PHQMD
(Parton-Hadron-Quantum-Molecular-Dynamics)
- a novel microscopic transport approach to study heavy ion reactions

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(E. Bratkovskaya, A. LeFèvre, Y. Leifels , V. Kireyev)

- ❑ 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

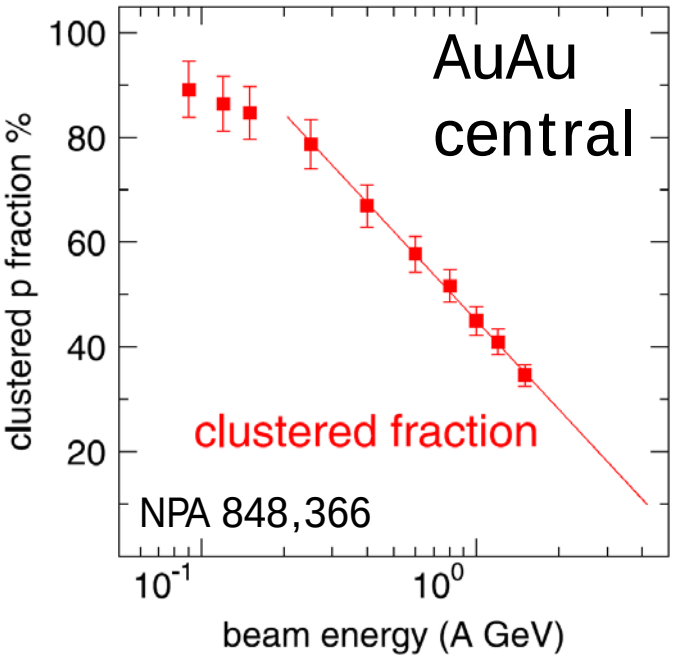
Subatech
Observables of Hadronization and the QCD Phase Diagram in the Cross-over Domain Oct 15-19, 2018

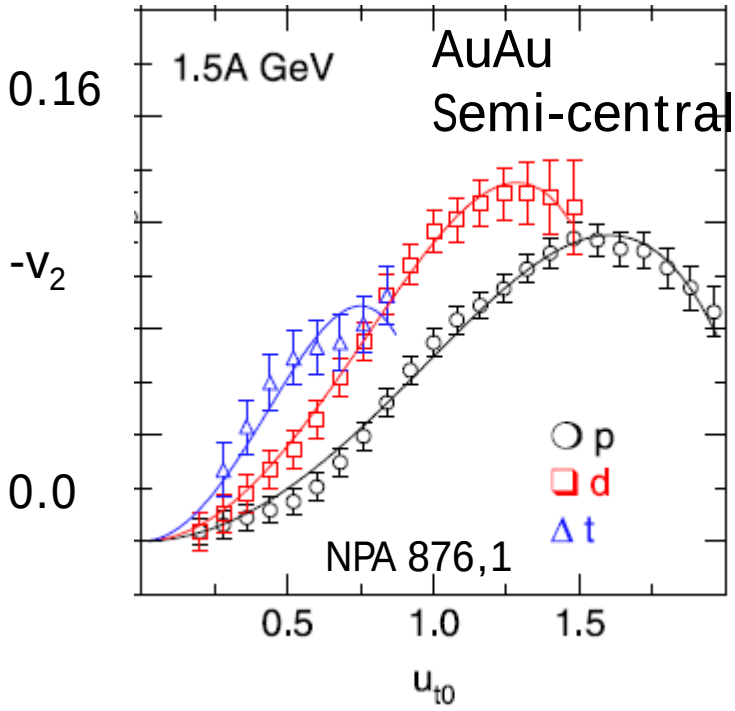
Why do we need a novel approach ?

At 3 AGeV, even in central collisions:

20% of the baryons are in clusters

... and baryons in clusters have quite different properties





Transverse velocity

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
  1st 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

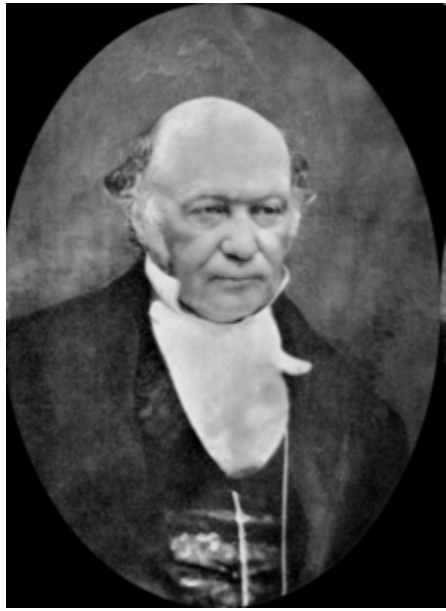
$$H(\mathbf{r}_1, .., \mathbf{r}_N, .., \mathbf{p}_1, .., \mathbf{p}_N, t)$$

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

For a given initial condition

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

the positions and momenta of all particles are predictible 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.

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

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 α, which is varied to find a lowest energy configuration:

$$\frac{d}{d\alpha} < \psi|\hat{H}|\psi >= 0 \rightarrow \alpha_{min}$$

determines α for which $\psi(q,\alpha)$ is closest to the true ground state and $< \psi(\alpha_{min})|\hat{H}|\psi(\alpha_{min}) >= E_0(\alpha_{min})$

Subatech

Extended Ritz variational principle (Koonin, TDHF)

Take trial wavefct with time dependent parameters and solve

$$\delta \int_{t_1}^{t_2} dt < \psi(t)|i\frac{d}{dt} - H|\psi(t) >= 0. \qquad (1)$$

QMD trial wavefct for particle I with p_{oi} (t) and q_{oi} (t)

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

For N particles:

$$\psi_N = \prod_{i=1}^{N} \psi_i(q_i, q_{0i}, p_{0i}) \qquad \text{QMD}$$

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

For the QMD trial wavefct eq. (1) yields

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

For Gaussian wavefct
eq. of motion very similar
to Hamilton's eqs.
(but only for Gaussians)

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

using a coalescence description for test particles

$$P_d(\mathbf{r_1}, \mathbf{r_2}, \mathbf{p_1}, \mathbf{p_2}, \mathrm{t}) = \underbrace{\rho_d^W(\mathbf{p_1} - \mathbf{p_2}, \mathbf{r_1} - \mathbf{r_2})}_{\text{deuteron Wigner density}}$$

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

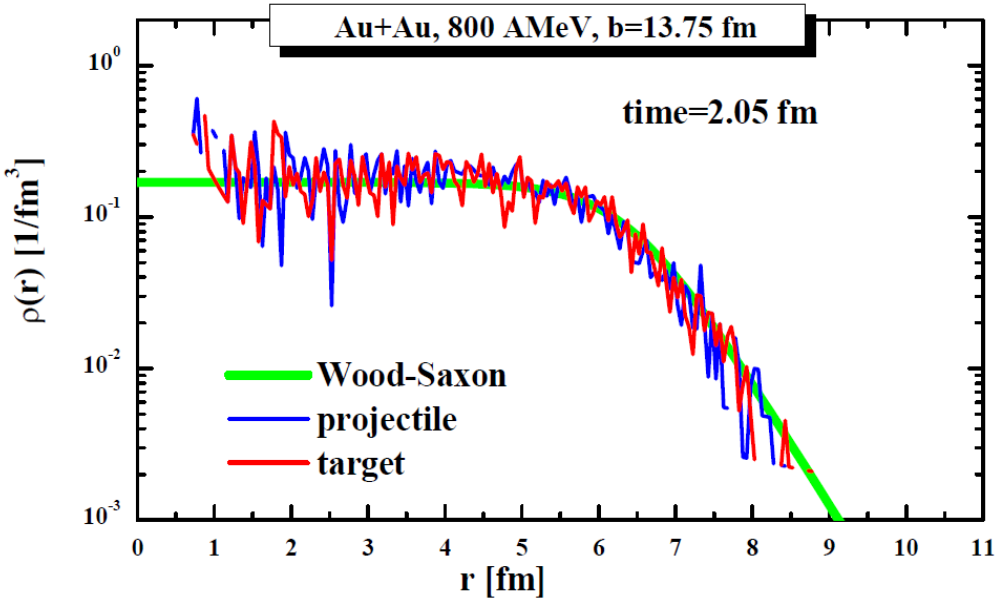
- result depends on the number of test particles
- result depends on time t when coalesce. is applied
- time is different for different particles: PRC56,2109
- no information about the formation process

PHQMD

Initial condition:
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

$$\begin{aligned}\mathbf{V}(\mathbf{r},\mathbf{r}',\mathbf{r_i},\mathbf{r_j}) &= V_{\rm Skyrme} + V_{\rm Coul} \\ &= \frac{1}{2}t_1\delta(\mathbf{r}-\mathbf{r}') + \frac{1}{\gamma+1}t_2\delta(\mathbf{r}-\mathbf{r}')\rho^{\gamma-1}(\mathbf{r}-\mathbf{r}',\mathbf{r_i},\mathbf{r_j}) \\ &\quad + \frac{1}{2}\frac{Z_iZ_je^2}{|\mathbf{r}-\mathbf{r}'|}.\end{aligned}$$

t_1, t_2 and γ adjusted to reproduce a given nuclear equation of state

$$\langle V(\mathbf{r_i},t)\rangle = \sum_{j\neq i}\int d^3r d^3r' d^3p d^3p' V(\mathbf{r},\mathbf{r'},\mathbf{r_i},\mathbf{r_j}) f(\mathbf{r},\mathbf{p},\mathbf{r_i},\mathbf{p_i},t) f(\mathbf{r'},\mathbf{p'},\mathbf{r_j},\mathbf{p_j},t)$$

$$\langle V_i^{Skyrme}(\mathbf{r_i},t)\rangle = \alpha\left(\frac{\rho_{int}(\mathbf{r_i},t)}{\rho_0}\right) + \beta\left(\frac{\rho_{int}(\mathbf{r_i},t)}{\rho_0}\right)^{\gamma}$$

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

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

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

All elastic and inelastic cross sections from PHSD – therefore at high energy the spectra of produced particles are similar to PHSD results

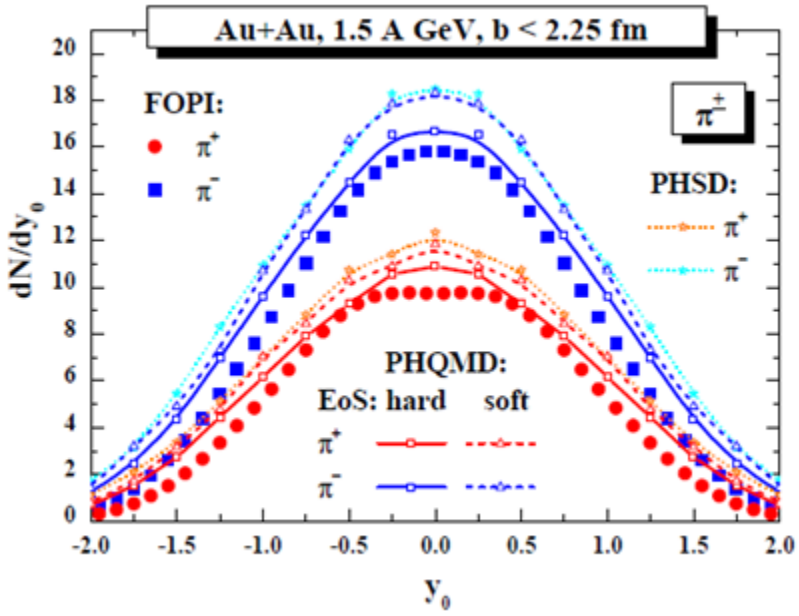
Results

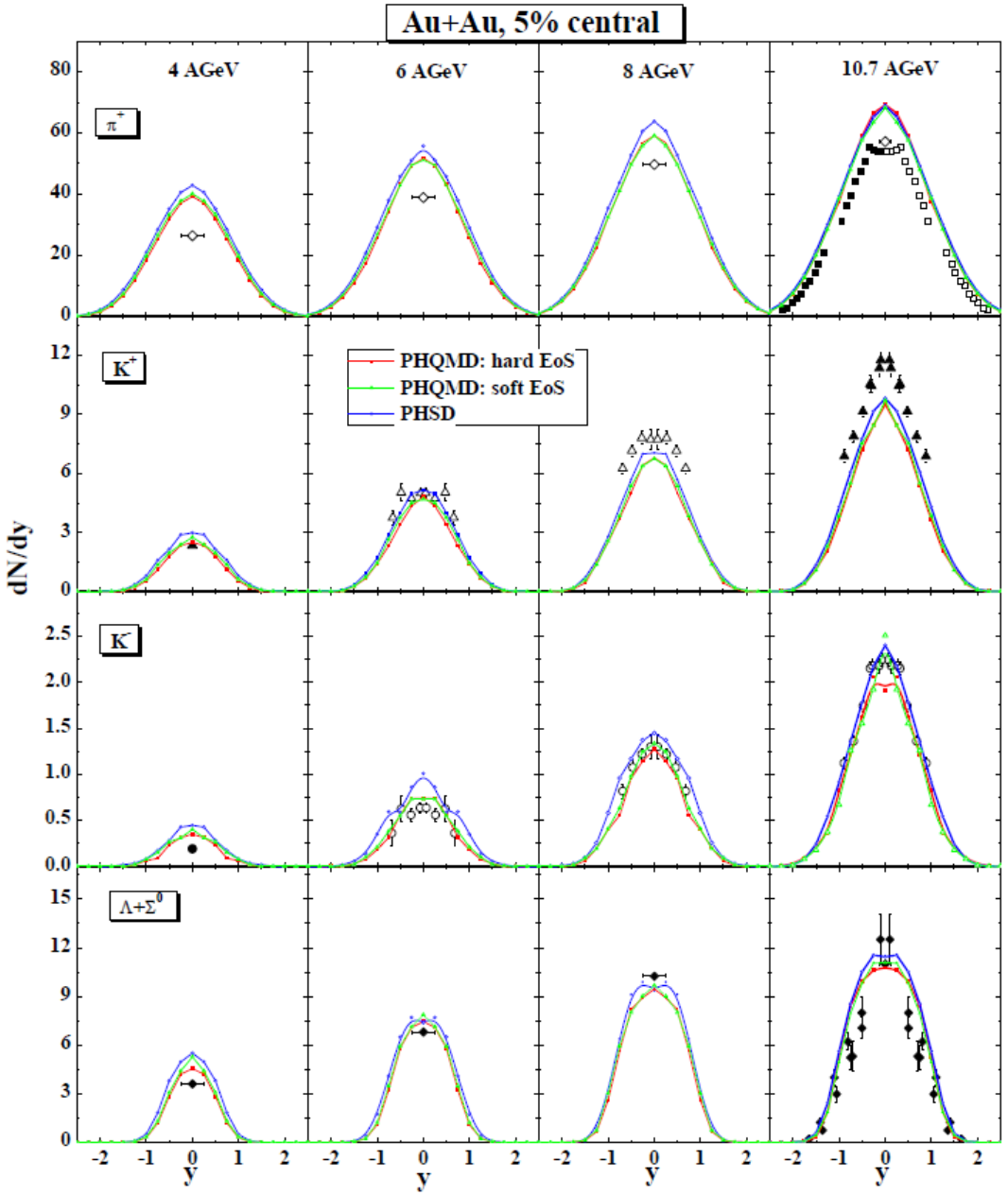
First Results of PHQMD

Produced particles

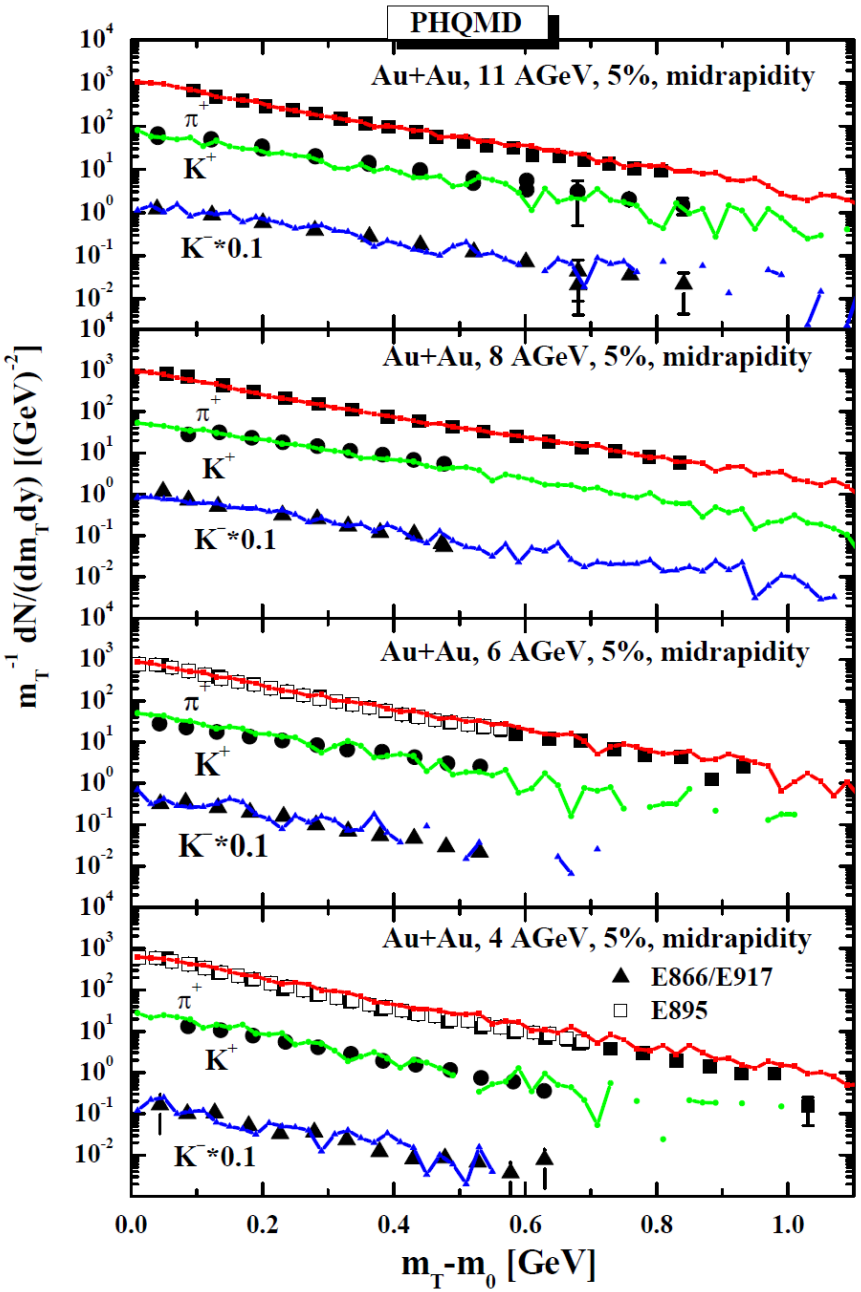
are well reproduced
at SIS/NICA/FAIR energies

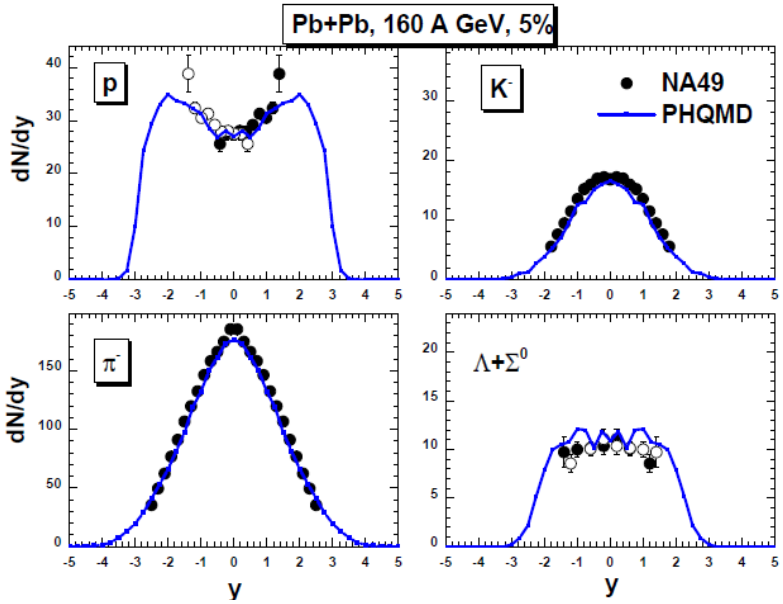
(dominated by collisions)

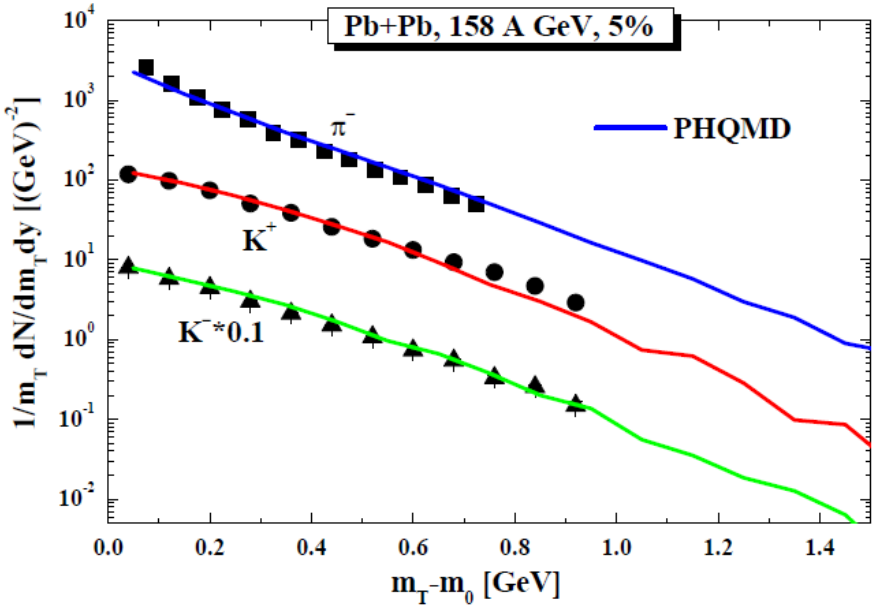




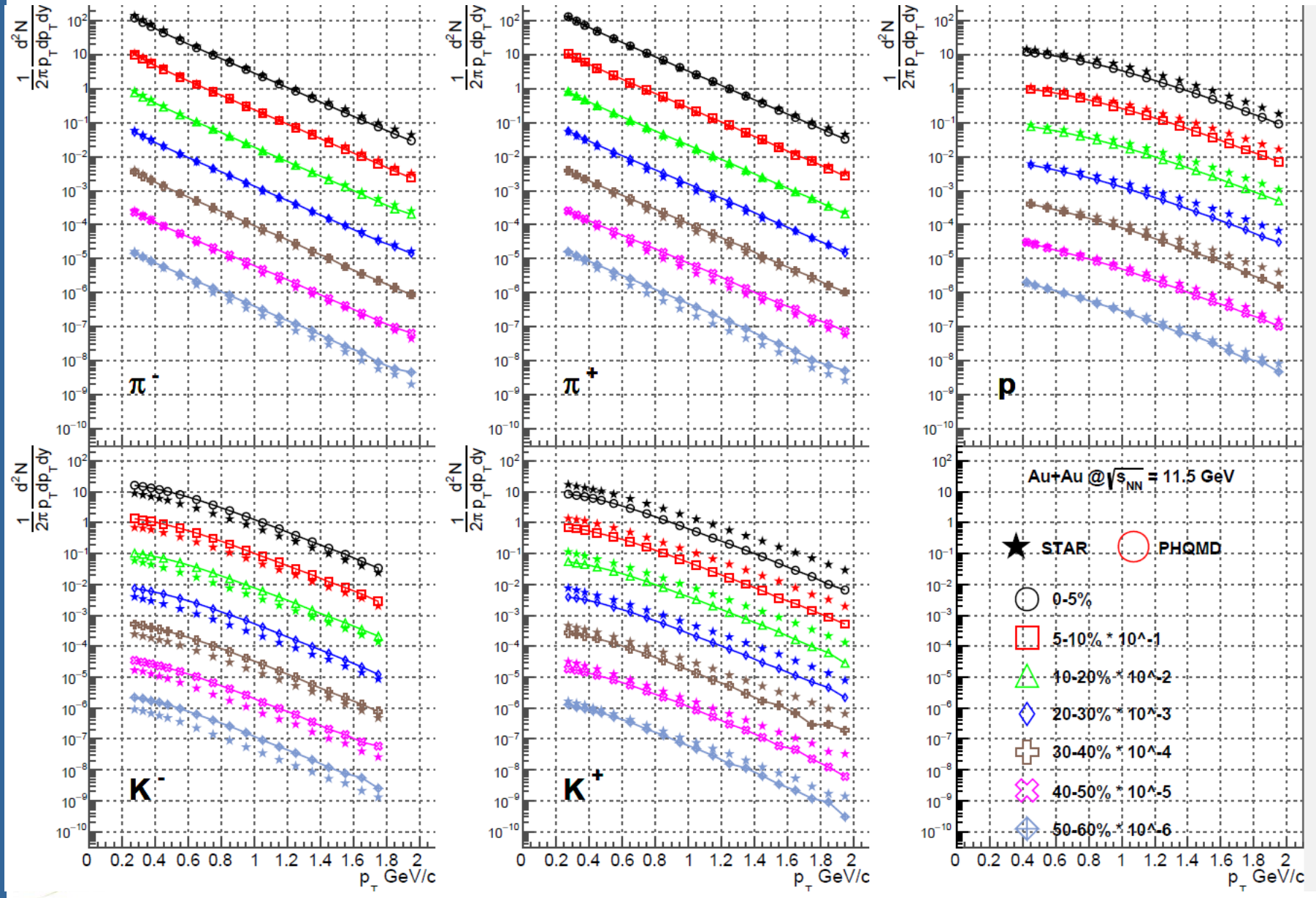
As well as at SPS energies







.. And also the most recent STAR data at 11.5 AGeV



How to define fragments in transport theories which propagate nucleons?

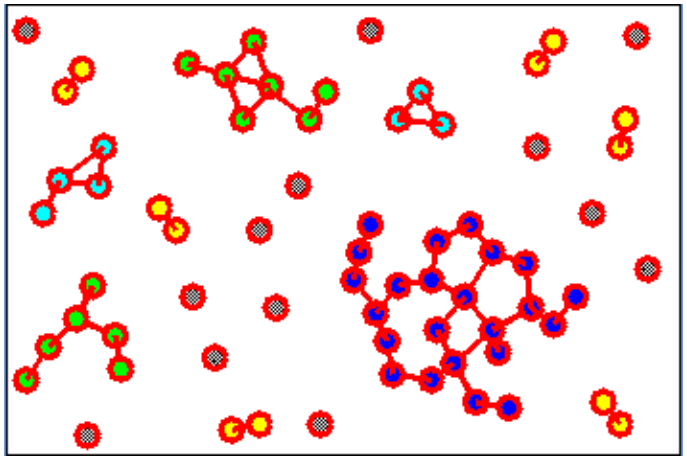
I. Minimum Spanning Tree (MST) is a cluster recognition method applicable for the (asymptotic) final state where coordinate space correlations may only survive for bound states.

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

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

$$\left|\vec{r}_i - \vec{r}_j\right| \leq 2.5\, fm$$

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

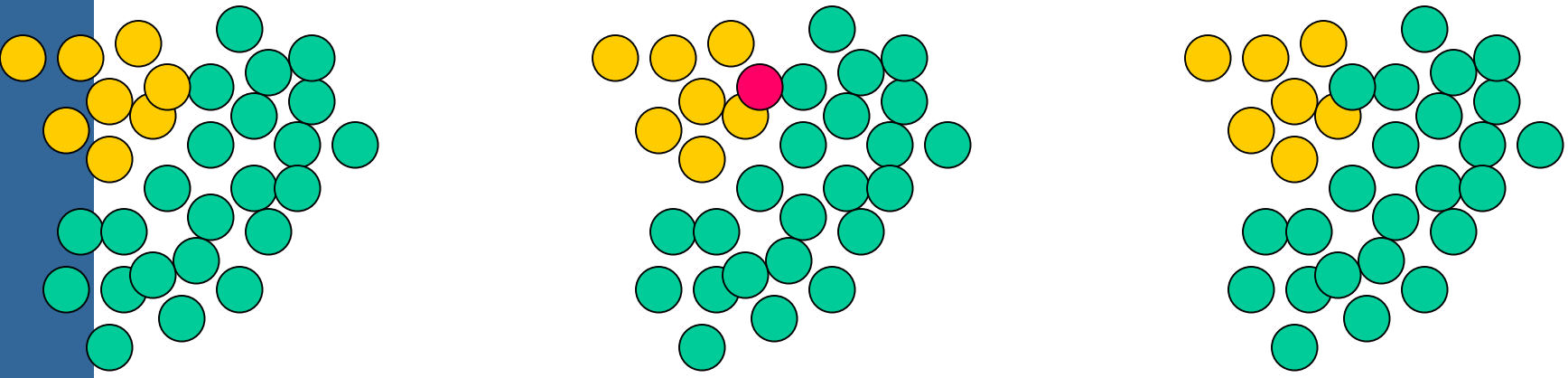
Simulations show: Clusters chosen that way at early times are the prefragments of the final state clusters.
(large persistent coefficient)

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

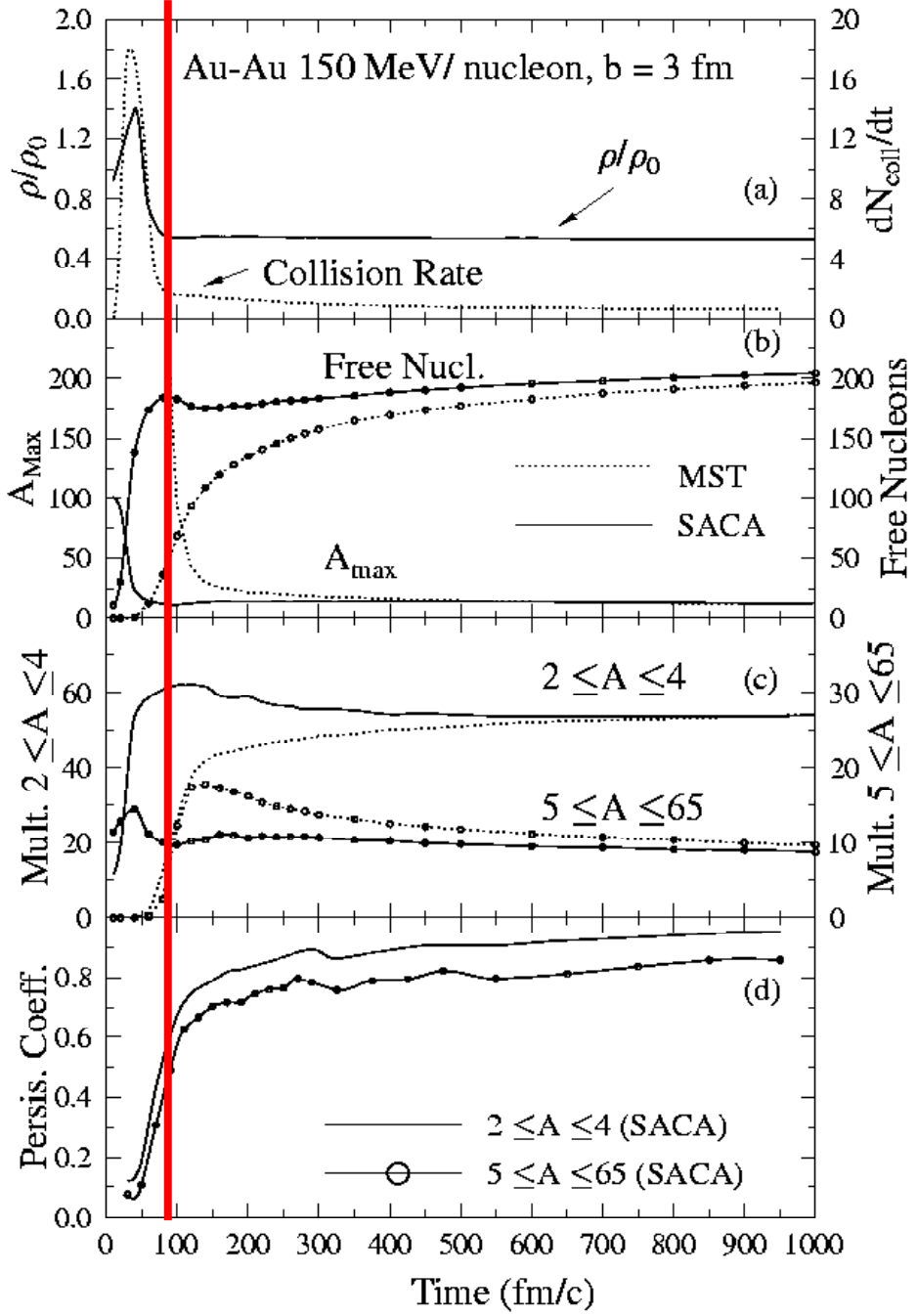
Add it randomly to another fragment



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

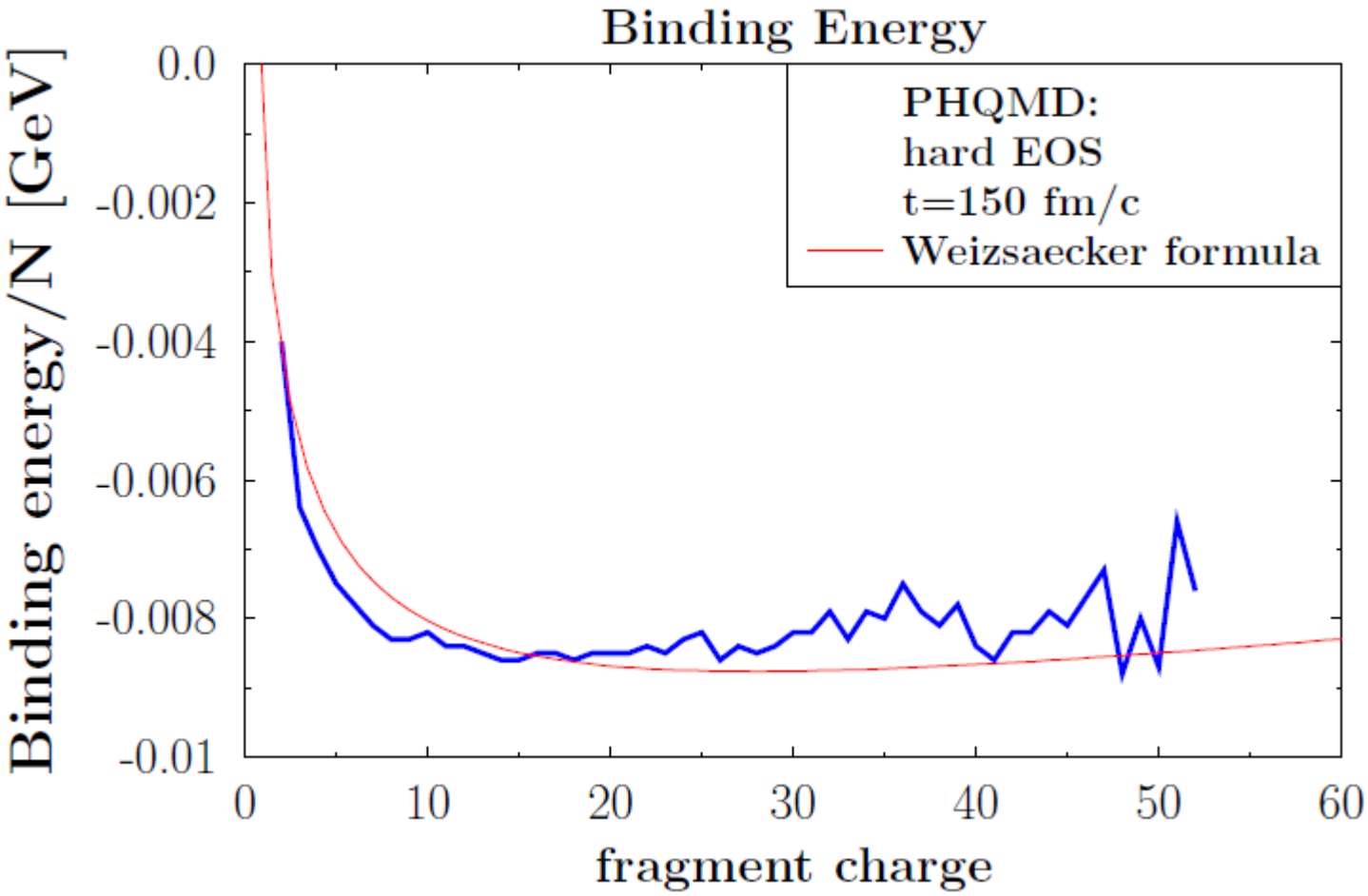
$E'=E^{1'}_{kin}+E^{2'}_{kin}+V^{1'}+V^{2'}$

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

At1.5t_{pass} Amax and multiplicities of intermediate mass fragments are determined



There are two kinds of fragments

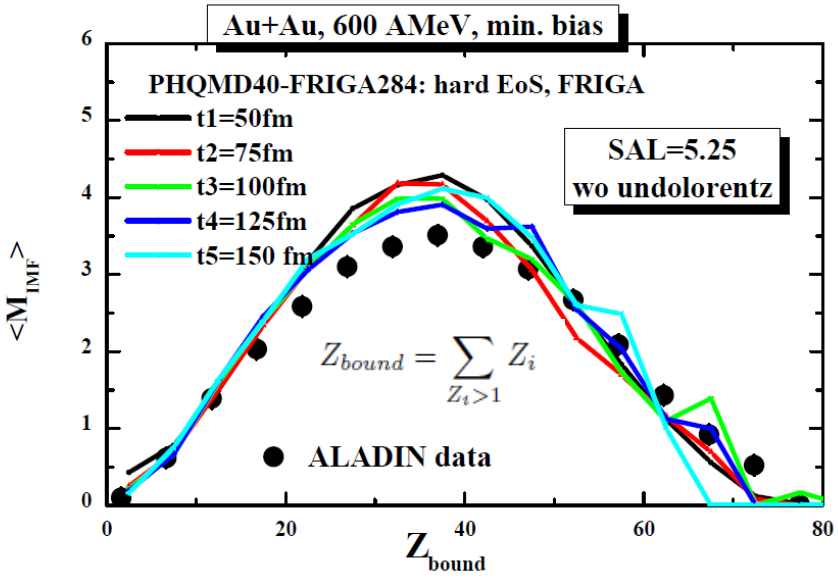
- formed from spectator matter
  close to beam and target rapidity
  initial-final state correlations
  HI reaction makes spectator matter unstable

- formed from participant matter
  created during the expansion of the fireball
  "ice" (E_{bind} ≈8 MeV/N) in "fire"(T≥ 100 MeV)
  origin not known yet
  seen from SIS to RHIC
  (quantum effects may be important)

First Results of PHQMD

Spectator Fragments

experm. measured up to E_{beam} =1 AGeV (ALADIN)

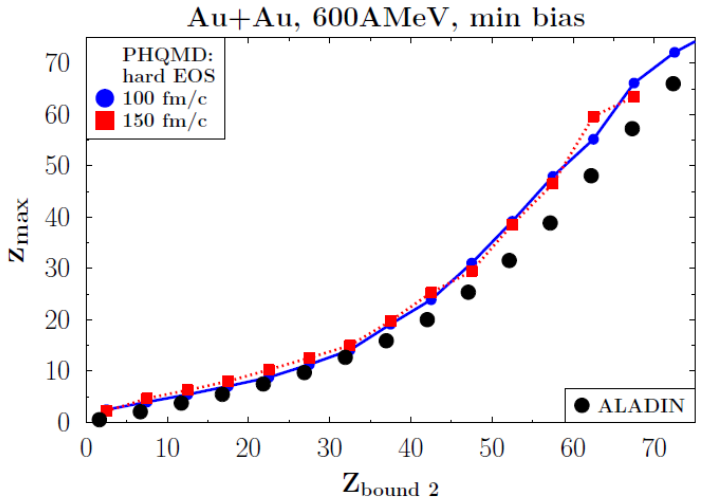


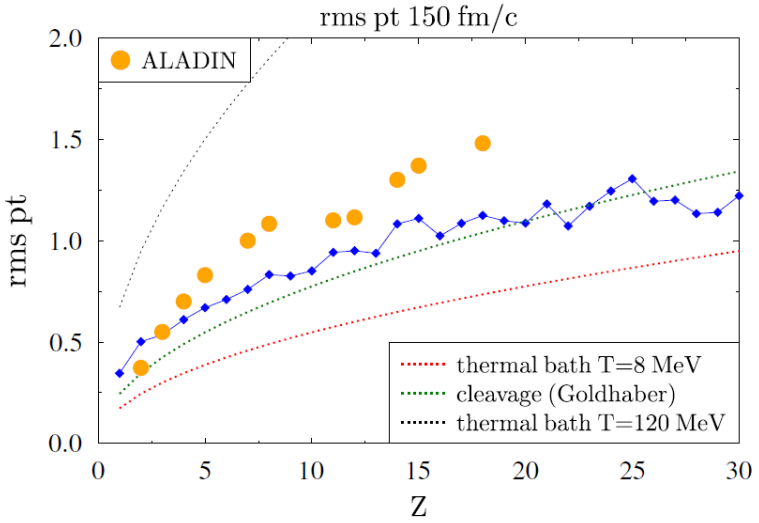
$$Z_{bound} = \sum_{Z_i>1} Z_i$$

agreement for very complex fragment observables like the

- ❑ energy independent "rise and fall"
- ❑ largest fragment (Z_{bound})

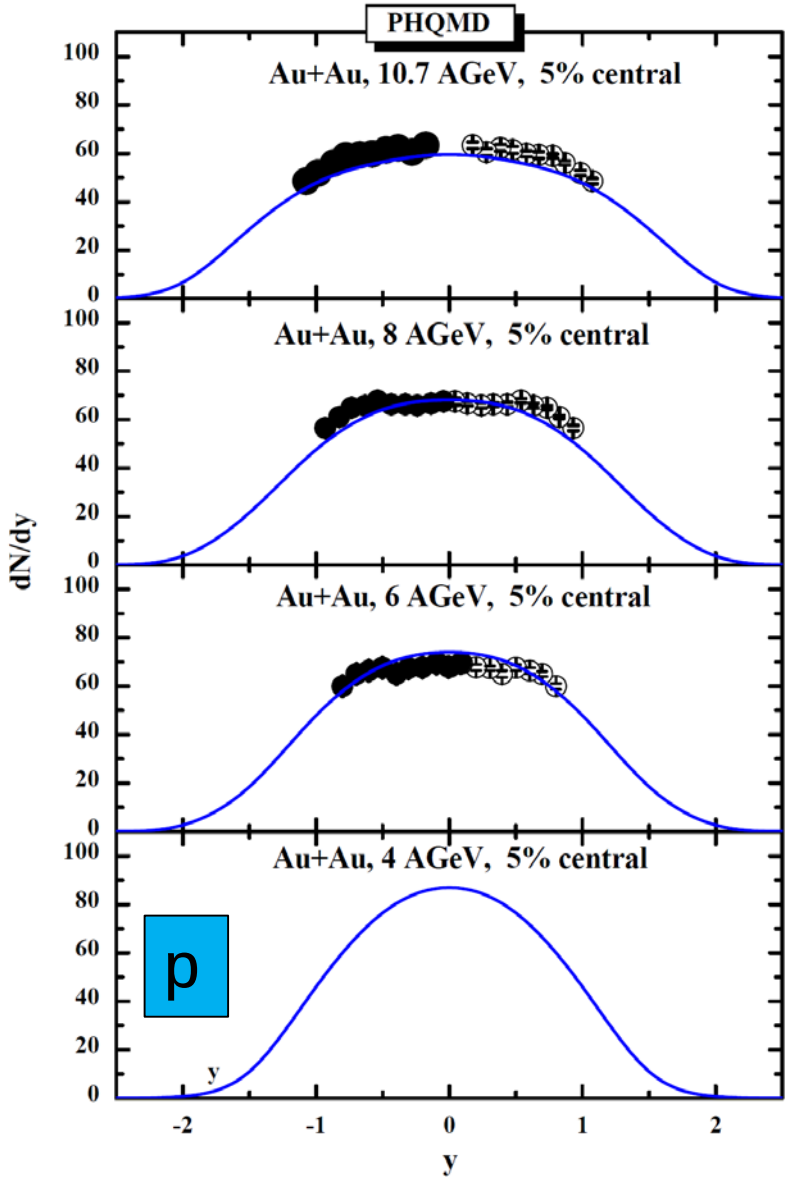
rms(p_t) shows $\sqrt{Z}$ dependence



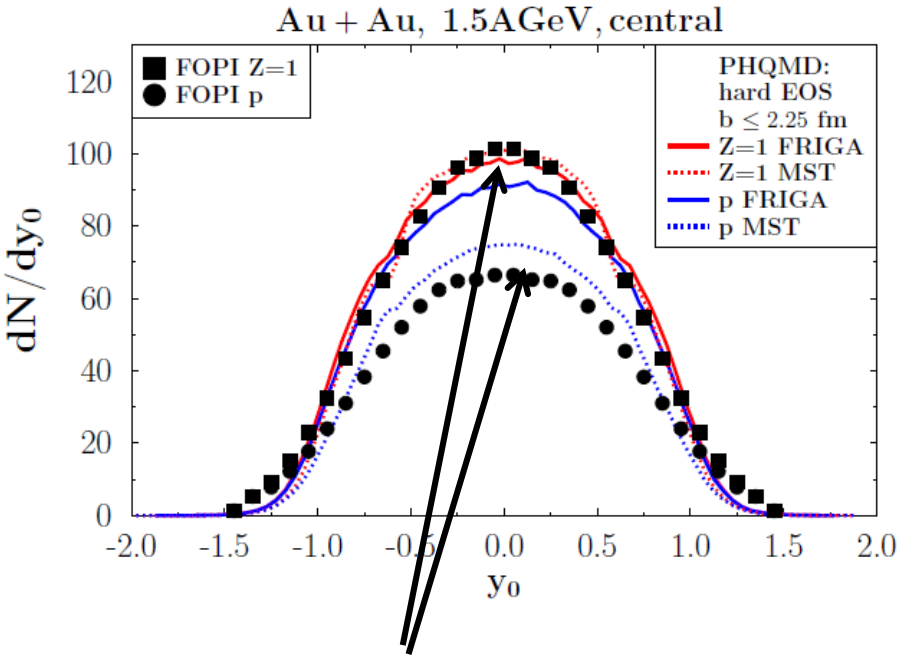


First Results of PHQMD

Protons at midrapidity well described



midrapidity fragment production increases with decreasing energy



1.5 AGeV central

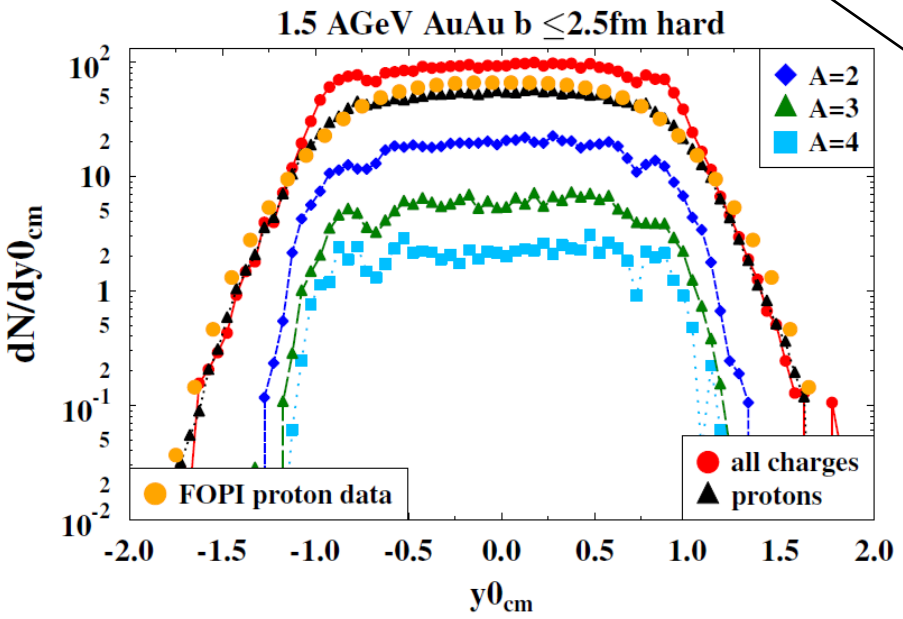
- 30% of protons bound in cluster

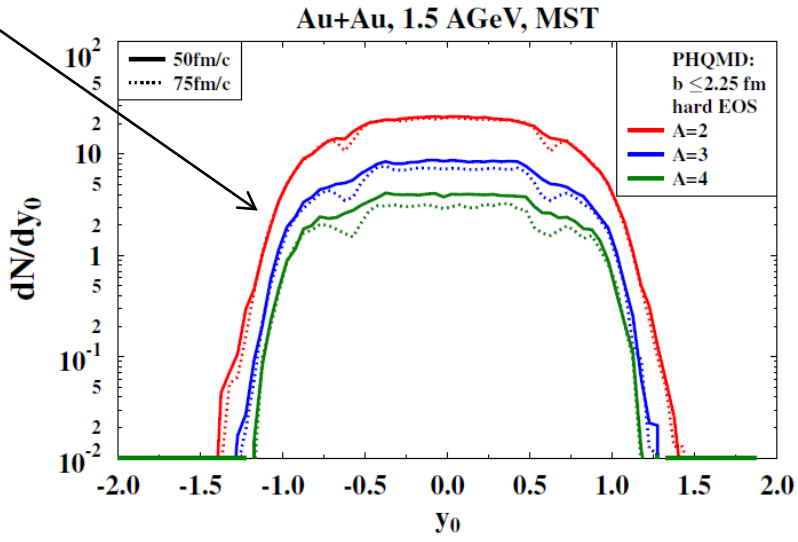
To improve: better potential for small clusters

First Results of PHQMD

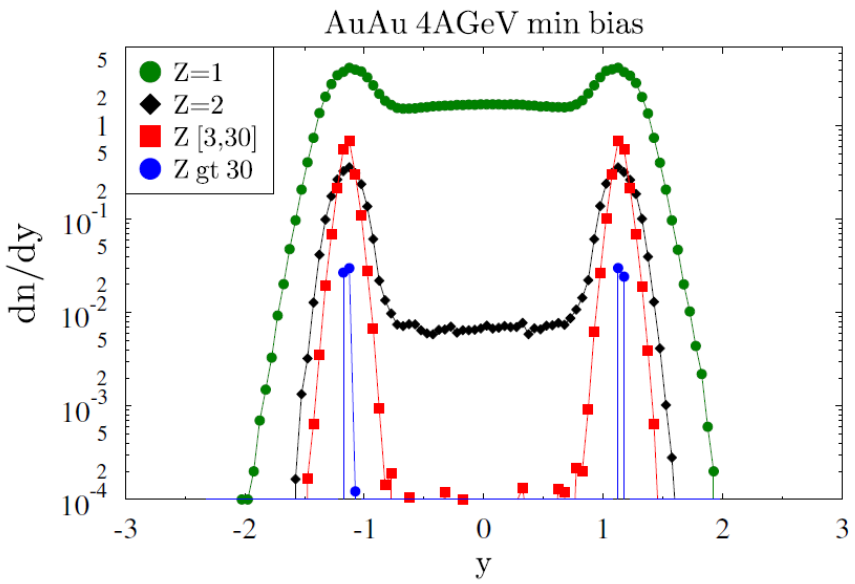
There are all kinds of dynamicall yproduced fragments at midrapidity and they are stable

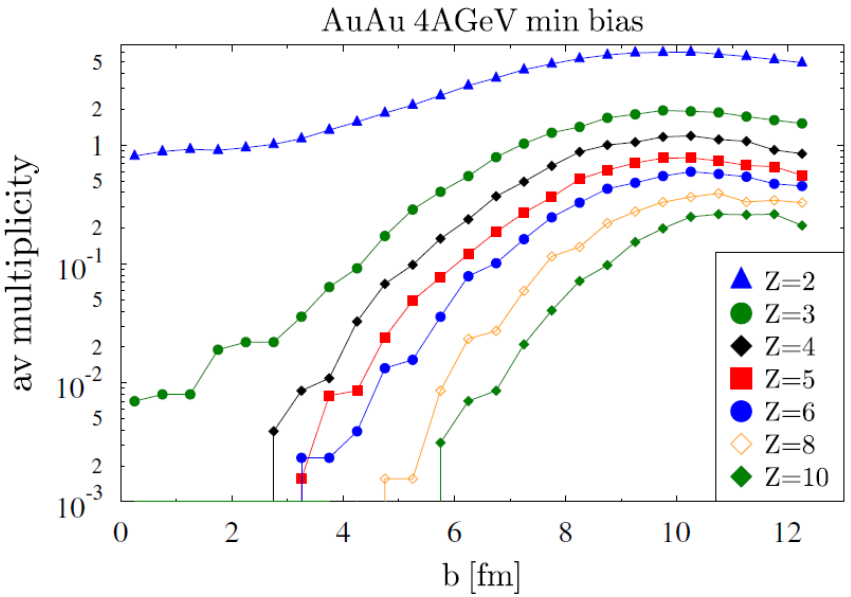
(MST finds at 60fm/c the same fragments as at 75fm/c)





First Results of PHQMD





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

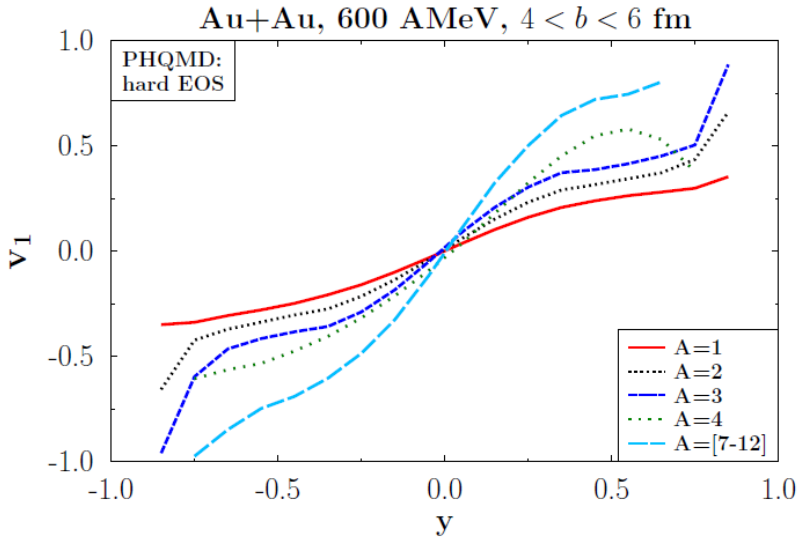
Dynamical variables - v_1

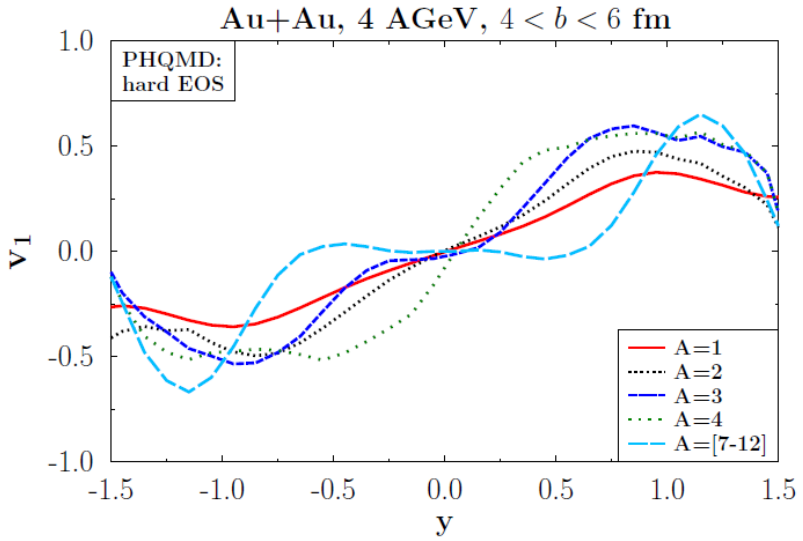
v_1 quite different for nucleons and fragments (as seen in experiments)

nucleons come from participant regions (-> small density gradient)

fragments from interface spectator-participant (strong density gradient)

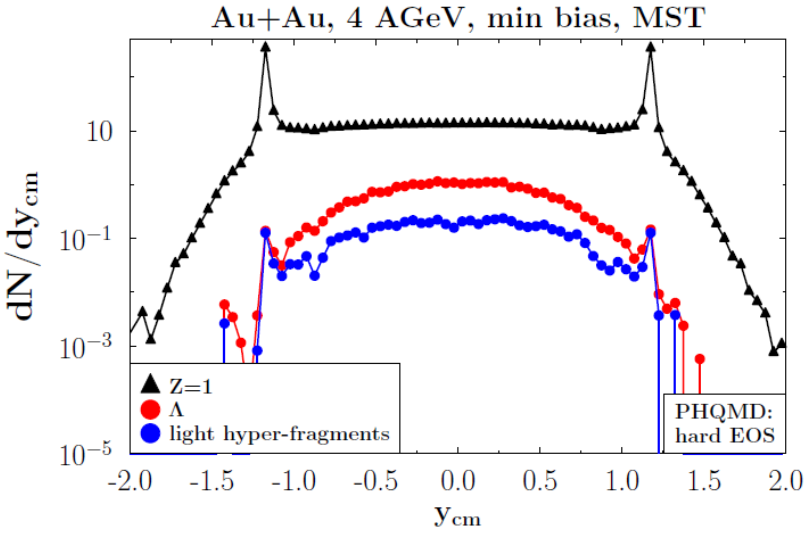
v_1 decreases with E_{beam}
smaller passing time t_p
→ F_T t_p = p_T smaller





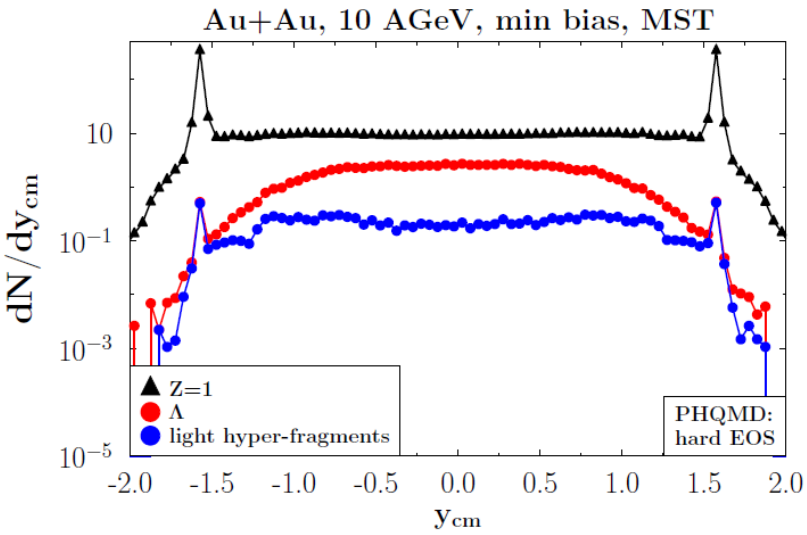
.. And what about hyper-nuclei ?

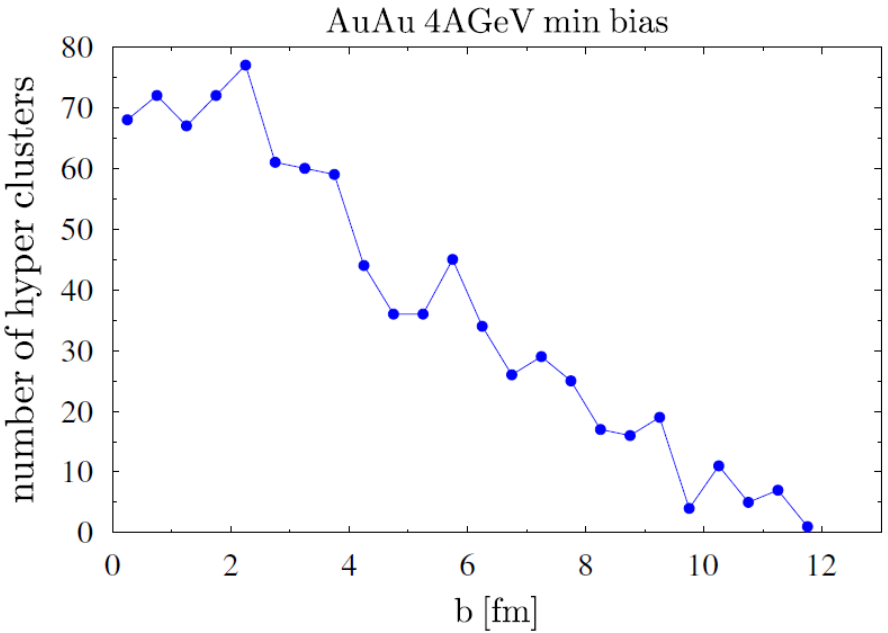
First Results of PHQMD



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

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

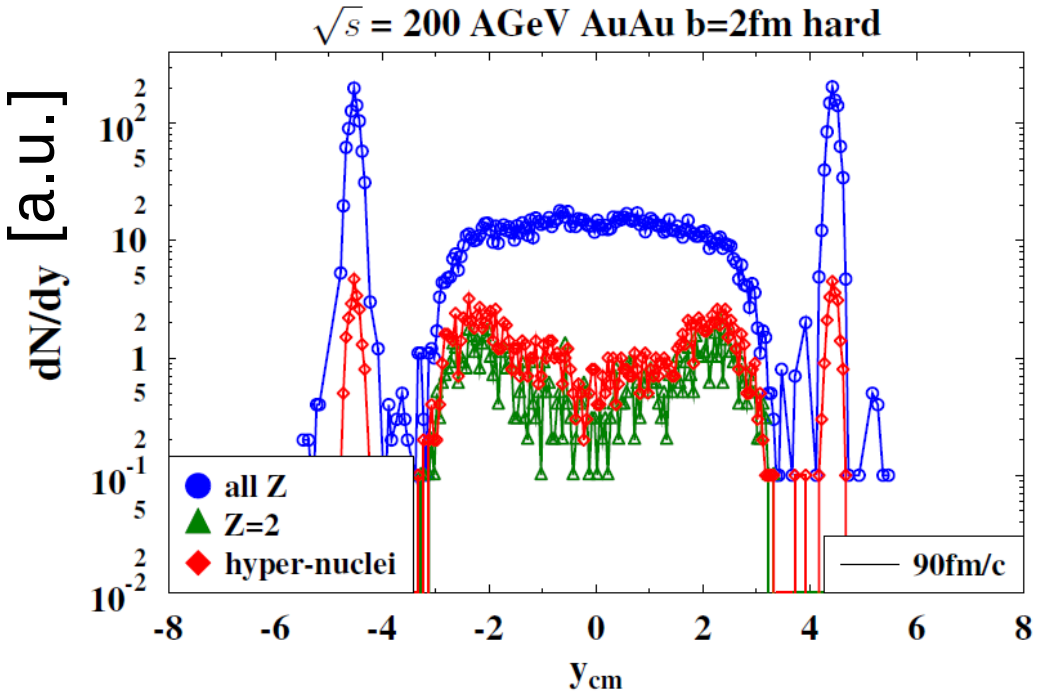




First Results of PHQMD

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 AMeV b=5fm

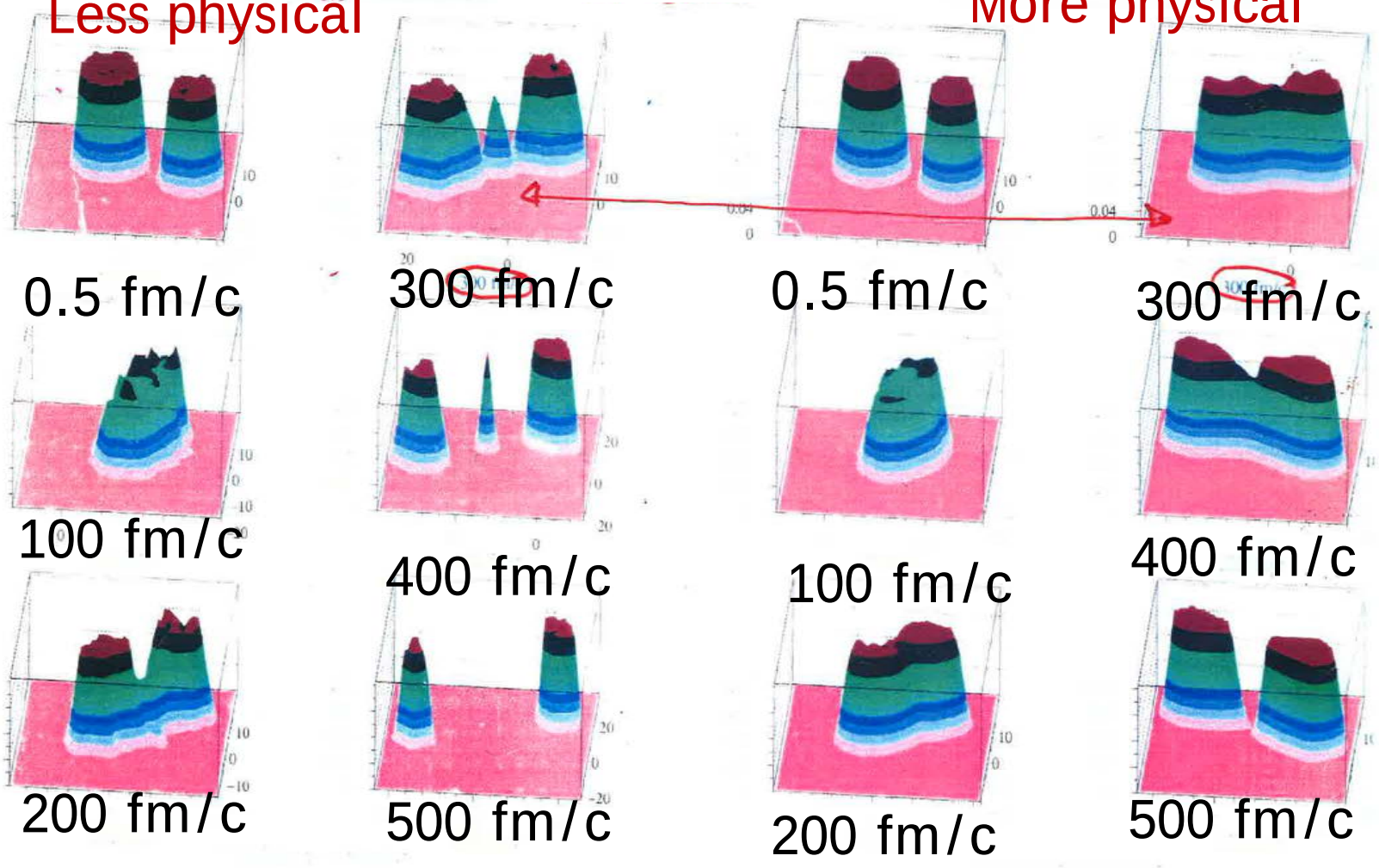
25 test particles/N

W. Bauer
U.Schröder

275 test paricles/N

Less physical

More physical

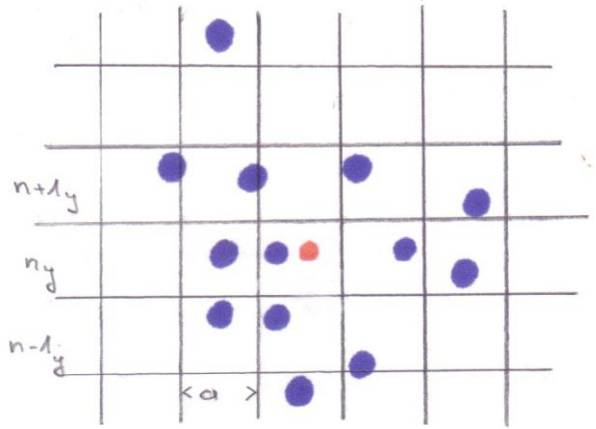


Numbers of test particles must be large enough

When is N sufficiently large?

One uses delta like forces: F(r) = δ(r) (Skyrme) but then point-like test particles f= Σ δ(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

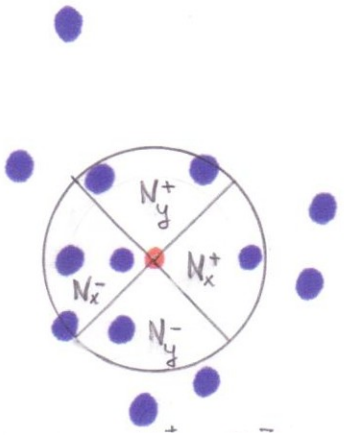


n_x-1 n_x n_x+1

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

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

Lagrange



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

Average distance between nucleons 2fm. Grid size ≈ 1fm (surface). Therefore very many test particles necessary to avoid numerical fluctuations: 100tp->12 in a cell->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

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int\int g I(g,\Omega)[f(\mathbf{p'}_A,t) f(\mathbf{p'}_B,t) - f(\mathbf{p}_A,t) f(\mathbf{p}_B,t)]\, d\Omega\, d^3\mathbf{p}_A\, d^3\mathbf{p}_B.$$

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

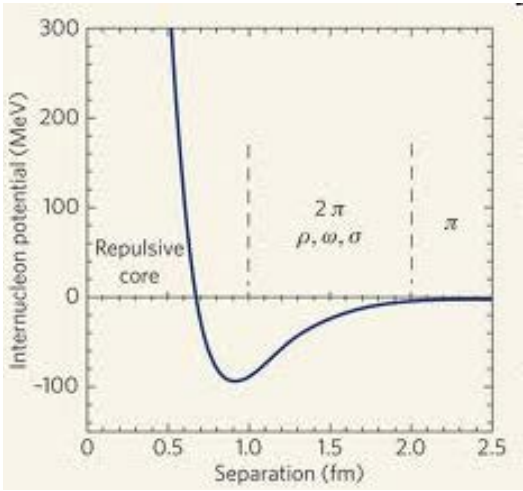
$$f(\mathbf{r},\mathbf{p},t) = \sum_{i=1}^{N\to\infty} \delta(\mathbf{r} - \mathbf{r}_i(t))\ \delta(\mathbf{p} - \mathbf{p}_i(t))$$

test particle ≠ nucleon

If N small unphysical fluctuations

What means N ->∞ in reality ?

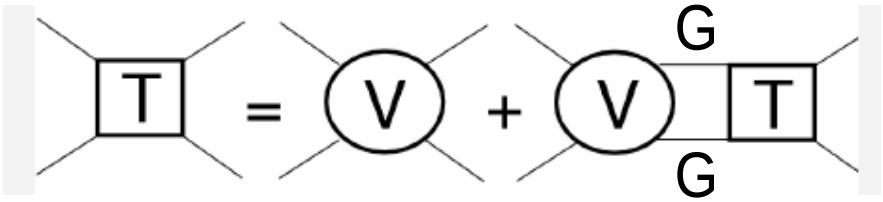
How does a collision term appear?



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)



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

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

Consequences:

V_{NN} is real → T is complex = ReT + i Im T

corresponds to V_{NN} in Hamiltonian (Skyrme)

σ_{elast} collisions done identically BUU (test-particles) and QMD (particles)

To this one adds inelastic collisions (BUU,HSD, SMASH and QMD – the same way)!

➔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 (σ,T,ρ) and mathematical fluctuations ($1=\frac{\tilde{N}}{\overline{N}}$) 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 Δr and Δp, dependence of T,ρ,(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) ≈ 2fm
- range of nuclear potential ≈ 2 fm

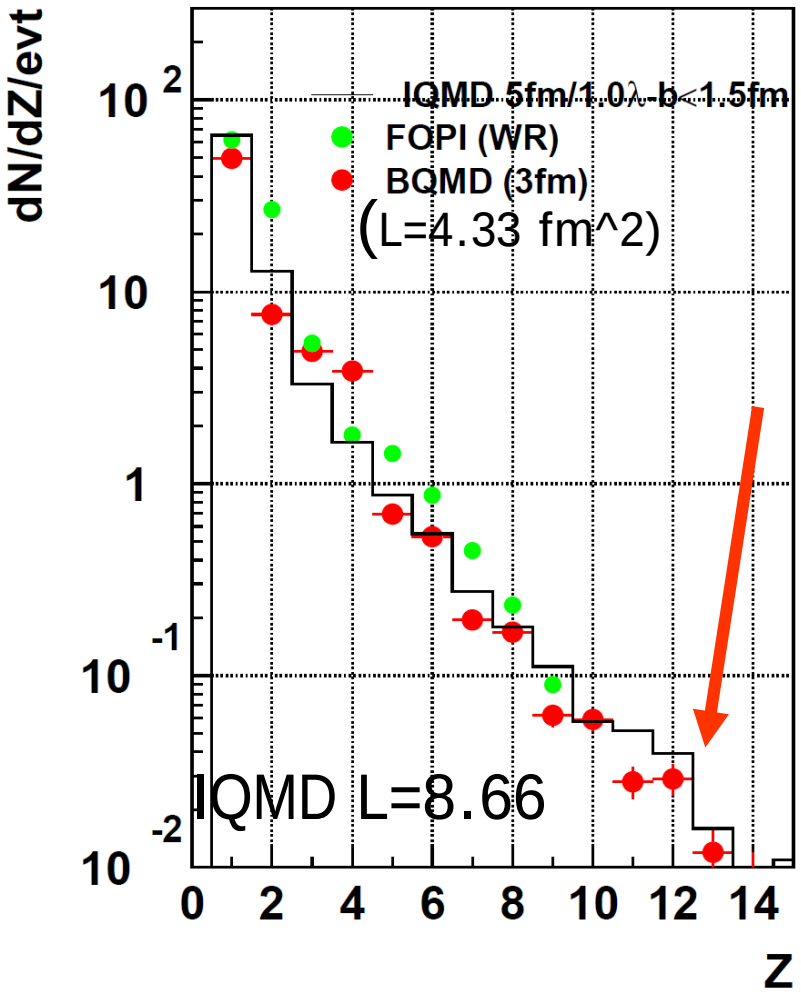
$$L = 4.33\ fm^2$$

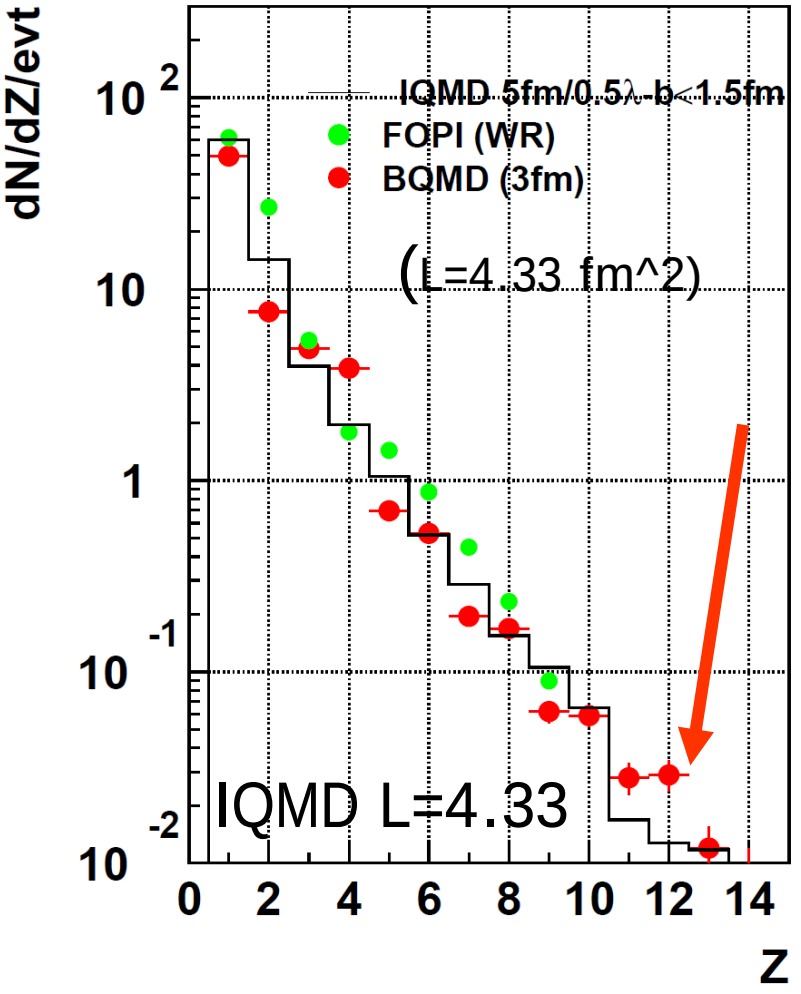
Where L shows up in the observables?

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

Influence of L on fragment yield (Y. Leifels)

AuAu 150 AMeV





There are differences but they are modest

Modeling of fragment and hypernucleus formation

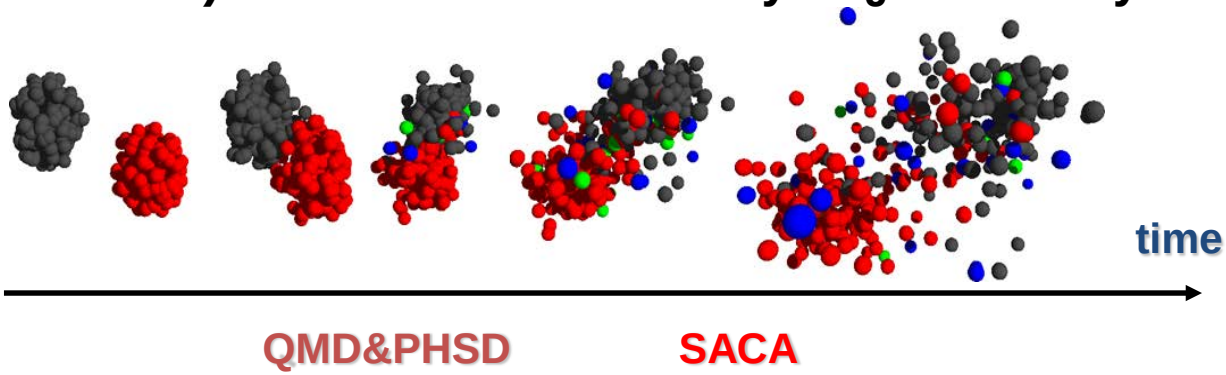
The goal: Dynamical modeling of cluster formation by a combined model

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 identity fragments very early during the reaction.



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