# Modeling of light nuclei formation at SIS energies


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**&**
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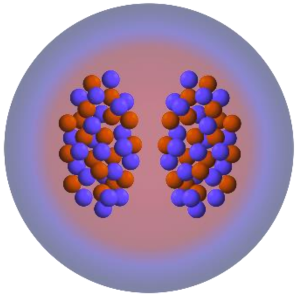
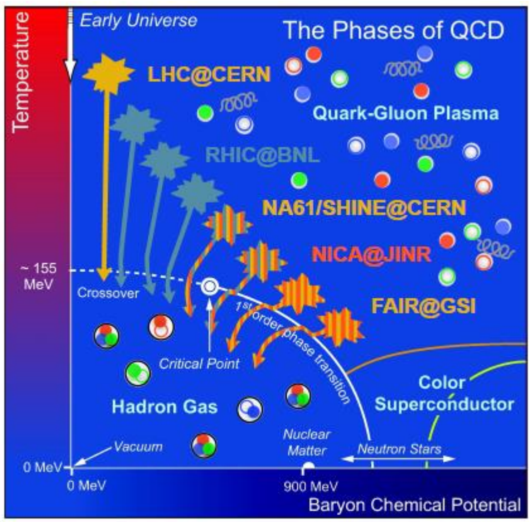
PHQMD

**EMMI Workshop "Probing dense baryonic matter with hadrons II: FAIR Phase-0",**
**19-21 February 2024, GSI, Darmstadt**

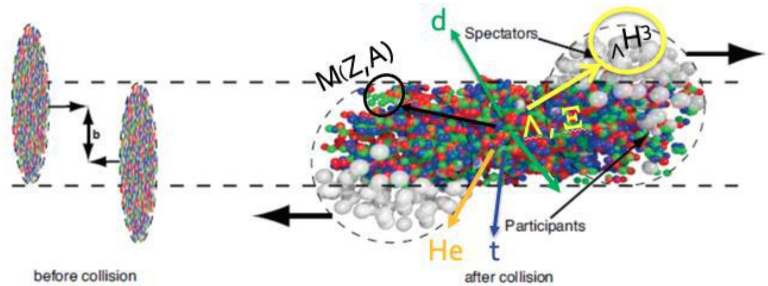


# Cluster production in heavy-ion collisions

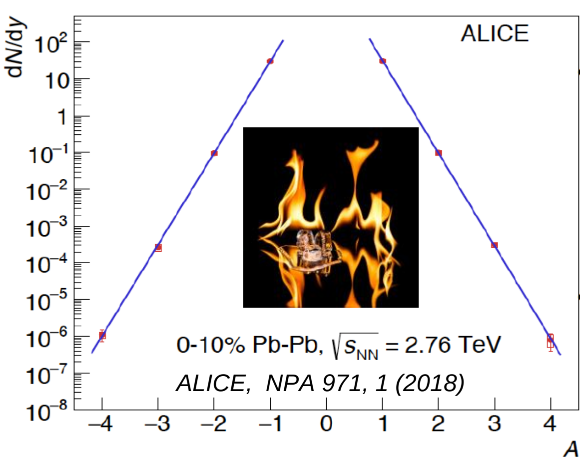
**The phase diagram of QCD**



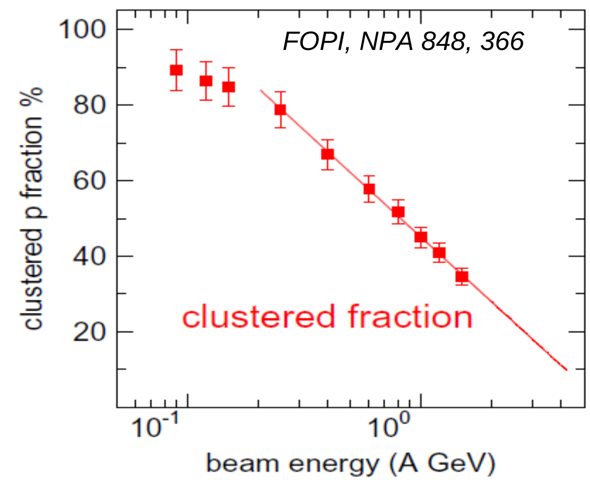

**Clusters and (anti-) hypernuclei**
**are observed experimentally at all energies**




Au+Au, central. midrapidity




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




- **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**

# Dynamical modeling of cluster and hypernuclei formation

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

**→ transport models:**
**dynamical modeling of cluster formation based on interactions:**

- **via potential interaction – ‘potential‘ mechanism**
- **by scattering (hadronic reactions) – ‘kinetic‘ mechanism**

PHQMD

- **PHQMD allows for a direct comparison of dynamical mechanisms for cluster formation to coalescence mechanism:**
  **- determination of clusters at a freeze-out time by coalescence radii in coordinate and momentum space**

# PHQMD

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

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

## Parton-Hadron-Quantum-Molecular Dynamics

PHSD mode

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

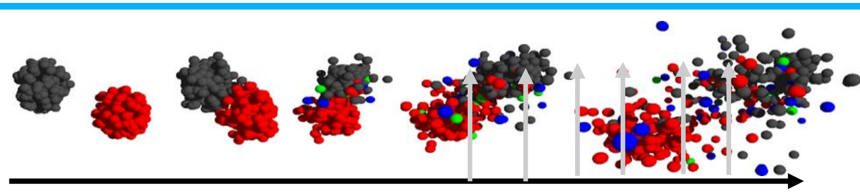
J.Aichelin, Phys. Rept. 202 (1991)

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

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

**Cluster recognition:**
**MST (Minimum Spanning Tree)**
**or SACA (Simulated Annealing Clusterization Algorithm)**

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




PHQMD:
J. Aichelin et al., PRC 101 (2020) 044905;
S. Gläßel et al., PRC 105 (2022) 1;
G. Coci et al., PRC 108 (2023) 1, 014902

# 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:**

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

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

**Ansatz: trial wave function for one particle "*i*" :**
**Gaussian 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 fm*$^2$

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

**2-body potential:** $V_{i,j} = V(\mathbf{r_i}, \mathbf{r_j}, \mathbf{r_{i0}}, \mathbf{r_{j0}}, t)$

# Local momentum dependent potential in PHQMD

New!

- Nucleon-nucleon local two-body momentum dependent potential:

$$V_{ij} = V(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_{i0}, \mathbf{r}_{j0}, \mathbf{p}_{i0}, \mathbf{p}_{j0}, t)$$
$$= V_{\text{Skyrme loc}} + V_{\text{mom}} + V_{\text{Coul}}$$
$$= \boxed{\frac{1}{2} t_1 \delta(\mathbf{r}_i - \mathbf{r}_j) + \frac{1}{\gamma+1} t_2 \delta(\mathbf{r}_i - \mathbf{r}_j)\, \rho^{\gamma-1}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_{i0}, \mathbf{r}_{j0}, t)} \quad \text{Skyrme}$$
$$+ \boxed{V(\mathbf{r}_i, \mathbf{r}_j, \mathbf{p}_{i0}, \mathbf{p}_{j0})} + \frac{1}{2} \frac{Z_i Z_j e^2}{|\mathbf{r}_i - \mathbf{r}_j|},$$

momentum dependent — Coulomb

- The single-particle potential <V> resulting from the convolution of the distribution functions $f_i$ and $f_j$ with the interactions $V_{Skyrme}$ + $V_{mom}$ (local interactions including their momentum dependence) for symmetric nuclear matter:

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 modified interaction density (with relativistic extension):

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

# Momentum dependent potential → EoS in PHQMD

New!

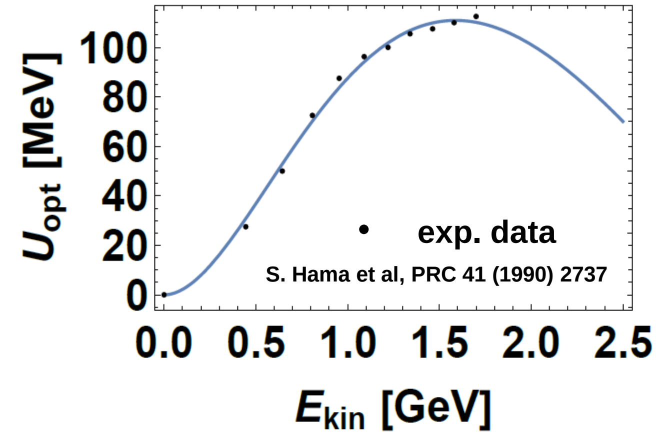
## 2) Momentum dependent potential :

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

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

**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 the EoS:**

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

$$V_{mom} = (a\Delta p + b\Delta p^2)\ exp(-c\sqrt{\Delta p})\ \frac{\rho}{\rho_0}$$

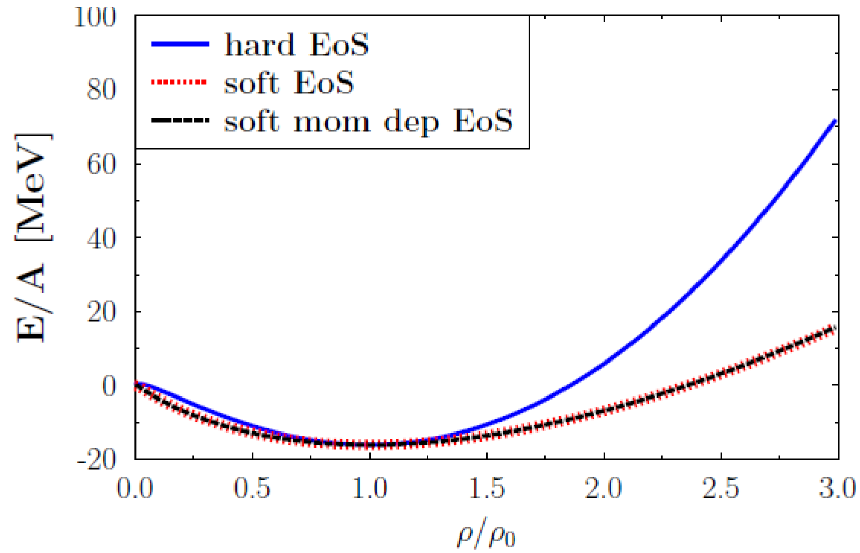
$$V_{Skyrme} = \alpha\frac{\rho}{\rho_0} + \beta\frac{\rho}{\rho_0}^{\gamma}$$

**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. | $\alpha[MeV]$ | $\beta[MeV]$ | $\gamma$ | 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**



# Mechanisms for cluster production in PHQMD:
# I. potential interactions (recongnized by MST)
# &
# II. kinetic reactions

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.**

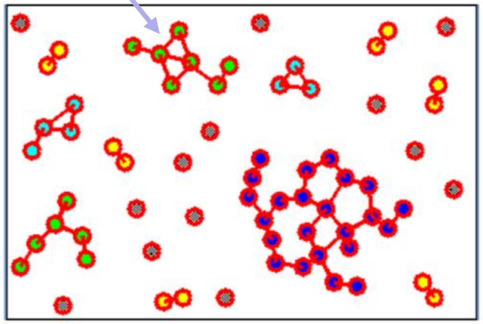
**The MST algorithm searches for accumulations of particles in coordinate space:**

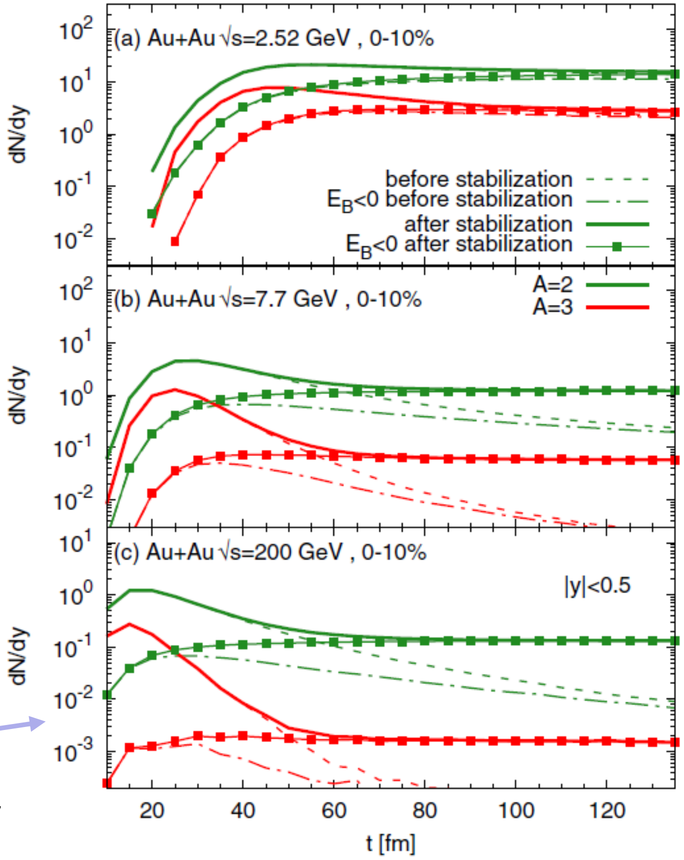
1. **Two particles are 'bound' if their distance in the cluster rest frame fulfills**

$$|\vec{r_i} - \vec{r_j}| \leq 4\ \mathrm{fm}$$

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 mostly not at the same position (V. Kireyeu, Phys.Rev.C 103 (2021) 5)






**New: 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 ⟷ d$\pi$ , $\pi$NN ⟷ d$\pi$ , NNN ⟷ dN
2) hadronic elastic $\pi$+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** $d^4x = dt*dV$
- With **test particle ansatz the transition rate for 3→2 reactions**:

W. Cassing, NPA 700 (2002) 618

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

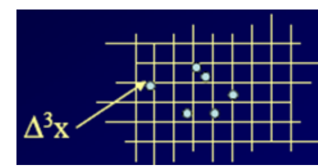
$$P_{3,2}(\sqrt{s}) = F_{spin} F_{iso} P_{2,3}(\sqrt{s}) \frac{E_1^f E_2^f}{2E_3 E_4 E_5} \frac{R_2(\sqrt{s}, m_1, m_2)}{R_3(\sqrt{s}, m_3, m_4, m_5)} \frac{1}{\Delta V_{cell}}$$

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: $\pi$+N+N⟷ d+$\pi$** 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

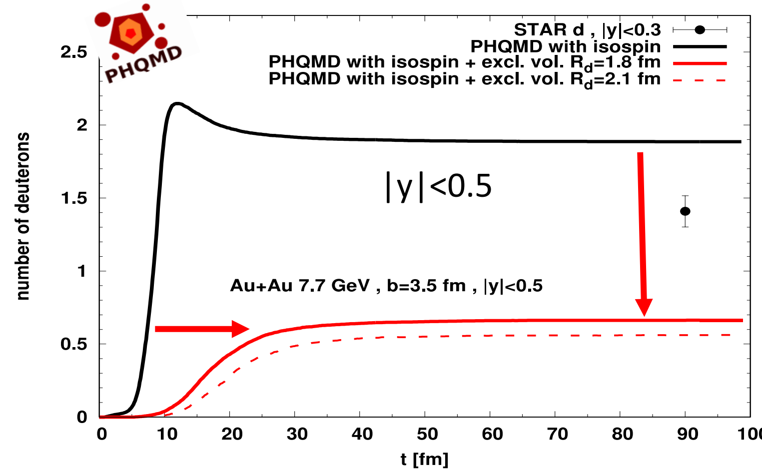
1) the **finite-size of *d* in coordinate space** (*d* is not a point-like particle) – for in-medium d production
2) the **momentum correlations of *p* and *n*** inside *d*

**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':

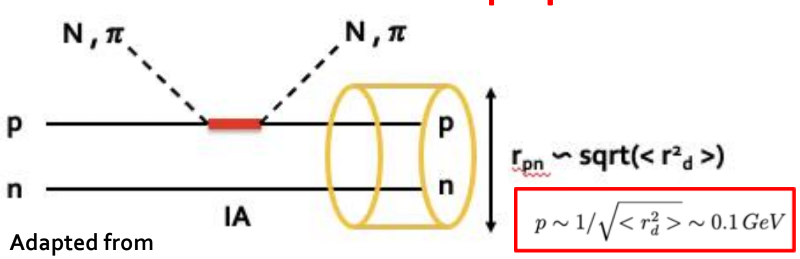
**Excluded-Volume Condition:** $|\vec{r}(i)^* - \vec{r}(d)^*| < R_d$

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

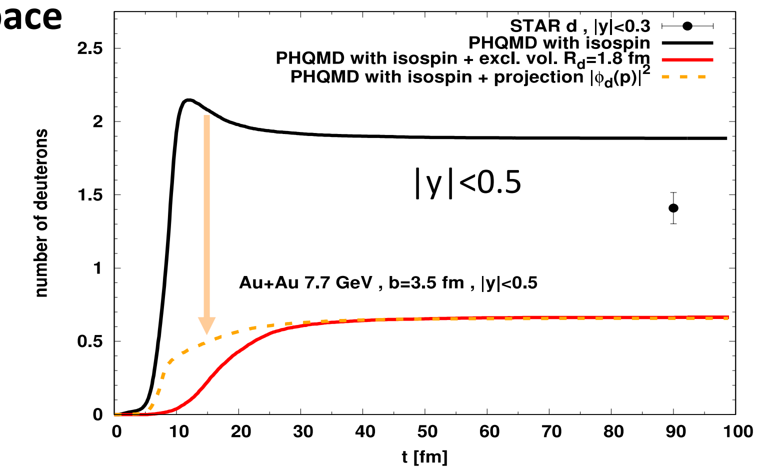



2) QM properties of deuteron must be also in momentum space

→ **momentum correlations of pn-pair**



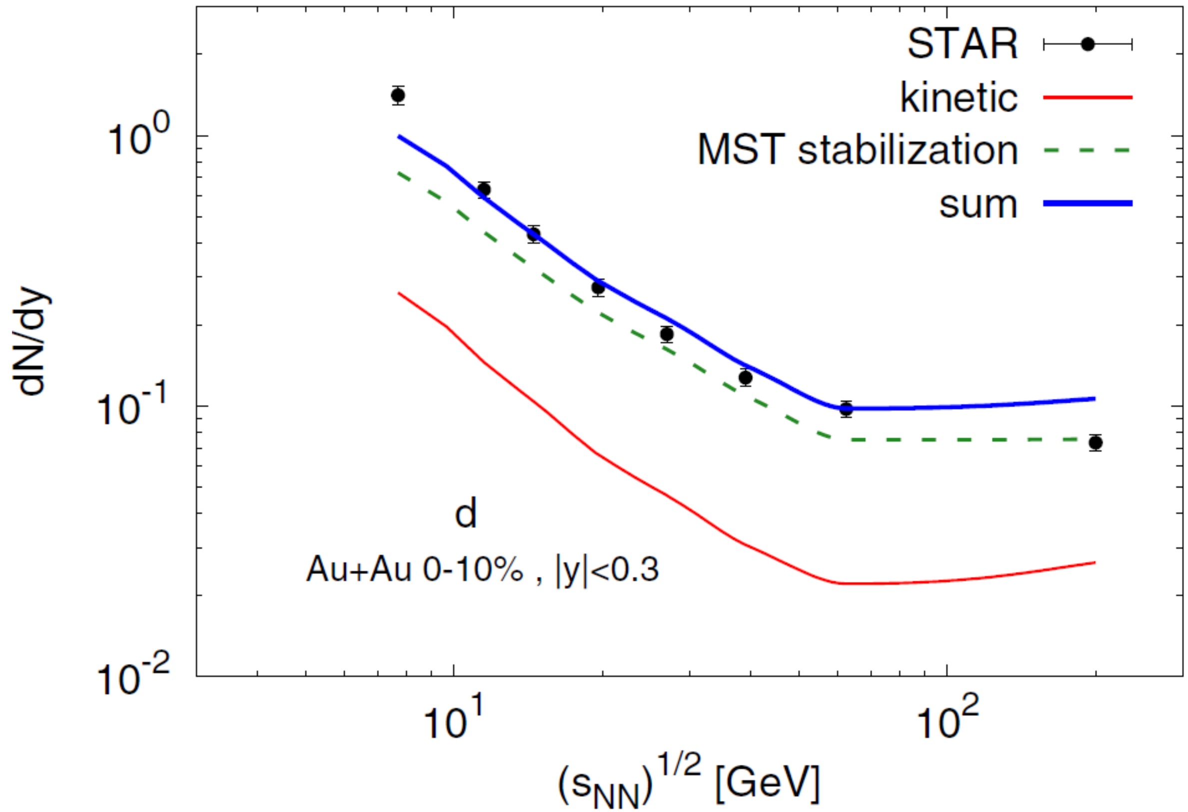

Adapted from
[Haidelbauer, Uzikov PLB 562(2003)]
[Hoftiezer et al. PRC23 (1981)]
Same spirit as AMPT [ K.-J. Sun, R. Wang, C.-M. Ko et al., 2106.12742]




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

# Kinetic vs. potential deuteron production

**Excitation function dN/dy of deuterons at midrapidity**




- **PHQMD provides a good description of STAR data**
- **The potential mechanism is dominant for d production at all energies!**

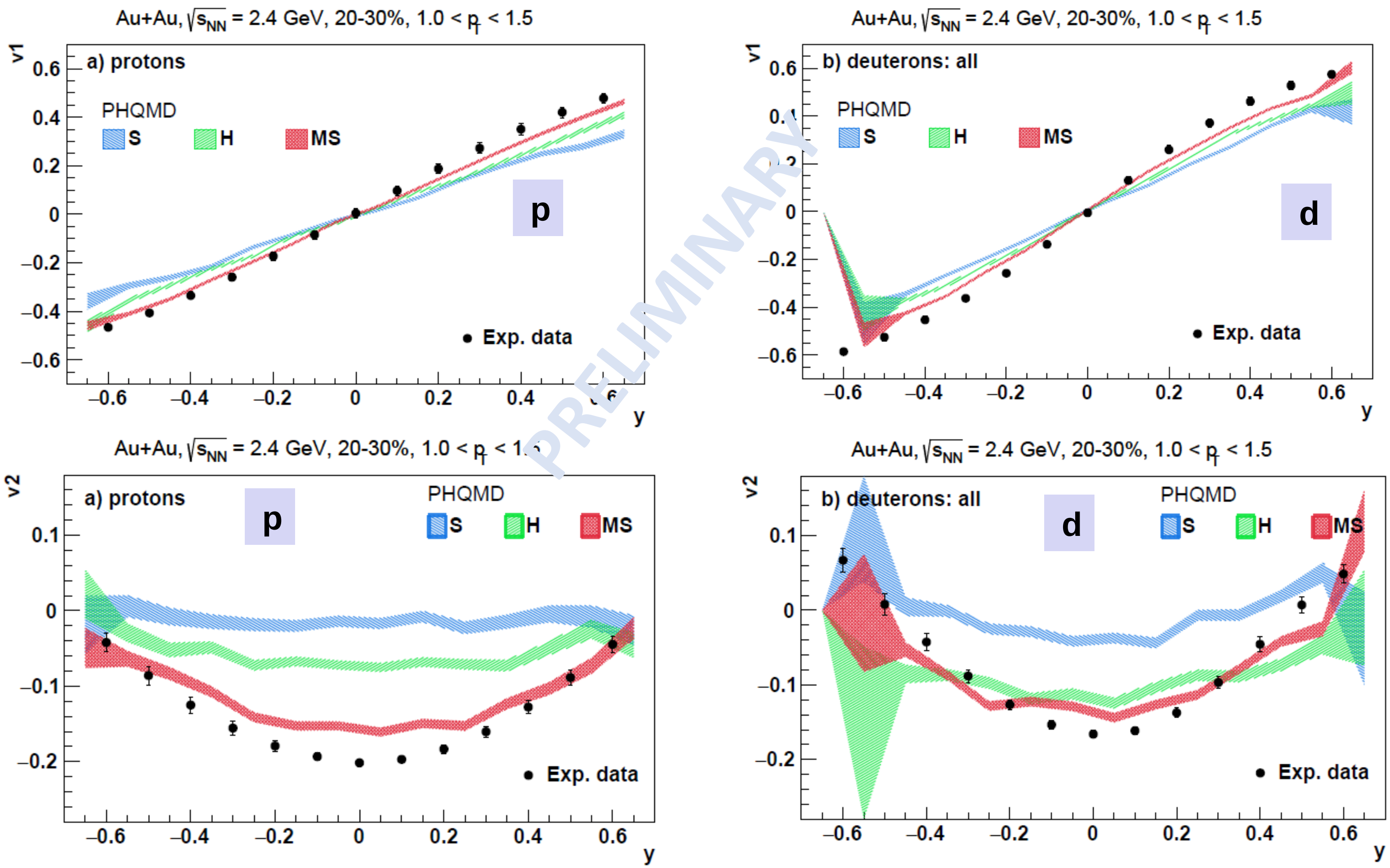
**G. Coci et al., Phys.Rev.*C* 108 (2023) 014902**

# $v_1$, $v_2$ with different EoS
# New in PHQMD: momentum dependent potential

PHQMD

# EoS dependence of $v_1(y)$, $v_2(y)$ at SIS energies: p,d

**Viktar Kireyeu, in progress**



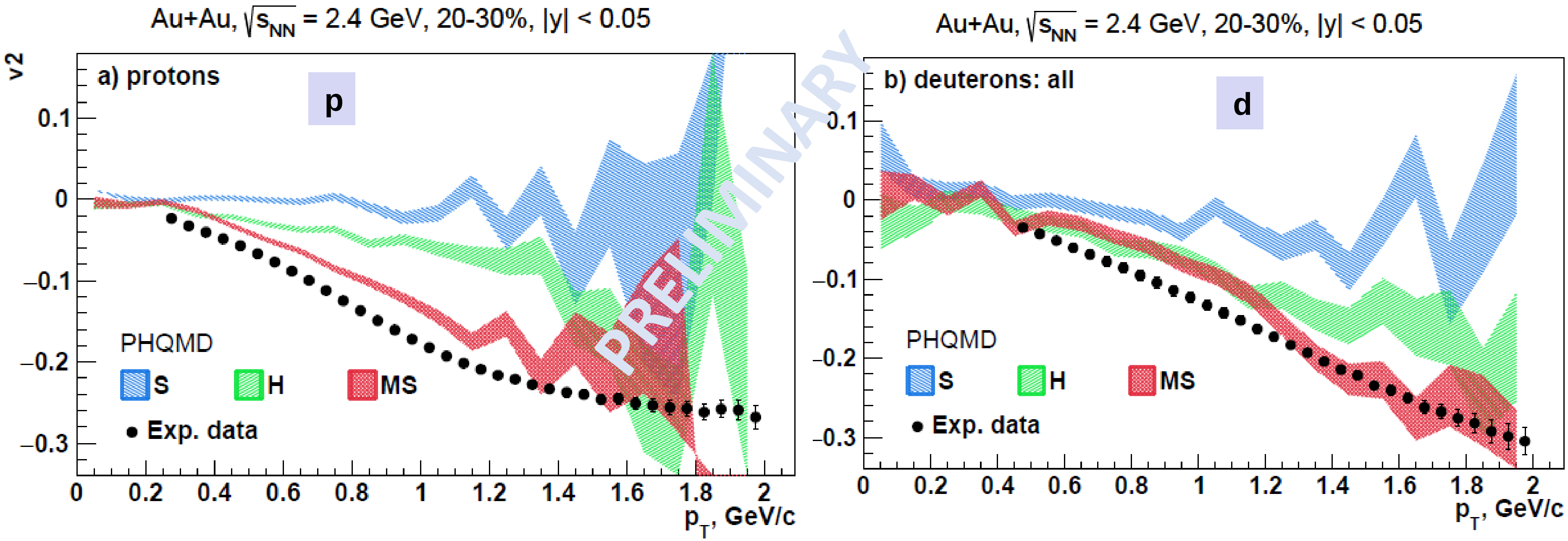

**PHQMD5.2W: S= soft EoS, H=hard EoS, MS = soft momentum dependent EoS**

**HADES data: of $v_1$, $v_2$ at high $p_T$: 1.0 < $p_T$ < 1.5 GeV/c** [HADES: Eur. Phys. J. A59 (2023) 80]

- **Strong EoS dependence of $v_1(y)$, $v_2(y)$ of protons and deuterons**
- **HADES data favor a soft momentum dependent potential (MS)**

# EoS dependence of $v_2(p_T)$ at SIS energies: p,d

Viktar Kireyeu, in progress

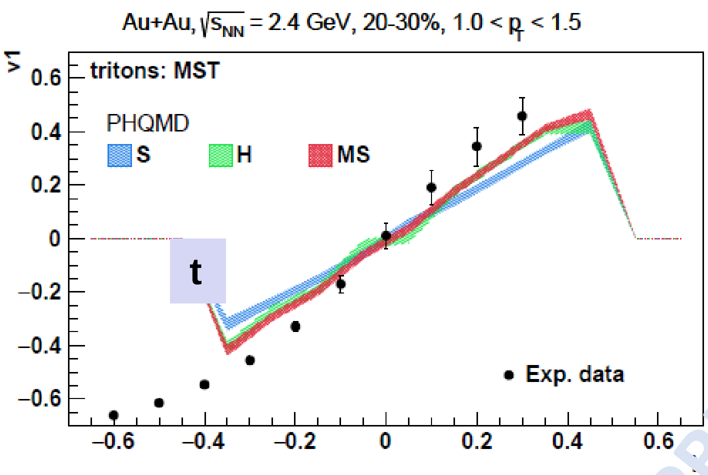


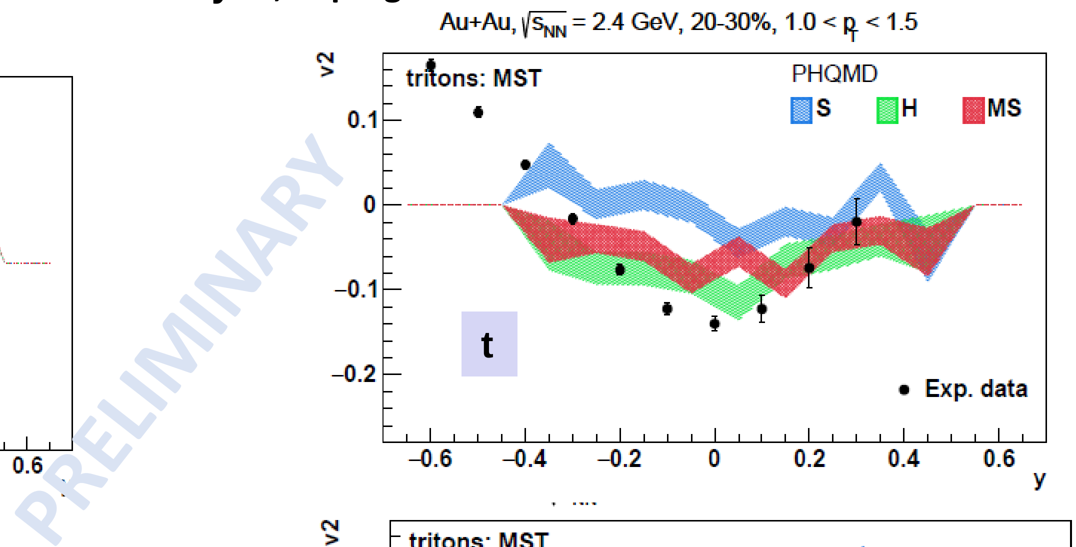

**PHQMD5.2W: S= soft EoS, H=hard EoS, MS = soft momentum dependent EoS**
**HADES data: of $v_2$ ($p_T$) at |y|<0.05** [HADES: Eur. Phys. J. A59 (2023) 80]

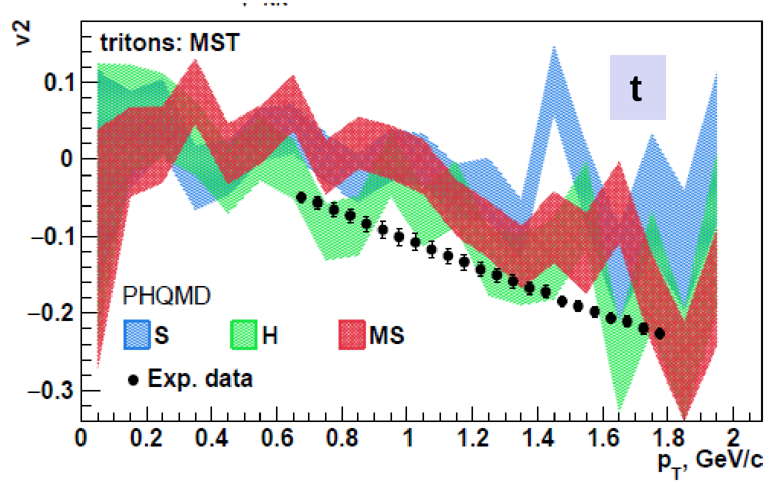
- **Strong EoS dependence of $v_2(p_T)$ of protons and deuterons**
- **HADES data favor a soft momentum dependent potential (MS)**

# EoS dependence of $v_1(y)$, $v_2(y)$, $v_2(p_T)$ at SIS energies: triton

Viktar Kireyeu, in progress



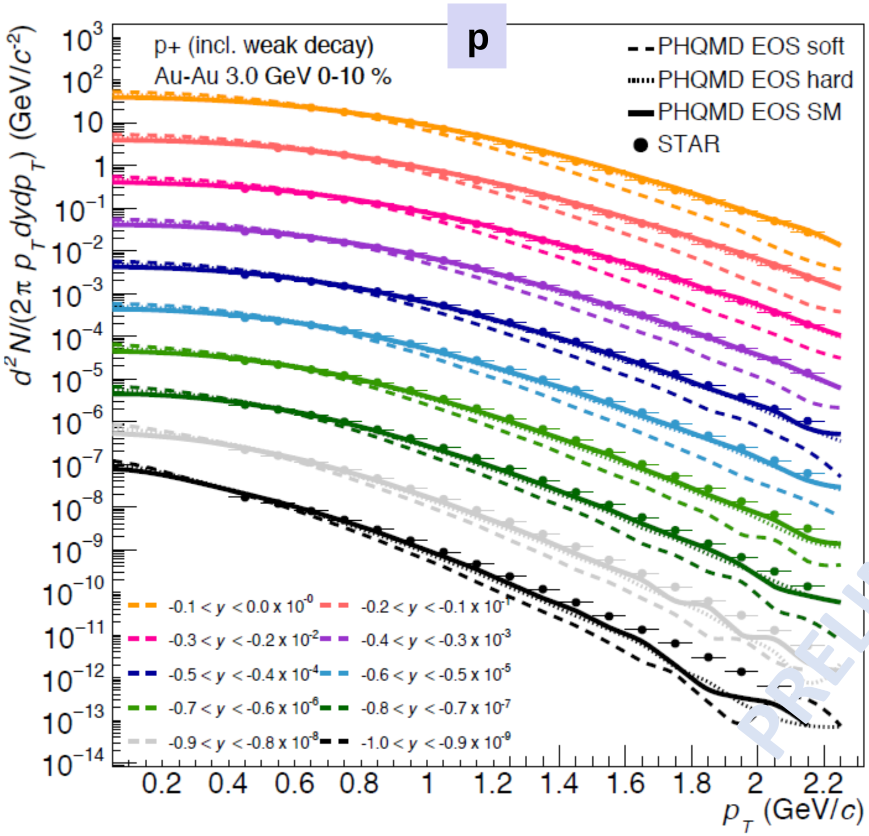



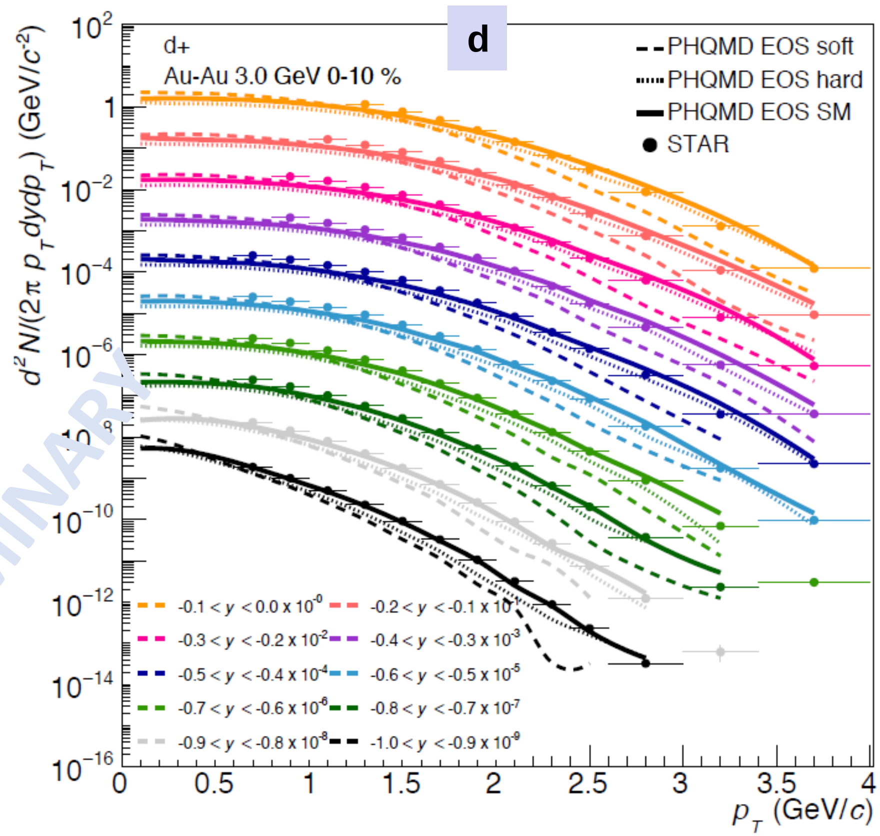

**PHQMD5.2W: S= soft EoS, H=hard EoS,**
**MS = soft momentum dependent EoS**
**HADES data: of $v_1$, $v_2$ at high $p_T$:**
**1.0 < $p_T$ < 1.5 GeV/c** [HADES: Eur. Phys. J. A59 (2023) 80]

- ❑ **Strong EoS dependence of $v_1(y)$, $v_2(y)$ of tritons**
- ❑ **HADES data favor a soft momentum dependent potential (MS)**

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

**Susanne Gläßel, in progress**



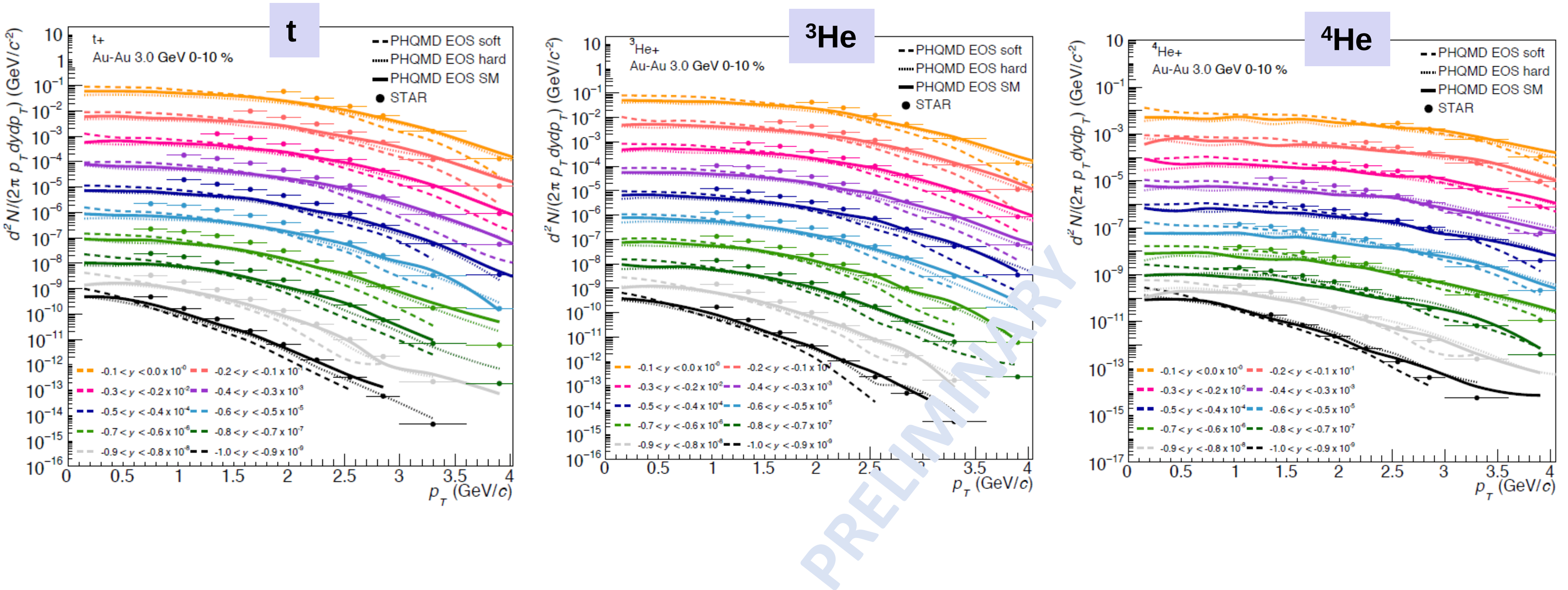

**S= soft EoS, H=hard EoS, SM = soft momentum dependent EoS**

- **Visible dependence of the $p_T$ spectra of protons and deuterons EoS**
- **STAR $p_T$ data favor a hard or soft-momentum dependent potential (H/SM)**

**STAR:H. Liu et al., 2208.04650, Acta Phys.Polon.Supp. 16 (2023) 1, 148**

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

Susanne Gläßel, in progress



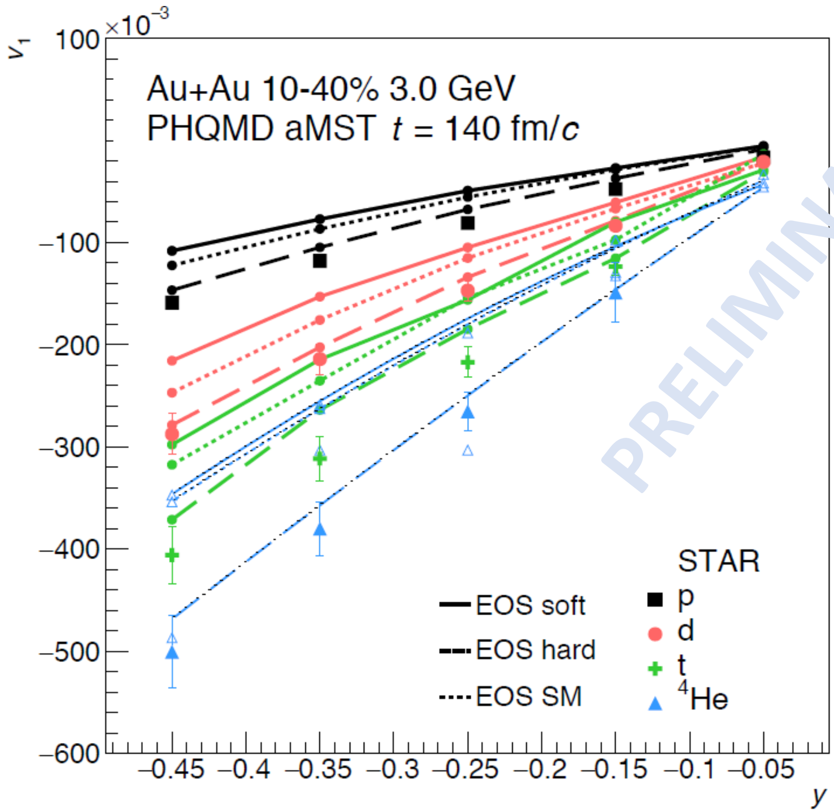

**S= soft EoS, H=hard EoS, SM = soft momentum dependent EoS**

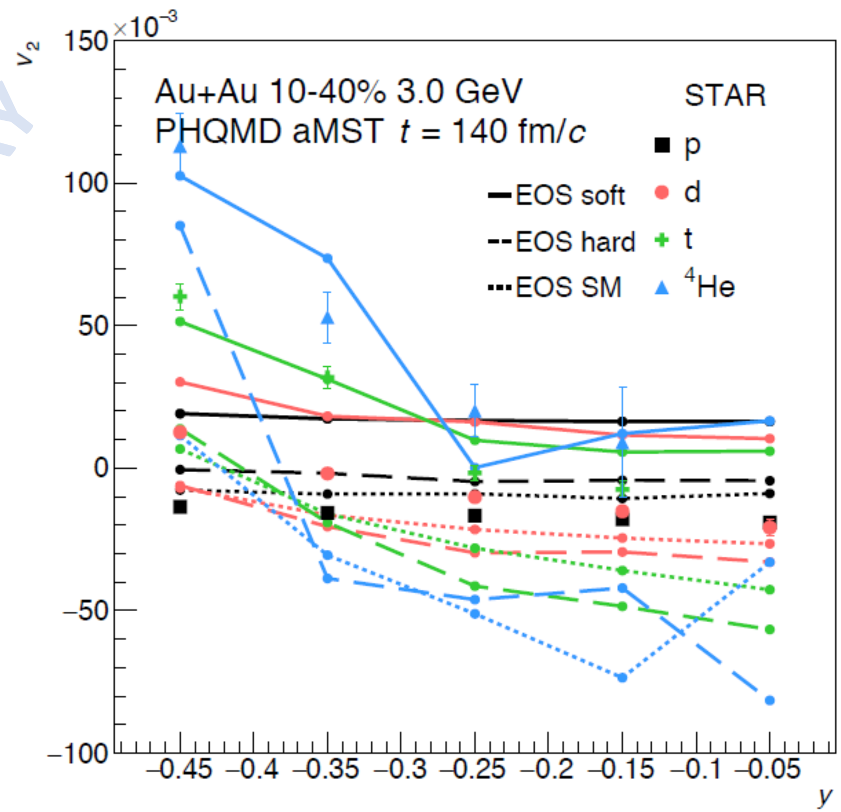
- **Visible dependence of $p_T$ spectra of t, $^3$He, $^4$He on EoS**
- **STAR $p_T$ data favor a hard or soft-momentum dependent potential (H/SM)**

STAR:H. Liu et al., 2208.04650, Acta Phys.Polon.Supp. 16 (2023) 1, 148

# EoS dependence of $v_1$, $v_2$ at at STAR : $s^{1/2}$=3 GeV

**Susanne Gläßel, in progress**




- **Strong EoS dependence of $v_1$, $v_2$**
- **STAR data favor a hard EoS or soft momentum dependent (H/SM)**
- **Influence of momentum dependent potential on flow $v_n$ decreases with increasing energy due to the decrease of U(p) for large p**

**Can the production mechanisms be identified experimentally?**

**Where the clusters are formed?**

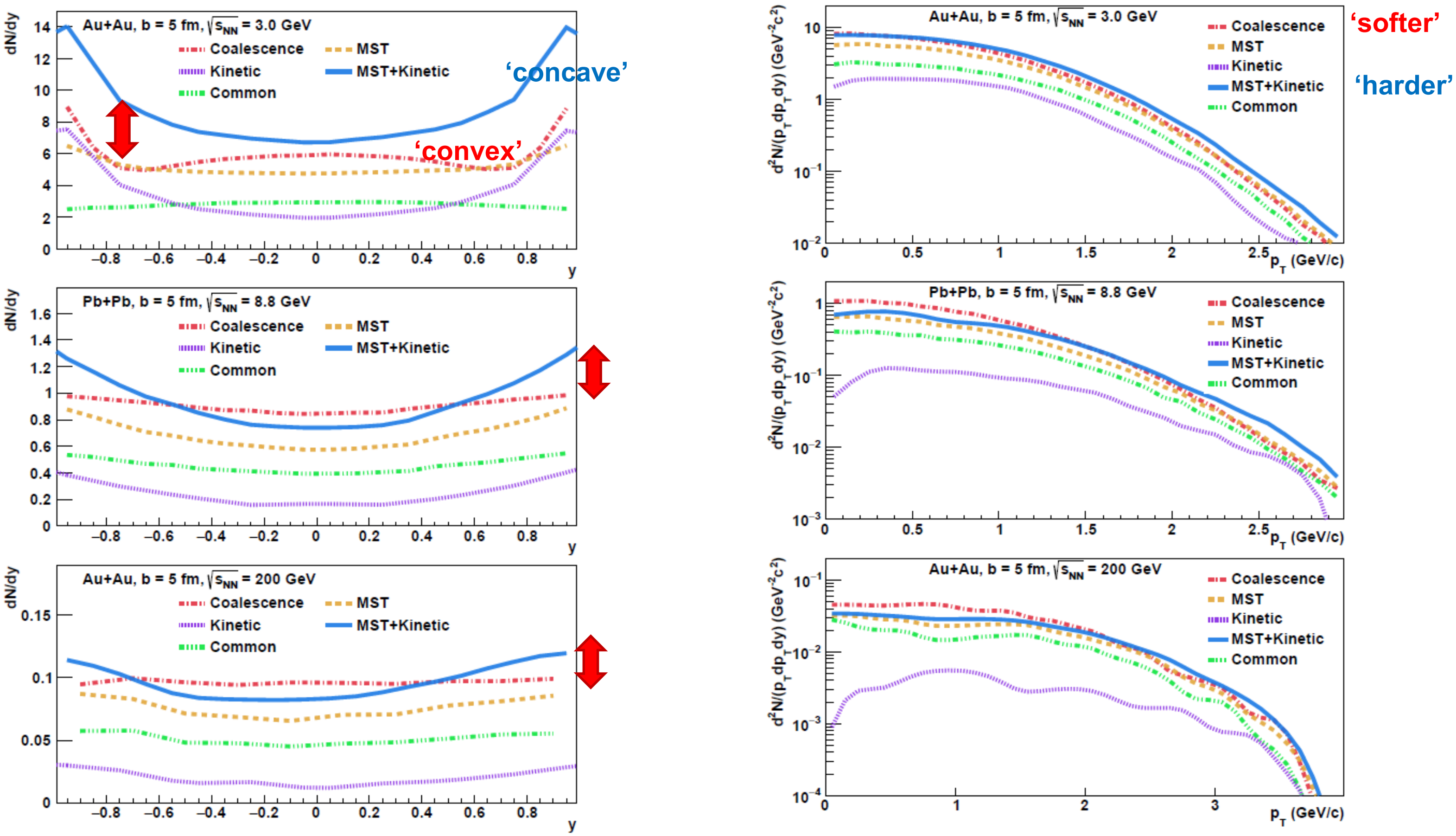
PHQMD

# Deuterons near midrapidity - can the production mechanism be identified experimentally?

PHQMD

**3 mechanisms: coalescence at kinetic freeze-out, kinetic and potential (MST) productions**

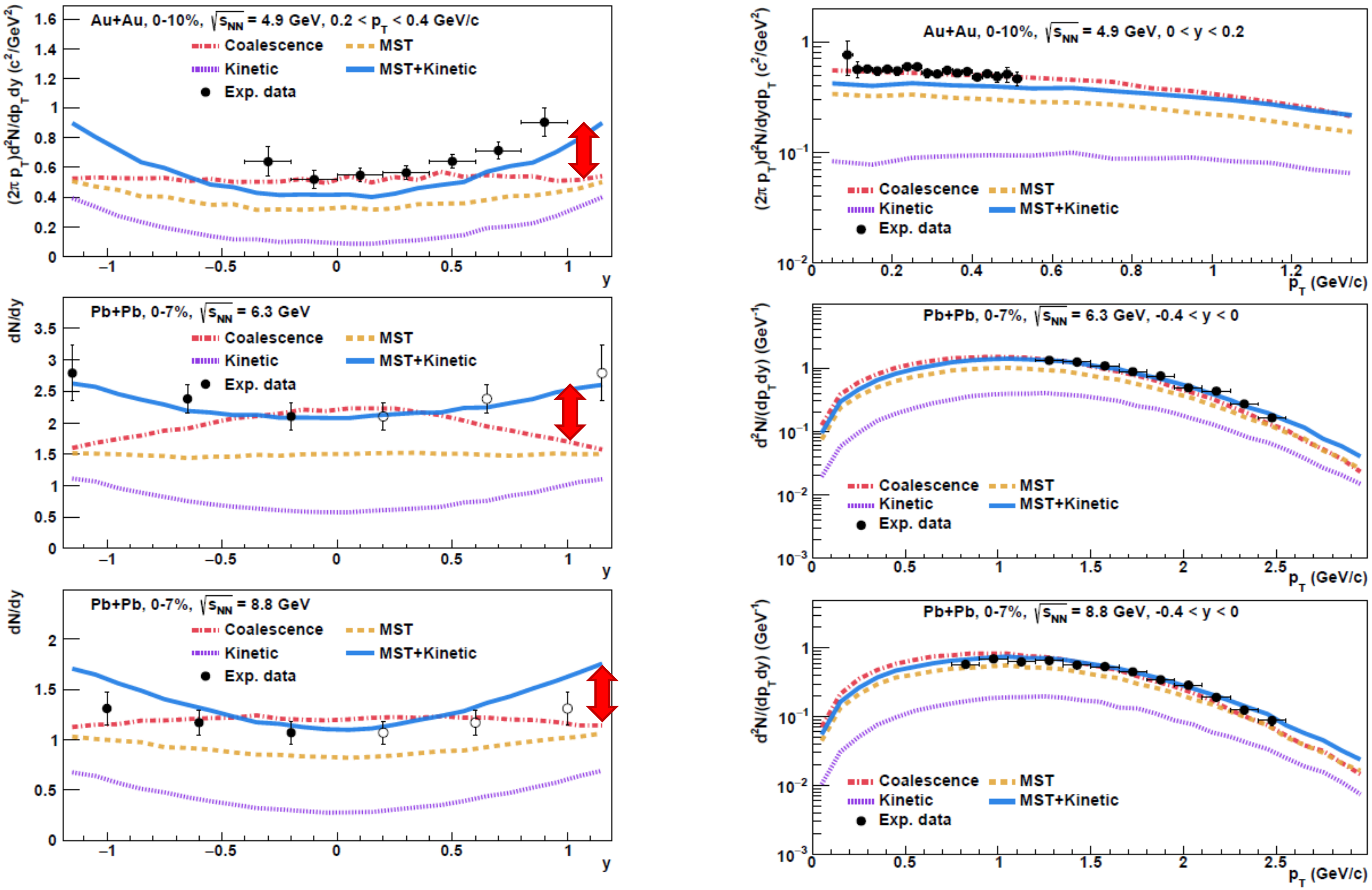
**“Common”: only about 20% of the MST deuterons are also identified as deuterons by coalescence**




**Observables, which are sensitive to the deuteron production mechanism: the rapidity distribution has a different form while the transverse momentum distribution has a different slope at low $p_T$**

**V. Kireyeu et al., 2304.12019**

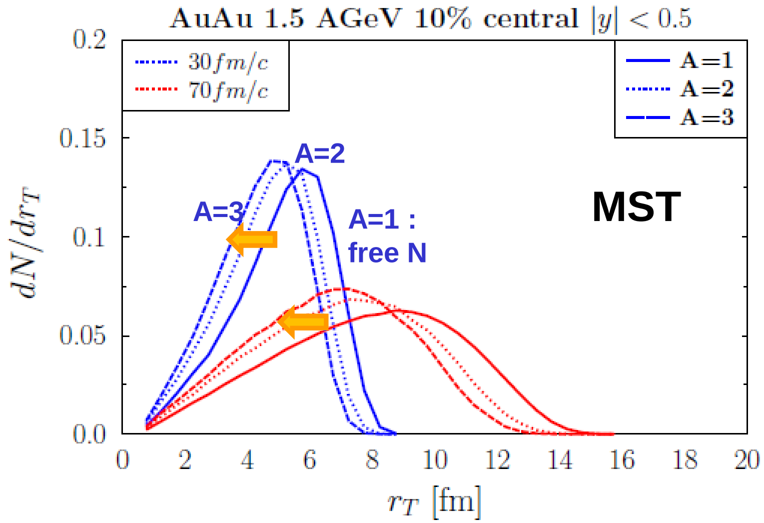
# Mechanism for cluster production: theory versus experimental data

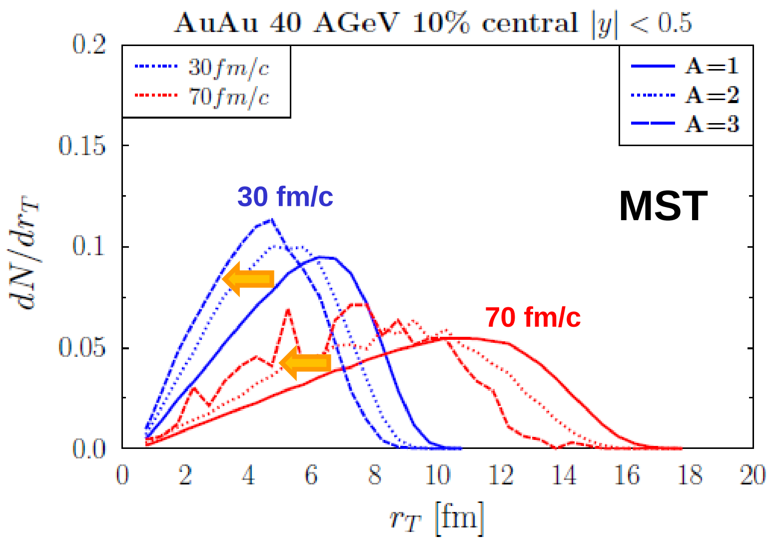


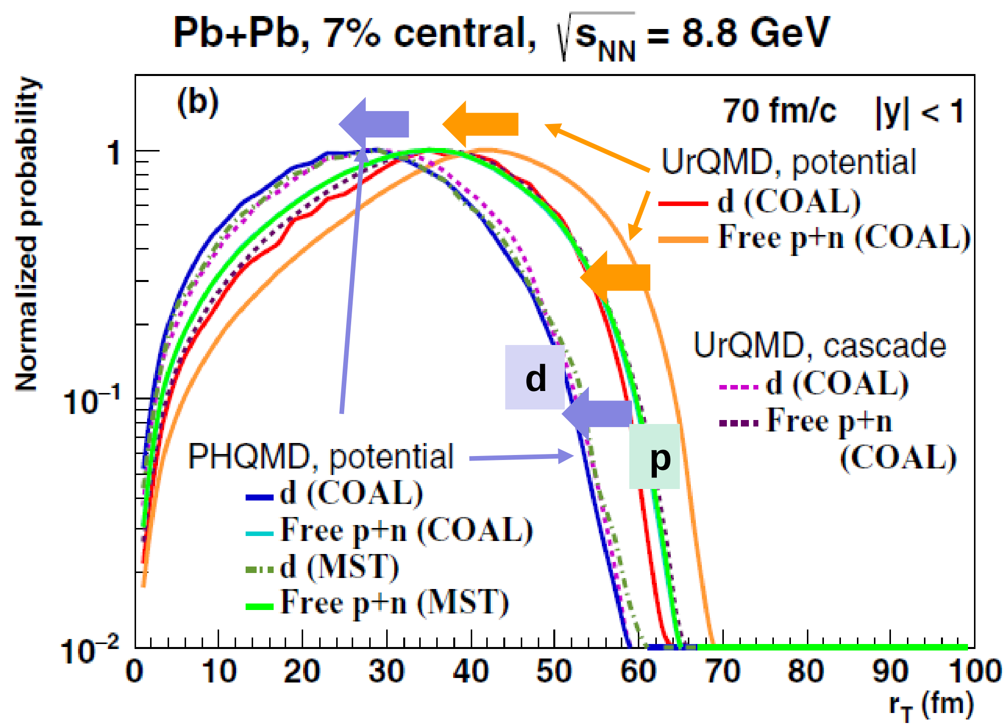

**The analysis of the presently available data points tentatively to the MST + kinetic scenario but further experimental data are necessary to establish this mechanism.**

**V. Kireyeu et al., 2304.12019**

# PHQMD and UrQMD: Where clusters are formed?




➔ **Coalescence as well as the MST procedure 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 pion wind)**

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 )

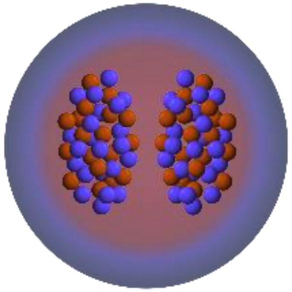
Clusters are formed dynamically

1) by potential interactions among nucleons and hyperons
   Novel development: momentum dependent potential with soft EoS
2) by kinetic mechanism for d : hadronic inelastic reactions NN $\leftrightarrow$ d$\pi$ , $\pi$NN $\leftrightarrow$ d$\pi$ , NNN $\leftrightarrow$ 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 reproduces cluster and hypernuclei data on dN/dy and dN/d$p_T$ as well as ratios d/p and $\bar{d}/\bar{p}$ for heavy-ion collisions from AGS to top RHIC energies.
- Measurement 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

- Strong dependencee of y- and $p_T$-spectra and $v_1$,$v_2$ on EoS - soft, hard, soft-mom. dependent - at SIS energies
- The influence of U(p) decreases with increasing collision energy since the modelled $U_{SEP}$(p) has a maximum at energy 1.5 GeV and decreases for large p ← no exp. data for extrapolation of $U_{SEP}$(p) to large p!
- HADES data data on $v_1$,$v_2$ favour a soft momentum dependent potential (SM)
- STAR data at 3 GeV favour a hard EoS or SM

- 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', cluster can survive



# Thank you for your attention !

# Thanks to the Organizers !