



Light cluster formation in the PHQMD transport approach

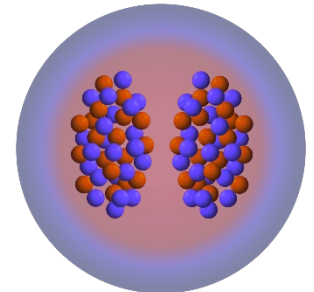
Jörg Aichelin
(Subatech/Nantes)

&

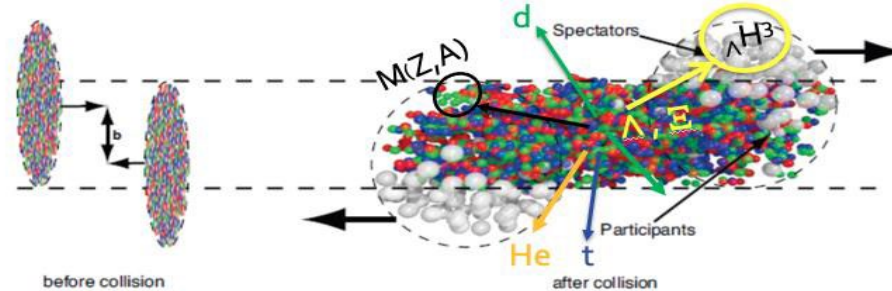
Elena Bratkovskaya, Susanne Glaessel, Gabriele Coci, Viktor Kireyeu,
Vadym Voronyuk, Christoph Blume, Vadim Kolesnikov, Michael Winn



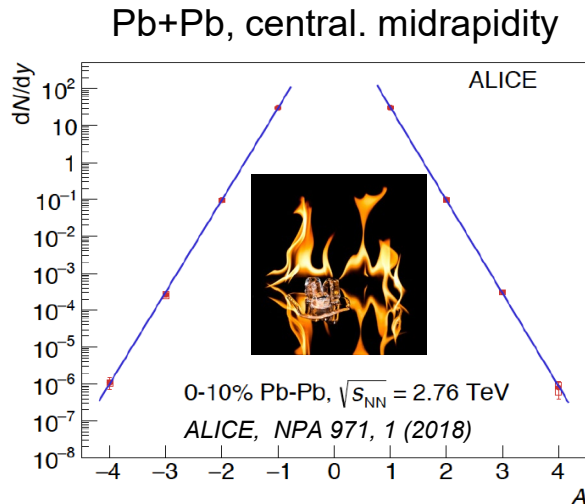
CPOD, Berkeley, May 20-25, 2024



Cluster production in heavy-ion collisions

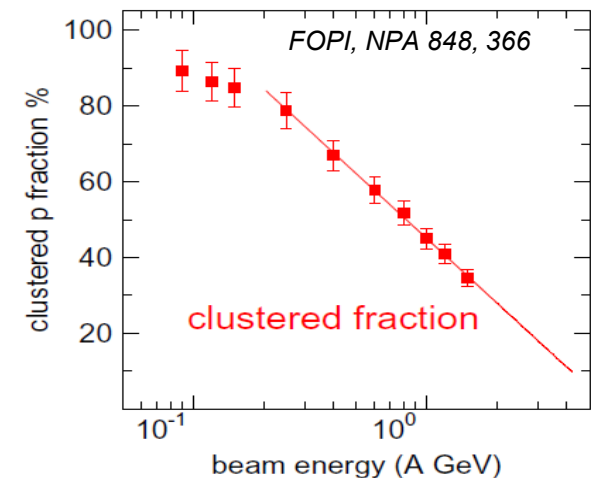


Clusters and (anti-) hypernuclei
are observed experimentally at all energies



- ❑ Clusters are **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 environment?!

Au+Au



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

Cluster production in heavy-ion collisions is a continuous process from $\sqrt{s} = 2$ GeV to $\sqrt{s} = 10$ TeV

Cluster formation at midrapidity happens from

$E_{\text{kin}} = 1$ GeV to $\sqrt{s} = 200$ GeV in a very continuous way

although environment changes drastically:

$E_{\text{kin}} = 1$ GeV 90% nucleons 10% pions

$\sqrt{s} = 200$ GeV 5% <(anti)baryons

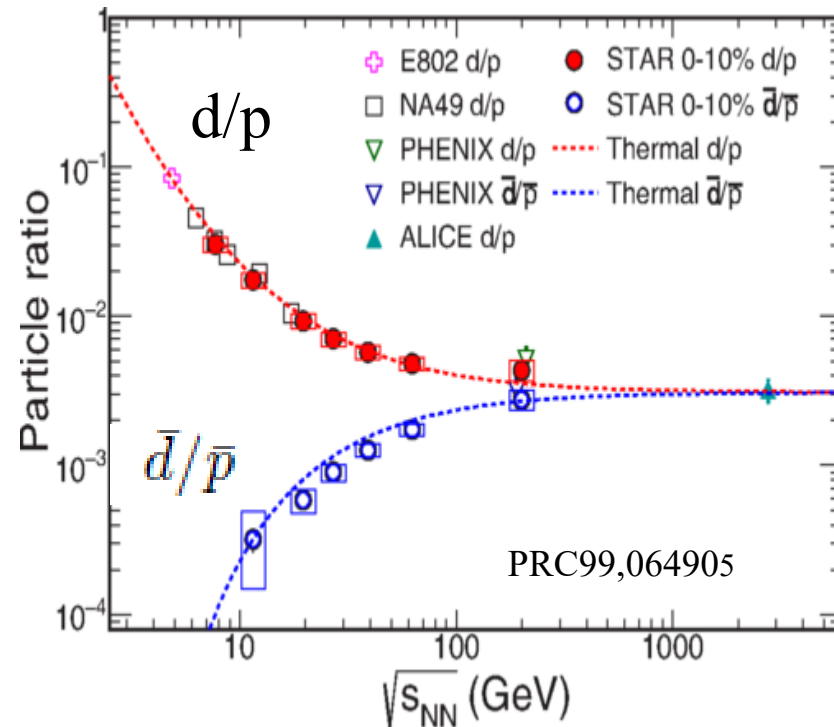
95% mesons

hadronic environment \rightarrow QGP

The slope of the transverse energy spectra
is rather similar

$T \approx 100$ MeV

\rightarrow To study cluster production we should explore all data
(which cover often a larger rapidity interval than at RHIC/LHC
and where models have to make less assumptions than at RHIC/LHC)



Models for cluster and hypernuclei formation

Existing models for cluster formation:

statistical model:

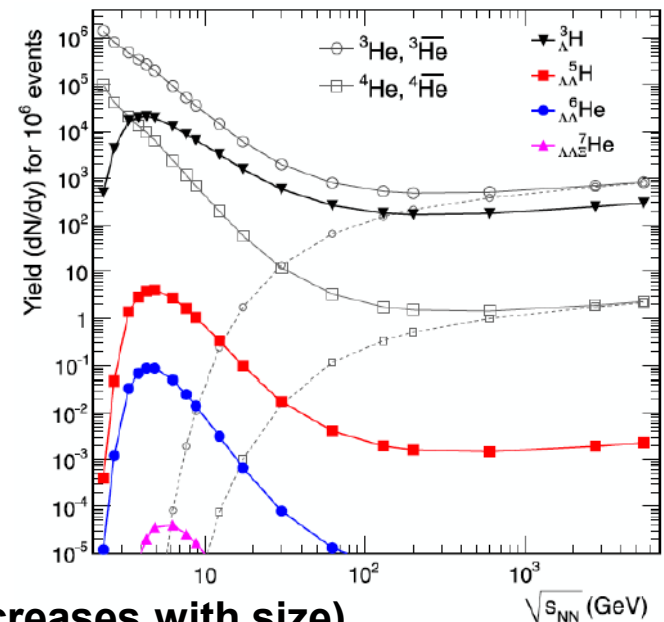
- assumption of thermal equilibrium
- no hadronic interactions → spectra wrong

Dynamical Models:

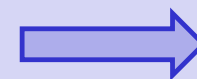
coalescence model:

- determination of clusters at a freeze-out time
- by coalescence radii in coordinate and momentum space
- ad hoc model with free parameters (number increases with size)
- third body for d-production?

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



- collisions $NNN \rightarrow dN$; $NN\pi \rightarrow d\pi$ (kinetic deuterons)
- corrections in the dense medium (d needs space)
- complicated 3 body process (detailed balance)
- only for deuterons



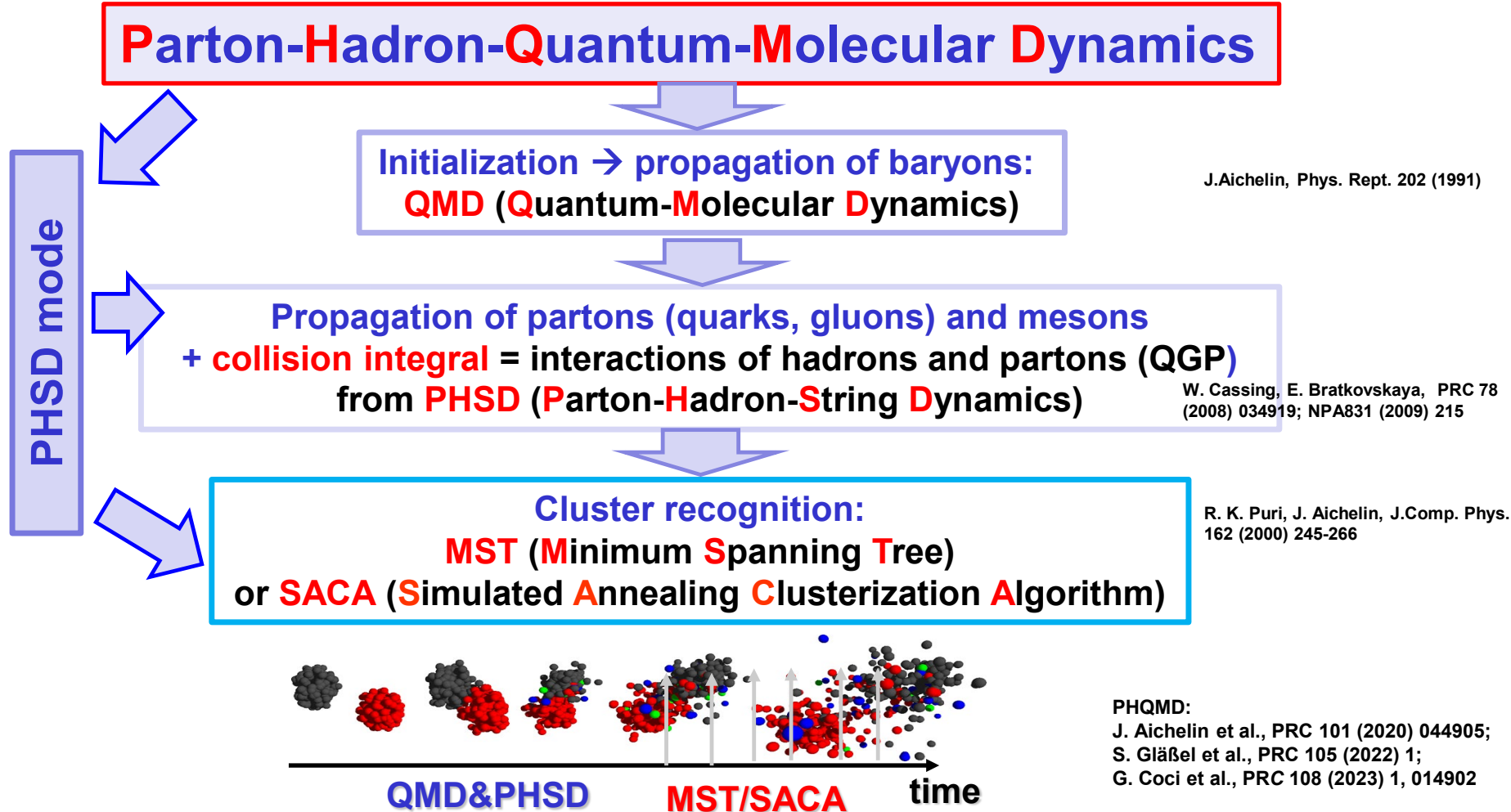
- formation by potential interactions (potential deuterons)
- (the same as applied during the whole HI collision)





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)**



QMD time evolution

□ **Generalized Ritz variational principle:**

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

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 !)

Ansatz: trial wave function for one particle "i":

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

Gaussian with width L centered at $\mathbf{r}_{i0}, \mathbf{p}_{i0}$

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

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

□ **Equations-of-motion (EoM) in coordinate and momentum space:**

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

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: $V_{i,j} = V(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_{i0}, \mathbf{r}_{j0}, t)$

Antisymmetrization is neglected since it would be impossible to formulate collision term

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

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

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

1) Skyrme potential ('static') :

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

with modified **interaction density** (with relativistic extension):

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

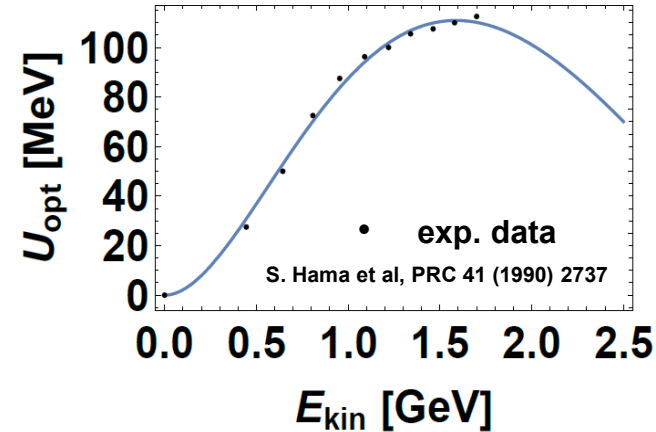
2) Momentum dependent potential :

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

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

Parameters **a**, **b**, **c** are fitted to the "optical" potential (Schrödinger equivalent potential U_{SEP}) extracted from elastic scattering data in pA:

$$U_{SEQ}(p) = \frac{\int^{p_F} V(\mathbf{p} - \mathbf{p}_1) d\mathbf{p}_1^3}{\frac{4}{3}\pi p_F^3}$$



❖ In infinite matter a potential corresponds to the EoS:

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

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

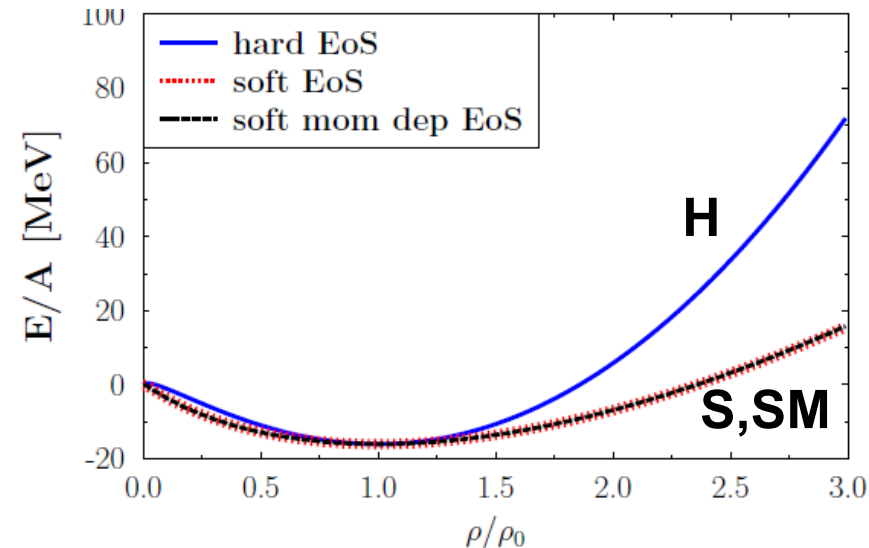
$$V_{Skyrme} = \alpha \frac{\rho}{\rho_0} + \beta \frac{\rho}{\rho_0}^\gamma$$

compression modulus **K** of nuclear matter:

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

E.o.S.	α [MeV]	β [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				

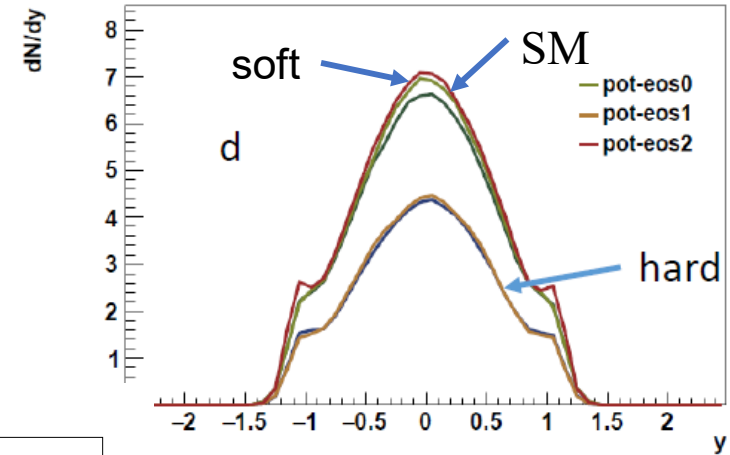
EoS for infinite cold nuclear matter at rest



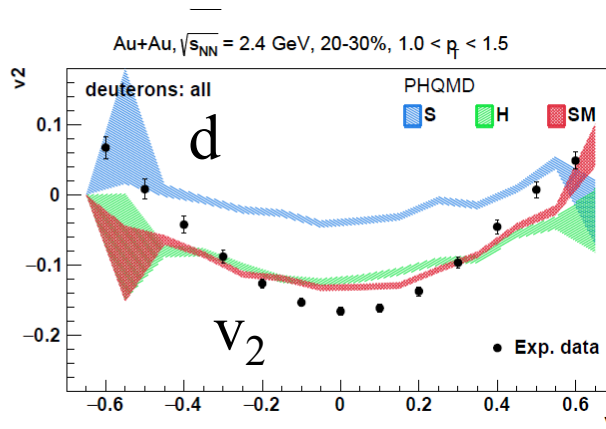
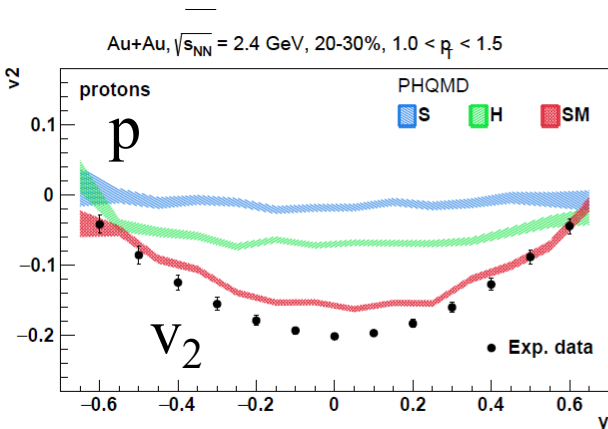
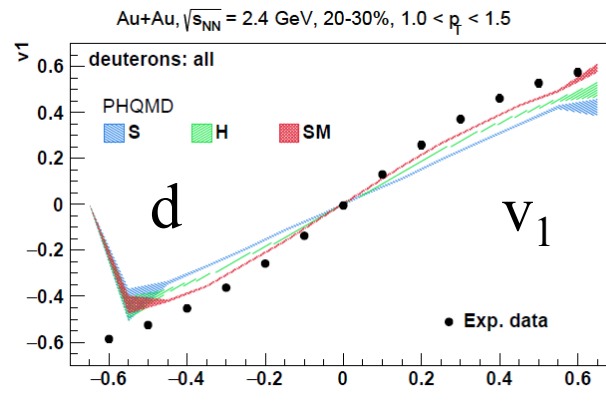
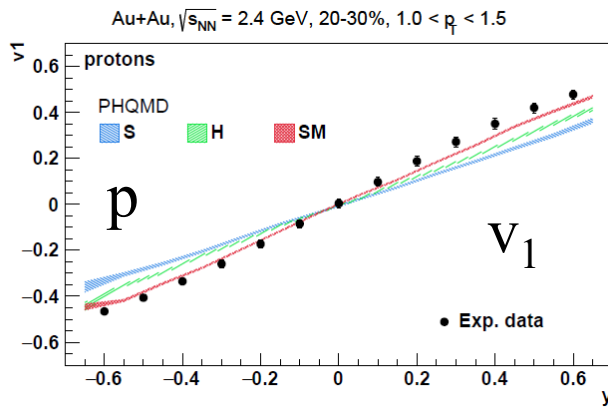
SM potential acts differently on different observables:

- yield (dN/dy) like a soft EoS
- flow harder than a hard EoS

Au+Au, $\sqrt{s_{NN}} = 3.0$ GeV, 1000010020



Au+Au, $\sqrt{s_{NN}} = 3.0$ GeV, 1000020030



Mechanisms for cluster production in PHQMD:

I. potential interactions
(recongized by MST)

&

II. kinetic reactions

III. Coalescence (discussed later)



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.

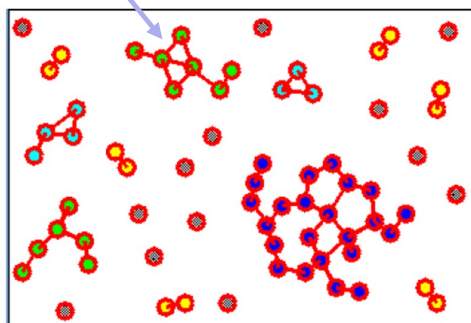
The MST algorithm searches for **accumulations of particles in coordinate space**:

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

$$|\vec{r}_i - \vec{r}_j| \leq 4 \text{ fm} \quad (\text{range of NN potential})$$

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)

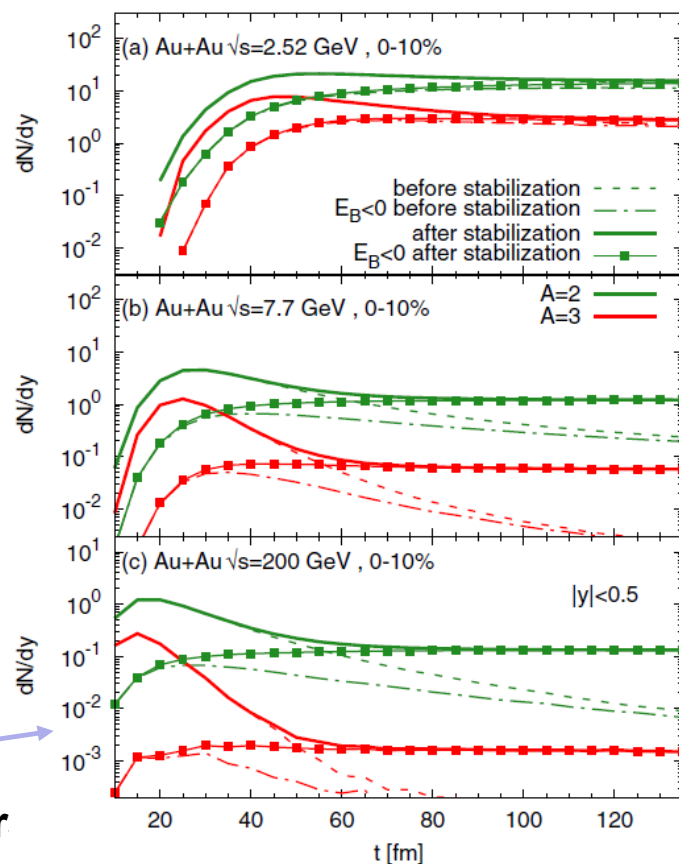
❑ **MST + extra condition: $E_B < 0$**

negative binding energy for identified clusters

❑ **Stabilization procedure** – to correct artifacts of

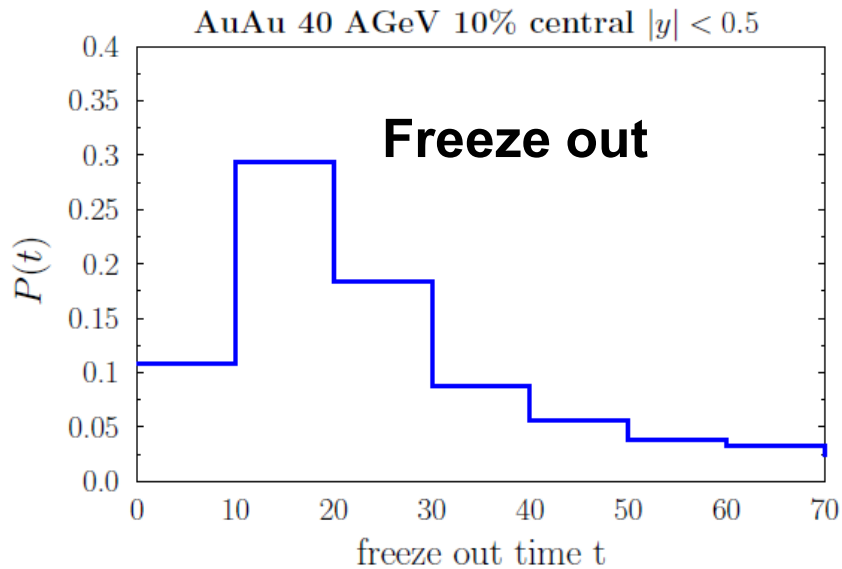
the semi-classical QMD:

recombine the final “lost” nucleons back into cluster if they left the cluster without rescattering

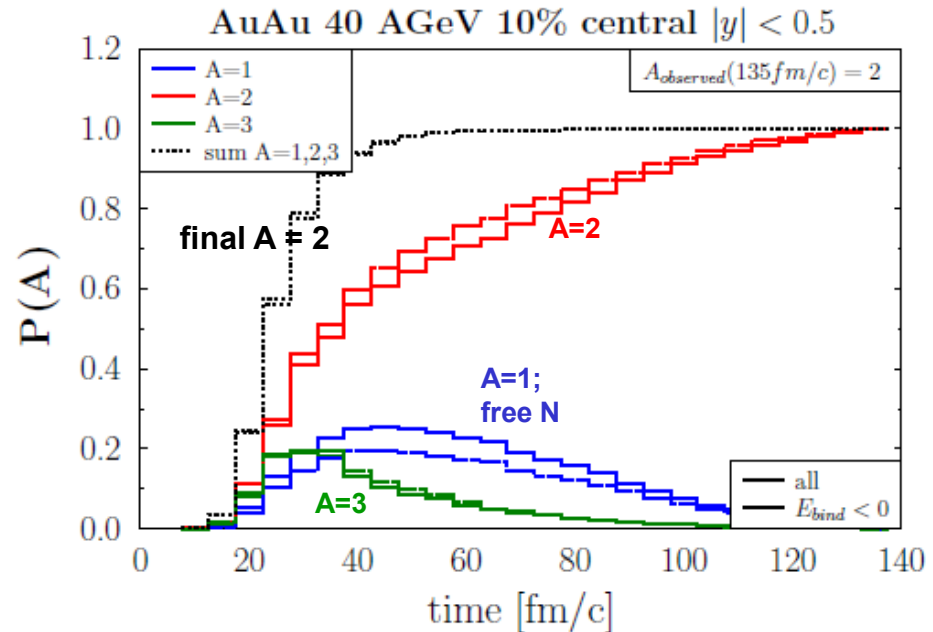


When are the $A=2$ clusters formed?

- The normalized distribution of the **freeze-out time of baryons** (nucleons and hyperons) which are finally observed at mid-rapidity $|y| < 0.5$



- The conditional probability $P(A)$ that the nucleons, which are finally observed in $A=2$ clusters at time 135 fm/c, were at time t members of $A=1$ (free nucleons), $A=2$ or $A=3$ clusters



➔ **Stable clusters** (observed at 135 fm/c) are formed shortly after the dynamical freeze-out

II. Deuteron production by hadronic reactions

“Kinetic mechanism”

- 1) hadronic inelastic reactions $NN \leftrightarrow d\pi$, $\pi NN \leftrightarrow d\pi$, $NNN \leftrightarrow dN$
- 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 $d^4x = dt \cdot dV$
- With test particle ansatz the transition rate for $3 \rightarrow 2$ reactions:

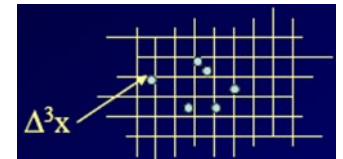
W. Cassing, NPA 700 (2002) 618

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

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

Energy and momentum of final particles

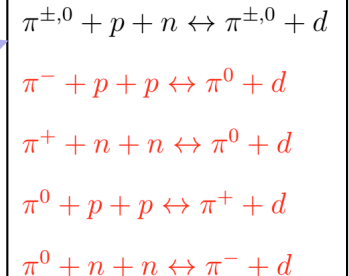
2,3-body phase space integrals
 [Byckling, Kajantie]



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

→ 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: $\pi+N+N \leftrightarrow d+\pi$ inclusion of all possible isospin channels allowed by total isospin T conservation → enhancement of the d production



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** in the entrance channel

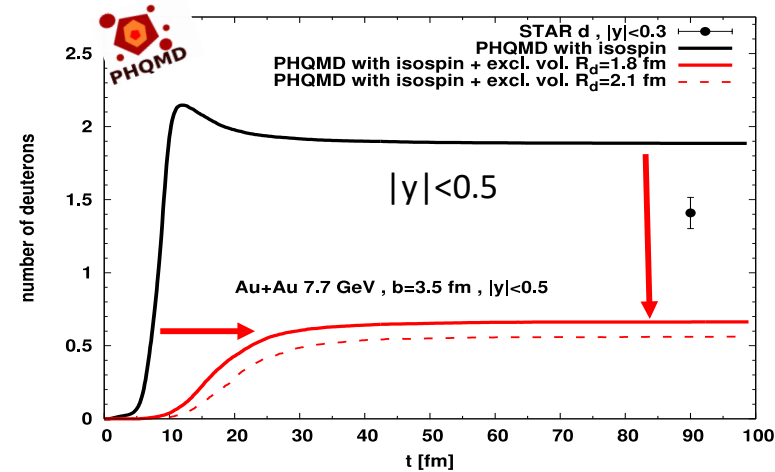
Realization:

- 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:

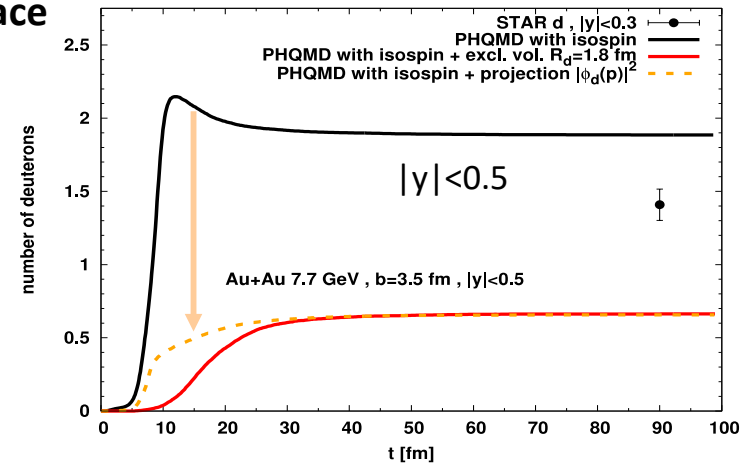
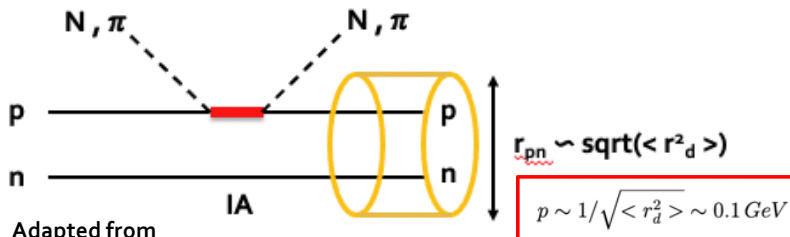
$$|\vec{r}(i)^* - \vec{r}(d)^*| < R_d$$

- ❑ **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

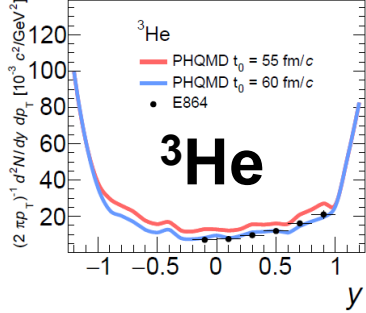
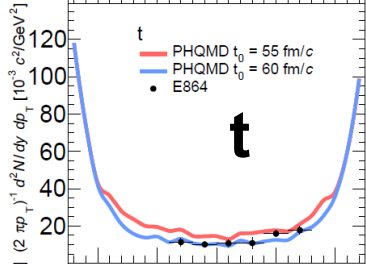
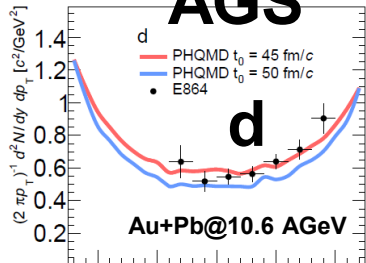
→ **momentum correlations of pn -pair**



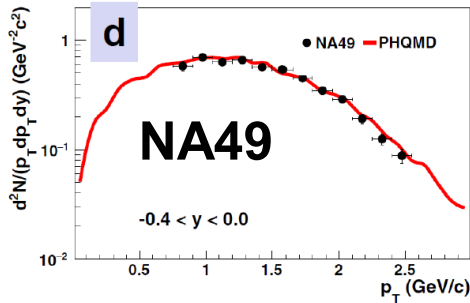
- ❑ **Strong reduction of d production at early times by projection on DWF $|\phi_d(p)|^2$**

Highlights: PHQMD cluster and hypernuclei dynamics from SIS to RHIC

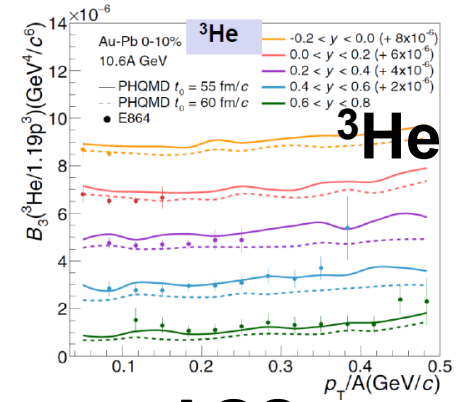
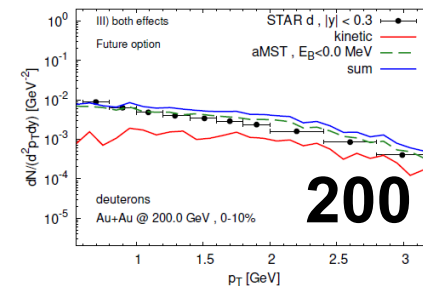
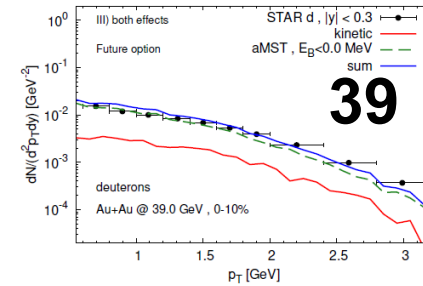
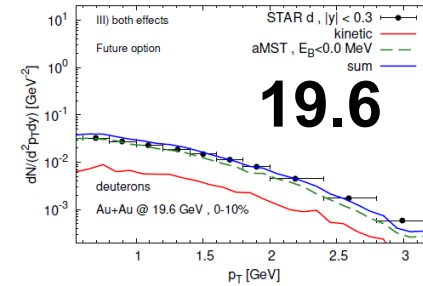
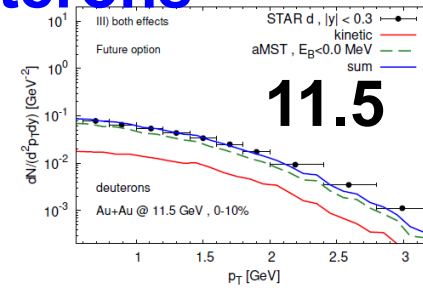
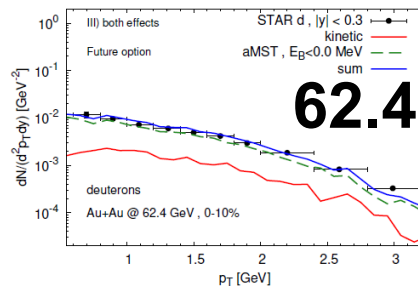
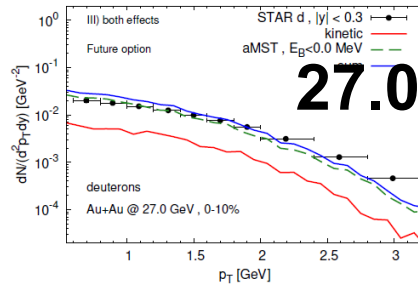
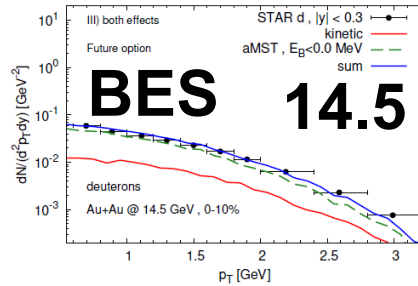
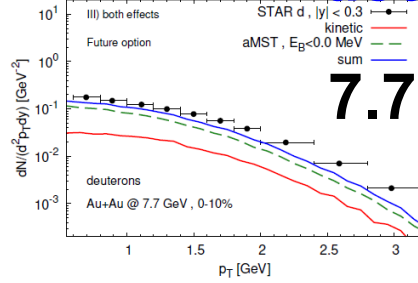
AGS



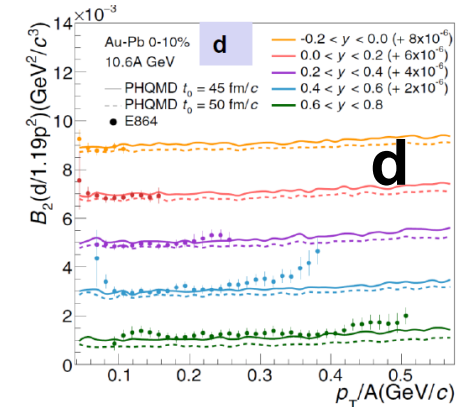
d, Pb+Pb, $\sqrt{s_{NN}} = 8.8$ GeV, $b = 0 - 5$ fm



deuterons



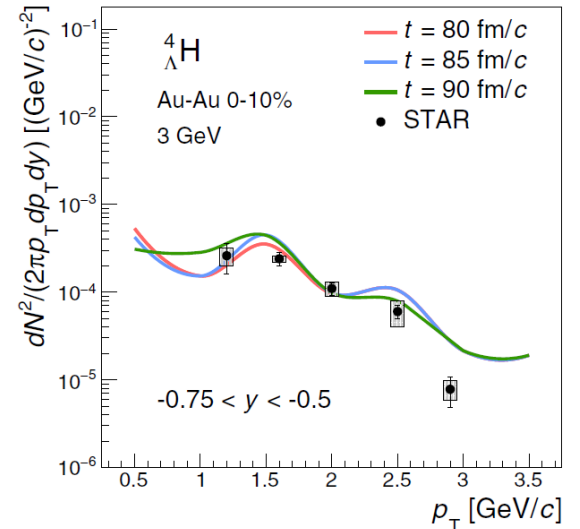
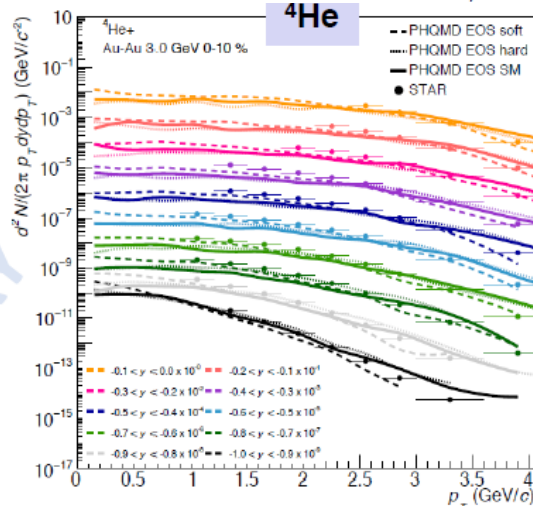
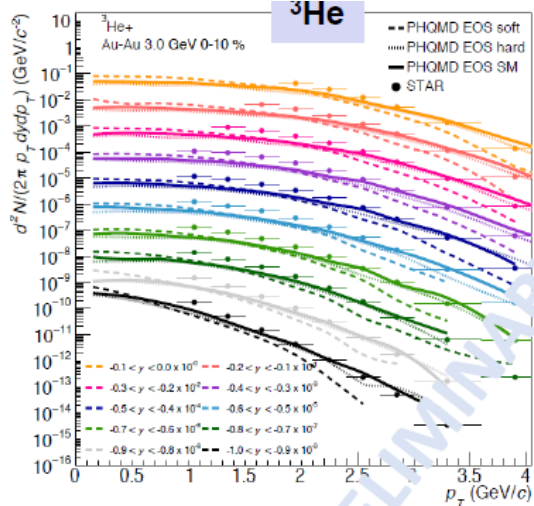
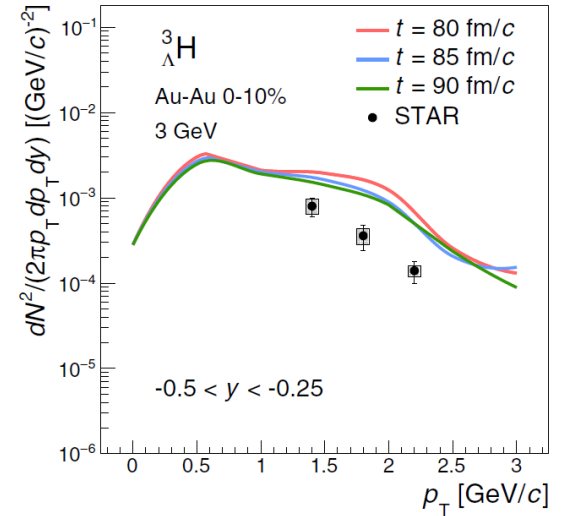
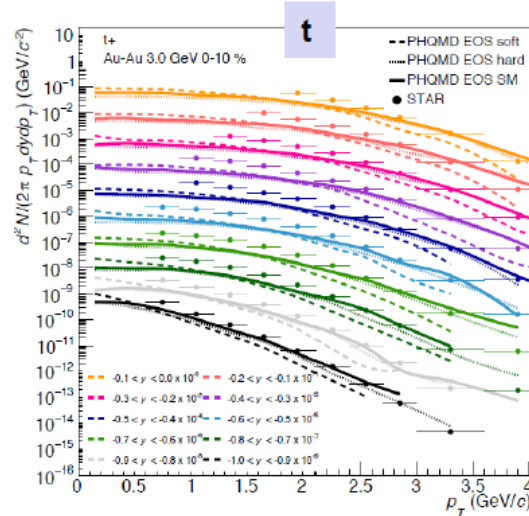
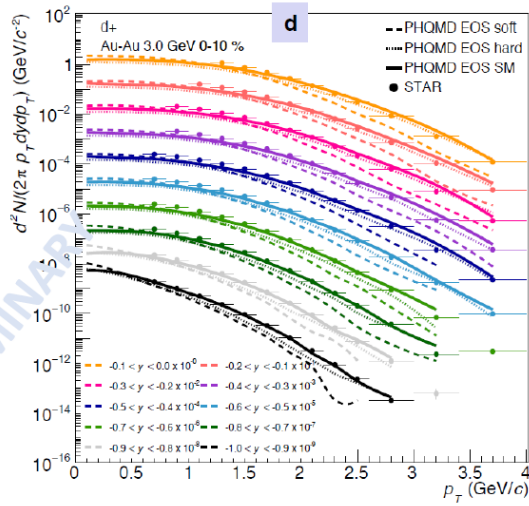
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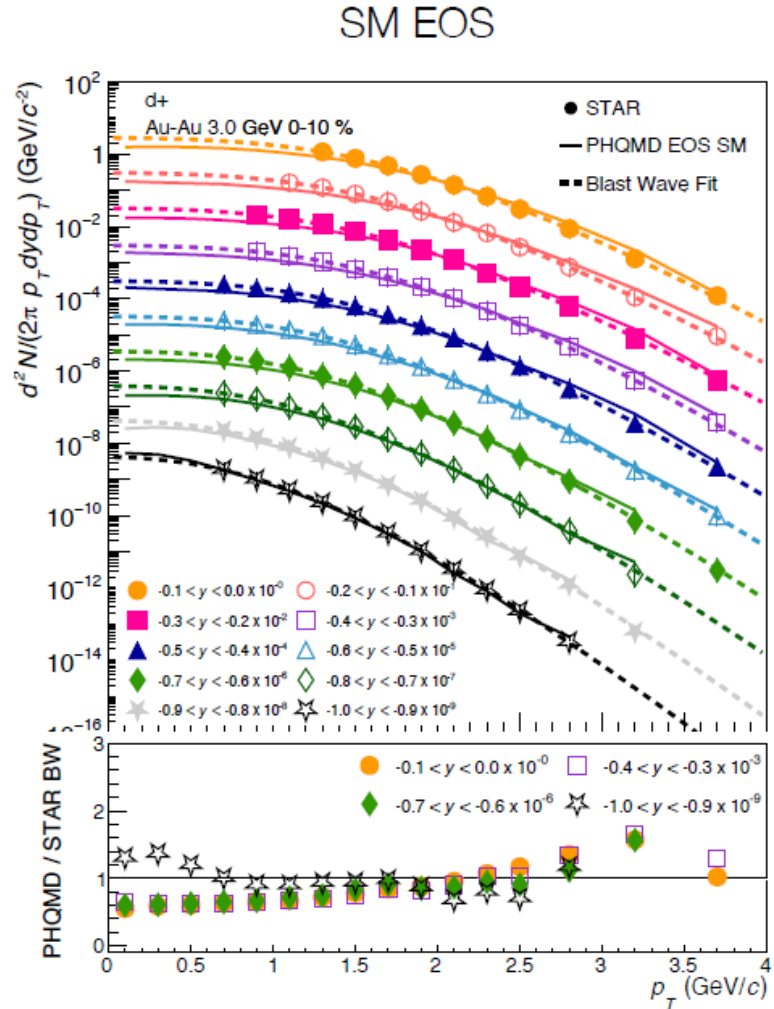
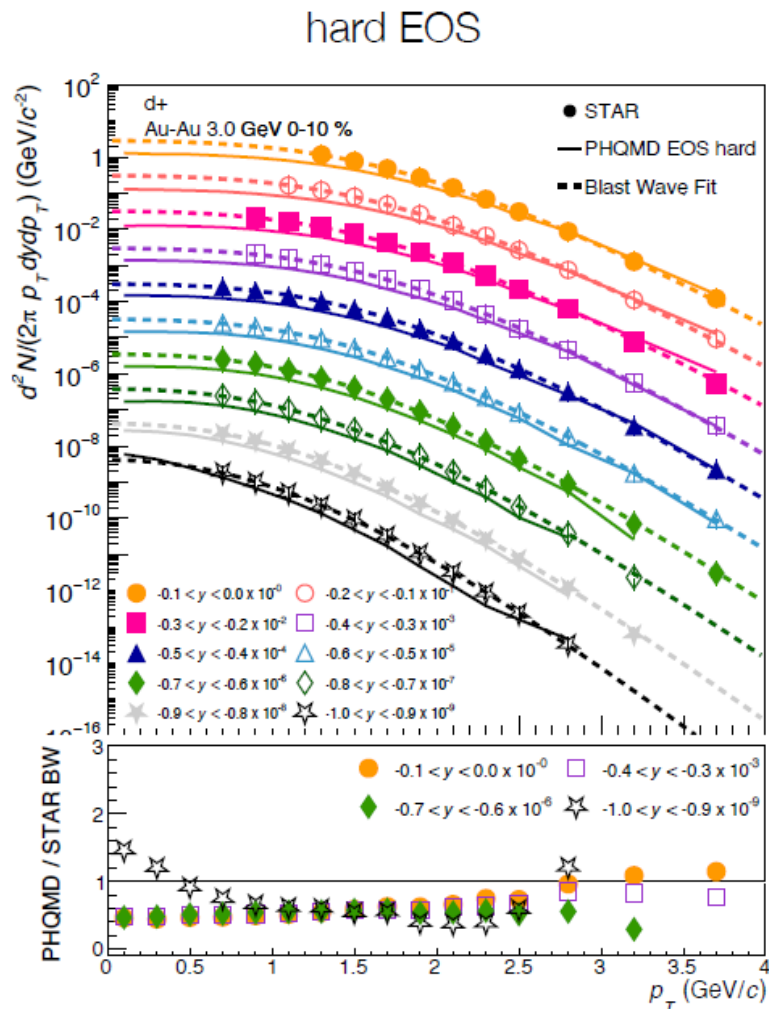


PHQMD:
J. Aichelin et al., PRC 101 (2020) 044905;
S. Gläsel et al., PRC 105 (2022) 1;
G. Coci et al., PRC 108 (2023) 1, 014902

Light cluster production at $s^{1/2} = 3$ GeV

The PHQMD comparison with recent STAR fixed target p_T distribution of p , d , t , ${}^3\text{He}$, ${}^4\text{He}$ from Au+Au central collisions at $\sqrt{s} = 3$ GeV

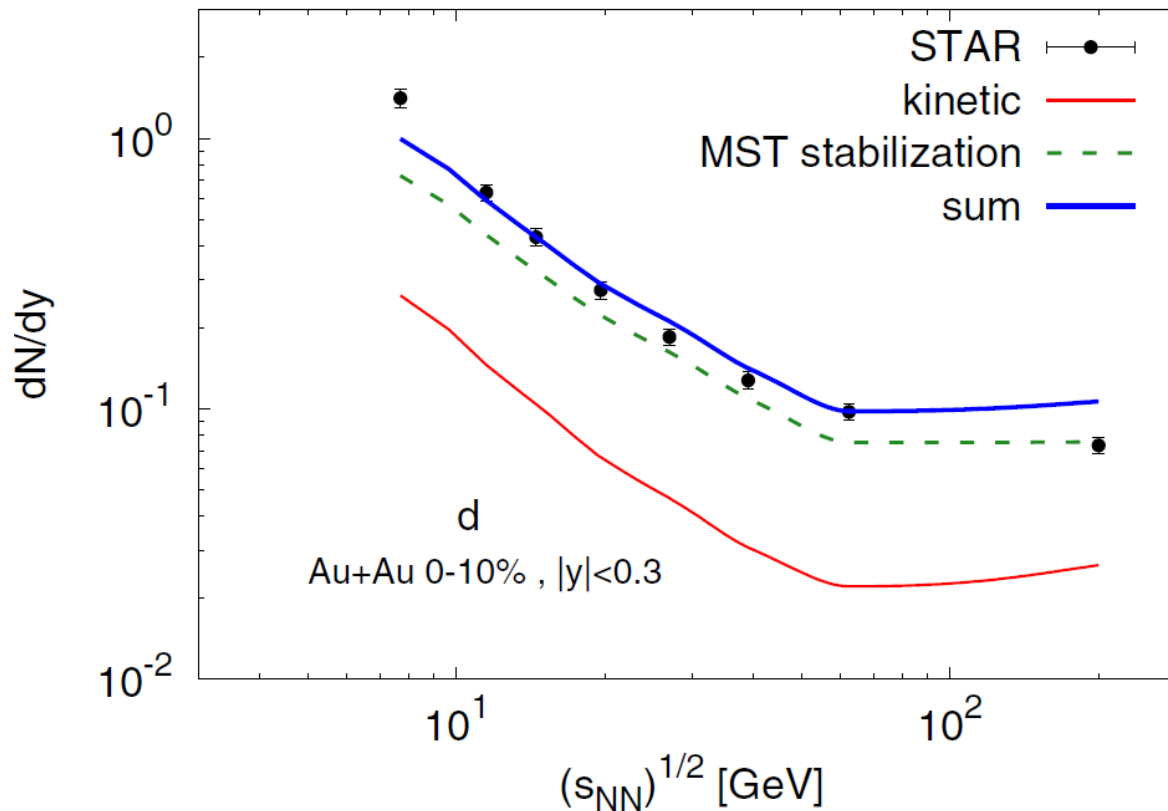




SM describes data best
difference PHQMD-data at low p_T → blast wave fits ok?

Kinetic vs. potential deuteron production

Excitation function dN/dy of deuterons at midrapidity

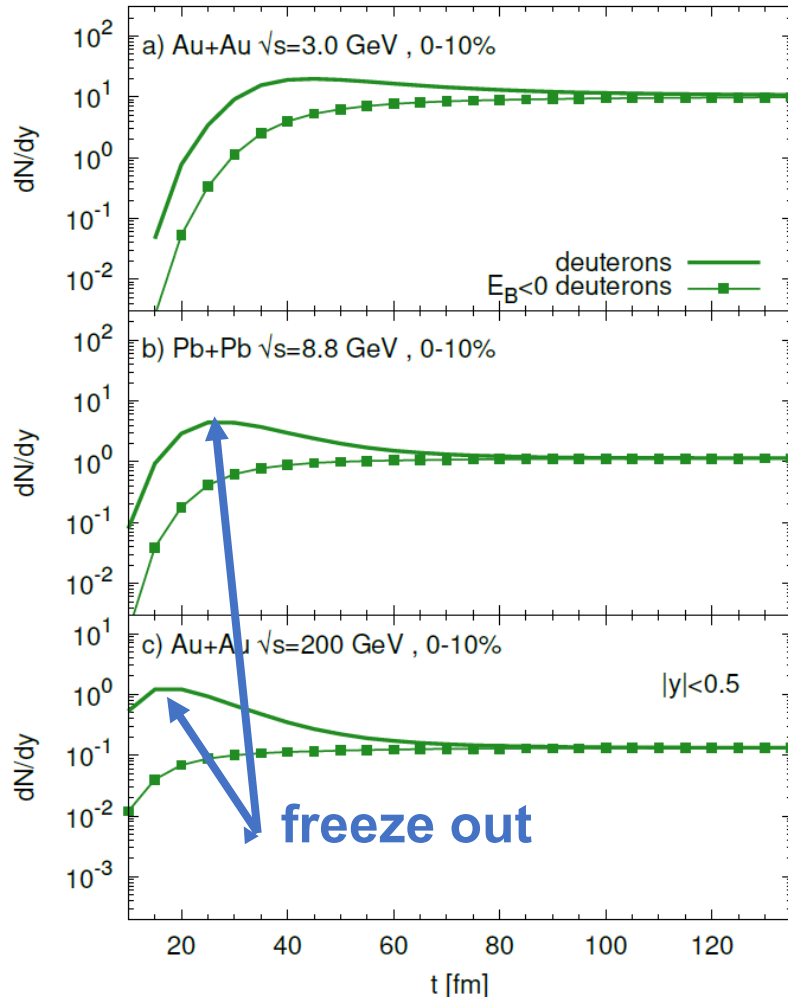


- ❑ Very continuous as a function of \sqrt{s}
- ❑ Functional form similar for kinetic and potential deuterons
- ❑ PHQMD provides a good description of STAR data
- ❑ **The potential mechanism is dominant for d production at all energies!**

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



MST deuterons



Why may the observables be different in coalescence and in MST?

Same simulation

- Coalescence deuterons produced earlier
- Most of the coalescence deuterons unbound
- Factor 3/8 brings them to the physical value
- Many surrounded by other hadrons when produced

Coalescence parameters from UrQMD
 → in PHQMD

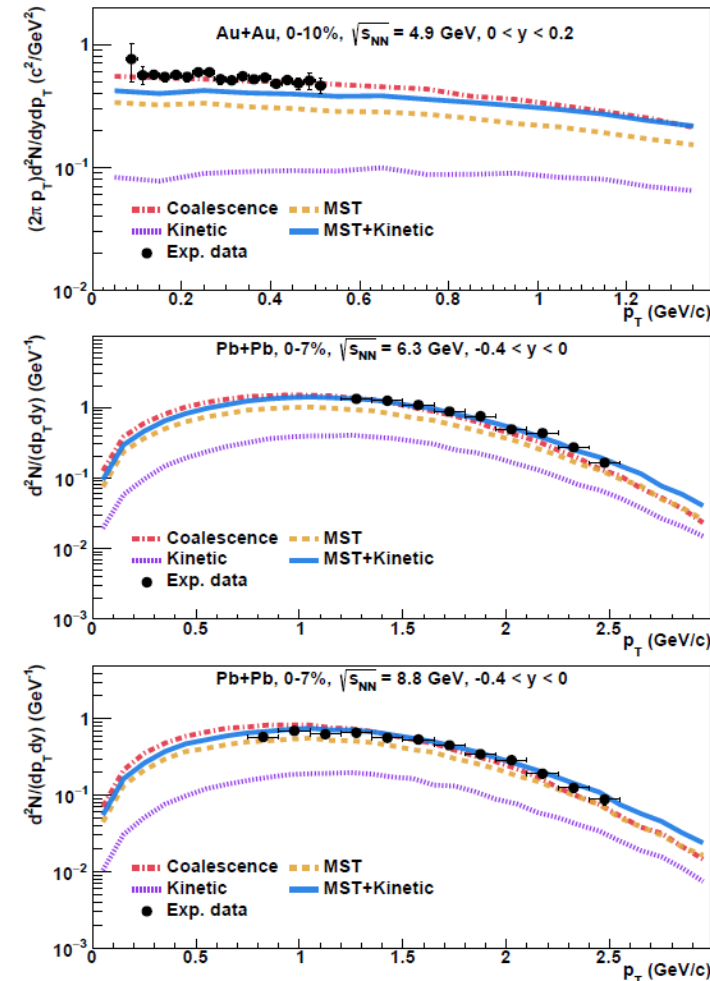
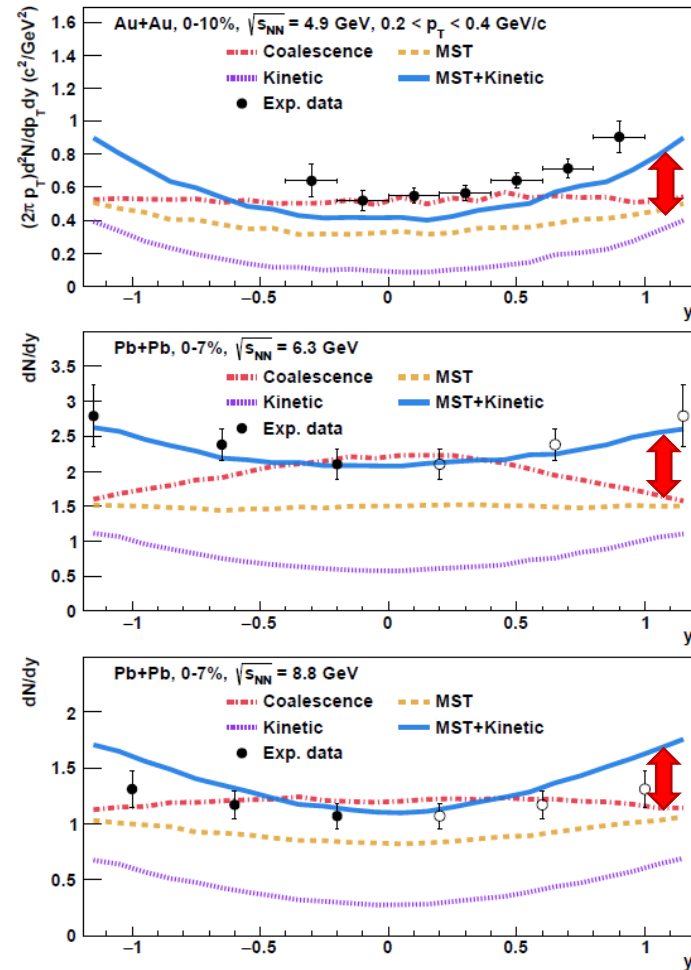
Coalescence and MST (potential) deuterons calculated in the same PHQMD run

Mechanism for cluster production

coalescence and MST ↔ experimental data

Deuterons:

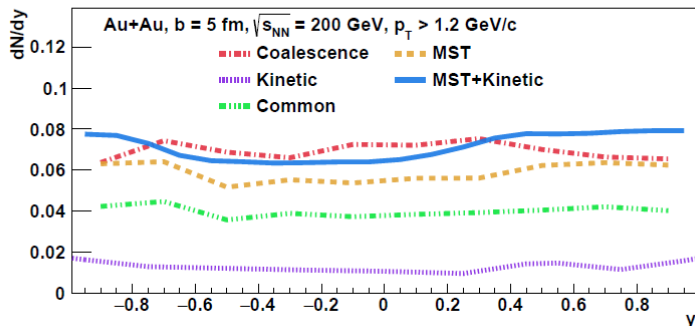
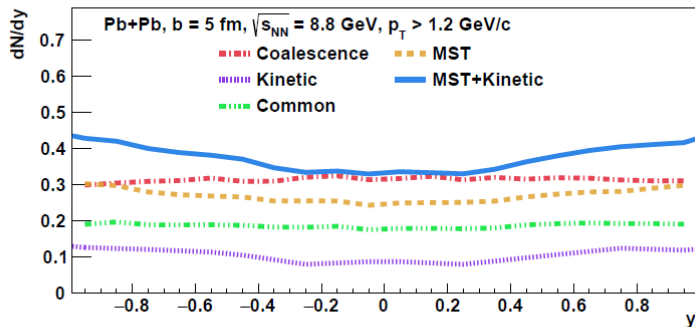
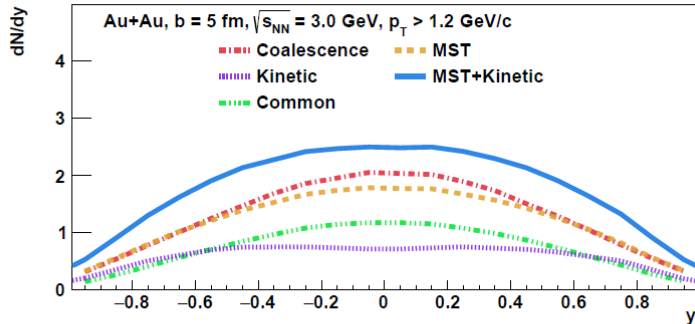
- p_T distributions similar for coalescence/ MST-kinetic
- y - distributions show differences



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

Difference big enough for an experimental decision?

$p_T > 1.2$ GeV (experimental acceptance)



Difference between COAL and MST
mostly at low p_T

In the measured p_T range signal is gone
for $\sqrt{s} = 3$ GeV

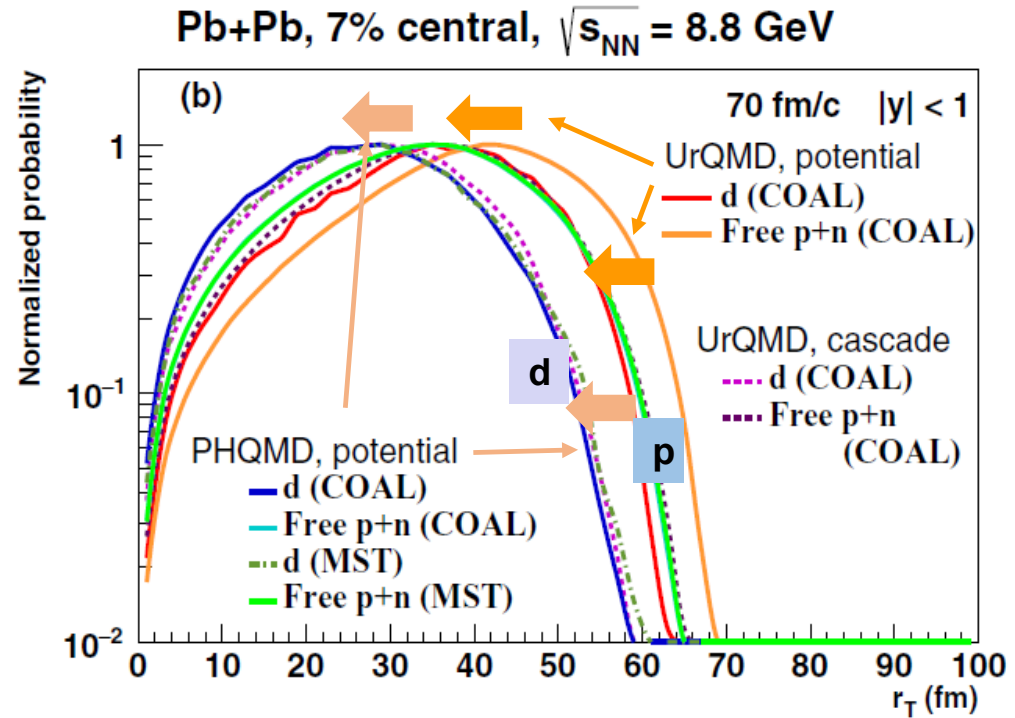
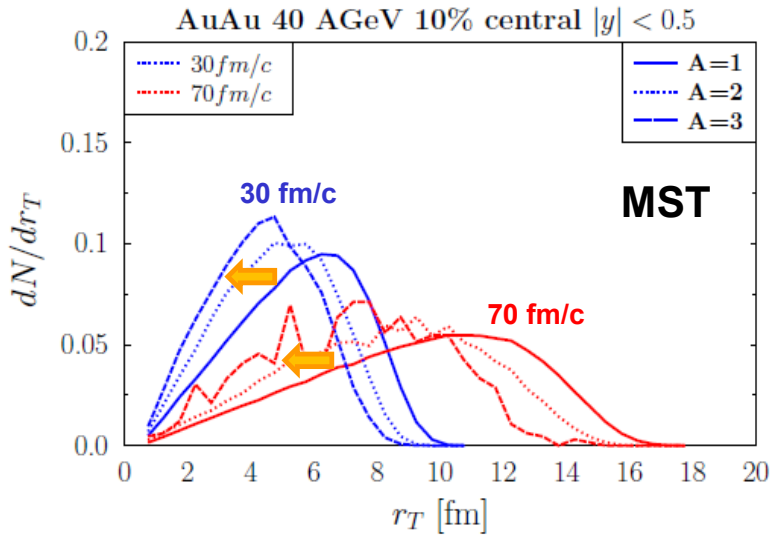
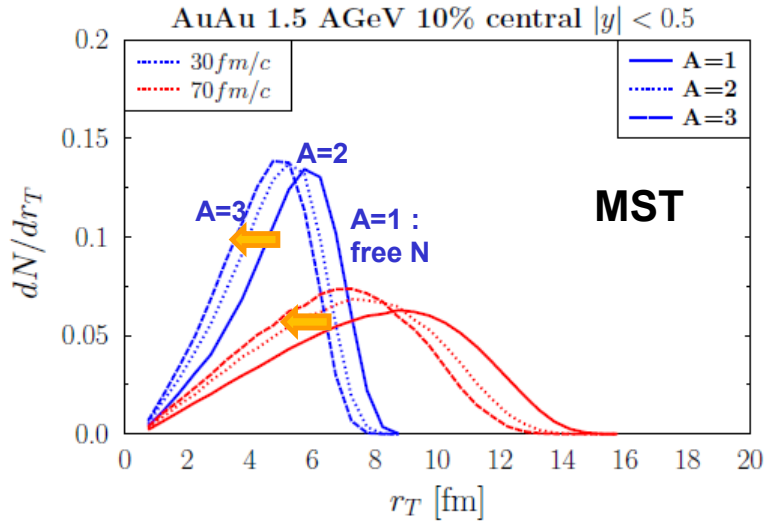
But: there seems to be a **sweet spot**
around $\sqrt{s} = [6 - 8]$ GeV
to identify the reaction mechanism

➔ We have to wait for more precise rapidity distributions

Where the clusters are formed?



PHQMD and UrQMD: Where clusters are formed?



- ➔ **COAL(escence) as well as the 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 the pion wind)

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) for d also by **kinetic mechanism**: 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 for **quantum properties of d**, modelled by the finite-size excluded volume effect in coordinate space and projection of relative momentum of p+n pairs on d wave-function in momentum space leads to a **strong reduction** of d production



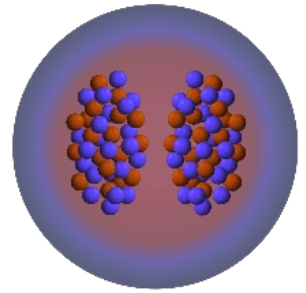
- ❑ PHQMD reproduces cluster and hypernuclei data of dN/dy and dN/dp_T as well as **ratios d/p** and \bar{d}/\bar{p} for heavy-ion collisions from AGS to top RHIC energies.
- ❑ Measurement of **dN/dy** beyond mid-rapidity seems to **distinguish the mechanisms for cluster production**: **coalescence versus dynamical cluster production** recognized by MST + kinetic mechanism for deuterons
- ❑ **Dependence 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 $p \leftarrow$ no exp. data for extrapolation of $U_{SEP}(p)$ to large p !
- ❑ HADES data data on v_1, v_2 STAR data at 3 GeV favour **a soft momentum dependent potential (SM)**

What did we learn (besides that PHQMD describes the data)?

- ❑ Cluster production at midrapidity is a **smooth process from \sqrt{s} 2.4 GeV to 5 TeV**
- ❑ Stable clusters are **formed (shortly) after elastic and inelastic collisions** have ceased
- ❑ They are formed **behind the front of the expanding energetic hadrons**
- ❑ They can survive the expansion because **“ ice does not meet the ‘fire’**
- ❑ This result is **the same for the PHQMD and UrQMD transport approaches**
(and very probably this is true for all other transport approaches)
- ❑ Coalescence as well as MST(+kinetic) can describe the data
however: to describe A[2-4] (and at low energy larger A)
MST does not need any (free) parameters for cluster production
Coalescence needs two for deuterons, 4 for ^3He ,t + problem of hadrons
close by

Major problem to be solved:

- **complete relativistic kinematics**
- **how to project classical phase space distributions on quantum states**



Thank you for your attention !

Thanks to the Organizers !