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GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Parton-Hadron-Quantum-Molecular Dynamics

PHQMD team

Susanne Glaessel, Gabriele Coci, Viktar Kireyeu, Joerg Aichelin, Elena Bratkovskaya, Vadym Voronyuk, Christoph Blume, Vadim Kolesnikov, Michael Winn, Taesoo Song;

In collaboration with Yvonne Leifels, Arnaud Le Fèvre

*HADES data benchmarking with PHQMD and other models

PHQMD

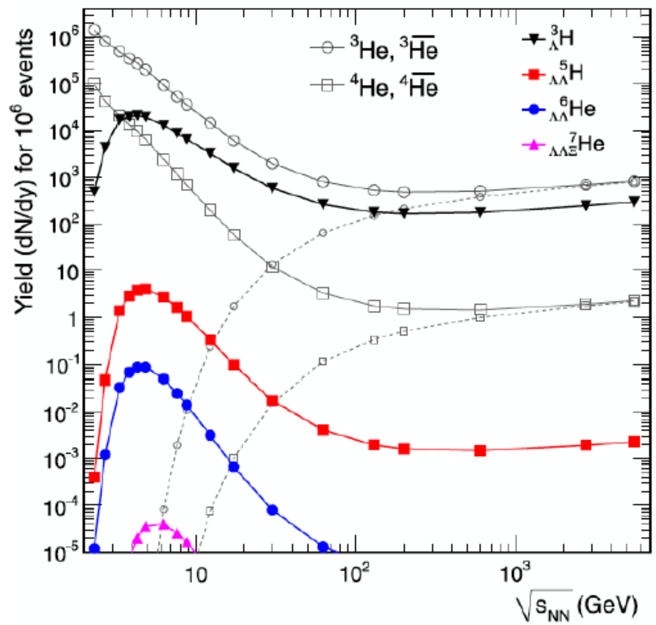
NuSym23: XIth International Symposium on Nuclear Symmetry Energy

GSI, Darmstadt, 18-22 September 2023

Modeling of cluster and hypernuclei formation

<u>**Existing models for cluster formation:**</u>

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



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

- **coalescence model:**
  - **determination of clusters at a freeze-out time by coalescence radii in coordinate and momentum space**

➔ **don‘t provide information on the dynamical origin of cluster formation**

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

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

– via potential interaction - potential mechanism

-- by scattering - kinetic mechanism

PHQMD

Cluster formation: QMD vs MF

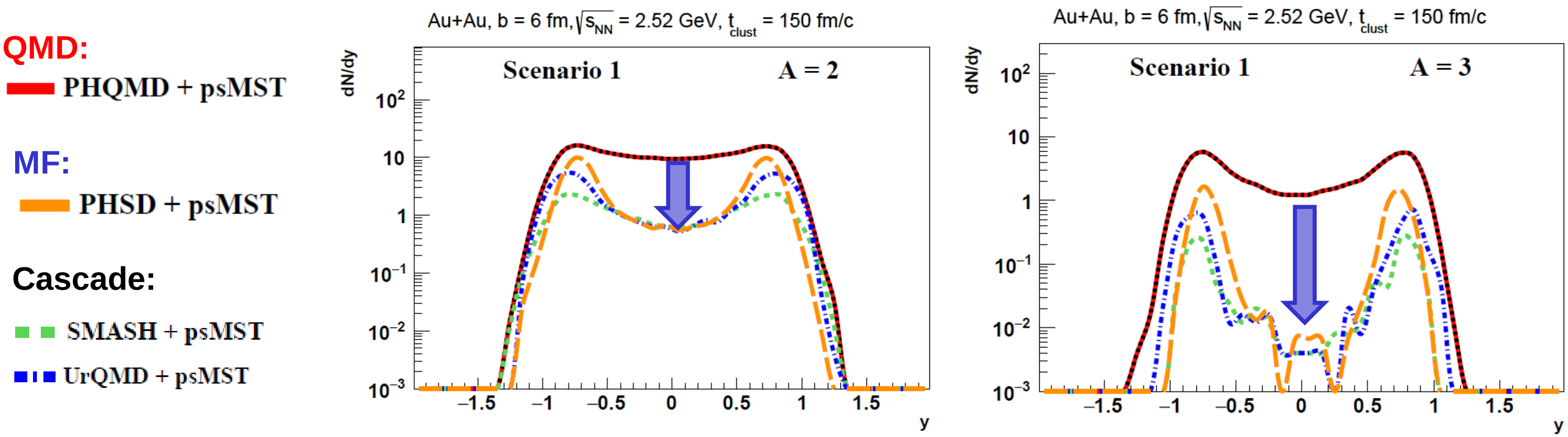
- Cluster formation is sensitive to nucleon dynamics

➔ One needs to keep the nucleon correlations (initial and final) by realistic nucleon-nucleon interactions in transport models:

- QMD (quantum-molecular dynamics) – allows to keep correlations
- MF (mean-field based models) – correlations are smeared out
- Cascade – no correlations by potential interactions

Example: Cluster stability over time:

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



➔ n-body QMD dynamics for the description of cluster production

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)

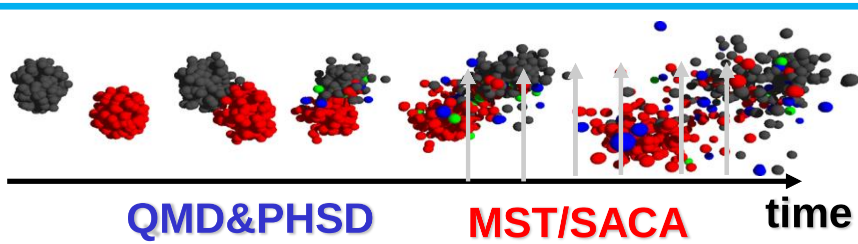
J.Aichelin, Phys. Rept. 202 (1991)

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



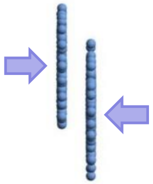
PHQMD:
J. Aichelin et al., PRC 101 (2020) 044905;
S. Gläßel et al., PRC 105 (2022) 1;
G. Coci et al., PRC 108 (2023) 1, 014902

PHQMD Collision Integral → from Parton-Hadron-String-Dynamics

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

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

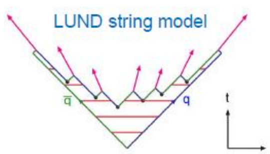
Initial A+A collision



→ Initialization of A-nuclei + QMD propagation of baryons

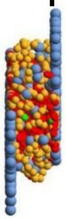
PHQMD

PHSD collision integral → PHQMD

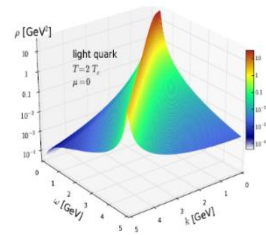


- **Initial A+A collisions :**
  N+N → string formation → decay to pre-hadrons + leading hadrons

Partonic phase

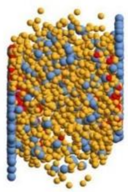


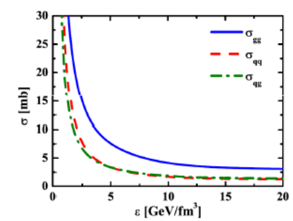
- **Formation of QGP stage** if local $\varepsilon > \varepsilon_{critical}$:
  dissolution of pre-hadrons → partons



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

Hadronization

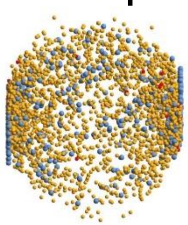


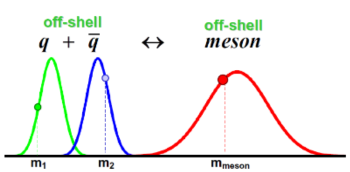


  - Degrees-of-freedom: strongly interacting quasiparticles: massive quarks and gluons (g,q,q_{bar}) with sizeable collisional widths in a self-generated mean-field potential

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

Hadronic phase





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

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

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

QMD propagation

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

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:**

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

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

Two-body potential in QMD

- Nucleon-nucleon density dependent two-body potential:

$$
\begin{aligned}
V(\mathbf{r_i},\mathbf{r_j},\mathbf{p_i},\mathbf{p_j}) &= G + V_{\mathrm{Coul}} \\
&= V_{\mathrm{Skyrme}} + V_{\mathrm{Yuk}} + V_{\mathrm{mdi}} + + V_{sym} + V_{\mathrm{Coul}} \\
&= \boxed{t_1\delta(\mathbf{r_i}-\mathbf{r_j}) + t_2\delta(\mathbf{r_i}-\mathbf{r_j})\rho^{\gamma-1}(\mathbf{r_i})} + \\
&\quad t_3\frac{\exp\{-|\mathbf{r_i}-\mathbf{r_j}|/\mu\}}{|\mathbf{r_i}-\mathbf{r_j}|/\mu} + \qquad (6) \\
&\quad \boxed{t_4 \ln^2(1+t_5(\mathbf{p_i}-\mathbf{p_j})^{\mathbf{2}})\delta(\mathbf{r_i}-\mathbf{r_j})} + \\
&\quad t_6\frac{1}{\varrho_0}T_3^i T_3^j\delta(\mathbf{r_i}-\mathbf{r_j}) + \frac{Z_i Z_j e^2}{|\mathbf{r_i}-\mathbf{r_j}|}.
\end{aligned}
$$

t_1 - t_4 depend on the EoS

t_4 contains the momentum dependence of the potential

- **Skyrme forces** and **momentum dependent interactions** corresponding to the volume energy. Their density dependence lead directly to the **nuclear EoS of symmetric matter**
- **Yukawa forces** corresponding to the surface energy
- **Coulomb forces** corresponding to the Coulomb energy
- **Isospin dependent forces** corresponding to the asymmetry energy and thus leading to the nuclear EoS of asymmetric matter.

Two-body potential in QMD

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

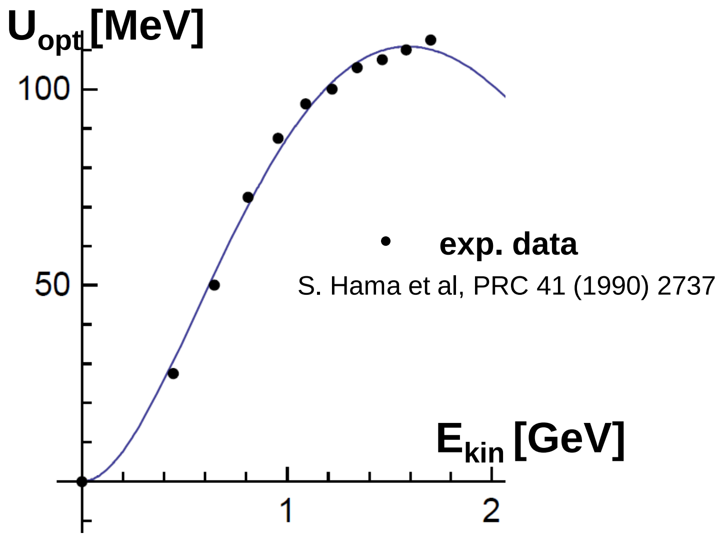
$$U_i(\mathbf{r}_{i0}, \mathbf{p}_{i0}, t) = \sum_j < V_{ij} > = \alpha\left(\frac{\rho_{int}(\mathbf{r}_{i0})}{\rho_0}\right) + \beta\left(\frac{\rho_{int}(\mathbf{r}_{i0})}{\rho_0}\right)^\gamma + \sum_j \delta \ln^2\left(\epsilon\,(\mathbf{p}_{i0}-\mathbf{p}_{j0})^2+1\right)\frac{\rho_{int}(\mathbf{r}_{i0})}{\rho_0}$$

- **Skyrme potential** ('static') :
  - Parameters t_1, t_2, t_4 correspond to α, β, γ

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

- **Momentum dependent potential** :
  - Parameters δ, ε are given by fits to the optical potential extracted from elastic scattering data in pA

J. Aichelin et al., Phys. Rev. Lett. 58 (1987) 1926



EoS in PHQMD

- modifed interaction density (with relativistic extension):

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

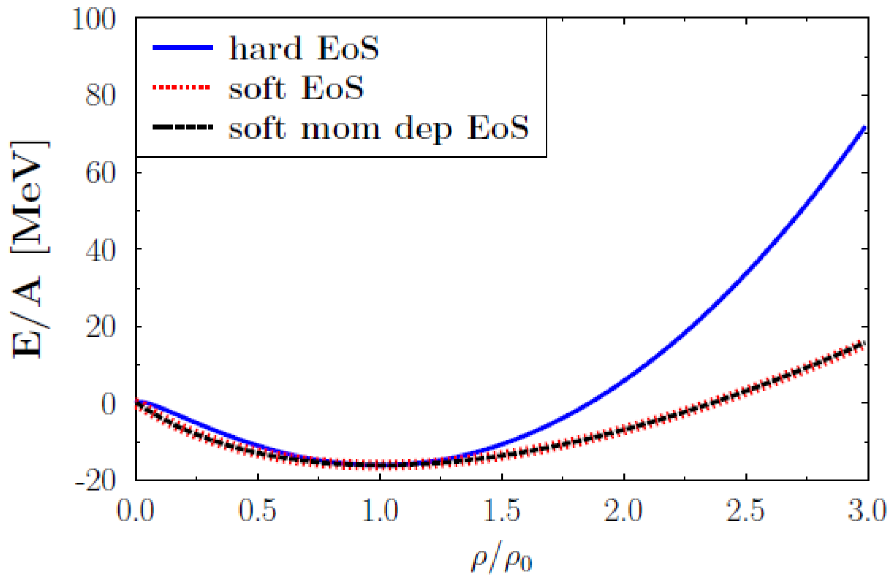
In infinite matter a potential corresponds to EoS

- HIC ←→ EoS for infinite matter at rest
  - compression modulus K of nuclear matter:

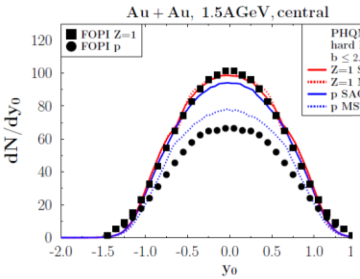
$$K = -V\frac{dP}{dV} = 9\rho^2\frac{\partial^2(E/A(\rho))}{(\partial\rho)^2}|_{\rho=\rho_0}.$$

	α (MeV)	β (MeV)	γ	K [MeV]
S	-390	320	1.14	200
H	-130	59	2.09	380
SM	-625	56	1.08	200

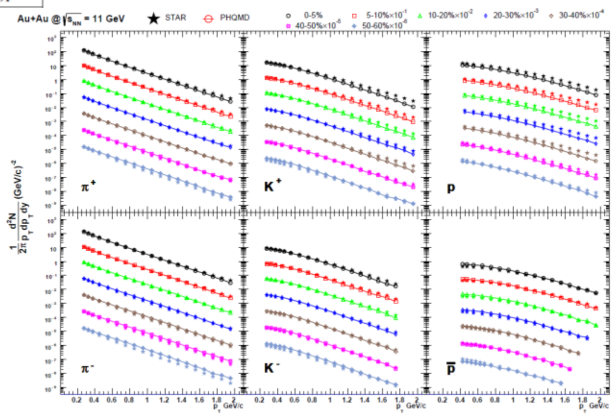
EoS for infinite matter at rest

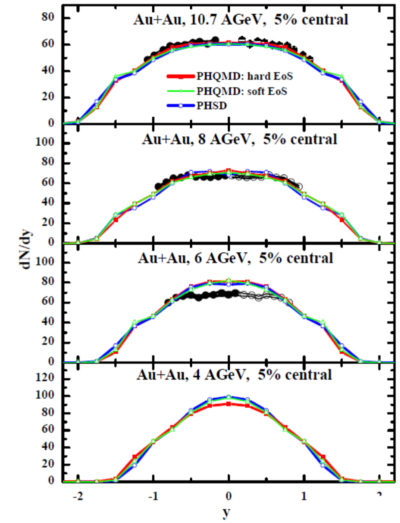


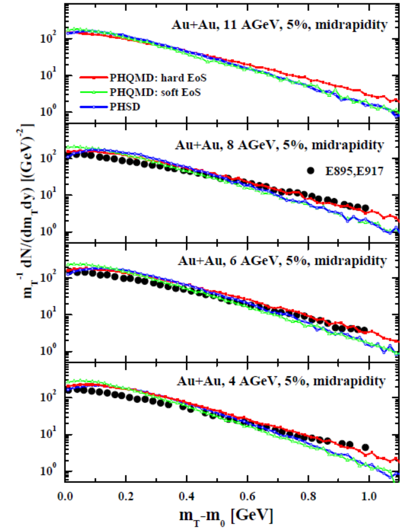
Highlights: PHQMD ‚bulk‘ dynamics from SIS to RHIC

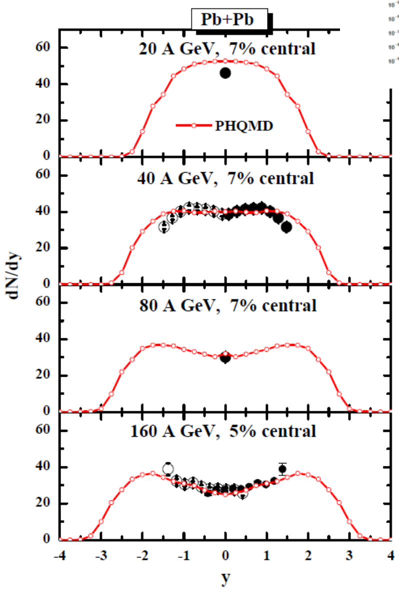


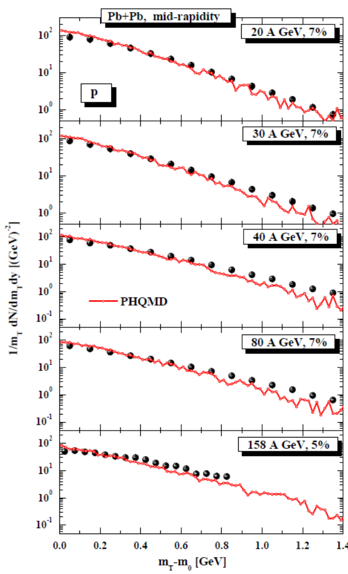
PHQMD: J. Aichelin et al., PRC 101 (2020) 044905

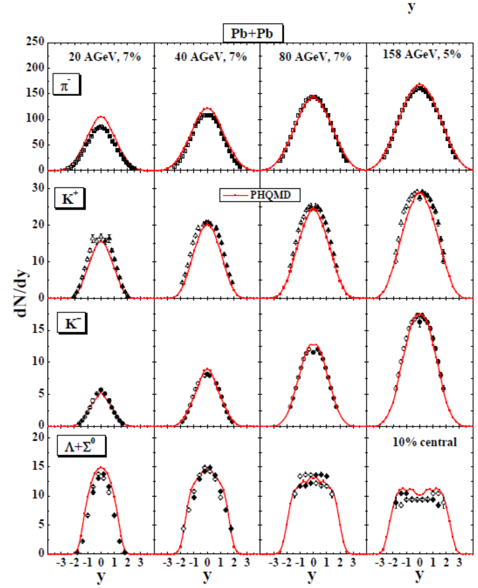


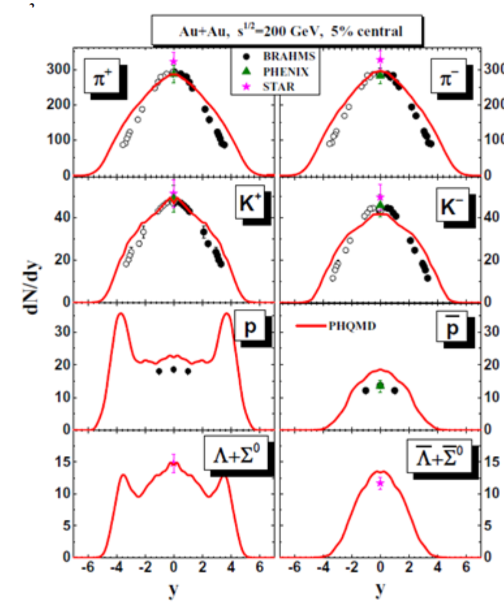












PHQMD provides a good description of hadronic ‘bulk’ observables from SIS to RHIC energies

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

PHQMD

I. Cluster recognition: Minimum Spanning Tree (MST)

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

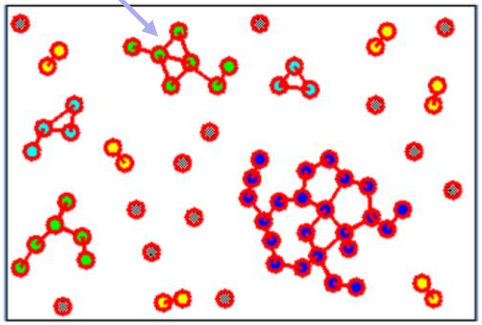
The Minimum Spanning Tree (MST) is a cluster recognition method applicable for the (asymptotic) final states where coordinate space correlations may only survive for bound states.

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

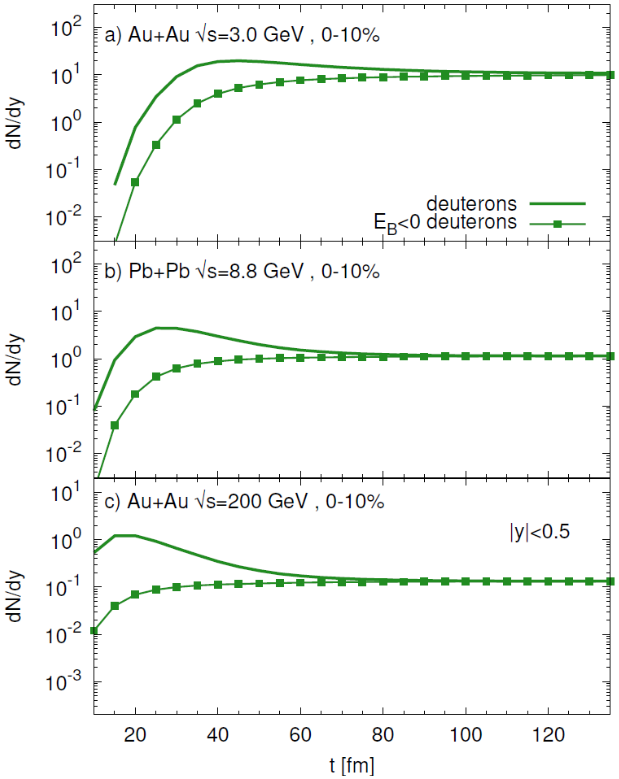
1. Two particles are 'bound' if their distance in the cluster rest frame fulfills

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

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)



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

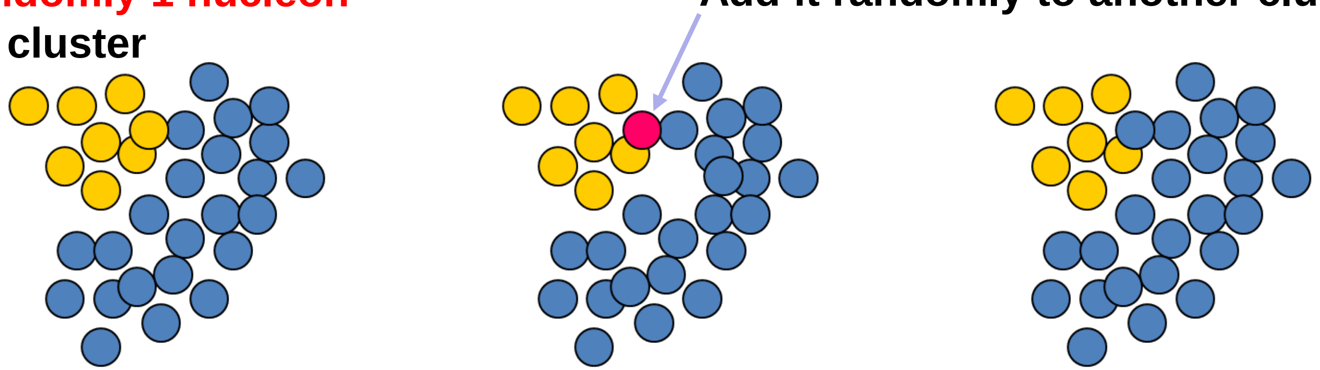
Simulated Annealing Clusterization Algorithm (SACA)

Basic ideas of clusters recognition by SACA:

Based on ideas by Dorso and Randrup (Phys.Lett. B301 (1993) 328)

- **Take the positions and momenta of all nucleons at time t**
- **Combine them in all possible ways into all kinds of clusters or leave them as single nucleons**
- **Neglect the interaction among clusters**
- **Choose that configuration which has the highest binding energy:**

Take randomly 1 nucleon out of a cluster — **Add it randomly to another cluster**



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

If E' < E take a new configuration
If E' > E take the old configuration with a probability depending on E'-E
Repeat this procedure many times

→ **Leads automatically to finding of the most bound configurations**

(realized via a Metropolis algorithm)

SACA: R. K. Puri, J. Aichelin, PLB301 (1993) 328, J.Comput.Phys. 162 (2000) 245-266;
P.B. Gossiaux, R. Puri, Ch. Hartnack, J. Aichelin, Nuclear Physics A 619 (1997) 379-390

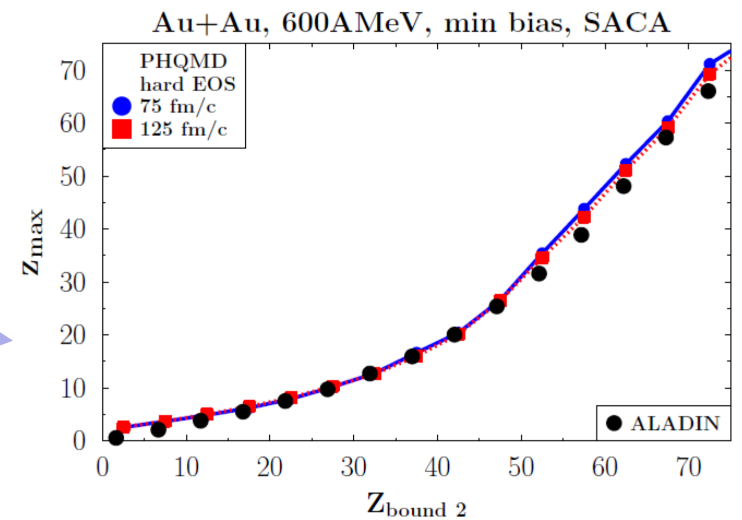
FRIGA: A. Le Fèvre, J. Aichelin, C. Hartnack, and Y. Leifels, Phys.Rev. C 100, 034904 (2019)

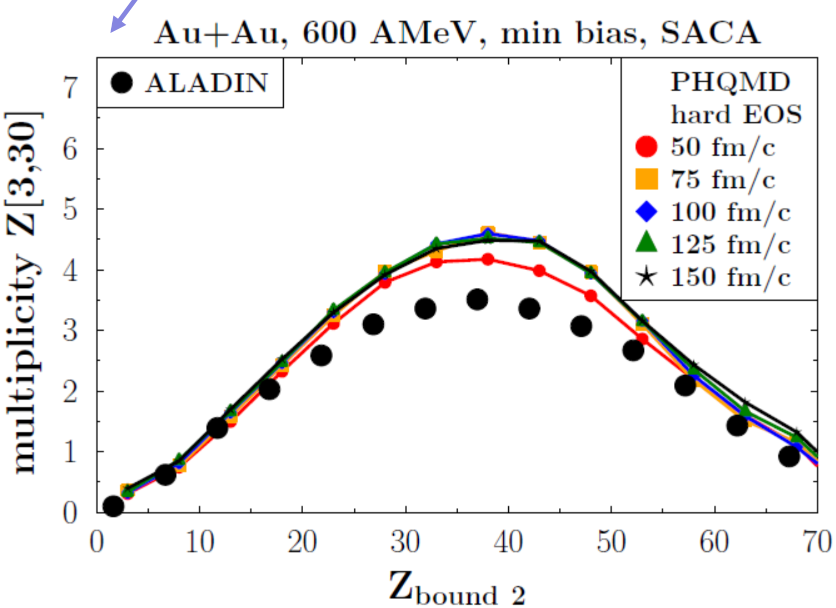
PHQMD: heavy clusters

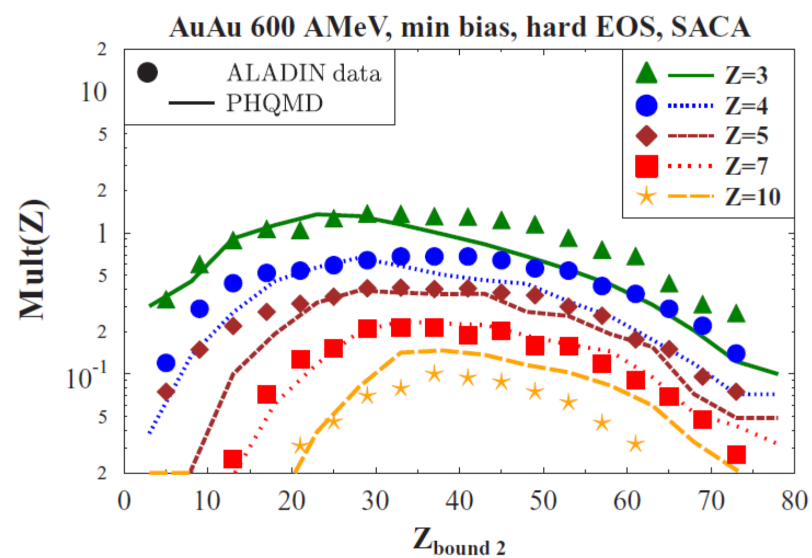
Heavy clusters (spectator fragments): experim. measured up to E_{beam} =1 AGeV (ALADIN Collab.)

PHQMD with SACA shows an agreement with ALADIN data for very complex cluster observables as

- Largest clusters (Z_{bound})
- Multiplicity (Z_{bound})
- Energy independent 'rise and fall'







$$Z_{\text{bound } 2} = \sum_i Z_i \,\Theta(Z_i - (1+\epsilon)) \quad (\epsilon < 1)$$

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

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

- 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. Casssing NPA 700 (2002) 618

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

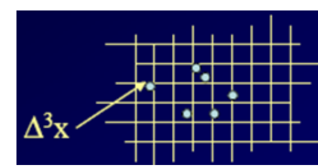
$$P_{3,2}(\sqrt{s}) = F_{spin} F_{iso} P_{2,3}(\sqrt{s}) \frac{E_1^f E_2^f}{2E_3 E_4 E_5} \frac{R_2(\sqrt{s}, m_1, m_2)}{R_3(\sqrt{s}, m_3, m_4, m_5)} \frac{1}{\Delta V_{cell}}$$

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: π+N+N⟷ d+π inclusion of all possible isospin channels allowed by total isospin T conservation

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

G. Coci et al., Phys.Rev.*C* 108 (2023) 1, 014902

Modelling finite-size effects in kinetic mechanism

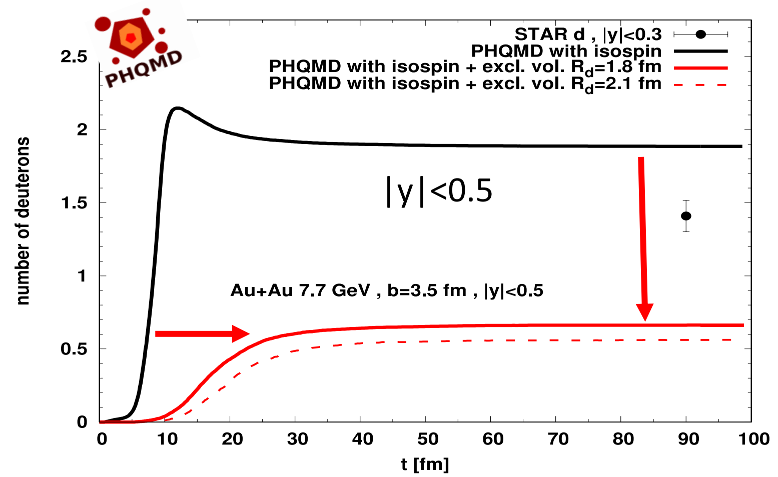
How to account for the quantum nature of deuteron, i.e. for
1) the finite-size of *d* in coordinate space (*d* is not a point-like particle) – for in-medium d production
2) the momentum correlations of *p* and *n* inside *d*

Realization:

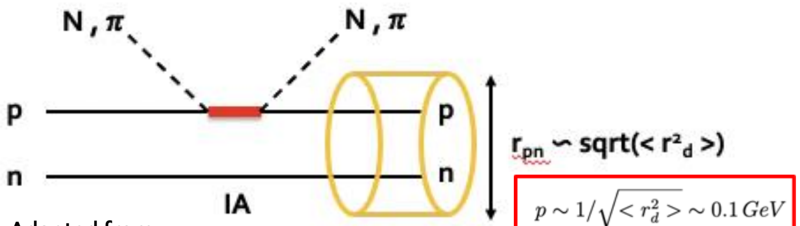
1) assume that a deuteron can not be formed in a high density region, i.e. if there are other particles (hadrons or partons) inside the 'excluded volume':

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

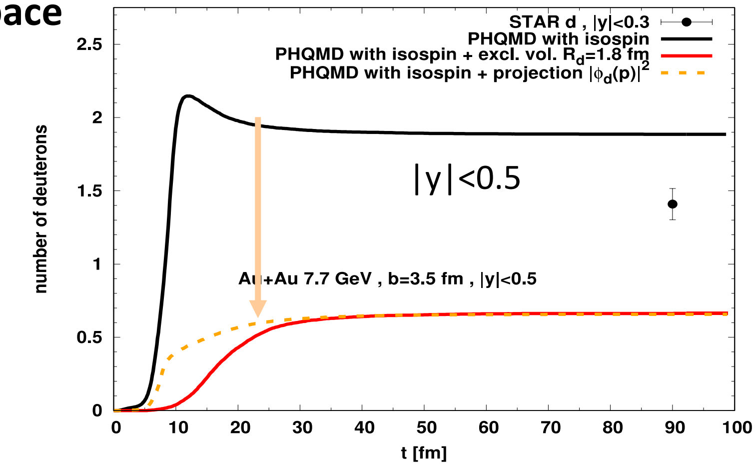
- Strong reduction of d production
- p_T slope is not affected by excluded volume condition



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



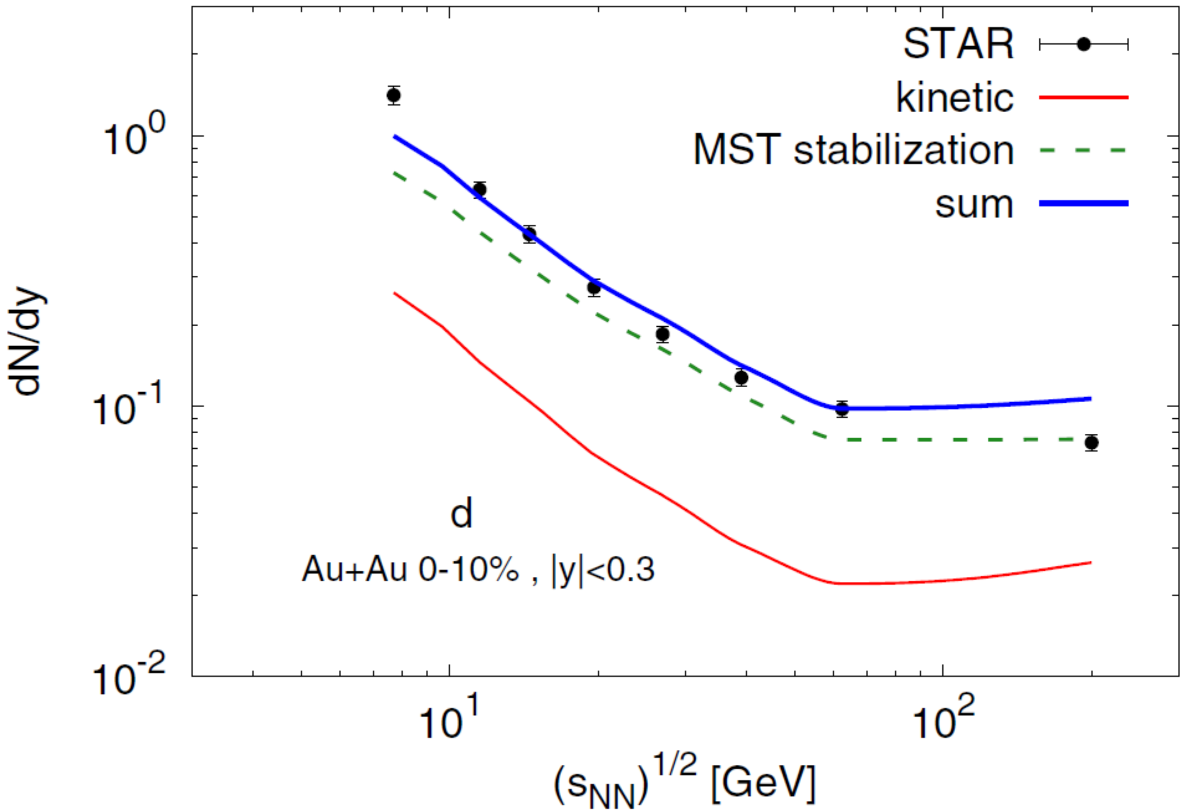
Adapted from
[Haidelbauer, Uzikov PLB 562(2003)]
[Hoftiezer et al. PRC23 (1981)]
Same spirit as AMPT [K.-J. Sun, R. Wang, C.-M. Ko et al., 2106.12742]



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

Kinetic vs. potential deuteron production

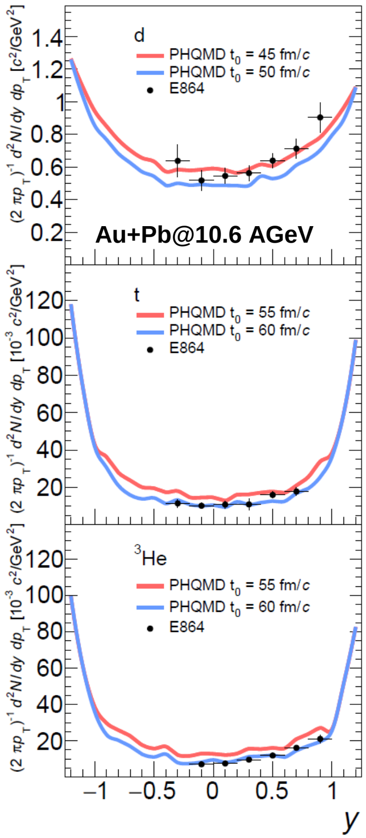
Excitation function dN/dy of deuterons at midrapidity



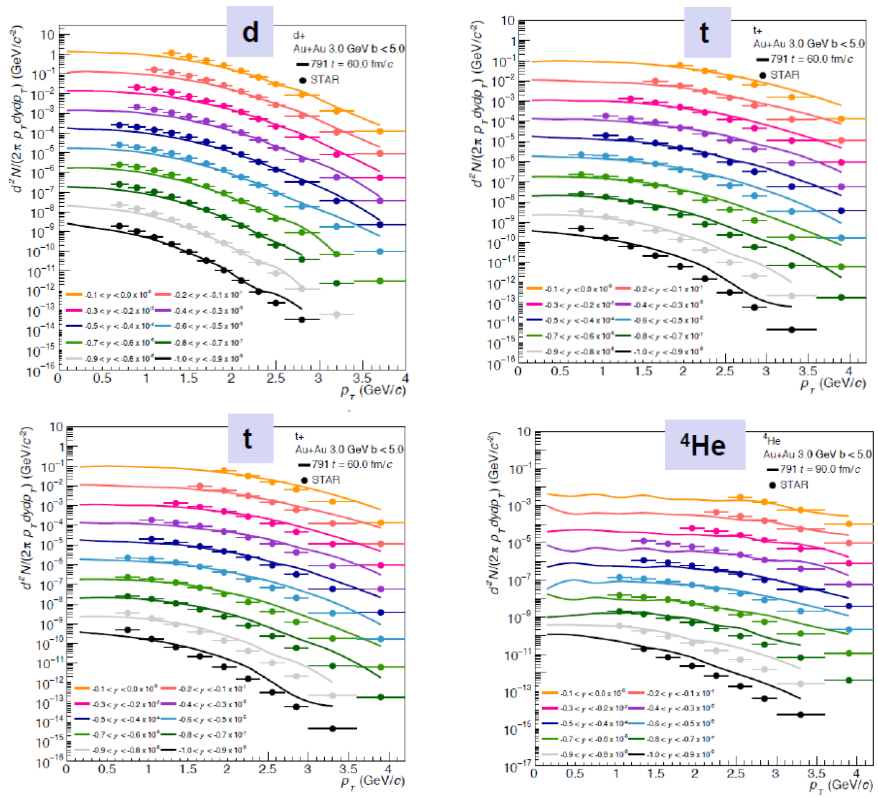
- **PHQMD provides a good description of STAR data**
- **The potential mechanism is dominant for d production at all energies!**

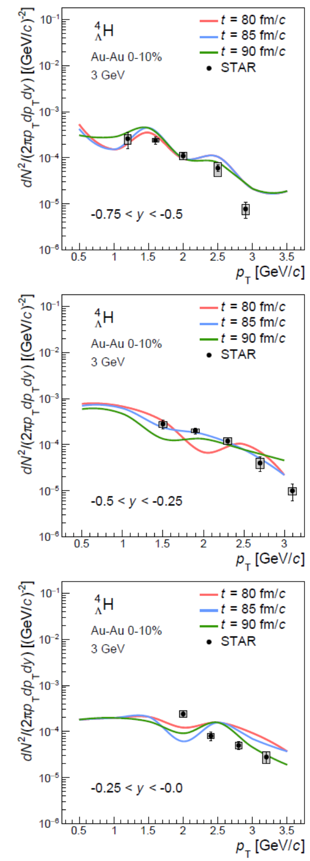
G. Coci et al., Phys.Rev.*C* 108 (2023) 1, 014902

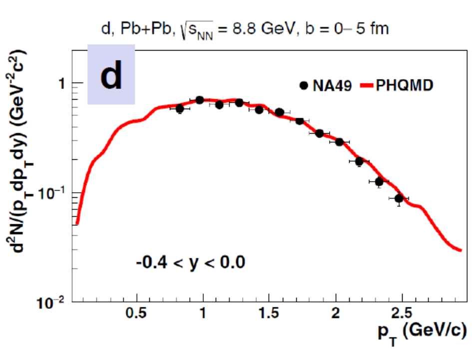
Highlights: PHQMD cluster and hypernuclei dynamics from SIS to RHIC

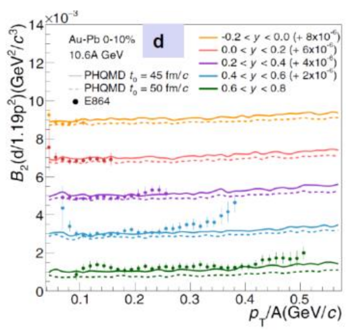


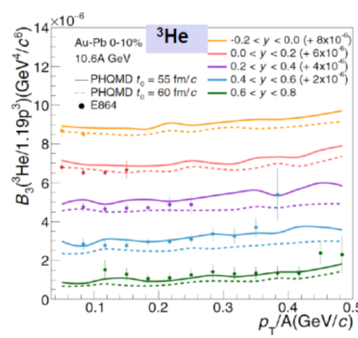
Au+Au central collisions at $\sqrt{s}$ =3 GeV





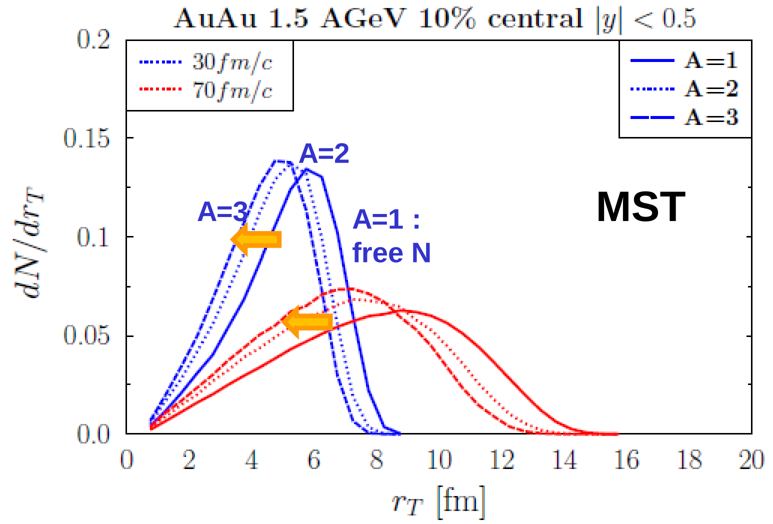


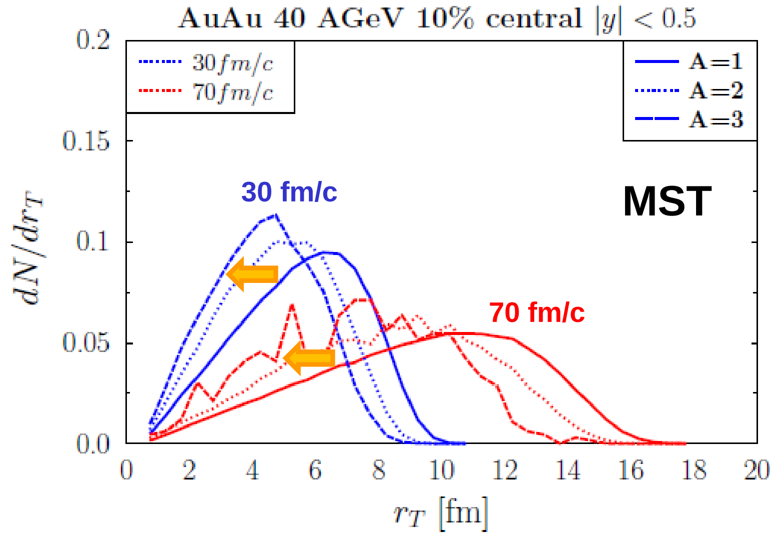


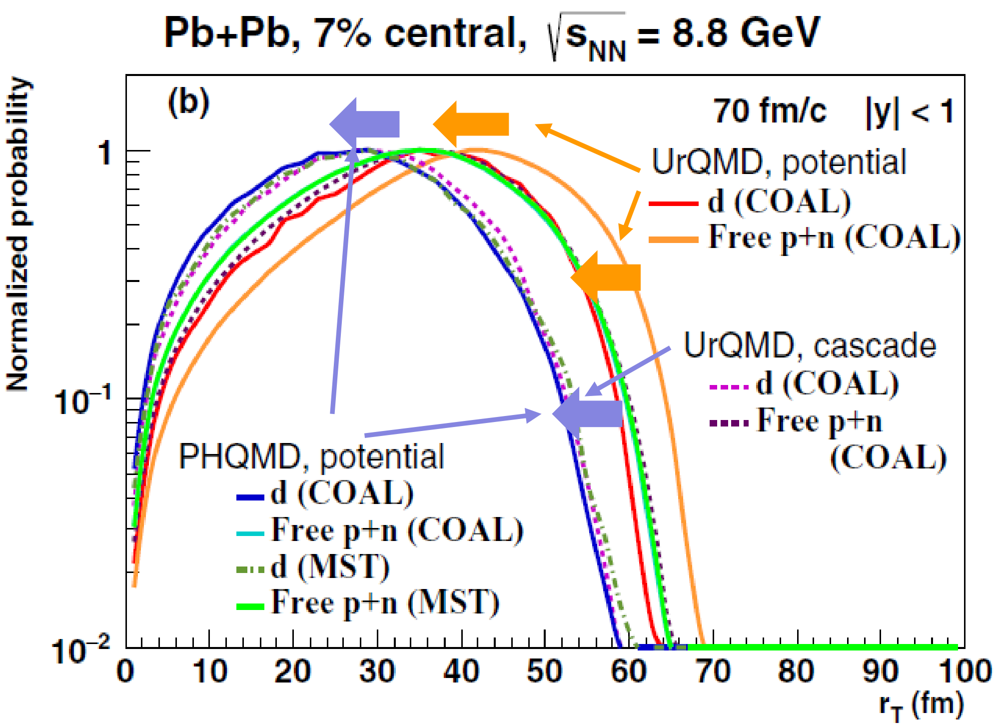


PHQMD:
J. Aichelin et al., PRC 101 (2020) 044905;
S. Gläßel et al., PRC 105 (2022) 1;
G. Coci et al., PRC 108 (2023) 1, 014902

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**

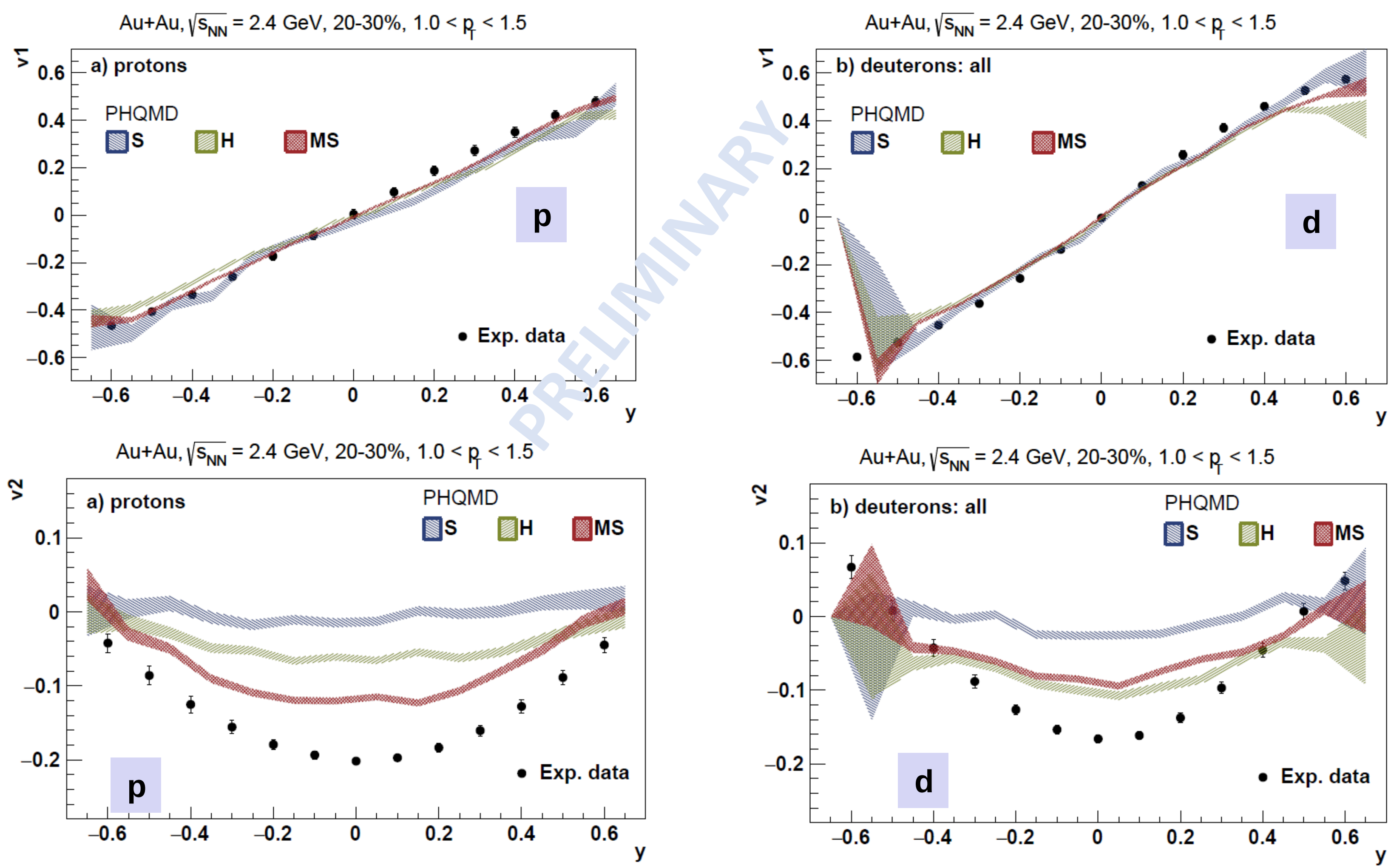
➔ **deuterons are behind the fast nucleons (and pion wind)**

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

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

v_1, v_2 with different EoS

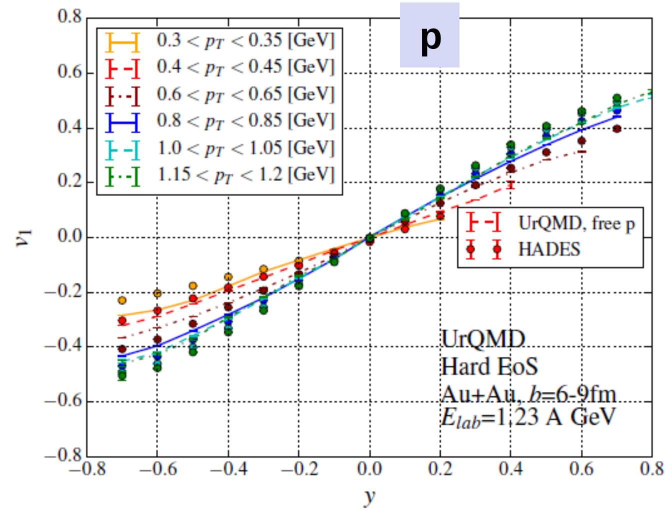
Viktar Kireyeu, in progress

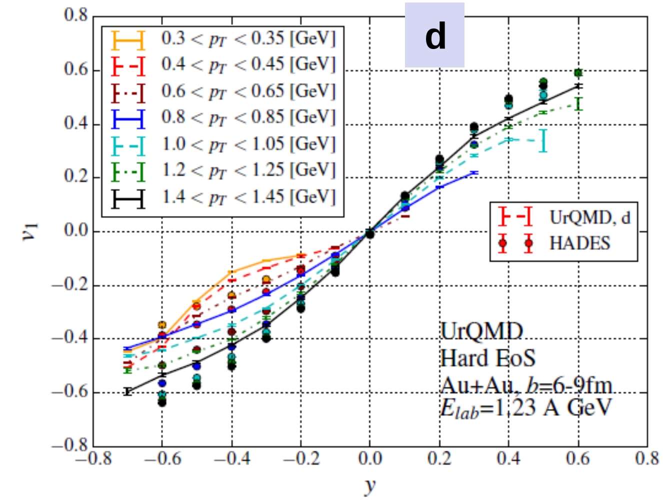


- Strong EoS dependence of v_2
- HADES data favor a momentum dependent potential

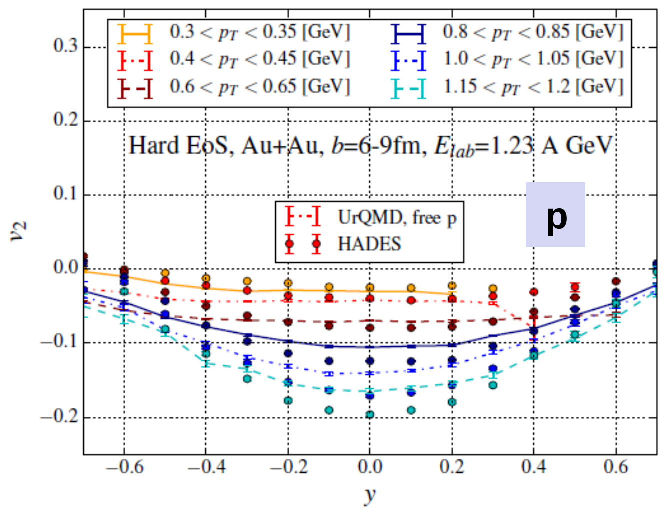
HADES: J. Adamczewski-Musch et al., Phys. Rev. Lett. 125, 262301 (2020), 2005.12217

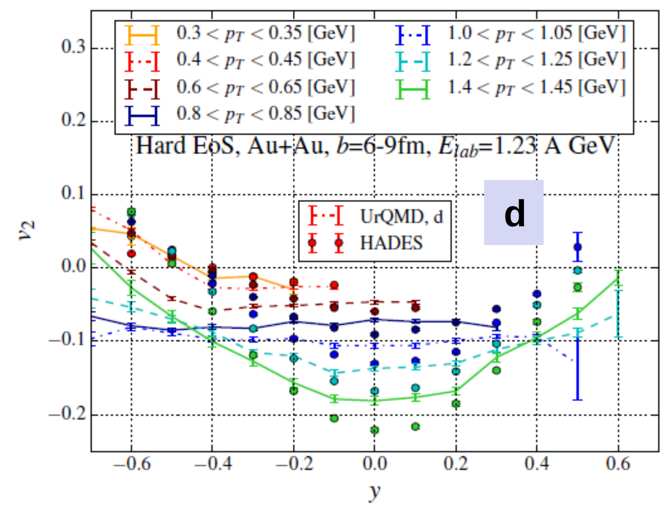
UrQMD: v_1, v_2 with hard EoS





d production by coalescence





UrQMD: P. Hillmann et al.,arXiv:1907.04571

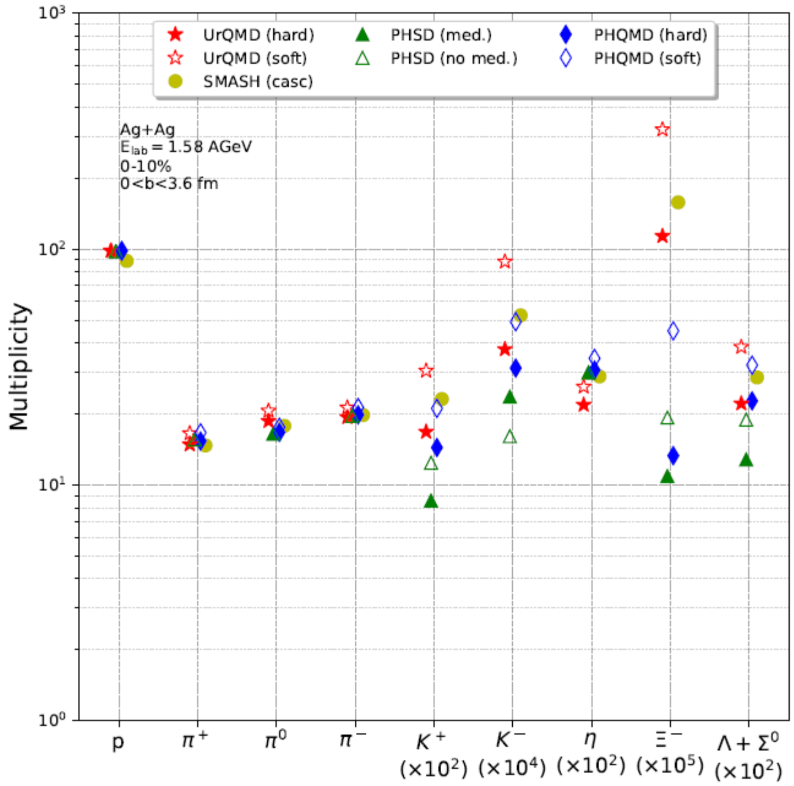
HADES: B. Kardan [HADES Collaboration], Nucl. Phys. A 982, 431 (2019)

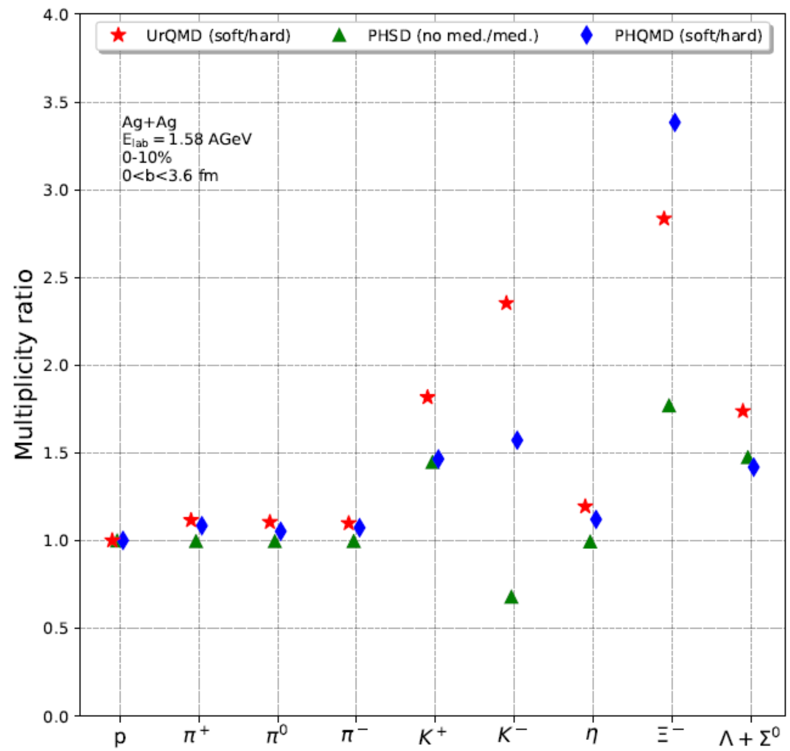
PHQMD & UrQMD & SMASH models: HADES data benchmarking

T. Reichert et al., J.Phys.G 49 (2022) 5, 055108

PHQMD & UrQMD & SMASH:

Comparison of heavy-ion transport simulations: Ag+Ag collisions at E_{lab} = 1.58A GeV





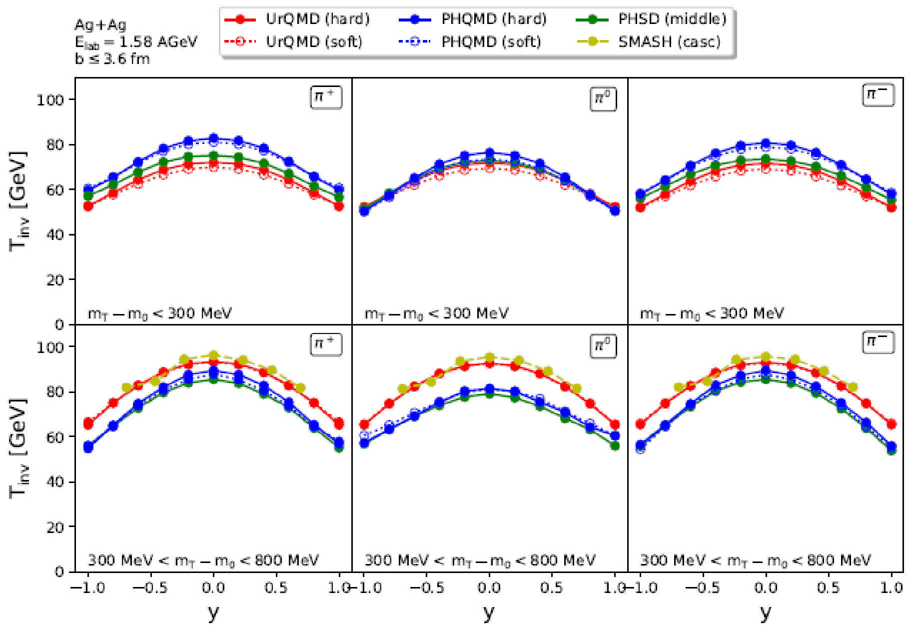
- ❑ **Reasonable agreement of transport models for the ‘bulk’ hadrons**
- ❑ **Strong influence of EoS and medium effects for strangeness production**
- ❑ **Sizable increase of strange particle yields for the soft EoS**

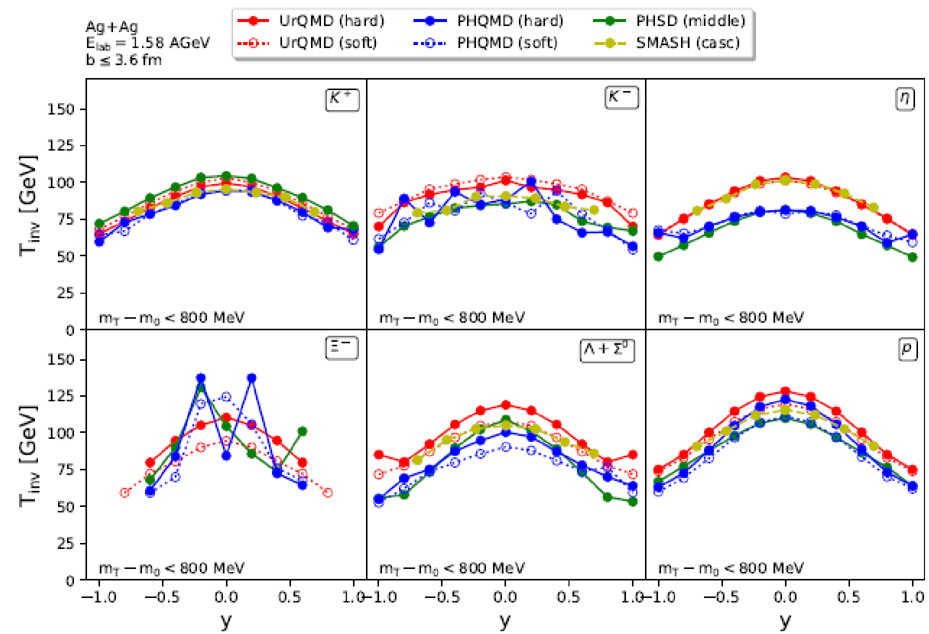
T. Reichert et al., J.Phys.G 49 (2022) 5, 055108

PHQMD & UrQMD & SMASH:

Comparison of heavy-ion transport simulations: Ag+Ag collisions at E_{lab} = 1.58A GeV

Inverse slope parameter T_{inv} in dependence of the rapidity extracted by fitting hadron m_T-spectra





$$T_{\rm inv}(y) = \frac{T_{\rm eff}}{\cosh(y)} \qquad T_{\rm eff} = T_{\rm source} + \frac{2}{3}\langle E_{\rm kin}\rangle = T_{\rm source} + \frac{1}{3}m\langle v_T\rangle^2$$

All models show similar source temperatures around $T_{\rm source} = 80 - 95$ MeV
and average transverse flow around $\langle v_T \rangle = 0.22c - 0.3c$

T. Reichert et al., J.Phys.G 49 (2022) 5, 055108