Cluster production in PHQMD

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&
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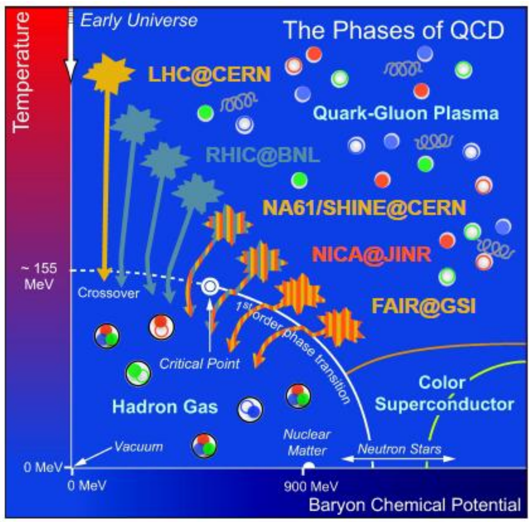
EMMI Workshop
'Collective phenomena and the Equation-of-State of dense baryonic matter'
10-13 November, 2025, GSI Darmstadt

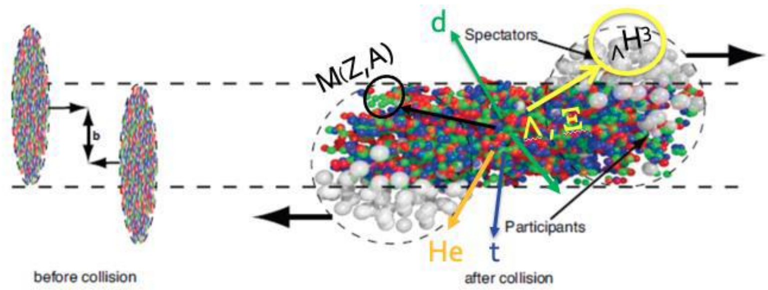
Cluster production in heavy-ion collisions

The phase diagram of QCD

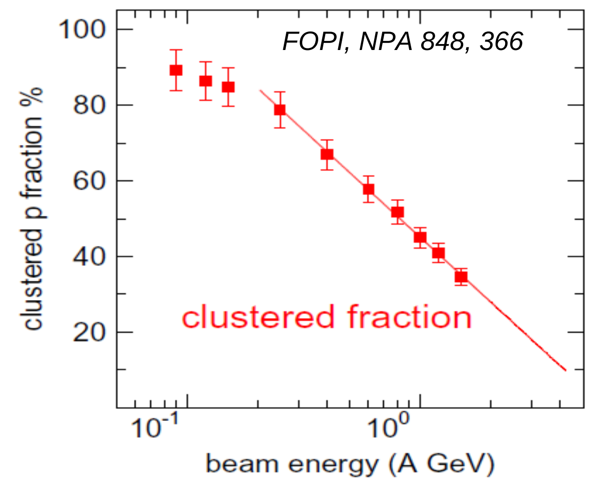


Clusters and (anti-) hypernuclei

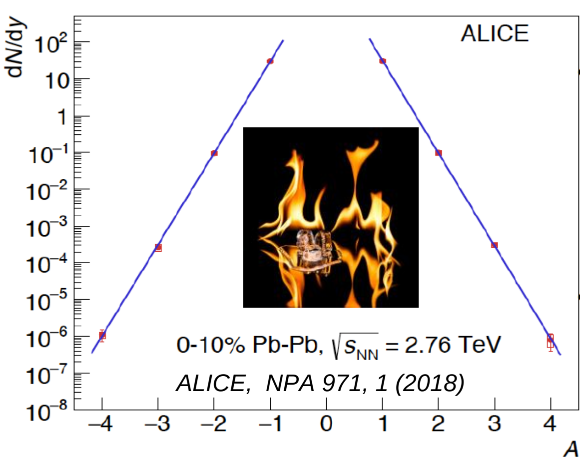
are observed experimentally at all energies



- **Clusters are very abundant at low energy**



Au+Au, central. midrapidity



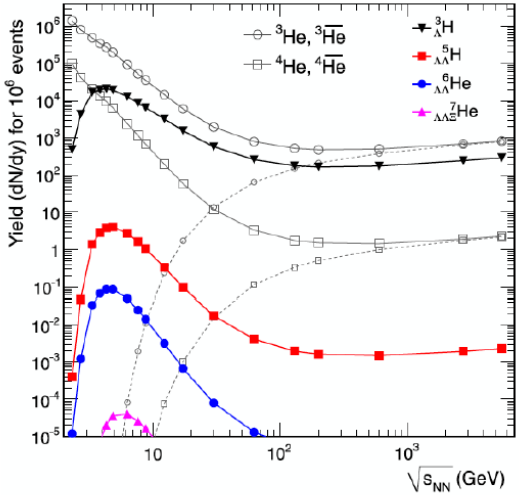
- **High energy HIC:**
  ‚Ice in a fire' puzzle:
  how the weakly bound objects can be formed and survive in a hot enviroment?!

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

Modeling of cluster and hypernuclei formation

Existing models for cluster formation:

A. Andronic et al., PLB 697, 203 (2011)



❑ **statistical model:**
- **assumption of thermal equilibrium**

In order to understand the microscopic origin of cluster formation one needs a realistic model for the dynamical time evolution of the HIC

Dynamical Models:

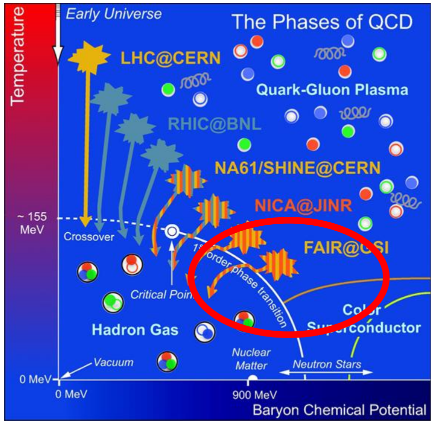
I. cluster formation by coalescence mechanism at a freeze-out time by coalescence radii in coordinate and momentum space

II. dynamical modeling of cluster formation - based on interactions – within microscopic transport models:

PHQMD

– perturbative‚potential‘ mechanism - via potential NN (NY) interactions (applied during the whole reaction time of HIC) + cluster recognition framework

– ‘kinetic‘ mechanism - by hadronic scattering (hadronic reactions as NNN→ dN ; NNπ→ dπ, NN→ dπ)



Study of QCD matter with heavy-ions

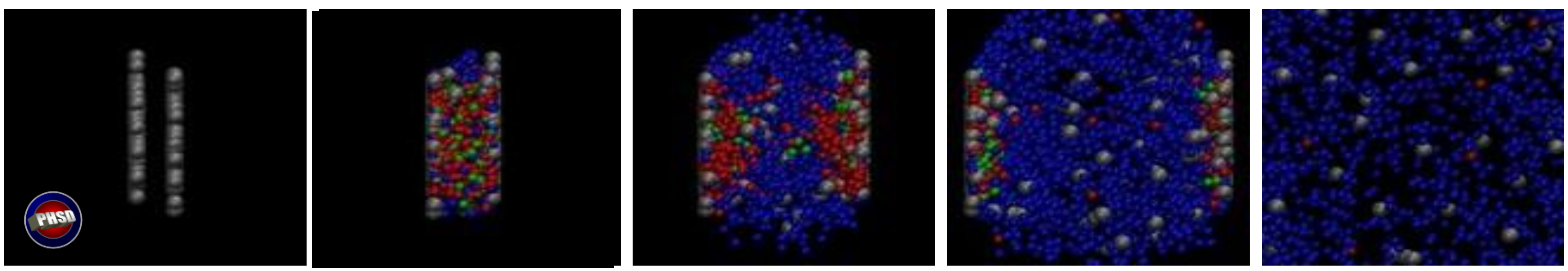
Goal: Microscopic modeling of heavy-ion collisions

PHSD & PHQMD

Parton-Hadron-String Dynamics & Parton-Hadron-Quantum-Molecular Dynamics

is a unified non-equilibrium microscopic transport approach for the description of the dynamics of strongly-interacting hadronic and partonic matter created in heavy-ion collisions and p+A, p+p, π+A reactions from SIS to LHC energies

Initial state: Au+Au	Quark-Gluon Plasma: lQCD EoS non-perturbative QCD - quasiaprticles	Dynamical Hadronization	Hadronic interactions ➔final hadrons + leptons



time

➔ **provides a continuous description of the HIC dynamics:**
– no artificial transition from micro- to macro-description as in hydro-type models, no jump in entropy and energy density

PHSD,PHQMD are the open source codes, available for all experimental collaborations (used by GSI/FAIR collaborations, linked to the exp. software) and upon registration for other users

PHSD/PHQMD code

Realization: parallel ensemble method

Computer language: Fortran

PHSD mode

Initialization A+A
+ propagation of baryons:
Mean Field dynamics
(BUU)

PHQMD mode

Initialization A+A
+ propagation of baryons:
Quantum Molecular dynamics
(QMD) – n-body model

Propagation of partons (quarks, gluons) and mesons:
Mean Field dynamics (Kadanoff-Baym, BUU)

↓

Collision integral = interactions of hadrons and partons (QGP)

↓

Optionally

Cluster recognition: MST (Minimum Spanning Tree)
or SACA (Simulated Annealing Clusterization Algorithm)
or coalescence mechanism + kinetic deuterons

↓

Final output – "events" : OSCAR, ROOT, Rivet formats

QMD propagation (EoM)

- **Generalized Ritz variational principle**:

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

Many-body wave function:

$$\psi(t) = \prod_{i=1}^{N} \psi(\mathbf{r}_i, \mathbf{r}_{i0}, \mathbf{p}_{i0}, t)$$

Ansatz:
Gaussian trial wave function (with width L) centered at r_{i0}, p_{i0}

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

L=4.33 fm²

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

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

Many-body Hamiltonian:

$$H = \sum_i H_i = \sum_i (T_i + V_i) = \sum_i (T_i + \sum_{j \neq i} V_{i,j})$$

[Aichelin, Phys. Rept. 202 (1991)]

- **Nucleon-nucleon local two-body potential:**

$$V_{ij} = V(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_{i0}, \mathbf{r}_{j0}, \mathbf{p}_{i0}, \mathbf{p}_{j0}, t) = V_{\mathrm{Skyrme\ loc}} + V_{\mathrm{mom}} + V_{\mathrm{Coul}}$$

momentum dependent potential

➔ **Single-particle potential <V> :**

1) Skyrme potential ('static') :

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

with relativistic extended interaction density:

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

Momentum dependent potential → EoS in PHQMD

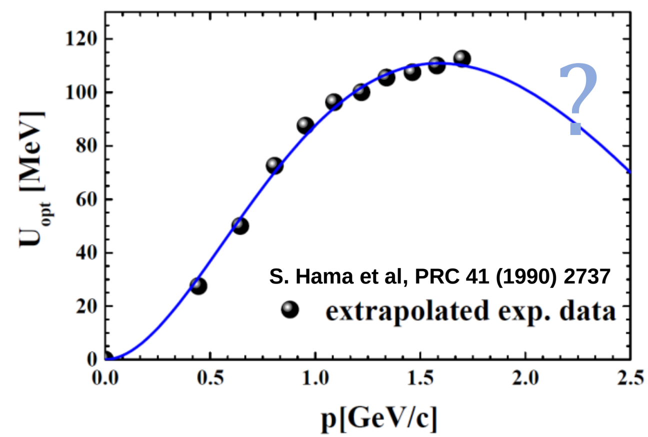
2) Momentum dependent potential :

V. Kireyeu et al., arXiv:2411.04969

$$V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{p}_{01}, \mathbf{p}_{02}) = (a\Delta p + b\Delta p^2)\ exp[-c\sqrt{\Delta p}]\ \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

$$\Delta p = \sqrt{(\mathbf{p}_{01} - \mathbf{p}_{02})^2}$$

Parameters a, b, c are fitted to the "optical" potential (Schrödinger equivalent potential U_{SEP}) extracted from elastic scattering data in pA: $U_{SEQ}(p) = \frac{\int^{p_F} V(\mathbf{p} - \mathbf{p}_1) dp_1^3}{\frac{4}{3}\pi p_F^3}$



- **In infinite matter a potential corresponds to an EoS:**

$$E/A(\rho) = \frac{3}{5}E_F + V_{Skyrme\ stat}(\rho) + V_{mom}(\rho)$$

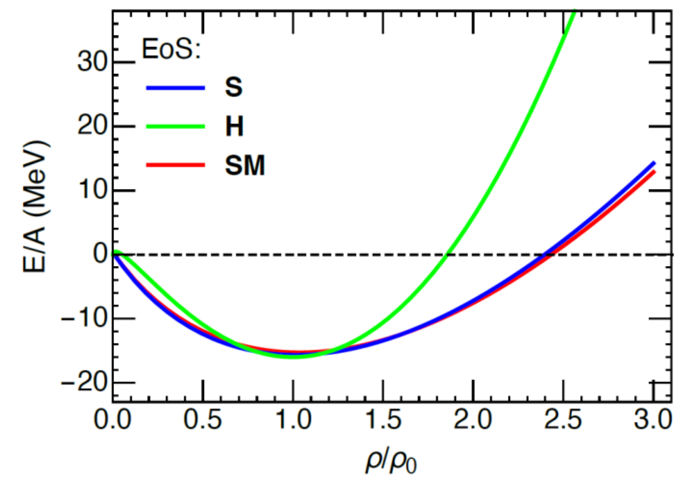
$$V_{Skyrme} = \alpha\frac{\rho}{\rho_0} + \beta\frac{\rho}{\rho_0}^{\gamma}$$

compression modulus K of nuclear matter:

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

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
	a $[MeV^{-1}]$	b$[MeV^{-2}]$	c$[MeV^{-1}]$	
	236.326	-20.73	0.901	

EoS for infinite cold nuclear matter at rest



Cf. talk by Jörg Aichelin (Tuesday, 11:00)

Mechanisms for cluster production in PHQMD:

I. MST: potential interactions, recongnized by MST

&

II. kinetic reactions for deuterons

III. Coalescence (to compare with I+II)

PHQMD

I. Cluster recognition: Minimum Spanning Tree (MST)

R. K. Puri, J. Aichelin, J.Comp. Phys. 162 (2000) 245-266

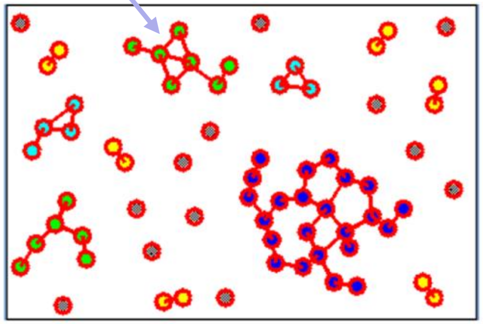
The Minimum Spanning Tree (MST) is a cluster recognition method applicable for the (asymptotic) final states where coordinate space correlations may only survive for bound states.

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

1. **Two particles are 'bound' if their distance in the cluster rest frame fulfills**

$$|\vec{r_i} - \vec{r_j}| \le 4 \text{ fm} \quad \text{(range of NN potential)}$$

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

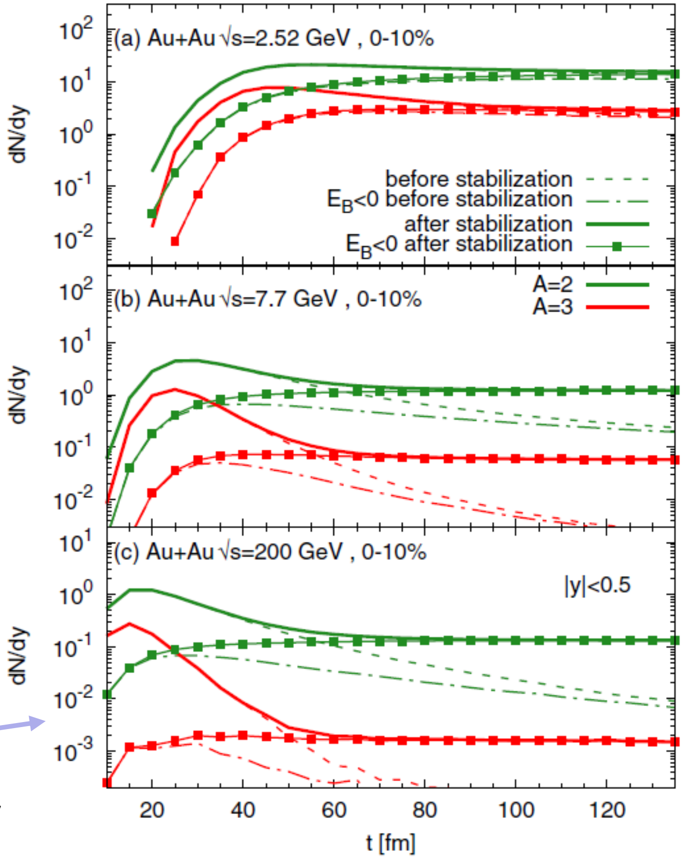


* Remark: inclusion of an additional momentum cut (coalescence) leads to small changes: particles with large relative momentum are almost never at the same position (V. Kireyeu, Phys.Rev.C 103 (2021) 5)

Advanced MST (aMST)

- **MST + extra condition: E_B<0 negative binding energy for identified clusters**

- **Stabilization procedure – to correct artifacts of the semi-classical QMD: recombine the final "lost" nucleons back into cluster if they left the cluster without rescattering**



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

II. Deuteron production by hadronic reactions

"Kinetic mechanism"

1) hadronic inelastic reactions NN ⟷ dπ , πNN ⟷ dπ , NNN ⟷ dN
2) hadronic elastic π+d, N+d reactions

SMASH: D. Oliinychenko et al., PRC 99 (2019) 044907;
J. Staudenmaier et al., PRC 104 (2021) 034908
AMPT: R.Q. Wang et al. PRC 108 (2023) 3

- **Collision rate** for hadron "*i*" is the number of reactions in the **covariant volume** d^{4}x = dt*dV
- With **test particle ansatz the transition rate for 3→2 reactions**:

W. Cassing, NPA 700 (2002) 618

$$\frac{\Delta N_{coll}[3+4+5 \to 1(d)+2]}{\Delta N_3 \Delta N_4 \Delta N_5} = P_{3,2}(\sqrt{s})$$

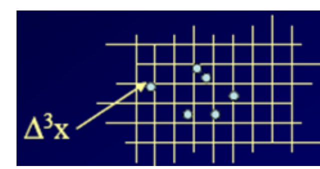
$$P_{3,2}(\sqrt{s}) = F_{spin} F_{iso} P_{2,3}(\sqrt{s}) \frac{E_1^f E_2^f}{2E_3E_4E_5} \frac{R_2(\sqrt{s}, m_1, m_2)}{R_3(\sqrt{s}, m_3, m_4, m_5)} \frac{1}{\Delta V_{cell}}$$

Energy and momentum of final particles

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

$$P_{2,3}(\sqrt{s}) = \sigma_{tot}^{2,3}(\sqrt{s}) v_{rel} \frac{\Delta t}{\Delta V_{cell}}$$

➔ solved by **stochastic method**



- Numerically tested in **"static" box**: PHQMD provides a good agreement with analytic solutions from rate equations and with SMASH for the same selection of reactions
- **New in PHQMD: π+N+N⟷ d+π** inclusion of **all possible isospin channels** allowed by total isospin T conservation ➔ enhancement of the d production

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

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

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

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

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

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

Modelling finite-size effects in kinetic mechanism

G. Coci et al., PRC 108 (2023) 014902

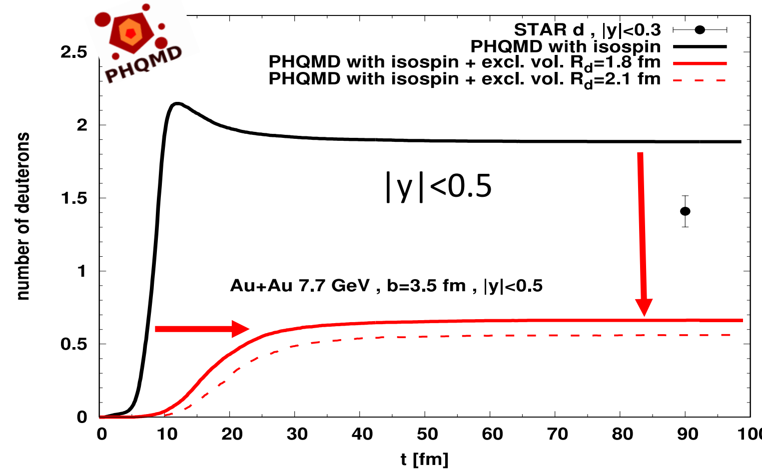
How to account for the **quantum nature of deuteron**, i.e. for

1) the **finite-size of *d* in coordinate space** (*d* is not a point-like particle) – for in-medium d production
2) the **momentum correlations of *p* and *n*** inside *d*

Realization:

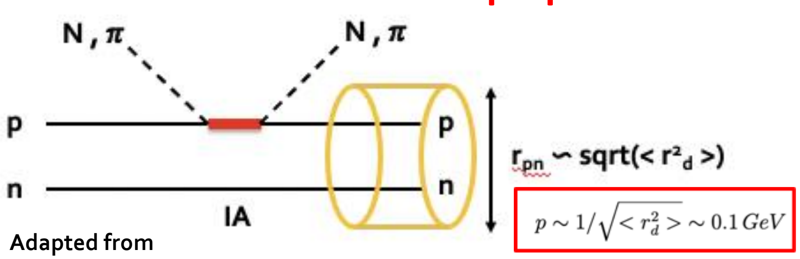
1) assume that a deuteron can not be formed in a high density region, i.e. if there are other particles (hadrons or partons) inside the 'excluded volume':

Excluded-Volume Condition: $|\vec{r}(i)^* - \vec{r}(d)^*| < R_d$

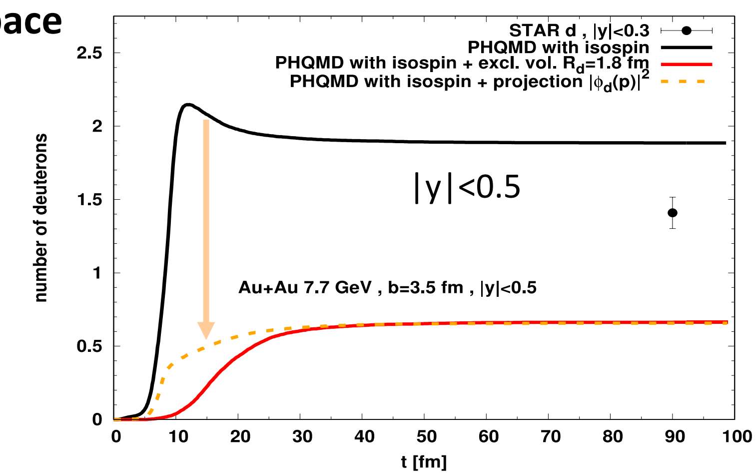


- ❑ **Strong reduction of d production**
- ❑ p_T slope is not affected by excluded volume condition

2) QM properties of deuteron must be also in momentum space
→ **momentum correlations of pn-pair**



Adapted from
[Haidelbauer, Uzikov PLB 562(2003)]
[Hoftiezer et al. PRC23 (1981)]
Same spirit as AMPT [K.-J. Sun, R. Wang, C.-M. Ko et al., 2106.12742]

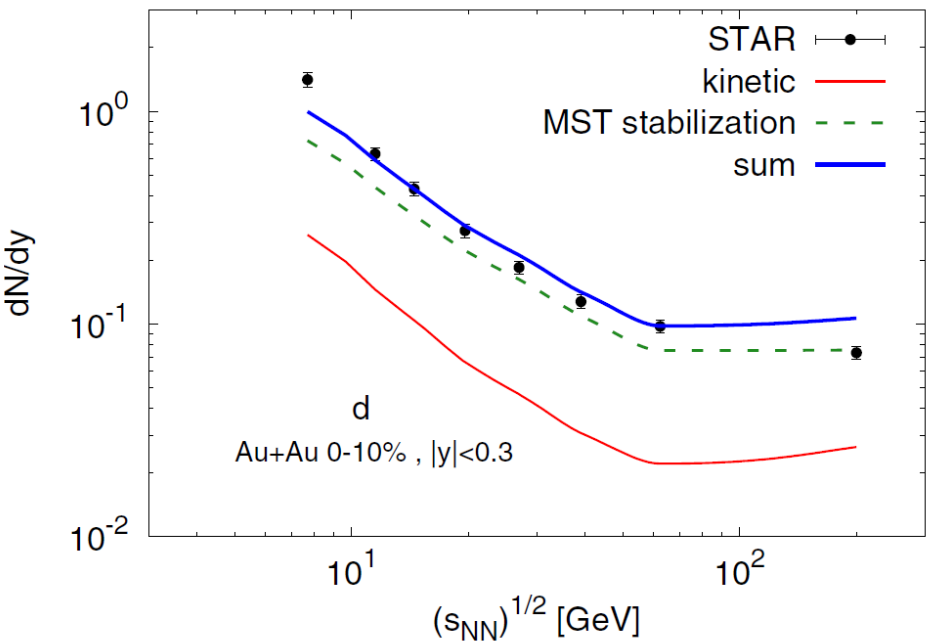


- ❑ **Strong reduction of d production** by projection on DWF $|\phi_d(p)|^2$

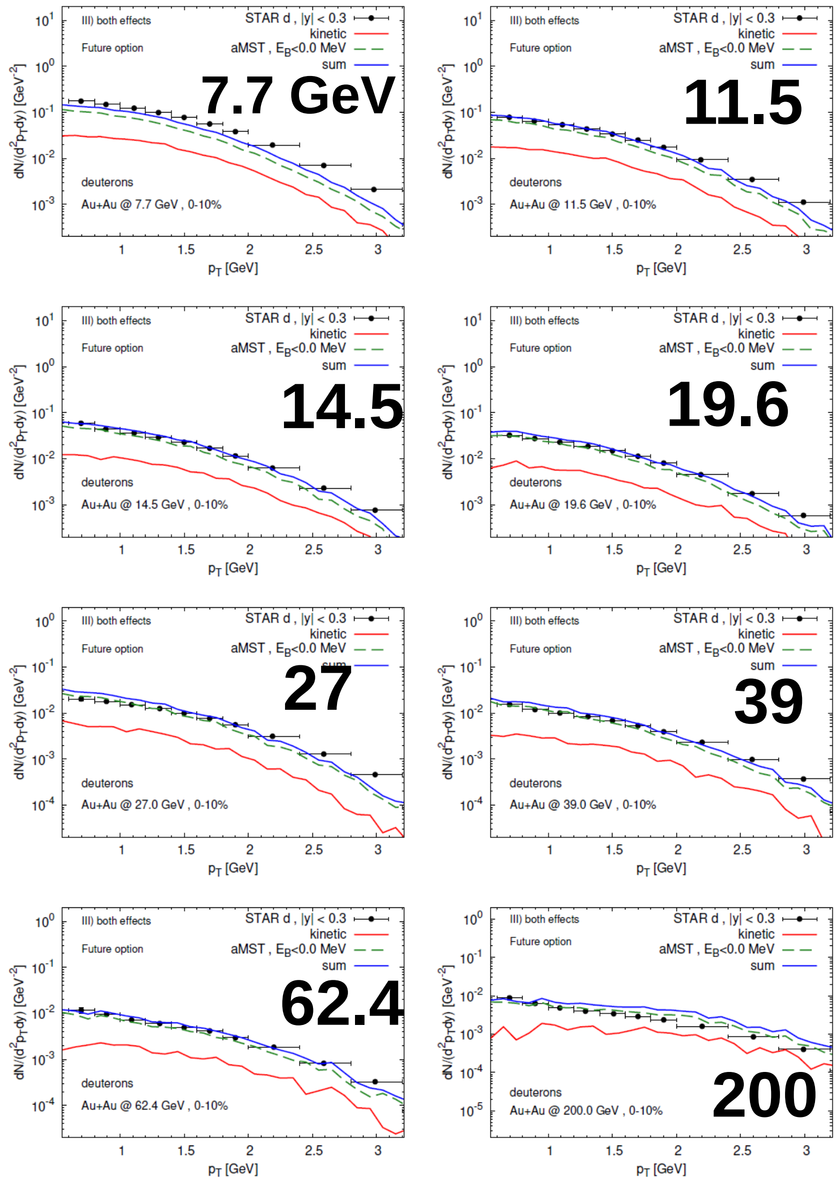
PHQMD

Kinetic vs. potential deuteron production

Excitation function dN/dy of deuterons at midrapidity



p_T – spectra (BES RHIC)

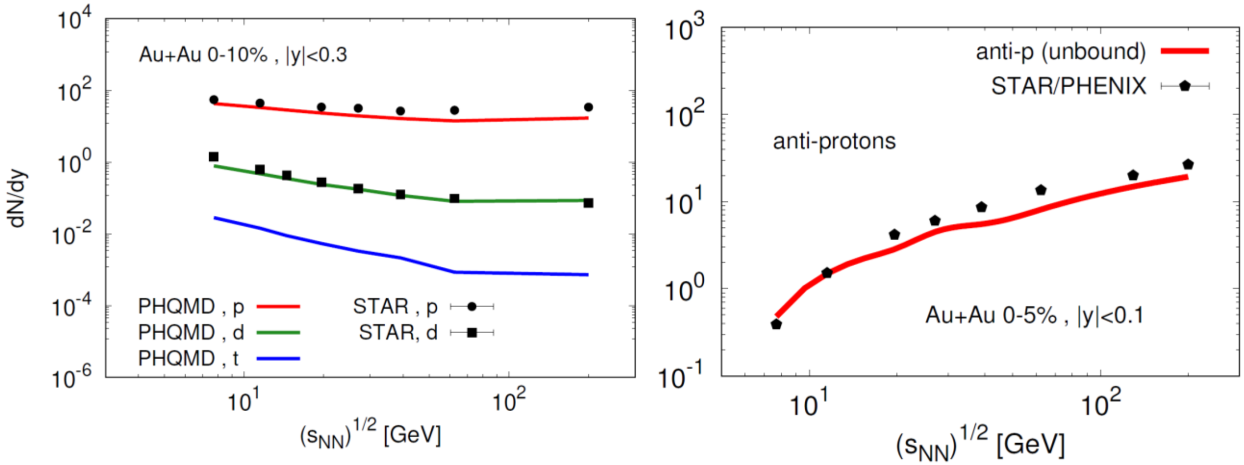


- PHQMD provides a good description of STAR data
- Functional forms of y- and p_T-spectra are slightly different for kinetic and potential deuterons
- **The potential mechanism is dominant for d production at all energies!**

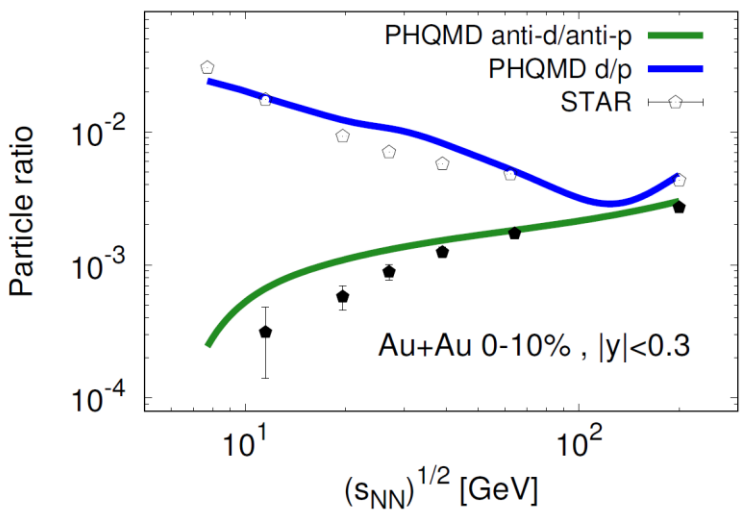
G. Coci et al., Phys.Rev.*C* 108 (2023) 014902

Anti-deuteron versus deuteron production

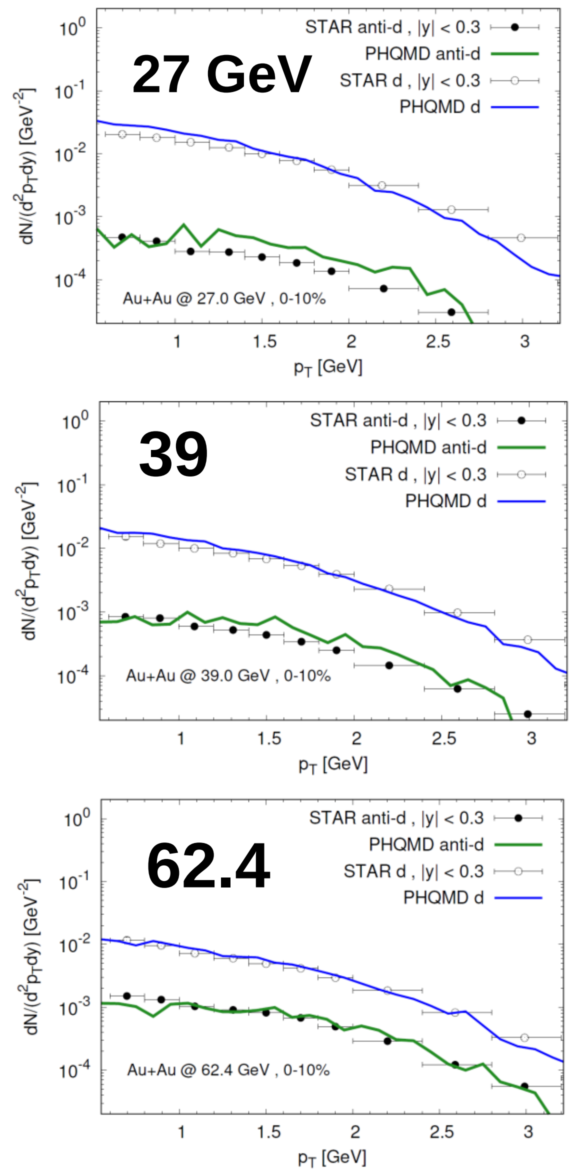
Excitation function dN/dy of p, d, anti-d at midrapidity



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



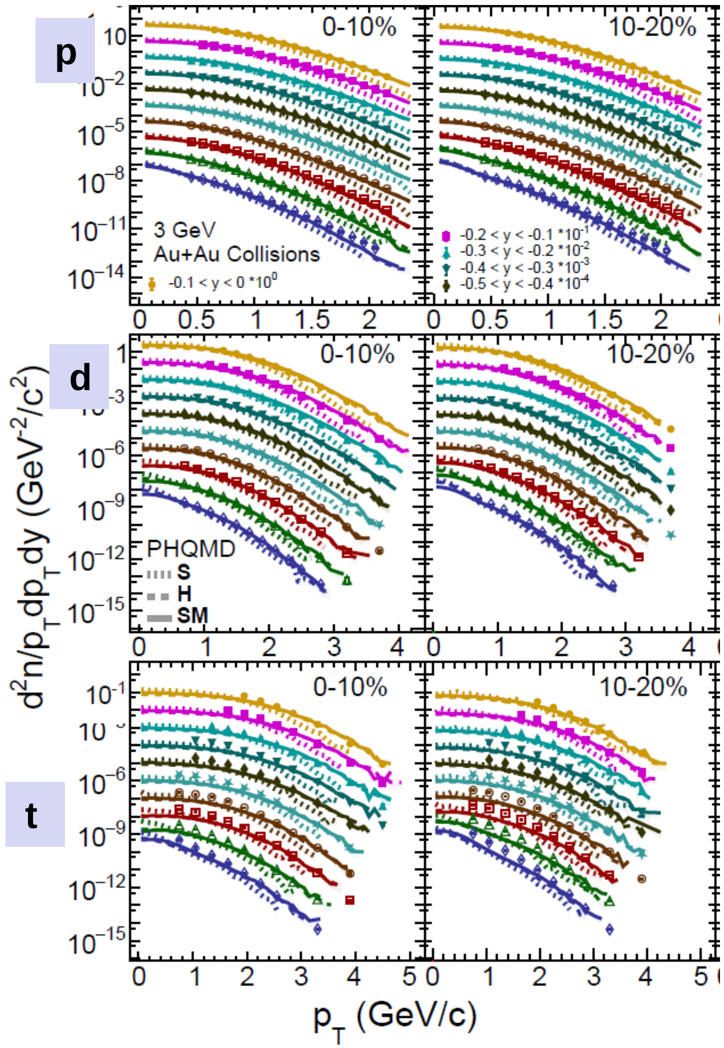
p_T – spectra (BES RHIC)

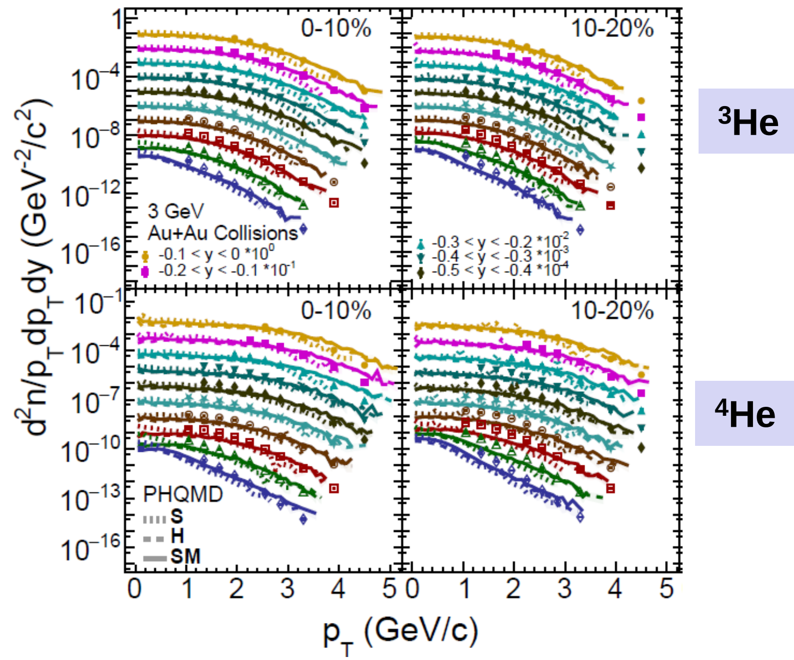


➔ **Exp. data on anti-d are well reproduced by the PHQMD**

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

EoS dependence of p_T-spectra at STAR : $s^{1/2}$=3 GeV





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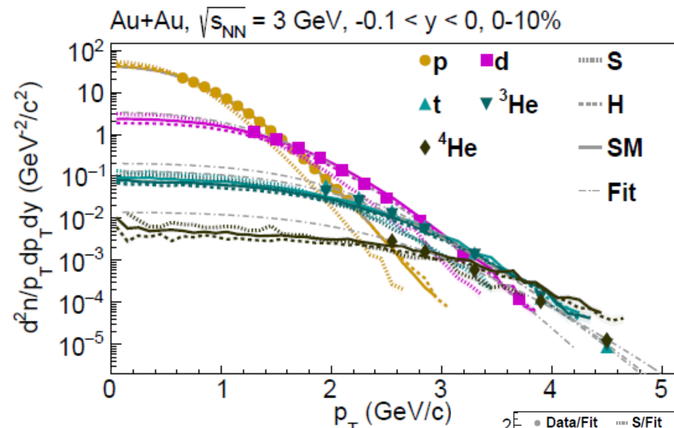
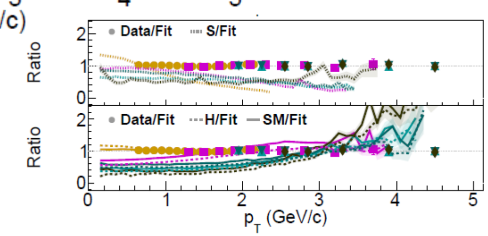


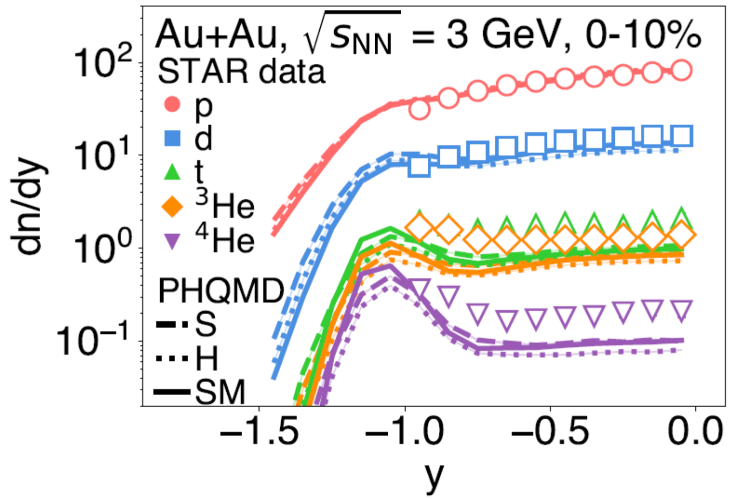


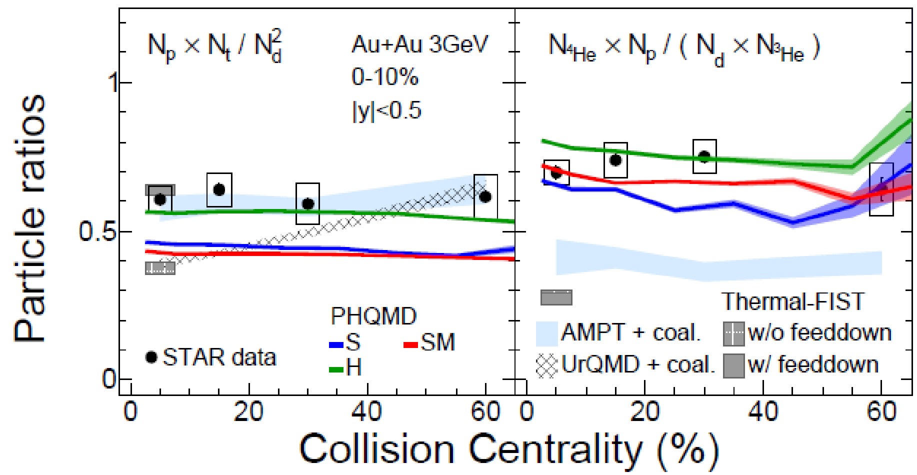
- STAR p_T data favor a hard or soft-momentum dependent potential (H/SM)

STAR: M. Abdulhamid et al., PRC 110 (2024) 5, 054911

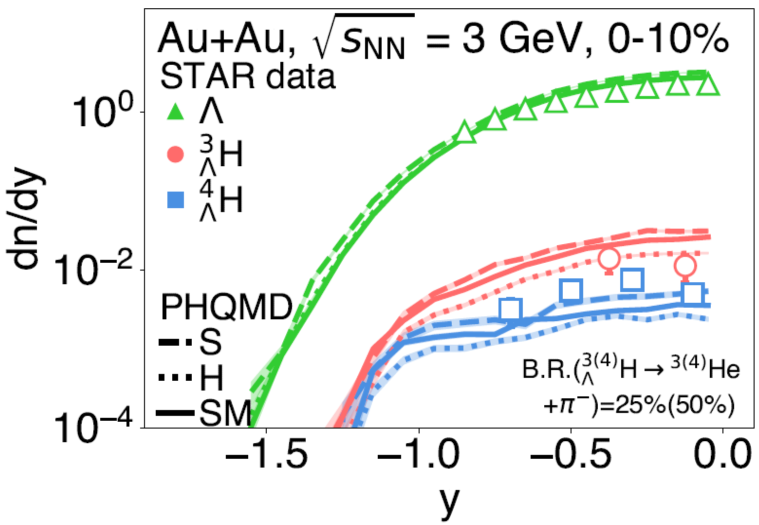
Yingjie Zhou et al., 2507.14255

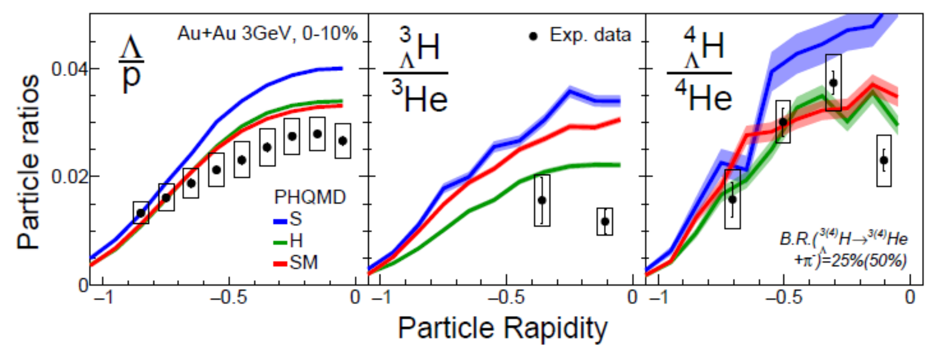
Cluster and hypernuclei at STAR : $s^{1/2}$=3 GeV





Hypernuclei:





❑ **STAR data on dn/dy favor a hard or soft-momentum dependent potential (H/SM)**

STAR: M. Abdulhamid et al., Phys.Rev.C 110 (2024) 5, 054911

Yingjie Zhou et al., 2507.14255

Can the production mechanisms be identified experimentally?
➔ potential interactions (MST) + kinetic reactions vs. coalescence

Where the clusters are formed?

PHQMD

III. Coalescence mechanism vs MST

➔ Clusters formation at a freeze-out time by coalescence radii in coordinate and momentum space

Coalescence parameters from UrQMD → in PHQMD:

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

- **PHQMD:**
  Coalescence and MST (potential) deuterons are calculated in the same PHQMD run (perturbatively)

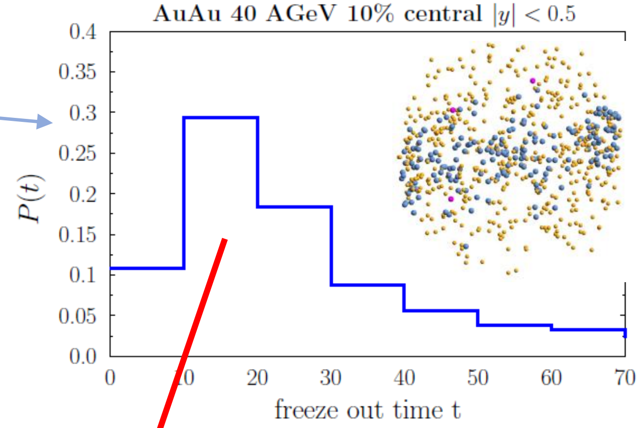
- **Why the observables can be different in coalescence and in MST?**

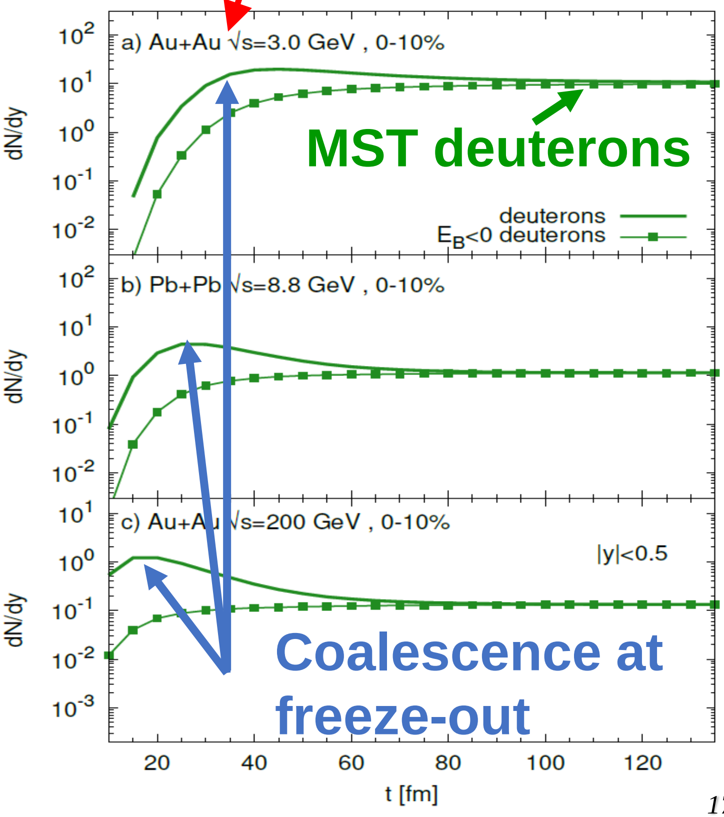
- The influance of the potential interaction after nucleon freeze-out

- Most of the coalescence deuterons are 'unbound'

- Many coalescence deuterons are surrounded by other hadrons when they are produced, in the MST they would not be identified as deuteron states rather as more heavy clusters

- N_d(MST)≈N_d(Coal) at mid-rapidity, but only 20% of coalescence deuterons (at freeze-out) are found by MST (asymptotically)

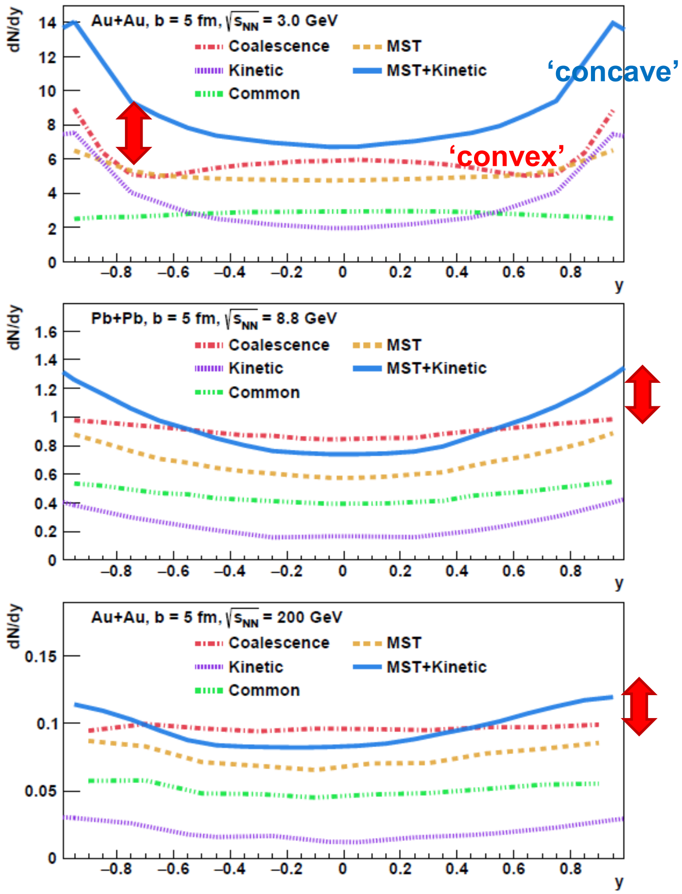




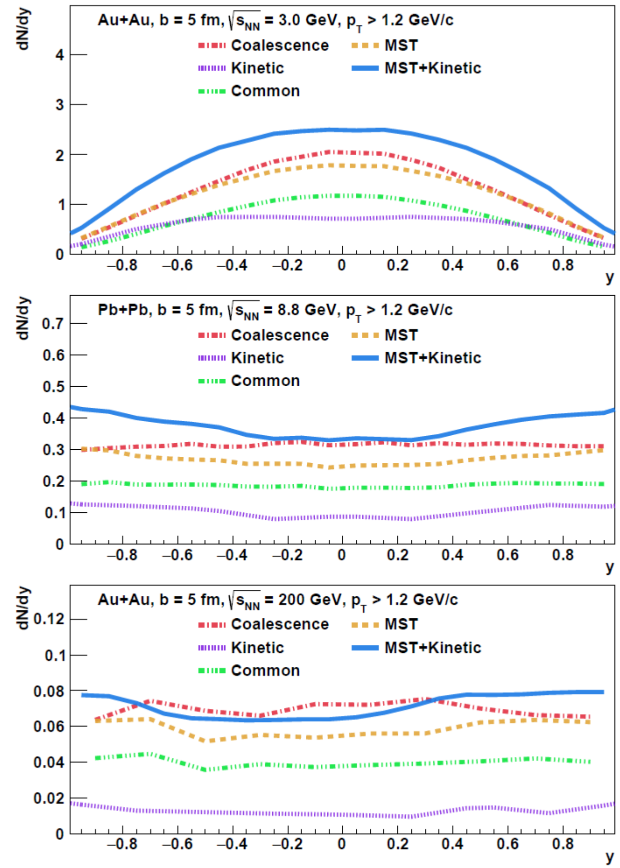
V. Kireyeu, et al., Phys. Rev. C 105 (2022) 044909

Can the production mechanism be identified experimentally? Deuteron y-ditribution. The influence of exp. acceptance

4π, no cuts in p_T



STAR acceptance: p_T > 1.2 GeV/c

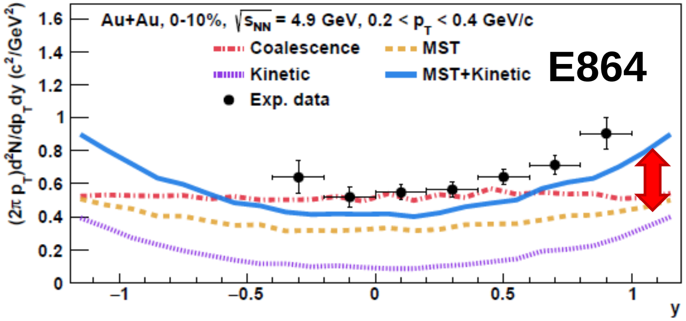


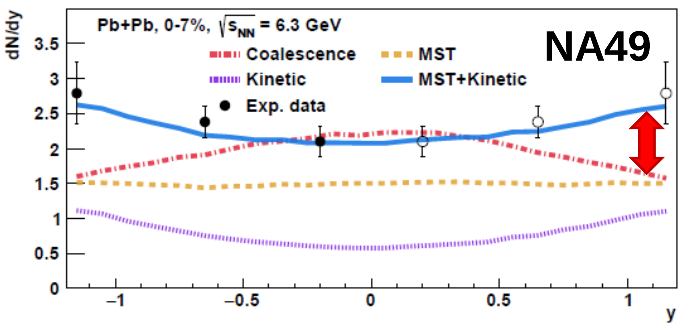
V. Kireyeu et al., PRC109 (2024), 044906

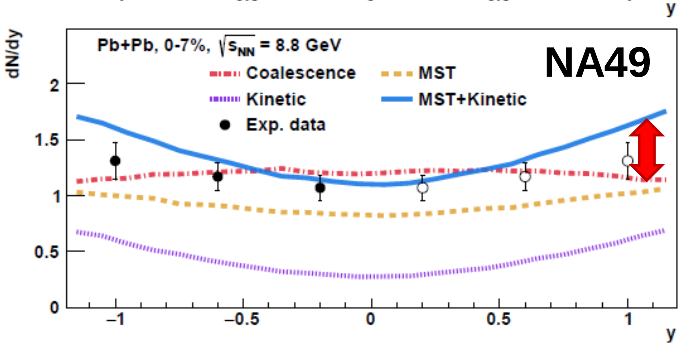
- Difference between coalescence and MST is mostly at low p_T
- In the measured p_T range signal is gone for $\sqrt{s}$ = 3 GeV
- But: there seems to be a 'sweet spot' around $\sqrt{s} = [6-8]$ GeV to identify the reaction mechanism

Mechanism for deuteron production: coalescence and MST+kinetic ⟺ experimental data

PHQMD

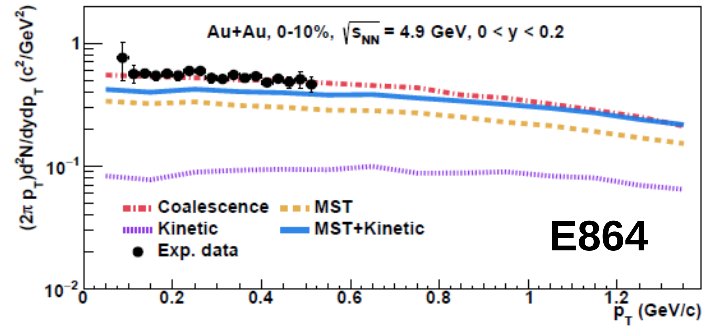


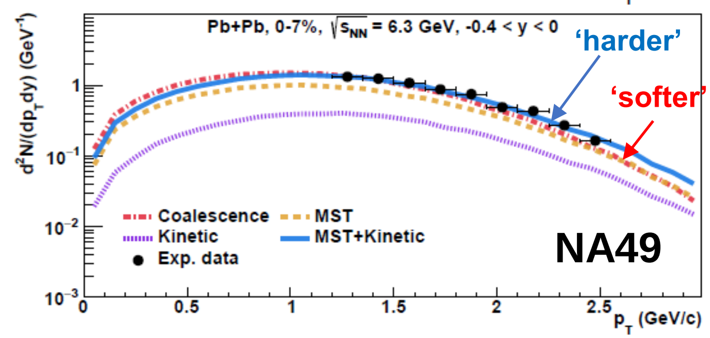


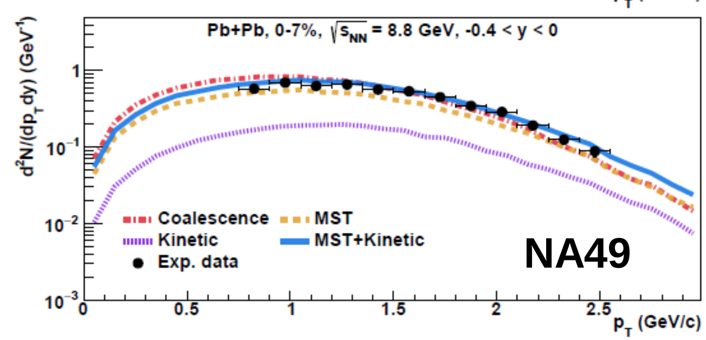


p_T **-distributions**
have a different slope for coalescence vs MST+kinetic mechanisms

y- distributions
show differences







➔ **The analysis of the presently available data points tentatively to the MST + kinetic scenario but further experimental data are necessary to establish the cluster production mechanism**

➔ **More precise experimental data on rapidity distributions are needed**

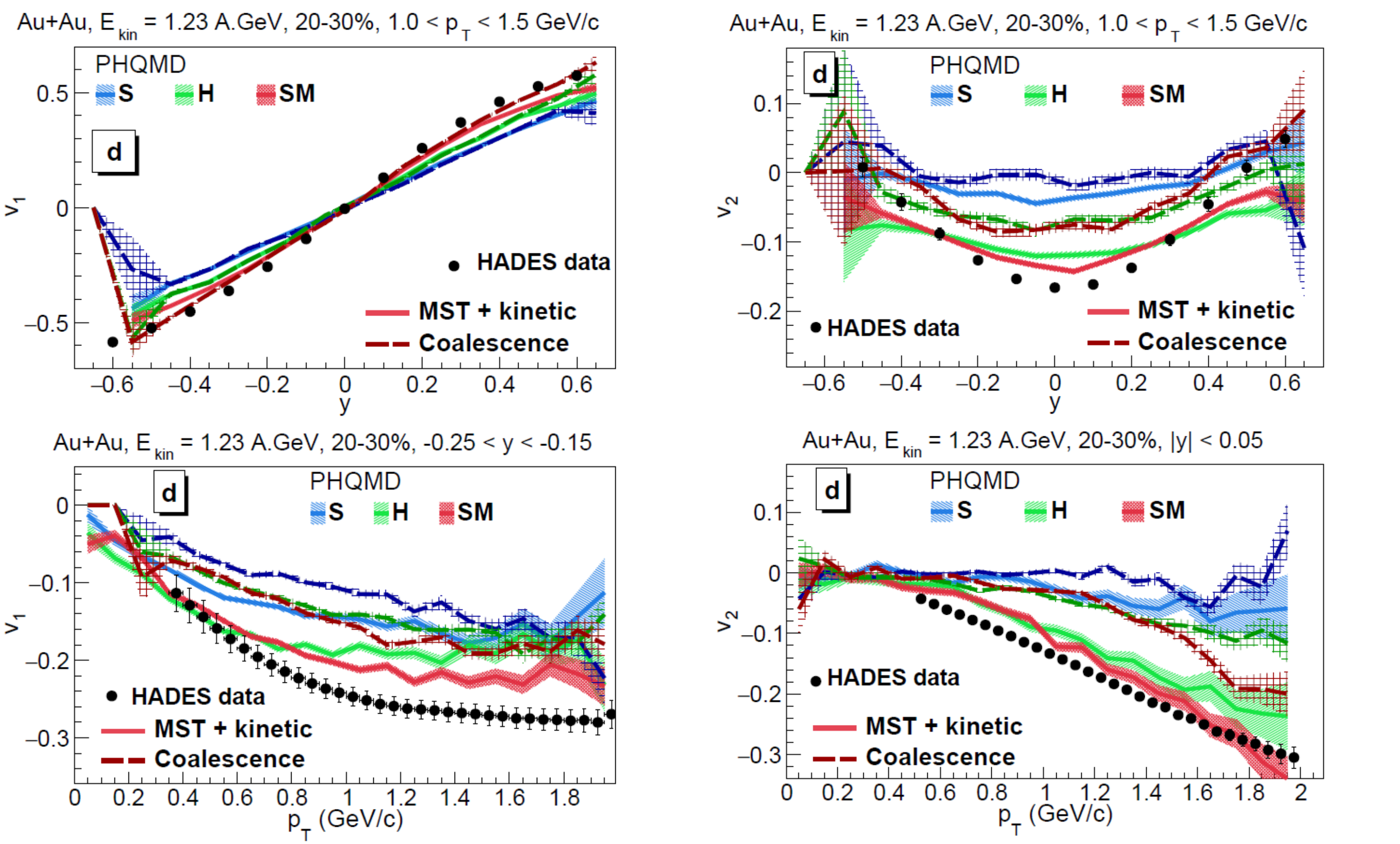
V. Kireyeu et al., PRC109 (2024), 044906

PHQMD

Influence of deuteron production mechanism on v_1, v_2 flows

EoS: soft (S), hard (H), soft momentum dependent (SM)

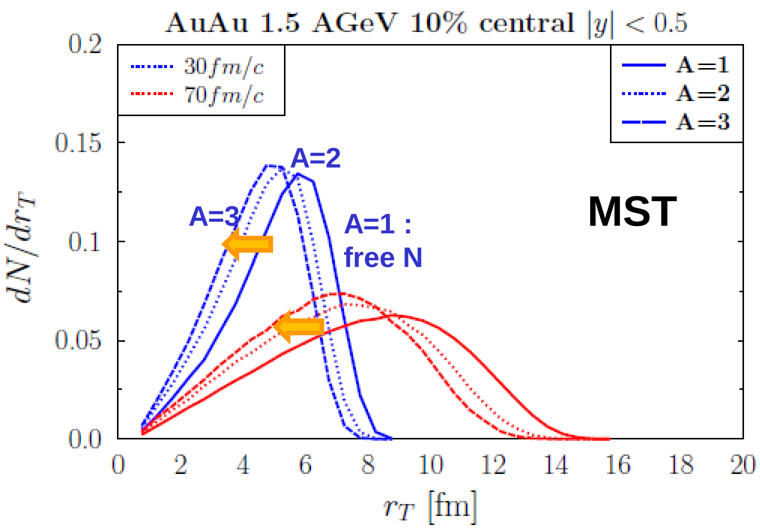
V. Kireyeu et al., arXiv:2411.04969

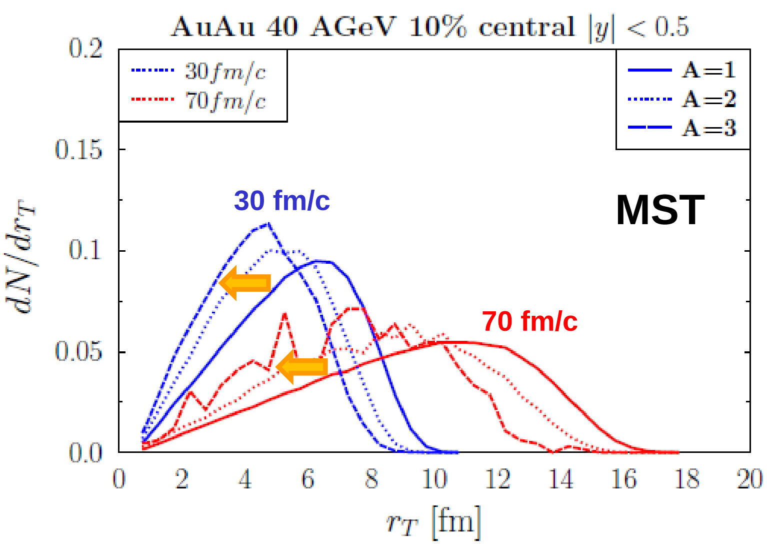


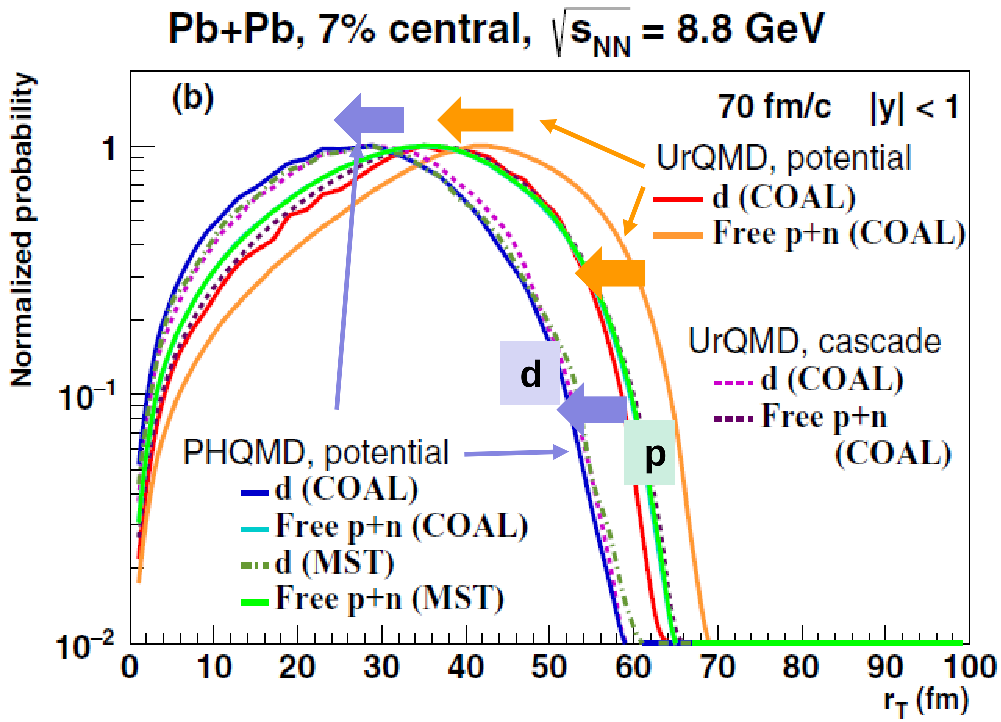
- **v_1, v_2 of deuterons are sensitive to the production mechanism:**
  absolute values of v_1, v_2 of coalescence deuterons are less than v_1, v_2 of MST+kinetic deuterons (v_1, v_2 of kinetic deuterons are only slightly larger than v_1, v_2 of MST deuterons)

- **Strong EoS dependence of v_1, v_2 of deuterons**

PHQMD and UrQMD: Where clusters are formed?







➔ **Coalescence (COAL) as well as MST show that the deuterons remain in transverse direction closer to the center of the heavy-ion collision than free nucleons**

➔ **deuterons are behind the fast nucleons (and pions)**

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

Summary

The PHQMD is a microscopic n-body transport approach for the description of heavy-ion dynamics and cluster and hypernuclei formation identified by Minimum Spanning Tree model

combined model PHQMD = (PHSD & QMD) & (MST | SACA)

Clusters are formed dynamically

1) by potential interactions among nucleons and hyperons and recognized (perturbatively) by MST
   Novel development: momentum dependent potential with soft EoS

2) by kinetic mechanism for d : hadronic inelastic reactions NN ↔ dπ , πNN ↔ dπ , NNN ↔ dN
   with inclusion of all possible isospin channels which enhance d production
   + accounting of quantum properties of d, modelled by the finite-size excluded volume effect in coordinate space and projection of relative momentum of p+n pair on d wave-function in momentum space which leads to a strong reduction of d production

- The PHQMD reasonably reproduces cluster and hypernuclei data on dN/dy and dN/dp_T, well as ratios d/p and $\bar{d}/\bar{p}$ for heavy-ion collisions from SIS to top RHIC energies

- Measurements of dN/dy beyond mid-rapidity will allow to distinguish the mechanisms for cluster production: coalescence versus 'dynamical' cluster production recognized by MST + kinetic mechanism for deuterons

- Flow observables v_1,v_2 are sensitive to the production mechanism

- Strong dependencee of y- and p_T-spectra and v_1,v_2 of light clusters on EoS (vs HADES, FOPI, and STAR data)

- Stable clusters are formed shortly after elastic and inelastic collisions have ceased and behind the front of the expanding energetic hadrons (similar results within PHQMD and UrQMD)
  ➔ since the 'fire' is not at the same place as the 'ice', clusters can survive

Thank you for your attention!

Thanks to the PHSD/PHQMD team!