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

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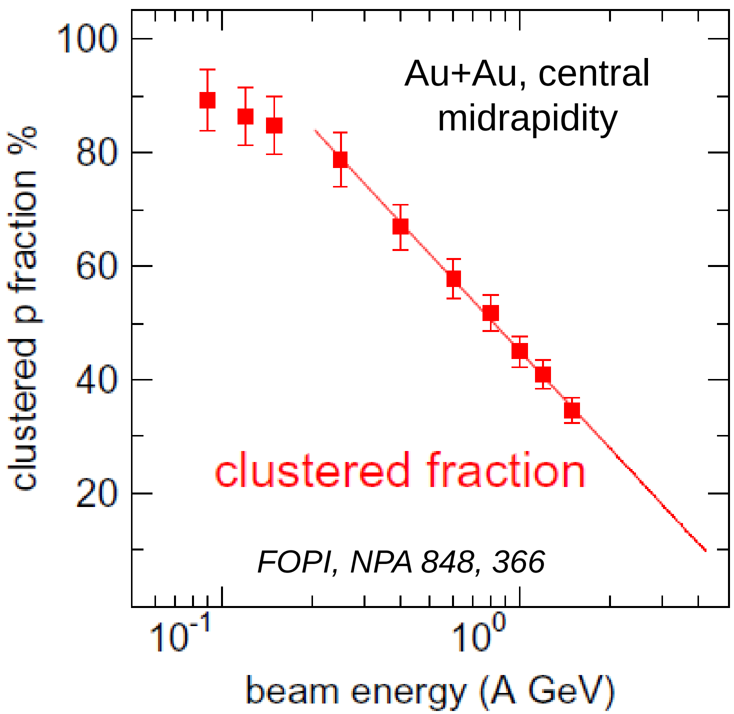
(E. Bratkovskaya, A. LeFèvre, Y. Leifels , V. Kireyev, V. Voronyuk)

- ❑ Why a novel approach?
- ❑ Basics of the QMD Transport theory
- ❑ Inherent Fluctuations and Correlations in QMD
- ❑ Fragment Formation

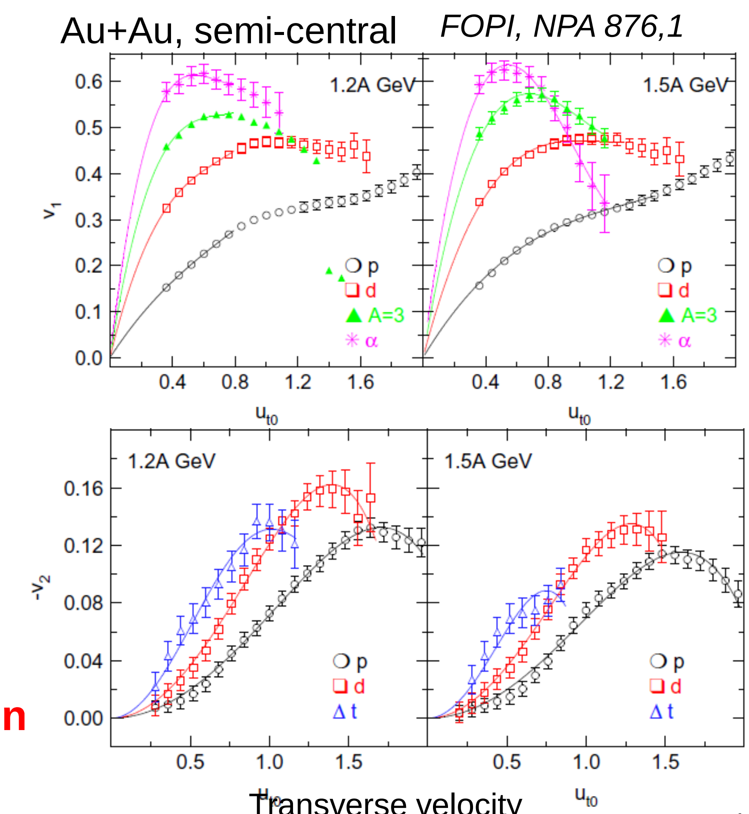
- ❑ Comparison with existing data
- ❑ Perspectives for BMN/NICA/FAIR/RHIC

Subatech

Clusters in HICs



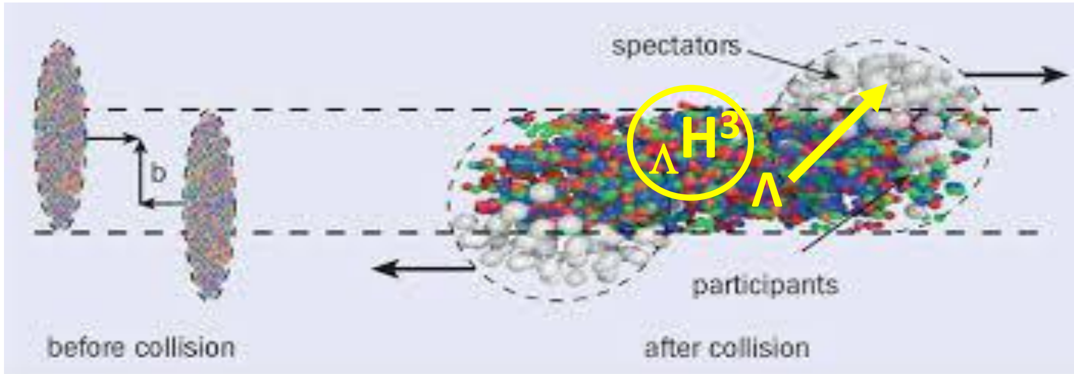
- Clusters are very **abundant at low energy;**
- at **3 AGeV** in central Au+Au collisions ~**20% of the baryons are in clusters!**
- … and baryons in clusters have quite different properties (v_1, v_2, dn/dp_T)



➔ **Understanding of cluster formation is needed**

- **for proper description of nucleon observables (v_1, v_2, dn/dp_T)**
- **to explore new physics opportunities like**
  - **hyper-nucleus formation**
  - **possible signals of the 1st order phase transition**
  - **cluster formation at midrapidity (RHIC, LHC)**

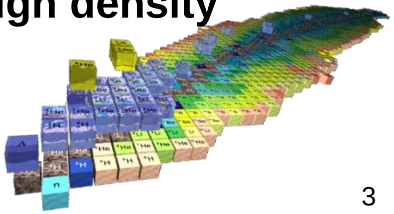
Why do we study especially hypermatter production?



- **Access to the nuclear dynamics:**
  different mechanisms for hypernucleus production vs. rapidity:
  - at mid-rapidity : Λ-coalescence - hypernuclei test the phase-space distribution of baryons in the expanding participant matter
  - at target/projectile y: Λ-absorption by spectators - elucidates the physics at the interface between spectator and projectile matter

Hypernuclei as bound objects:

- **give access to the third dimension of the nuclear chart (strangeness)**
- **give information on hyperon-nucleon and hyperon-hyperon interactions**
- **important e.g. for neutron stars (production of hypermatter at high density and low temperature)**
- **new field of hyperon spectroscopy**



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Modelling of fragment and hypernucleus formation

Present microscopic approaches:

- **VUU(1985), BUU(1985), (P)HSD(96), SMASH(2016) solve the time evolution of the one-body phase-space density in a mean field→ no dynamical fragments**
- **UrQMD is a n-body model but makes clusterization via coalescence and a statistical fragmentation model**
- **QMD is a n-body model but is limited to energies < 1.5 AGeV**
  → describes fragments at SIS energies,
  but conceptually not adapted for NICA/FAIR energies and higher

In order to understand the cluster formation from a microscopic origin one needs:
- **a realistic model for the dynamical time evolution of HICs**
- **dynamical modelling of cluster formation based on interactions**

Dynamical modelling of cluster formation is a complex task which involves: the fundamental nuclear properties, quantum effects, variable timescales

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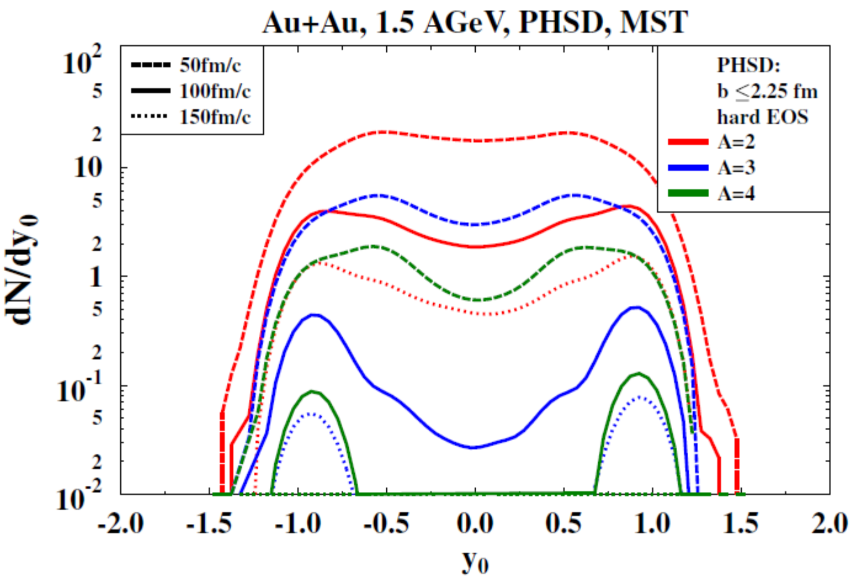
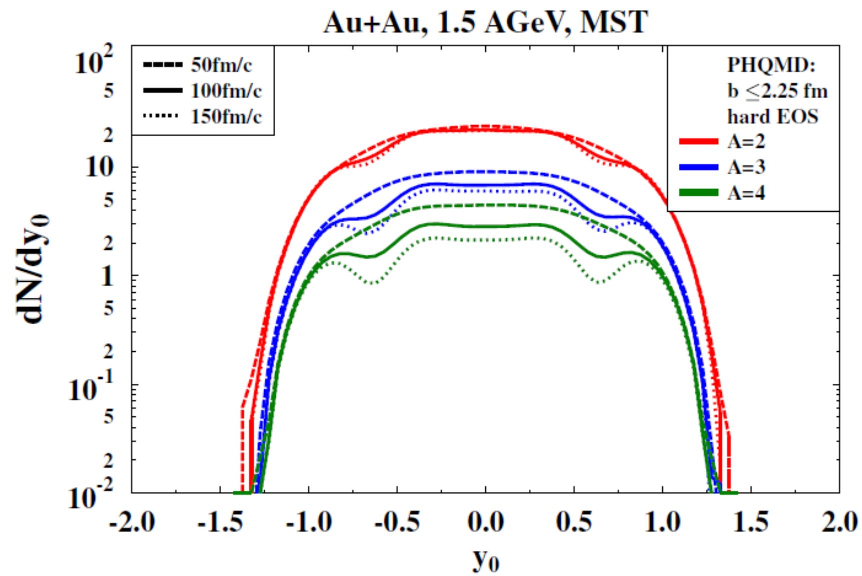
Time dependence of cluster formation: QMD vs. MF

mean field propagation



QMD propagation



QMD propagation: **number of clusters are stable vs. time**
(MST finds at 50 fm/c almost the same clusters as at 150fm/c)

MF propagation:
- -- **number of fragments strongly time dependent**
- -- **fragments disappear with time**
- -- **midrapidity fragments disappear early, projectile/target fragments later**
  → **no common time for coalescence**

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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 the lowest energy expectation value:

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

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

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 !!)

The PHQMD approach is designed to fill this gap

- still under construction
  but
- validated by comparison with experiments
  and other transport approaches
- first pertinent results available

PHQMD

The goal: to develop a **unified n-body microscopic transport approach** for the description of heavy-ion dynamics and dynamical cluster formation from low to ultra-relativistic energies

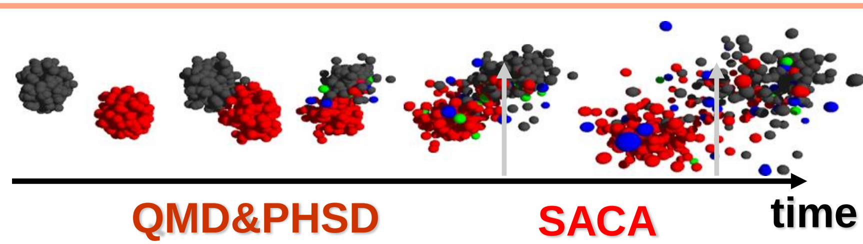
Realization: combined model **PHQMD = (PHSD & QMD) & SACA**

Parton-Hadron-Quantum-Molecular Dynamics

Initialization → propagation of baryons:
QMD (Quantum-Molecular Dynamics)

Propagation of partons (quarks, gluons) and mesons
+ collision integral = interactions of hadrons and partons (QGP)
from PHSD (Parton-Hadron-String Dynamics)

Clusters recognition:
SACA (Simulated Annealing Clusterization Algorithm)
vs. MST (Minimum Spanning Tree)



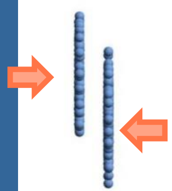
Parton-Hadron-String-Dynamics (PHSD)

collision integral → PHQMD

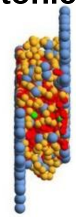
PHSD is a **non-equilibrium microscopic transport approach** for the description of **strongly-interacting hadronic and partonic matter** created in heavy-ion collisions

Dynamics: based on the solution of **generalized off-shell transport equations** derived from Kadanoff-Baym many-body theory

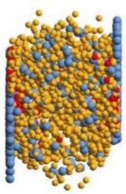
Initial A+A collision



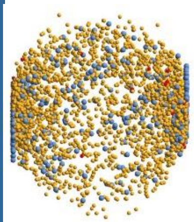
Partonic phase



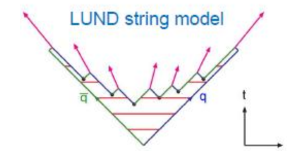
Hadronization



Hadronic phase

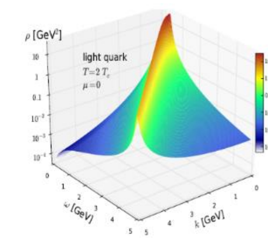


- ❑ **Initial A+A collisions** :
  N+N → string formation → decay to pre-hadrons + leading hadrons



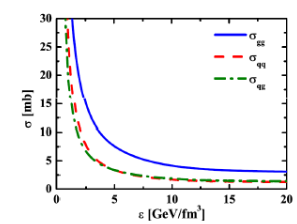
- ❑ **Formation of QGP stage** if local $\varepsilon > \varepsilon_{critical}$:
  dissolution of pre-hadrons → partons

- ❑ **Partonic phase - QGP:**
  QGP is described by the Dynamical QuasiParticle Model (DQPM) matched to reproduce lattice QCD EoS for finite T and μ_B (crossover)

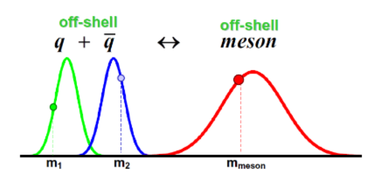


- Degrees-of-freedom: strongly interacting quasiparticles: massive quarks and gluons (g,q,q_{bar}) with sizeable collisional widths in a self-generated mean-field potential

- Interactions: (quasi-)elastic and inelastic collisions of partons



- ❑ **Hadronization** to colorless off-shell mesons and baryons:
  Strict 4-momentum and quantum number conservation



- ❑ **Hadronic phase: hadron-hadron interactions – off-shell HSD**

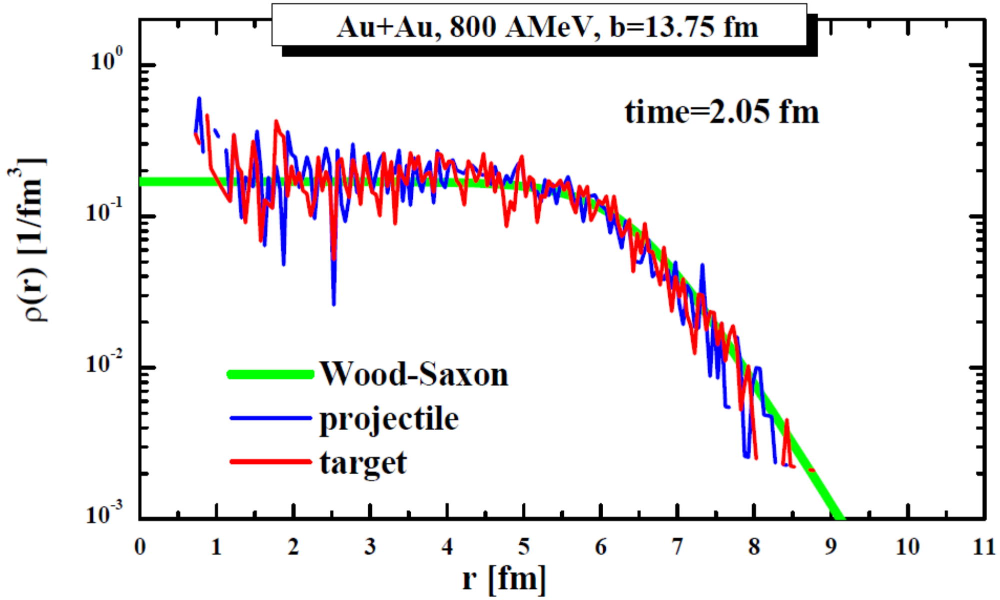
W. Cassing, E. Bratkovskaya, PRC 78 (2008) 034919; NPA831 (2009) 215; W. Cassing, EPJ ST 168 (2009) 3

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

above ε=0.5 GeV/fm³ transition to QGP like in PHSD

Below:

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 the 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

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

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

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

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

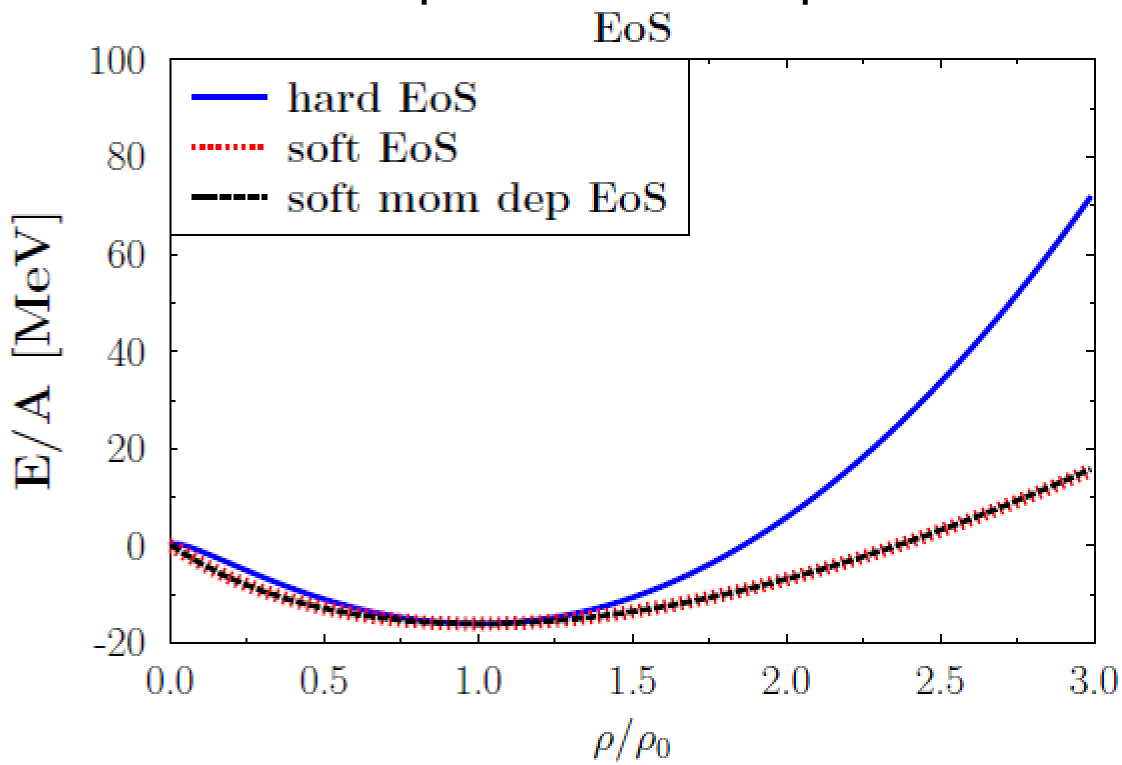
$$\rho_{int}(\mathbf{r_i},t) \rightarrow C\sum_j \left(\frac{4}{\pi L}\right)^{3/2} e^{-\frac{4}{L}(\mathbf{r_i^T}(t)-\mathbf{r_j^T}(t))^2}$$
$$\cdot e^{-\frac{4\gamma_{cm}^2}{L}(\mathbf{r_i^L}(t)-\mathbf{r_j^L}(t))^2}.$$

For the midrapidity region γ → 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 (however initial distribution is different in PHSD and PHQMD)

How to fix the strength of the potential?

In infinite matter a potential corresponds to an equation of state (EoS)



Equation of state cannot be calculated:
Brückner G-matrix is a low density expansion:
Expansion parameter : $a \cdot k_F$ a=hard core range (.6 *fm*)

$$k_F = p_F/\text{hbar} = 1.28\,(\rho/\rho_0)^{1/3}\,\frac{1}{fm}$$

fixing by experiments (K^+, v_1, v_2, cluster……)

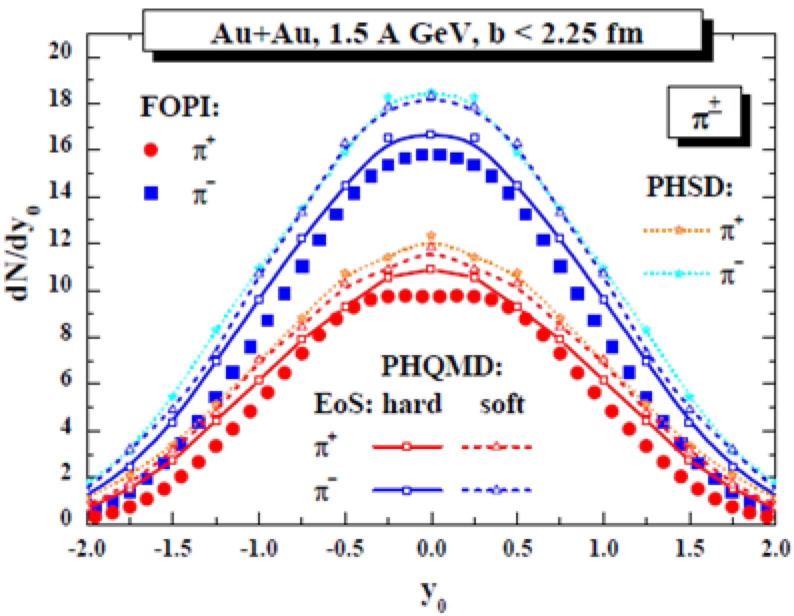
Results

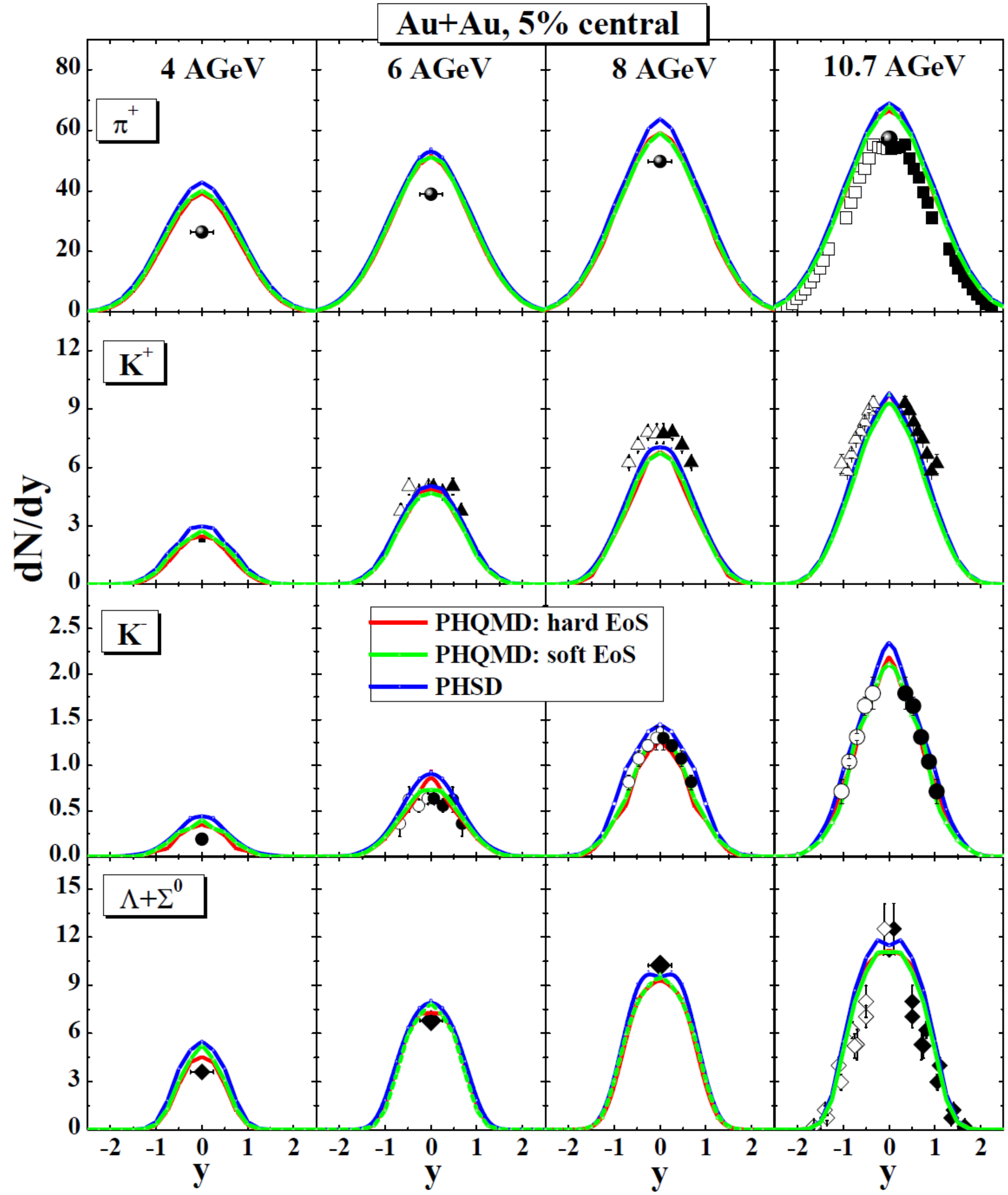
First Results of PHQMD

Produced particles

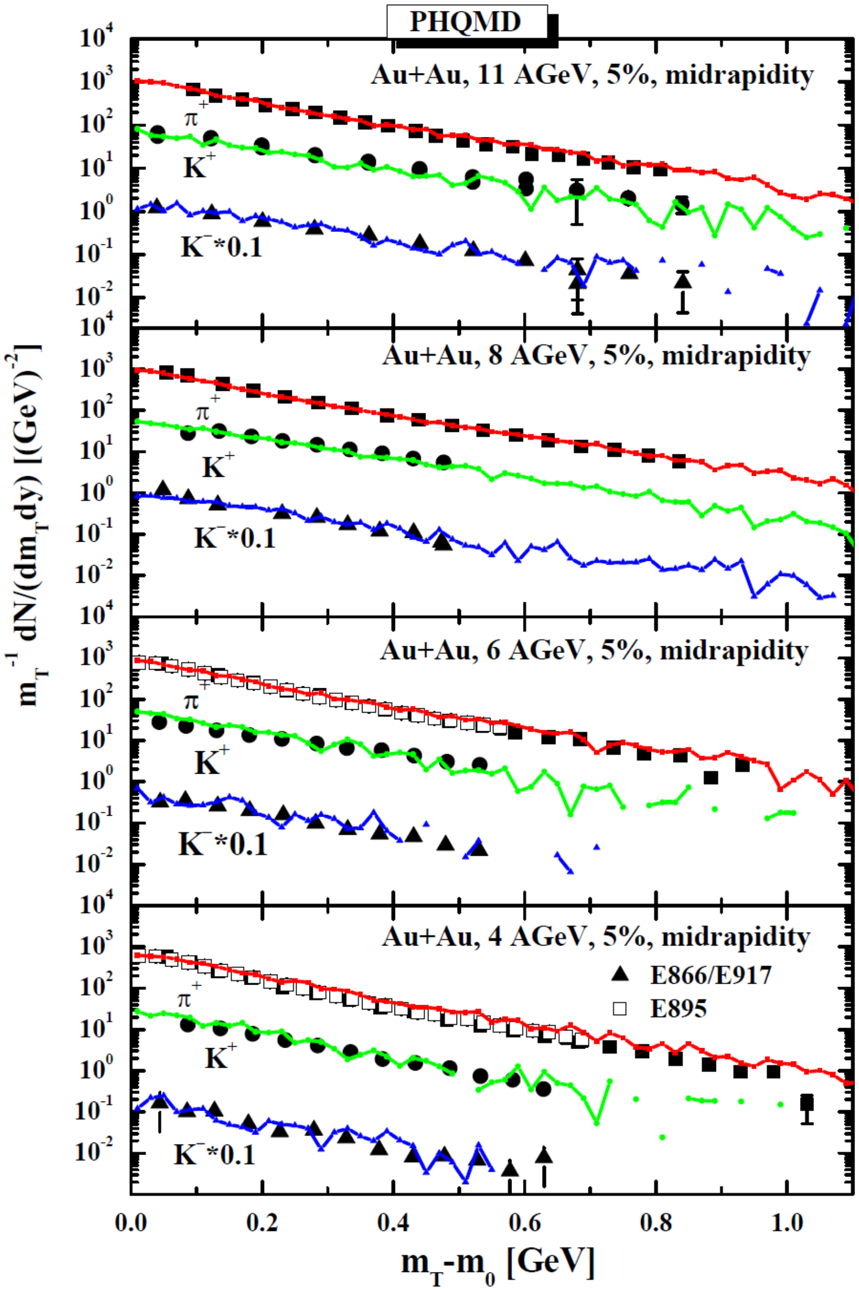
are well reproduced
at SIS/NICA/FAIR energies

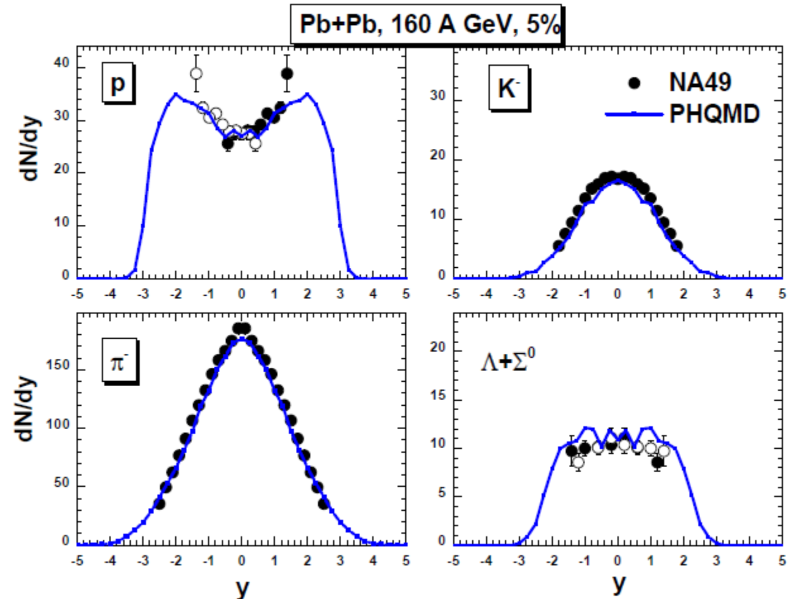
(dominated by collisions)

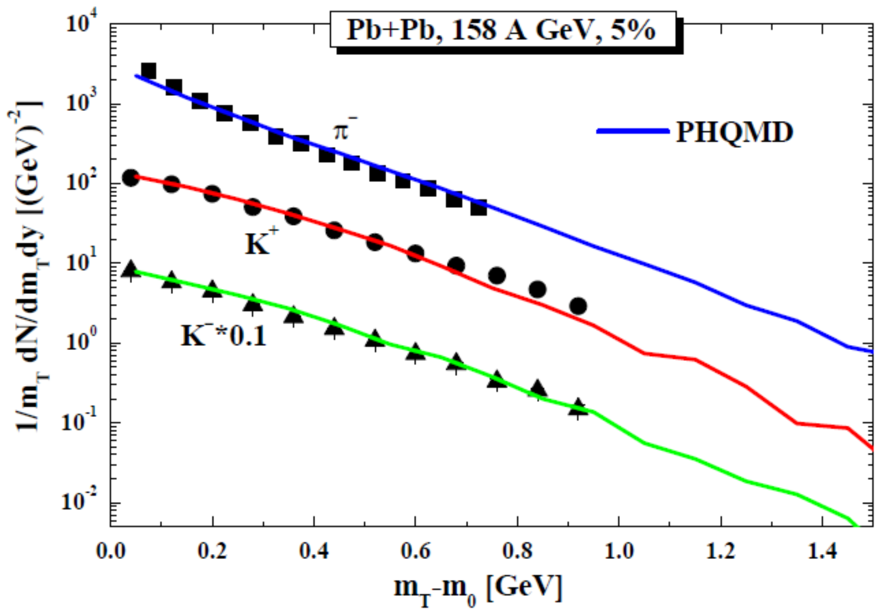




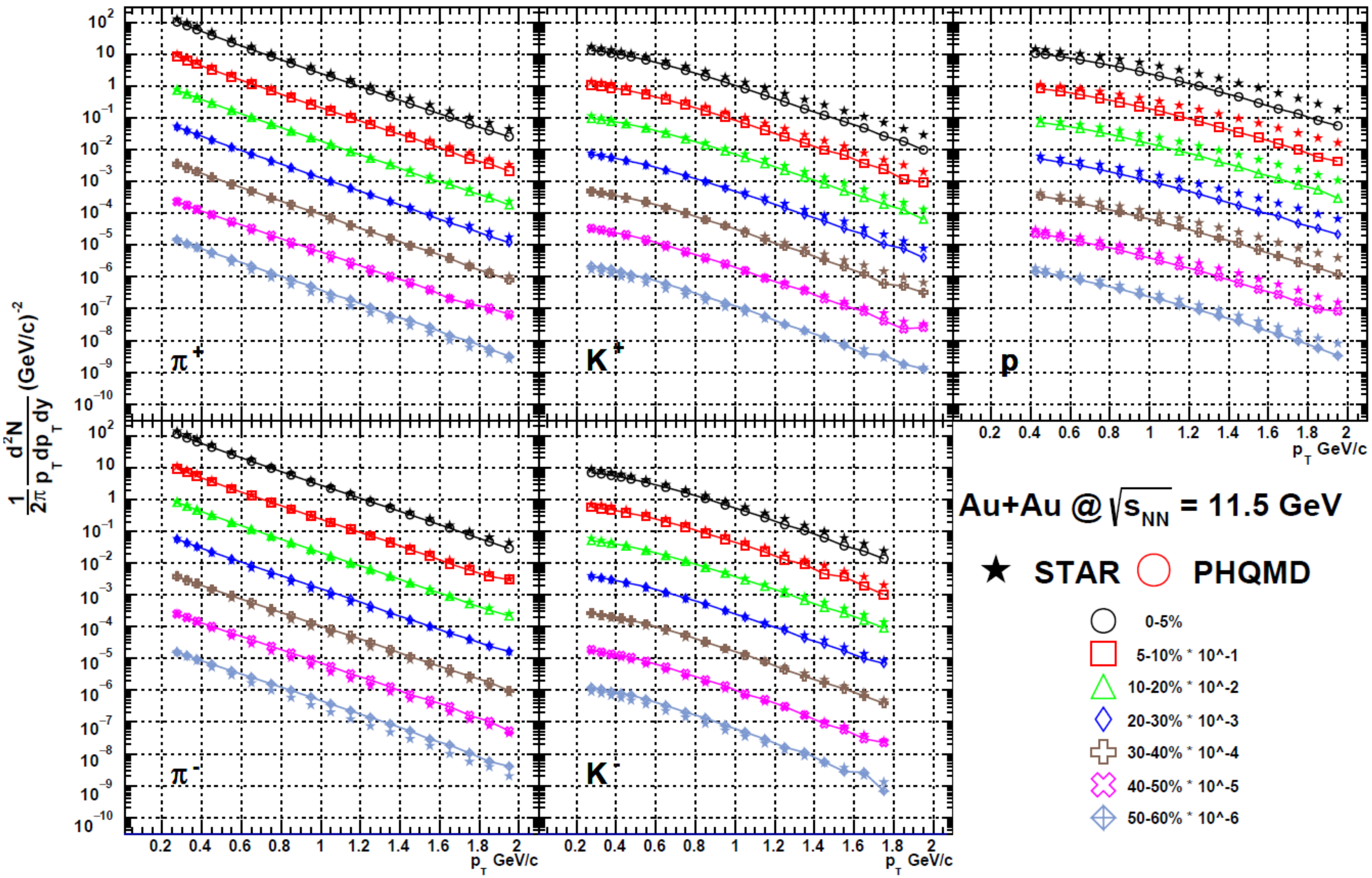
As well as at SPS energies







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



Methods to identify fragments in theories which propagate nucleons:

Static approaches:

means fragment multiplicity determined at a fixed time point

-- coalescence (early, assumption: no coll. later)

-- statistical model (V,T,N) very late $\rho << \rho_0$

Dynamical approaches:

means fragment multiplicity is fct. of time

-- minimum spanning tree (correlation in coord. space)

-- simulated annealing (correlation in mom and coord. space)

-- time dep. perturbation theory using Wigner densities

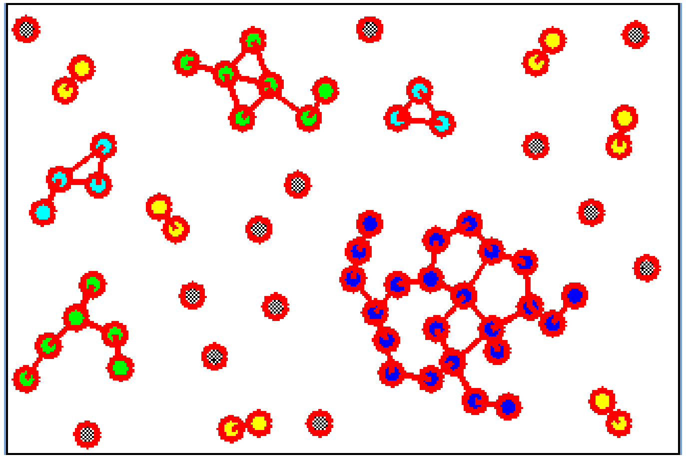
I. Minimum Spanning Tree (MST) is a cluster recognition method applicable for the (asymptotic) final state where coordinate space correlations may only survive for bound states.

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 preclusters of the final state clusters.

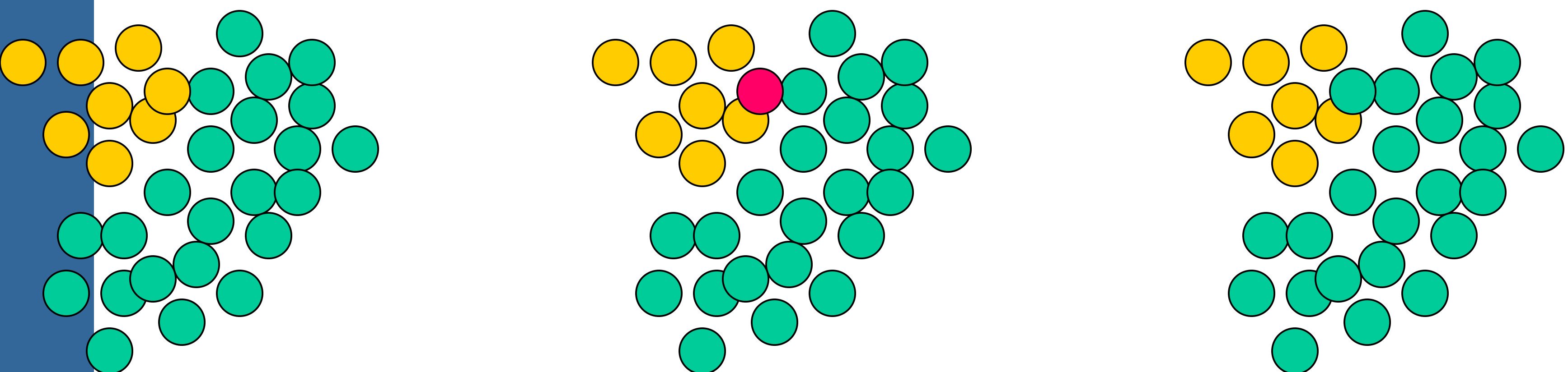
(large persistent coefficient)

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

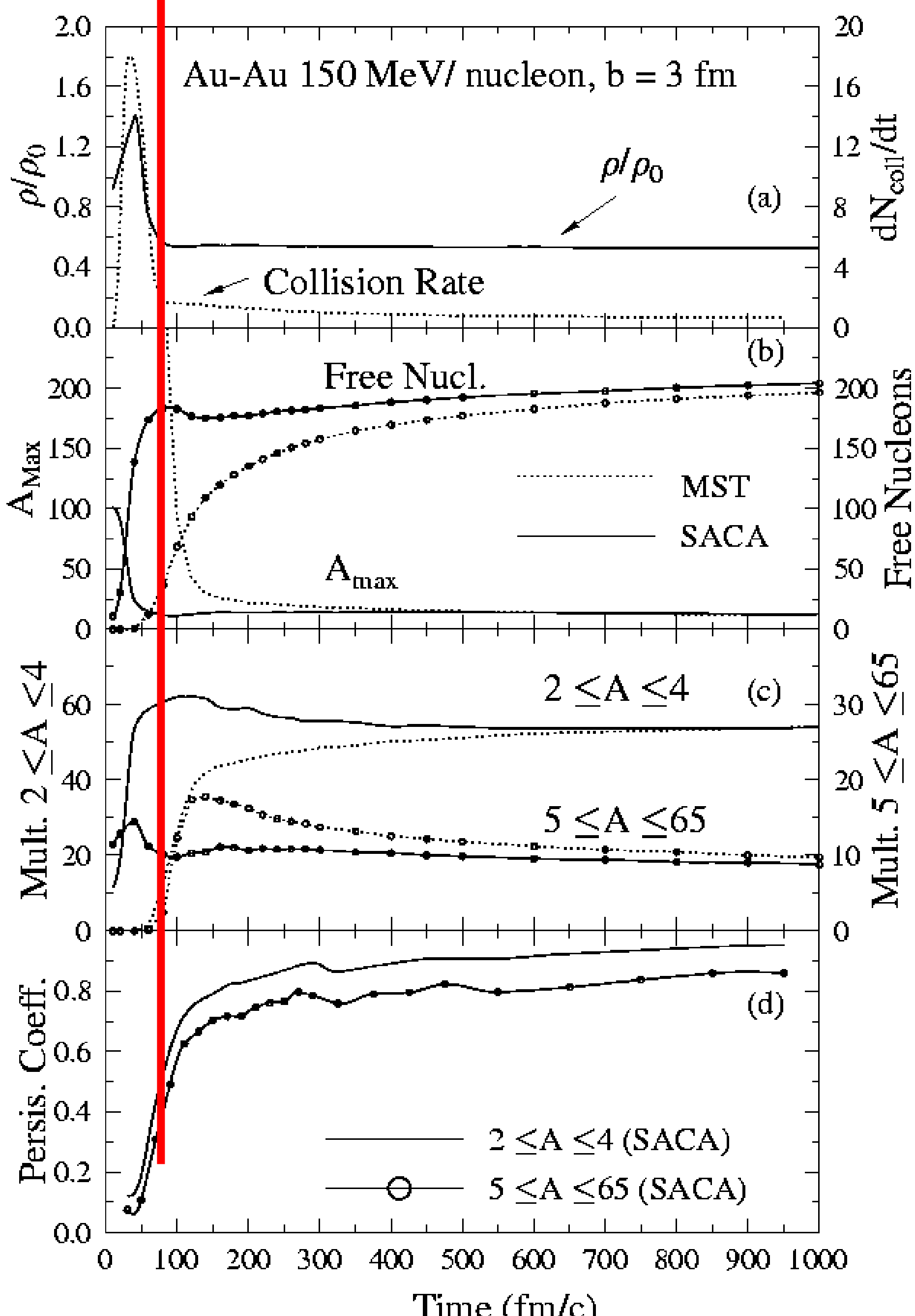
Add it randomly to another fragment



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

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

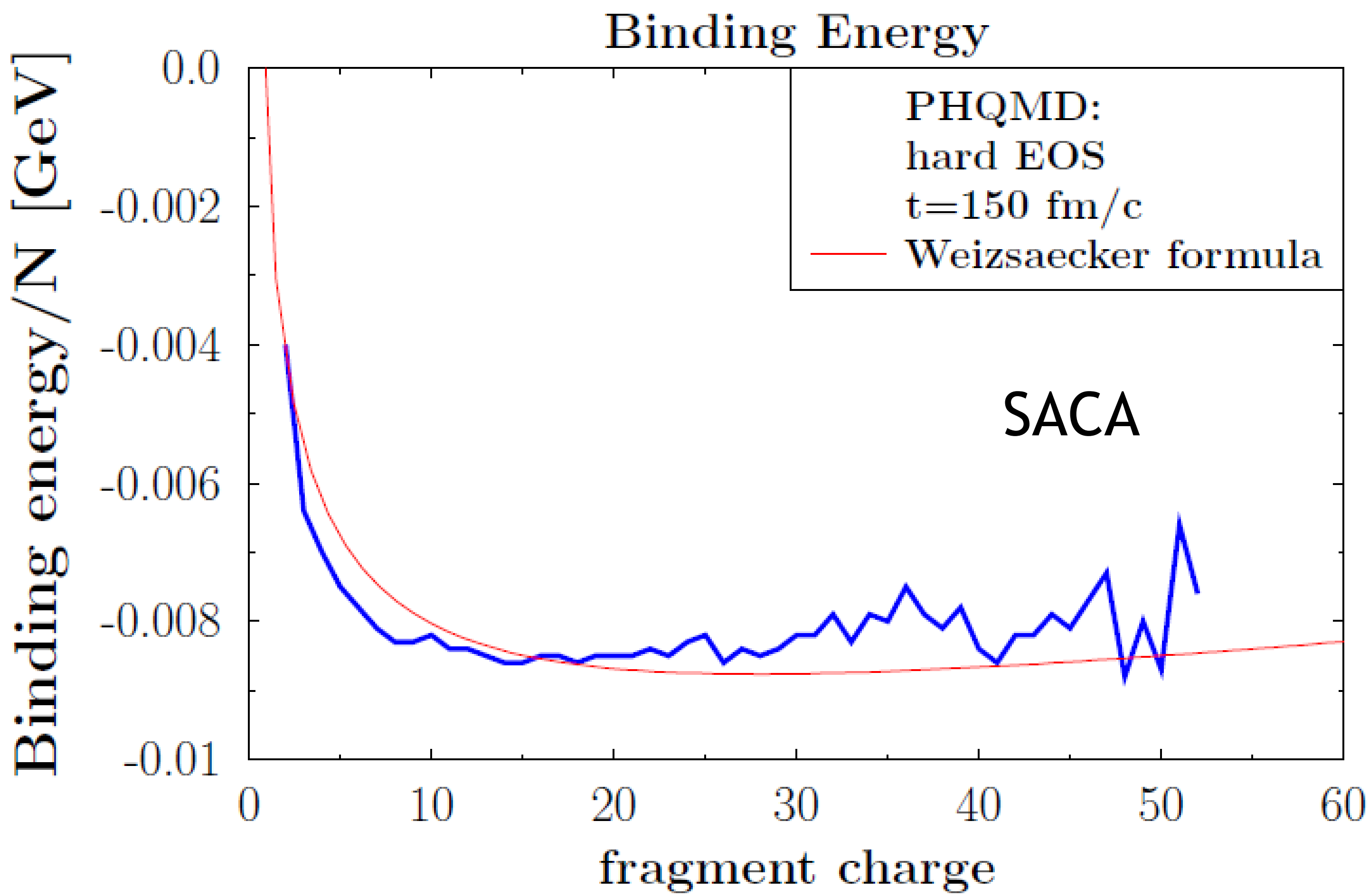
If E’ < E take the new configuration
If E’ > E take the old with a probability depending on E’-E
Repeat this procedure very many times
→ Leads automatically to the most bound configuration



SACA 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 $1.5t_{pass}$ Amax and multiplicities of intermediate mass fragments are determined

Fragment formation in PHQMD



There are two kinds of fragments

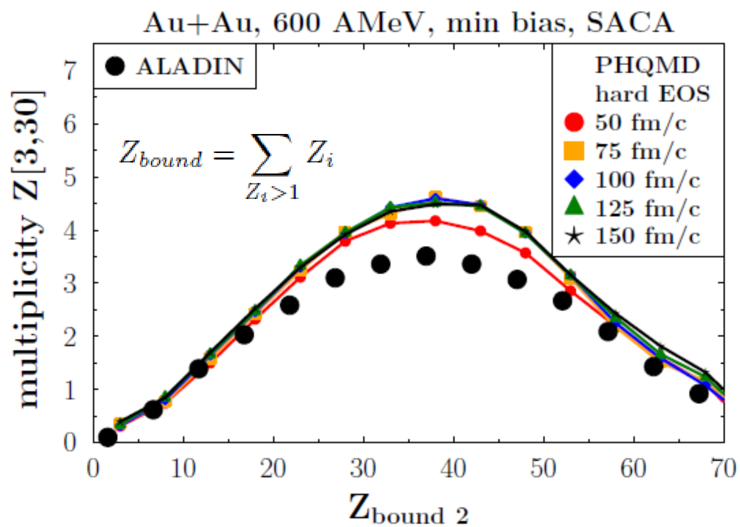
- formed from spectator matter
  close to beam and target rapidity
  initial-final state correlations
  HI reaction makes spectator matter unstable

- 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

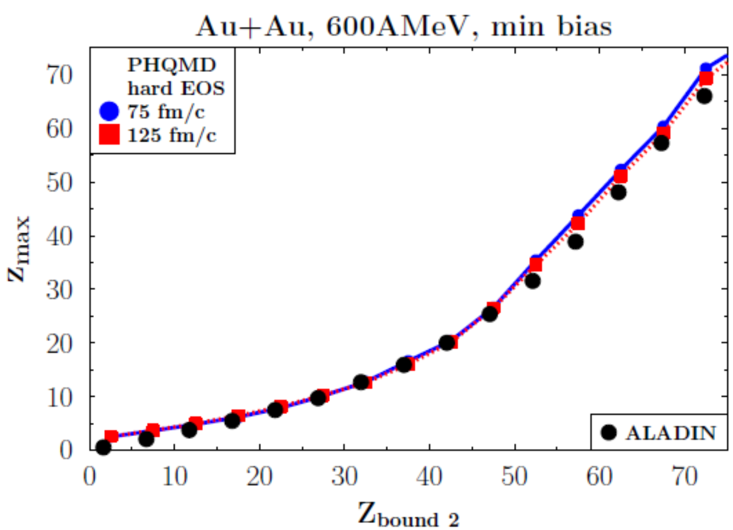
experm. measured up to E_{beam} =1 AGeV (ALADIN)

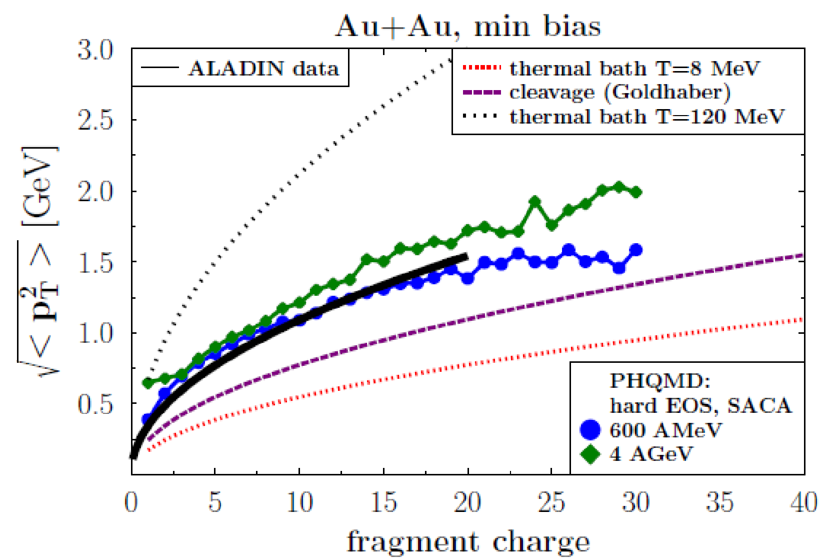


agreement for very complex fragment observables like the

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

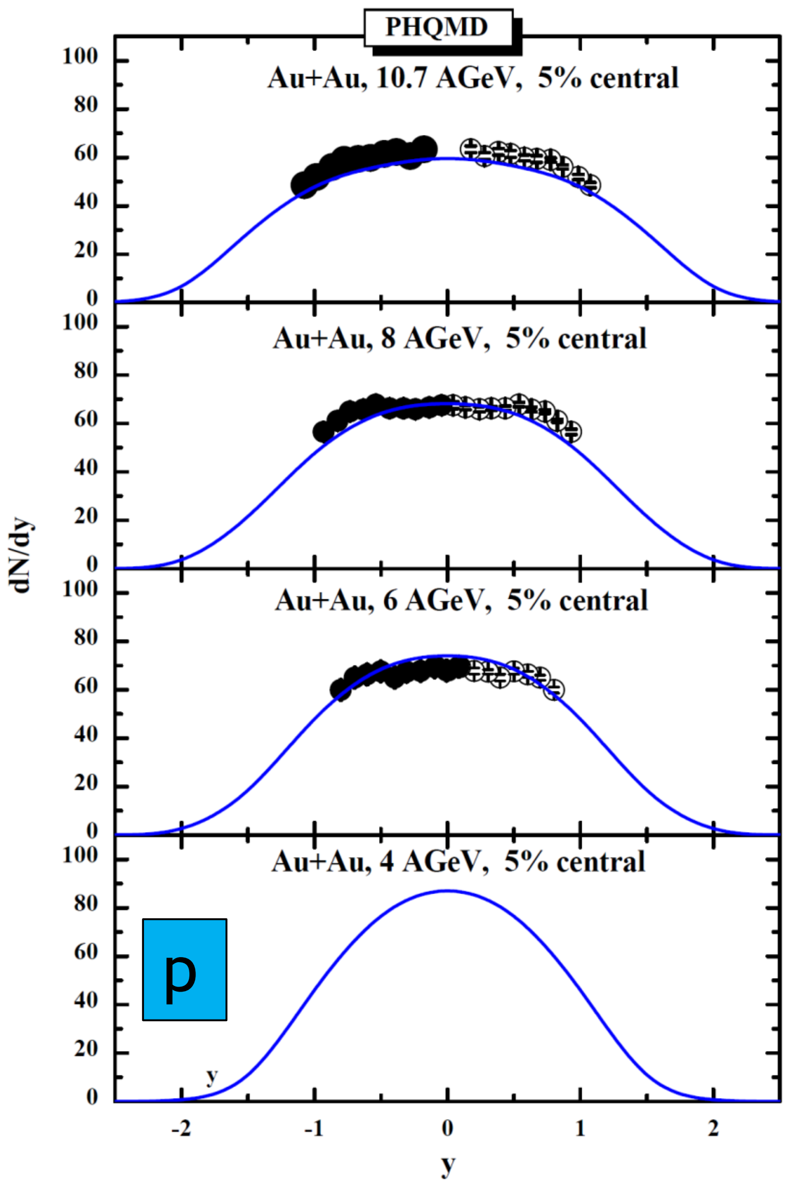
rms(p_t) shows $\sqrt{Z}$ dependence



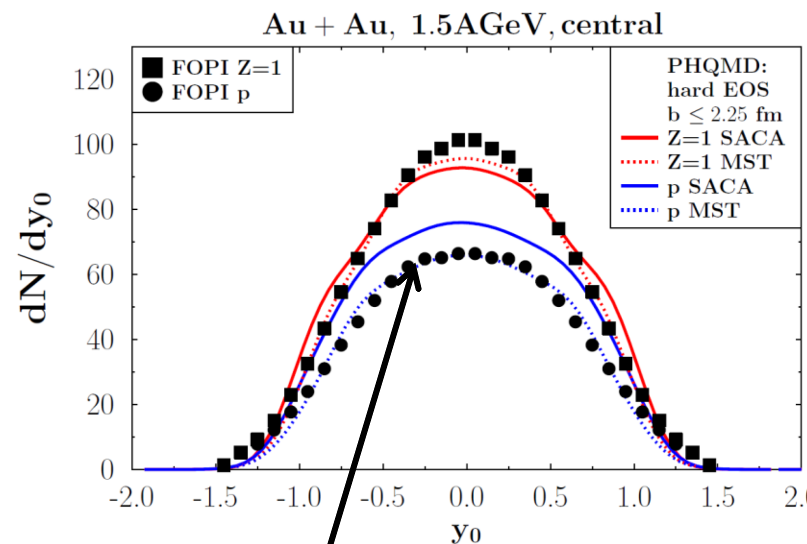


First Results of PHQMD

Protons at midrapidity well described



midrapidity fragment production increases with decreasing energy



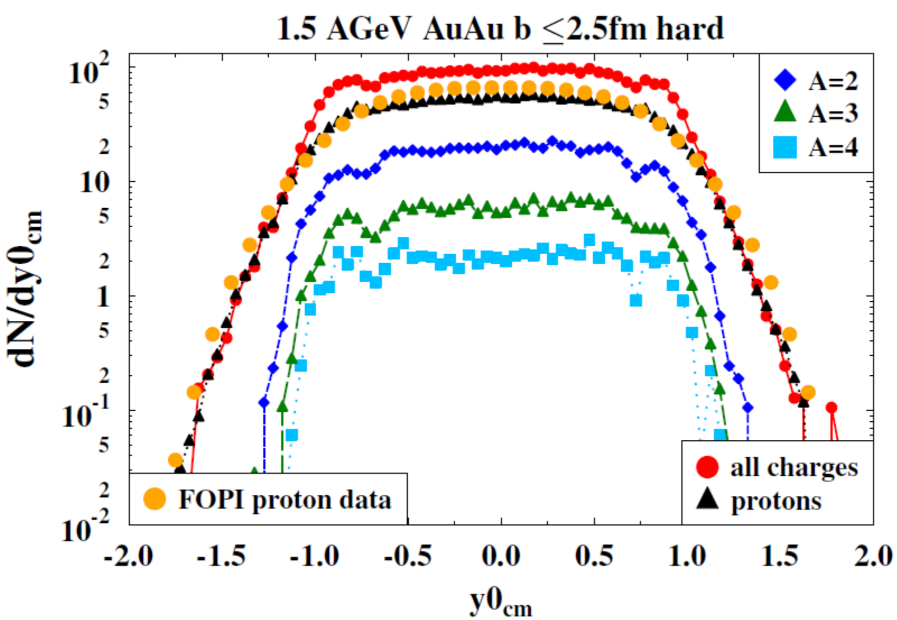
1.5 AGeV central

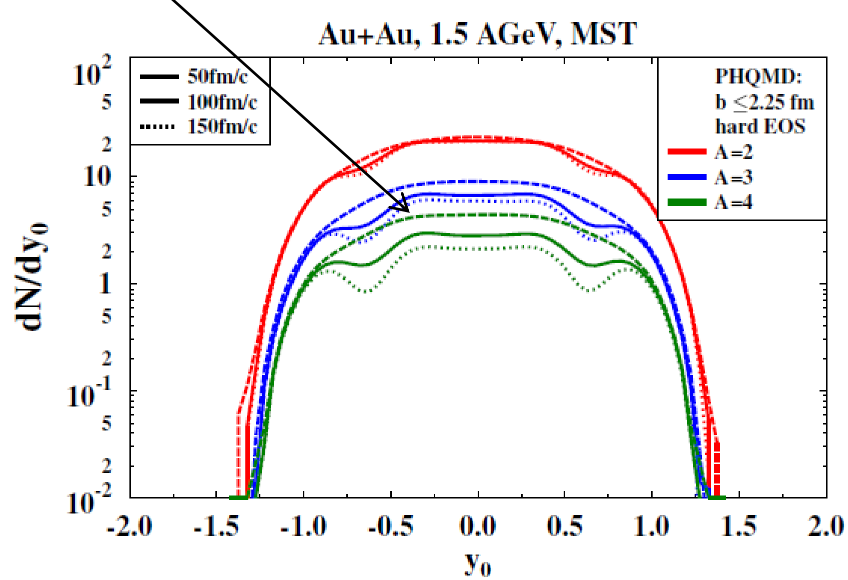
- 30% of protons bound in cluster

To improve: better potential for small clusters

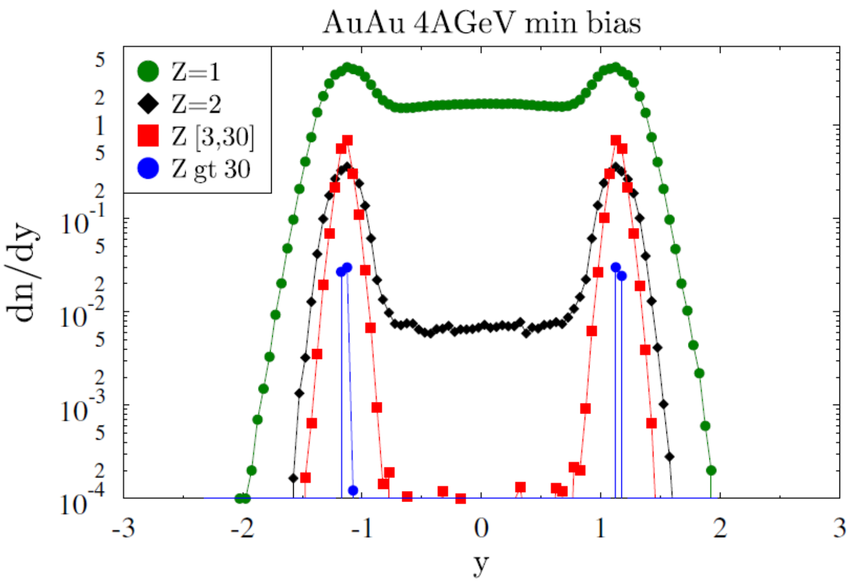
First Results of PHQMD

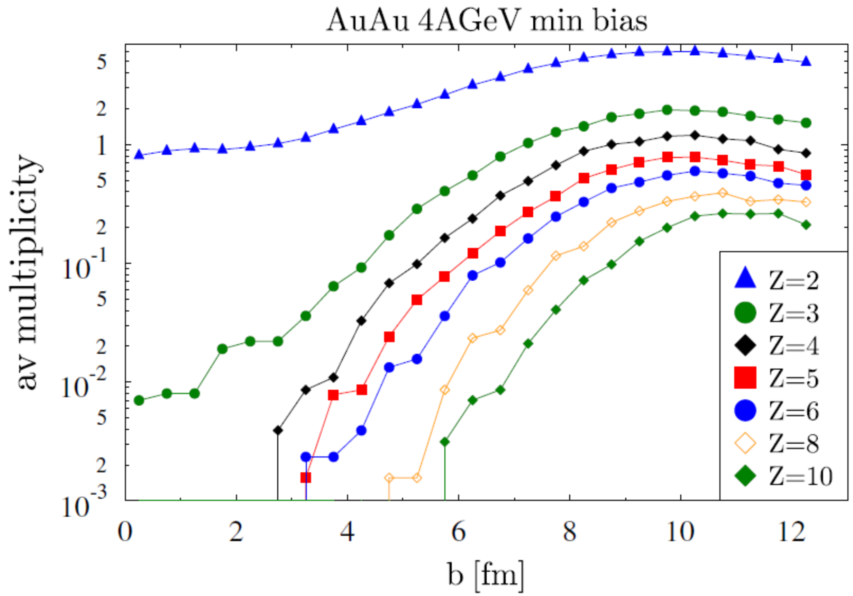
There are all kinds of dynamically produced fragments at midrapidity and they are stable
(MST finds at 50fm/c almost the same fragments as at 150fm/c)





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

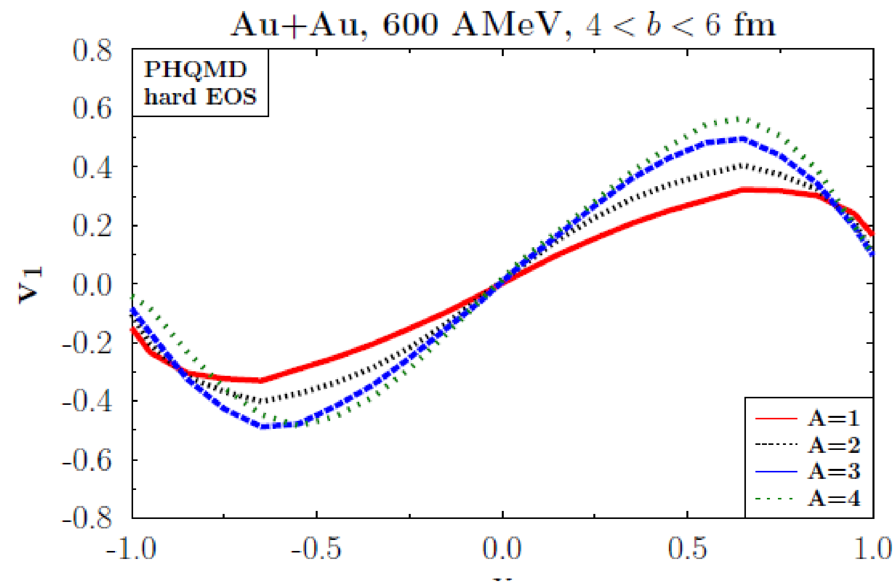
Dynamical variables - v_1

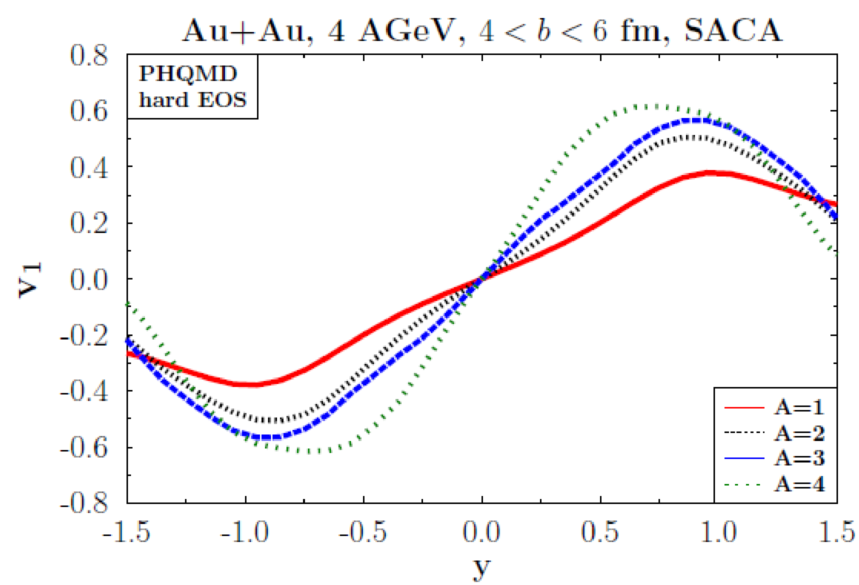
v_1 quite different for nucleons and fragments (as seen in experiments)

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

fragments from interface spectator-participant (strong density gradient)

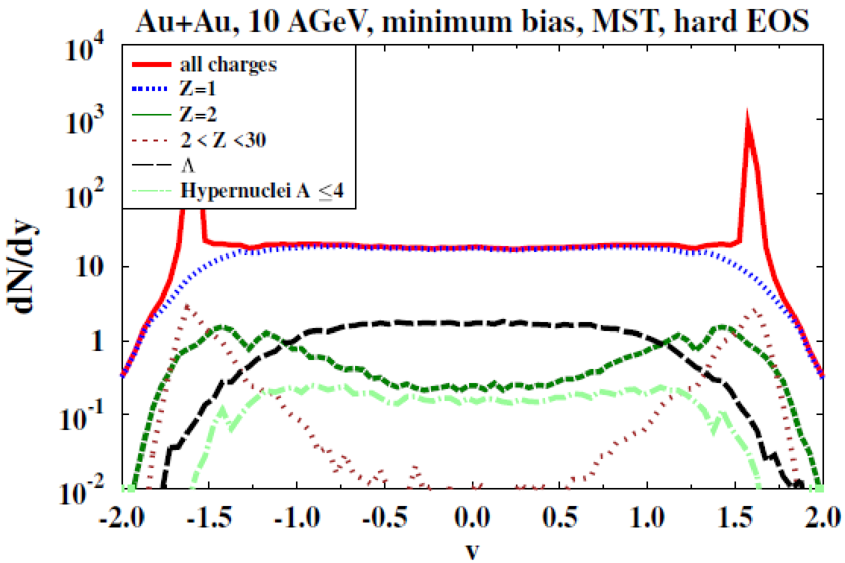
v_1 increases with E_{beam}
larger density gradient
→ $F_T\, t_p = p_T$ larger



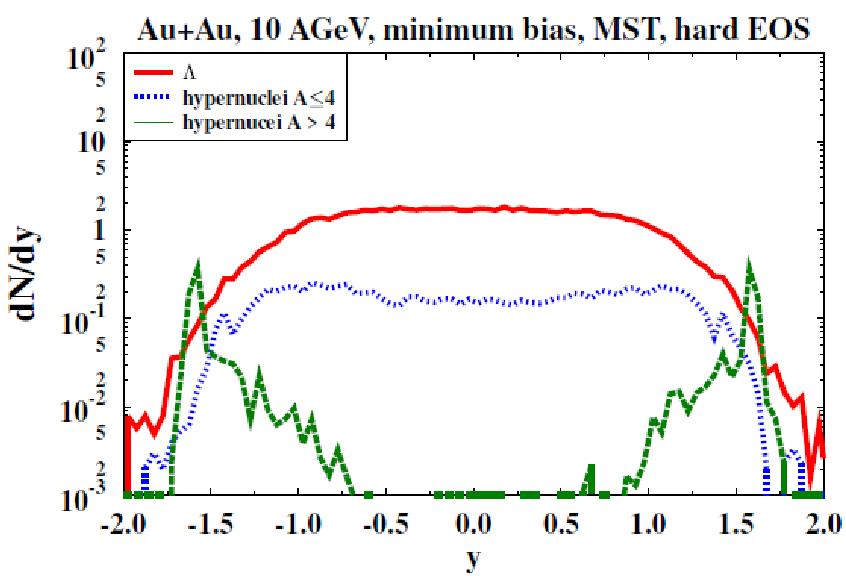


.. and what about hyper-nuclei ?

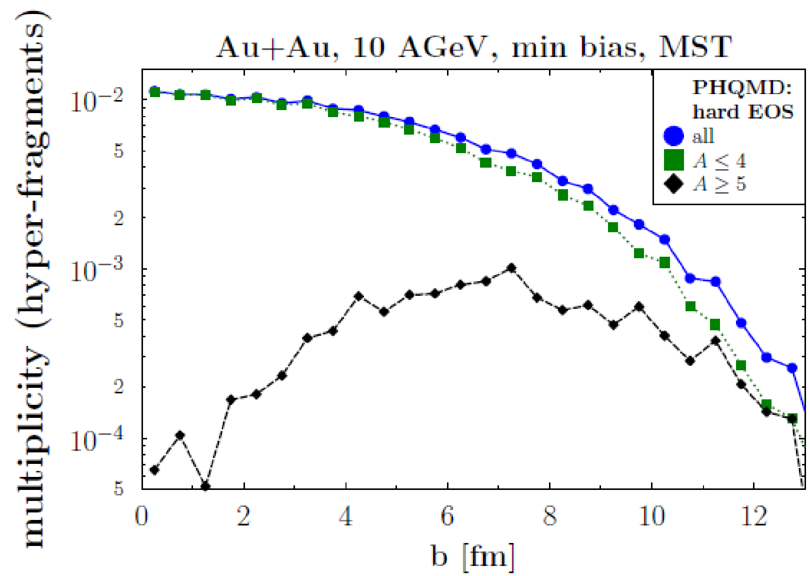
First Results of PHQMD



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



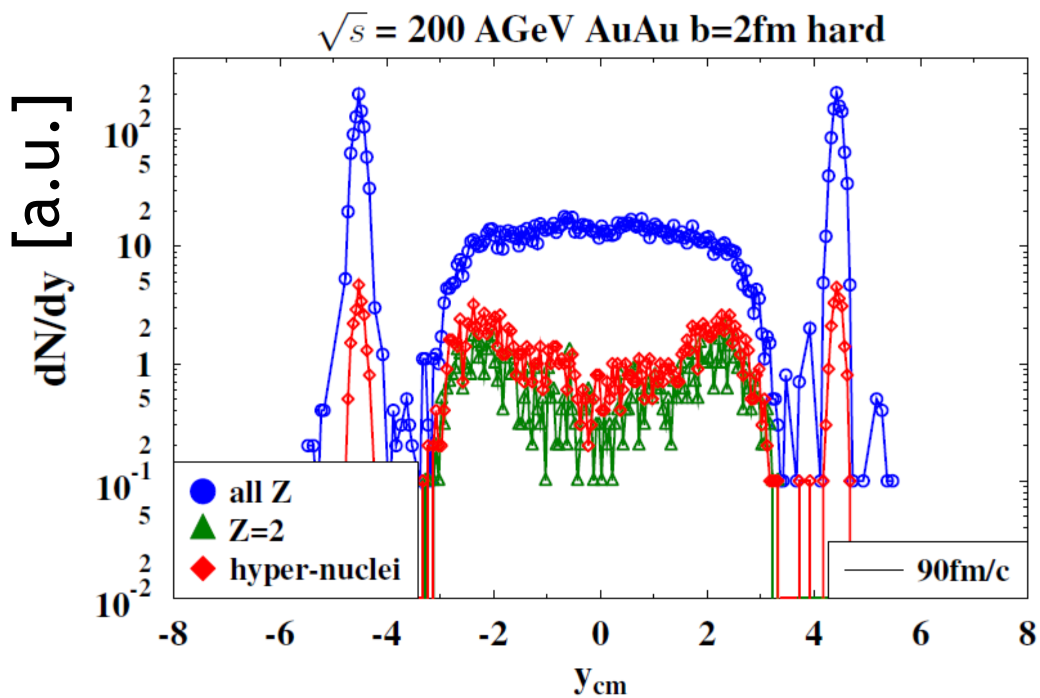
Central collisions → light hyper-nuclei
Peripheral collisions → heavy hyper-nuclei



First Results of PHQMD

At RHIC

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



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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!!