Nuclear production mechanism studies using the PHQMD model

Susanne Glaessel

& Gabriele Coci, Viktar Kireyeu, Elena Bratkovskaya, Joerg Aichelin, Christoph Blume, Vadym Voronyuk, Vadim Kolesnikov

5th EMMI workshop on anti-matter, hyper-matter and exotica production
Salerno, Italy, November 10-14, 2025

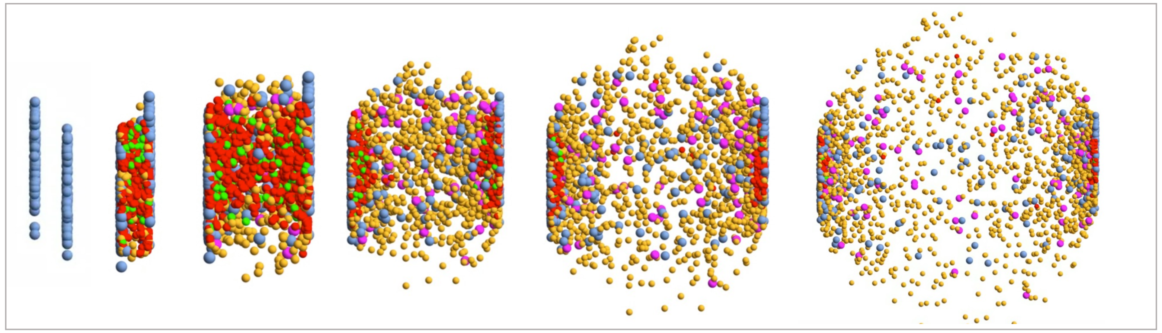
Agenda

PHQMD model

Mechanisms for cluster production in PHQMD

Can the production mechanisms be identified experimentally?

Where are the clusters formed?



Cluster and hyper-cluster production in HICs with PHQMD

Motivation

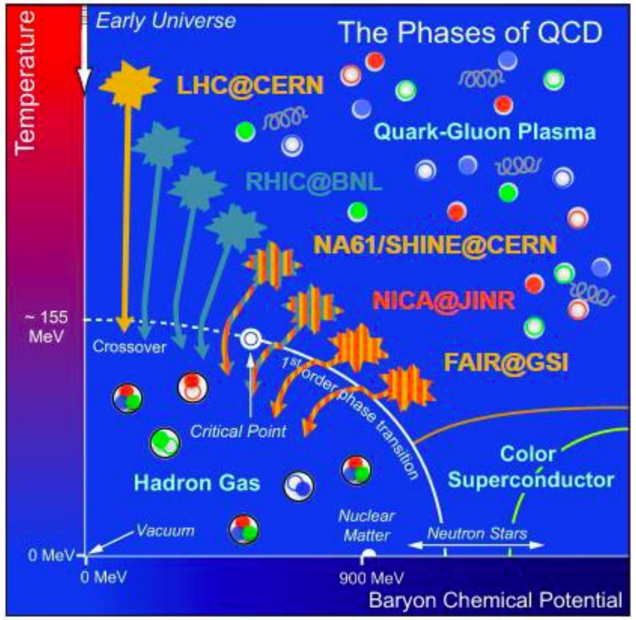
Exploring the **QCD-phase-diagram** with clusters as **experimental observables.**

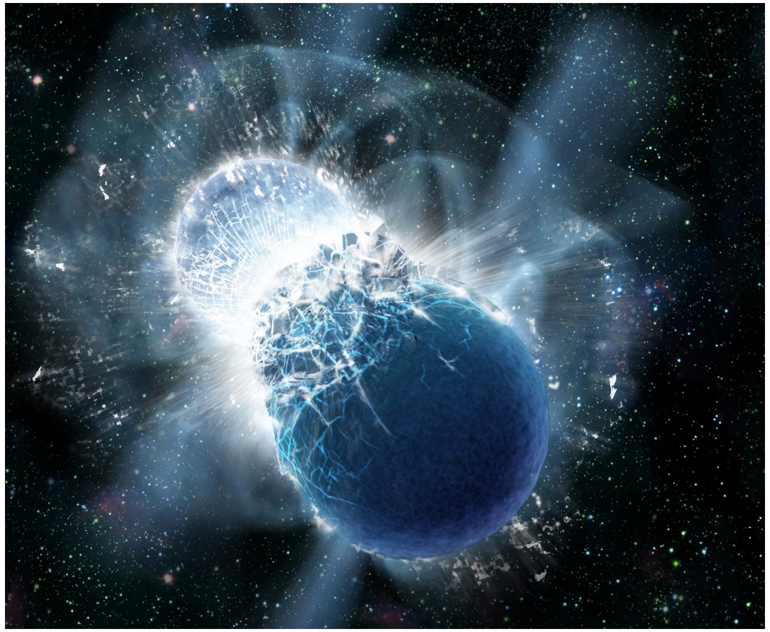
Mechanisms of cluster formation in strongly interacting matter are not well understood

How can **weakly bound** clusters survive

in the **hot and dense** environment of a HICs?

'**Ice in fire puzzle**'





Challenge

Modeling the **time evolution of cluster formation** and the origin of their production.

Modelling of cluster formation in HIC

Statistical models

- Production of nuclei depending on T and μ_B at chemical freeze-out & particle mass
- Assumption of thermal equilibrium

Dynamical models within microscopic transport models:

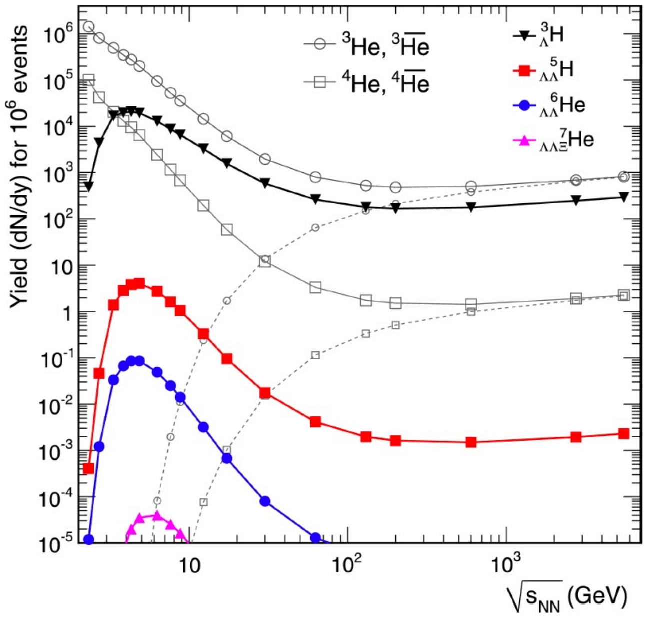
Coalescence models

- formation of nuclei by nucleons & hyperons that are close in coordinate and momentum spaces at freeze-out time (coalescence radii)

Interaction mechanism in transport models

- potential mechanism - via potential NN (NY) interactions
- kinetic mechanism - by hadronic scattering (e.g. NNπ → dπ)

PHQMD



A. Andronic et al., Phys. Lett. B697 (2011) 203-207.

Parton-Hadron-Quantum-Molecular Dynamics

= n-body microscopic transport approach for the description of heavy-ion collisions with dynamical cluster formation

PHSD + QMD + MST

Relativistic considerations

but: mean-field potentials
=> correlations are smeared out

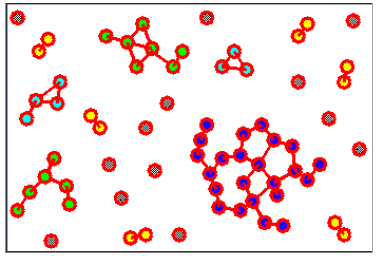
Correlations between baryons

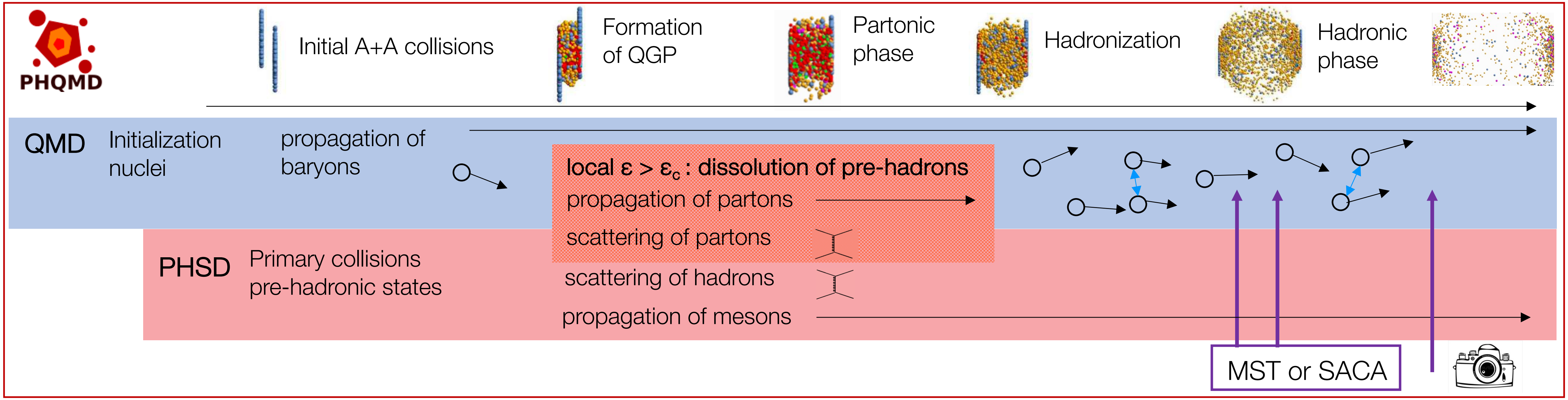
n-body transport approach

=> formation of clusters due to potential interactions

Cluster recognition

search for accumulations of particles in coordinate space





J. Aichelin et al., PRC 101 (2020) 044905 PHSD: W. Cassing, E. Bratkovskaya, PRC 78 (2008) 034919; NPA831 (2009) 215; W. Cassing, EPJ ST 168(2009)

Cluster formation within different transport approaches

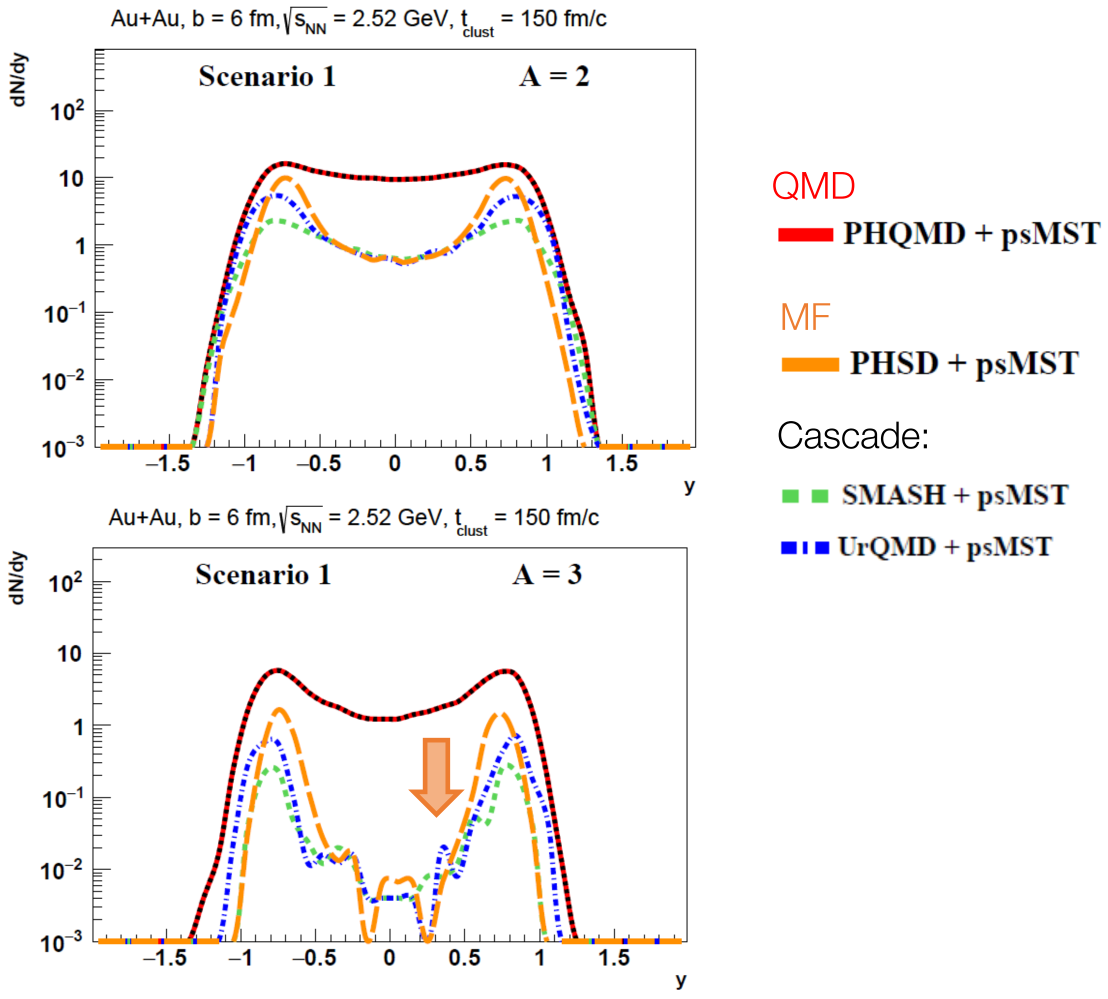
Cluster formation is sensitive to nucleon dynamics.

Modeling of nucleon-nucleon potential interactions:

- QMD (quantum-molecular dynamics) – allows to keep correlations
- MF (mean-field based models) – correlations are smeared out
- Cascade – correlations by potential interactions missing

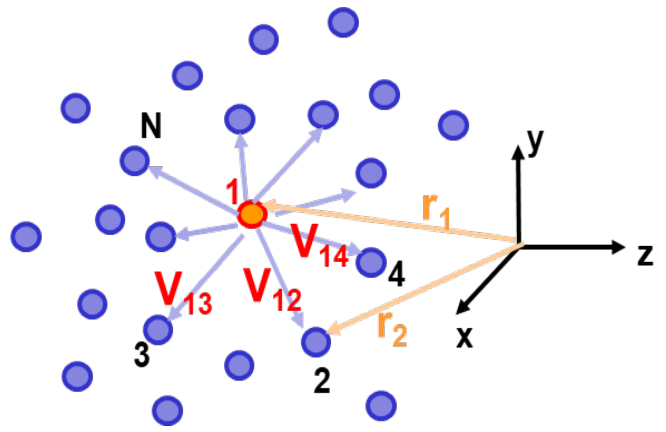
At late times: only simulations including the nucleon-nucleon potential keep the clusters bound.

Clusters at final time



V. Kireyeu, Phys.Rev.C 103 (2021) 5.

QMD propagation



= n-body transport approach

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

Ansatz: trial wave function for one particle "i" : Gaussian with width L centered at r_{i0}, p_{i0} Aichelin Phys. Rept. 202 (1991)

$$\psi(\mathbf{r}_i, \mathbf{r}_{i0}, \mathbf{p}_{i0}, t) = C\ \mathrm{e}^{-\frac{1}{4L}\left(\mathbf{r}_i - \mathbf{r}_{i0}(t) - \frac{\mathbf{p}_{i0}(t)}{m}t\right)^2} \cdot\ \mathrm{e}^{i\mathbf{p}_{i0}(t)(\mathbf{r}_i - \mathbf{r}_{i0}(t))} \cdot\ \mathrm{e}^{-i\frac{\mathbf{p}_{i0}^2(t)}{2m}t}$$

L=4.33 fm^2

Assume that $\psi(t) = \prod_{i=1}^{N} \psi(\mathbf{r}_i, \mathbf{r}_{i0}, \mathbf{p}_{i0}, t)$ for N particles (neglecting antisymmetrization!)

Equations-of-motion (EoM) for Gaussian centers in coordinate and momentum space:

$$\dot{r_{i0}} = \frac{\partial \langle H \rangle}{\partial p_{i0}} \qquad \dot{p_{i0}} = -\frac{\partial \langle H \rangle}{\partial r_{i0}}$$

J. Aichelin et al., PRC 101 (2020) 044905

QMD potentials and EoS

expectation value of Hamiltonian

$$\langle H\rangle = \sum_i \langle H_i\rangle = \sum_i (\langle T_i\rangle + \sum_{j\neq i}\langle V_{i,j}\rangle) \qquad V_{ij} = V_{\mathrm{Skyrme\ loc}} + V_{\mathrm{mom}} + V_{\mathrm{Coul}}$$

Skyrme interaction ('static'): Effective density dependent nucleon-nucleon interactions

$$\langle V_{Skyrme}(\mathbf{r_{i0}},t)\rangle = \alpha\left(\frac{\rho_{int}(\mathbf{r_{i0}},t)}{\rho_0}\right) + \beta\left(\frac{\rho_{int}(\mathbf{r_{i0}},t)}{\rho_0}\right)^{\gamma}$$

Interaction density (with relativistic extension):

$$\rho_{int}(\mathbf{r_{i0}},t) \rightarrow C\sum_j \left(\frac{4}{\pi L}\right)^{3/2} e^{-\frac{4}{L}(\mathbf{r^T_{i0}}(t)-\mathbf{r^T_{j0}}(t))^2}\ e^{-\frac{4\gamma_{cm}^2}{L}(\mathbf{r^L_{i0}}(t)-\mathbf{r^L_{j0}}(t))^2}$$

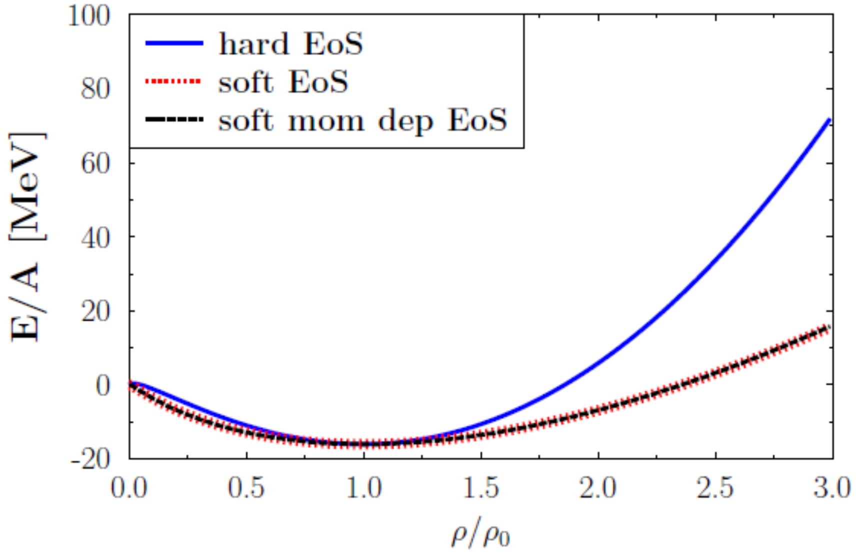
Parameter of the nuclear equation of state in PHQMD

E.o.S.	$\alpha[MeV]$	$\beta[MeV]$	γ	K [MeV]
S	-383.5	329.5	1.15	200
H	-125.3	71.0	2.0	380
SM	-478.87	413.76	1.10	200

compression modulus K of nuclear matter

$$K = -V\frac{dP}{dV} = 9\rho^2\frac{\partial^2(E/A(\rho))}{(\partial\rho)^2}|_{\rho=\rho_0}.$$

EoS for infinite matter at rest

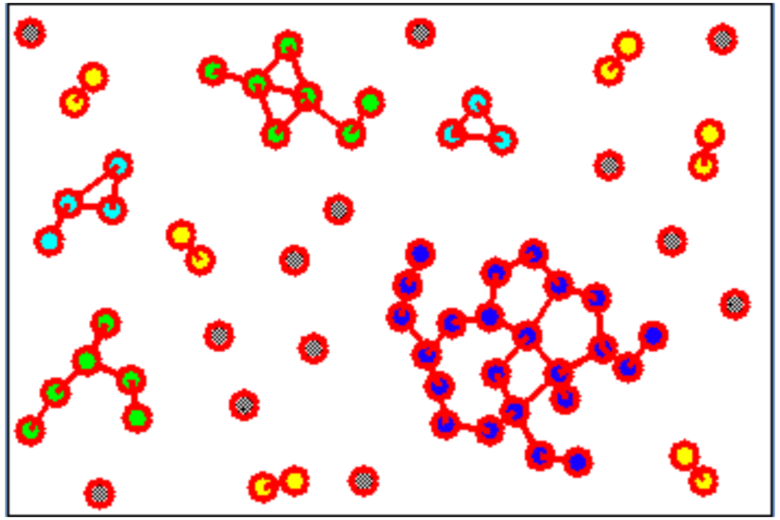


Implementation of momentum-dependent potential: talk by Yue Hang Leung on Thursday, 13.11, 14.30 pm.

Minimum Spanning Tree (MST)

Cluster criterion: distance of nuclei

Algorithm: search for accumulations of particles in coordinate space



1. Two particles i & j are bound if:

$$|r_i - r_j| < 4.0 \text{ fm}$$

2. Particle is bound to cluster if bound with at least one particle of cluster

Application at different times → study development of clusters

Application at final time → get stable clusters multiplicites

Remark: additional momentum cuts lead to a small changes: particles with large relative momentum are mostly not at the same position (V. Kireyeu, Phys.Rev.C 103 (2021) 5)

Cluster stability over time

Decrease of cluster multiplicity with time:

- at early times: baryons collide with other baryons & escape cluster
- at all times: artificial dissolving of clusters, because:

<u>QMD is a semiclassical model:</u>

Clusters not described as ‘quantum objects

with minimal average kinetic energy for nucleons

=> cluster-nucleon can accumulate kinetic energy to escape cluster

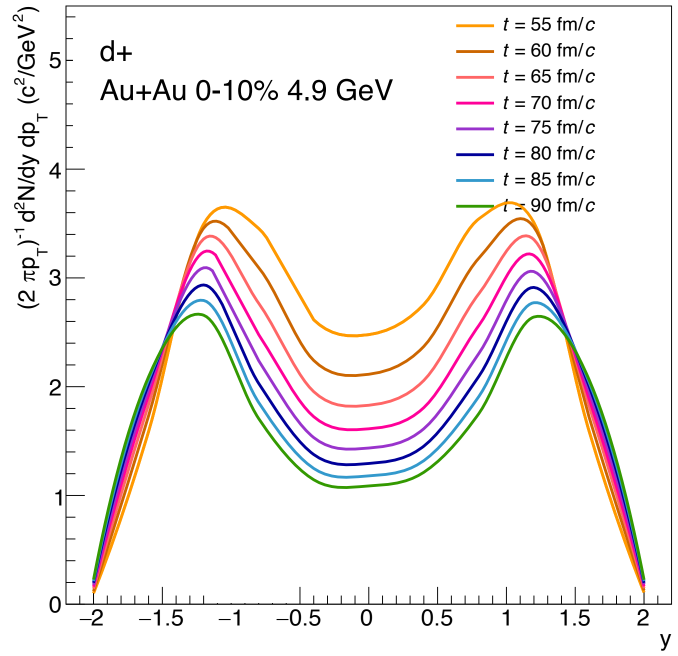
Skyrme potential is not relativistic

calculation of cluster binding energy in cluster-system after Lorentz-boost from computational frame

=> baryons have different times in cluster-frame

=> binding energy can change

Deuterons identified with MST



Stabilisation procedure Advanced MST (aMST)

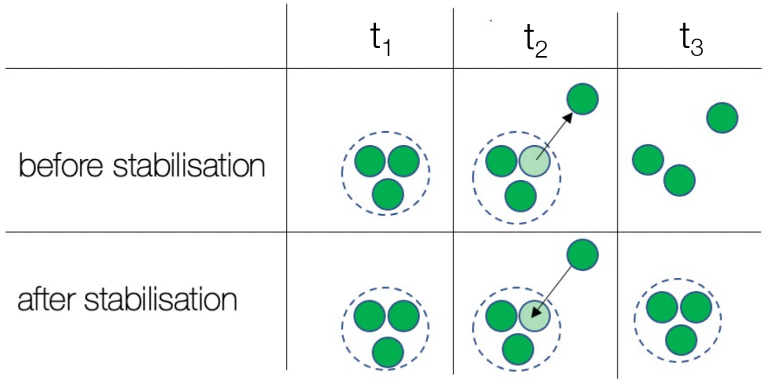
Correction of artifacts of the semi-classical QMD:

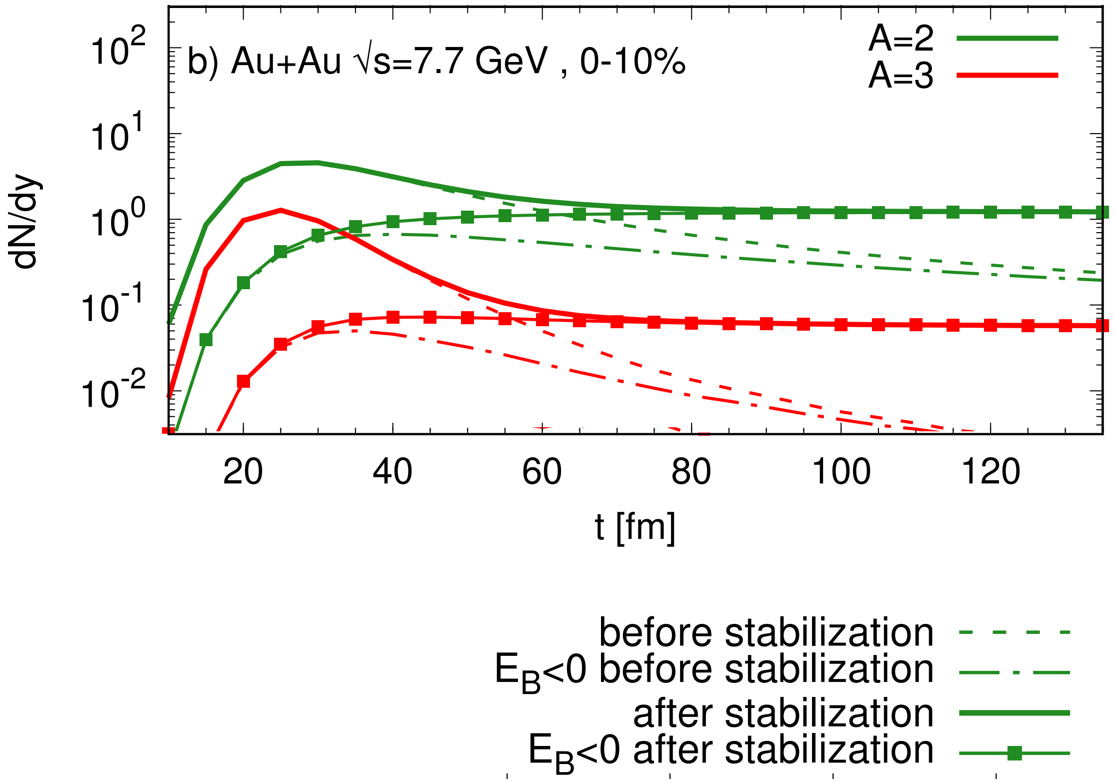
Consider a cluster as stable after all baryons in the cluster are frozen

1) Check if time of cluster disintegration > baryon freeze-out time.
2) Restore cluster

+ extra condition: $E_B<0$

negative binding energy for identified clusters





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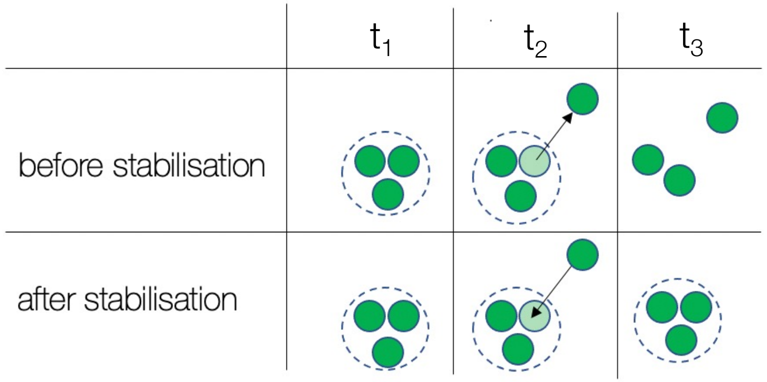
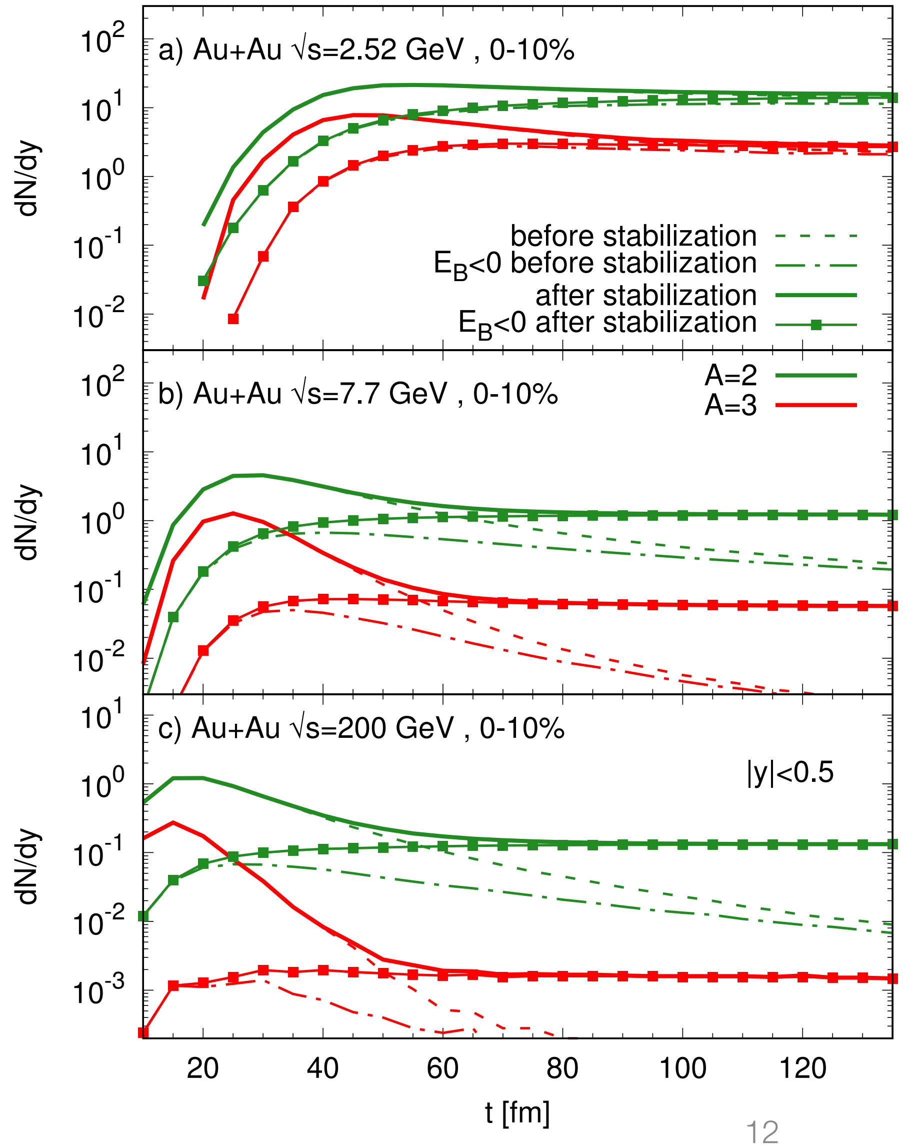
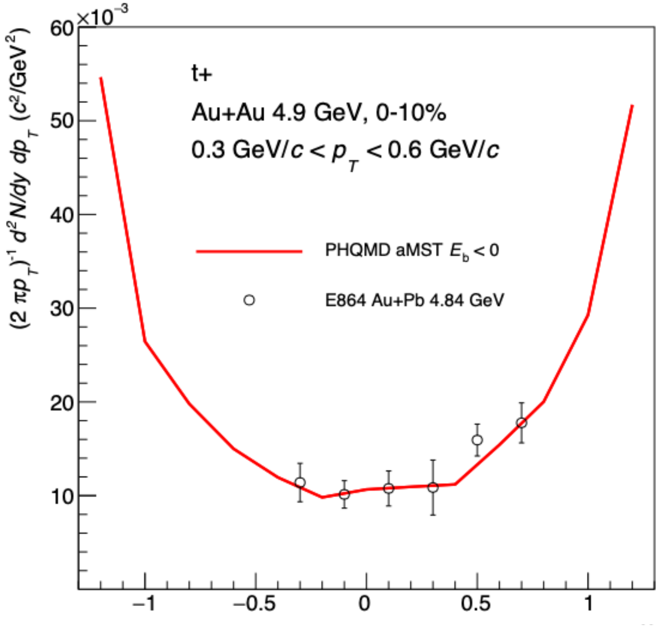
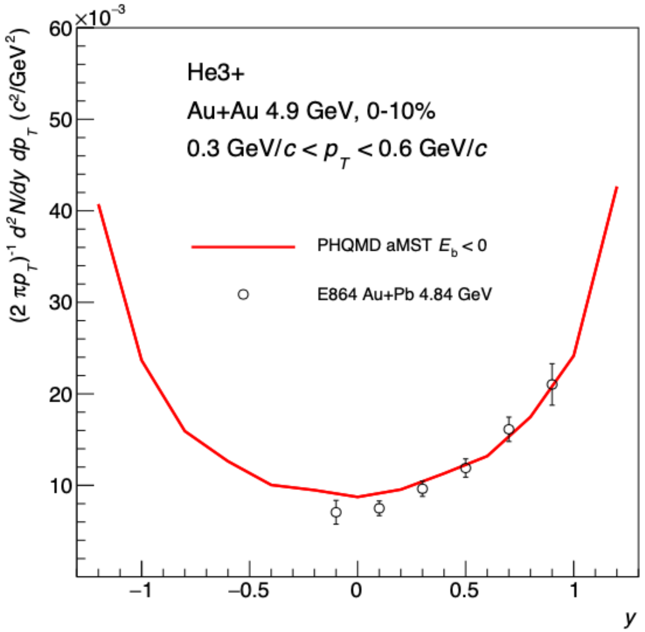
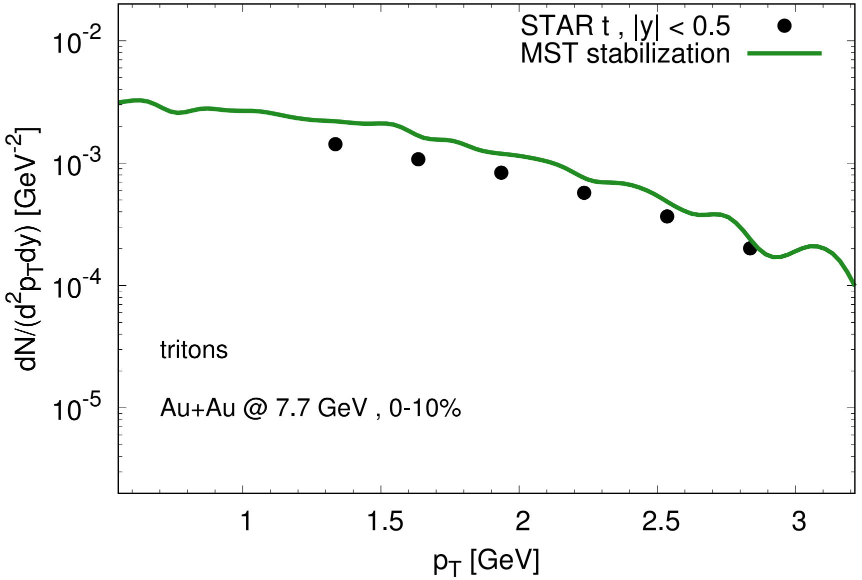




Stable light nuclei at $\sqrt{s_{NN}}$ = 4.9 and 7.7 GeV with aMST







PHQMD with stabilisation procedure fits the experimental data at $\sqrt{s_{NN}}$ = 4.9 and 7.7 GeV very well for triton and ^{3}He.

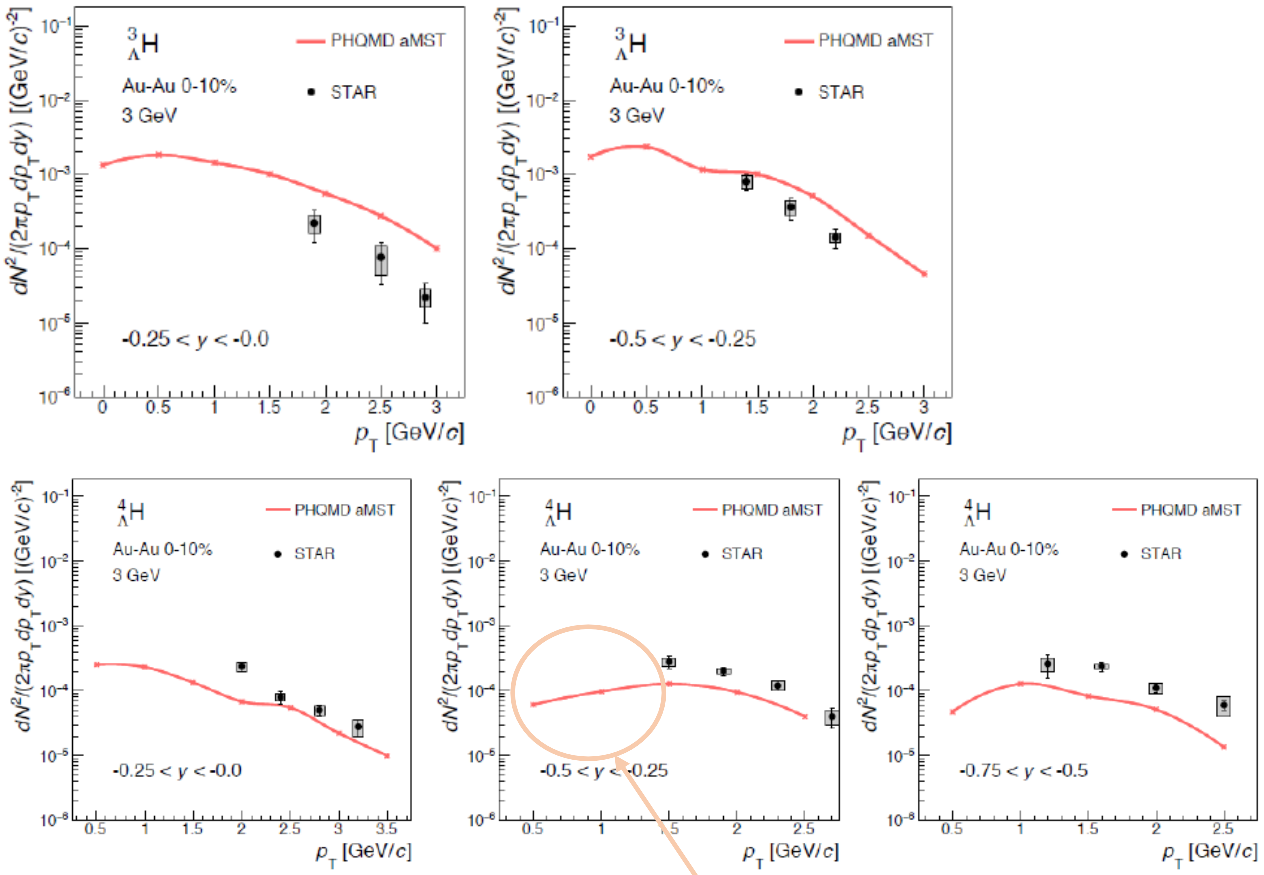
Deuterons are underestimated => contribution of deuterons formed by inelastic scattering.

T. A. Armstrong et al (E864), Phys Rev. C, 61, 064908 (2002)

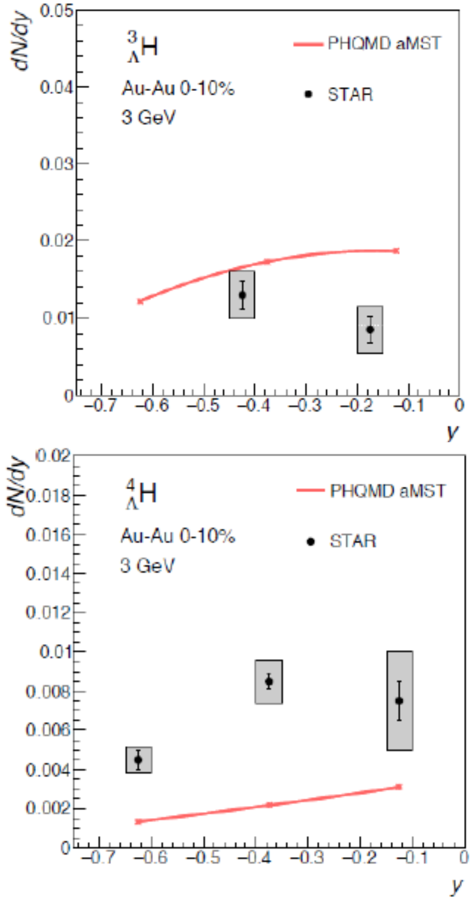
J. Adam et al. (STAR), Phys. Rev. C 99, 064905 (2019)

Hypernuclei production at STAR $\sqrt{s}$=3 GeV

p_T-spectra



y-spectra



Low p_T – exp. data are needed for reliable estimation of y-spectra.

Yue-Hang Leung: First results of H3L & H4L (dN/dy, c_T, v_1) from 3 GeV Au+Au collisions with the STAR detector (CPOD2021).

Kinetic deuterons: Hadronic reactions

1) Hadronic inelastic reactions:

NN $\leftrightarrow$ dπ , πNN $\leftrightarrow$ dπ , NNN $\leftrightarrow$ dN

- d+π and d+N scattering: large cross sections $\sigma_{peak} \approx$ 200 mb
- RHIC and LHC energies: large π abundance
  $\rightarrow$ deuterons formed by π-catalysis.
- consider all π-channels allowed by total isospin conservation:
  $\rightarrow$ enhancement compared to SMASH

$$\pi^{\pm,0} + p + n \leftrightarrow \pi^{\pm,0} + d$$

$$\pi^- + p + p \leftrightarrow \pi^0 + d$$

$$\pi^+ + n + n \leftrightarrow \pi^0 + d$$

$$\pi^0 + p + p \leftrightarrow \pi^+ + d$$

$$\pi^0 + n + n \leftrightarrow \pi^- + d$$

2) Hadronic elastic reactions: π+d, N+d

PHQMD: G. Coci et al., Phys.Rev.C 108 (2023) 014902

Kinetic deuterons in PHQMD

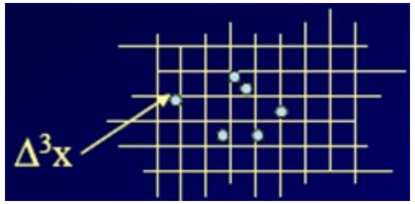
Collision rate $\frac{dN_{coll}[n(i)\to m]}{dtdV}$ for the scattering process i: Number of reactions in the covariant volume $d^4x = dt*dV$:

Test particle ansatz for f(p,x) to solve numerically in ΔV_{cell} and Δt: rates are sampled stochastically

- With n=2 initial particles: the covariant rate / probability can be expressed in terms of the reaction cross section

$$\frac{\Delta N_{coll}[1(d)+2\to 3+4+5]}{\Delta N_1 \Delta N_2} = P_{2,3}(\sqrt{s}) = v_{rel}\sigma_{2,3}(\sqrt{s})\frac{\Delta t}{\Delta V_{cell}}$$

W. Cassing, NPA 700 (2002) 618



- With n > 2 initial particles: covariant rate can be expressed in terms of cross section of inverse reaction

$$\frac{\Delta N_{coll}[3+4+5\to 1(d)+2]}{\Delta N_3 \Delta N_4 \Delta N_5} = P_{3,2}(\sqrt{s}) = F_{spin}F_{iso}P_{2,3}(\sqrt{s})\frac{E_1^f E_2^f}{2E_3E_4E_5}\frac{R_2(\sqrt{s},m_1,m_2)}{R_3(\sqrt{s},m_3,m_4,m_5)}\frac{1}{\Delta V_{cell}}$$

Energy and momentum of final particles

2,3-body phase space integrals [Byckling, Kajantie]

Numerically tested in “static” box: good agreement with analytic solutions from rate equations and with SMASH.

PHQMD: G. Coci et al., Phys.Rev.C 108 (2023) 014902

SMASH: D. Oliinychenko et al., PRC 99 (2019) 044907; J. Staudenmaier et al., PRC 104 (2021) 034908.

Modelling finite-size effects in kinetic mechanism

How to account for the quantum nature of deuteron:

1) Finite-size of d in coordinate space (d is not a point-like particle)

Deuteron can not be formed in a high density region, i.e. if there are other particles inside the 'excluded vc $|\vec{r}(i)^* - \vec{r}(d)^*| < R_d$

-> Strong reduction of d production

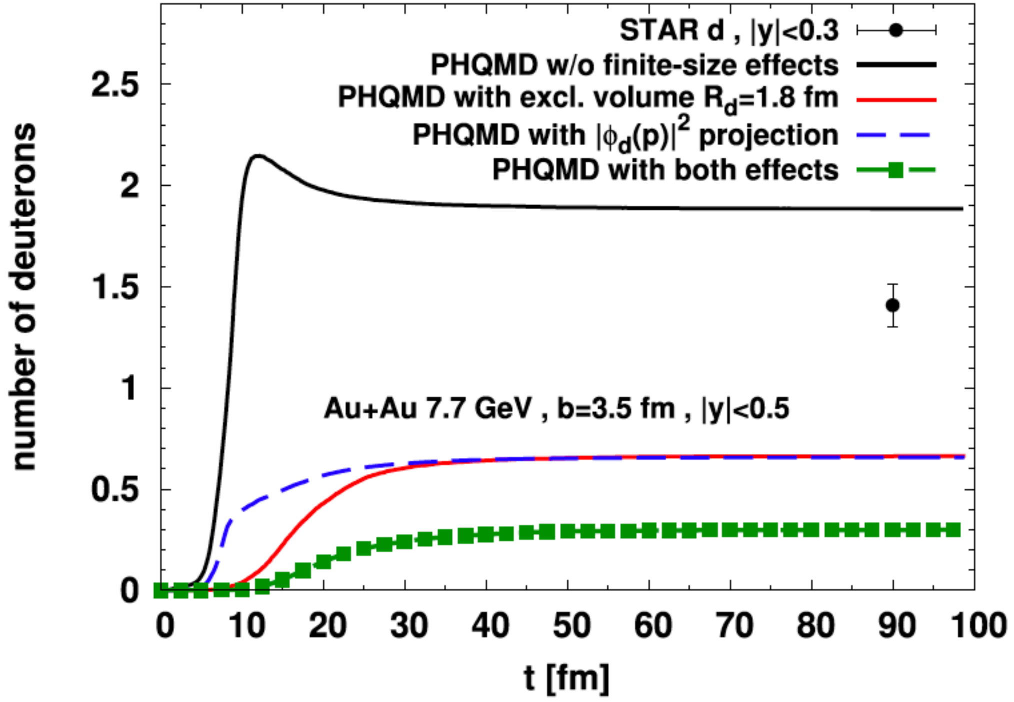
2) Momentum correlations of p and n inside d

Highest probability to form a deuteron for p-n-pair with relative momentum $p \sim 1/\sqrt{<r_d^2>} \sim 0.1\,GeV$

Bound pn-pairs selected by projection on DWF $|\phi_d(p)|^2$

-> Strong reduction of d production

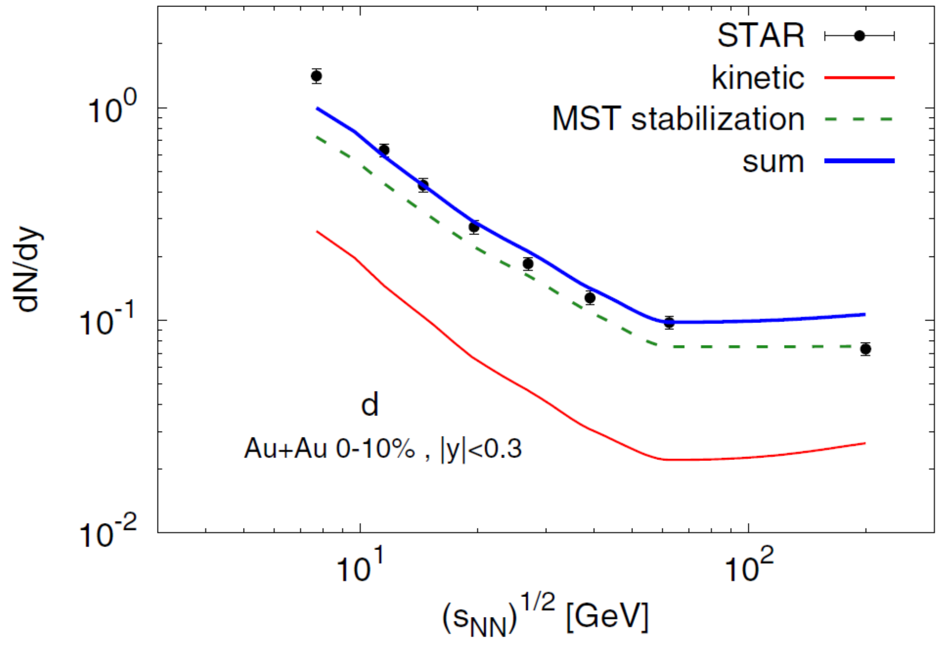
-> p_T slope is not affected by finite size effects



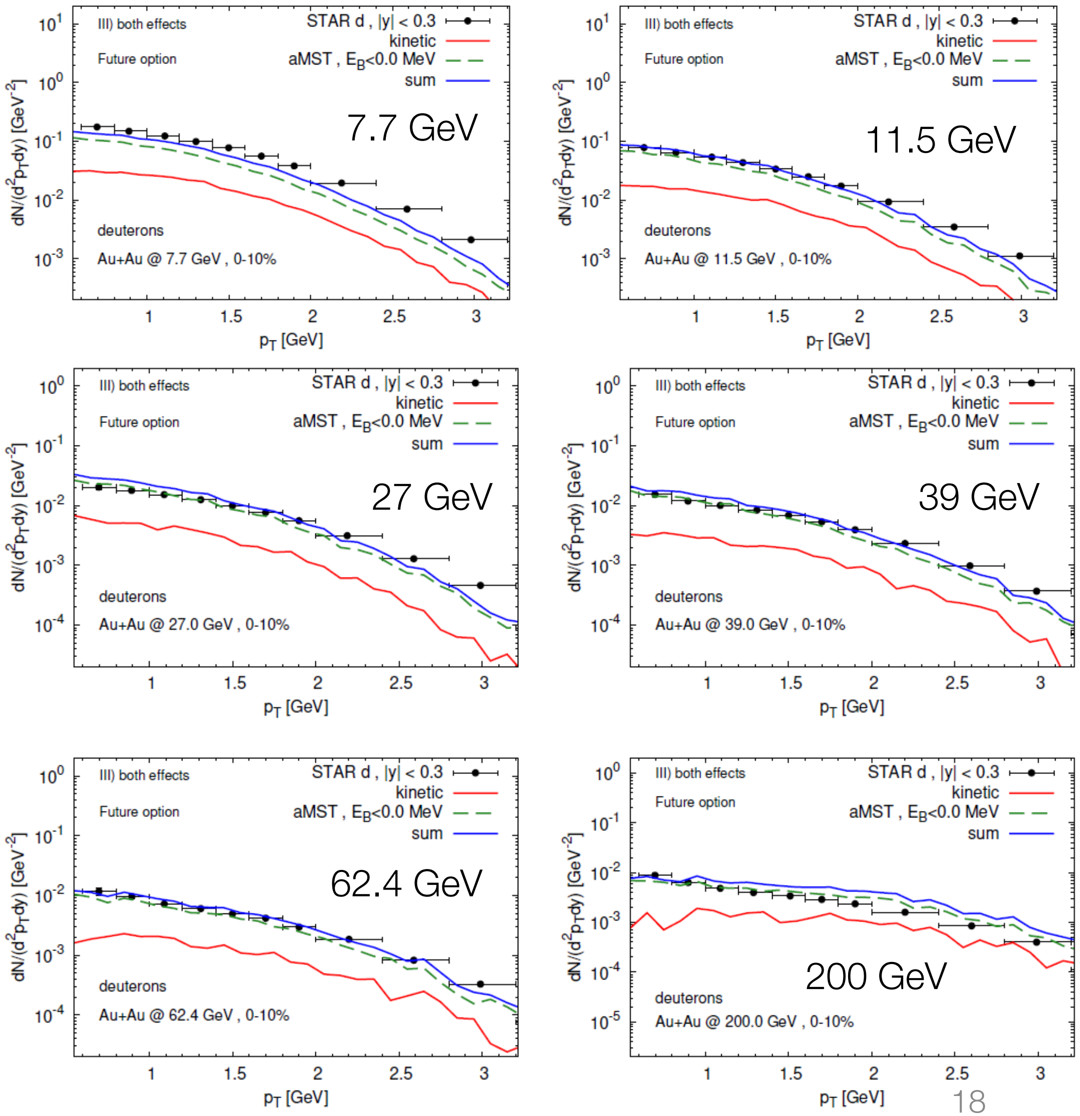
G. Coci et al., Phys.Rev.C 108 (2023) 014902.

Deuteron production compared to STAR data

Excitation function dN/dy of deuterons at midrapidity



p_T – spectra (BES RHIC)



PHQMD provides a good description of STAR data.

Functional forms of p_T-spectra are similar for kinetic and potential d.

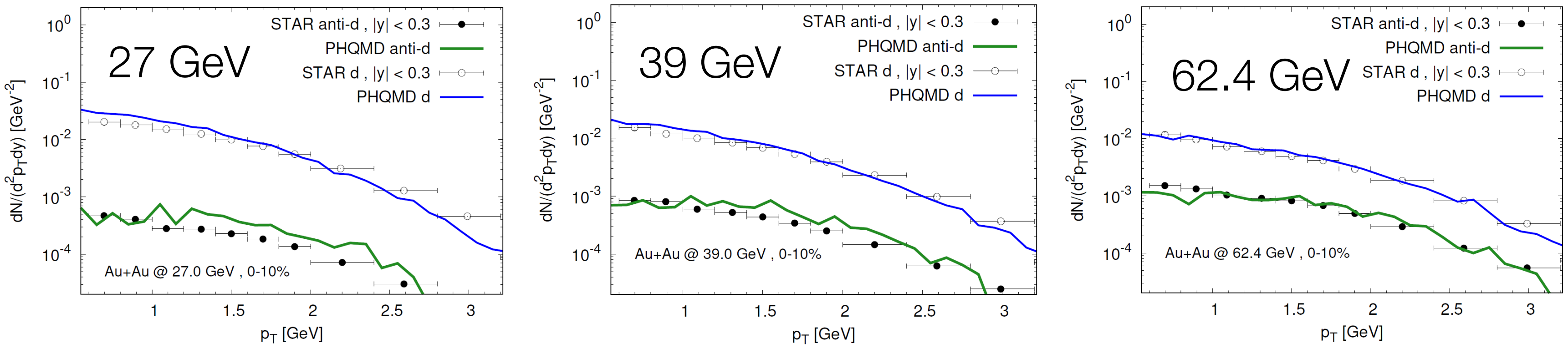
The potential mechanism is dominant for d production at all energies.

G. Coci et al., Phys.Rev.C 108 (2023) 014902.

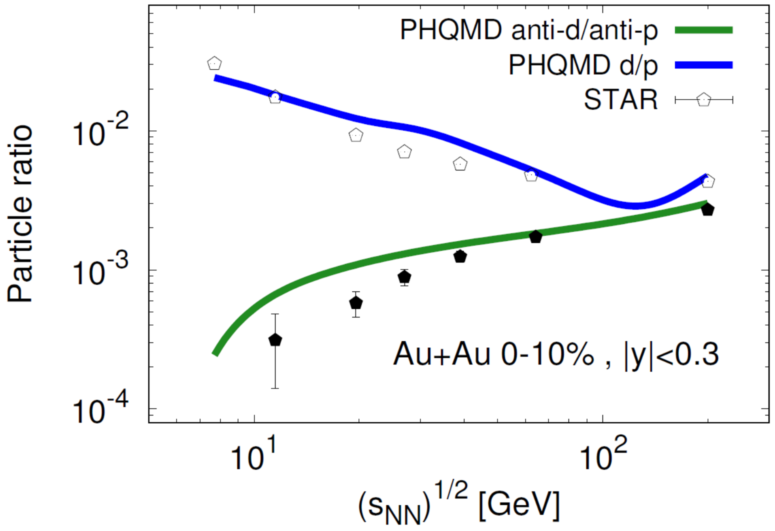
J. Adam et al. (STAR), Phys. Rev. C 99, 064905 (2019)

Anti-deuteron production and deuteron/proton ratio

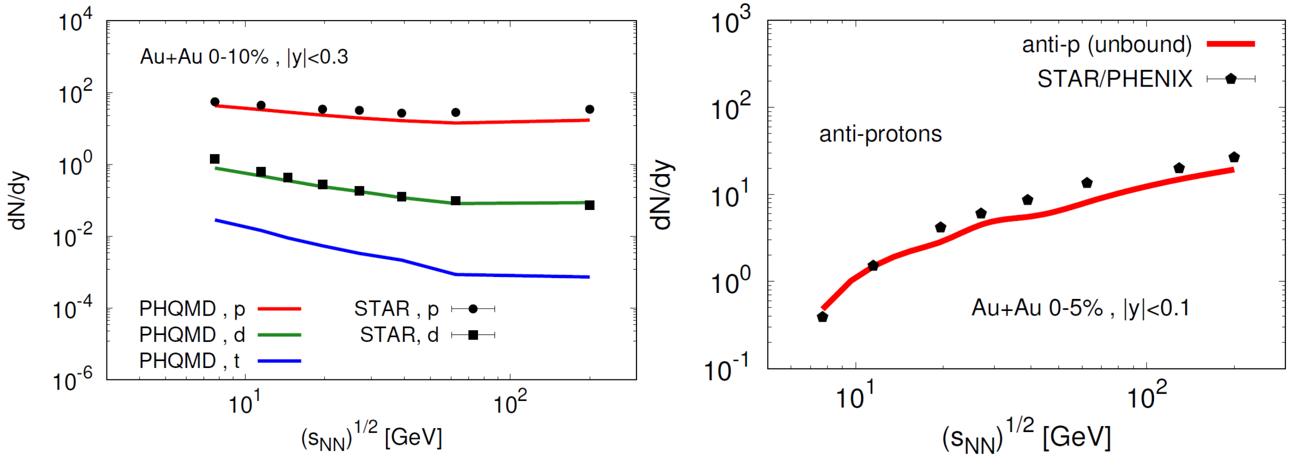
p_T – spectra (BES RHIC)



Excitation function of d/p and anti-d/p ratio at y=0



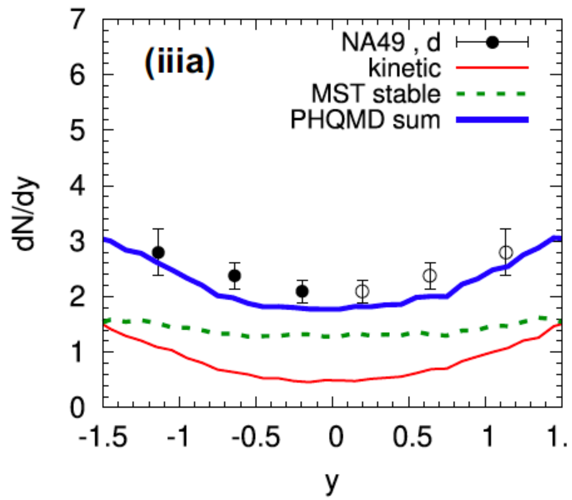
Excitation function dN/dy of p, d, anti-p at midrapidity



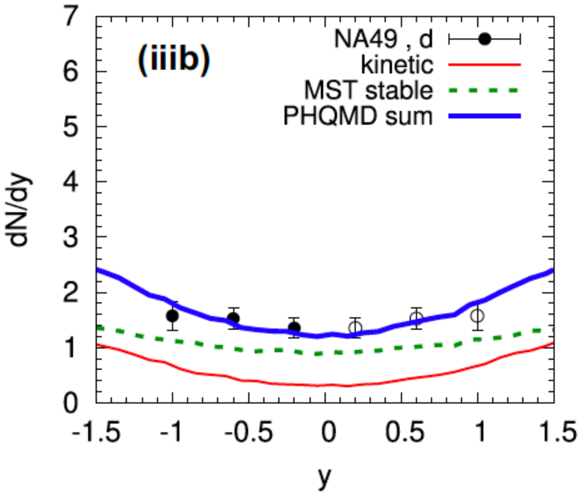
Experimental data on anti-d are well reproduced by the PHQMD

Deuteron rapidity spectra compared to NA49 data

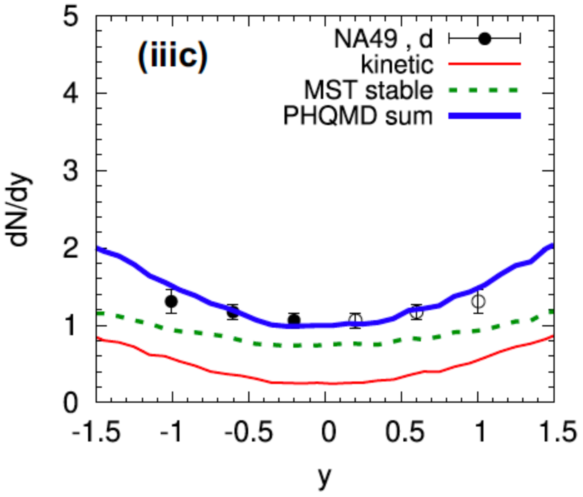
6.3 GeV



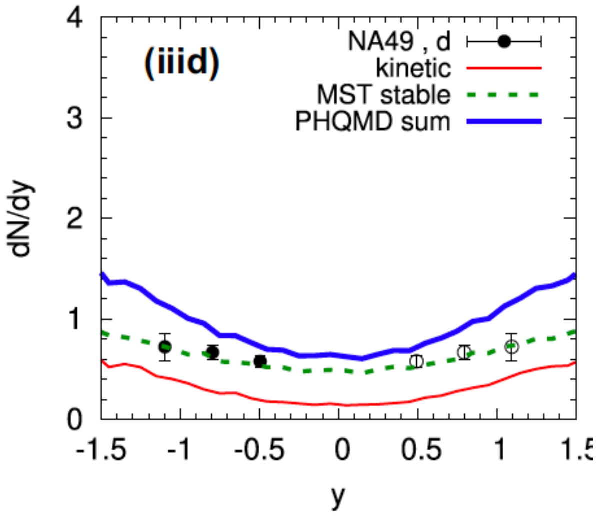
7.6 GeV



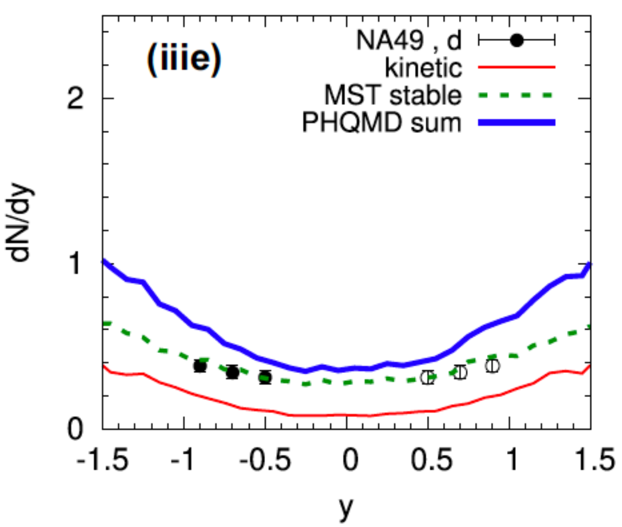
8.8 GeV



12.3 GeV



17.3 GeV



Rapidity spectra are nicely reproduced for energies below 10 GeV.

For higher energies the experimental data are slightly overestimated for |y |> 0.5

(No experimental data for |y| < 0.5.)

T. Anticic et al. (NA49), Phys. Rev. C 94, 044906 (2016).

Coalescence mechanism vs. MST

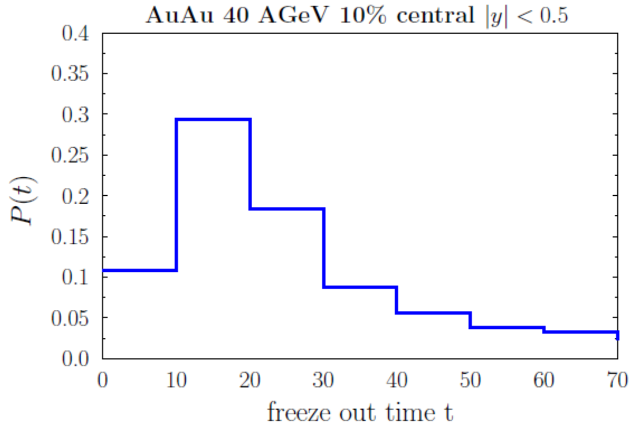
Comparison of coalescence and dynamic clusters (MST+kinetic) in PHQMD:

Coalescence and MST deuterons calculated in the same PHQMD run

Coalescence: Cluster formation at freeze-out time by coalescence radii in coordinate and momentum space

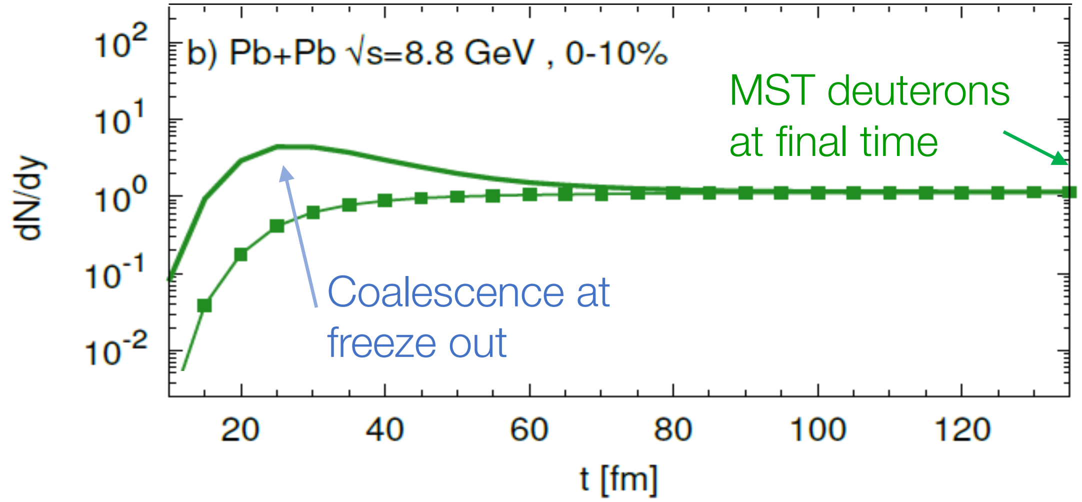
Coalescence parameters from UrQMD:

$\Delta P < 0.285$ GeV and $\Delta R < 3.575$ fm



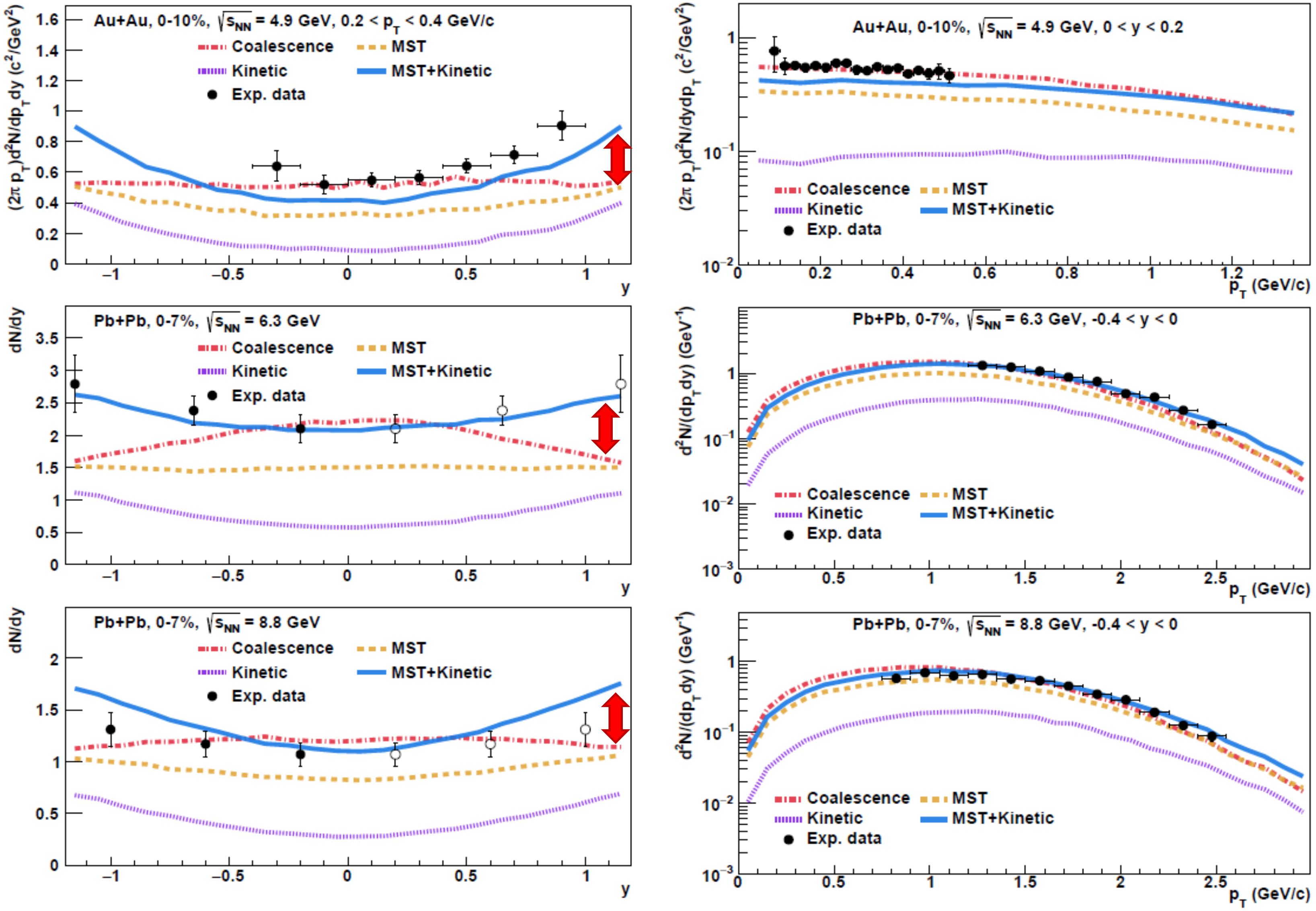
Why can the observables be different in coalescence and MST?

- influence of the potential interaction after nucleon freeze-out
- most of the coalescence deuterons are unbound at freeze-out
- p-n pairs surrounded by other hadrons are part of bigger cluster in MST



V. Kireyeu, et al., Phys. Rev. C 105 (2022) 044909

Mechanism for deuteron production: Coalescence vs. dynamic clusters (aMST+ kinetic)



y- distributions show differences for coalescence/dynamic.

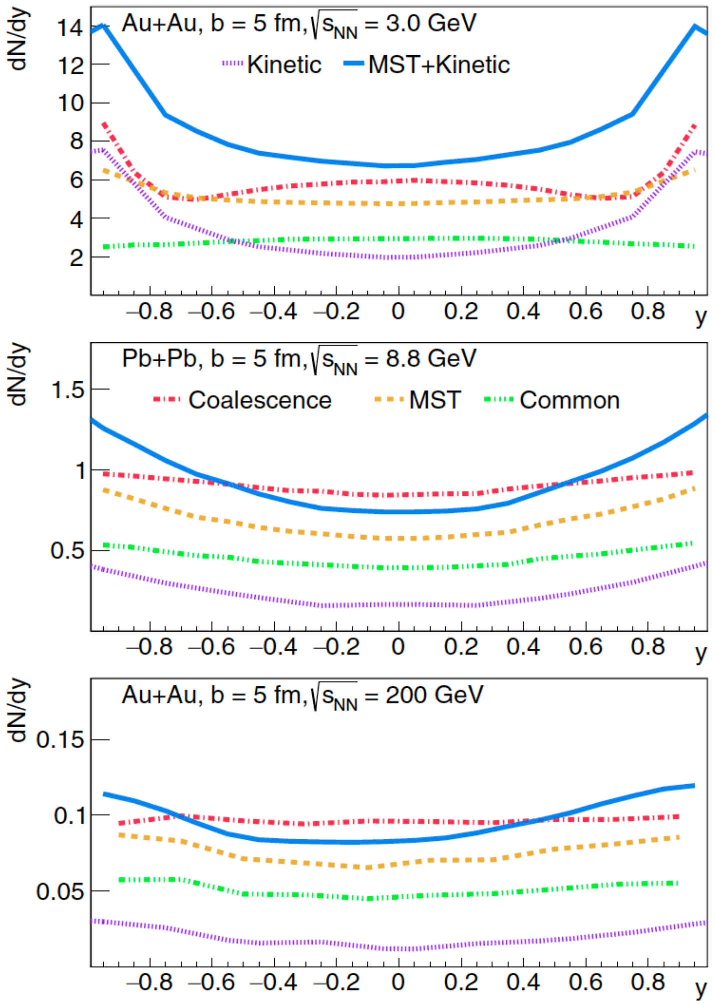
p_T-distributions have a different slope.

The analysis points tentatively to the MST + kinetic scenario but further experimental data are necessary.

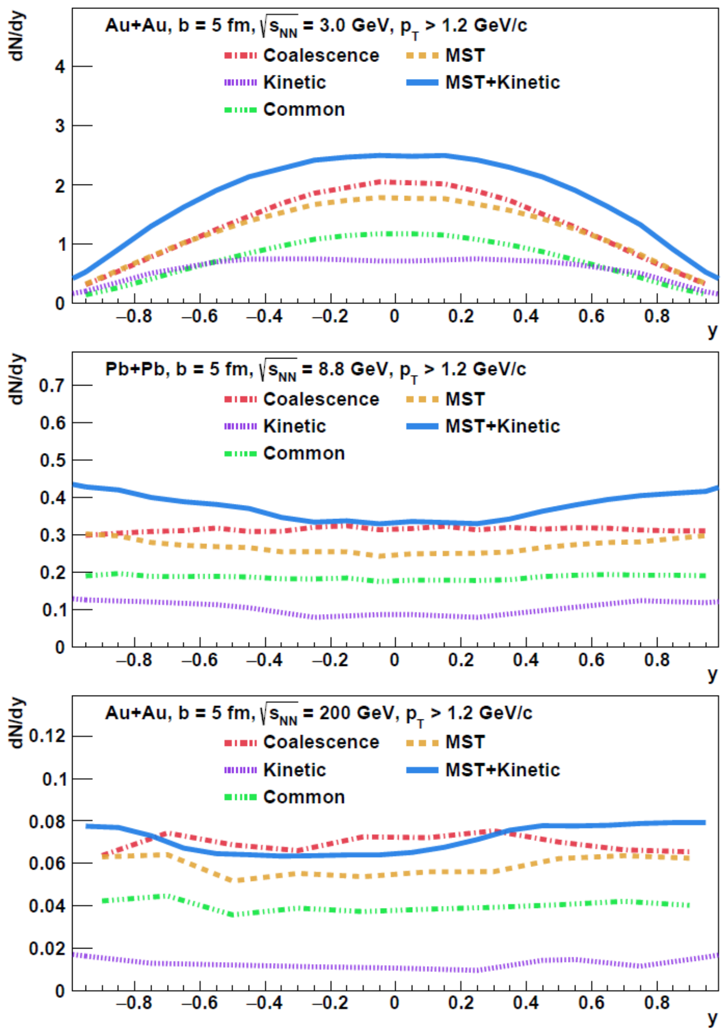
V. Kireyeu et al., PRC109, 044906.

Is the difference big enough for experimental decision?

no p_T cut



p_T > 1.2 GeV/c (STAR experimental acceptance)



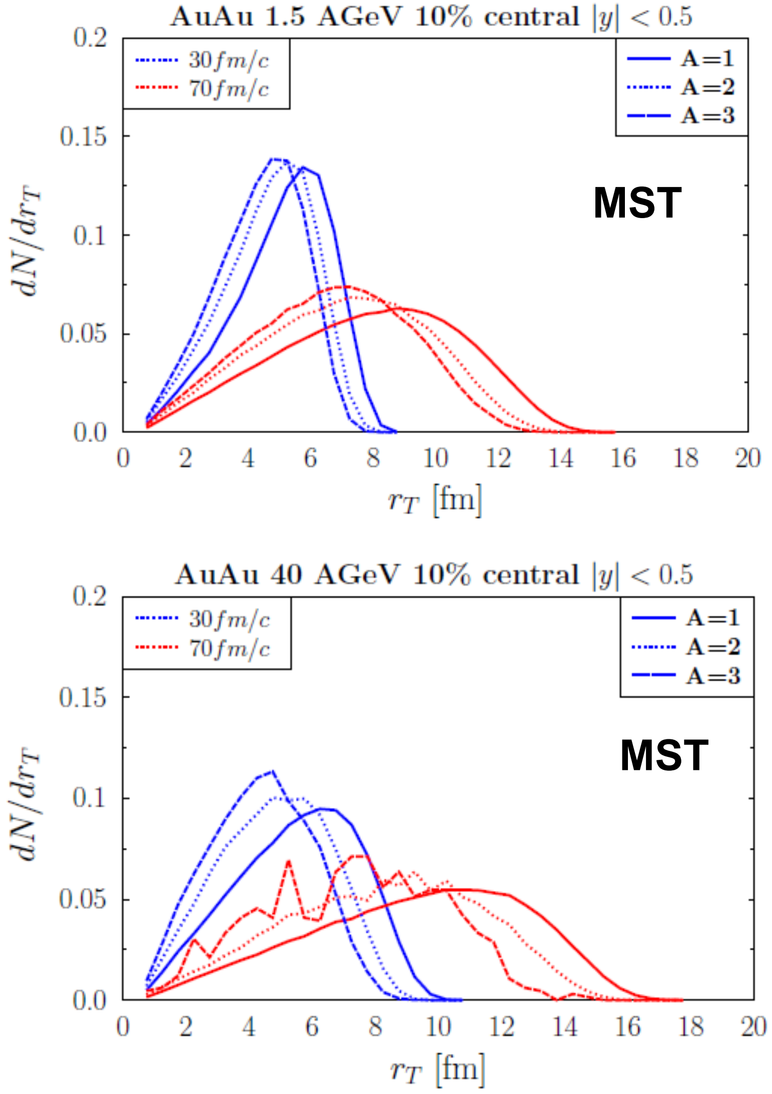
Difference between coalescence and dynamic deuterons is mostly at low p_T.

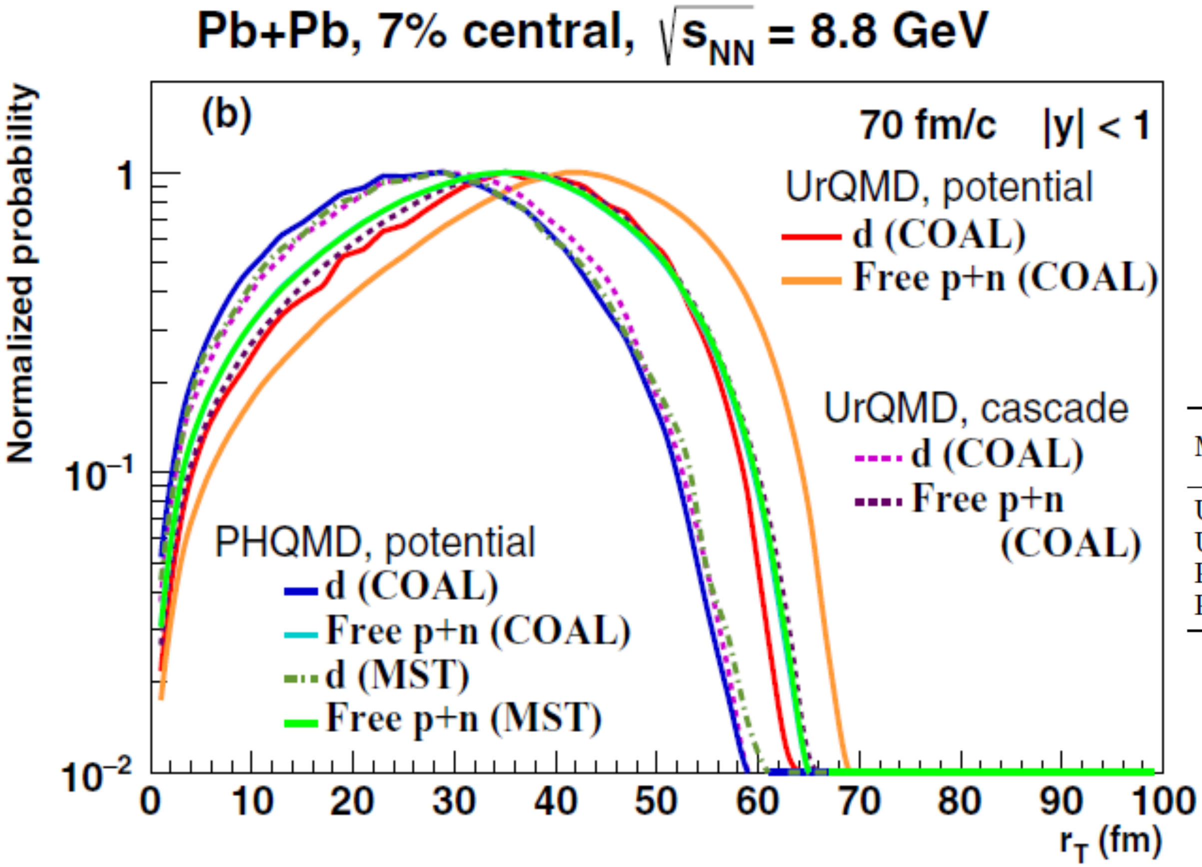
In the measured p_T range signal is gone.

More precise experimental data on rapidity distributions are needed.

V. Kireyeu et al., PRC109, 044906.

PHQMD and UrQMD: Where clusters are formed?





Model mode	r_T (fm) at P_{max} d	p
UrQMD potential	35	41
UrQMD cascade	29	35
PHQMD potential	27	35
PHQMD potential (MST)	29	35

→ Clusters remain closer to the center of the HIC than free nucleons.

V. Kireyeu, J. Steinheimer, M. Bleicher, J. Aichelin, E.B., Phys. Rev. C 105 (2022) 044909

Summary & Conclusion

PHQMD

- is a microscopic n-body transport approach to describe HIC and dynamical cluster formation
- is a combined model: $\boxed{\text{PHSD + QMD + MST | SACA}}$

Clusters are formed dynamically

1) by potential interactions among nucleons and hyperons
   Novel development: momentum dependent potential with soft EoS (talk on Thursday, 14.30 pm by Yue Hang)
2) by kinetic mechanism for d : hadronic inelastic reactions incl. all isospin channels NN $\leftrightarrow$ dπ , πNN $\leftrightarrow$ dπ , NNN $\leftrightarrow$ dN
   + accounting of quantum properties of d: excluded volume & momentum projection condition

The PHQMD reproduces nuclei and hypernuclei dN/dy, dN/dp$_T$, ratios d/p and $\bar{\mathrm{d}}/\bar{\mathrm{p}}$ from SIS to top RHIC energies.

Distinguish mechanisms for cluster production - coalescence or dynamical cluster production – by measurements of dN/dy beyond mid-rapidity and for low pT.

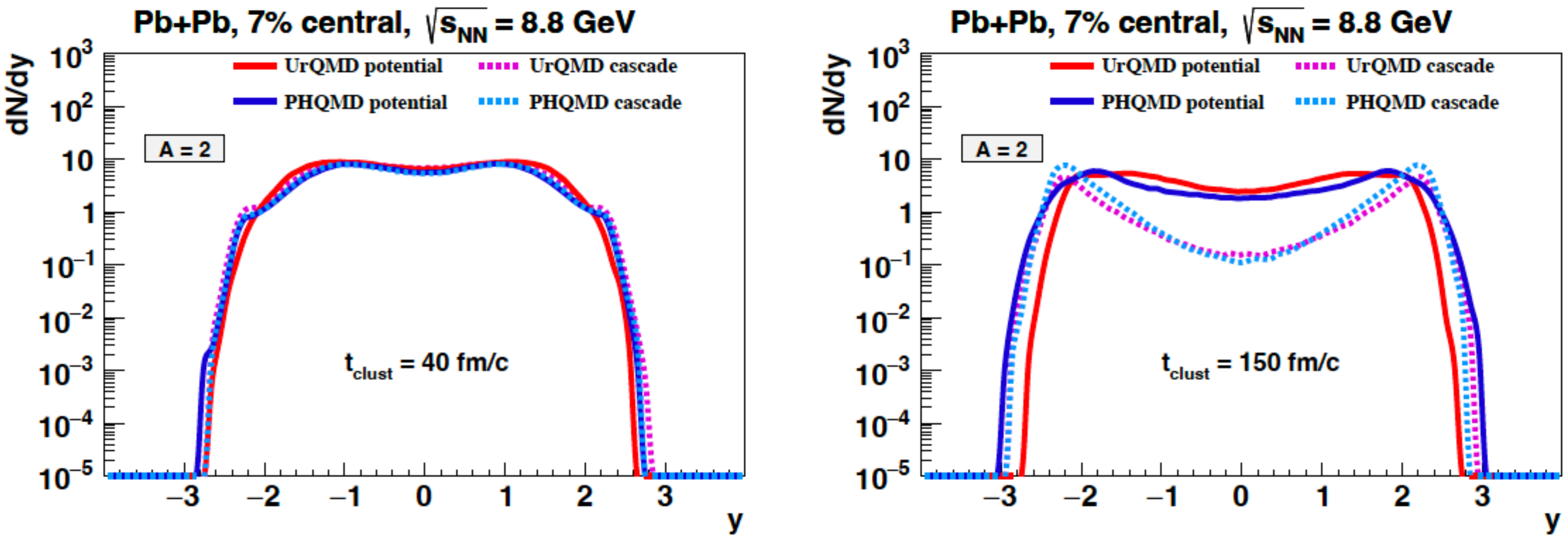
Stable clusters are formed behind the front of the energetic hadrons ➔ since the 'fire' is not at the same place as the 'ice', cluster can survive.

THANK YOU FOR YOUR ATTENTION.

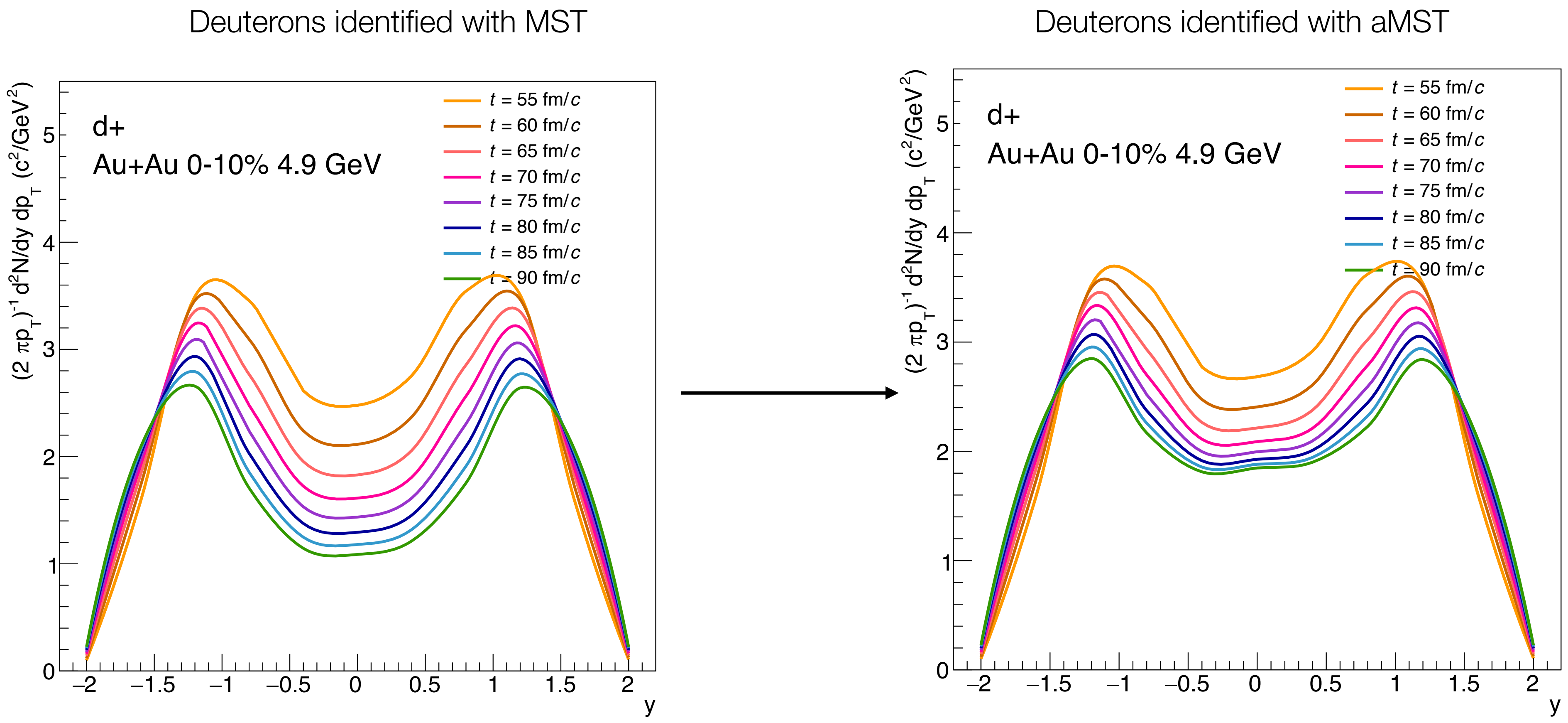
Modeling of dynamic cluster formation in HIC

At t=40 fm/c: the yields and the shape of the deuteron distribution are nearly identical
-> 2-particle correlations are similar with and without potential interaction.

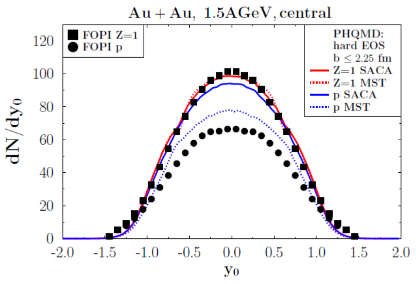
At later times: only simulations including the nucleon-nucleon potential keep the clusters bound, for the simulations without potential the deuteron yield decreases at central rapidities.

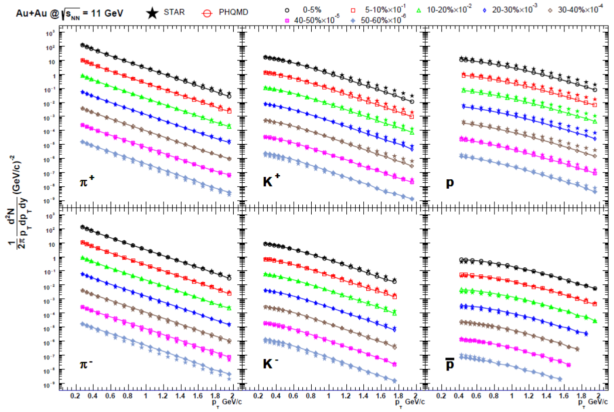


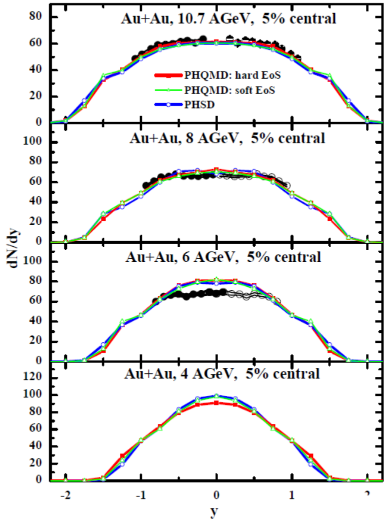
Cluster stability over time with and without stabilisation

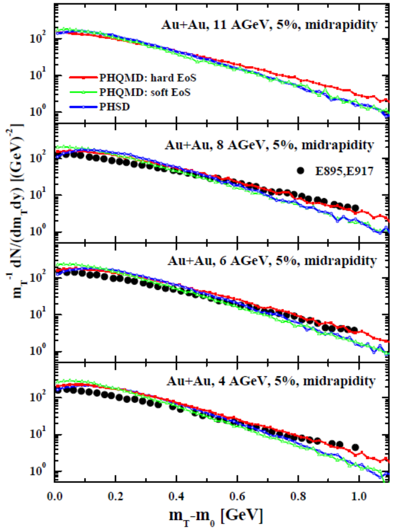


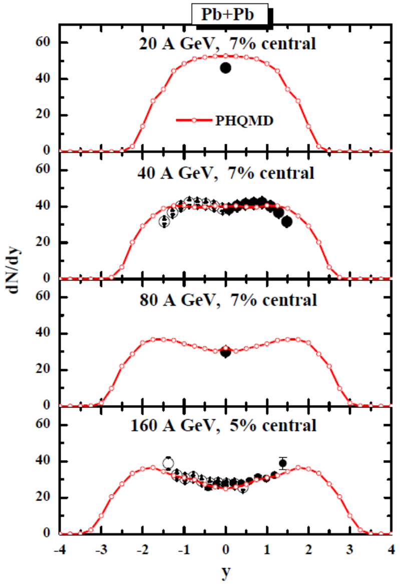
Highlights: PHQMD ‚bulk‘ dynamics from SIS to RHIC

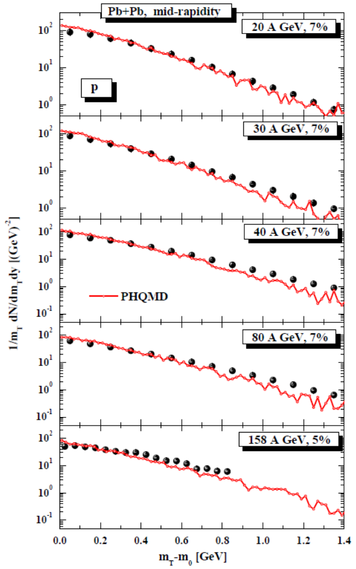


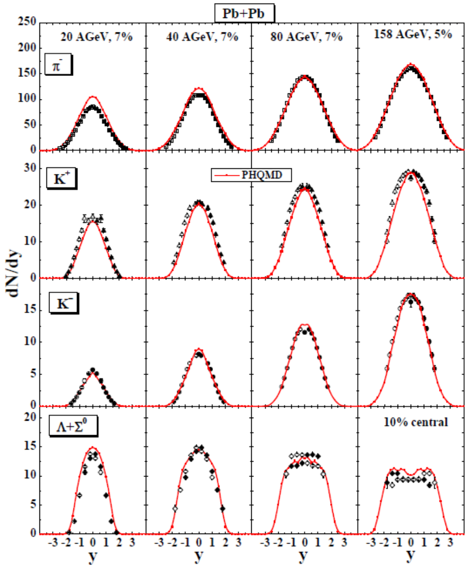


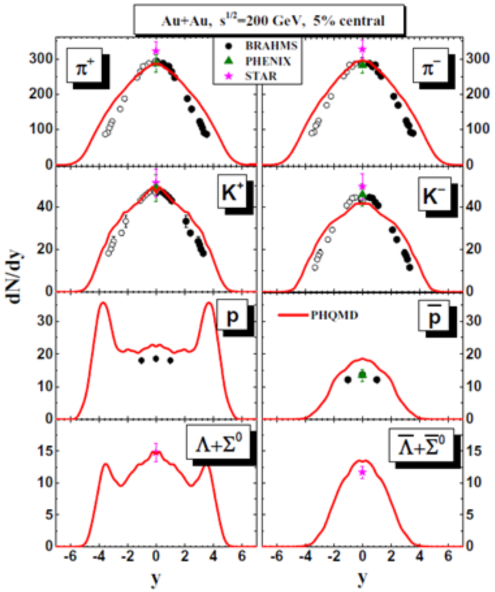












PHQMD: J. Aichelin et al., PRC 101 (2020) 044905

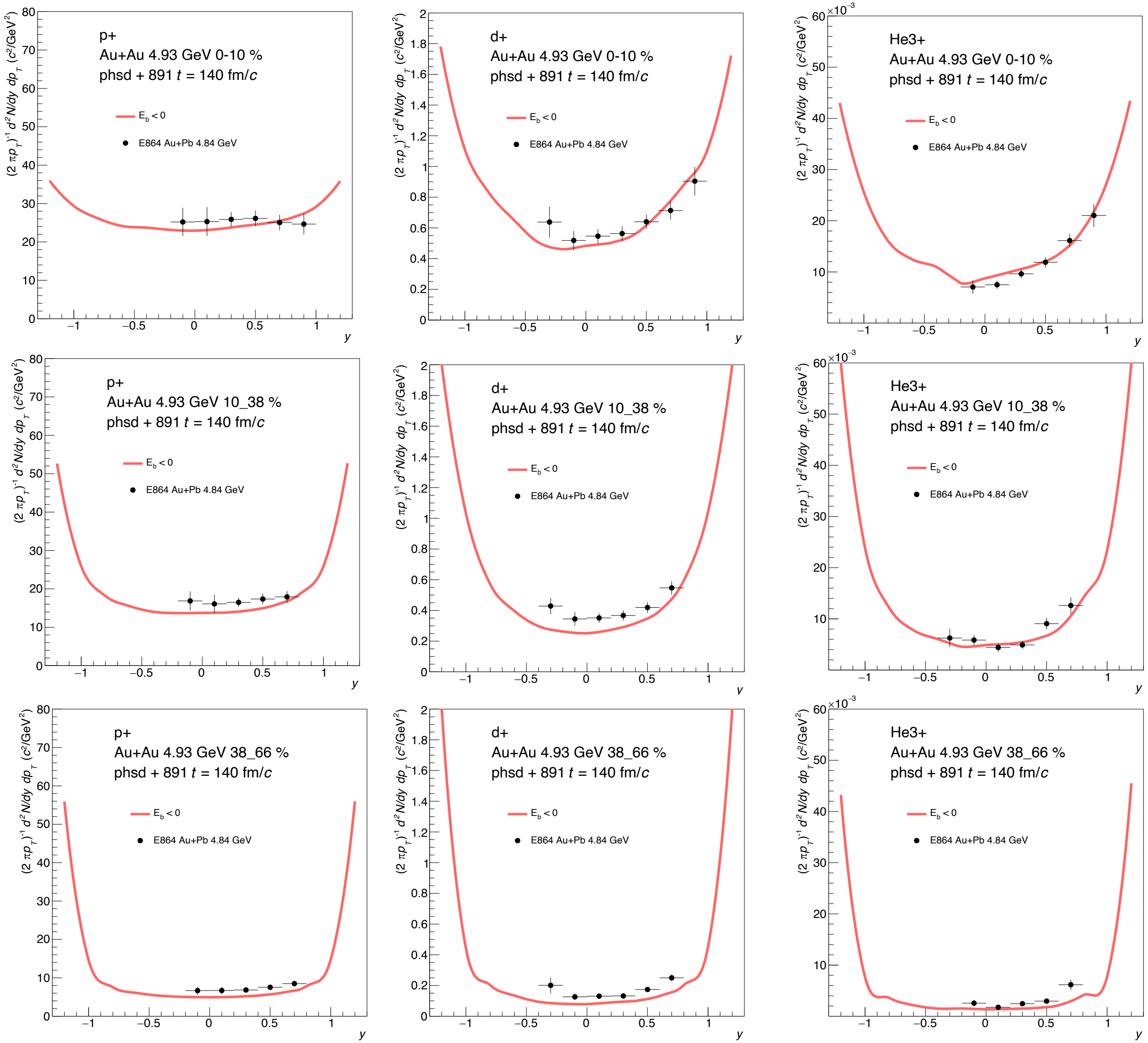
=> PHQMD provides a good description of hadronic ‘bulk’ observables from SIS to RHIC energies.

Rapidity spectra compared to experimental data at 4.9 GeV

0-10 %

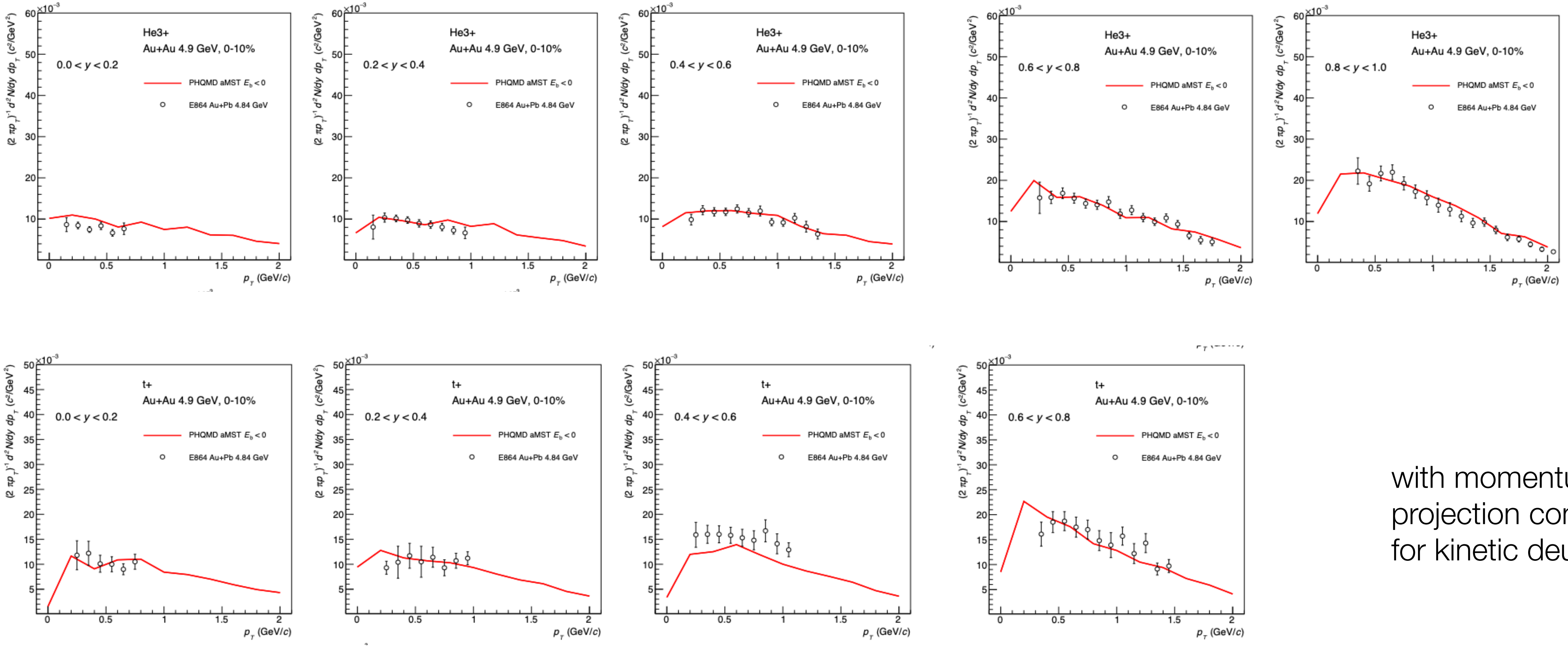
10-38 %

38-66 %



with momentum projection condition for kinetic deuterons

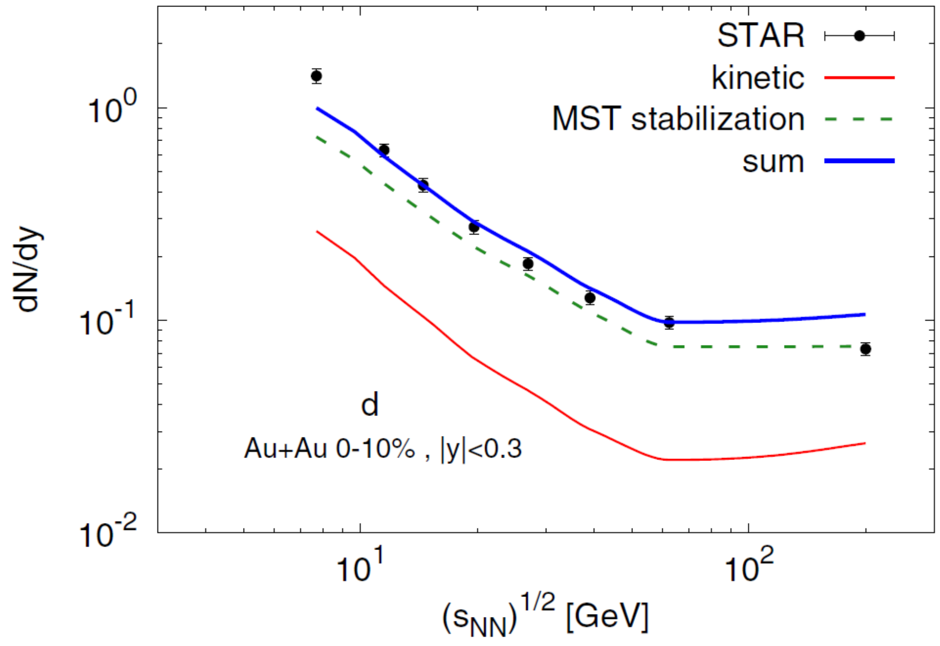
p_T spectra compared to experimental data at 4.9 GeV



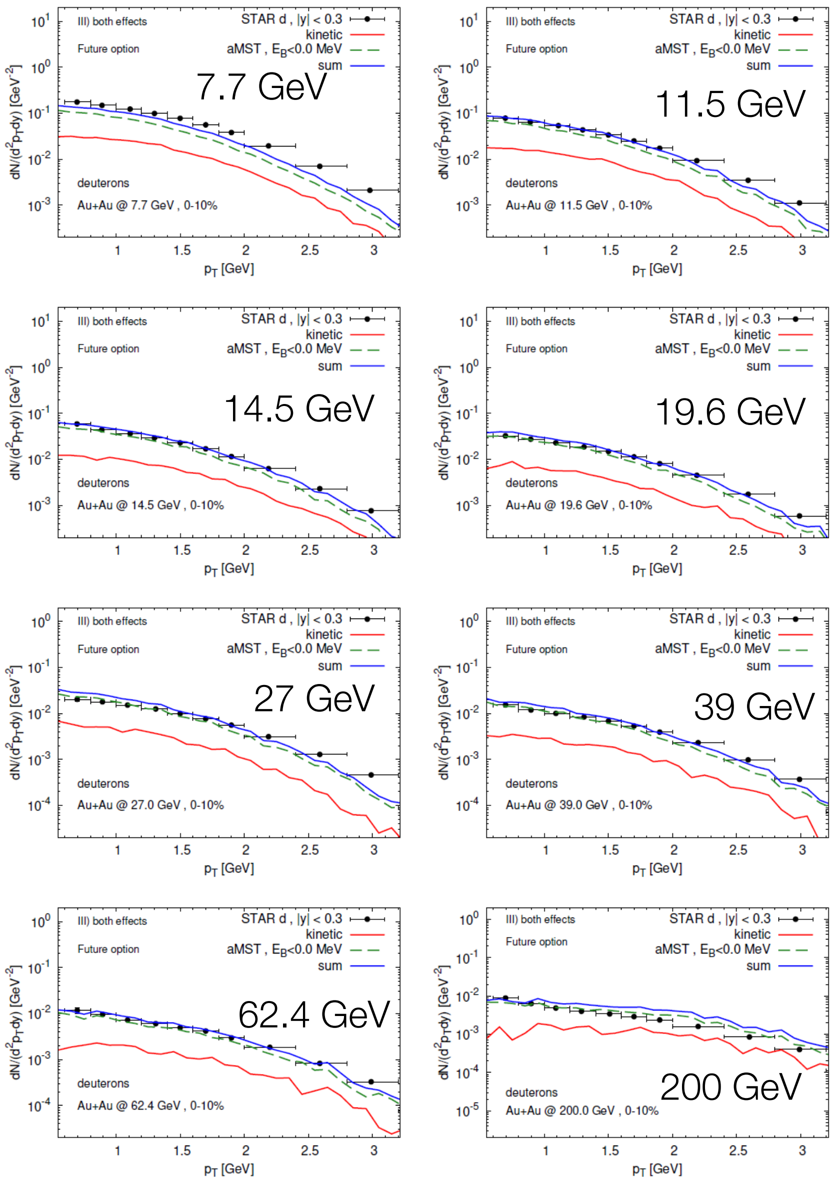
with momentum projection condition for kinetic deuterons

Deuteron production compared to STAR data

Excitation function dN/dy of deuterons at midrapidity



p_T – spectra (BES RHIC)



PHQMD provides a good description of STAR data.

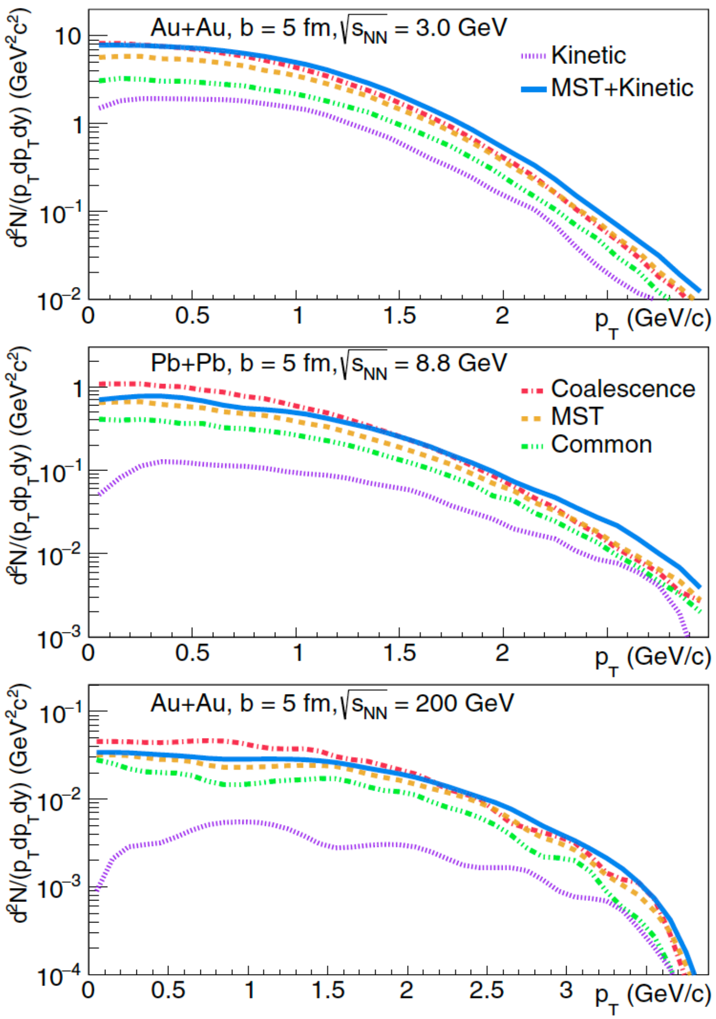
Functional forms of p_T-spectra are similar for kinetic and potential d.

The potential mechanism is dominant for d production at all energies.

G. Coci et al., Phys.Rev.C 108 (2023) 014902.

J. Adam et al. (STAR), Phys. Rev. C 99, 064905 (2019)

p_T-spectra of coalescence and dynamic clusters



p_T cut can change the form of the rapidity distributions at both, low and high energies. measurement of low pT deuterons is necessary to identify the production mechanism.

Distribution of 'coalescence' and 'potential' deuterons agree at large p_T for the two lower energies.
at small p_T the spectra differ.

Clusters, which are produced by coalescence but which are not bound at the end (and therefore do not appear as 'potential' deuterons), are concentrated at low pT