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

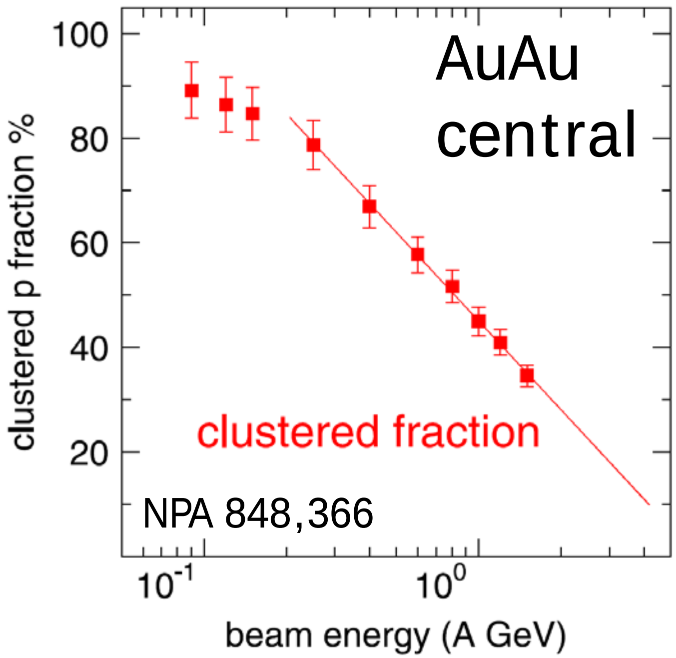
- ❑ Comparison with existing data
- ❑ Perspectives for BMN/NICA/FAIR/RHIC

Subatech

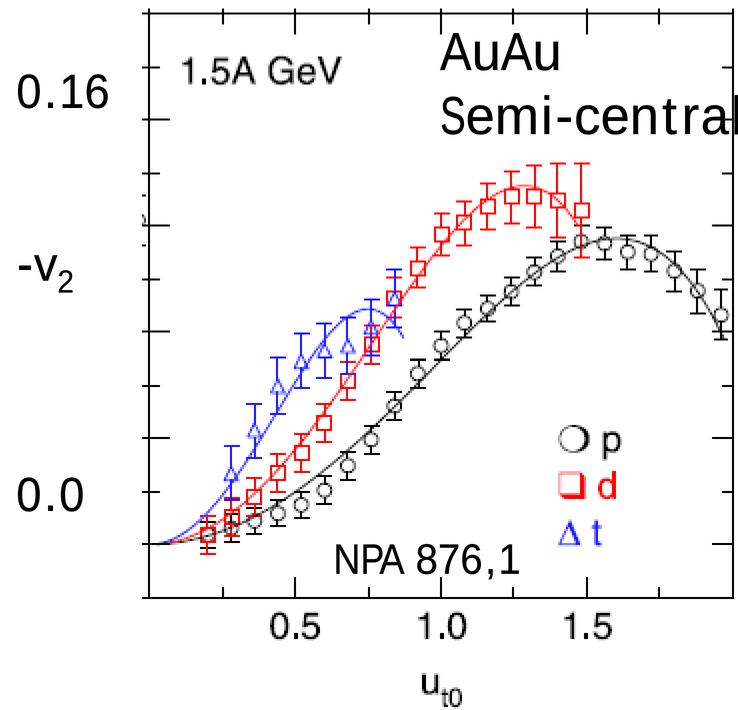
Why do we need a novel approach ?

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
  1st order phase transition
  time development of the phase space density

Present micoscopic approaches fail to describe fragments at NICA/FAIR energies

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

UrQMD solves the n-body theory but has no potential
→ nucleons cannot be bound to fragments

(I)QMD solves the 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

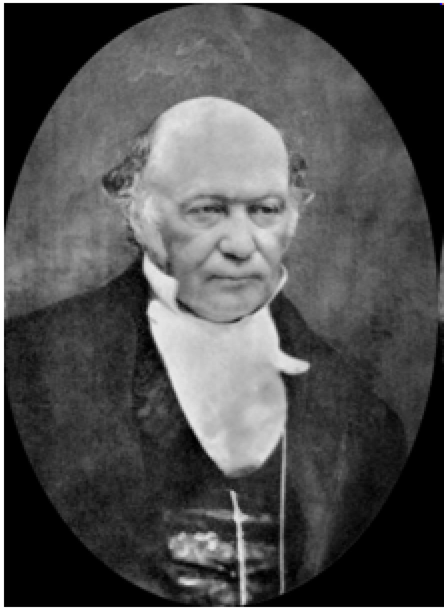
$$H(\mathbf{r}_1,..,\mathbf{r}_N,..,\mathbf{p}_1,..,\mathbf{p}_N,t)$$

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

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:

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

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

Extended Ritz variational principle (Koonin, TDHF)

Take trial wavefct with time dependent parameters and solve

$$\frac{< \psi_N | i\frac{d}{dt}\hat{H} | \psi_N >}{< \psi_N | \psi_N >} = 0 \qquad (1)$$

QMD trial wavefct for one particle (Gaussian):

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

For N particles:

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

QMD

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

AMD / FMD

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.

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

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

Same interaction, not possible classically

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

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

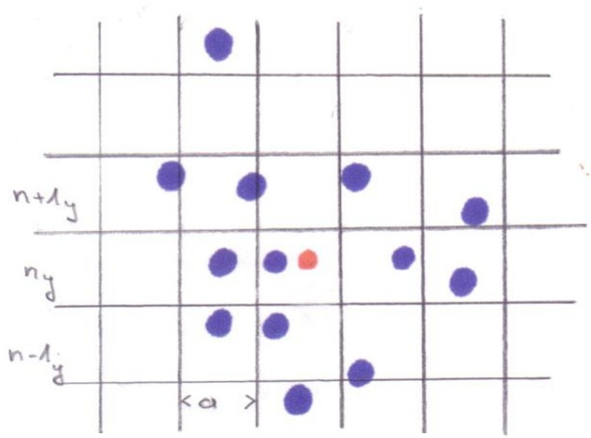
If N small unphysical fluctuations

What means N ->∞ in reality ?

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).

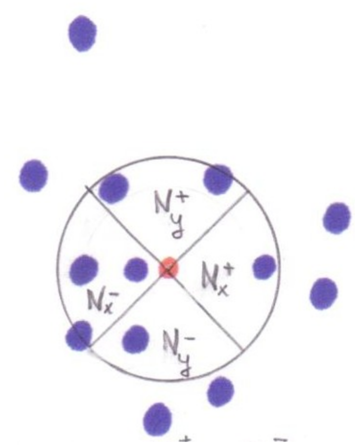
Euler



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

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

Lagrange

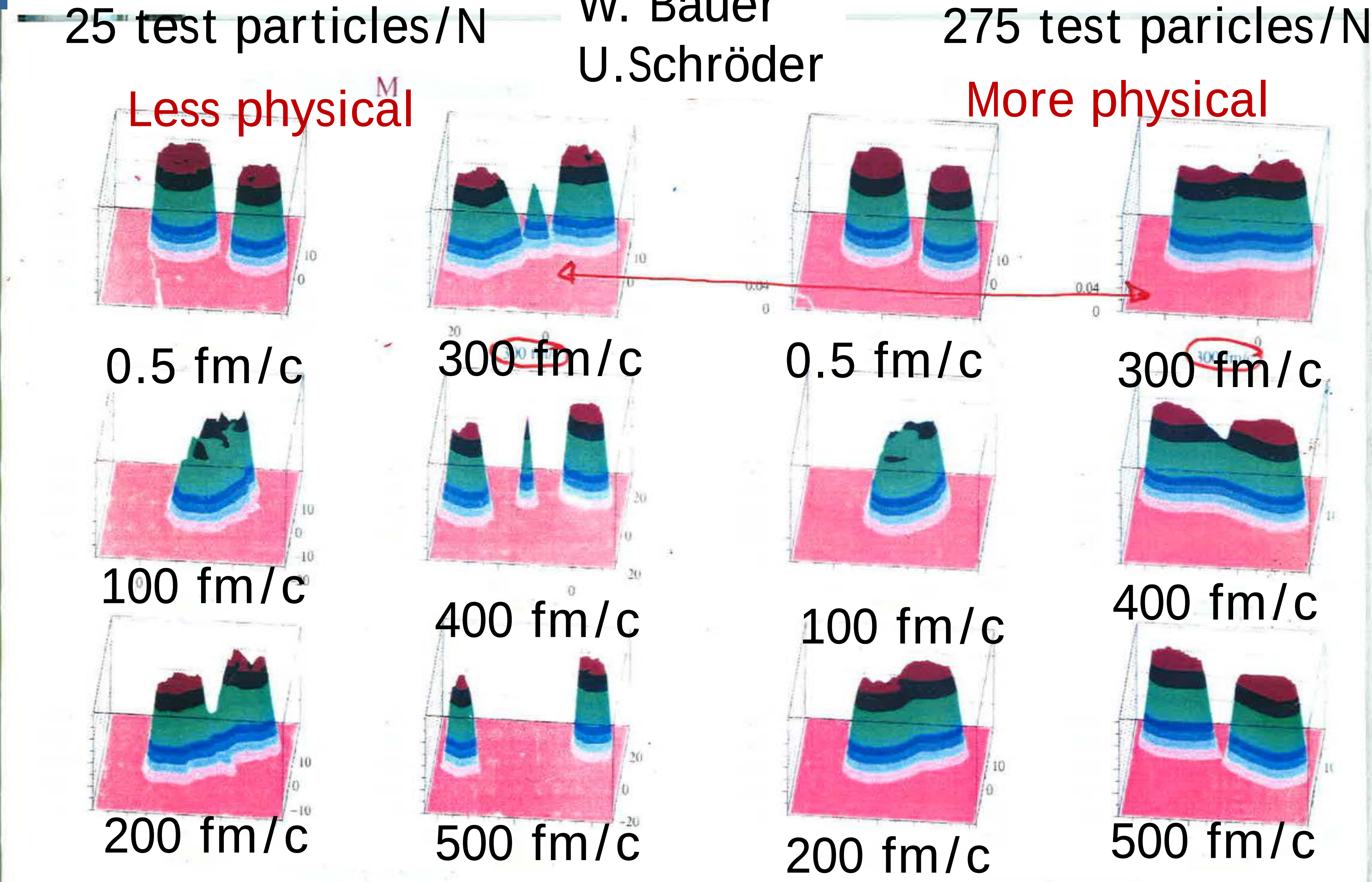


$$F_x = \frac{U_{x\ right}(\rho) - U_{x\ left}(\rho)}{2a}$$

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

Bi+Xe, 28 AMeV b=5fm

W. Bauer
U.Schröder



Numbers of test particles must be large enough

Attempts have been made to form clusters in the test particle BUU approach

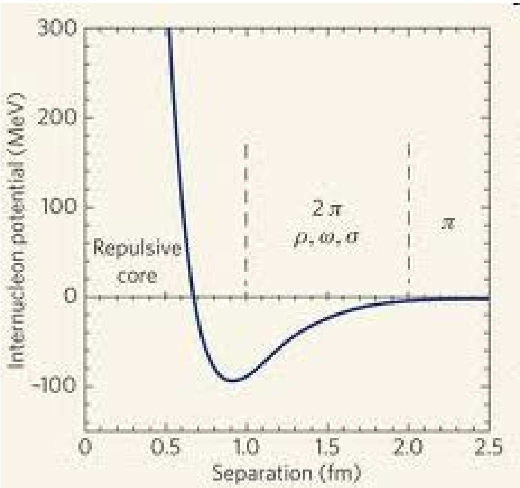
using a coalescence description for test particles

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

but 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 eq. is applied
- time is different for different particles: PRC56,2109
- no information about the formation process

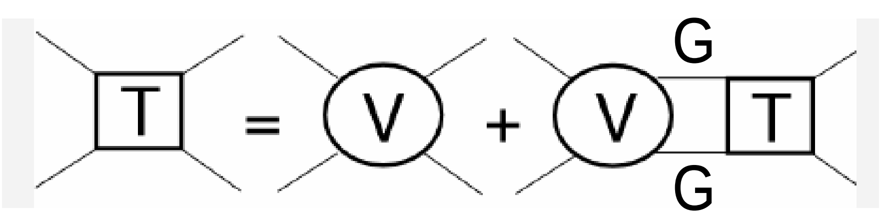
How does a collision term appear?



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)



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

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

Consequences:

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

ReT → corresponds to V_{NN} in Hamiltonian (Skyrme)

Im T → 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)

Modeling of fragment and hypernucleus formation

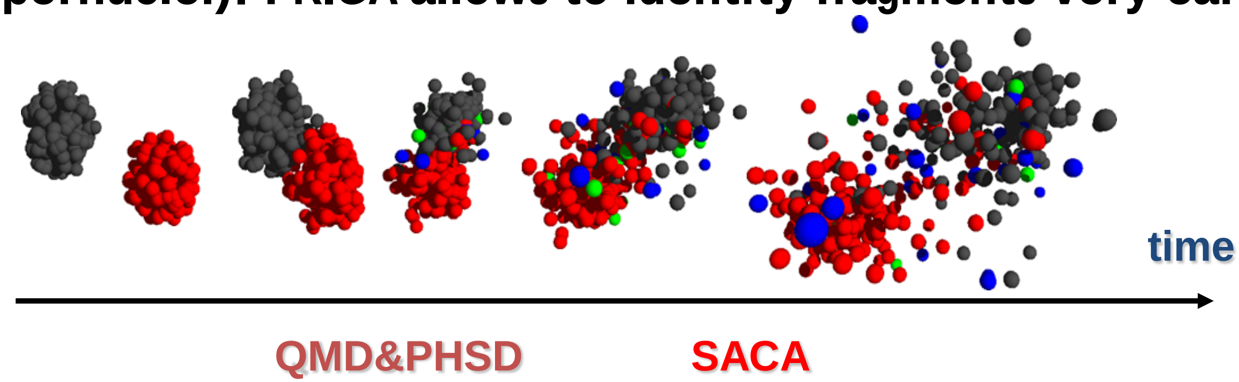
The goal: **Dynamical modeling of cluster formation by a combined model**

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.**



Potential in PHQMD

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 are small and therefore nonrelativistic kinematics can be applied.

Potential interaction between nucleons

$$\begin{aligned} U_{ij}(\mathbf{r},\mathbf{r}') &= U_{\text{Skyrme}} + U_{\text{Coul}} \\ &= \frac{1}{2} t_1 \delta(\mathbf{r}-\mathbf{r}') + \frac{1}{\gamma+1} t_2 \delta(\mathbf{r}-\mathbf{r}') \rho^{\gamma-1}(\mathbf{r}) \\ &\quad + \frac{1}{2} \frac{Z_i Z_j e^2}{|\mathbf{r}-\mathbf{r}|}. \qquad (3) \end{aligned}$$

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

Subatech

$$< U(\mathbf{r_i}) > \; = \; \sum_j \int d^3r d^3r' d^3p d^3p'$$
$$U_{ij}(\mathbf{r},\mathbf{r'}) f_i(\mathbf{r},\mathbf{p},t) f_j(\mathbf{r'},\mathbf{p'},t)$$

$$< U_i(\mathbf{r_i},t) > = \alpha \left(\frac{\rho_{int}}{\rho_0}\right) + \beta \left(\frac{\rho_{int}}{\rho_0}\right)^{\gamma}$$

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

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

For the midrapidity region γ → 1. and we can apply nonrelativisitic kinematics as well

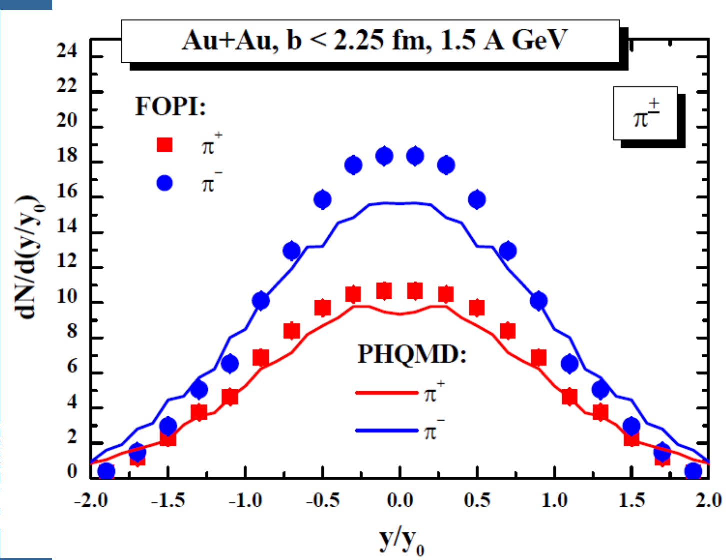
All elastic and inelastic collisions are treated as in PHSD - therefore the spectra of produced particles are very similar to PHSD results

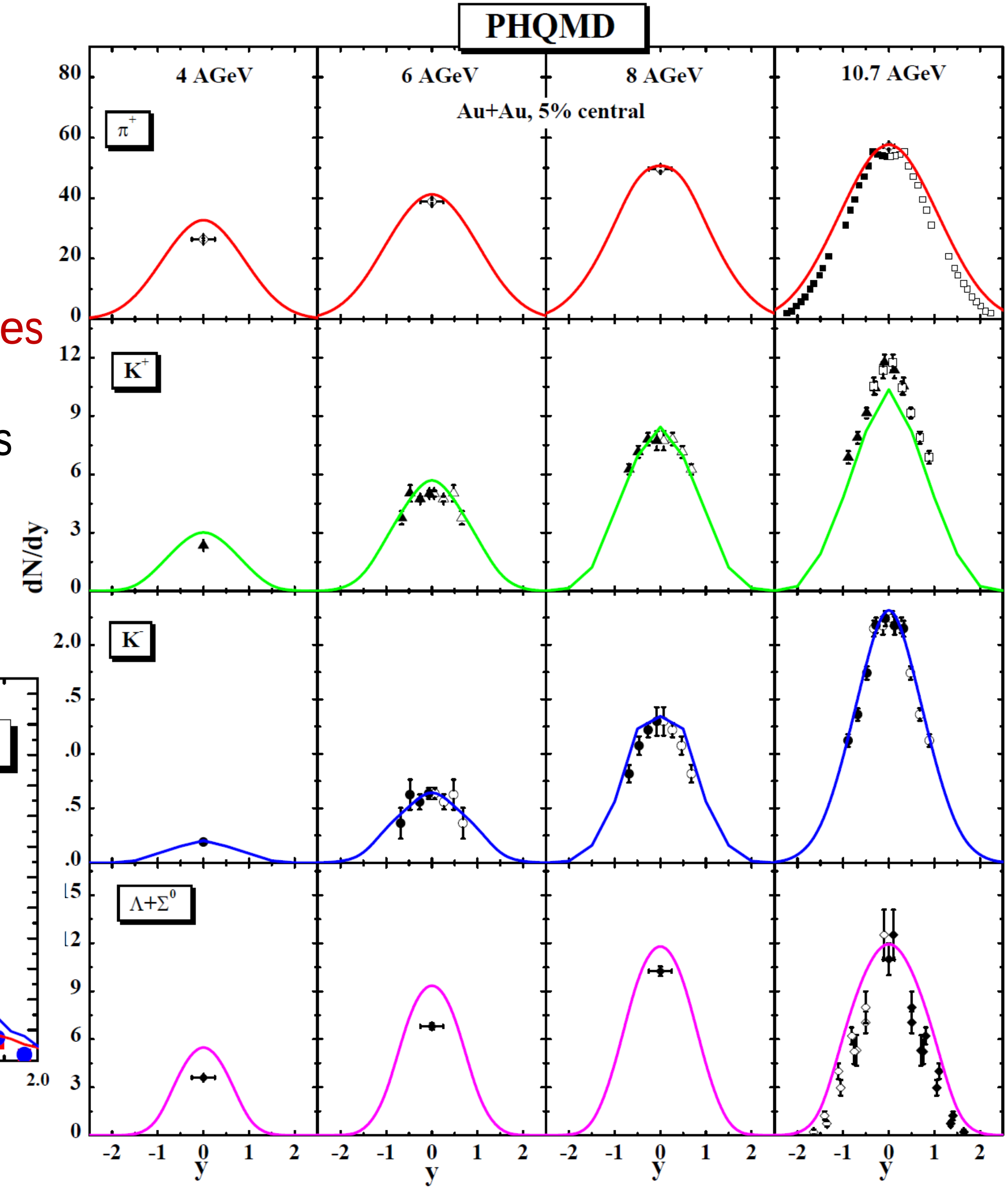
Results

First Results of PHQMD

Produced particles
are well reproduced
at SIS/NICA/FAIR energies

(dominated by collisions
→ similar to PHSD)





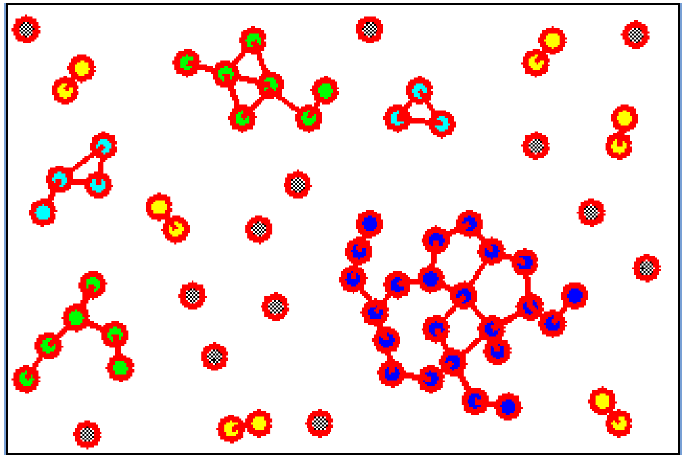
How to define fragments in transport theories which propagate nucleons?

A) 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

B) SACA and FRIGA see talk of V. Kireyev

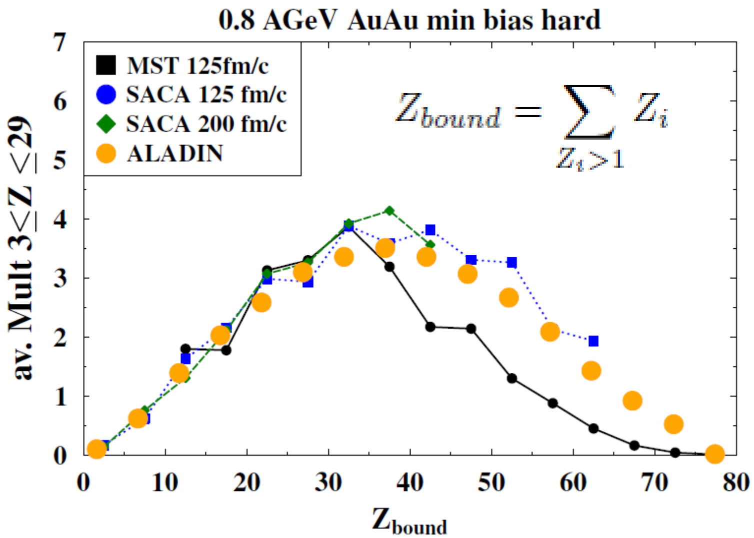
There are two kinds of fragments

- formed from spectator matter
  - close to beam and target rapidity
  - initial-final state correlations
  - HI reaction makes spectator matter unstable
    - can be identified by MST or SACA → Kireyev

- 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
    - can be only identified by MST presently
    - (quantum effects are important)

First Results of PHQMD

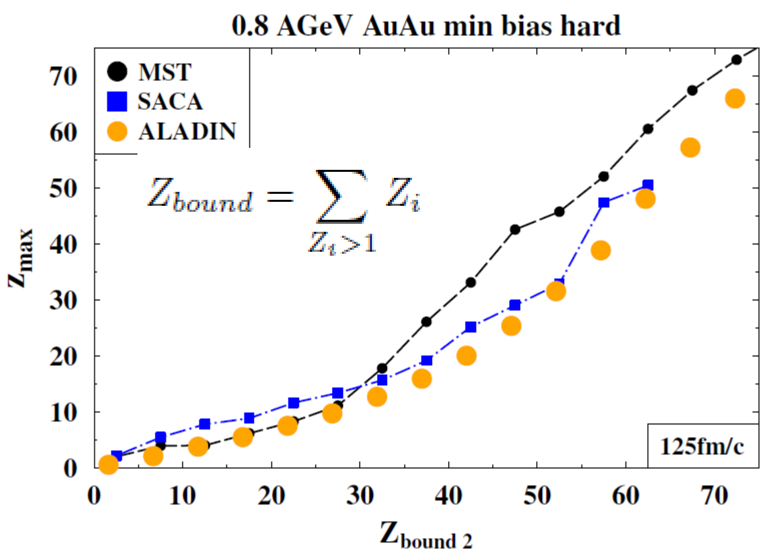
Spectator Fragments
experm. measured up to E_{beam} =1AGeV (ALADIN)

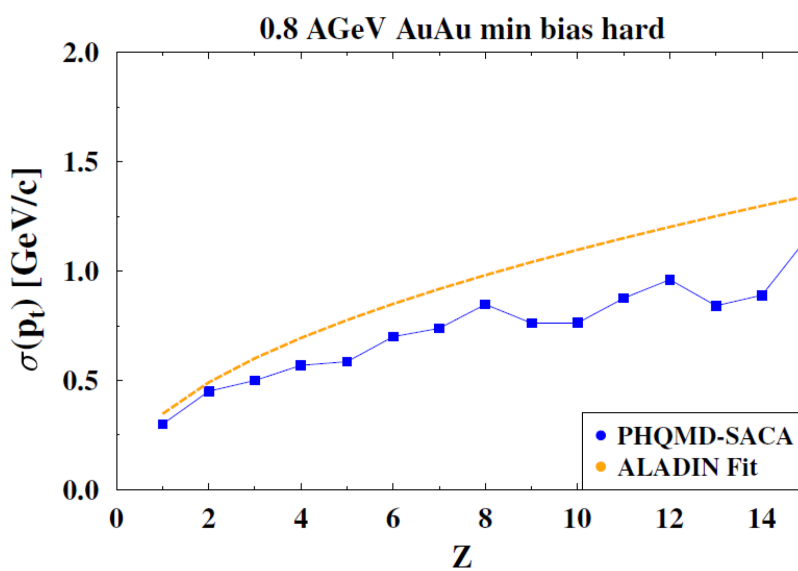


agreement for very complex fragment observables like the

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

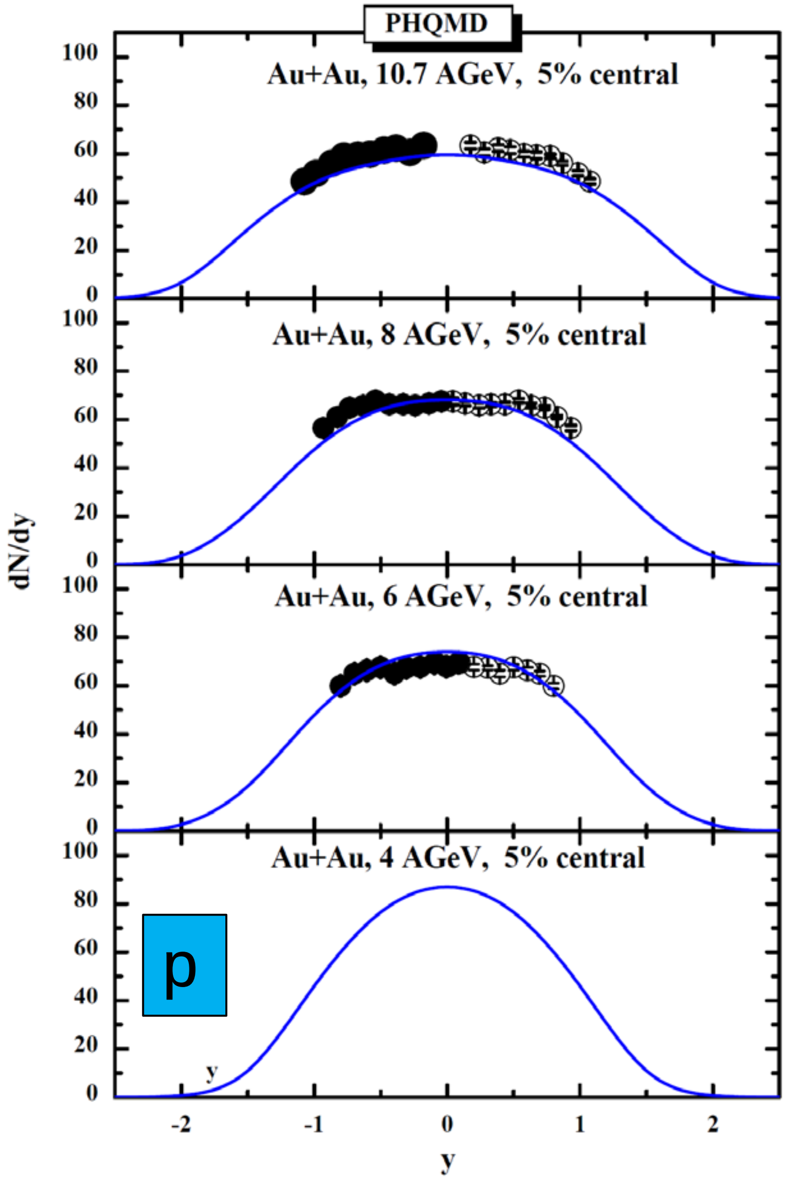
rms(p_t) shows $\sqrt{Z}$ dependence



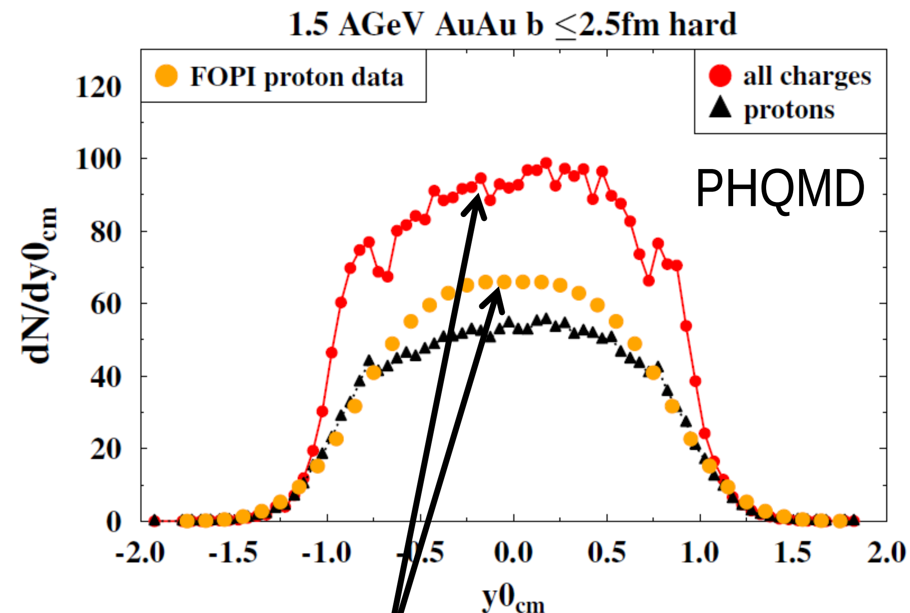


First Results of PHQMD

Protons at midrapidity well described



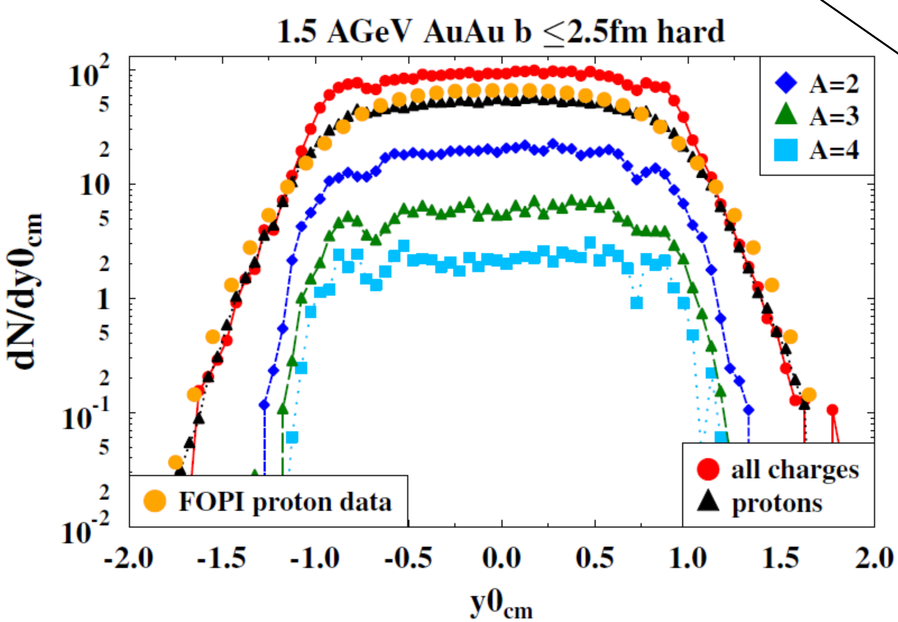
midrapidity fragment production increases with decreasing energy

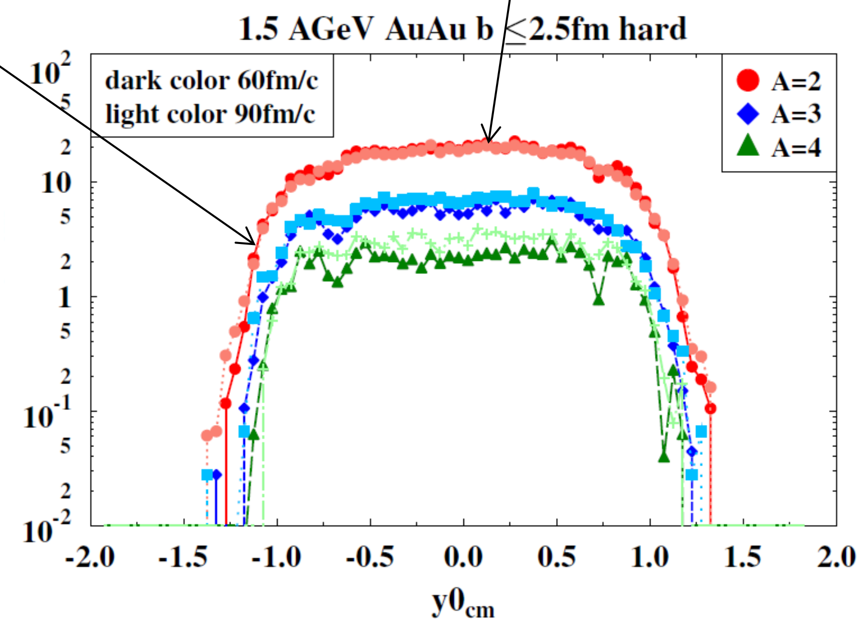


1.5 AGeV central
> 30% of protons bound in cluster

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)

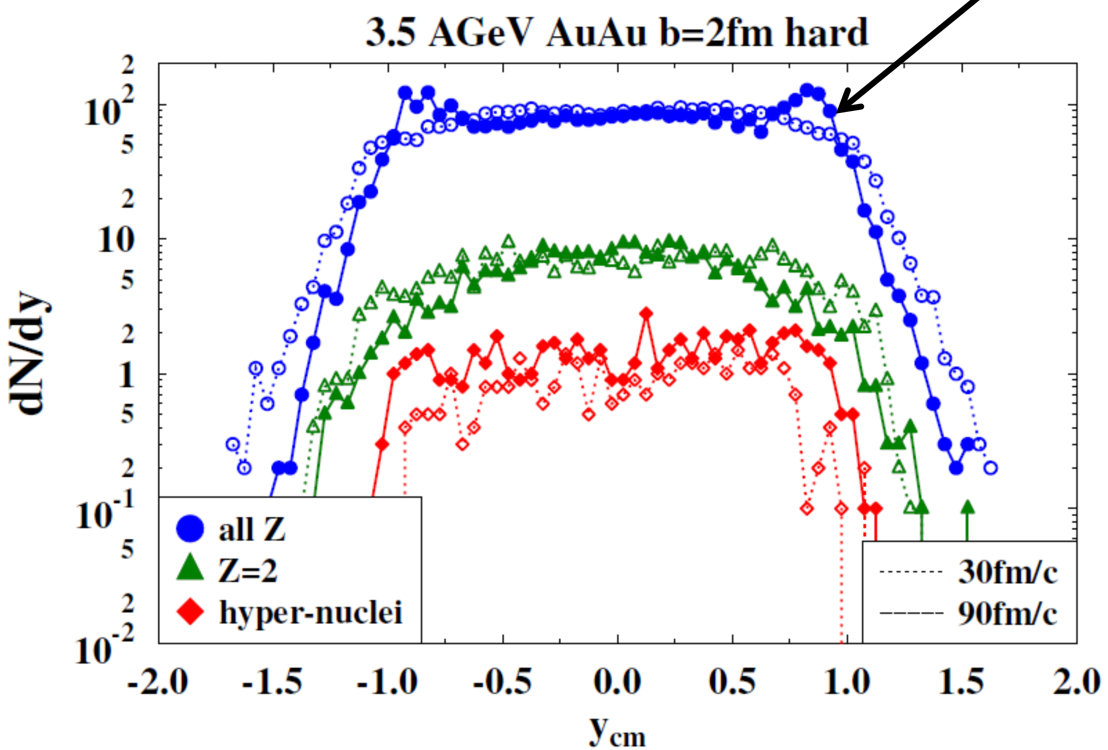




First Results of PHQMD

BMN energy

Still activity in spectator matter after 30 fm/c

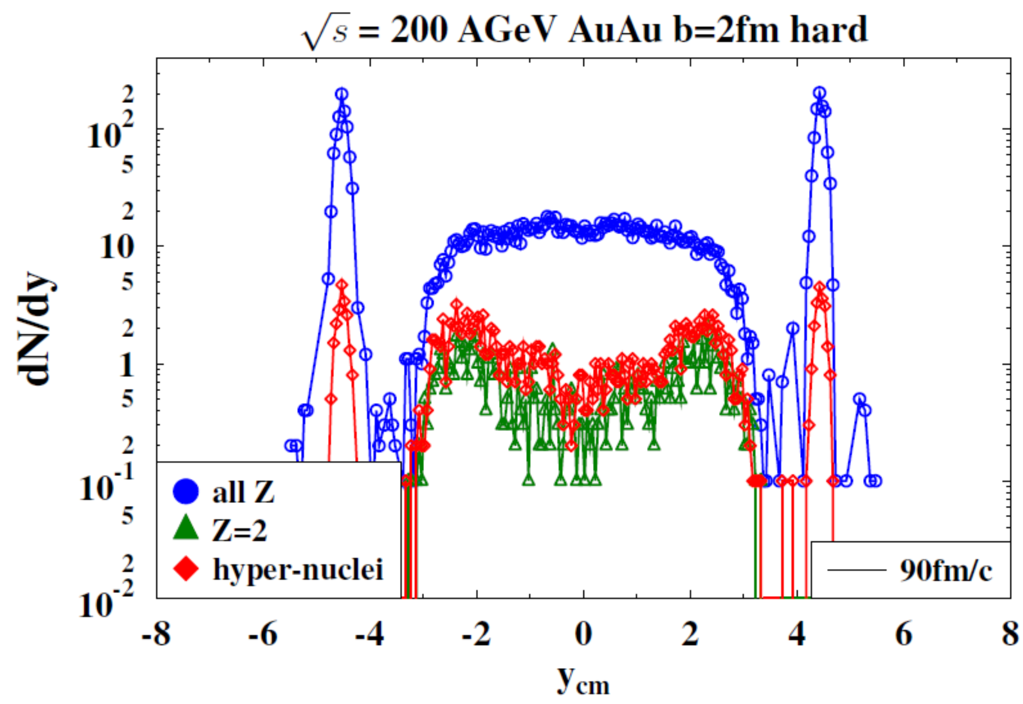


- fragments are stable from 30fm/c -> 90 fm/c
- hyper-nuclei are produced in number

First Results of PHQMD

At RHIC

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



Subatech

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

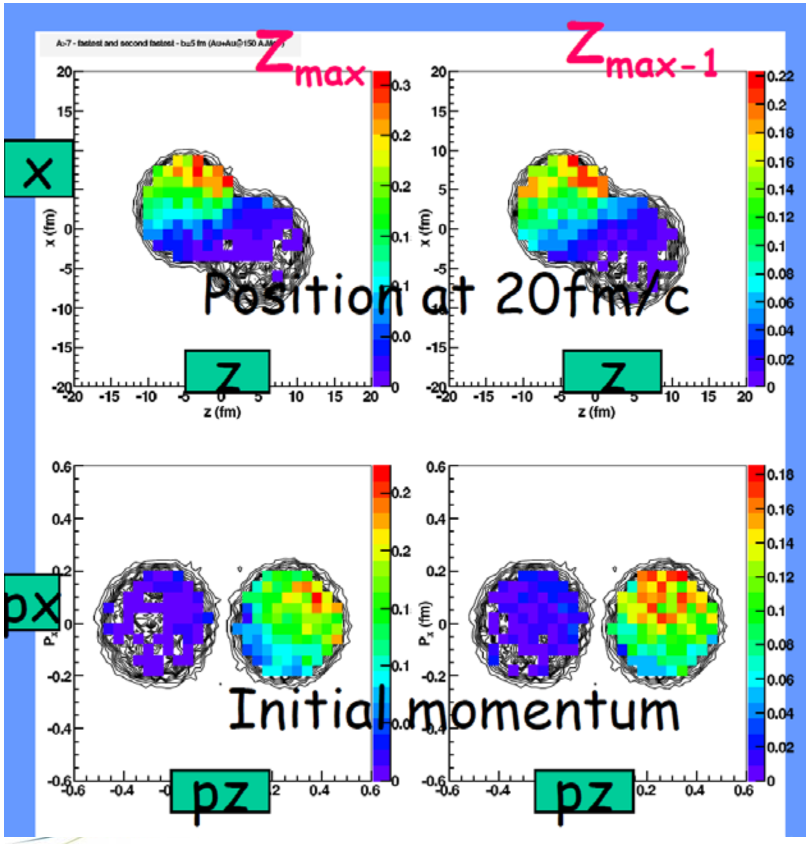
Very good agreement with the presently available fragment data as well as with the AGS single particle spectra

But a lot has still to be done!!

Back up

Fragments - the most interesting n-body observables

QMD has been constructed to study multifragmention
Fragments are N-body correlations -> not accessible in BUU



In QMD fragments are preserved initial state correlations.

Fragment nucleons come from a well defined subspace of the initially populated phase space

How to define fragments in transport theories which propagate nucleons?

History:

- Minimum spanning tree (possible at the end of the reaction)
  -> Study of fragmentation mechanism impossible
- SACA or ECRA determines fragments very early
  -> possible to study reaction mechanism
- New SACA (talk of A. LeFevre) allows for studying isotope yields and hypernuclei (including symmetry energy, pairing and shell effects)

SACA or ECRA

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

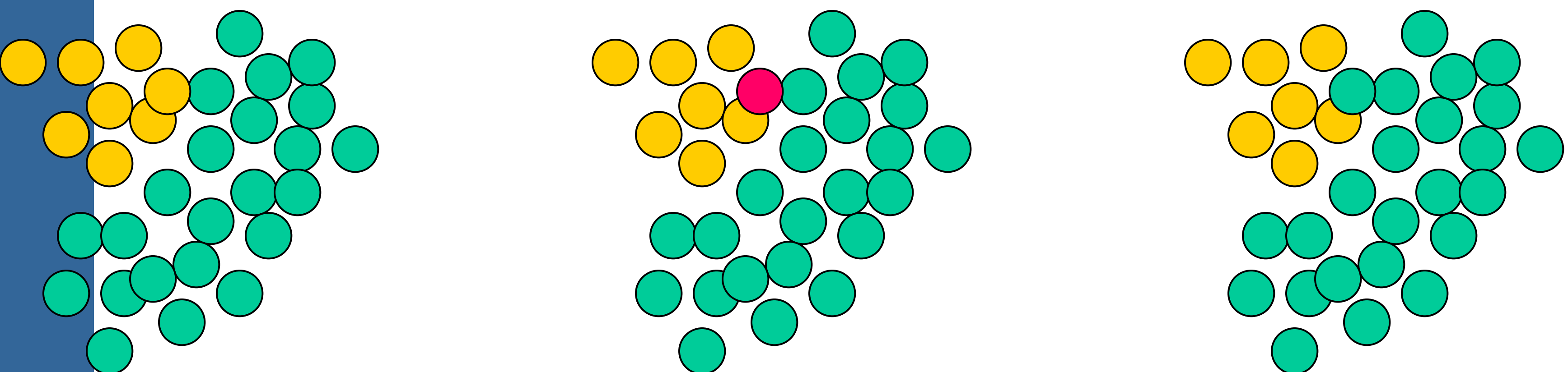
Simulations show: Clusters chosen that way at early times are the prefragments of the final state clusters because fragments are not a random collection of nucleons at the end but initial-final state correlations

How does this work?

Simulated Annealing Procedure: PLB301:328,1993
later SACA

Take randomly 1 nucleon out of a fragment

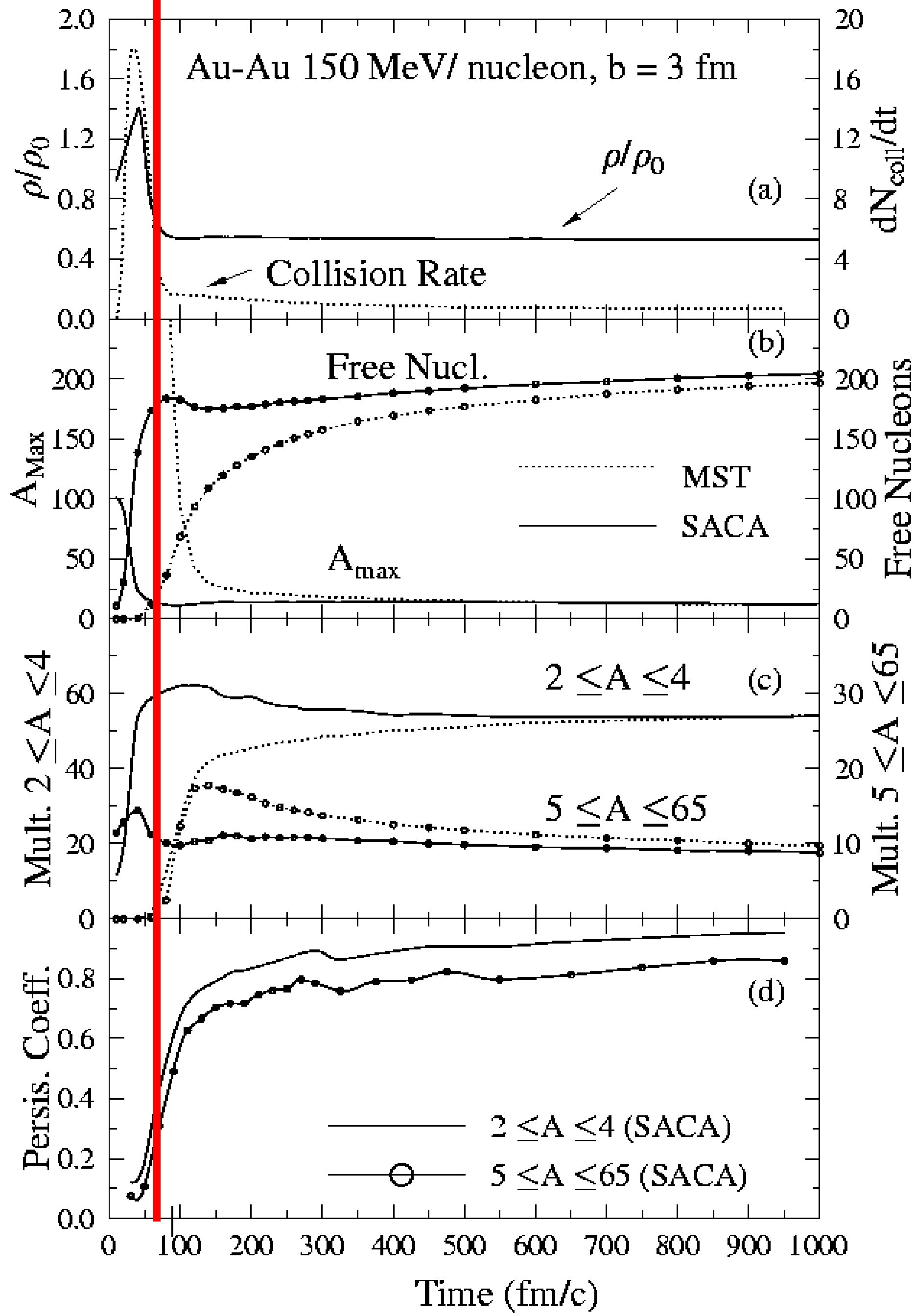
Add it randomly to another fragment



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

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

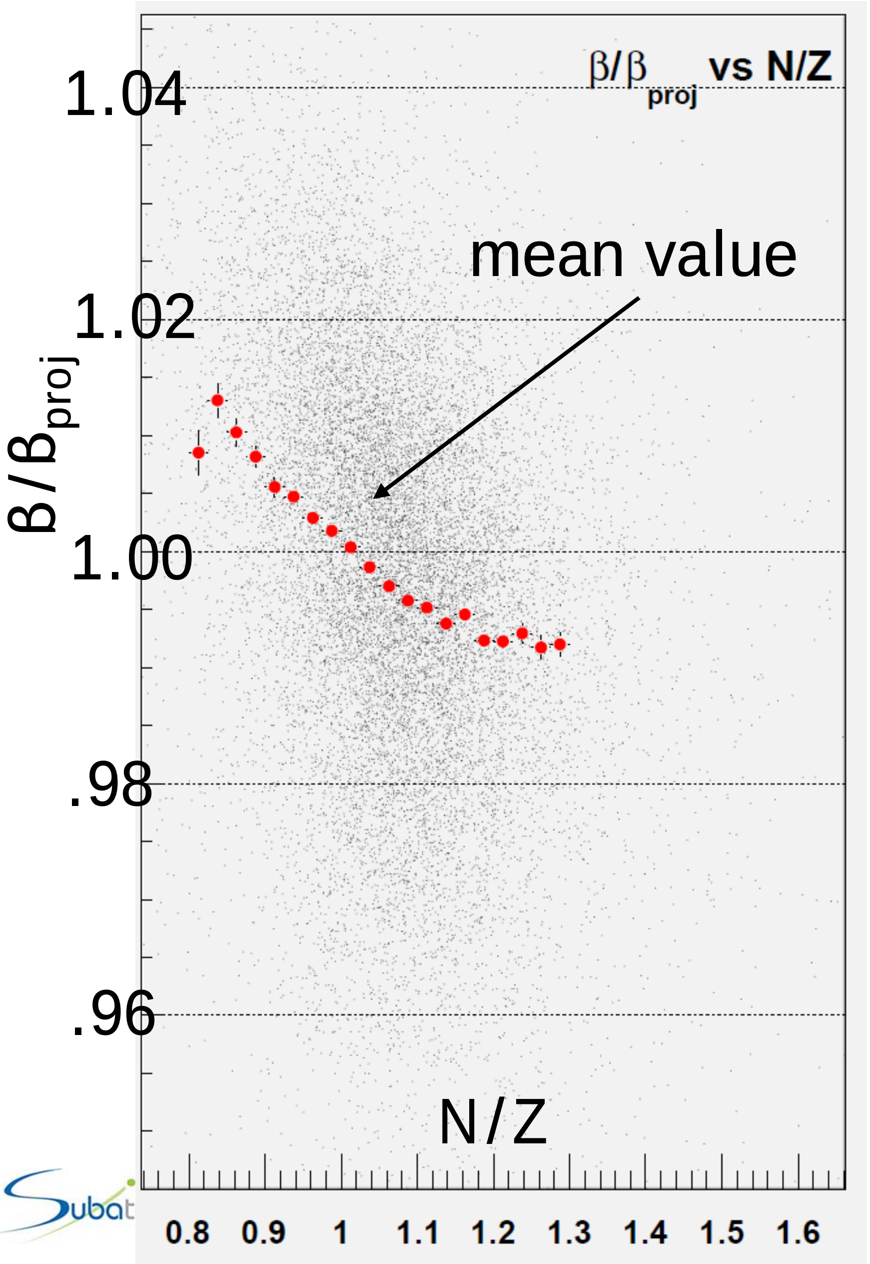
If E’ < E take the new configuration
If E’ > E take the old with a probability depending on E’-E
Repeat this procedure very many times
→ Leads automatically to the most bound configuration



ECRA or SACA 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 60 fm/c Amax and multiplicities of intermediate mass fragments are determined

Evidence for early cluster formation



Fragment separator
Strong correlation between β/β_{proj} and N/Z
Aladin supports this (LeFevre)

Can only be explained if fragments are formed early and gets therefore full Coulomb boost

Statistical models cannot at all explain this result

Fluctuations due to collision term

The collisions term causes fluctuations (in density and momentum space) because it removes particles from their phase space cell

In BUU these fluctuations are 1/N times smaller than in QMD and therefore negligible for large N (number of test particles)

In QMD these fluctuations are responsible for fragmentation (especially for spectator fragmen. dominant for E> 100 AMeV)

(and also for single nucleon spectra because one has to subtract fragment nucleons to obtain measured single part spectrum)

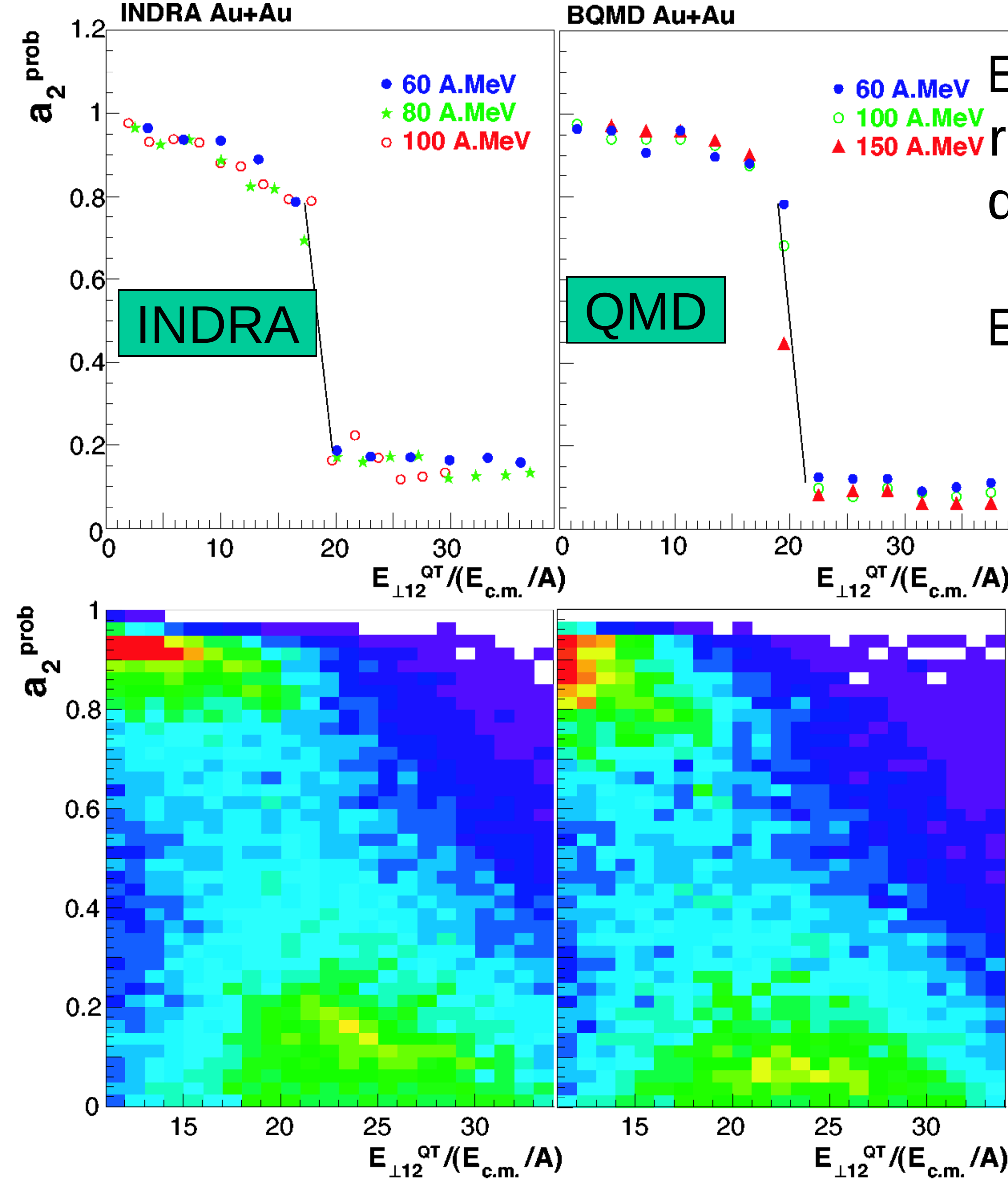
Because fluctuations are important: attempts to introduce additional fluctuations in BUU

- 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 ($1/\sqrt{N}$) 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.)

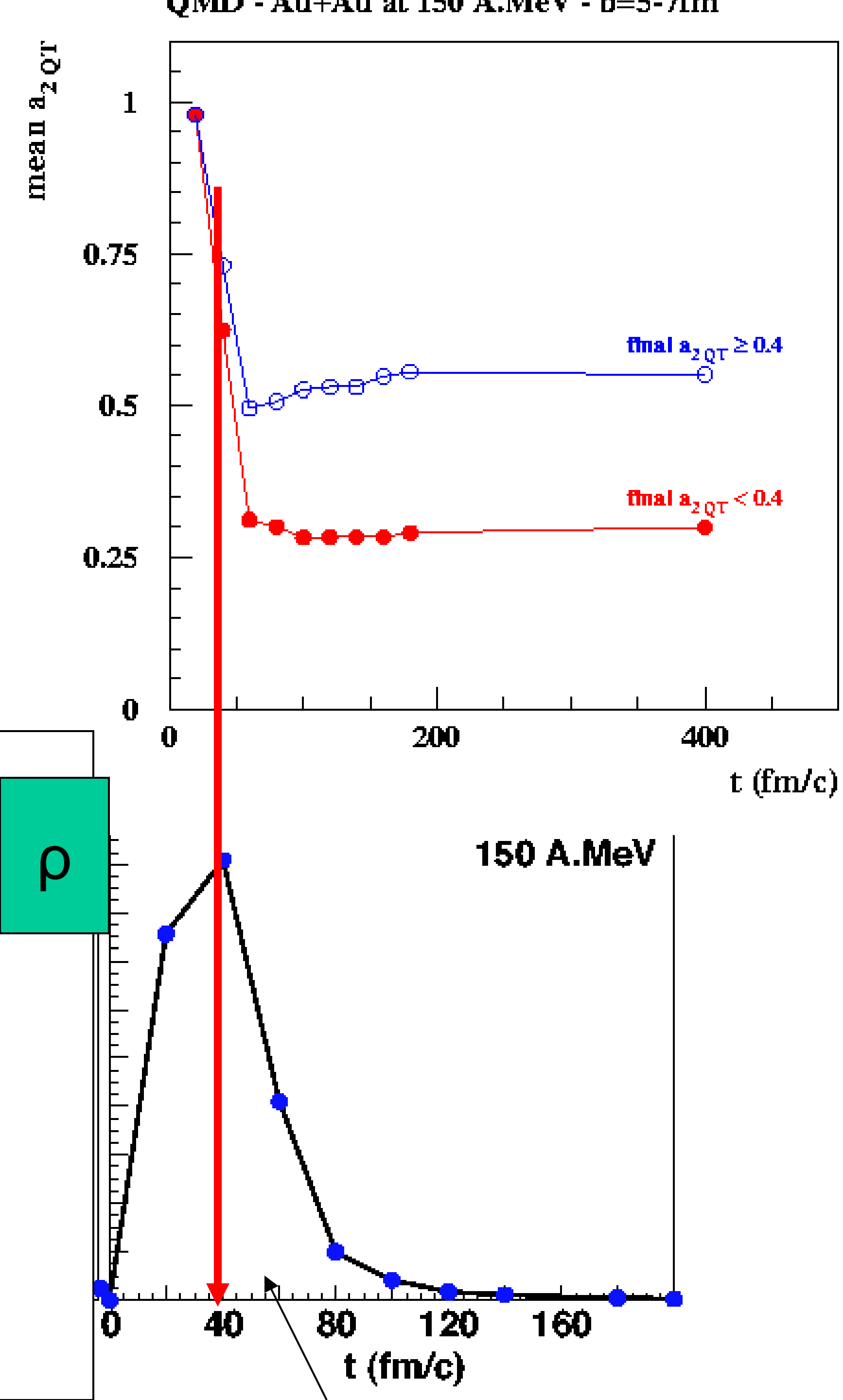


Early fragment formation reproduces data quantitatively

Example: Bimodality

$$a_{2(t)} = \frac{Z_{max(t)} - Z_{max-1(t)}}{Z_{max(t)} + Z_{max-1(t)}}$$

mean value
as well as
the distribution
(arXiv:0708.3639)



With ECRA we can trace back the fragment formation
Can calculate $a_2(t)$

$$a_{2(t)} = \frac{Z_{\max(t)} - Z_{\max-1(t)}}{Z_{\max(t)} + Z_{\max-1(t)}}$$

Fragment pattern is created very early

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

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

Where L shows up in the observables?

- initially the average over many simulations gives the same ρ(r) as BUU '`d^{3}pf (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)

The QMD trial wavefct eq. (1) yields

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

very similar to classical Hamilton eq. (H-><H>)
AMD/FMD equations much more complicated

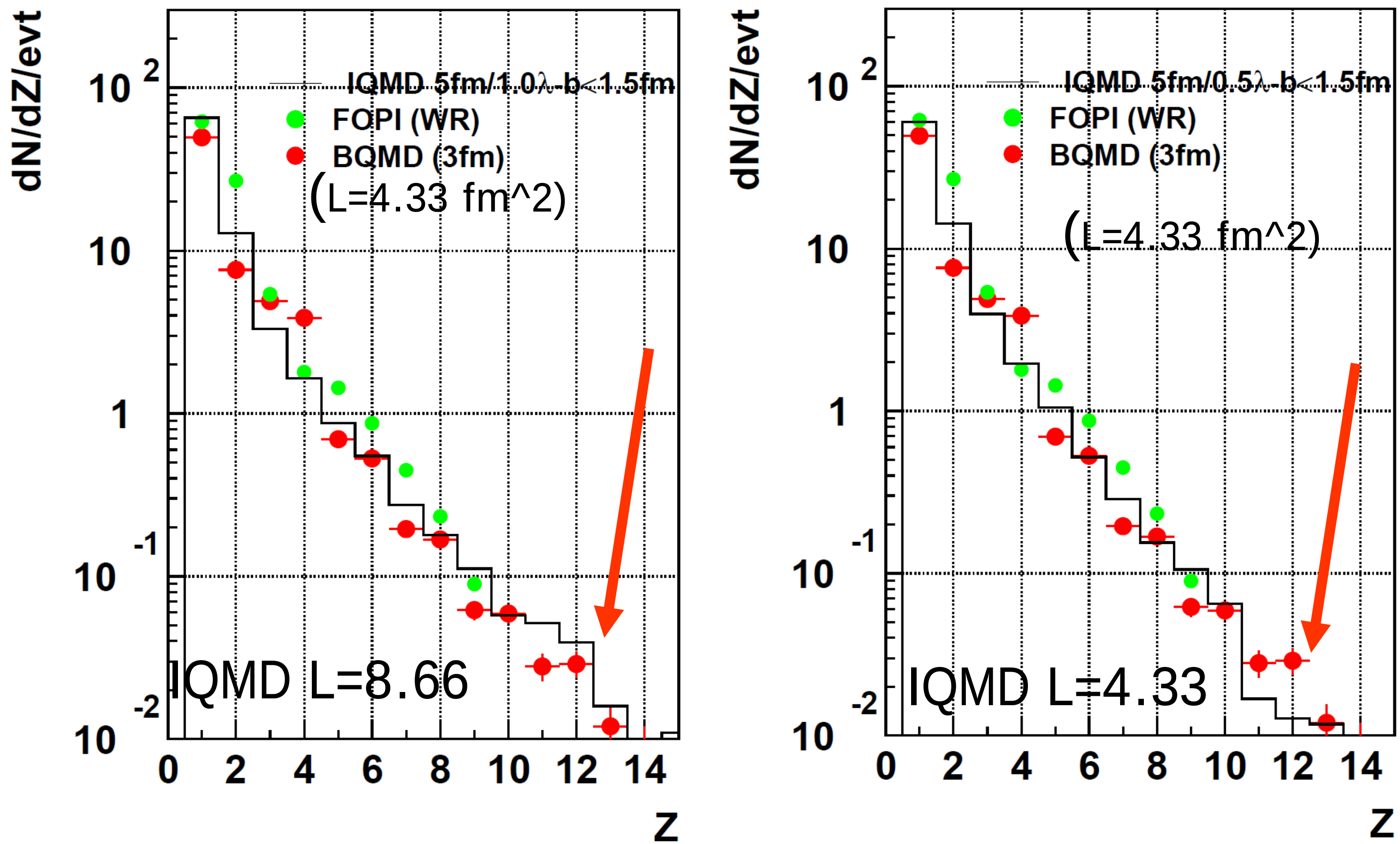
Of course trial wavefct is our choice and nothing prevents us to assume that also the width L is time dependent.

In QMD L is assumed to be constant

It's value has not changed since the first publication in 1985

Influence of L on fragment yield (Y. Leifels)

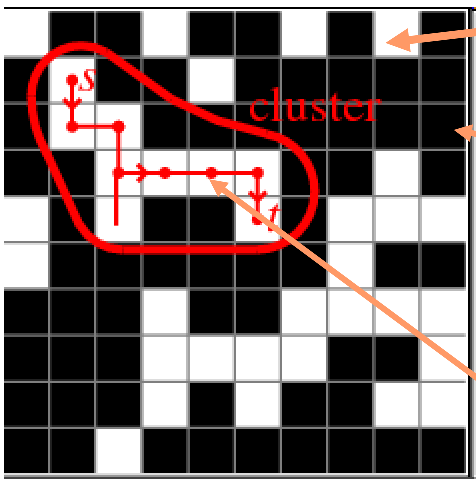
AuAu 150 AMeV



There are differences but they are modest

How one should this imagine?
Easiest Way: percolation model (Bauer)

Divide the nucleus in phase space cells. Inside the nucleus initially all cells are filled by a nucleon.



Filled cell (model in 2 dim)

Collisions with large mom transfer between proj and targ nucleons remove nucleons from their orig.cells

Connected occupied cells become prefragments

Completely opposite to statistical models:
No initial final state correlations, nucleons are formed very late at densities less than < 0.2 ρ_0.

Collisions in BUU and QMD

BUU and QMD describe the (measured) one particle density

$$\rho(r) = \int d^3p\, f(r;p;t) = \cdots = \sum_{i=1}^{N} \phi_i(r;t)$$

BUU QMD

and the measured Fermi distribution with

$$\phi_i(r; r_{i0}(t); p_{i0}(t); t) = \exp[-(r - r_{i0}(t) - p_{i0}(t)t/m)^2/4L] \cdot \exp[i(p_{i0}(t)(r - r_{i0}(t)) - p_{i0}(t)^2 t/2m]$$

Therefore $f(r;p_1;t) f(r;p_2;t) \sigma(p_1;p_2 \to p_3;p_4)$ is the same and consequently the collisions should be very similar

Parallel ensemble method: subroutines are even identical

BUT: In AMD and FMD cross section cannot be defined that way -> FMD: no coll, AMD rather arbitrary

Summary

BUU/LV/VUU

$f(r_1; p_1; t) = f^{(1)}$

Can predict correlations only if

$$f^{(2)} = f^{(1)} f^{(1)}$$

- deuteron density if neutron dens*proton dens (what is rarely the case)
- if the system is in global equilibrium

QMD/IQMD/AMD

$f^{(N)}(r_1; r_2; ::r_N; p_1; p_2; ::p_N; t) = f^{(N)}$

Can predict any correlation

$$f^{(2)} = \int \prod_{i=3}^{N} d^3r_i \, d^3p_i \, f^{(N)}$$

allows predictions of fragments

HBT correlations

Parameters: grid size (BUU/LV/VUU); width L (QMD/IQMD/AMD)

consequences: Trento workshop

We expect that

- 1 body observables like (p,n),Λ,K,π spectra are identical
  This has extensively been checked (Init. Fluc not important)
- N body observables differ

PHQMD