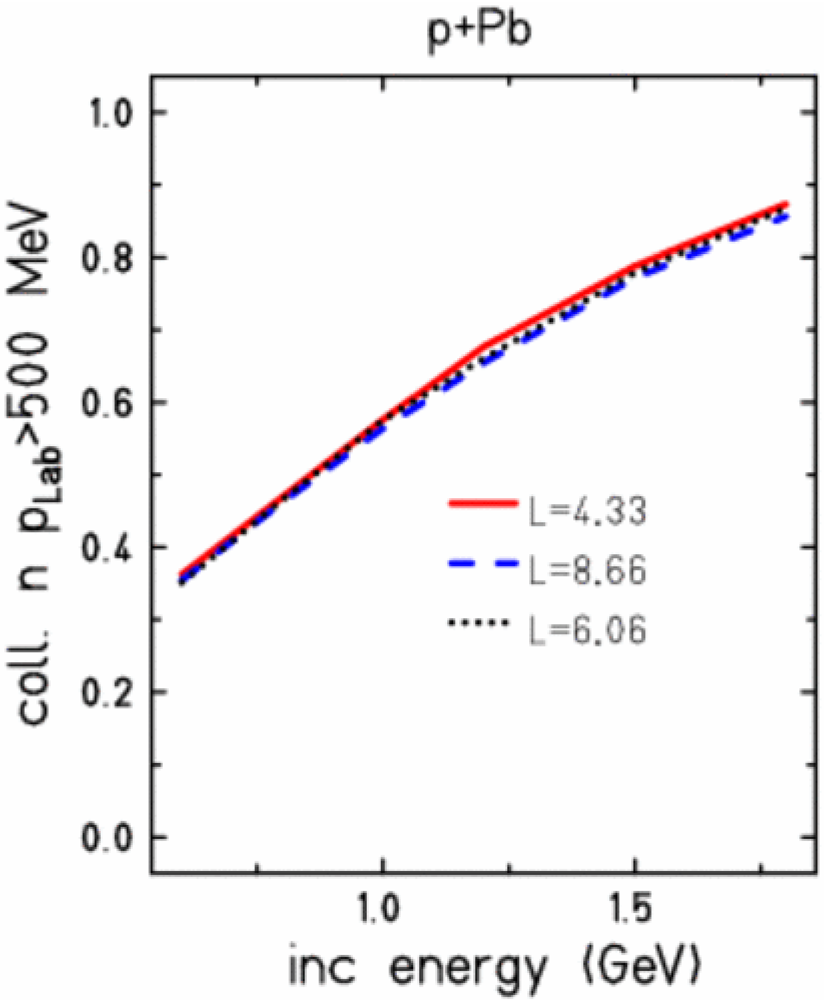


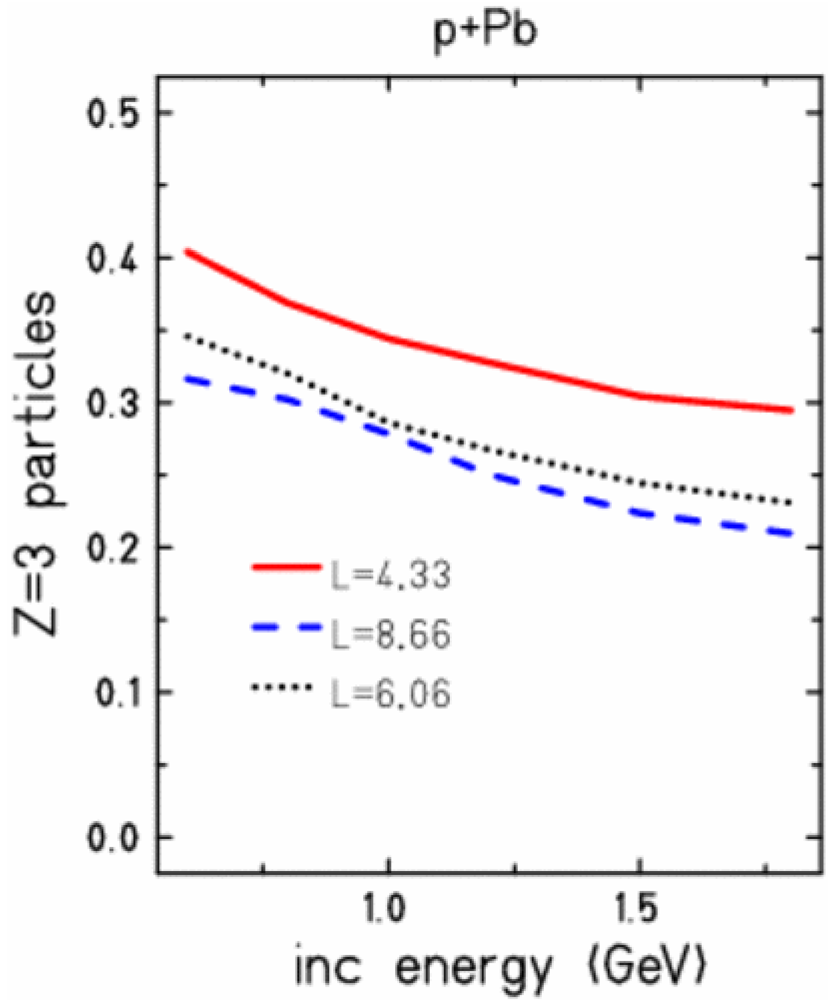
## …but Fermi momentum is needed for explaining subthreshold kaon production



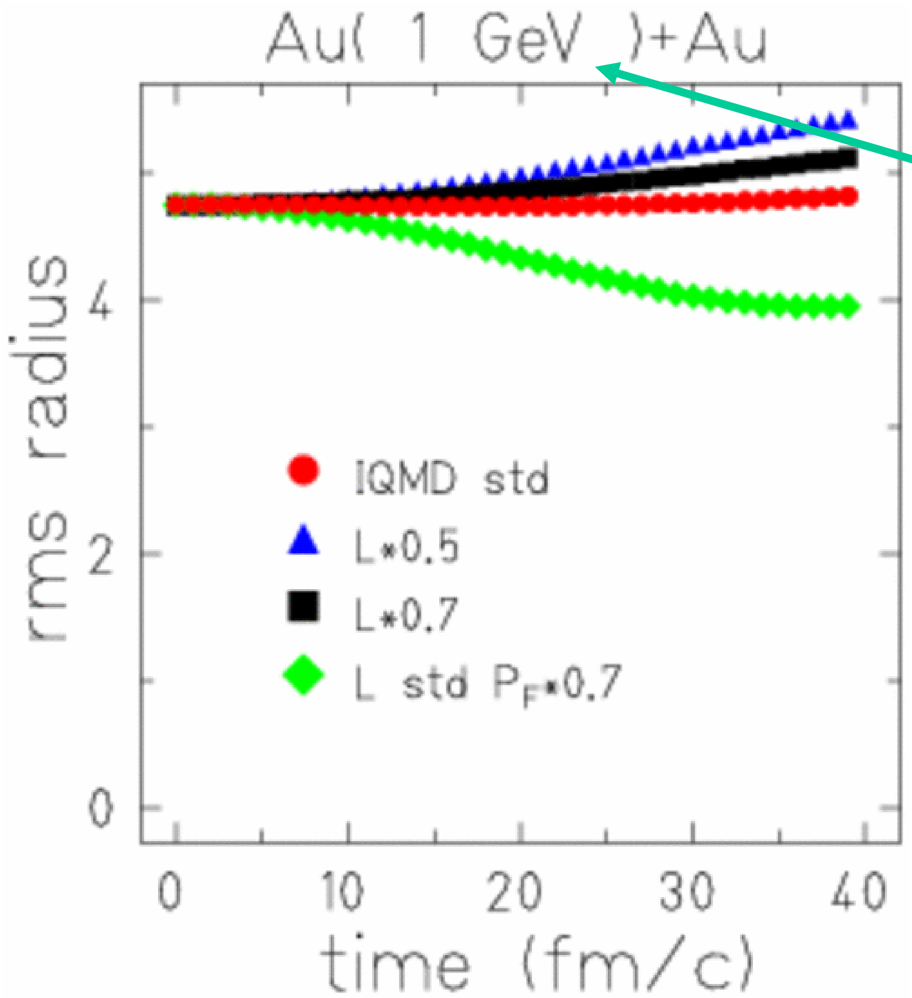



# Gaussian width in potential range: no effects on pions+high E but on fragmentation



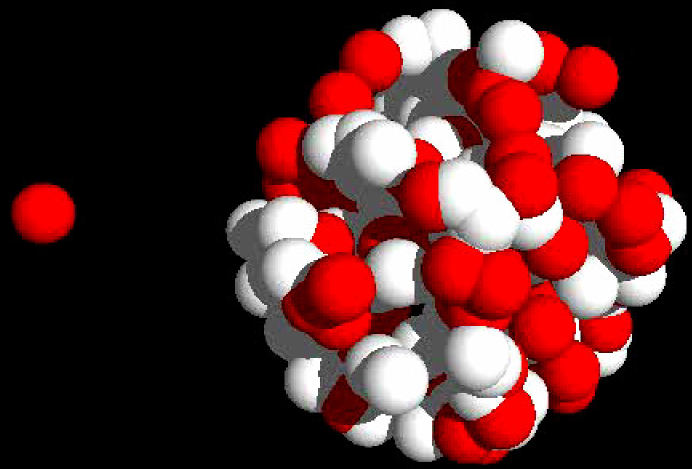
# Choice of parameters



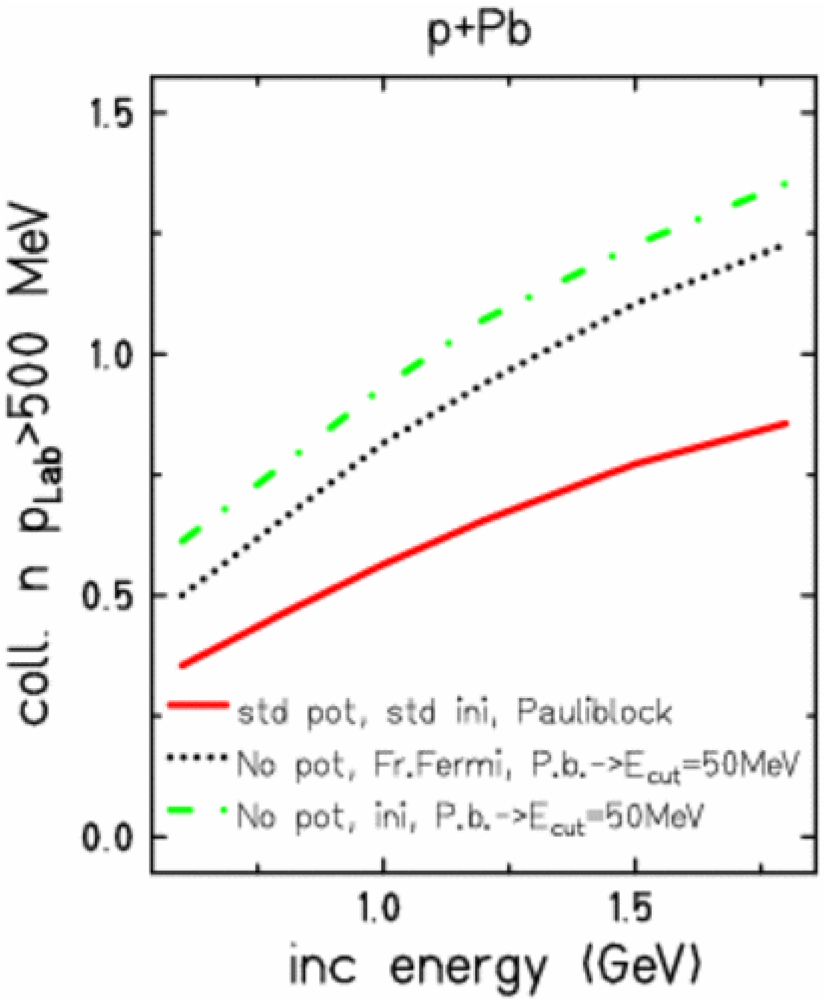

**Issued from physics at higher energies:**

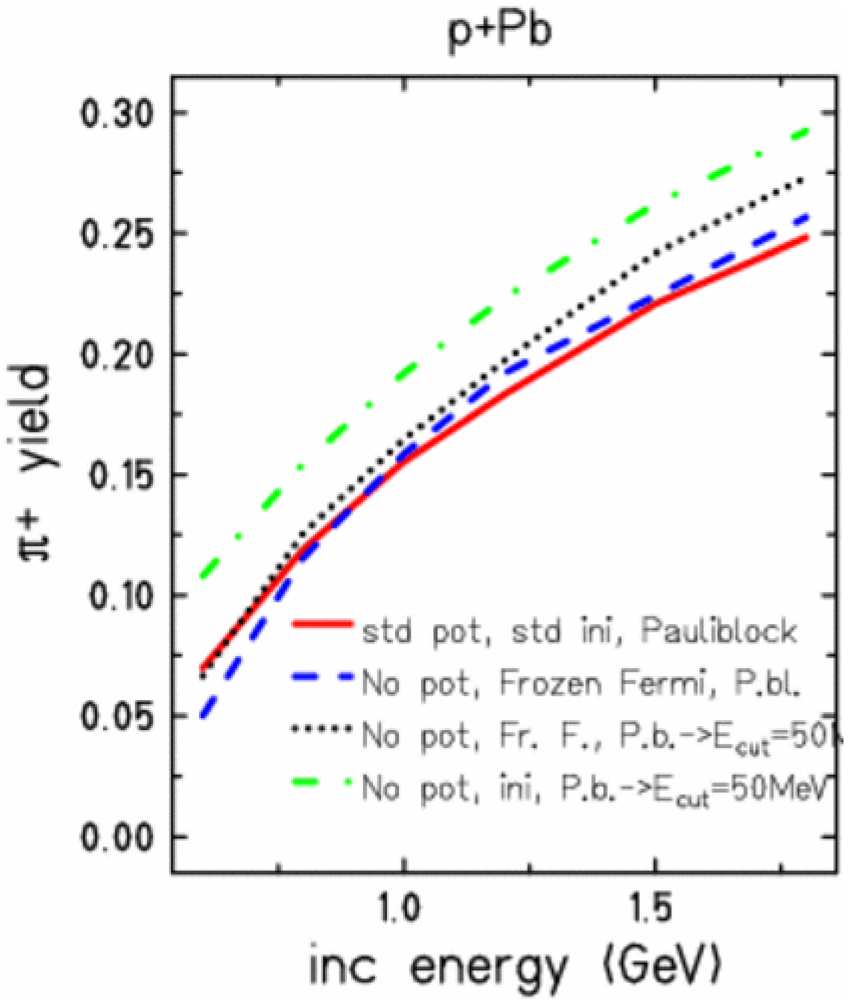
**Maximum stability during reaction time**

## If you choose not the correct parameters the system might become less stable



# Pseudo-stability: no potentials+frozen Fermi



# A « genealogy » of QMD (by head, not exhaustive nor precise)

| *(int.)* Name | 1st auth.+sup. | birth | based on | specials, purpose |
|---|---|---|---|---|
| *Dino*-QMD | Aichelin+Stöcker | 1986 | BUU | 1st QMD, N, Δ, no isospin |
| QMD-*N14* | Peilert+A+St | 1987 | DinoQMD | fragmentation, Pl.Ball |
| IQMD | Hartnack+St | 1987 | VUU | isospin, pions, flow Pl.Ball |
| *B*QMD | Bohnet +A | 1989 | QMDN14 | fragmentation, ALADIN |
| *K*QMD | Konopka+St | 1990 | *from scratch* | low energy, spallation |
| *P*QMD | Peilert+St | 1991 | QMDN14 | transmutation, LLNL |
| RQMD | Sorge+St | 1991 | IQMD | relat. Transport, AGS,SPS |
| *H*QMD | Huber+A | 1991 | BQMD | isospin, pions, N* |
| *T*RQMD | Lehmann,Fuchs | 1992 | BQMD | rel. Transport, high E |
| MQMD | Li ??? | 1993?? | IQMD?? | Stability, fragmentation |
| UrQMD | Bass+St | 1997 | *from scratch* | rel. Transport, RHIC |

# Different models of similar type

**VUU (Kruse, Jacak, Stoecker)**

**one body model, testparticles on a Lagrangian grid**
**comparisons to Streamerchamber, Plasticball**

**IQMD (Bass, Hartnack, Stoecker)**

**N-body model using Gaussians**
**comparisons to Pl.ball, FOPI, TAPS, KaoS, Hades**

**BQMD (Aichelin, Bohnet)**

**N-body model using Gaussians**
**comparisons to MSU, ALADIN, INDRA**

**For further details see:**

**C. Hartnack et al. Eur. Phys. J A1 (1998) 151**

# VUU vs. IQMD

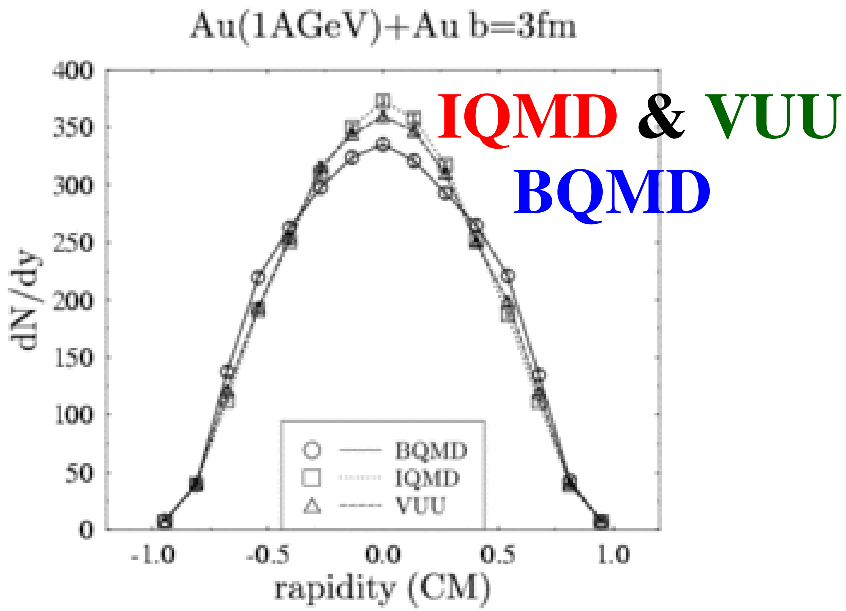
- **Very similar treatment of the initialisation: hard spheres in coordinate and momentum space**
- **Quasi-identical treatment of the collisions in event-by-event handling, IQMD cross sections majorly from VUU**
- **Different treatment of the potential term**
    - **VUU uses pointparticle spheres in parallel ensembles and applies only Skyrme forces**
    - **IQMD uses Gaussians in single events and apply additional forces: Yukawa, Coulomb, symmetry**

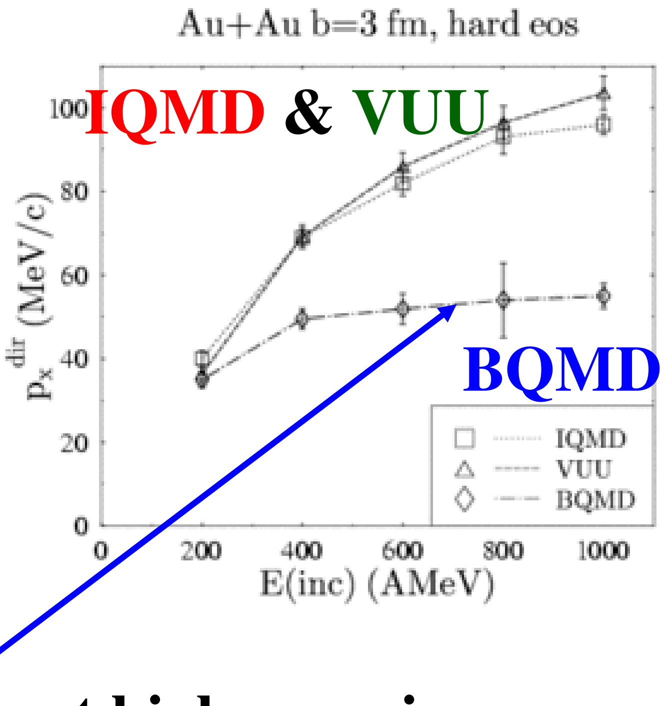
# BQMD vs. IQMD

- **Different initialisations:**
  - **BQMD uses Wood-Saxon distributions in coordinate space and reduced Fermi momenta, default reference frame CM**
  - **IQMD uses hard spheres in coordinate and momentum space default reference frame « equal speed » (NN-CM)**
- **Different cross section parametrizations**
  - **BQMD uses Cugnon parametrization**
  - **IQMD bases on VUU parametrization**
- **Potential treatment rather similar in its principles but different parameters (like default Gaussian width) are used.**

**IQMD has explicit Coulomb interactions and symmetry energy.**

# Comparison at higher energy (but A+A)

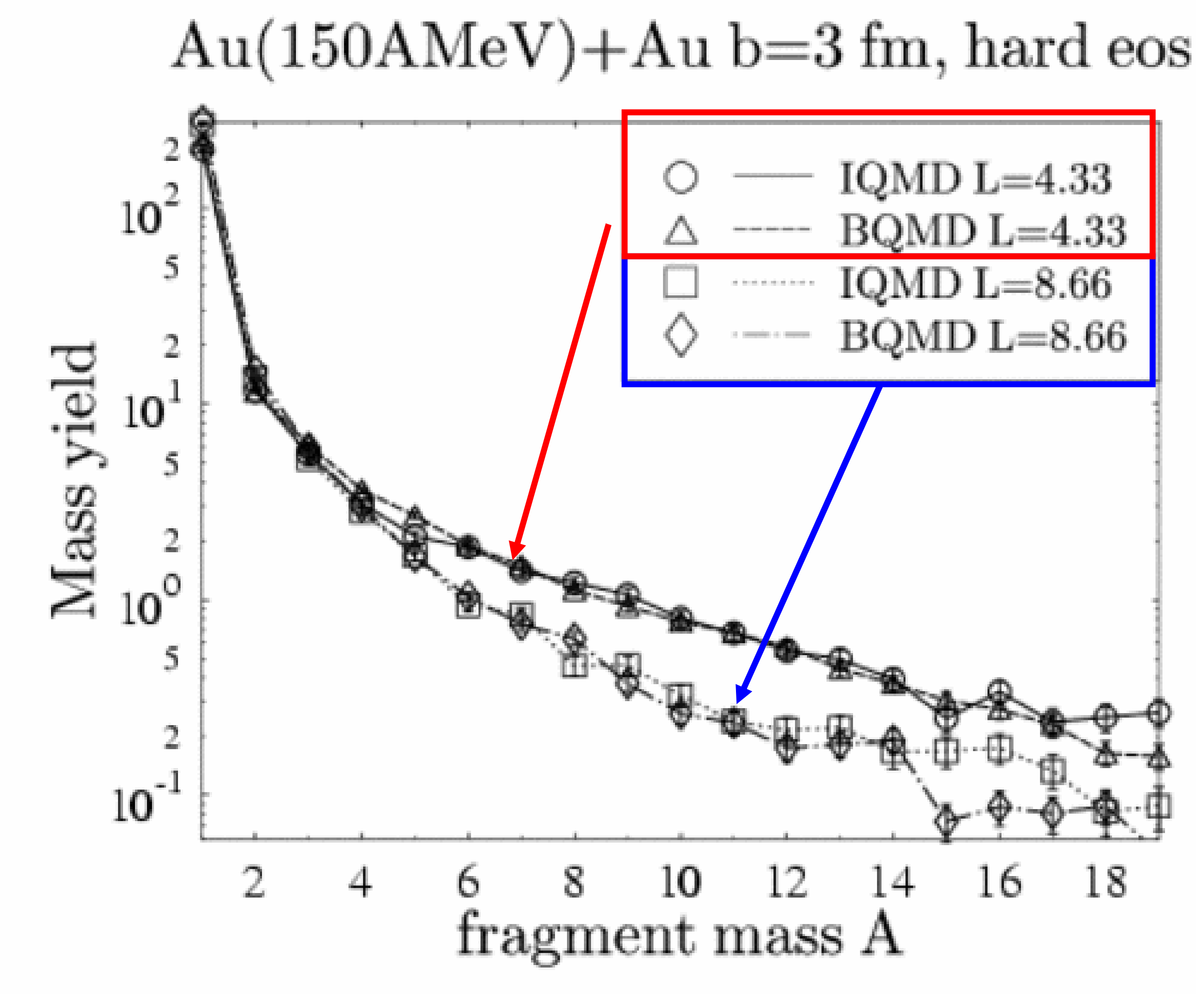



**VUU and IQMD quite similar at high energies**

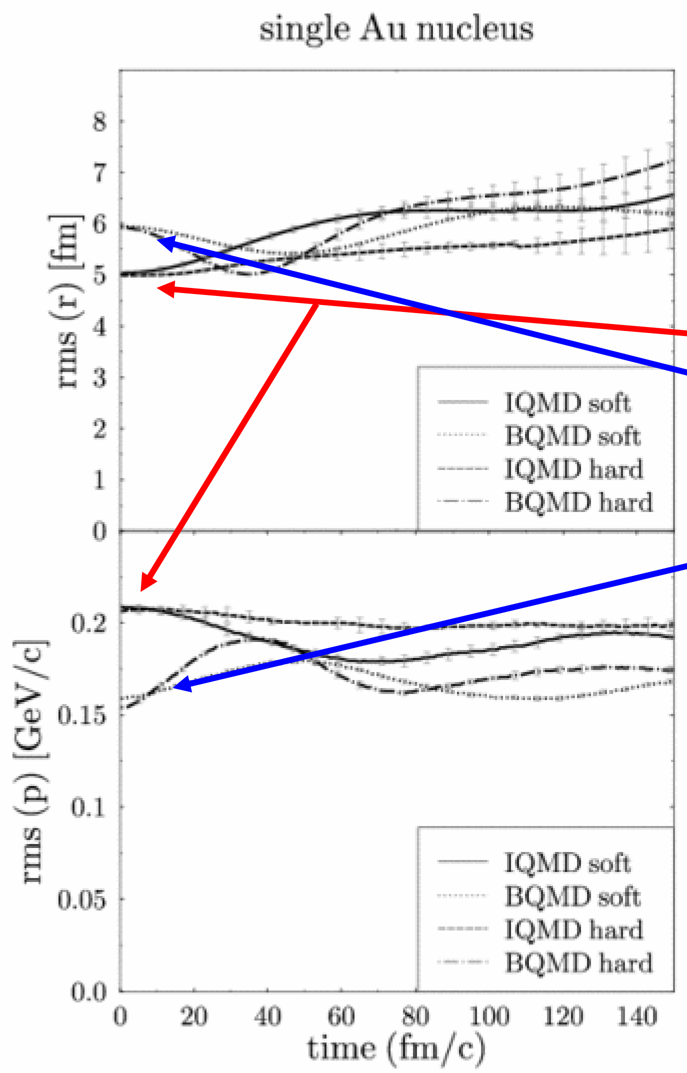
**BQMD yields less flow**

# Fragment production at lower energies




**Differences can be explained by used internal parameters:**
**Gaussian width**

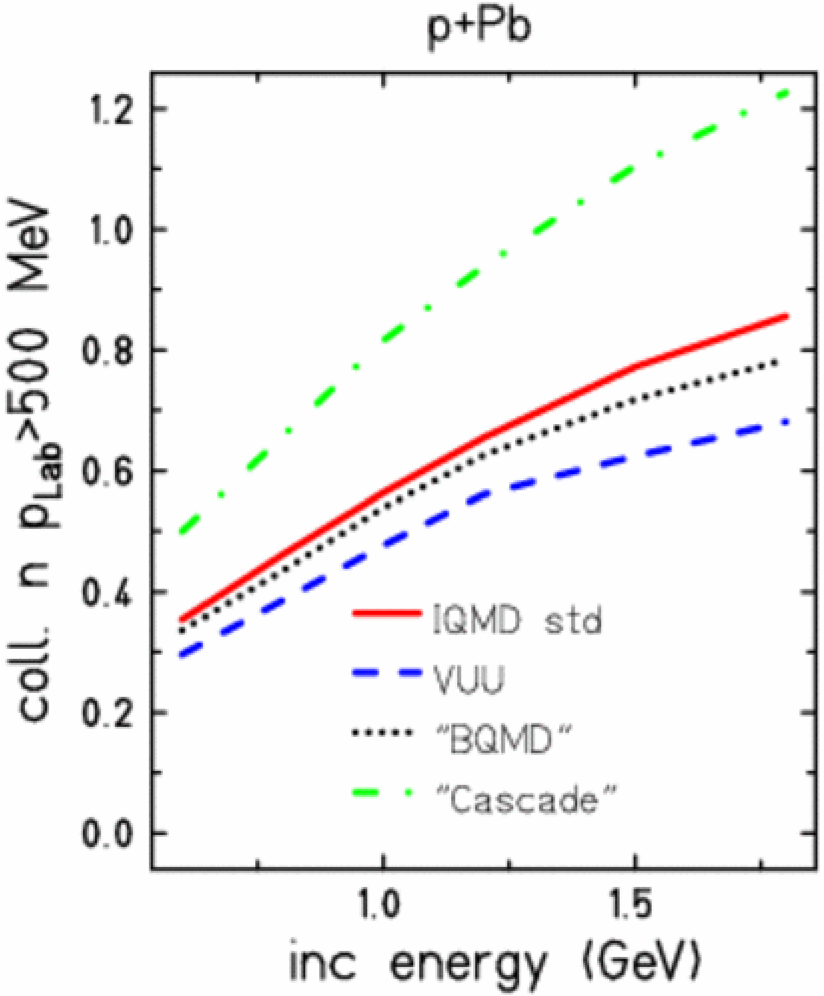
# Stability

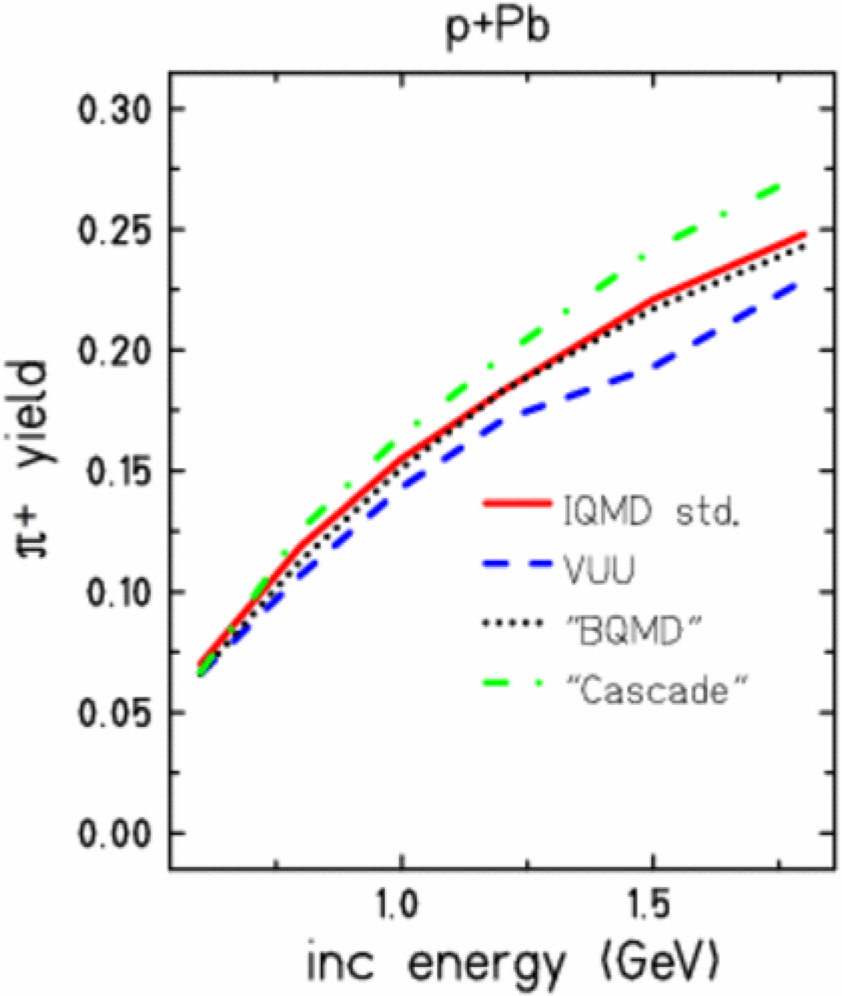



**Due to different initialisation**
**IQMD tends to evaporation**
**while BQMD tends to breathing modes**

**IQMD is used in default mode but could be switched to a BQMD type mode**

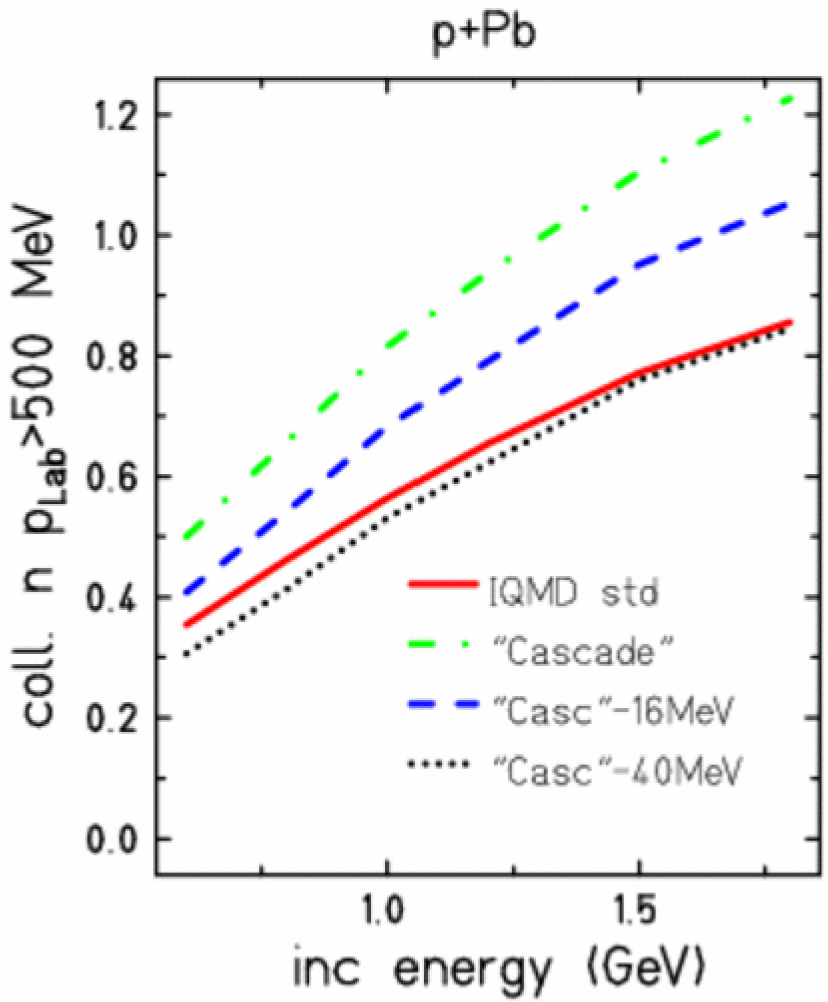
# Preliminary p+A comparison




**« BQMD » and « Cascade » are IQMD-emulations of the codes**

# Cascade: question of potential




**If we subtract the missing potential energy "by hand" we become comparable to IQMD**

# Limits of the models

- **Versions (or parametrizations) « for particle production » or « for fragmentation »**
- **No higher resonances than the Delta**
- **Highest energy at around 2-3 AGeV,<br>lowest energy at around 40-60 MeV**
- **for lower energies take AMD (Ono), FMD(Schnack)<br>for higher energies take UrQMD …**

# UrQMD

Ultrarelativistic Quantum Molecular Dynamics

- contains higher mass resonances and strings
- could be used up to RHIC energies
- succesfully used for cosmic rays
- functionalities similar to IQMD
- partly included into the GEANT4 package
- OSCAR-interface (97 and 99)
- potential mode (up to 10 GeV) and cascade mode

Details http:// th.physik.uni-frankfurt.de/~urqmd

S.A. Bass et al. Prog. Part. Nucl. Phys. 41(1998)225

M. Bleicher et al. J. Phys. G 25 (1999) 1859

# URQMD: included Particles

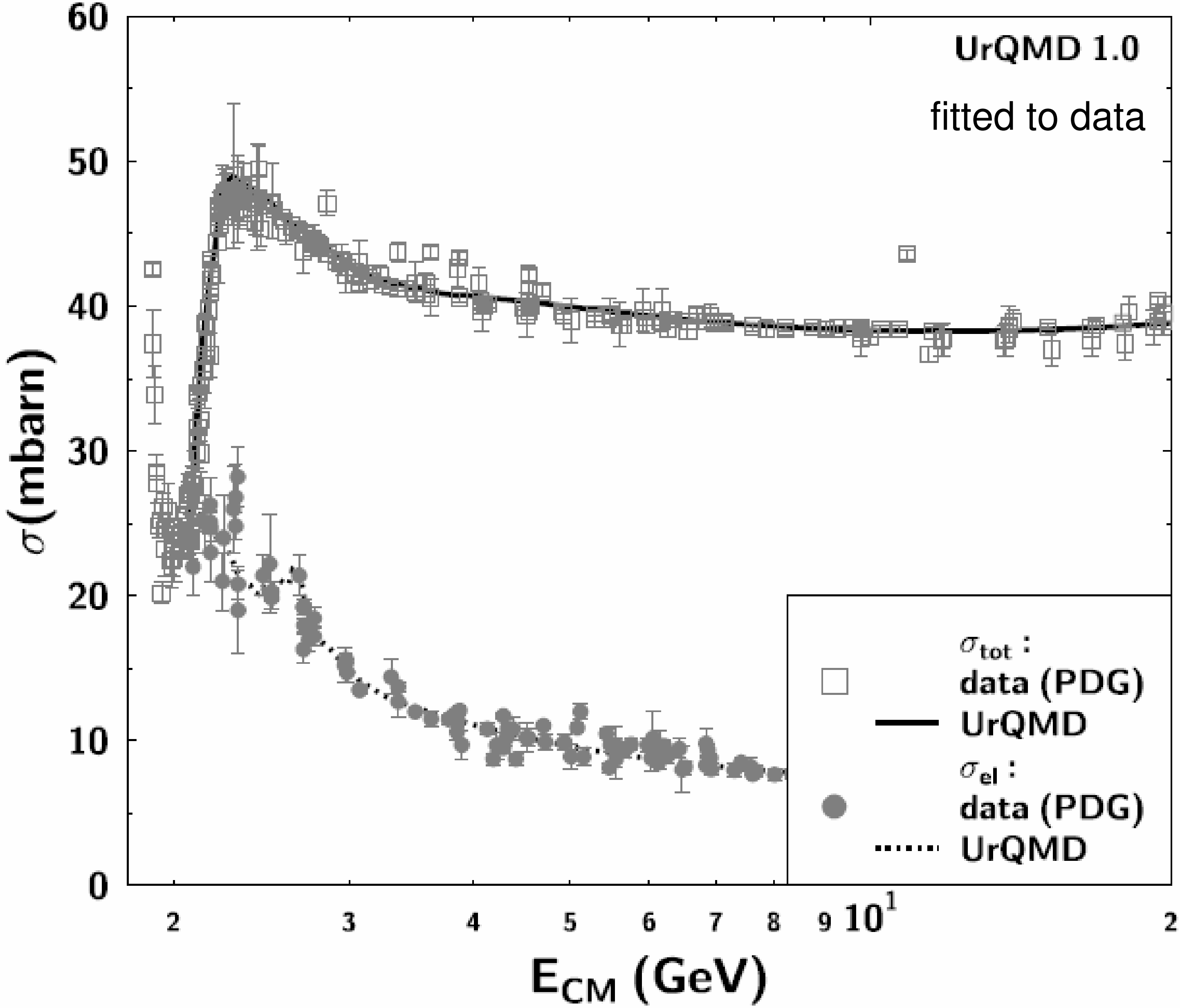
| N | Δ | Λ | Σ | Ξ | Ω |
|---|---|---|---|---|---|
| 938 | 1232 | 1116 | 1192 | 1317 | 1672 |
| 1440 | 1600 | 1405 | 1385 | 1530 | |
| 1520 | 1620 | 1520 | 1660 | 1690 | |
| 1535 | 1700 | 1600 | 1670 | 1820 | |
| 1650 | 1900 | 1670 | 1790 | 1950 | |
| 1675 | 1905 | 1690 | 1775 | 2025 | |
| 1680 | 1910 | 1800 | 1915 | | |
| 1700 | 1920 | 1810 | 1940 | | |
| 1710 | 1930 | 1820 | 2030 | | |
| 1720 | 1950 | 1830 | | | |
| 1990† | | 2100 | | | |
| 2080 | | 2110 | | | |
| 2190 | | | | | |
| 2200 | | | | | |
| 2250 | | | | | |

| $0^{-+}$ | $1^{--}$ | $0^{++}$ | $1^{++}$ |
|---|---|---|---|
| $\pi$ | $\rho$ | $a_0$ | $a_1$ |
| $K$ | $K^*$ | $K_0^*$ | $K_1^*$ |
| $\eta$ | $\omega$ | $f_0$ | $f_1$ |
| $\eta'$ | $\phi$ | $f_0^*$ | $f_1'$ |

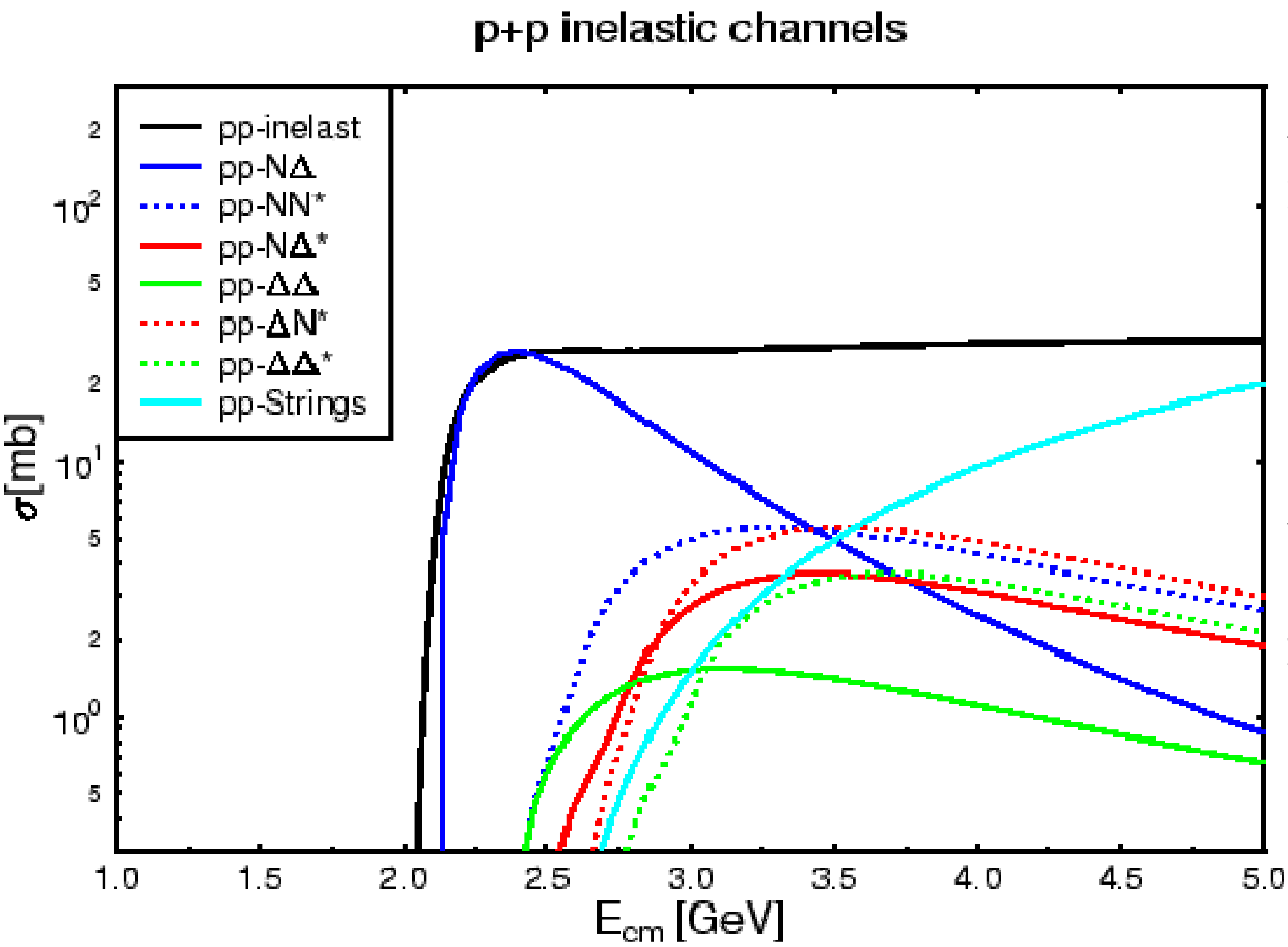
| $1^{+-}$ | $2^{++}$ | $(1^{--})^*$ | $(1^{--})^{**}$ |
|---|---|---|---|
| $b_1$ | $a_2$ | $\rho_{1450}$ | $\rho_{1700}$ |
| $K_1$ | $K_2^*$ | $K^*_{1410}$ | $K^*_{1680}$ |
| $h_1$ | $f_2$ | $\omega_{1420}$ | $\omega_{1662}$ |
| $h_1'$ | $f_2'$ | $\phi_{1680}$ | $\phi_{1900}$ |

Problem: at least 60x60 cross sections needed
→need to group into classes

# pp cross sections



# Inelastic cross sections




**At low energies: inelastic cross section is filled up by known hadron resonances**

**At higher energies: string fragmentation**

# Meson-baryon scattering: resonance region

| resonance | mass | width | $N\gamma$ | $N\pi$ | $N\eta$ | $N\omega$ | $N\varrho$ | $N\pi\pi$ | $\Delta_{1232}\pi$ | $N^*_{1440}\pi$ | $\Lambda K$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $N^*_{1440}$ | 1.440 | 200 | | 0.70 | | | | 0.05 | 0.25 | | |
| $N^*_{1520}$ | 1.520 | 125 | | 0.60 | | | | 0.15 | 0.25 | | |
| $N^*_{1535}$ | 1.535 | 150 | 0.001 | 0.55 | 0.35 | | | 0.05 | | 0.05 | |
| $N^*_{1650}$ | 1.650 | 150 | | 0.65 | 0.05 | | | 0.05 | 0.10 | 0.05 | 0.10 |
| $N^*_{1675}$ | 1.675 | 140 | | 0.45 | | | | | 0.55 | | |
| $N^*_{1680}$ | 1.680 | 120 | | 0.65 | | | | 0.20 | 0.15 | | |
| $N^*_{1700}$ | 1.700 | 100 | | 0.10 | 0.05 | | 0.05 | 0.45 | 0.35 | | |
| $N^*_{1710}$ | 1.710 | 110 | | 0.15 | 0.20 | | 0.05 | 0.20 | 0.20 | 0.10 | 0.10 |
| $N^*_{1720}$ | 1.720 | 150 | | 0.15 | | | 0.25 | 0.45 | 0.10 | | 0.05 |
| $N^*_{1900}$ | 1.870 | 500 | | 0.35 | | 0.55 | 0.05 | | 0.05 | | |
| $N^*_{1990}$ | 1.990 | 550 | | 0.05 | | | 0.15 | 0.25 | 0.30 | 0.15 | 0.10 |
| $N^*_{2080}$ | 2.040 | 250 | | 0.60 | 0.05 | | 0.25 | 0.05 | 0.05 | | |
| $N^*_{2190}$ | 2.190 | 550 | | 0.35 | | | 0.30 | 0.15 | 0.15 | 0.05 | |
| $N^*_{2220}$ | 2.220 | 550 | | 0.35 | | | 0.25 | 0.20 | 0.20 | | |
| $N^*_{2250}$ | 2.250 | 470 | | 0.30 | | | 0.25 | 0.20 | 0.20 | 0.05 | |
| $\Delta_{1232}$ | 1.232 | 115. | 0.01 | 1.00 | | | | | | | |
| $\Delta^*_{1600}$ | 1.700 | 200 | | 0.15 | | | | | 0.55 | 0.30 | |
| $\Delta^*_{1620}$ | 1.675 | 180 | | 0.25 | | | | | 0.60 | 0.15 | |
| $\Delta^*_{1700}$ | 1.750 | 300 | | 0.20 | | | 0.10 | | 0.55 | 0.15 | |
| $\Delta^*_{1900}$ | 1.850 | 240 | | 0.30 | | | 0.15 | | 0.30 | 0.25 | |
| $\Delta^*_{1905}$ | 1.880 | 280 | | 0.20 | | | 0.60 | | 0.10 | 0.10 | |
| $\Delta^*_{1910}$ | 1.900 | 250 | | 0.35 | | | 0.40 | | 0.15 | 0.10 | |
| $\Delta^*_{1920}$ | 1.920 | 150 | | 0.15 | | | 0.30 | | 0.30 | 0.25 | |
| $\Delta^*_{1930}$ | 1.930 | 250 | | 0.20 | | | 0.25 | | 0.25 | 0.30 | |
| $\Delta^*_{1950}$ | 1.950 | 250 | 0.01 | 0.45 | | | 0.15 | | 0.20 | 0.20 | |

# Conclusion?

**Rather a discussion  than a conclusion...**

**IQMD is working well for A+A but not well tested for p+A.**

**Problems when describing fragmentation, particle production and collectif effects (flow) at the same time.**

**There are several parameters which might be used for finetuning, but the observables have to be discussed.**

**Maximum energy of application is around 2-3 GeV:**

**Above, use UrQMD**