Mechanisms for deuteron production in HICs with PHQMD transport approach.

Gabriele Coci

In collaboration with the PHQMD group:
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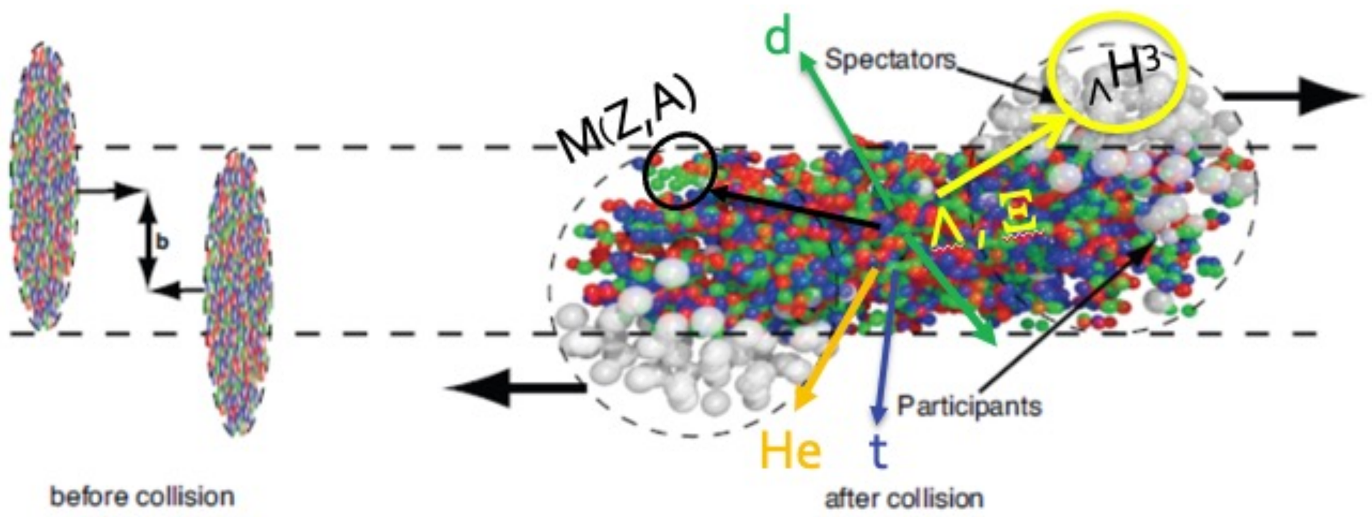
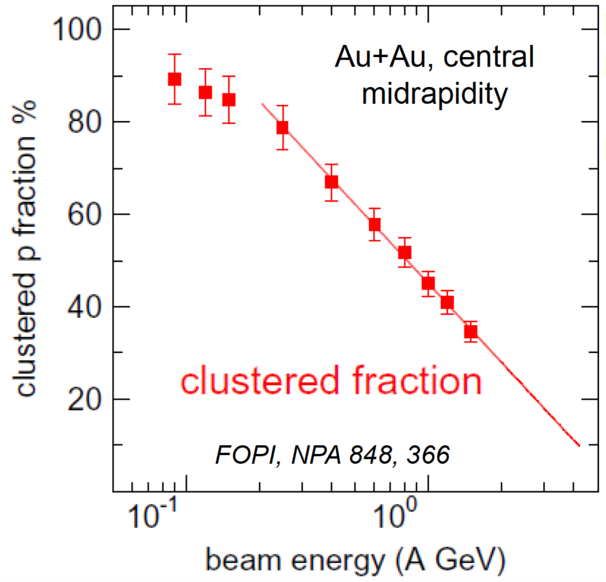


Many clusters produced at low energy !



Theoretical models describing clusters production:

- Coalescence model → multiplicity of clusters from f_N(x,p) of nucleons at freeze-out time.
- Thermal model → assumption of thermal equilibrium source. Parameters (T_f, μ_B) tuned to hadron yields.
  - ➢ Deuteron binding energy $E_B \approx 2$ MeV << $T_f \approx 150$ MeV.
    How can such fragile object survive in the fireball ?

To study the microscopic origin of cluster a realistic description of HICs dynamical evolution is necessary !
→ transport models

- ➢ Potential interaction → gathering of nucleons during time evolution tracked by clusterization algorithms.
- ➢ Kinetic mechanism → deuteron production by 3⟶2 hadronic reactions (development in PHQMD: this talk!)

SMASH group:
[D. Oliinychenko PRC 99 (2019) 4, 044907]
[J. Staudenmaier et al., PRC 104 (2021) 3, 034908]

Parton-Hadron Quantum Molecular Dynamics

- Model: A **unified n-body microscopic transport approach** for the description of HICs and **dynamical cluster formation** from low to ultra-relativistic energies.
- Realization: (**PHSD** + **QMD**) & **MST/SACA**.

[J. Aichelin et al. PRC 101 (2020) 044905]

Quantum Molecular Dynamics (QMD)
Initialization & Propagation of baryons

↓

Parton-Hadron-String-Dynamics (PHSD)
Propagation and interaction of partons and mesons
QGP phase by Dynamical Quasi-Particle Model (DQPM)

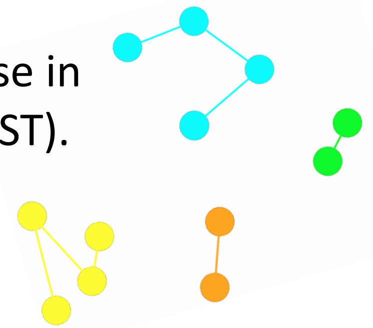
↓

Cluster Identification
Minimum Spanning Tree (MST)
Simulated Annealing Clusterization Algorithm (SACA)

Baryons described by *n*-body Wigner functions, preserve many-body correlations.
J. Aichelin Phys. Rep. 202, (1991) 233
C. Hartnack, Puri, Aichelin et al. EPJ A 1, (1998)

Collision Integral → reactions of partons and hadrons (also **deuterons**: this work!)
W. Cassing, E. Bratkovskaya, NPA 831, (2009)
P. Moreau, O. Soloveva, et al. PRC 100 (2019)

Identify clusters as baryons close in coordinate space (PHQMD + MST).
S. Gläßel et al. PRC 105, (2022) 01498.
V. Kireyeu et al. PRC 105, (2022) 04909



QMD propagation

Equation of Motion (EoM) derived from generalized Ritz variational principle:

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

- *ψ(t)* is the quantum wavefunction for the N-particles system.
  - *Assume* $$\psi(t) = \prod_{i=1}^{N} \psi(\mathbf{r_i}, \mathbf{r_{i0}}, \mathbf{p_i}, \mathbf{p_{i0}}, t)$$ *(neglect N-antisymmetrization)*
  - *Ansatz* $$\psi(\mathbf{r_i}, \mathbf{r_{i0}}, \mathbf{p_i}, \mathbf{p_{i0}}, t) = C e^{\frac{-1}{4L}(\mathbf{r_i} - \mathbf{r_{i,0}}(t) - \frac{\mathbf{p_{i0}}(t)}{m} t)^2} e^{i\mathbf{p_{i0}(t)} \cdot (\mathbf{r_i} - \mathbf{r_{i0}})} e^{-i\frac{\mathbf{p_{i0}(t)}^2}{2m} t}$$

  the single particle "trial" wavefunction is a Gaussian centered at phase space coordinate (r_{i0} , p_{i0}) with width L.
- EoM for the Gaussian centroids:

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

  - The expectation value of Hamiltonian appears: $$\langle H \rangle = \sum_i \langle H_i \rangle = \sum_i (\langle T_i \rangle + \sum_{j \neq i} \langle V_{i,j} \rangle)$$
  - The two-body potential part has a Coulomb and a Skyrme contribution.
  - The expectation of Skyrme potential realized by a static density dependent expression with parameters tuned to the Equation of State of infinite nuclear matter

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

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

[J. Aichelin et al. PRC 101 (2020) 044905]

Collision Integral: covariant rate formalism

- In Boltzmann Equation the Collision Integral accounts for all dissipative processes (hadronic reactions ...)

$$p_{1,\mu}\partial_x^\mu f_i(x,p_1) = I^i_{coll} = \sum_n \sum_m \; I^i_{coll}[n \leftrightarrow m]$$

$$I^i_{coll}[n \leftrightarrow m] = \frac{1}{2}\frac{1}{N_{id}!}\sum_\nu \sum_\lambda \left(\frac{1}{(2\pi)^3}\right)^{n+m-1} \left(\prod_{j=2}^{n}\int \frac{d^3\vec{p}_j}{2E_j}\right)\left(\prod_{k=n+1}^{n+m}\int \frac{d^3\vec{p}_k}{2E_k}\right)$$
$$\times (2\pi)^4 \delta^4(p_1^\mu + \sum_{j=2}^{n} p_j^\mu - \sum_{k=1}^{n+m} p_k^\mu)\, W_{n,m}(p_1, p_j; i, \nu \mid p_k; \lambda)$$
$$\times \left[\prod_{k=n+1}^{n+m} f_k(x,p_k) - f_i(x,p_1)\prod_{j=2}^{n} f_j(x,p_j)\right]$$

(n-1) initial + m final integrations

Transition amplitude

Gain - Loss

[W. Cassing NPA 700 (2000)]

- Collision rate for hadron "i" is the number of reactions in the covariant volume $d^4x = dt*dV$

$$\frac{dN_{coll}[n(i) \to m]}{dtdV} \propto \int \frac{d^3p_1}{2E_1} f_i(x,p_1) \int \left(\prod_{j=2}^{n}\frac{d^3p_j}{2E_j} f_j(x,p_j)\right) \int \left(\prod_{k=n+1}^{n+m}\frac{d^3p_k}{2E_k}\right)$$
$$\times (2\pi)^4 \delta^4(\sum_{j=1}^{n} p_j^\mu - \sum_{k=n+1}^{n+m} p_k^\mu)\, W_{n,m}(p_j; \tau(i), \nu \mid p_k; \lambda)$$

... similar for m→n(i)

Collision Integral: covariant rate formalism

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

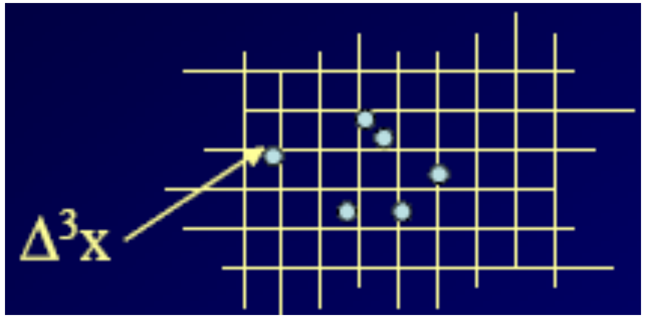
$$\frac{dN_{coll}[1(d)+2\to 3+4]}{dtdV} \propto \frac{1}{(2\pi)^6}\int\frac{d^3p_1}{2E_1}f_1(x,p_1)\int\frac{d^3p_2}{2E_2}f_4(x,p_4)\times$$

$$\int\frac{d^3p_3}{(2\pi)^3 2E_3}\int\frac{d^3p_4}{(2\pi)^3 2E_4}W_{2,2}(p_1,p_2;p_3,p_4)(2\pi)^4\,\delta^4(p_1+p_2-p_3-p_4) \rightarrow 4E_1E_2v_{rel}\sigma_{2,2}(\sqrt{s})$$

- Using test-particle ansatz for *f(x,p)* the collision integral is numerically solved dividing the coordinate space in cells of volume ΔV_{cell} where the reaction rate at each time step Δt are sampled stochastically with probability.

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

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



- $\Delta t \rightarrow 0$, $\Delta v_{cell} \rightarrow 0$ convergence to exact solution

Collision Integral: covariant rate formalism

- With n > 2 initial particles , the covariant rate cannot be expressed in terms of the reaction cross section

$$\frac{dN_{coll}[3+4+5 \to 1(d)+2]}{dtdV} \propto \int \left(\prod_{k=3}^{5} \frac{d^3p_k}{(2\pi)^3} f_k(x,p_k) \right) \times$$
$$\int \frac{d^3p_1}{(2\pi)2E_1} \int \frac{d^3p_2}{(2\pi)2E_2} W_{2,3}(p_1,p_2;p_3,p_4,p_5)(2\pi)^4\, \delta(p_1+p_2-p_3-p_4-p_5)$$

- With the ASSUMPTION for the TRANSITION AMPLITUDE: $W(\sqrt{s})$ **[W. Casing NPA 700 (2002)]**

the covariant collision rate can be still expressed in terms of the reaction probability:

$$\frac{dN_{coll}[3+4+5 \to 1(d)+2]}{dtdV} = \int \left(\prod_{k=3}^{5} \frac{d^3p_k}{(2\pi)^3} f_k(x,p_k) \right) P_{3,2}(\sqrt{s})$$

→ With test particle ansatz

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

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

Deuteron reactions in the box

π+p+n ⟷ d+π , d+N ⟷ p+n+N , N+N ⟷ d+π , d+X elastic

SMASH group:
[J. Staudenmaier et al., PRC 104 (2021) 3, 034908]

- 2 ⟶ 2 and 2 ⟶ 3 either by geometric criterium or stochastic method.

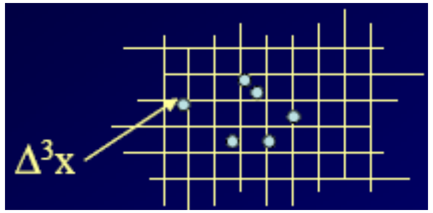
[Kodama et al. Phys. Rev. C 29 (1984)]

$$d_T < \sqrt{\frac{\sigma^{2,3}_{tot}(\sqrt{s})}{\pi}}$$

$$P_{2.3}\left(\sqrt{s}\right) = \sigma^{2,3}_{tot}(\sqrt{s})v_{rel}\frac{\Delta t}{\Delta V_{cell}}$$

- 2 ⟵ 3 realized via **covariant rate formalism.** [W. Cassing NPA 700 (2002)]

- Numerically tested in "static" box.



- Compared to solutions from rate equations.

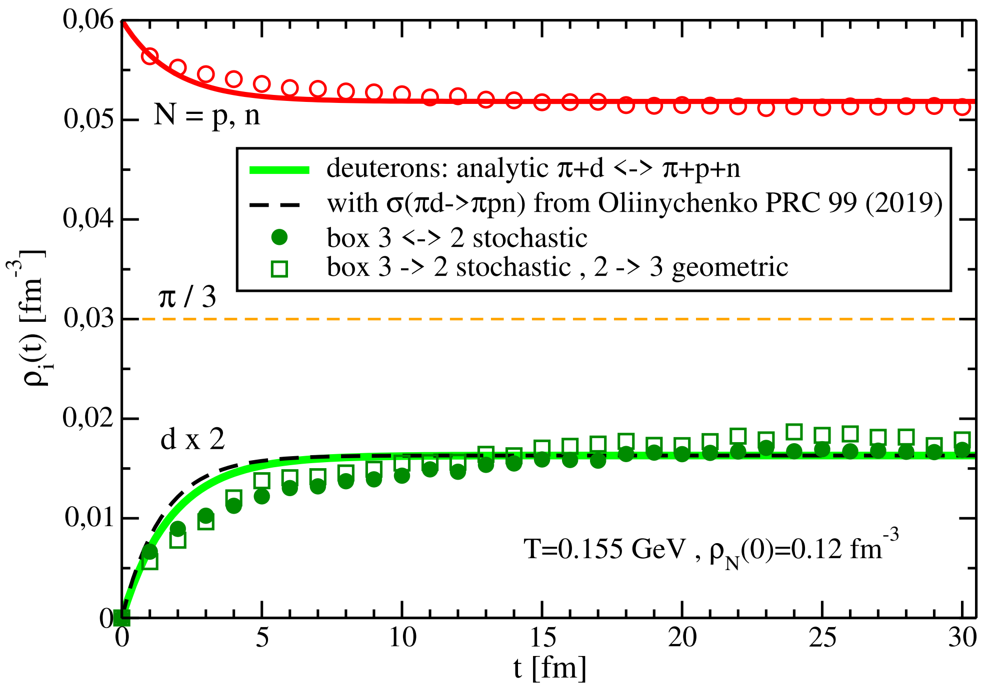
[Y. Pan S. Pratt, PRC 89 (2014), 044911]

$$\begin{cases} \dot{\lambda}_d = \sum < v_{rel}\sigma_{\pi d} > \left(\frac{g_d g_\pi}{g_N^2 g_\pi}\lambda_N^2 - \lambda_d\right) n_\pi^{eq}\lambda_\pi \\ \dot{\lambda}_N = -\sum < v_{rel}\sigma_{\pi d} > \left(\frac{g_d g_\pi}{g_N^2 g_\pi}\lambda_N^2 - \lambda_d\right) n_\pi^{eq}\lambda_\pi \\ \dot{\lambda}_\pi = 0 \end{cases}$$

+ initial conditions

Density inside the box at temperature T: $\rho_i = n^{eq}(T) * \lambda_i(t)$.

$F_{iso} = 1$



Deuteron reactions in the box

π+N+N⟷ d+π , d+N ⟷ p+n+N , N+N ⟷ d+π , d+X elastic

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

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

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

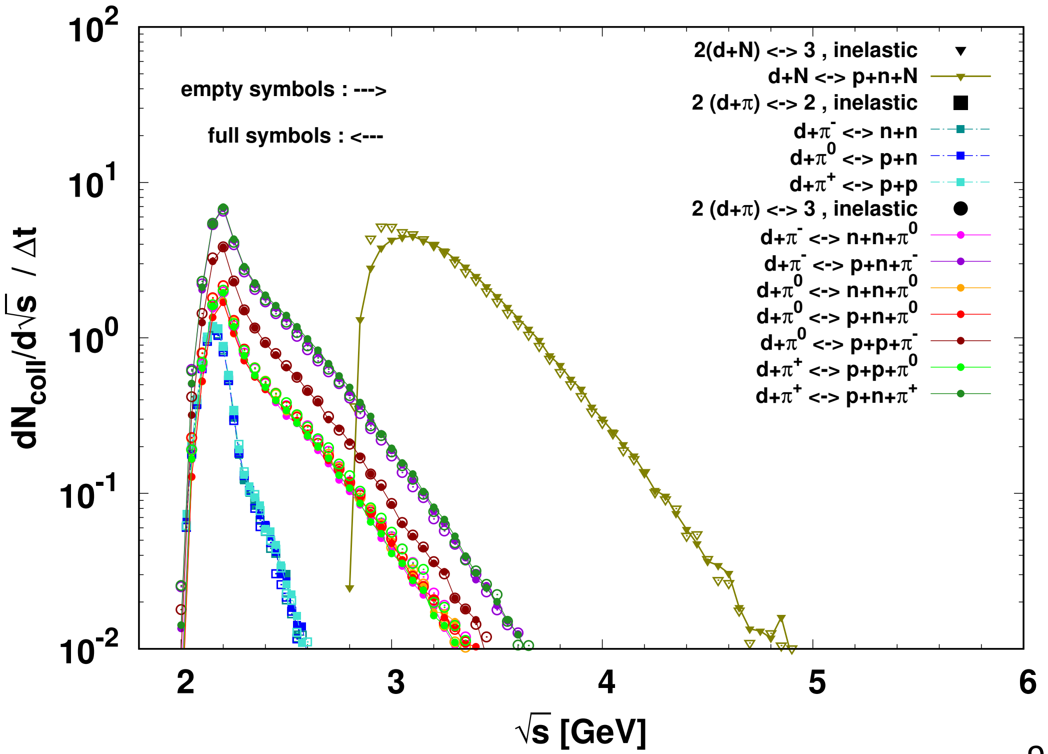
- NNπ expanded as superposition of eigenstates of total isospin T

$$|N, N, \pi\rangle = \sum_T \sum_{T_3=-T}^{-T} \langle T, T_3 | N, N, \pi\rangle \, |T, T_3\rangle$$

- Fourier coefficient of eigenstate of total isospin 1 (= T(d π)=T(π))

$$F_{iso} = |\langle N, N, \pi | T(d+\pi) = 1, T_3\rangle|^2$$

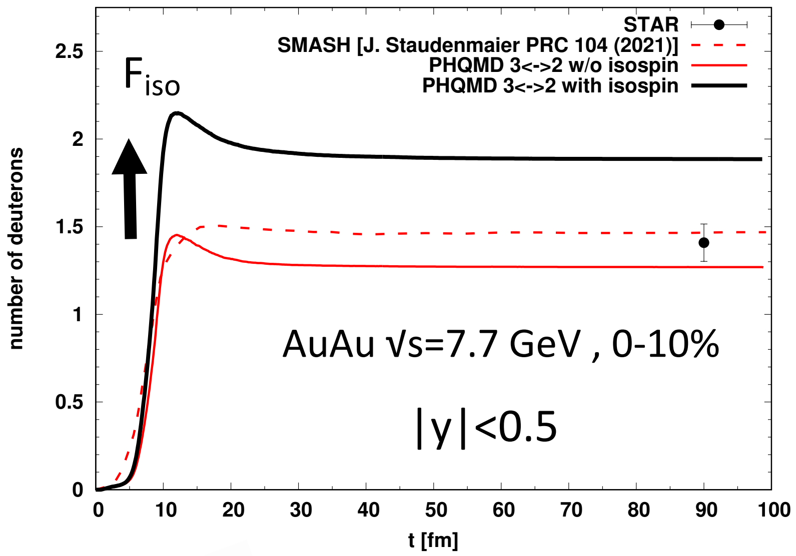
→ Detailed balance condition fulfilled.

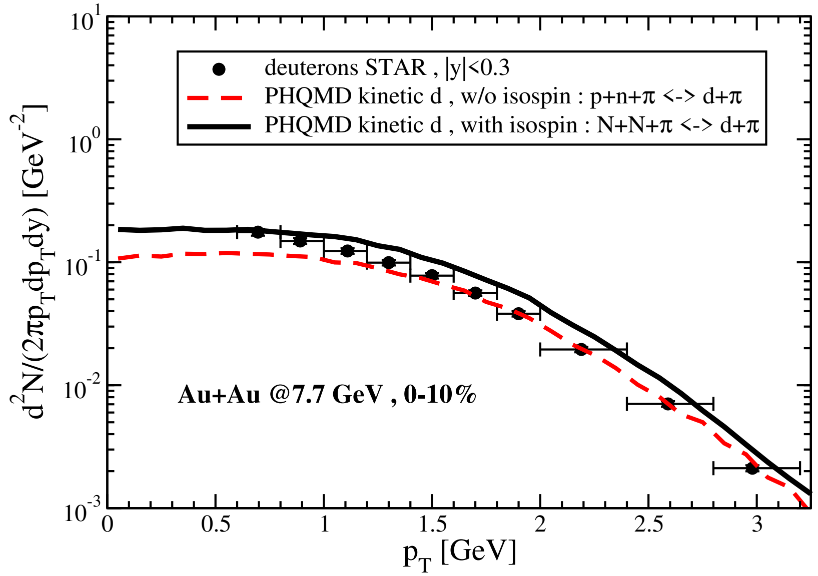


Kinetic deuterons in PHQMD

RHIC BES energy √s = 7.7 GeV:

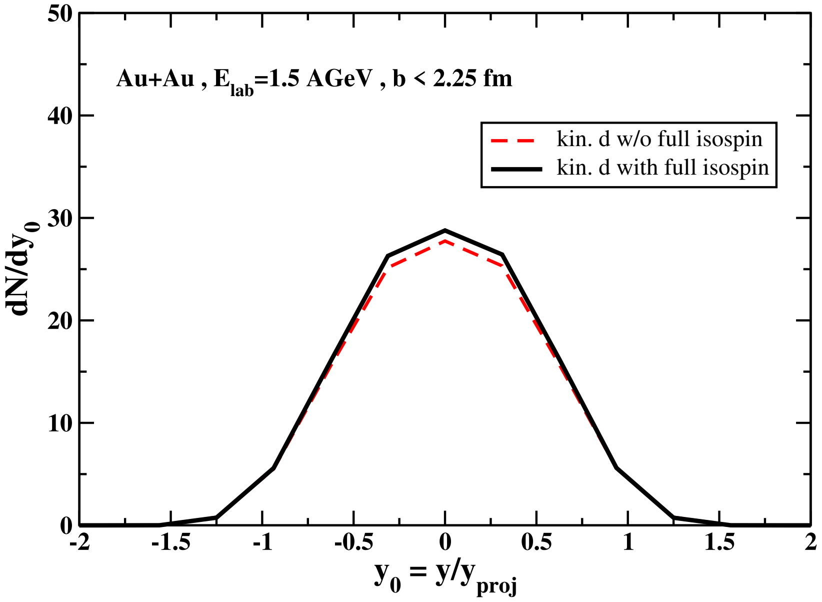
- Hierarchy due to large π abundance
  π+N+N→π+d >> N+p+n→N+d
- Inclusion of all channels enhances deuteron yield ~ 50%.
- p_T slope is not affected.





GSI SIS energy √s < 3GeV :

- Baryonic dominated matter.
- Enhancement due to inclusion of isospin channels is negligible.



Modelling finite-size effects in kinetic mechanism

In QM the deuteron is a broad p-n bound system. It is reasonable to assume that, as soon as a deuteron is formed, it is immediately destroyed in high density regions.

We model this effect implementing an Excluded-Volume Condition:

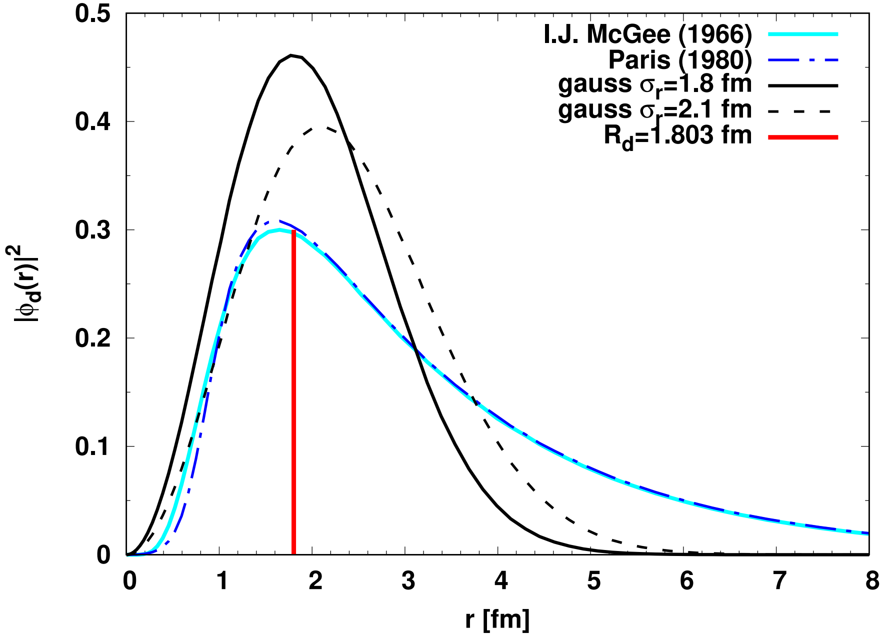
$$|\vec{r}(i)^* - \vec{r}(d)^*| < R_d$$

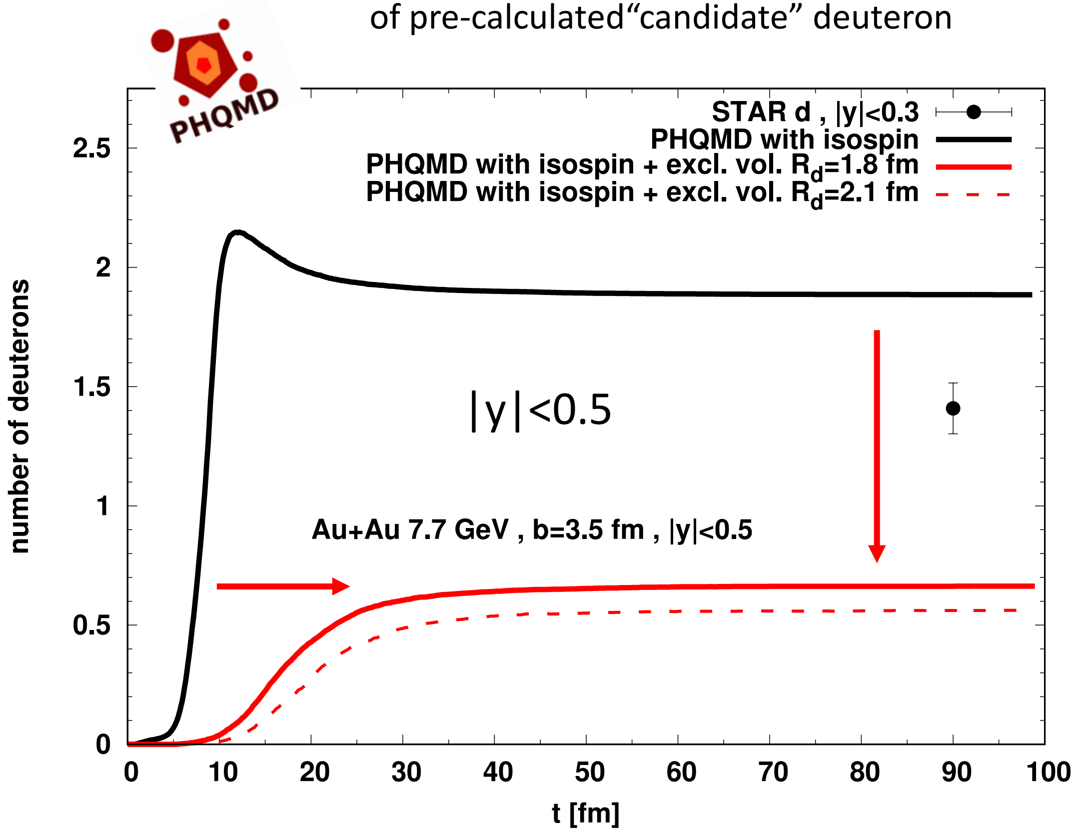
"i" is any particle not participating in πNN→ πd , NNN→ Nd , NN→ dπ

* means that positions are in the cms of pre-calculated"candidate" deuteron

The exclusion parameter R_d is tuned to the physical radius

$$\langle r_d^2 \rangle = \int_0^\infty r^2 |\phi_d(r)|^2 dr \sim 1.8\, fm$$

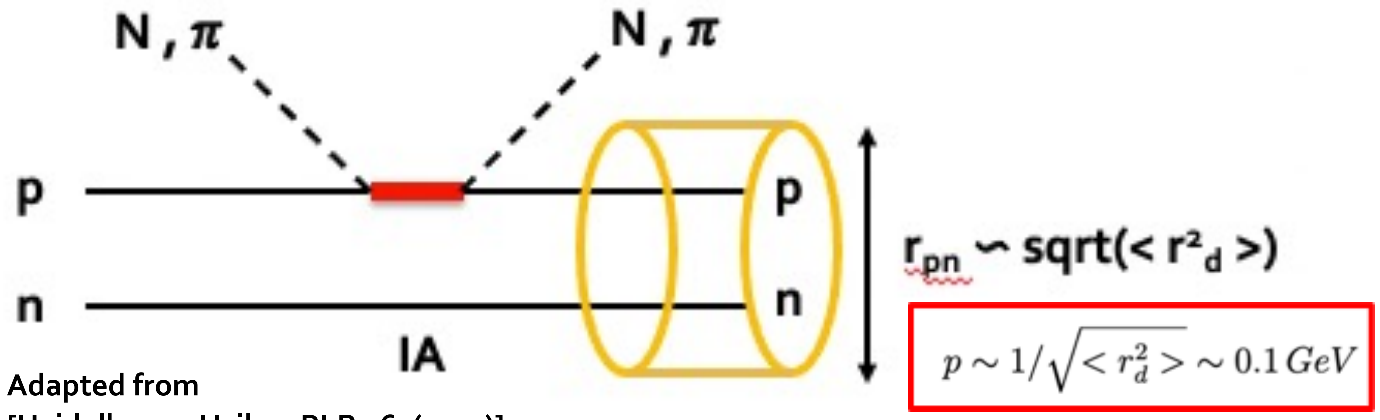




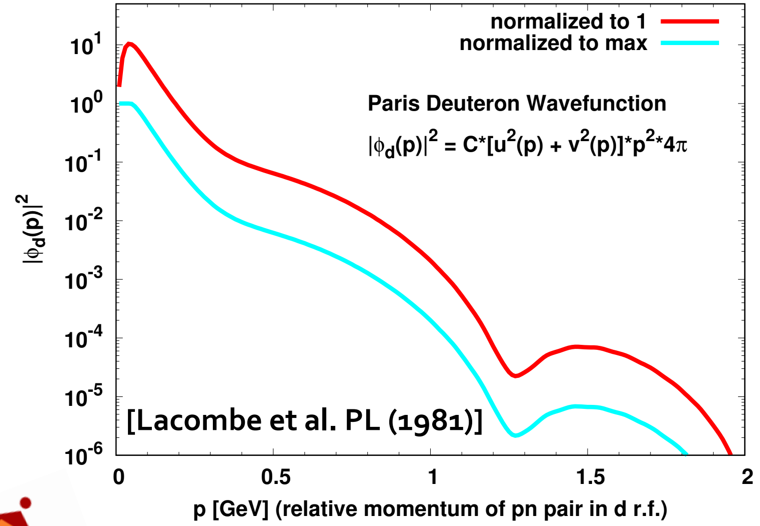
p_T slope is not affected!

Modelling finite-size effects in kinetic mechanism

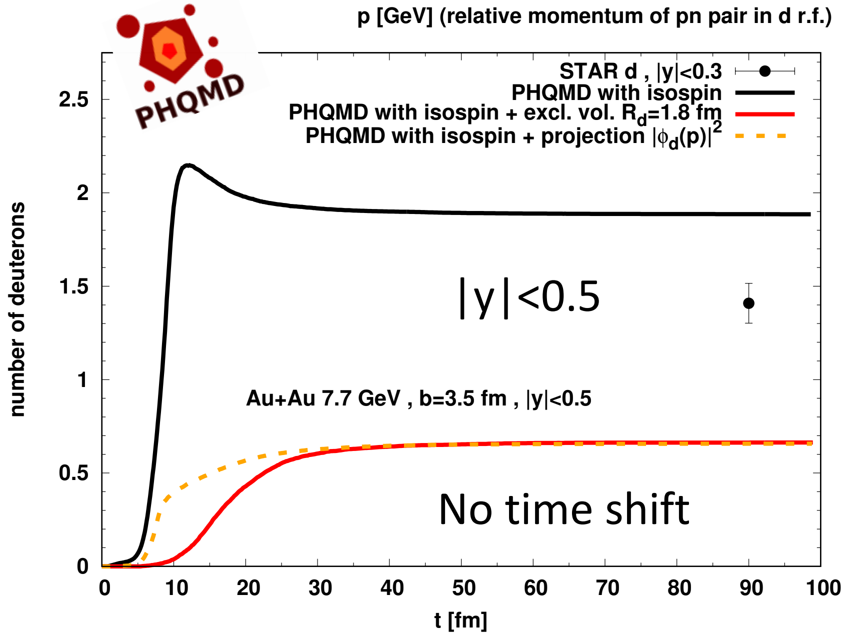
QM properties of deuteron must be also in momentum space → momentum correlations of NN-pairs



Adapted from
[Haidelbauer, Uzikov PLB 562(2003)]
[Hoftiezer et al. PRC23 (1981)]



- For a “candidate” deuteron calculate the relative momentum p of the interacting pn-pair in the deuteron rest frame.
- The probability of the pn-pair to bound into a final deuteron with momentum p is given by the DWF $|\phi_d(p)|^2$.
- Bound pn-pairs are selected by projection on DWF $|\phi_d(p)|^2$.



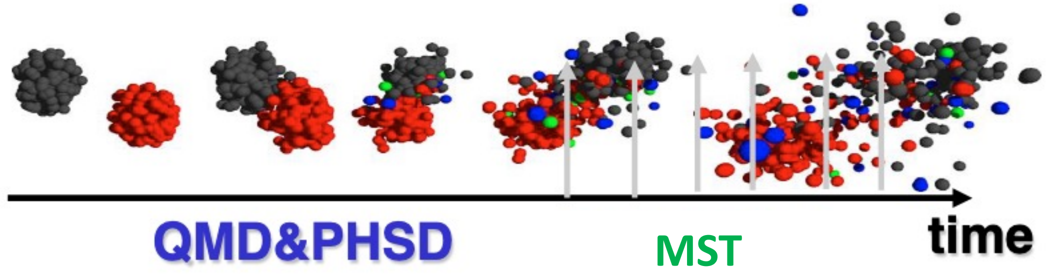
Cluster identification via Minimum-Spanning Tree (MST)

The Minimum Spanning Tree (MST) is a cluster recognition algorithm which is applied in the asymptotic final state.

- At time snapshots MST searches for correlations of nucleons in coordinate space:

[Puri, Aichelin, J.Comp. Phys. 162 (2000) 245]

[J. Aichelin Phys. Rept. 202, 233 (1991)]



1. Two baryons are part of a cluster if their distance in the cluster rest frame fulfills: $|\vec{r_i} - \vec{r_j}| \leq 4$ fm

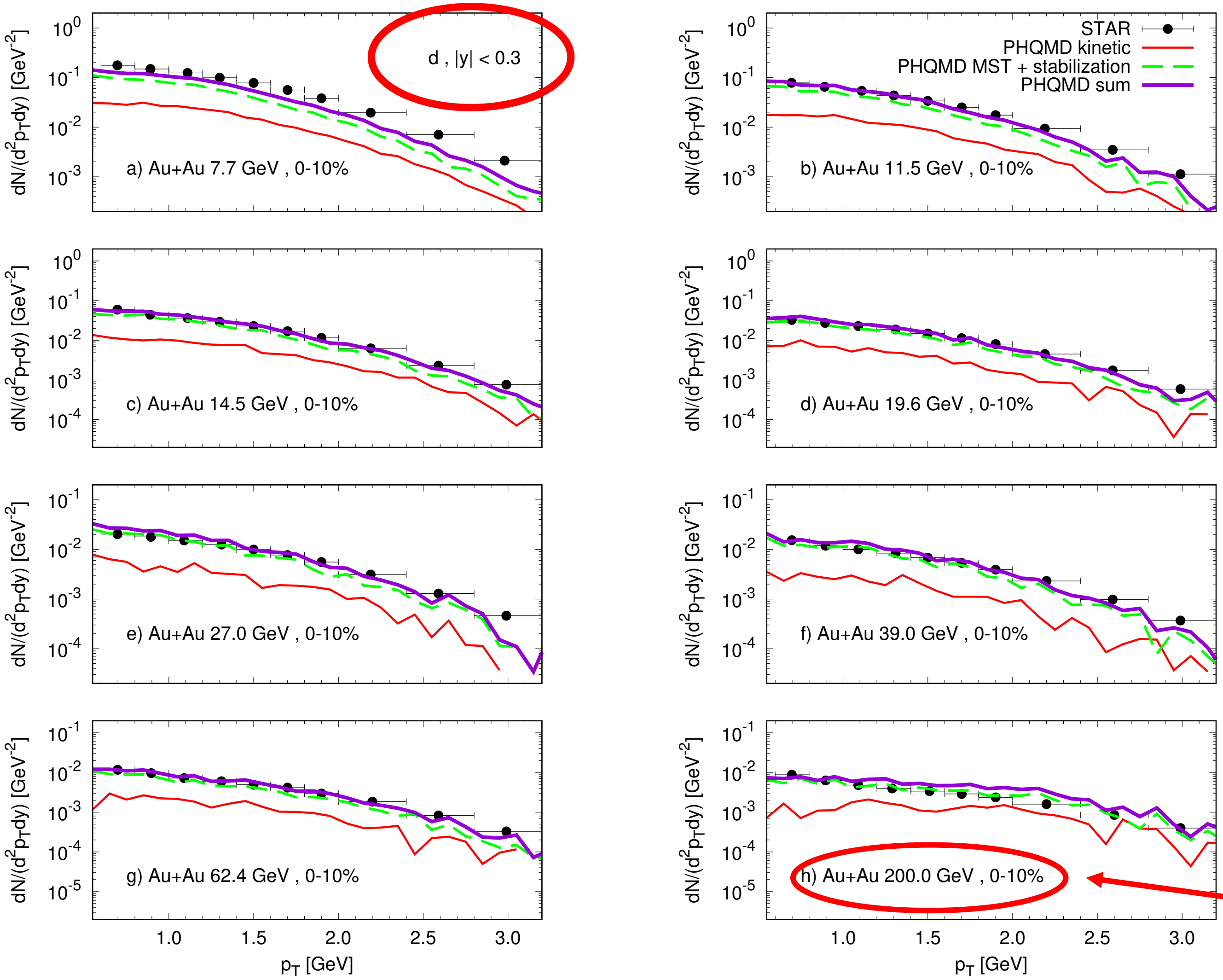
2. A baryon belongs to some cluster if it is “bound” at least to one baryon which is already part of that cluster.

- In semiclassical approach (as QMD) a cluster which is “bound” at time *t* can spontaneously dissolve at *t + Δt* .

  ✓ Numerical artifact… loose clusters at relativistic energies → Solution through Stabilization Procedure:

  - For each nucleon in MST track the freezout-time = time at which last collision occurred.

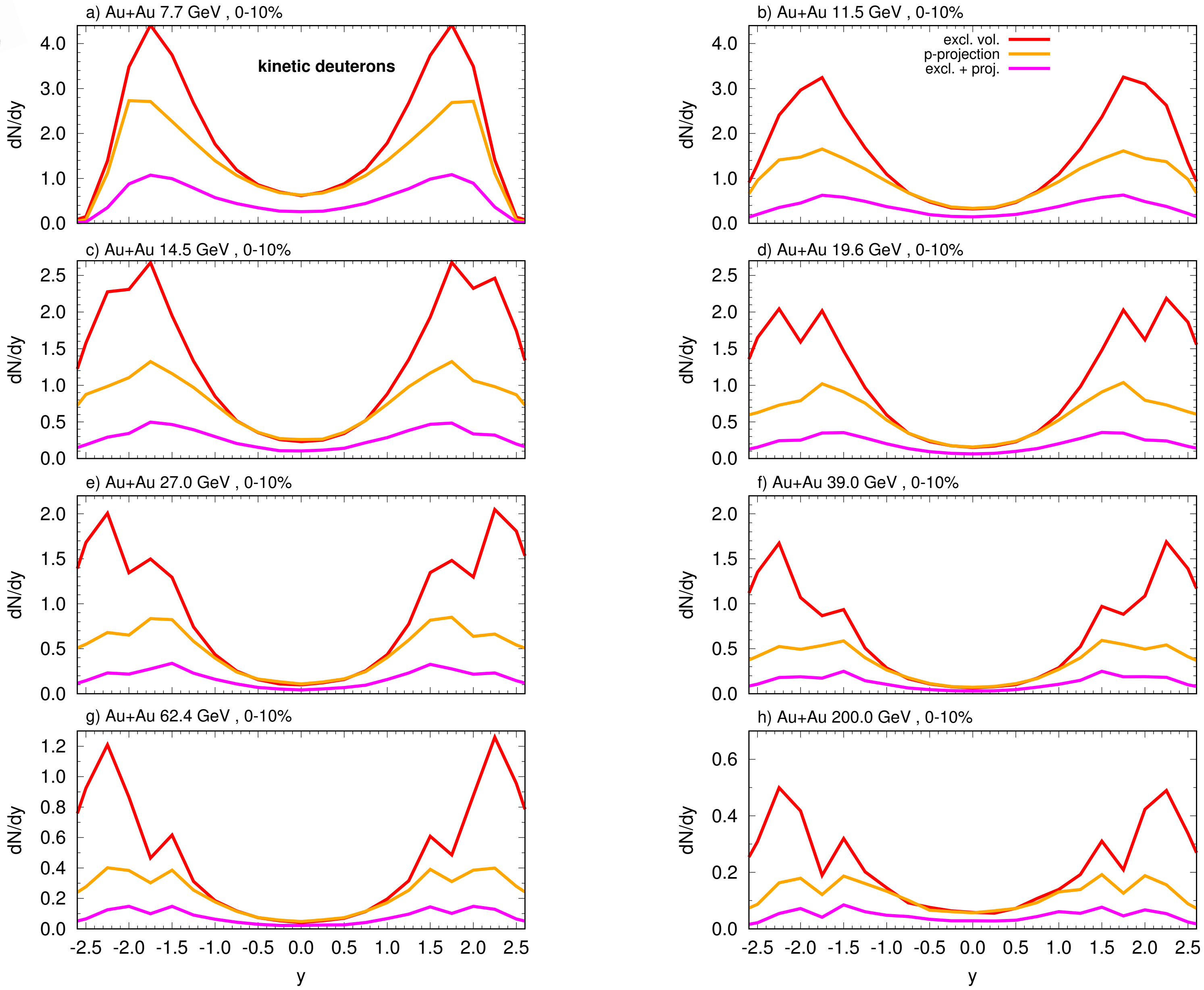
  - Recombine nucleons into cluster with $E_B < 0$ if time of disintegration is larger than nucleons freeze-out time.



top RHIC energy

kinetic mechanism with finite-size effects + MST identification of “stable” bound (E_B<0) A=2 , Z=1 clusters.

- Coupling two dynamical processes for deuteron formation: no double counting !
- Good description of mid-rapidity STAR data [PRC 99, (2019)].

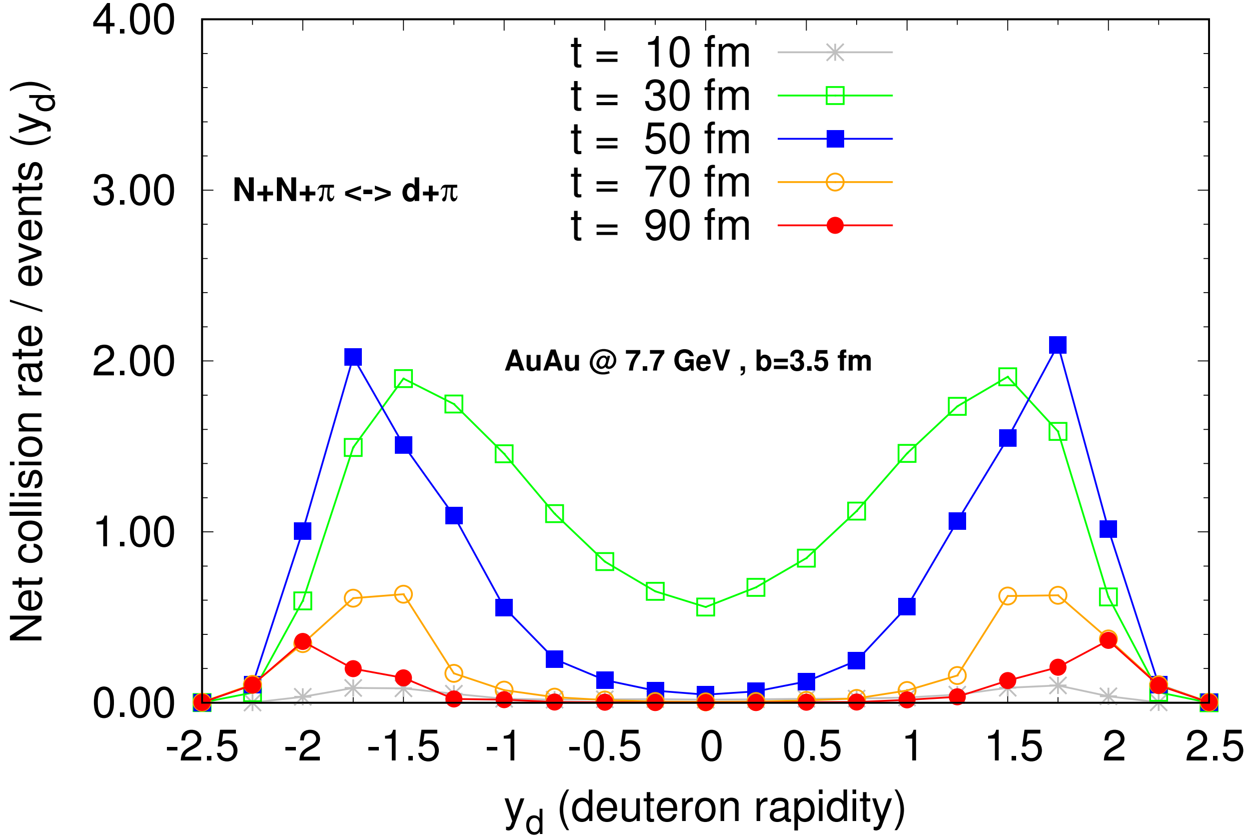


Comparison between models:

- dN/dy only kinetic deuterons.
- Excluded-volume effect (Model 1) and projection of NN rel. p on DWF (Model 2) have similar effect at mid-rapidity.
- At |y|>1 the two models start to behave differently (why?)
- Including both finite-size effects gives the largest suppression (dN_d/dy almost flat).
- Which model is more correct?

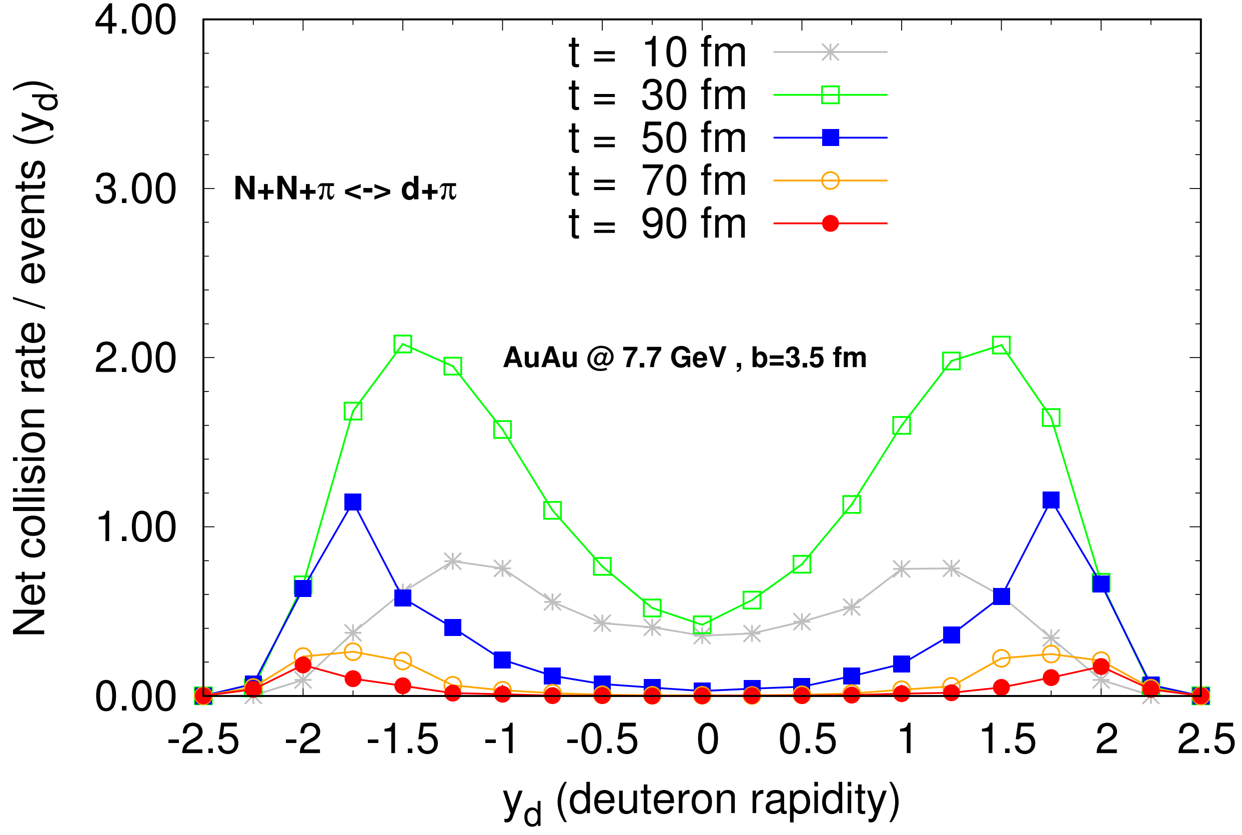
Model 1

kinetic mechanism + excluded-volume R_d=1.8 fm



Model 2

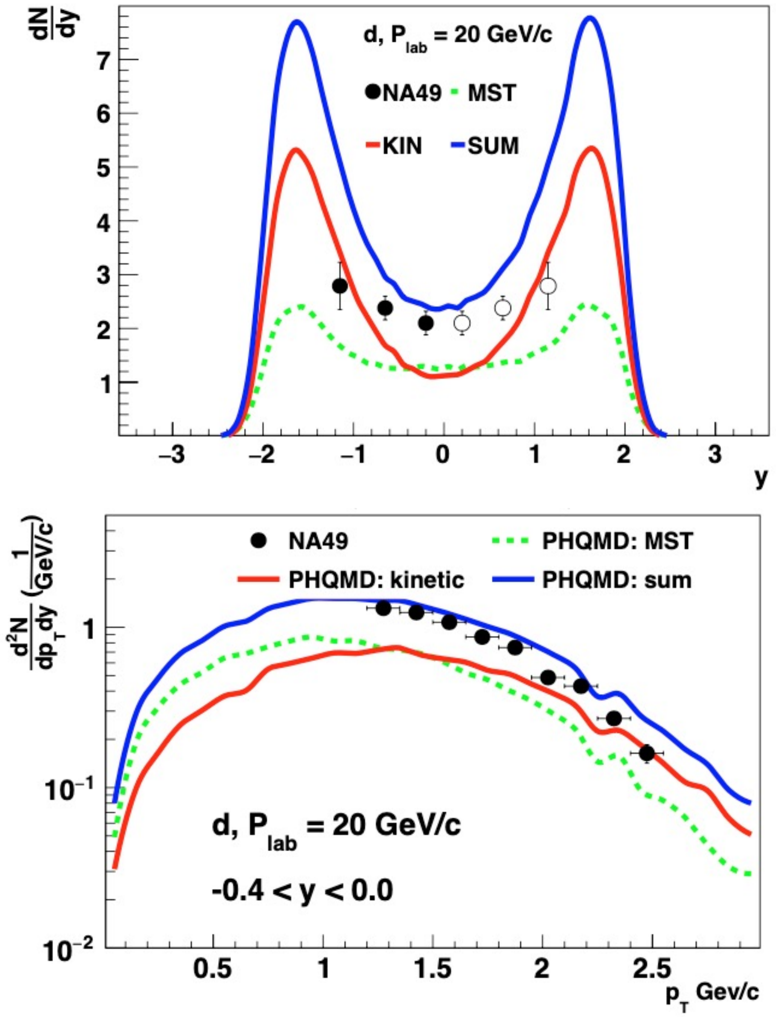
kinetic mechanism + momentum projection



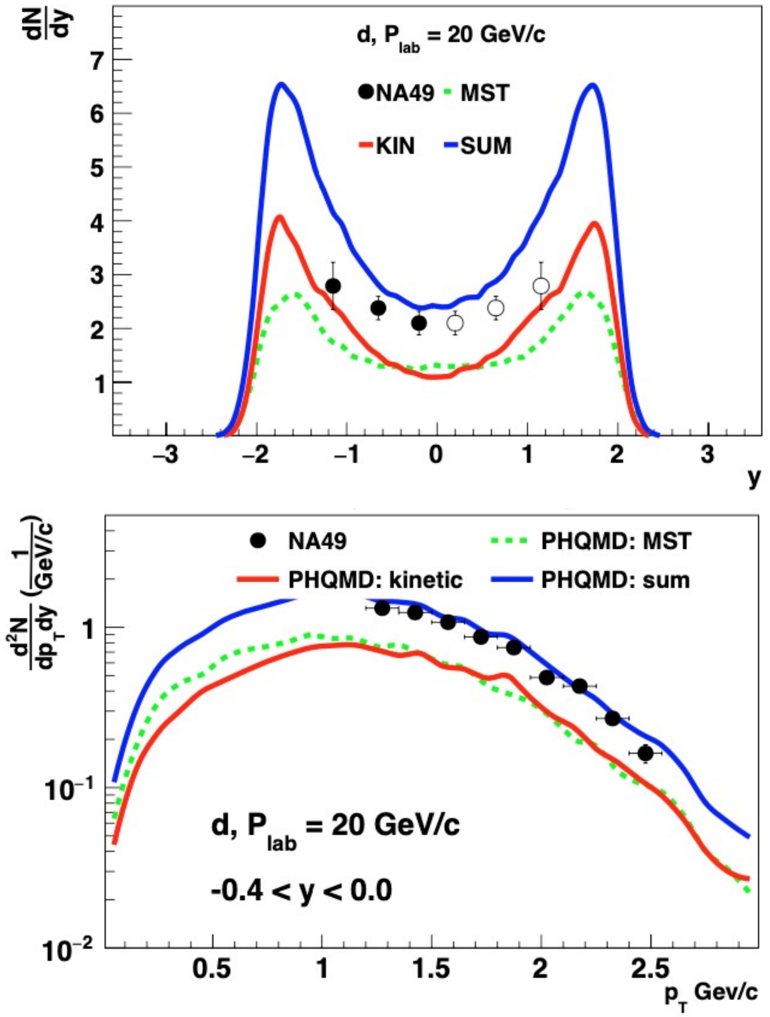
- Deuteron formation near target/projectile rapidity happens at later time compared to mid-rapidity.
- Momentum projection of NN-pair suppresses deuterons more effectively than excluded-volume at |y|>1.

PHQMD results: combine kinetic + potential deuterons

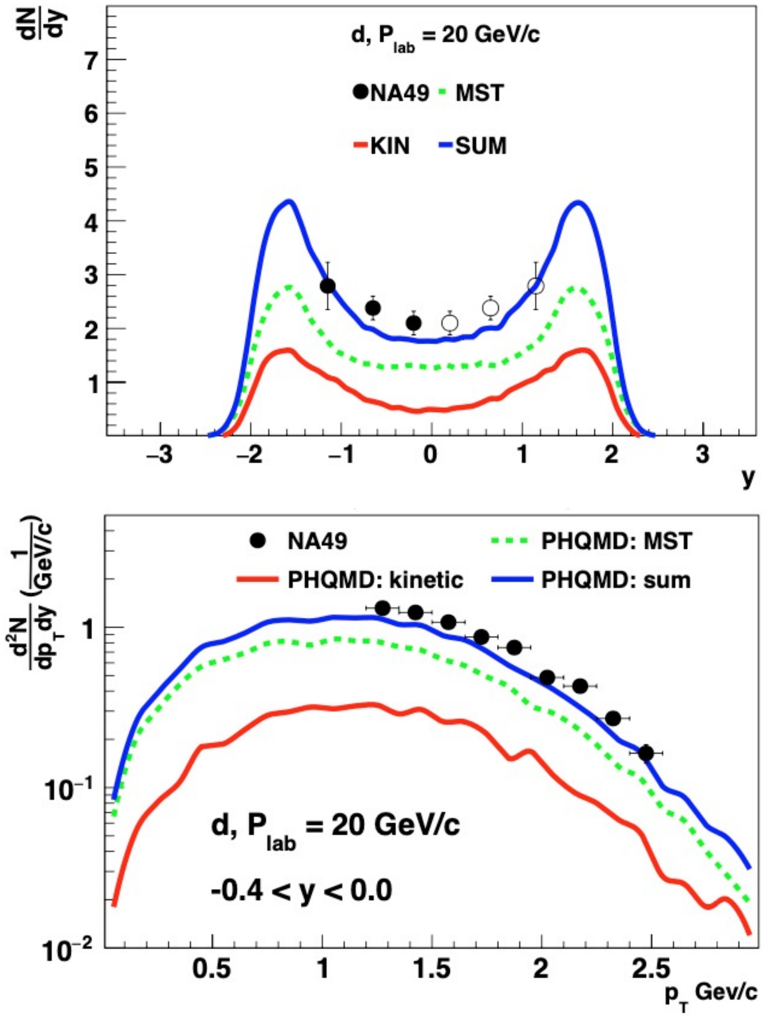
1) excluded-volume



2) Momentum projection



3) both effects



PHQMD results: combine kinetic + potential deuterons

1) excluded-volume

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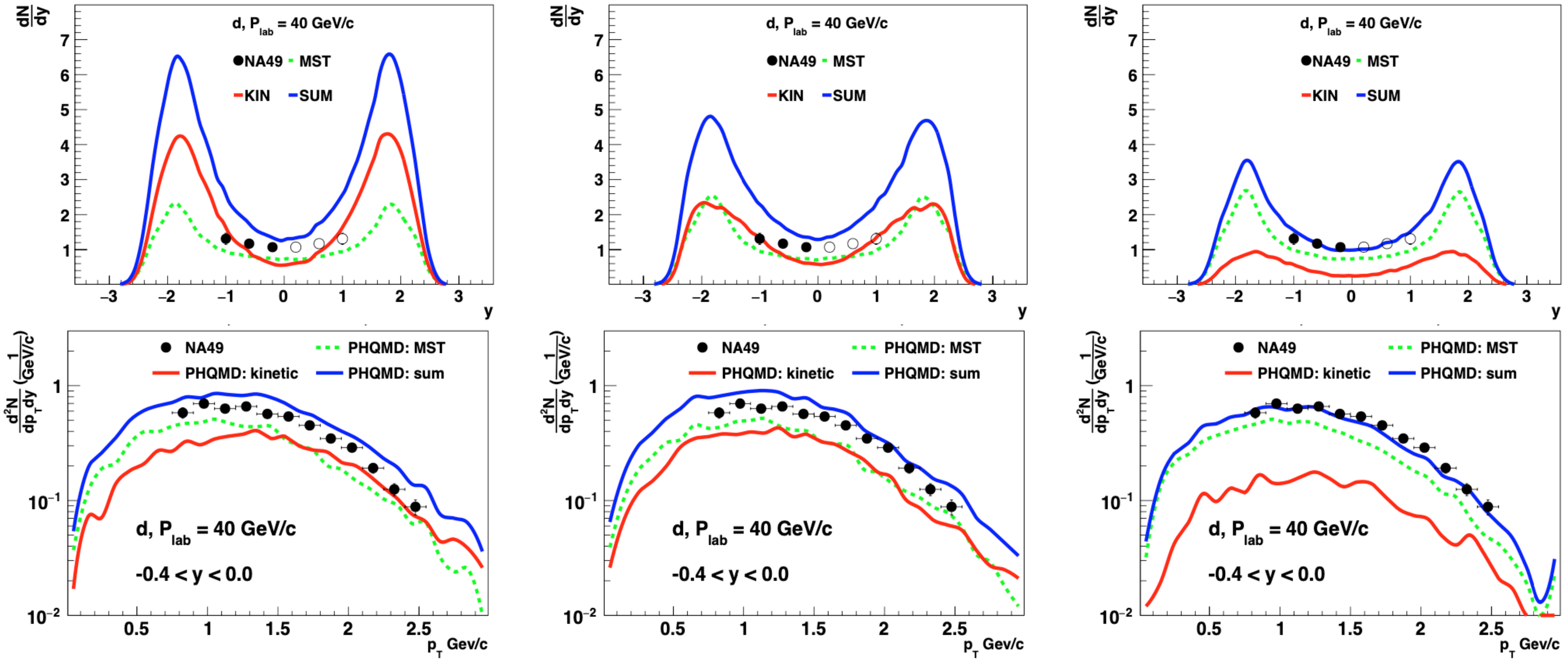


Summary:

- Hadronic reactions for deuteron production are now implemented in PHQMD collision integral including full isospin decomposition.
- Modelling finite-size effects in order to capture QM properties of deuteron shows sensitivity to different rapidity regions.
- Combined kinetic and potential mechanisms for deuteron production in good agreement with available exp. data dN_d/dy and p_T spectra.

[GC , J. Aichelin , E. Bratkovskaya et al. in preparation]

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

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

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

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

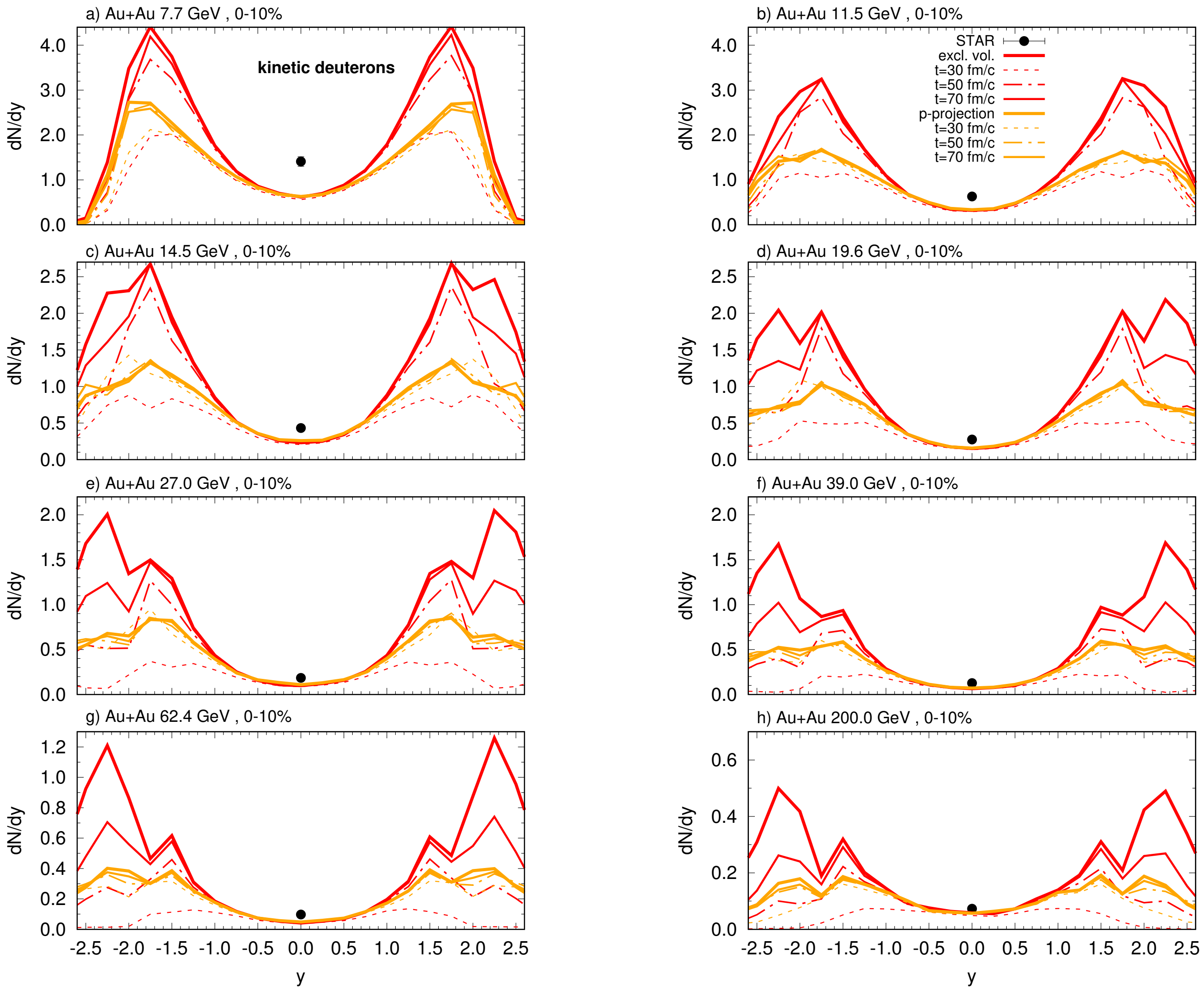
$$\pi^{0} + n + n \leftrightarrow \pi^{-} + d$$

Outlook:

- Treatment of the deuteron as a quantum state?

Thank you for your attention!

Backup

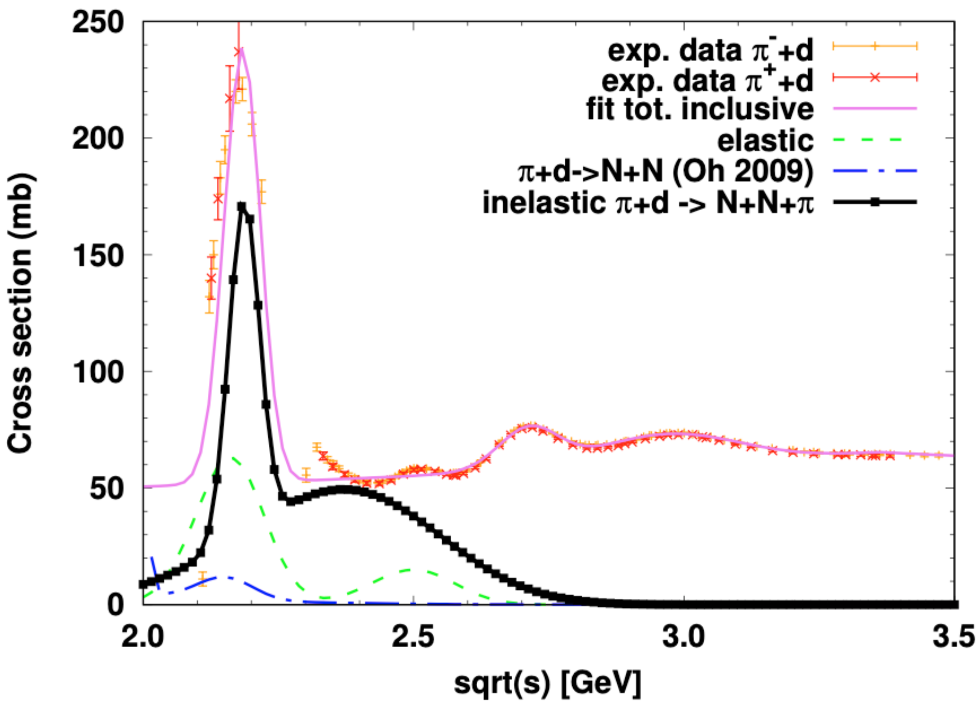


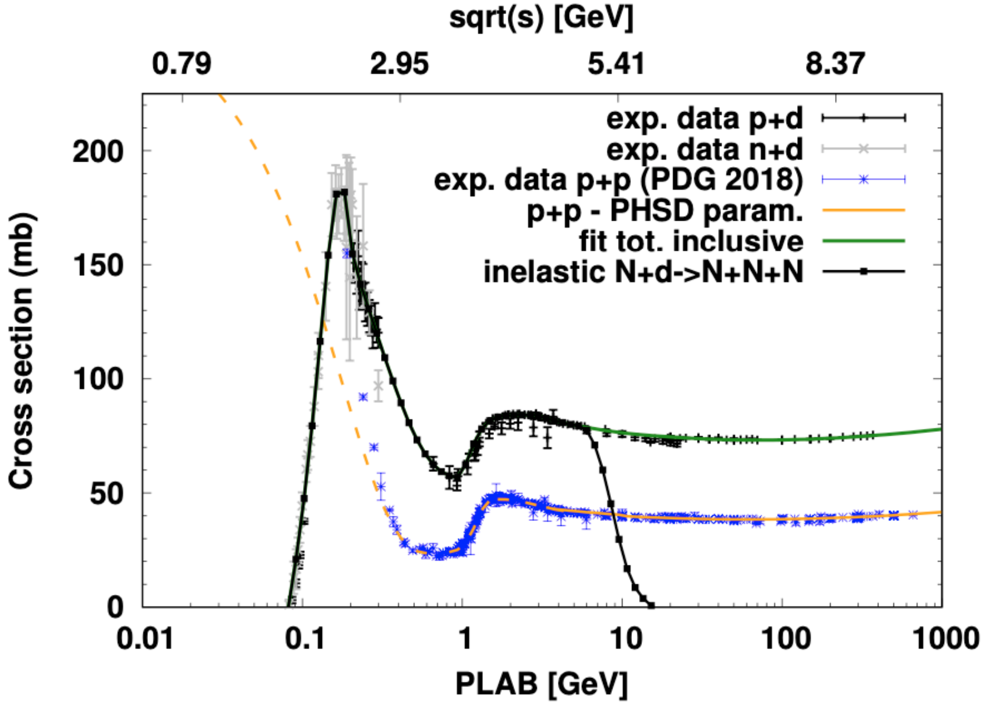
Time evolution of dN/dy of kinetic deuterons: excluded-volume vs momentum projection

Cross sections

- Hadronic reactions for d+π and d+N scattering characterized by inclusive cross sections $\sigma_{peak} \approx 200$ mb .
- Inverse reactions X+N+N → X+d (X=π,N with X catalyzer) important for d formation in HICs .
- At relativistic HICs π-catalysis >> N-catalysis due to large π abundance .
- Cross sections parametrized according to exp. data [PDG PRD 98 (2018)] .

[J. Kapusta PRC 21 (1980) 1301]
[D. Oliinychenko PRC 99 (2019) 4, 044907]





Fit exp.

$$\sigma_{tot}^{incl}(\pi d) = \sum_{n\geq 1} \sigma_{inel}(NN + n*\pi) + \sigma(\pi d \rightarrow NN) + \sigma_{el}(\pi d)$$

n=1

Fit exp.

$$\sigma_{tot}^{incl}(Nd) = \sum_{n\geq 1} \sigma_{inel}(NNN + n*\pi) + \sigma(Nd \rightarrow NNN) + \sigma_{el}(Nd)$$