

# PHQMD

(Parton-Hadron-Quantum-Molecular-Dynamics)

- a novel microscopic transport approach to study heavy ion reactions

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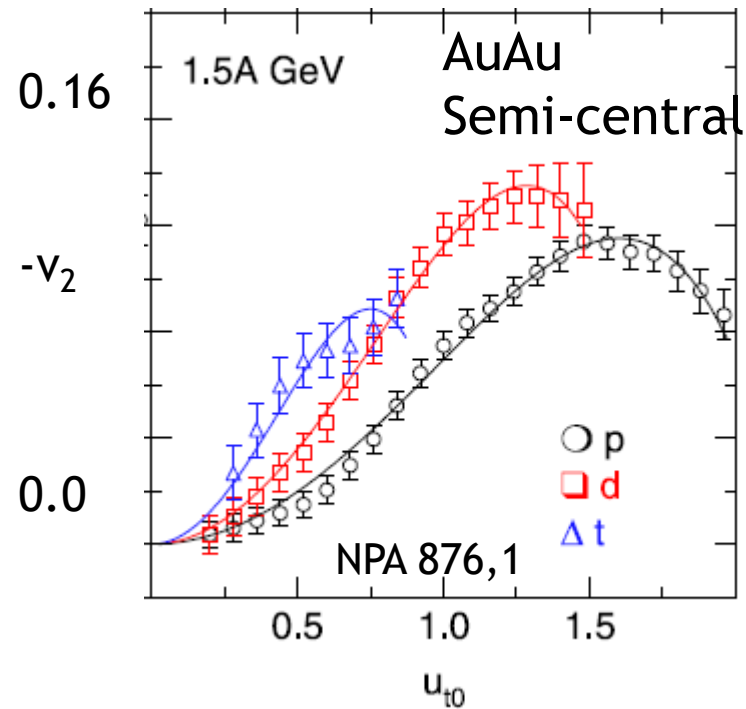
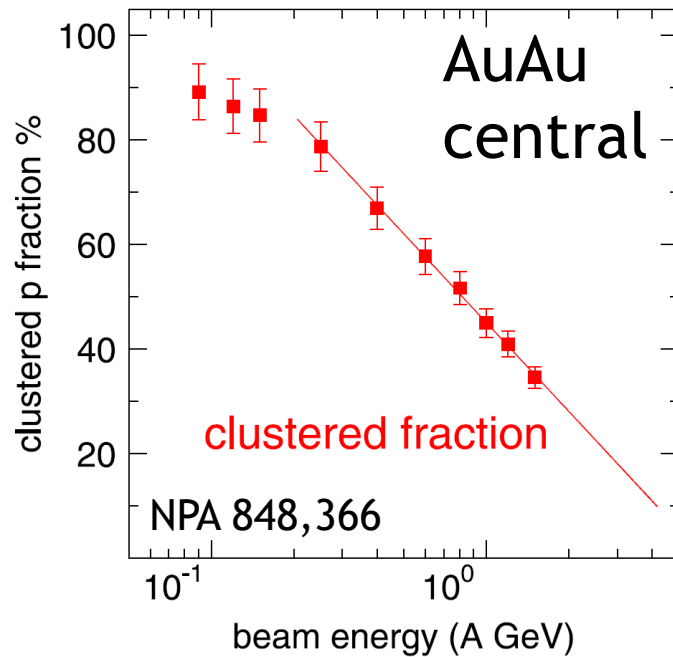
- Why a novel approach?
- Basics of the QMD Transport theory
- Inherent Fluctuations and Correlations in QMD
- Fragment Formation
  
- Comparison with existing data
- Perspectives for BMN/NICA/FAIR/RHIC

# Why do we need a novel approach ?

At 3 AGeV, even in central collisions:

20% of the baryons are in clusters

... and baryons in clusters have quite different properties



If we do not describe the **dynamical formation** of fragments

- we cannot describe the nucleon observables ( $v_1, v_2, dn/dp_T$ )
- we cannot explore the new physics opportunities like  
**hyper-nucleus formation**  
**1<sup>st</sup> order phase transition**  
**fragment formation at midrapidity (RHIC, LHC)**

**Present microscopic approaches** fail to describe fragments at NICA/FAIR (and higher) energies

VUU(1983), BUU(1983), (P)HSD(96), SMASH(2016) solve the time evolution of the one-body phase space density → **no fragments**

UrQMD is a n-body theory but has no potential  
→ **nucleons cannot be bound to fragments**

(I)QMD is a n-body theory but is limited to energies  $< 1.5$  AGeV  
→ **describes nicely fragments at SIS energies,**  
**but conceptually not adapted for NICA/FAIR**

QMD (like AMD and FMD) are true N-body theories.

**N-body theory:** Describe the exact time evolution of a system of N particles. All correlations of the system are correctly described and fluctuations correctly propagated.

**Roots in classical physics:**

A look into textbooks on classical mechanics:  
If one has a given Hamiltonian

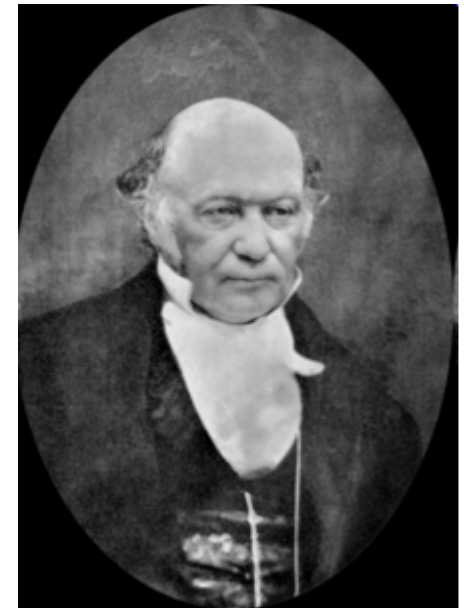
$$H(\mathbf{r}_1, \dots, \mathbf{r}_N, \dots, \mathbf{p}_1, \dots, \mathbf{p}_N, t)$$

$$\frac{d\mathbf{r}_i}{dt} = \frac{\partial H}{\partial \mathbf{p}_i}; \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial H}{\partial \mathbf{r}_i}$$

For a given initial condition

$$\mathbf{r}_1(t=0), \dots, \mathbf{r}_N(t=0), \mathbf{p}_1(t=0), \dots, \mathbf{p}_N(t=0)$$

the positions and momenta of all particles  
are predictable for all times.



William Hamilton

## Roots in Quantum Mechanics

Remember QM cours when you faced the problem

- we have a Hamiltonian  $\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + V$
- the Schrödinger eq.

$$\hat{H}|\psi_j\rangle = E_j|\psi_j\rangle$$

has no analytical solution

- we look for the ground state energy



Walther Ritz

### Ritz variational principle:

Assume a trial function  $\psi(q, \alpha)$  which contains one adjustable parameter  $\alpha$ , which is varied to find a lowest energy configuration:

$$\frac{d}{d\alpha} \langle \psi | \hat{H} | \psi \rangle = 0$$

determines  $\alpha$  for which  $\psi(q, \alpha)$  is closest to the true ground state wfct and  $\langle \psi | \hat{H} | \psi \rangle > E_0$

Extended Ritz variational principle (Koonin, TDHF)

Take **trial wavefct** with **time dependent** parameters and solve

$$\frac{\langle \psi_N | i \frac{d}{dt} \hat{H} | \psi_N \rangle}{\langle \psi_N | \psi_N \rangle} = 0 \quad (1)$$

QMD **trial wavefct** for one particle (Gaussian):

$$\psi_i(q_i, q_{0i}, p_{0i}) = C \exp[-(q_i - q_{0i} - \frac{p_{0i}}{m}t)^2 / 4L] \cdot \exp[ip_{0i}(q_i - q_{0i}) - i \frac{p_{0i}^2}{2m}t]$$

For N particles:  $\psi_N = \prod_{i=1}^N \psi_i(q_i, q_{0i}, p_{0i})$  **QMD**

$$\psi_N^F = \text{Slaterdet} \left[ \prod_{i=1}^N \psi_i(q_i, q_{0i}, p_{0i}) \right] \quad \text{AMD/FMD}$$

The QMD trial wavefct eq. (1) yields

$$\frac{dq}{dt} = \frac{\partial \langle H \rangle}{\partial p} \quad ; \quad \frac{dp}{dt} = - \frac{\partial \langle H \rangle}{\partial q}$$

For Gaussian wavefct eq. of motion very similar to Hamilton's eqs.

Attempts have been made to form clusters in the BUU approach (which uses test particle method)

using a **coalescence** description for test particles

$$P_d(\mathbf{r}_1, \mathbf{r}_2, \mathbf{p}_1, \mathbf{p}_2, t) = \underbrace{\rho_d^W(\mathbf{p}_1 - \mathbf{p}_2, \mathbf{r}_1 - \mathbf{r}_2)}_{\text{deuteron Wigner density}}$$

**This is theoretically not consistent** because 1 and 2 are test particles, no nucleons.

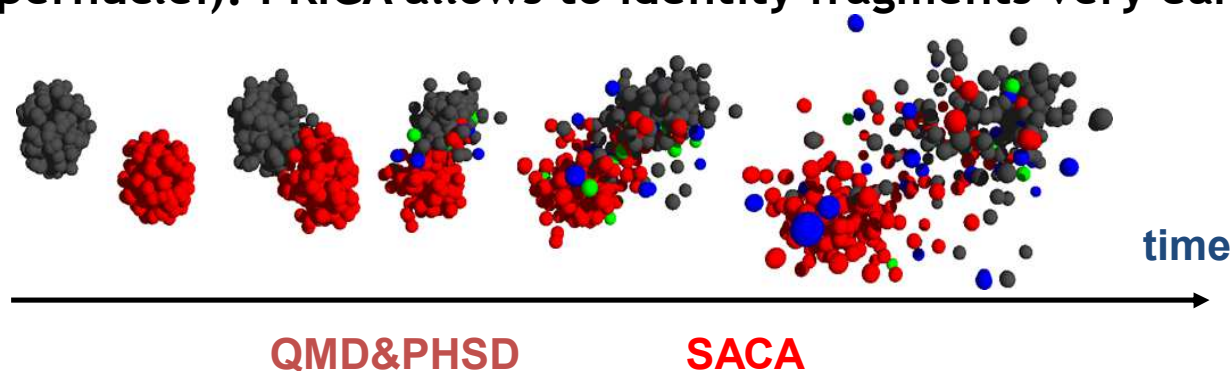
In addition:

- result depends on the **number of test particles**
- result depends on **time** t when coalesce. is applied
- time is **different for different particles**: PRC56,2109
- no information about the formation process**

# Modeling of fragment and hypernucleus formation

The goal: Dynamical modeling of cluster formation by a combined model  
**PHQMD = (QMD & PHSD) & SACA (FRIGA)**

- ❑ **Parton-Hadron-Quantum-Molecular-Dynamics** - a non-equilibrium microscopic transport model which describes **n-body dynamics** based on **QMD propagation** with **collision integrals from PHSD** (Parton-Hadron-String Dynamics) and **cluster formation by the SACA model** or by the Minimum Spanning Tree model (MST).
- ❑ MST can determine clusters only at the end of the reaction.
- ❑ **Simulated Annealing Clusterization Algorithm** - cluster selection according to the largest binding energy (**extension of the SACA model** -> **FRIGA** which includes hypernuclei). FRIGA allows to identify fragments very early during the reaction.



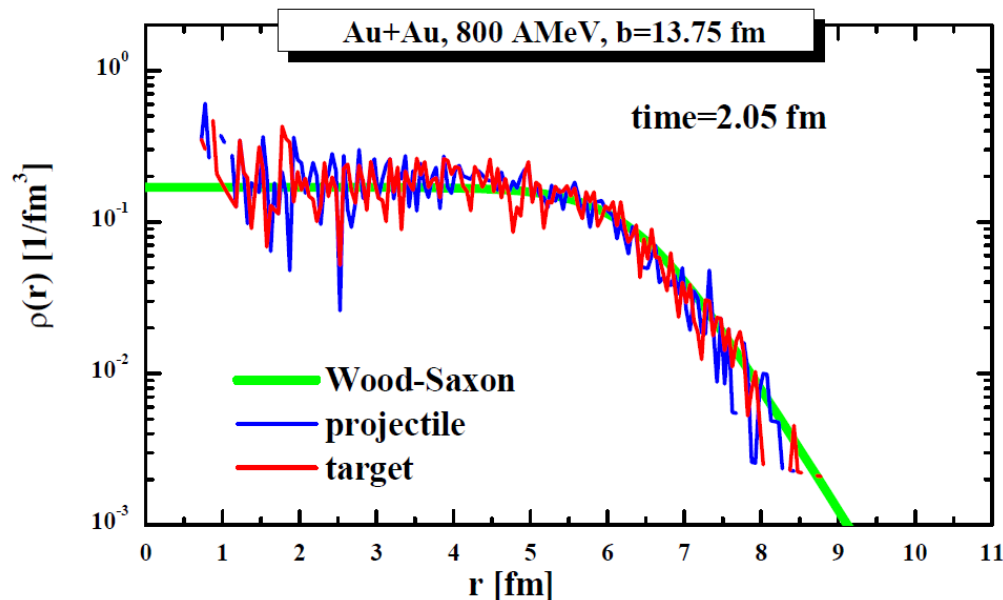


## Initial condition in PHQMD

to describe fragment formation and  
to guaranty the stability of nuclei

The initial distributions of nucleons in proj and targ has to be carefully modelled:

- Right density distribution
- Right binding energy



local Fermi gas model  
for the momentum  
distribution

## Potential in PHQMD

Relativistic molecular dynamics (PRC 87, 034912) too time consuming

The **potential interaction** is most **important in two rapidity intervals**:

- ❑ at **beam and target rapidity** where the fragments are **initial - final state correlations** and created from spectator matter
- ❑ at **midrapidity** where - at a late stage - the phase space density is sufficiently high that small fragments are formed

In both situations we profit from the fact that the **relative momentum between neighboring nucleons is small** and therefore **nonrelativistic kinematics can be applied**. Potential interaction between nucleons

$$\begin{aligned}U_{ij}(\mathbf{r}, \mathbf{r}') &= U_{\text{Skyrme}} + U_{\text{Coul}} \\ &= \frac{1}{2}t_1\delta(\mathbf{r} - \mathbf{r}') + \frac{1}{\gamma + 1}t_2\delta(\mathbf{r} - \mathbf{r}')\rho^{\gamma-1}(\mathbf{r}) \\ &\quad + \frac{1}{2}\frac{Z_i Z_j e^2}{|\mathbf{r} - \mathbf{r}'|}.\end{aligned}$$

$t_1$ ,  $t_2$  and  $\gamma$  adjusted to reproduce a given **nuclear equation of state**

$$\langle U(\mathbf{r}_i) \rangle = \sum_j \int d^3r d^3r' d^3p d^3p' U_{ij}(\mathbf{r}, \mathbf{r}') f_i(\mathbf{r}, \mathbf{p}, t) f_j(\mathbf{r}', \mathbf{p}', t)$$

$$\langle U_i(\mathbf{r}_i, t) \rangle = \alpha \left( \frac{\rho_{int}}{\rho_0} \right) + \beta \left( \frac{\rho_{int}}{\rho_0} \right)^\gamma$$

To describe the potential interactions in the **spectator matter** we transfer the Lorentz-contracted nuclei back into the **projectile and target rest frame**, neglecting the small time differences

$$\rho_{int}(\mathbf{r}_i, t) \rightarrow C \sum_j \left( \frac{4}{\pi L} \right)^{3/2} e^{-\frac{4}{L} (\mathbf{r}_i^T(t) - \mathbf{r}_j^T(t))^2} \cdot e^{-\frac{4\gamma_{cm}^2}{L} (\mathbf{r}_i^L(t) - \mathbf{r}_j^L(t))^2}$$

For the midrapidity region  $\gamma \rightarrow 1$ . and we can apply nonrelativistic kinematics as well

All elastic and inelastic collisions are treated as in PHSD - therefore the spectra of produced particles are similar to PHSD results

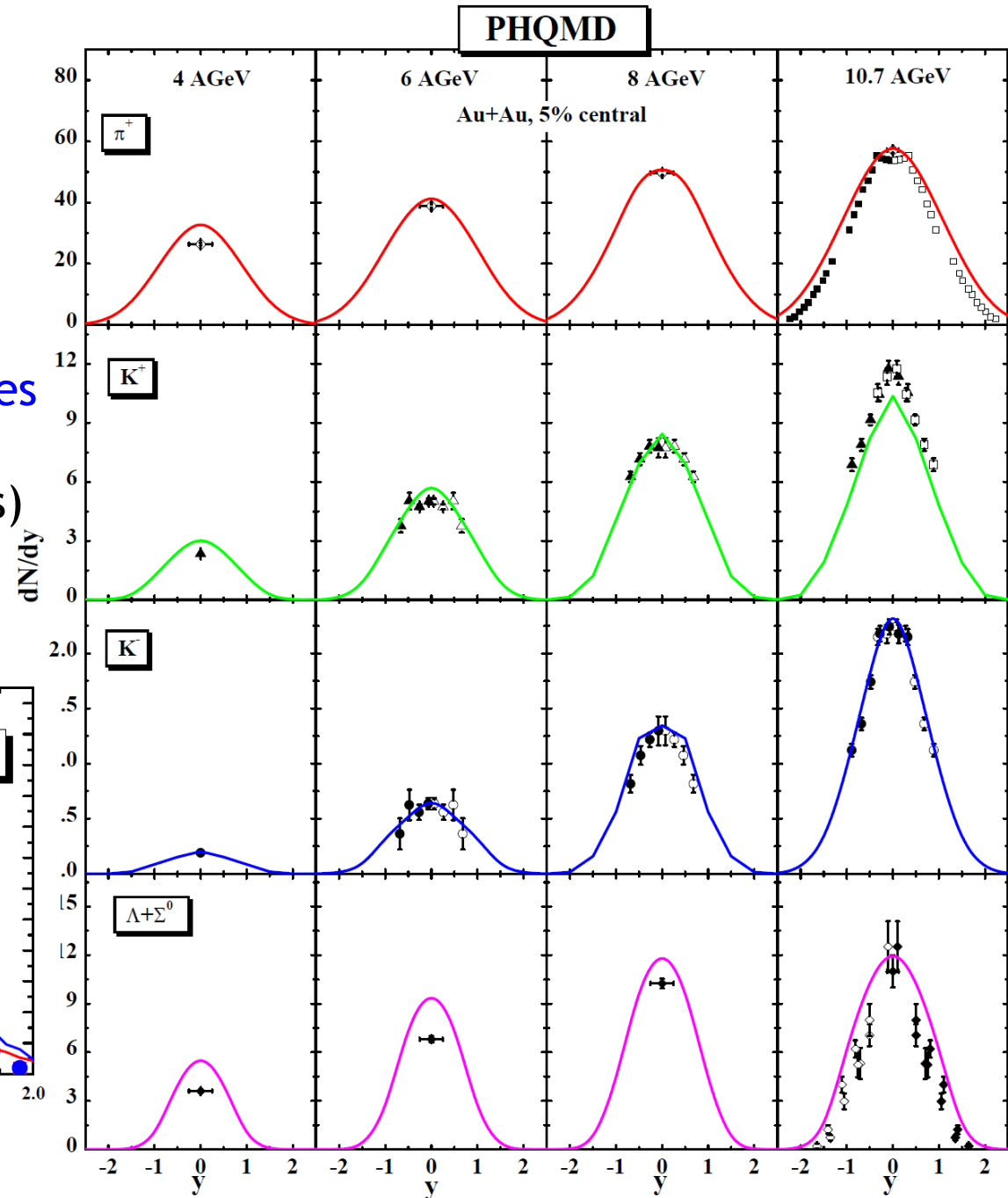
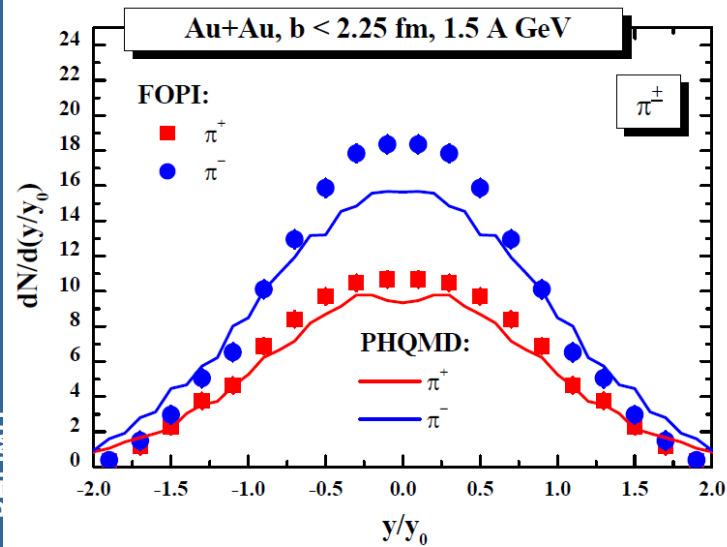
# Results

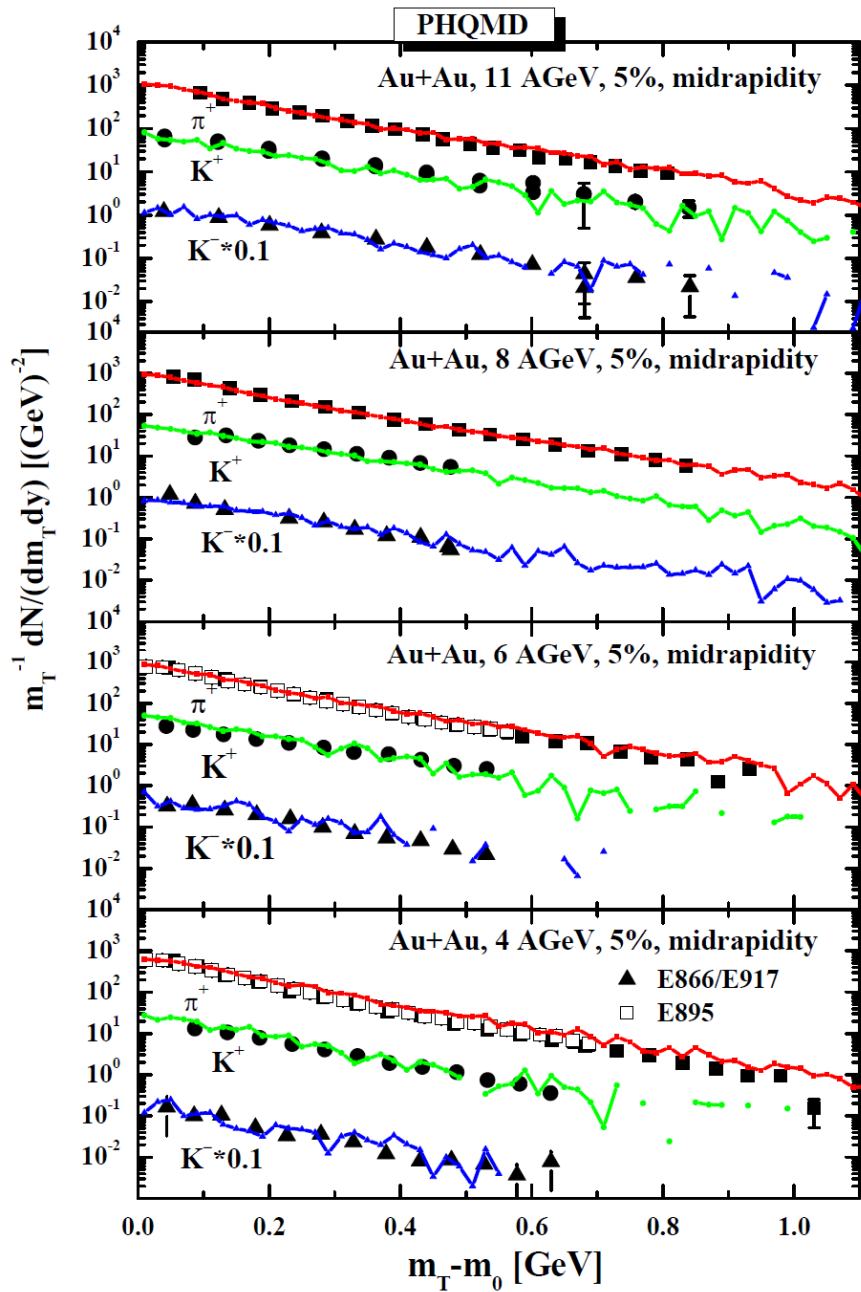
# First Results of PHQMD

Produced particles

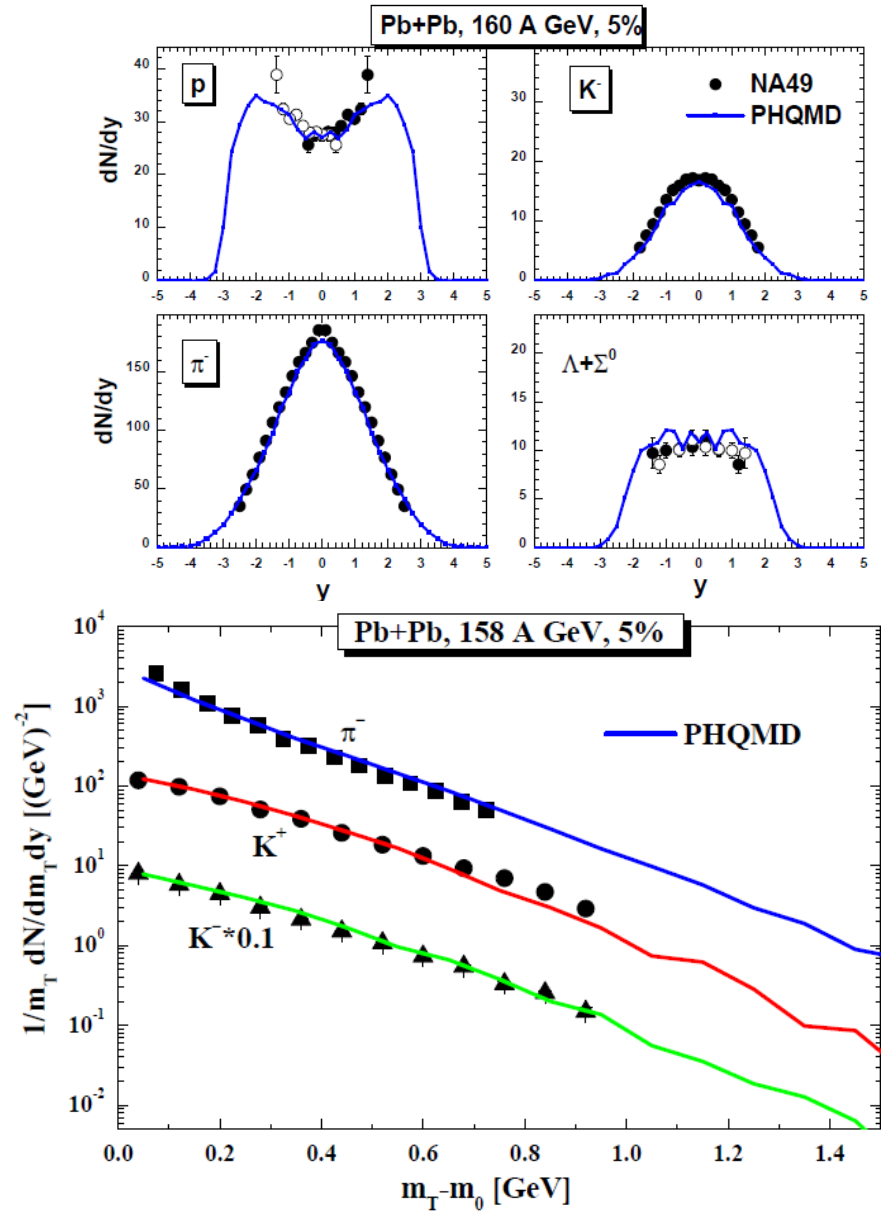
are well reproduced  
at SIS/NICA/FAIR energies

(dominated by collisions)





# As well as at SPS energies





## How to define fragments in transport theories which propagate nucleons?

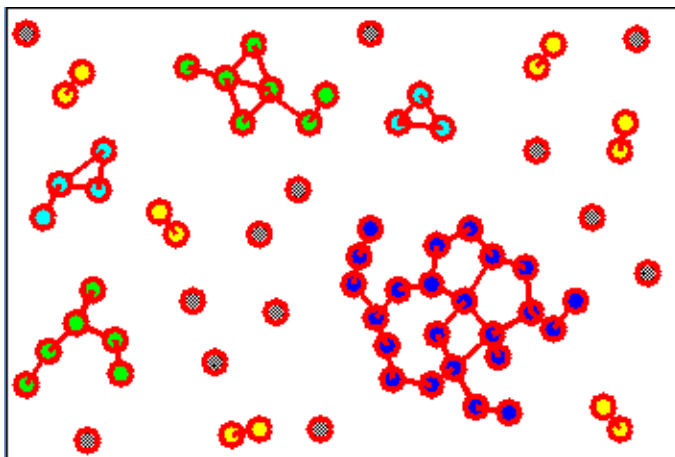
1. **Minimum Spanning Tree (MST)** is a **cluster recognition** method applicable for the (asymptotic) **final state** where coordinate space **correlations may only survive for bound states**.

The **MST algorithm** searches for accumulations of particles in coordinate space:

1. Two particles are **bound** if their distance in coordinate space fulfills

$$|\vec{r}_i - \vec{r}_j| \leq 2.5 \text{ fm}$$

2. A particle is **bound to a cluster** if it is **bound with at least one particle** of the cluster.



Additional momentum cuts (coalescence) change little:  
Large relative momentum  
-> finally not at the same position

## II.SACA or ECRA now FRIGA

If we want to identify fragments earlier one has to use momentum space info as well as coordinate space info

Idea by Dorso et al. (Phys.Lett.B301:328,1993) :

- a) Take the positions and momenta of all nucleons at time  $t$ .
- b) Combine them in all possible ways into all kinds of fragments or leave them as single nucleons
- c) Neglect the interaction among clusters
- d) Choose that configuration which has the highest binding energy

Simulations show: Clusters chosen that way at early times are the **prefragments** of the final state clusters.

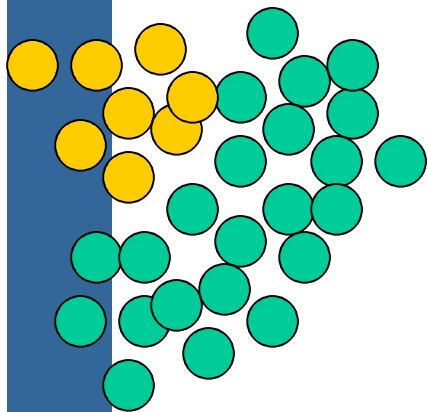


# How does this work?

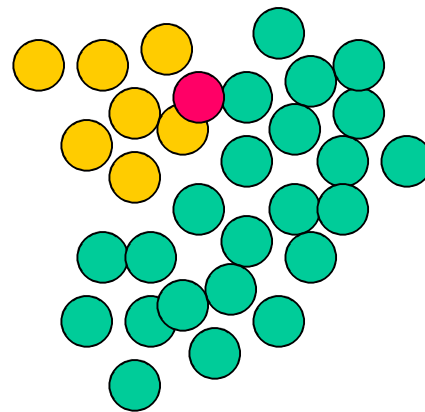
Simulated Annealing Procedure: PLB301:328, 1993  
later SACA , now FRIGA :Nuovo Cim. C39 (2017) 399

Take randomly 1 nucleon  
out of a fragment

Add it randomly to another  
fragment



$$E = E_{kin}^1 + E_{kin}^2 + V^1 + V^2$$



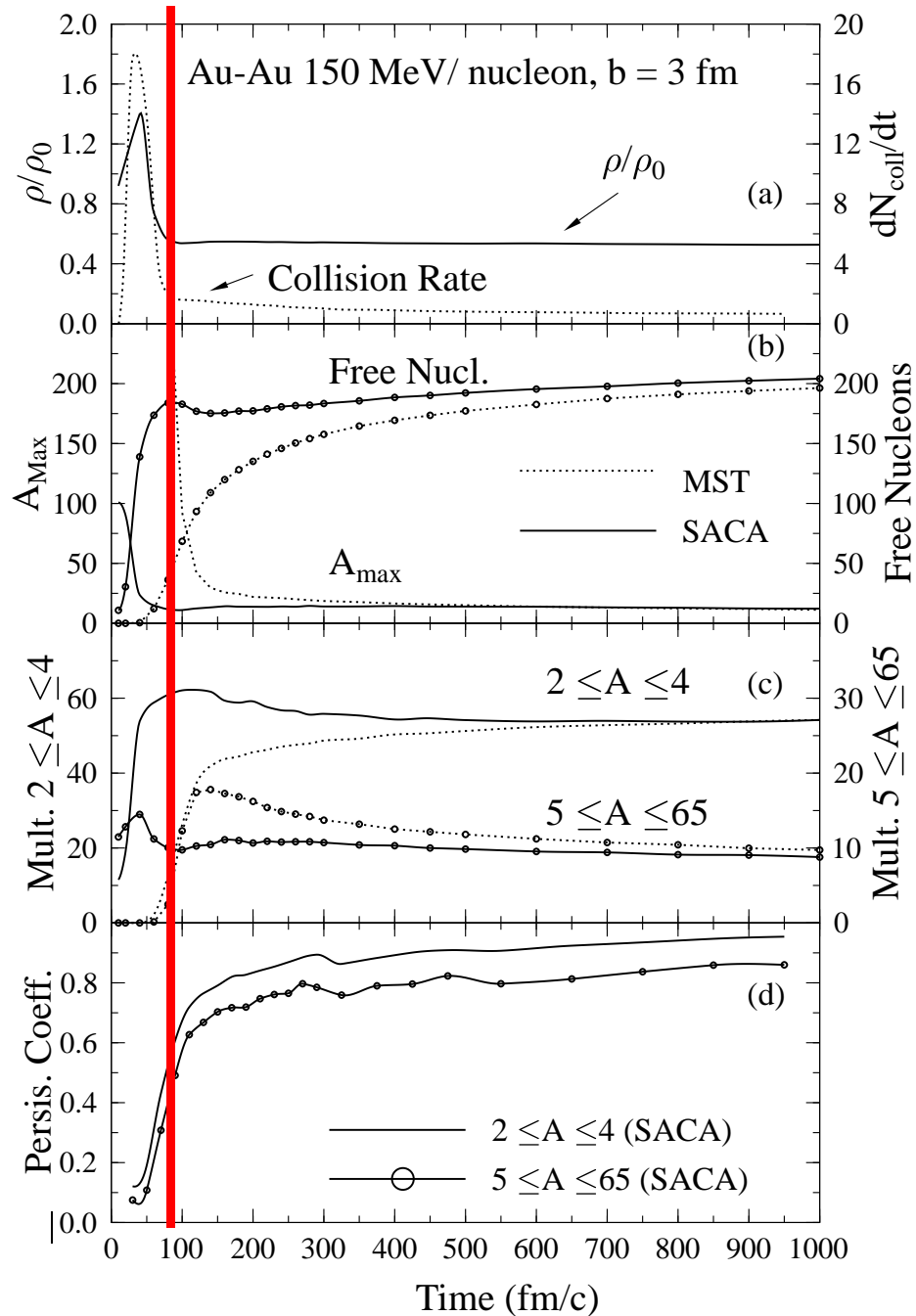
$$E' = E_{kin}^{1'} + E_{kin}^{2'} + V^{1'} + V^{2'}$$

If  $E' < E$  take the new configuration

If  $E' > E$  take the old with a probability depending on  $E' - E$

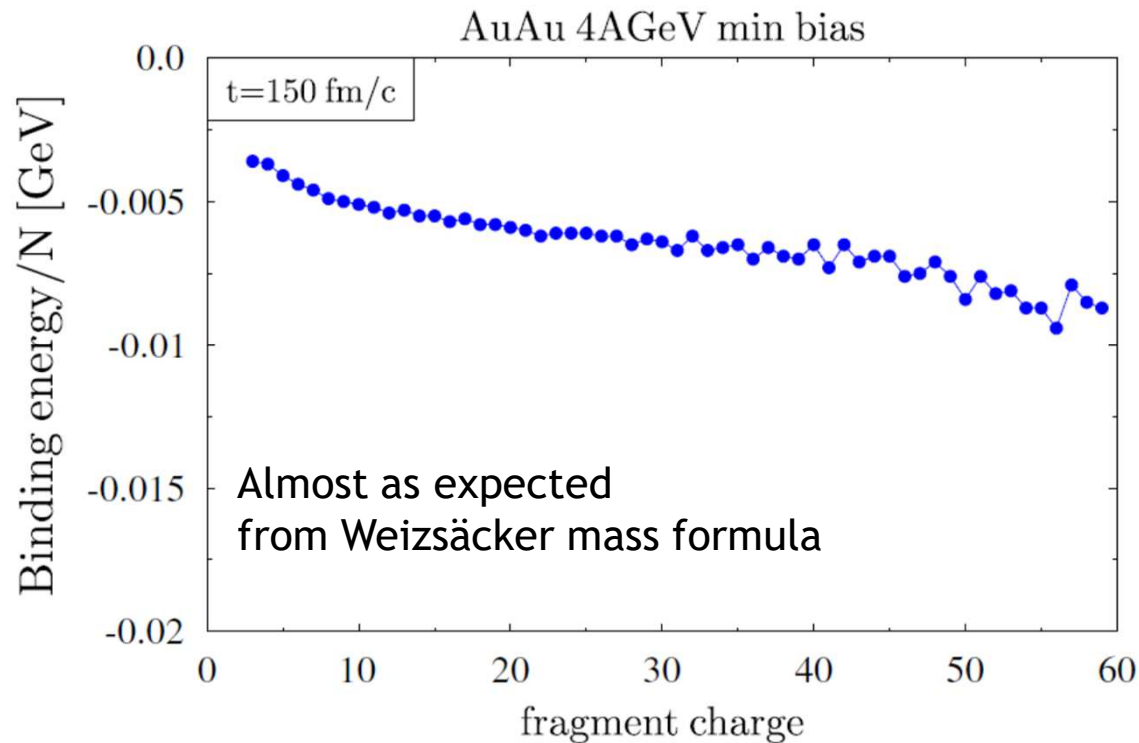
Repeat this procedure very many times

→ Leads automatically to the most bound configuration



SACA/FRIGA can really identify the fragment pattern very early as compared to the Minimum Spanning Tree (MST) which requires a maximal distance in coordinate space between two nucleons to form a fragment

At  $1.5t_{\text{pass}}$   $A_{\text{max}}$  and multiplicities of intermediate mass fragments are determined



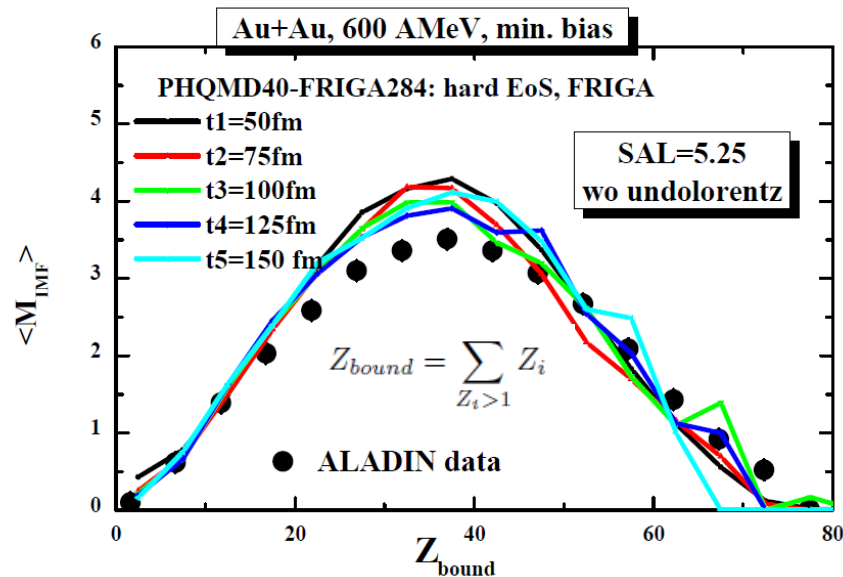
There are two kinds of fragments

- formed from **spectator matter**  
 close to beam and target rapidity  
 initial-final state correlations  
 HI reaction makes spectator matter unstable
- formed from **participant matter**  
 created during the expansion of the fireball  
 “ice” ( $E_{\text{bind}} \approx 8 \text{ MeV/N}$ ) in “fire” ( $T \geq 100 \text{ MeV}$ )  
 origin not known yet  
 seen from SIS to RHI  
 (quantum effects are important)

# First Results of PHQMD

## Spectator Fragments

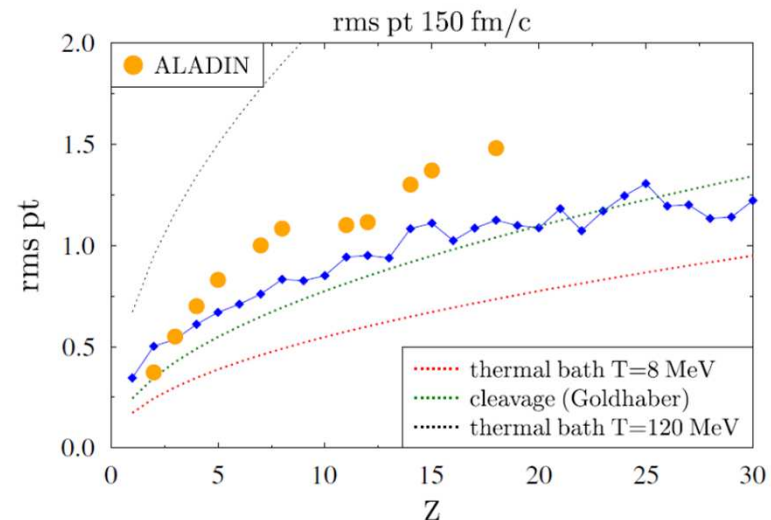
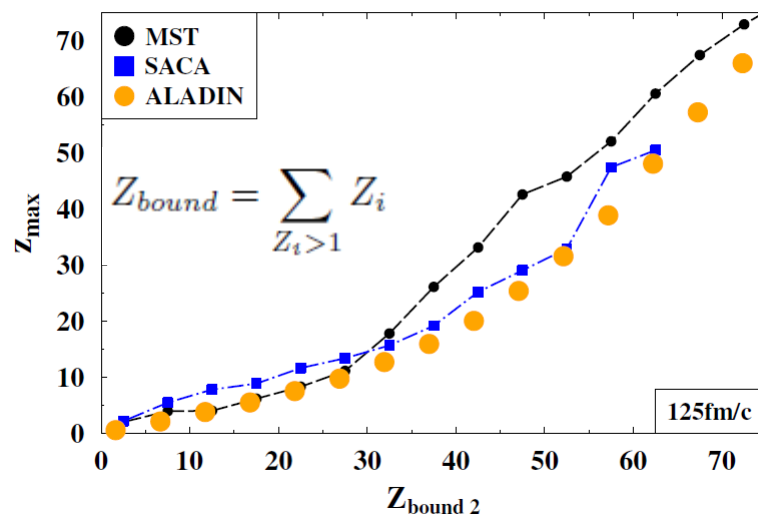
experim. measured up to  $E_{\text{beam}} = 1$  AGeV (ALADIN)



agreement for **very complex fragment observables** like the

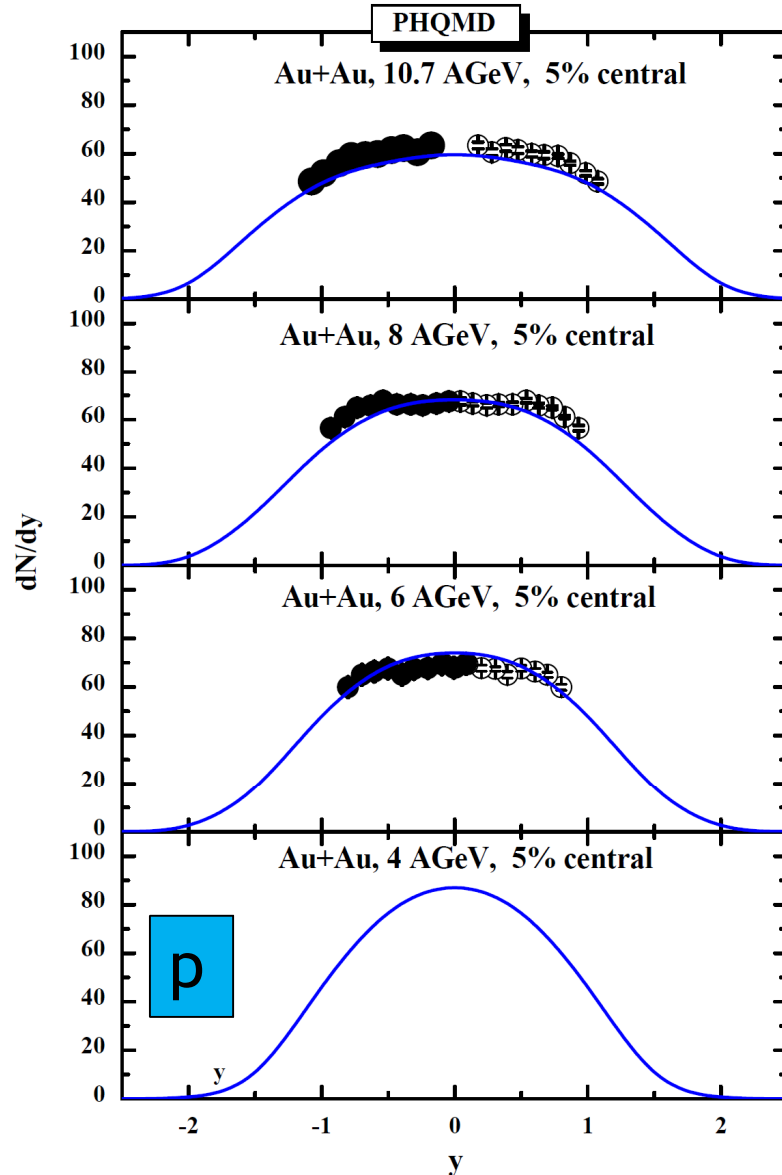
- energy independent “rise and fall”
- largest fragment ( $Z_{\text{bound}}$ )

rms( $p_t$ ) shows  $\sqrt{Z}$  dependence

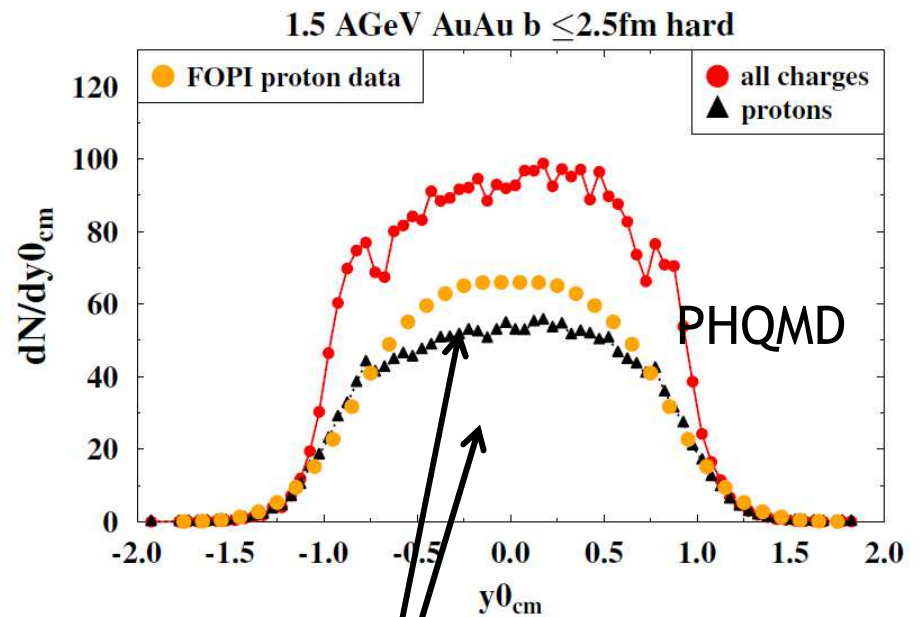


# First Results of PHQMD

Protons at **midrapidity** well described



midrapidity fragment production increases with decreasing energy

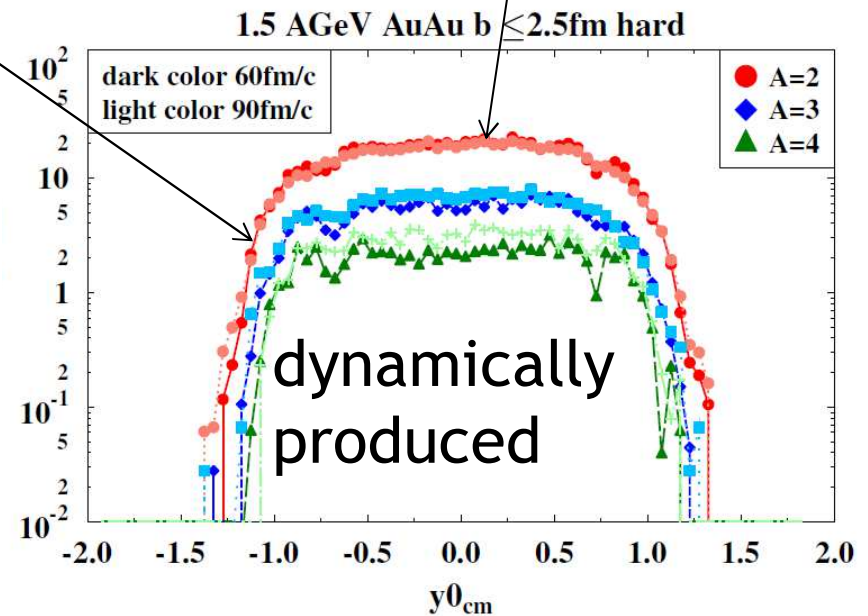
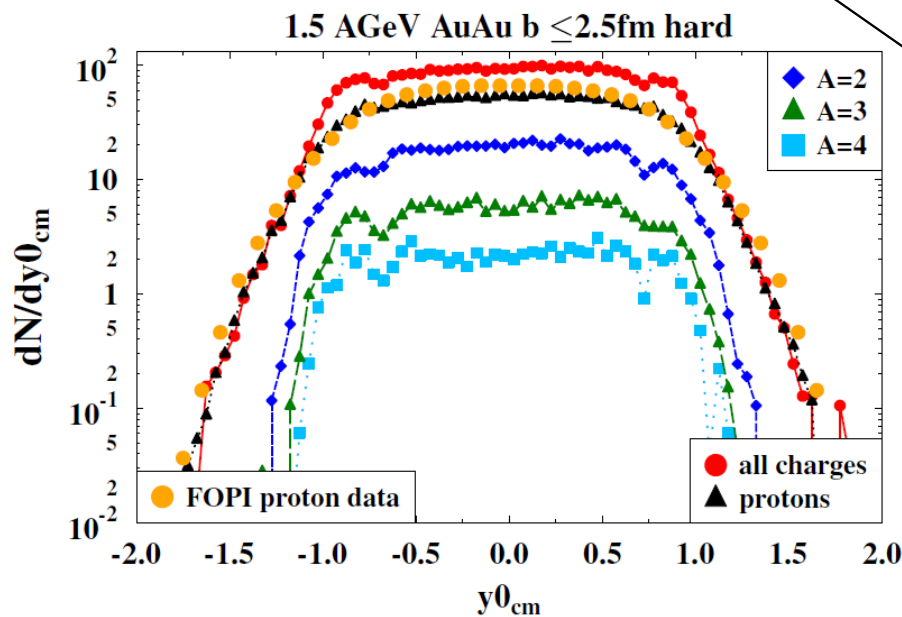


1.5 AGeV **central**

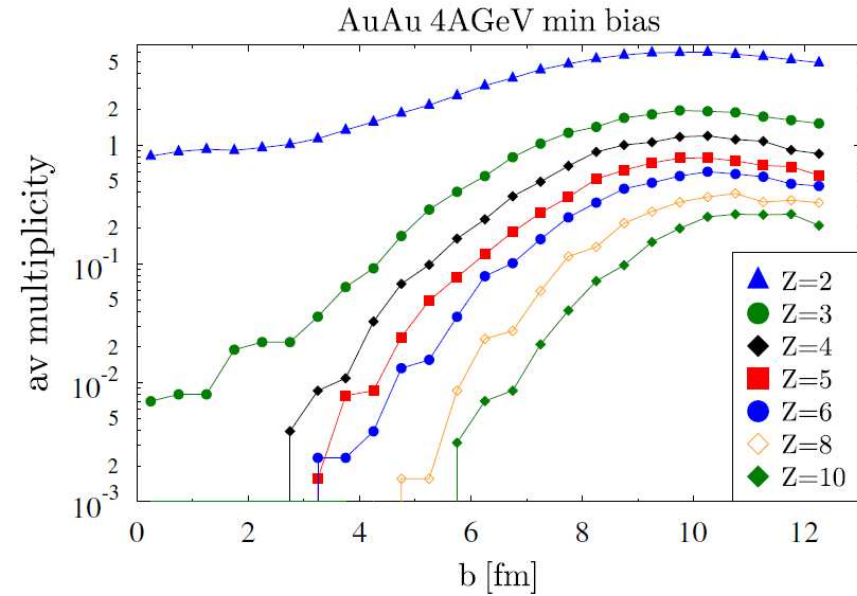
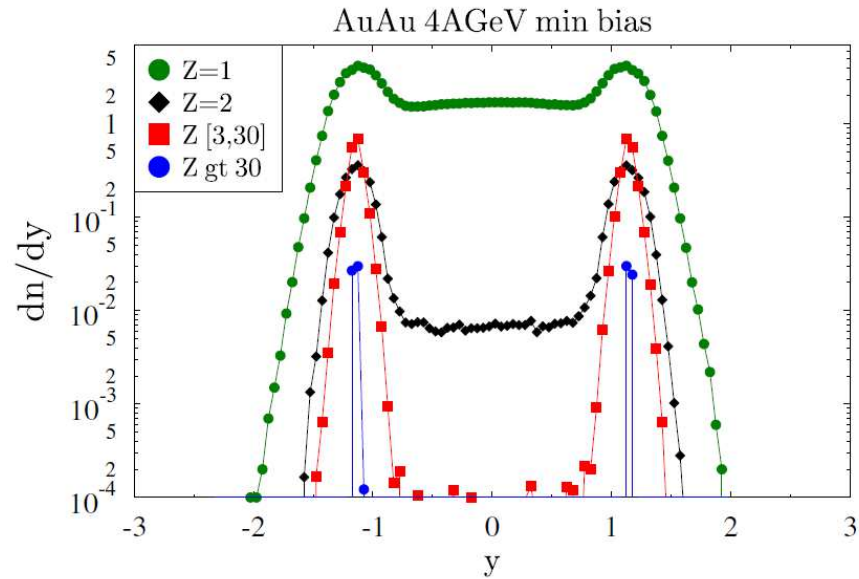
- 30% of protons bound in cluster
- To improve: better potential for small clusters

# First Results of PHQMD

There are all kinds of fragments at midrapidity  
and **they are stable**  
(MST finds at 60fm/c the same fragments as at 90fm/c)

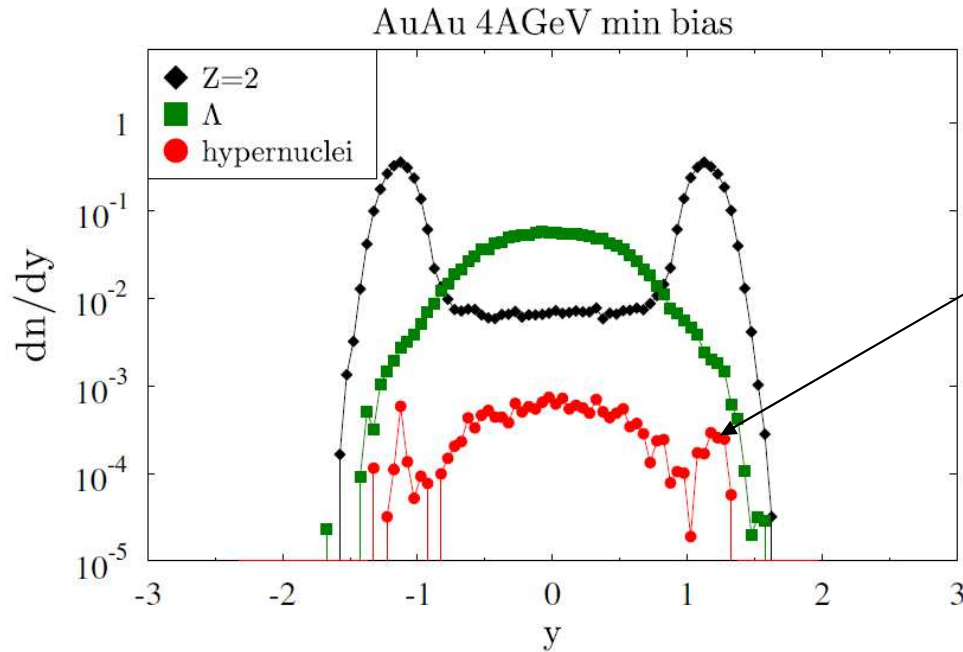


# First Results of PHQMD



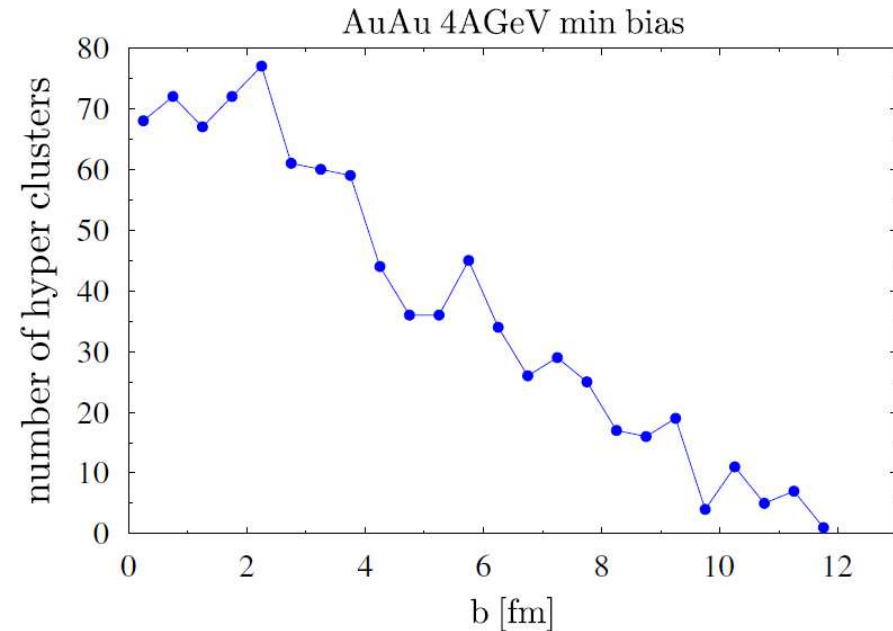
- Only for most central events fragments do not play a role
- Heavy fragments appear only in the residue rapidity range
- Complicated fragment pattern for larger impact parameters (acceptance??)
- $M_z(b)$  is different for each fragment charge

.. And what about hyper-nuclei ?



There are hyper-nuclei  
 - at midrapidity (small)  
 - at beam rapidity (large)  
 few in number but  
 more than in other reactions  
 to create hyper-nuclei

Central collisions → light hyper-nuclei  
 Peripheral collisions → heavy hyper-nuclei

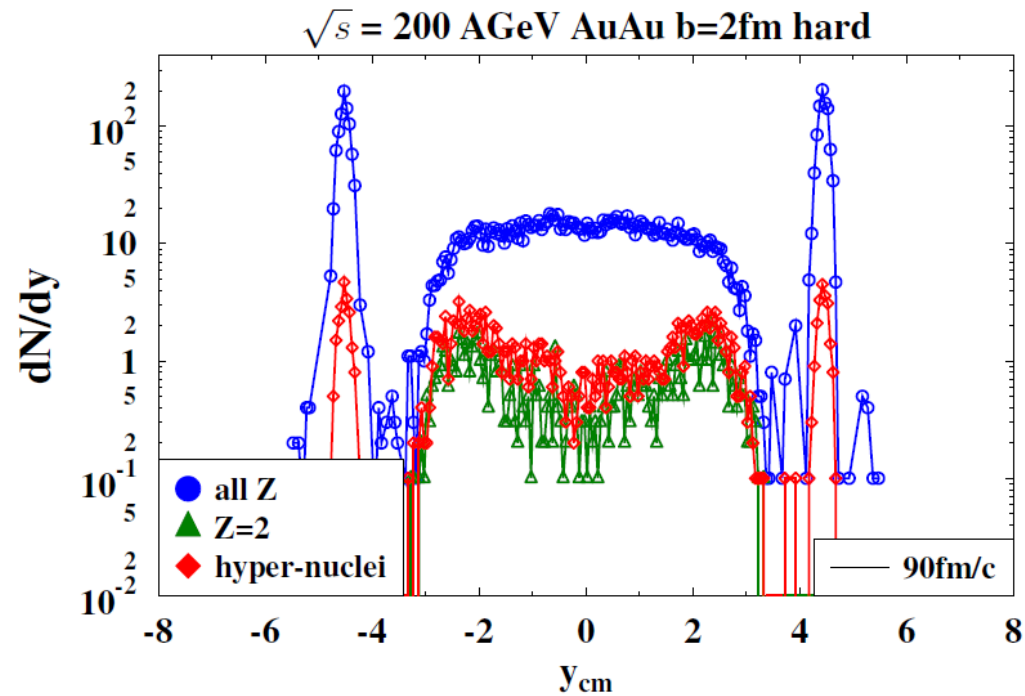




# First Results of PHQMD

At RHIC

hyper-nuclei also from spectator matter  
Z=2 fragments at midrapidity



## Conclusions

We presented a new model, PHQMD, for the NICA/CBM energies which allows - **in contrast to all other models** - to predict the

### **dynamical formation of fragments**

- allows to understand the proton spectra and the properties of light fragments ( $dn/dp_T dy$ ,  $v_1, v_2$ , fluctuations)
- allows to understand fragment formation in participant and spectator region
- allows to understand the formation of hypernuclei
- should allow to understand fragment formation at RHIC/LHC

Very good agreement with the presently available fragment data as well as with the AGS/SPS single particle spectra

But a lot has still to be done!!

Back up

Bi+Xe, 28 A MeV

b=5fm

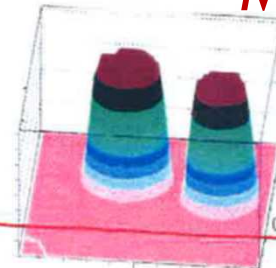
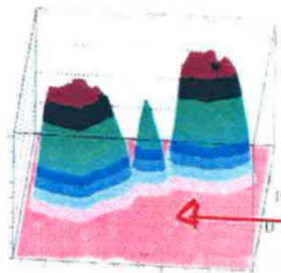
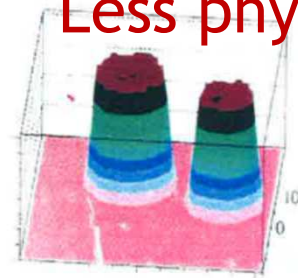
25 test particles/N

W. Bauer  
U.Schröder

275 test particles/N

Less physical<sup>M</sup>

More physical

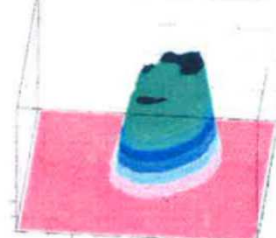
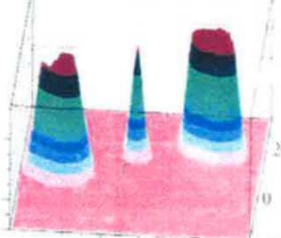
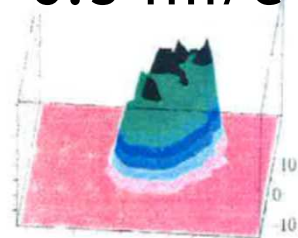


0.5 fm/c

300 fm/c

0.5 fm/c

300 fm/c

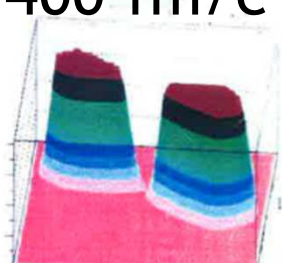
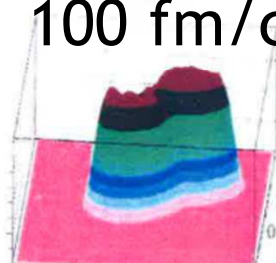
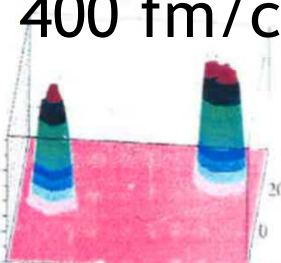
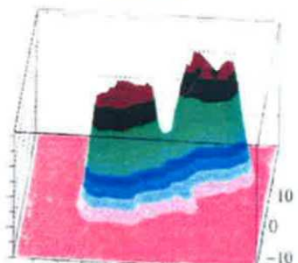


100 fm/c

400 fm/c

100 fm/c

400 fm/c



200 fm/c

500 fm/c

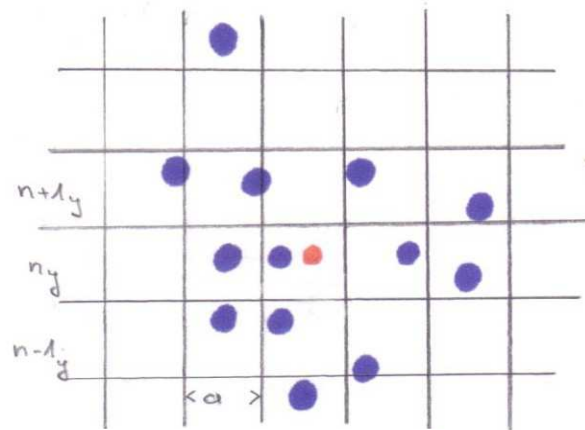
200 fm/c

500 fm/c

## When is N sufficiently large?

One uses delta like forces:  $F(r) = \delta(r)$  (Skyrme) but then point-like test particles  $f = \sum \delta(r-r_i(t))$  do **almost never interact**. Solution: one uses grids (and introduces the grid size  $a$  which plays a similar role as the width in QMD).

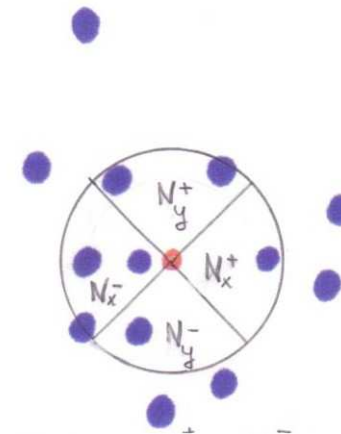
Euler



$$F_x = \frac{U_{n_x-1}(\rho) - U_{n_x+1}(\rho)}{2a}$$

Result  
different  
if number  
of test  
particles  
is finite  
(usually  
 $N=100$ )

Lagrange



$$F_x = \frac{U_{x \text{ right}}(\rho) - U_{x \text{ left}}(\rho)}{2a}$$

Average distance between nucleons 2fm. Grid size  $\approx$  1fm (surface).

Therefore **very many test particles necessary** to **avoid numerical**

**fluctuations:** 100tp  $\rightarrow$  12 in a cell  $\rightarrow$  30% fluctuation

VUU, BUU, HSD, SMASH solve a Boltzmann type eq.

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{p}} = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}$$

Same interaction, not possible classically

$$\left( \frac{\partial f}{\partial t} \right)_{\text{coll}} = \iint \underbrace{gI(g, \Omega)}_{\text{v} \cdot \text{differential cross section}} [f(\mathbf{p}'_A, t)f(\mathbf{p}'_B, t) - f(\mathbf{p}_A, t)f(\mathbf{p}_B, t)] d\Omega d^3\mathbf{p}_A d^3\mathbf{p}_B.$$

v · differential cross section

Only the **test particle method** made it possible to solve the BUU equations in complex situations

Test particle method -> replace integrals by sums (MC) integration

$$f(\mathbf{r}, \mathbf{p}, t) = \sum_{i=1}^{N \rightarrow \infty} \delta(\mathbf{r} - \mathbf{r}_i(t)) \delta(\mathbf{p} - \mathbf{p}_i(t)) \quad \text{test particle} \neq \text{nucleon}$$

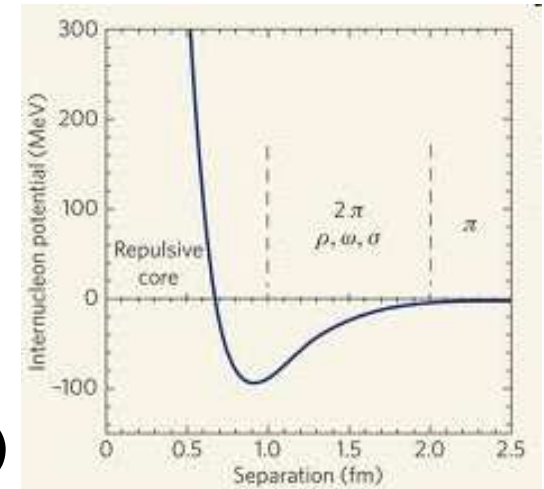
If N small unphysical fluctuations

What means N -> ∞ in reality ?

## How does a collision term appear?

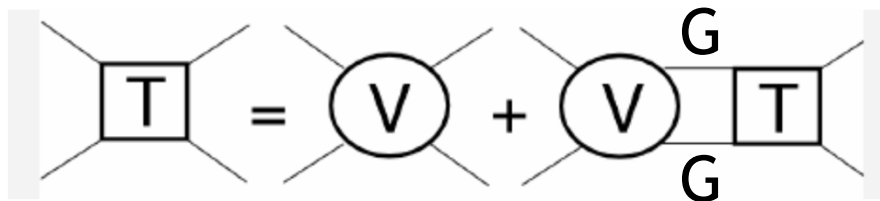
The Hamiltonian (Schrödinger and Boltzmann eq.) contains  $V = NN$  potential

The **NN potential has a hard core**, would make **transport calculations very unrealistic** (Bodmer 75) (independent of the beam energy the participants would **thermalize** like in a cascade calculation without Pauli blocking)



**Solution** (taken over from TDHF):

Replace the NN potential  $V_{NN}$  by the solution of the Bethe-Salpeter eq. in T-matrix approach (Brueckner)



$$T_{\alpha}(E; q, q') = V_{\alpha}(q, q') + \int k^2 dk V_{\alpha}(q, k) G_{Q\bar{Q}}^0(E, k) T_{\alpha}(E; k, q')$$

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## Consequences:

$V_{NN}$  is real  $\rightarrow$  **T is complex** = **ReT** + **i Im T**

$\swarrow$   $\searrow$

corresponds to  $V_{NN}$   $\sigma_{\text{elast}}$   
 in Hamiltonian **collisions**  
 (Skyrme) done identically  
BUU (test-particles)  
and QMD (particles)

To this one adds inelastic collisions

**(BUU, HSD, SMASH and QMD - the same way)!**

$\rightarrow$  Therefore in BUU and QMD the spectra of produced particles are (almost) identical (intensively checked in the past)



- take a small number of test particles ( $N_1$ ):
  - mathematically this is then **not a correct solution** of the differential (BUU) equation
  - in practise problems with **energy and momentum conserv.**
  - assumes, relations between physical ( $\sigma, T, \rho$ ) and mathematical fluctuations ( $1 = \overline{N}$ ) which are difficult to justify
- add a fluctuating force to the BUU equation  
Colonna, Suraud, Ayik.....
  - mathematically correct
  - difficult to determine these fluctuations  
size in  $\Delta r$  and  $\Delta p$ , dependence of  $T, \rho$ , (as effectively in QMD)..???
- move in BUU several testparticles simultaneously (Bertsch..)
  - how many and which ones?
  - in which way?

**Question: Why not start directly from a N-body theory where fluctuations are (better) under control ?  
(Width L fixed by nucl. density profile etc.)**

## How to determine the width L?

- **surface** of the nucleus -> L not too large
- **correlations** of the relative 2-part. wavefct in a nucleus (healing distance)  $\approx 2\text{fm}$
- **range** of nuclear potential  $\approx 2\text{ fm}$

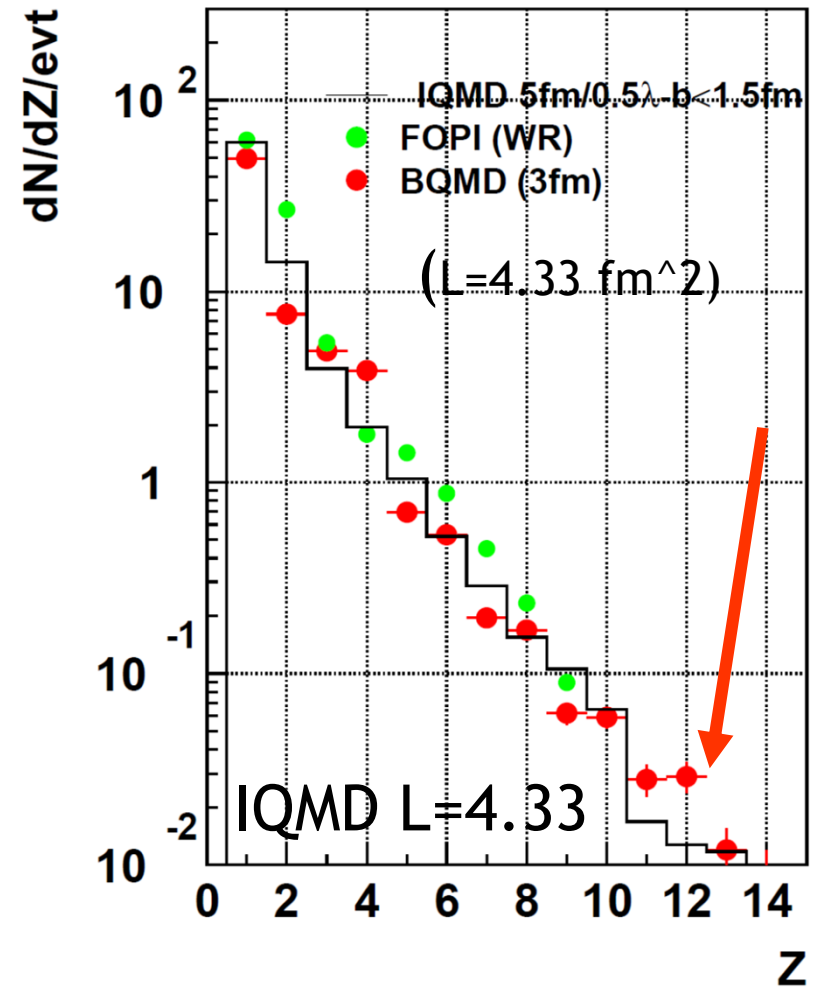
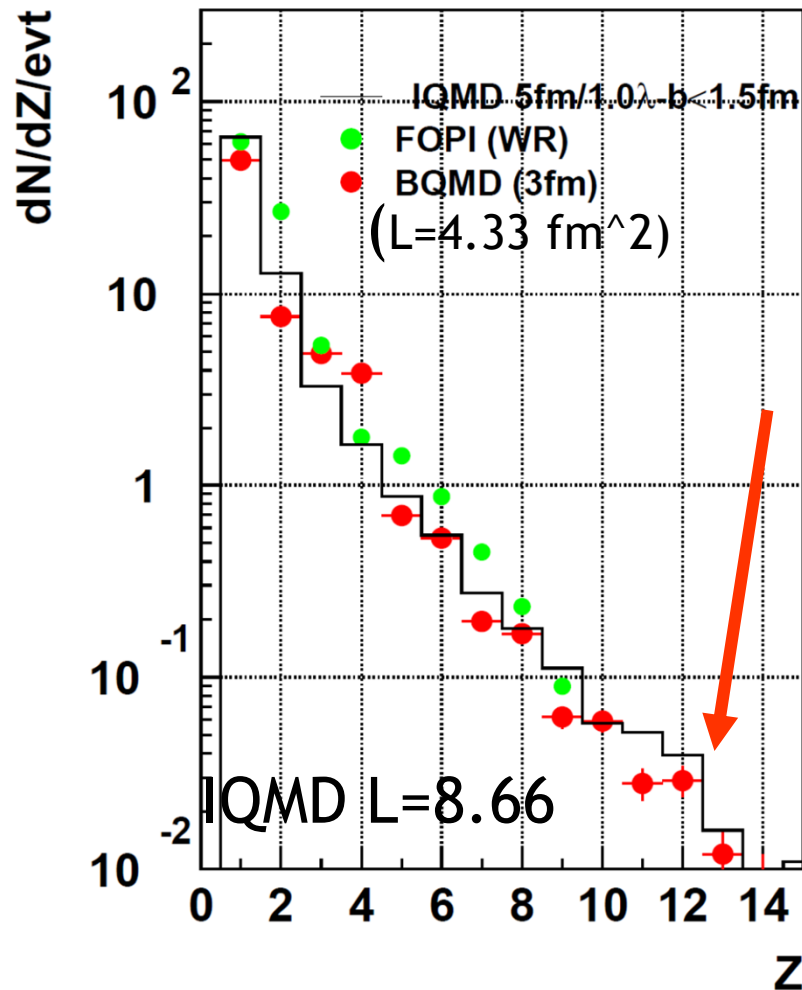
$$L = 4.33 \text{ fm}^2$$

## Where L shows up in the observables?

- initially the **average over many simulations** gives the same  $\rho(r)$  as BUU  $\int d^3p f(r; p; t)$   
**but** the density in each simulation fluctuates around  $\rho(r)$   
**Initial state fluctuations depend on L**
- L determines the local density change if a nucleon is kicked out by a hard collision (spectator fragmentation)  
**L influences spectator fragmentation**
- L plays also a role when fragments are formed from prefer.  
**in participant fragmentation** (via binding energies)

# Influence of L on fragment yield (Y. Leifels)

AuAu 150 AMeV



There are differences but they are modest