The reaction-based nuclear production model in PYTHIA 8.3

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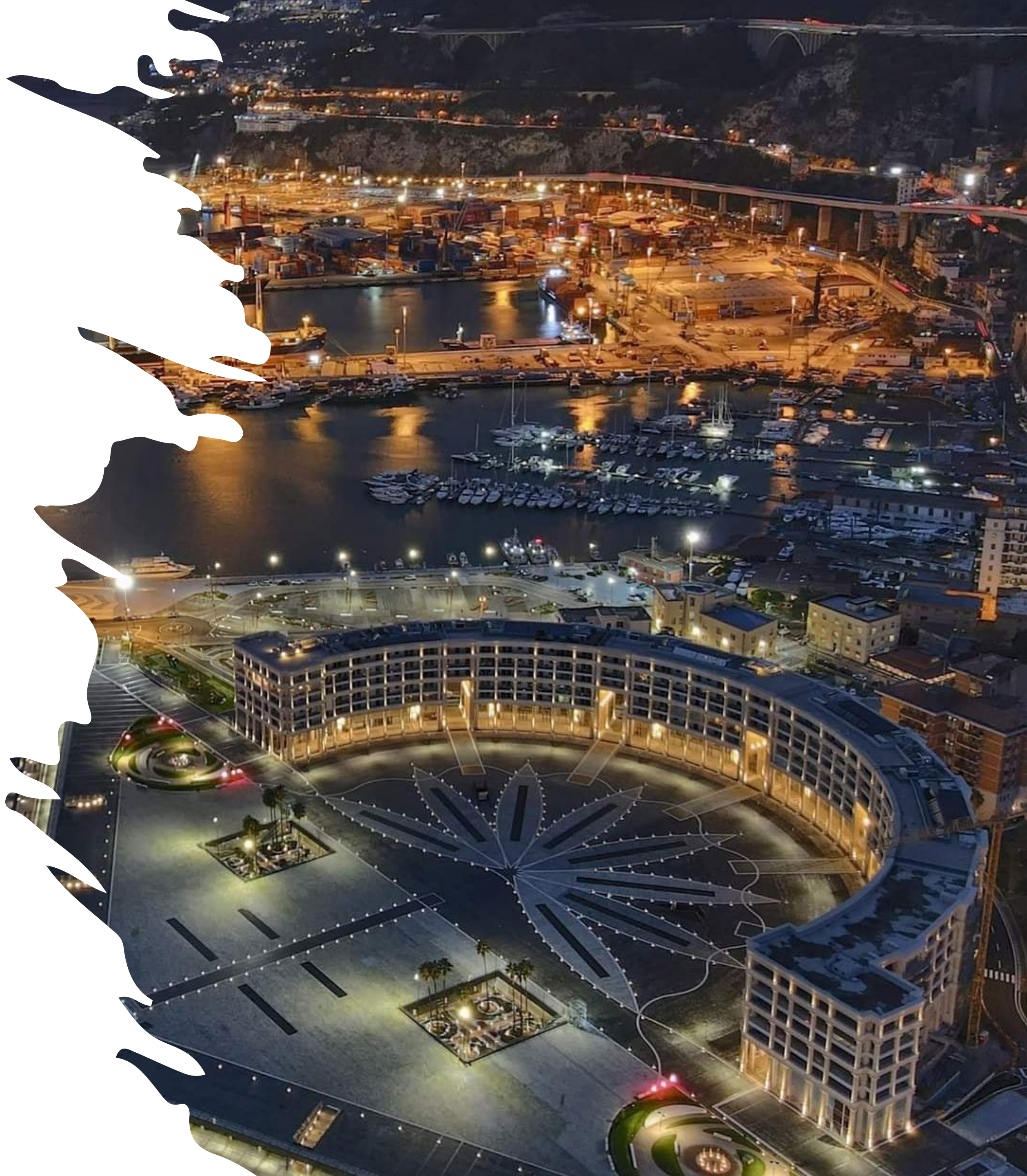
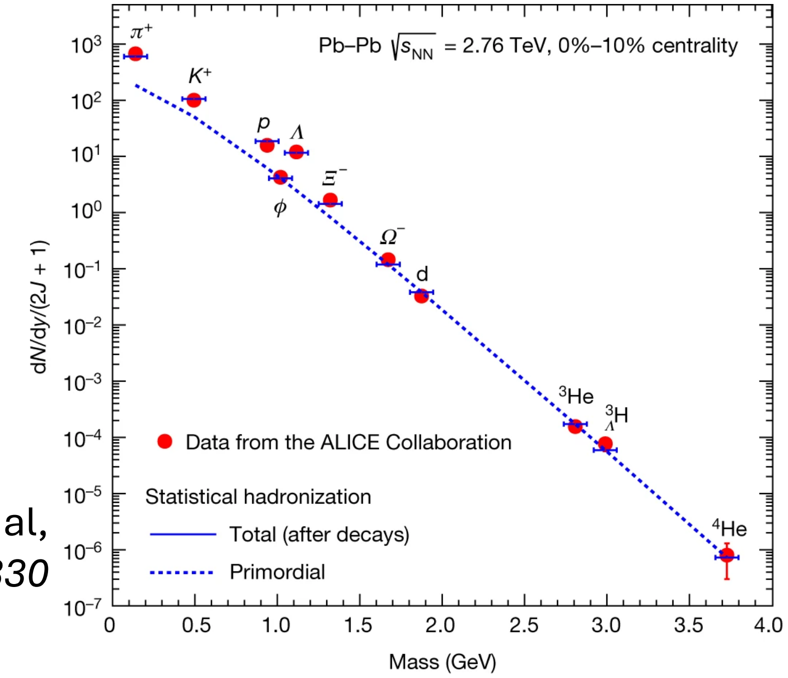
5th workshop on Anti-Matter, Hyper-Matter and Exotica Production



Light (anti)nuclei production models

Statistical Hadronization Model (SHM)

- Hadrons emitted from a system in statistical and chemical equilibrium with temperature T_{chem}
- $dN/dy \propto \exp(-m/T_{chem})$ → nuclei are sensitive to T_{chem} due their large mass
- Particle yields well described with a common T_{chem} of ~ 156 MeV



A. Andronic et al,
Nature vol. 561 (2018) 321-330

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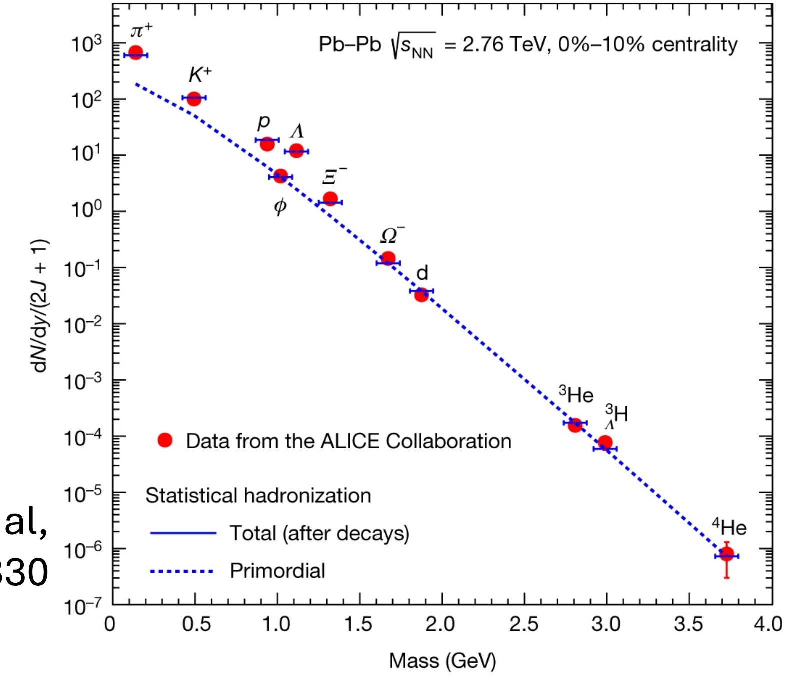
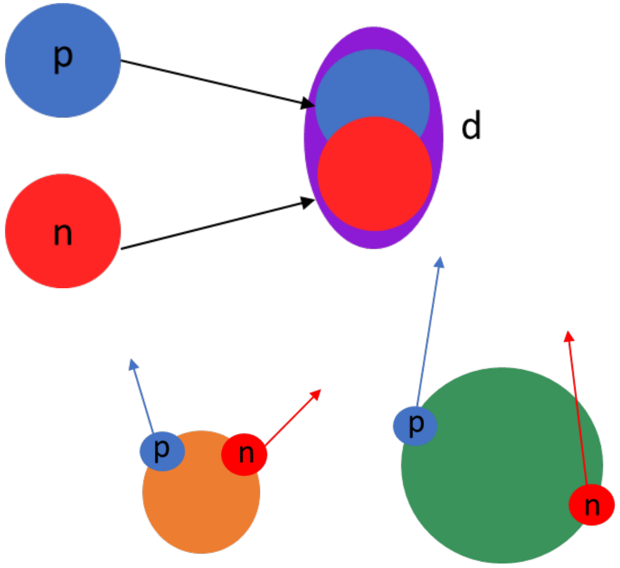


A. Andronic et al, Nature vol. 561 (2018) 321-330

Baryon Coalescence

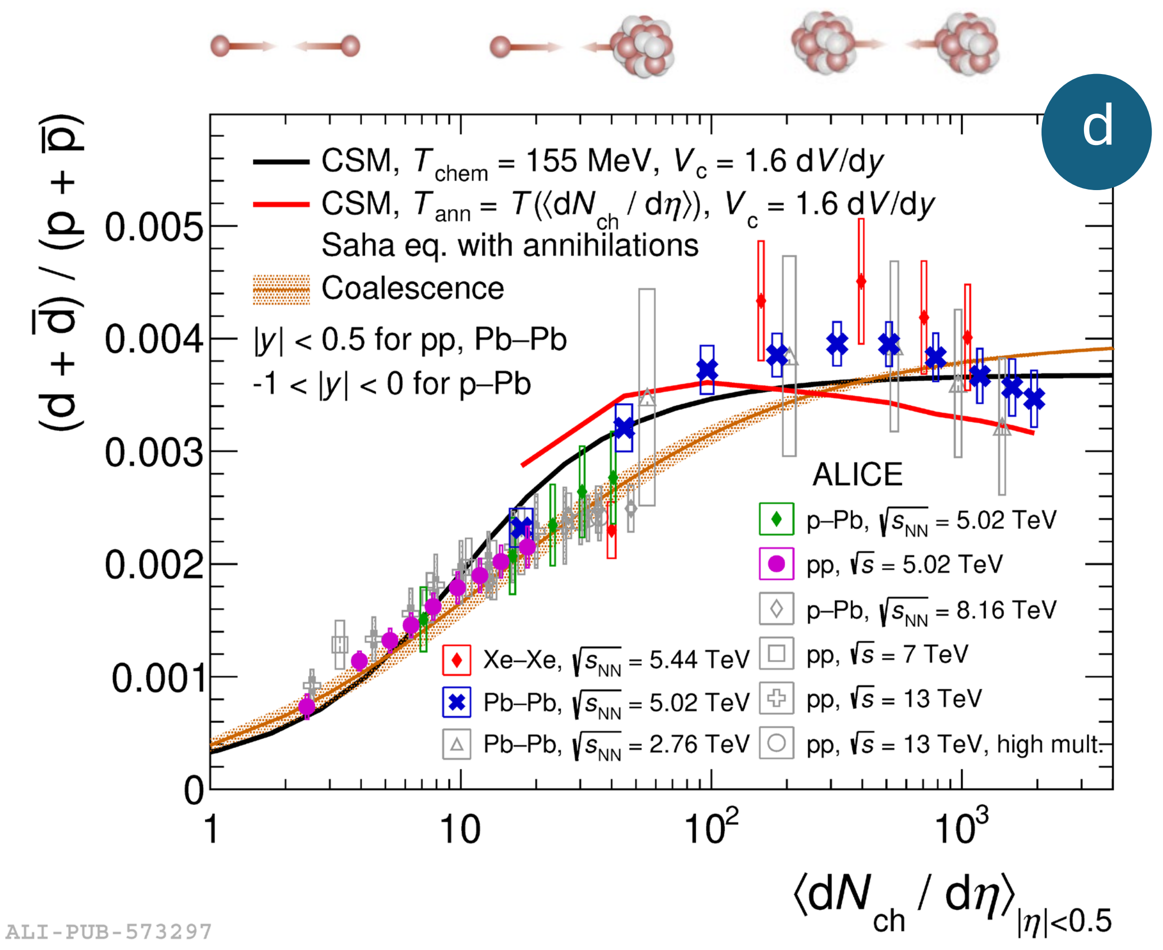


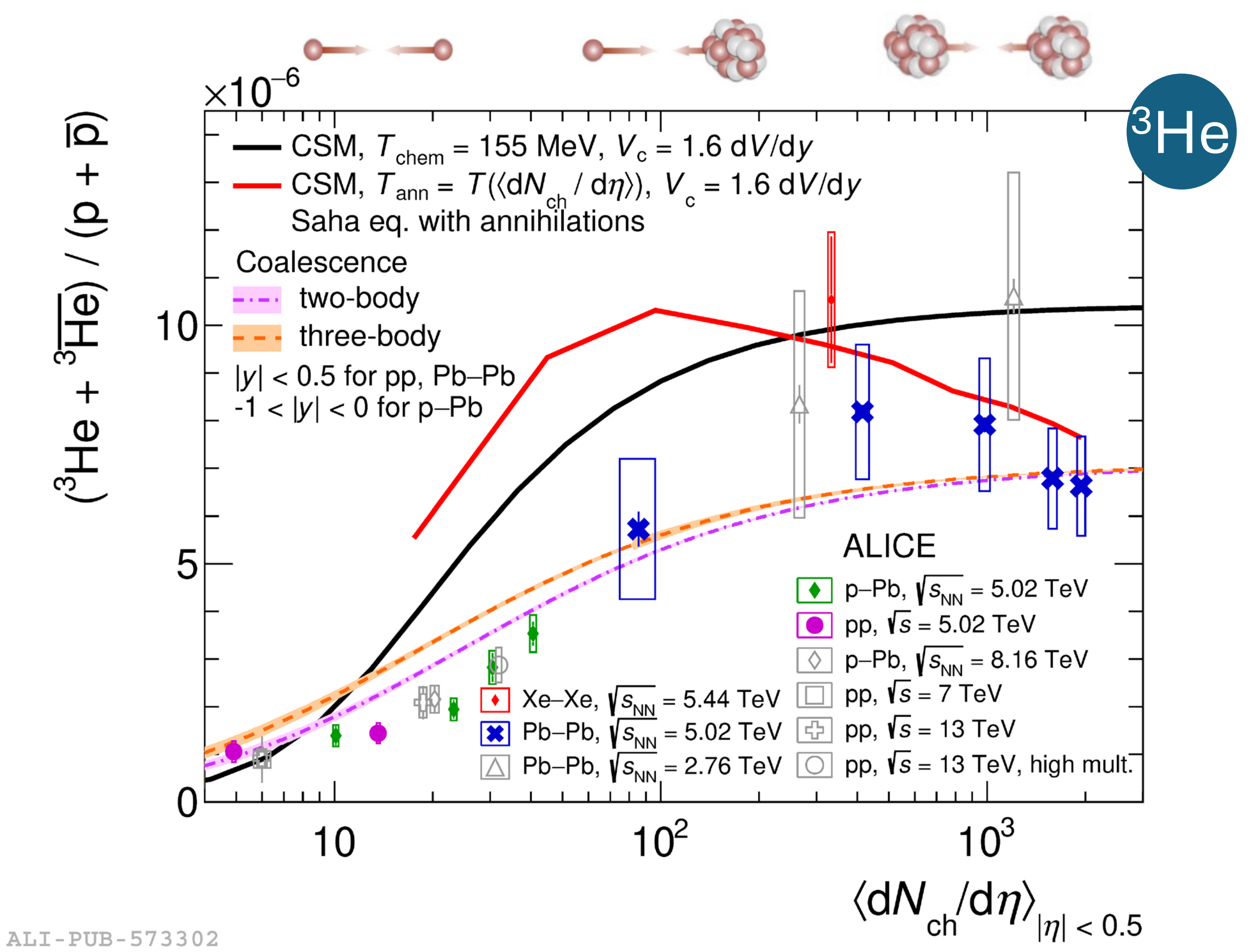
- (Anti)nuclei arise from the overlap of the (anti)nucleons phase-space distributions with the Wigner density of the bound state
- Dependence on the source size
- Coalescence parameter B_A proportional to the coalescence probability

$$E_A \frac{d^3N_A}{dp_A^3} = B_A \cdot \left(E_p \frac{d^3N_p}{dp_p^3}\right)^A \qquad p_p = p_A/A$$

S. T. Butler et al., *Phys. Rev. 129 (1963) 836*
M. Mahlein et al., *Eur. Phys. J. C 83 (2023) 804*

The current status





ALICE Collaboration, *Phys. Rev. C* 110 (2024) 064901

- No definitive answer from data (models too close, data not enough precise) → *we need something more*

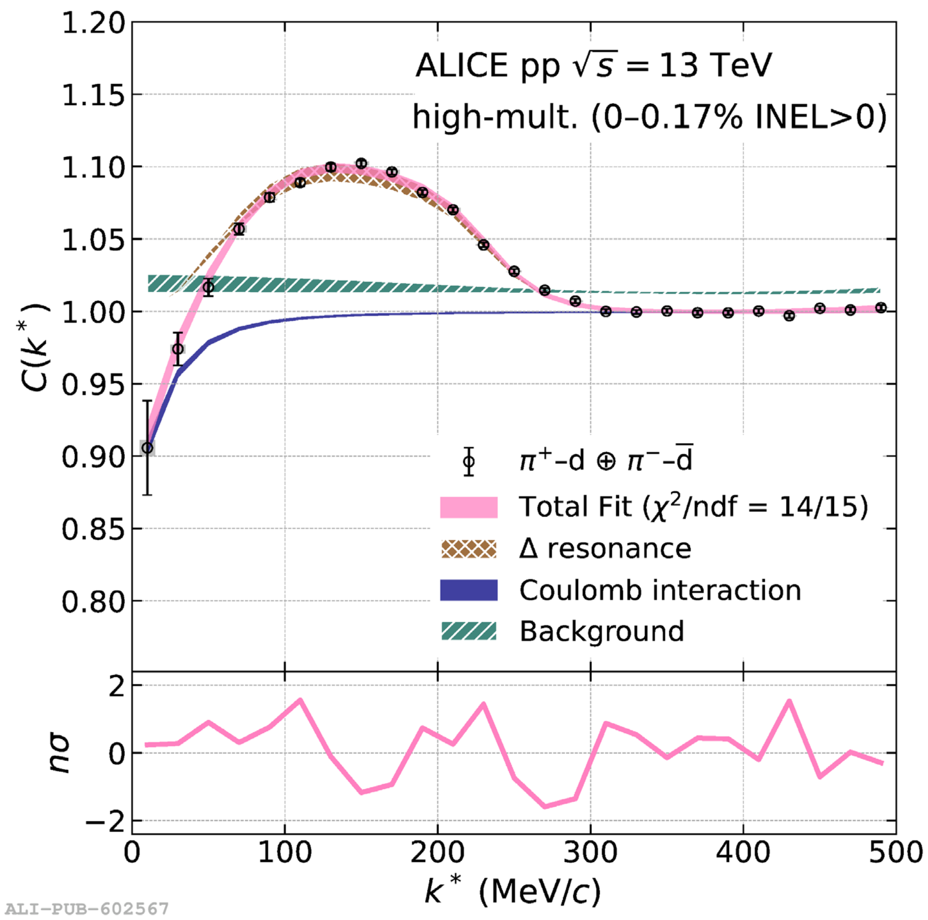
What's new?

See Maximilian's talk for more details!

- Recent results from the ALICE collaboration show the contribution of the Δ(1232) resonance in the deuteron formation

- Measurements achieved studying the deuteron-pion correlation functions in HM pp collisions

- Model independent evidence
  - About 80% of the (anti)deuterons are produced in nuclear fusion reactions following the decay of short lived resonances
  - About the 60% of them derive from the Δ(1232)



ALICE Collaboration, *arXiv:2504.02393 [nucl-ex]*

Nuclei production in event generators

- Different event generators are available for simulate high energy hadronic collisions

- In the majority of them, the nuclear production is not directly implemented

- The results on nuclei production are then evaluated in relation to the SHM and the baryon coalescence using thermal predictions or coalescence afterburners

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- Different event generators are available for simulate high energy hadronic collisions
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- The results on nuclei production are then evaluated in relation to the SHM and the baryon coalescence using thermal predictions or coalescence afterburners
- ***In PYTHIA 8.3 the (anti)deuteron production is implemented using a reaction-based production***

The reaction-based model in PYTHIA 8.3

C. Bierlich et al., *SciPost Phys.Codeb. 2022 (2022) 8*

- The default implementation is based on the Dal-Raklev model:
  - The nucleon binding cross section is not a uniform distribution up to a cutoff value (still available in the model), but it is determined from fits to nucleon-scattering data from different experiments
  - Different reactions are considered:

$pn \rightarrow \gamma d$	$pn \rightarrow \pi^0 d$	$pp \rightarrow \pi^+ d$	$nn \rightarrow \pi^- d$
$pn \rightarrow \pi^- \pi^+ d$	$pn \rightarrow \pi^0 \pi^0 d$	$pp \rightarrow \pi^+ \pi^0 d$	$nn \rightarrow \pi^- \pi^0 d$

  - Similar implementation for the antideuteron
  - Channels can be removed, added or modified
  - Each channel must have a two-body initial state and a n-body final state with n > 1 and at least one of the outgoing particles must be a deuteron
  - The kinematics of the final state is determined by an isotropic decay of the initial state pair

The Dal-Raklev empirical model

- **Base hypothesis of the model**: the probability that a combination of a N_1N_2 pair with a k momentum difference in the centre-of-mass frame form a deuteron is a random event with a value:

$$P(N_1N_2 \rightarrow dX_i|k) = \frac{\sigma_{N_1N_2 \rightarrow dX_i}(k)}{\sigma_0}$$

- With σ_0 a free normalization factor assumed the same for all the processes

- Which process dominates as a function of k?

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

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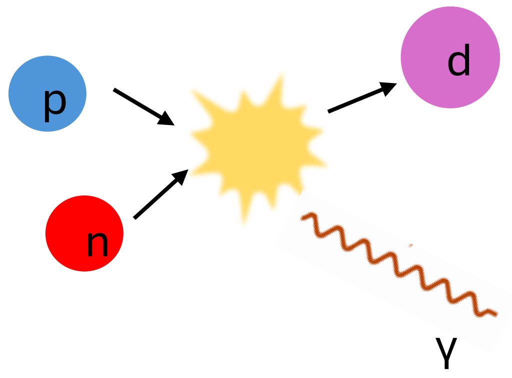

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

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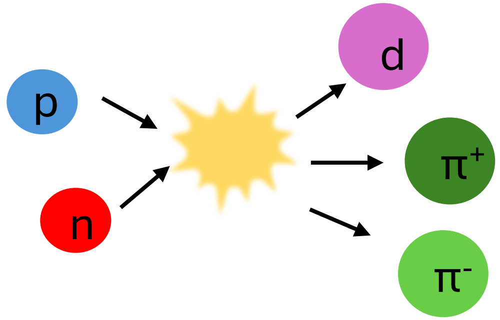

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- Which process dominates as a function of k?
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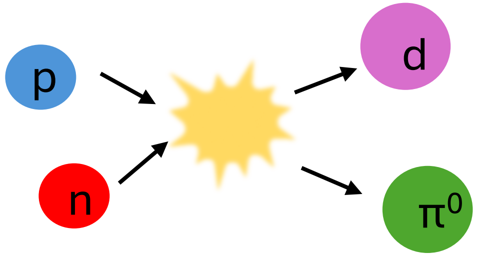

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

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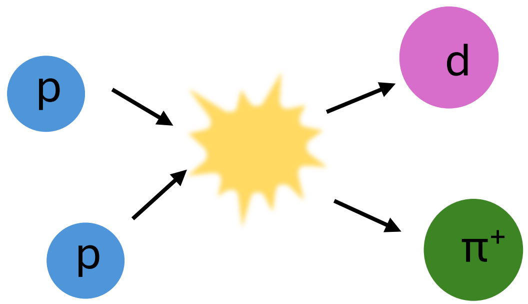

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  - At the same energies the pp and nn processes are more efficient for deuteron production, hence must be considered

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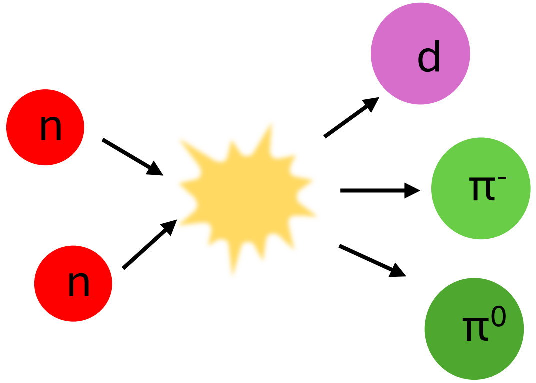

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  - At the same energies the pp and nn processes are more efficient for deuteron production, hence must be considered
  - The cross section decreases with increasing the products in the final state

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

pn → dγ process

- Little to no data for pn → dγ process, no fit possible in this condition

- But plenty of data for the inverse process dγ → pn that can be used thanks to the principle of the detailed balance:

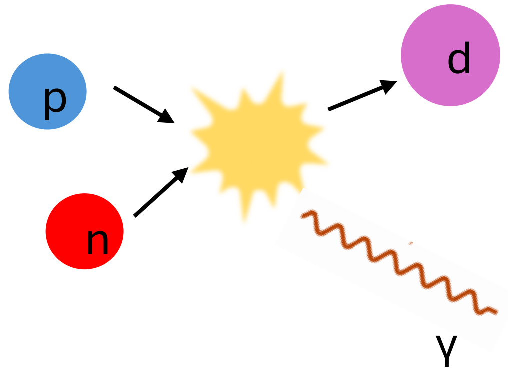
$$\sigma(Aa \to Bb) = \frac{g_B g_b}{g_A g_a}\frac{p_b^2}{p_a^2}\sigma(Bb \to Aa)$$

- With p_i the particle momentum, g_i the number of spin (for massive particles $g_i = 2s_i + 1$)

- Cross sections are invariant under Lorentz boost in the beam direction

- In our case:

$$\sigma(pn \to d\gamma) = \frac{3}{2}\frac{p_\gamma^2}{p_n^2}\,\sigma(d\gamma \to pn)$$



L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

pn → dγ process

- In some range of energies, experimental data are in tension
  - Keep only the most recent dataset
  - If a experiment dataset is discarded in one region, all data of the same experiment are discarded

- Final fit:

$$\frac{\sigma_{pn\to d\gamma}}{(1\mu b)} = \begin{cases} \sum_{n=-1}^{10} a_n \kappa^n & \kappa < 1.28 \\ \exp(-b_1\kappa - b_2\kappa^2) & \kappa \geq 1.28 \end{cases}$$

- $\kappa = k/1$ GeV

- Fit over 6 order of magnitude → parameters finely tuned

Parameter	Value
a_{-1}	2.30346
a_0	-9.366346×10^1
a_1	2.565390×10^3
a_2	-2.5594101×10^4
a_3	1.43513109×10^5
a_4	-5.0357289×10^5
a_5	1.14924802×10^6
a_6	-1.72368391×10^6
a_7	1.67934876×10^6
a_8	-1.01988855×10^6
a_9	3.4984035×10^5
a_{10}	-5.1662760×10^4
b_1	−5.1885
b_2	2.9196

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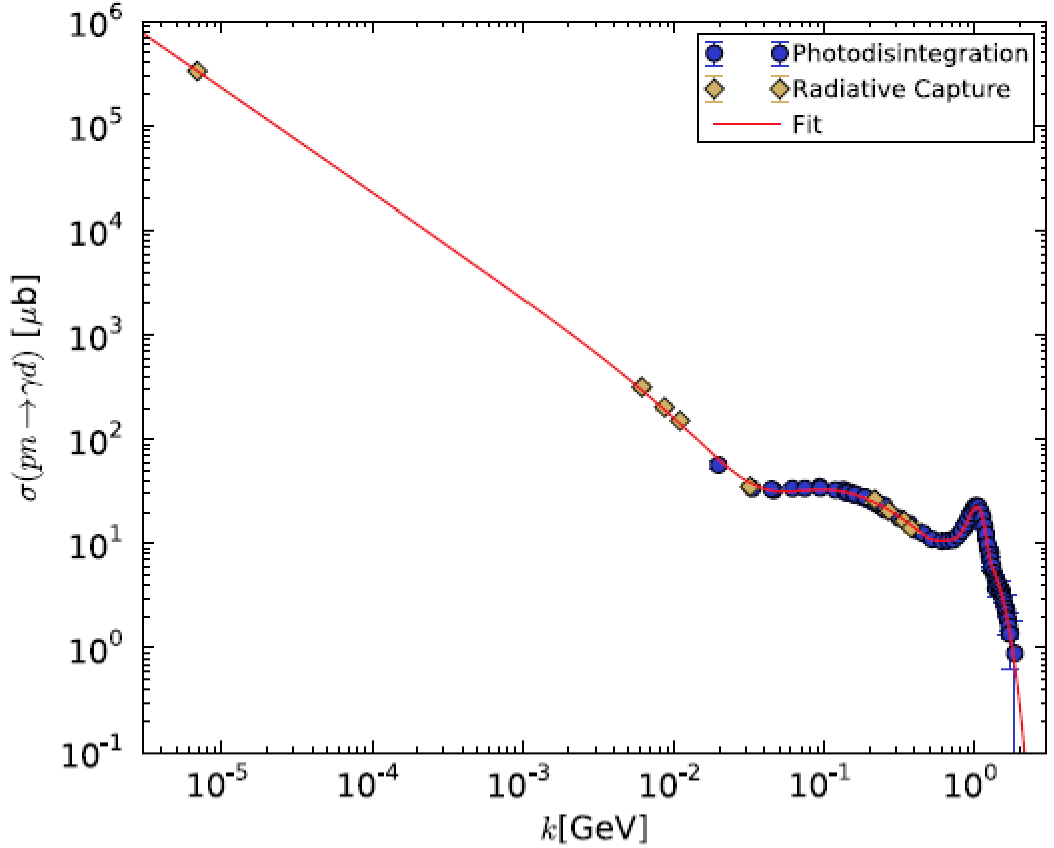
- $\kappa = k/1$ GeV
- Fit over 6 order of magnitude → parameters finely tuned
- Peak at ~ 1 GeV → Δ resonance contribution



L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

$N_1N_2 \rightarrow d\pi$ processes

- Look at three different reactions:

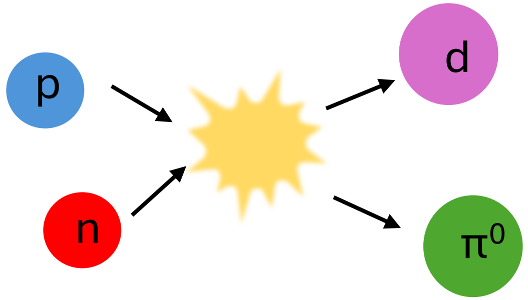
  $pn \rightarrow \pi^0 d$ $pp \rightarrow \pi^+ d$ $nn \rightarrow \pi^- d$

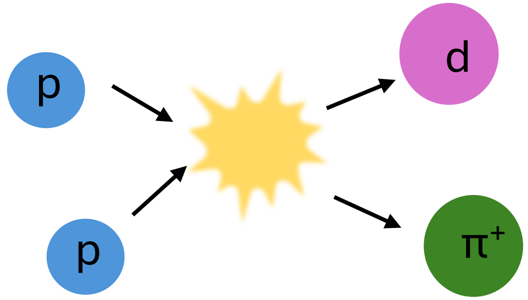
- Isospin invariance relations

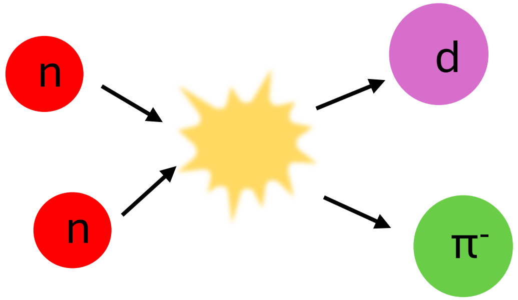
$$\sigma_{pn \rightarrow d\pi^0} = \frac{1}{2}\sigma_{pp \rightarrow d\pi^+}$$

$$\sigma_{nn \rightarrow d\pi^-} = \sigma_{pp \rightarrow d\pi^+}$$

- *Not exact relations due to broken isospin symmetry*
- Very little data for $pn \rightarrow \pi^0 d$, no data for $nn \rightarrow \pi^- d$
- Use of the plenty of data for $pp \rightarrow \pi^+ d$ plus isospin relations







H. Machner and J. Niskanen, *Nucl. Phys. A776, 172 (2006)*

$N_1N_2 \rightarrow d\pi$ processes

- Experimental data fitted by

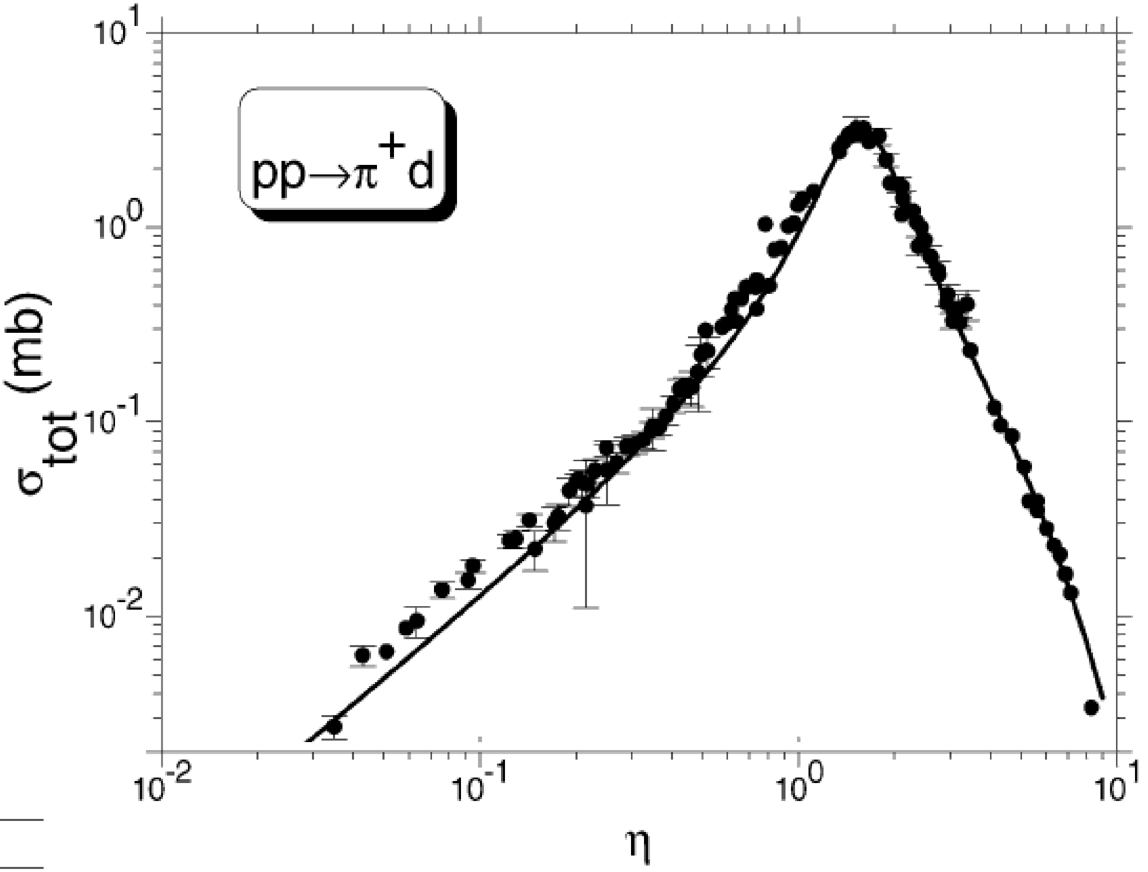
$$\sigma(\eta) = \frac{a\eta^b}{\left(c - \exp(d\eta)\right)^2 + e}$$

- Where $\eta = q/m_\pi$ and q the pion momentum in the c.m frame

- Applied corrections for Coulomb repulsion and phase space difference of nucleon and pions, to be revoked or reapplied in other reactions

- Total effects are negligible (slight change of threshold value, % different in the peak) → neglected

a (mb)	*b*	*c*	*d*	*e*
0.17 ± 0.03	1.34 ± 0.06	1.77 ± 0.04	0.38 ± 0.02	0.096 ± 0.02



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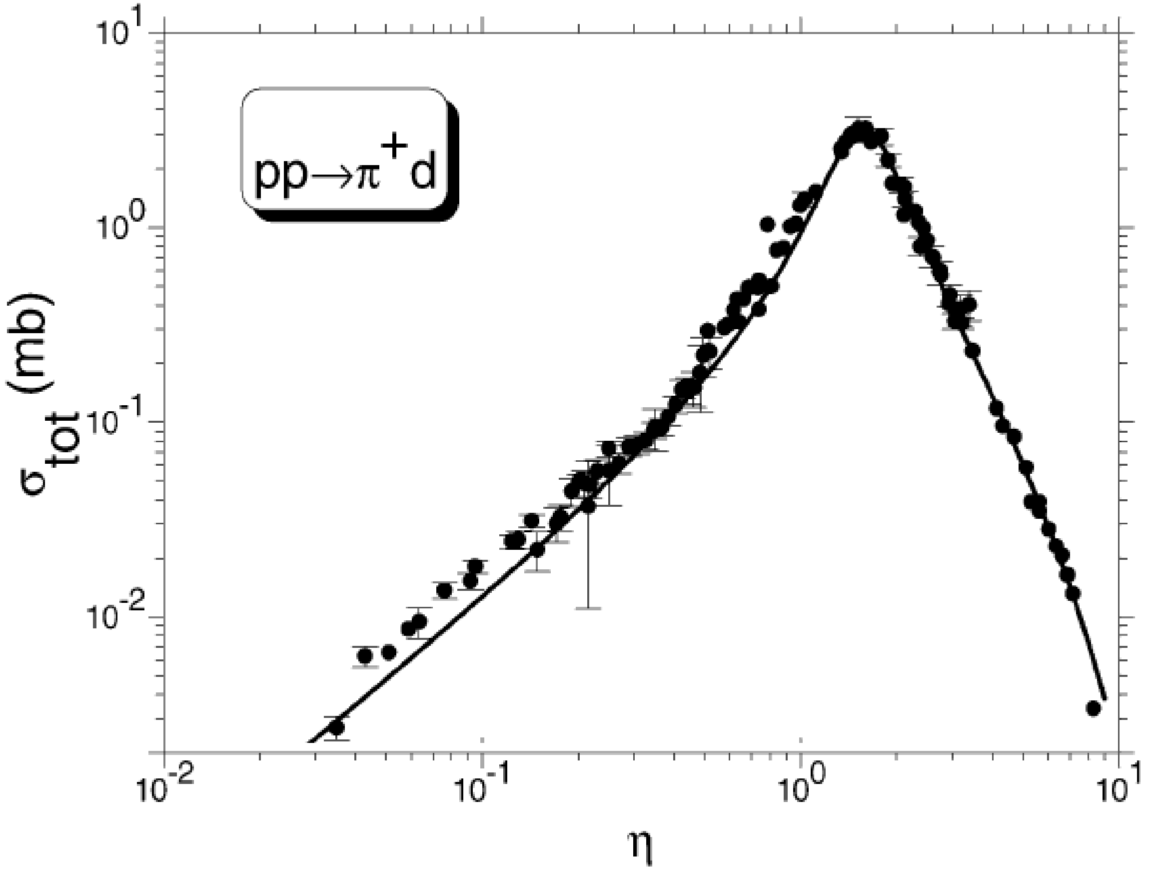
- Also in this case, the peak of the Δ resonance is present



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$N_1N_2 \rightarrow d\pi\pi$ processes

- Look of four different reactions:

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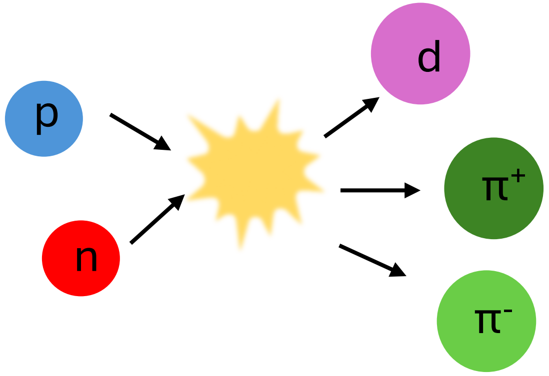
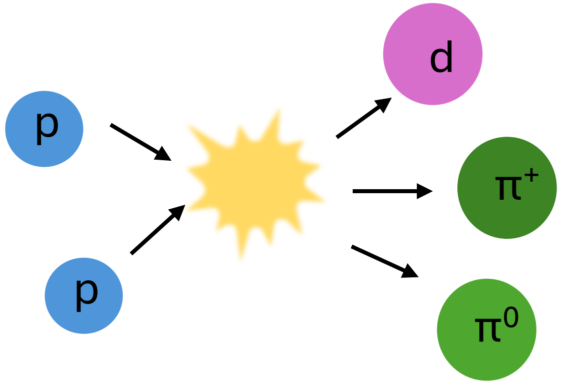
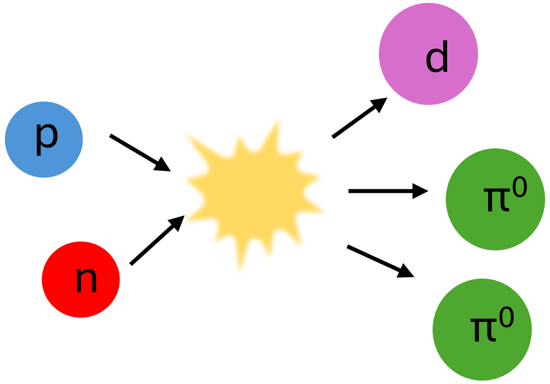
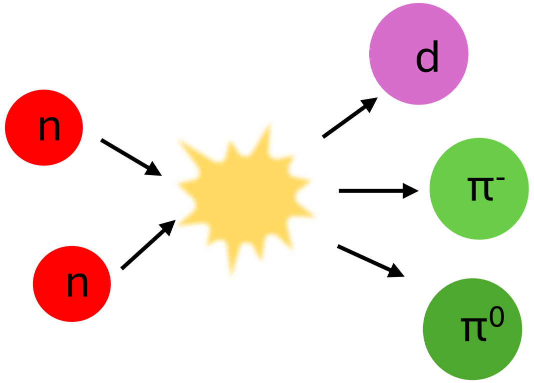








L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

$N_1N_2 \rightarrow d\pi\pi$ processes

- Look of four different reactions:

  $pn \rightarrow \pi^-\pi^+d$ $pn \rightarrow \pi^0\pi^0d$ $pp \rightarrow \pi^+\pi^0d$ $nn \rightarrow \pi^-\pi^0d$

- Some constraints:
  - No data for $nn \rightarrow \pi^-\pi^0d$
  - Very little data for all the other reactions at $\sqrt{s}$ > 2.5 GeV/c
  - Presence of resonanance peak at around $\sqrt{s}$ > 2.5 GeV/c that challenge the fit procedure

- Use of the isospin invariance to maximize the results:

$$\sigma_{pn\rightarrow d\pi^+\pi^-} = 2\,\sigma_{pn\rightarrow d\pi^0\pi^0} + \frac{1}{2}\sigma_{pp\rightarrow d\pi^+\pi^0}$$

$$\sigma_{nn\rightarrow d\pi^-\pi^0} = \sigma_{pp\rightarrow d\pi^+\pi^0}$$

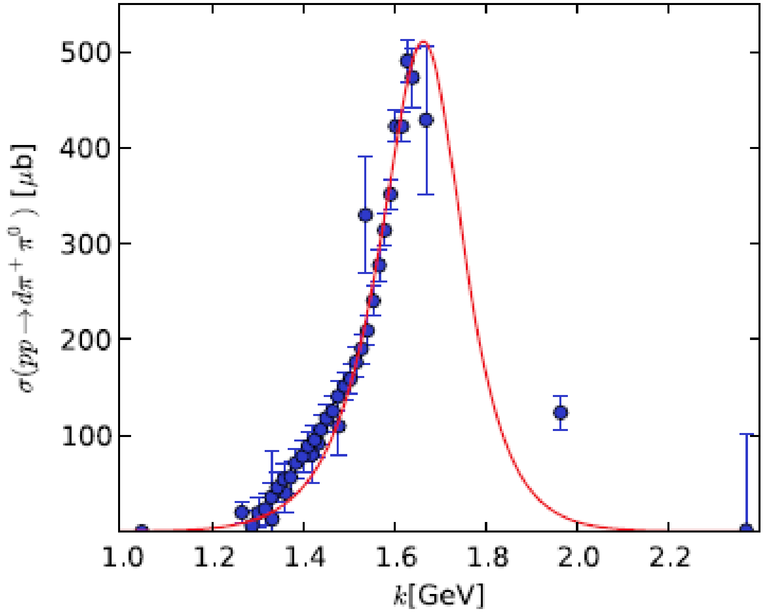
- Big influence of isospin breaking effects (~ 25%) → individual fit for each process with data of the other processes included but weighted down (1/100 in the χ^2) + dummy points at kinematic cutoff

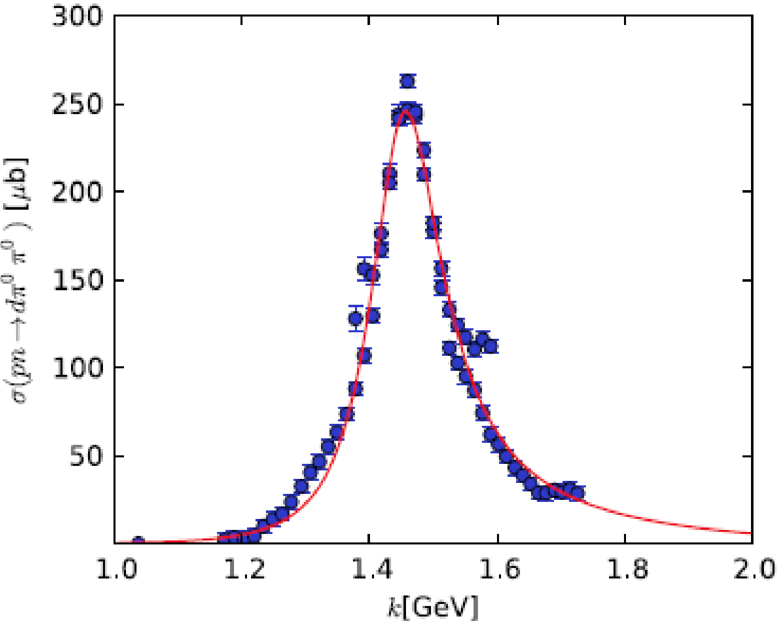
L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

$N_1N_2 \rightarrow d\pi\pi$ processes

- For the $pp \rightarrow \pi^+\pi^0 d$ and $pn \rightarrow \pi^0\pi^0 d$ reactions the experimental data are fitted by:

$$\sigma(\kappa) = \frac{a\kappa^{b}}{\left(c - \exp(d\kappa)\right)^{2} + e}$$





Parameter	Value
a [μb]	5.099×10^{15}
b	1.656×10^{1}
c	2.333×10^{7}
d	1.133×10^{1}
e	2.868×10^{16}

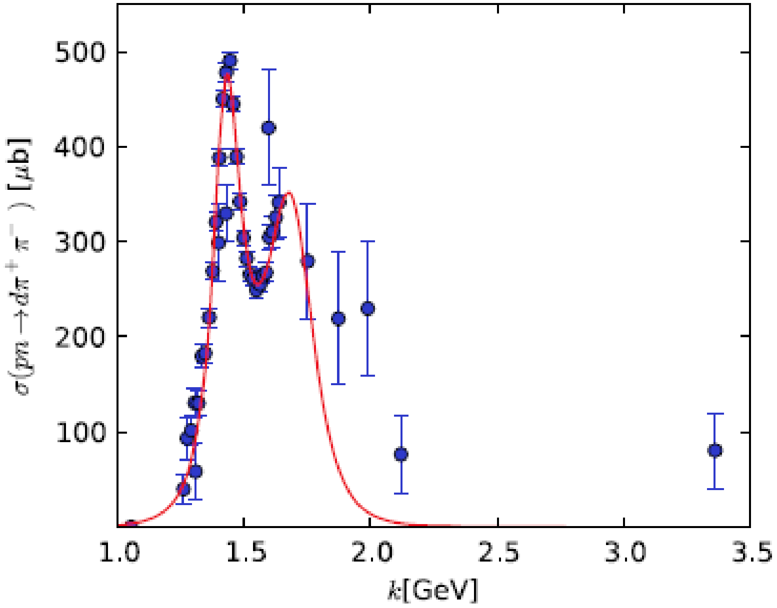
Parameter	Value
a [μb]	2.855×10^{6}
b	1.311×10^{1}
c	2.961×10^{3}
d	5.572×10^{0}
e	1.461×10^{6}

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

$N_1N_2 \rightarrow d\pi\pi$ processes

- For the $pn \rightarrow \pi^-\pi^+d$ reactions the experimental data are fitted by:

$$\sigma(\kappa) = \frac{a_1\kappa^{b_1}}{(c_1 - \exp(d_1\kappa))^2 + e_1} + \frac{a_2\kappa^{b_2}}{(c_2 - \exp(d_2\kappa))^2 + e_2}$$



Parameter	Value
a_1 [μb]	6.465×10^6
b_1	1.051×10^1
c_1	1.979×10^3
d_1	5.363×10^0
e_1	6.045×10^5
a_2 [μb]	2.549×10^{15}
b_2	1.657×10^1
c_2	2.330×10^7
d_2	1.119×10^1
e_2	2.868×10^{16}

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

$N_1N_2 \rightarrow d\pi\pi$ processes

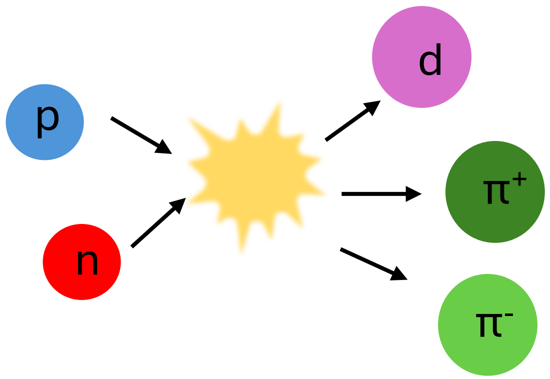
- Having a 3-body final state, the kinematic here is more involved

- Not enough data to parametrize the deuteron momentum distribution in the c.m. frame

  - Assumption of no angular correlation between the deuteron and the pions
  - The distributions are made considering the phase space alone

- The deuteron momentum is calculated as:

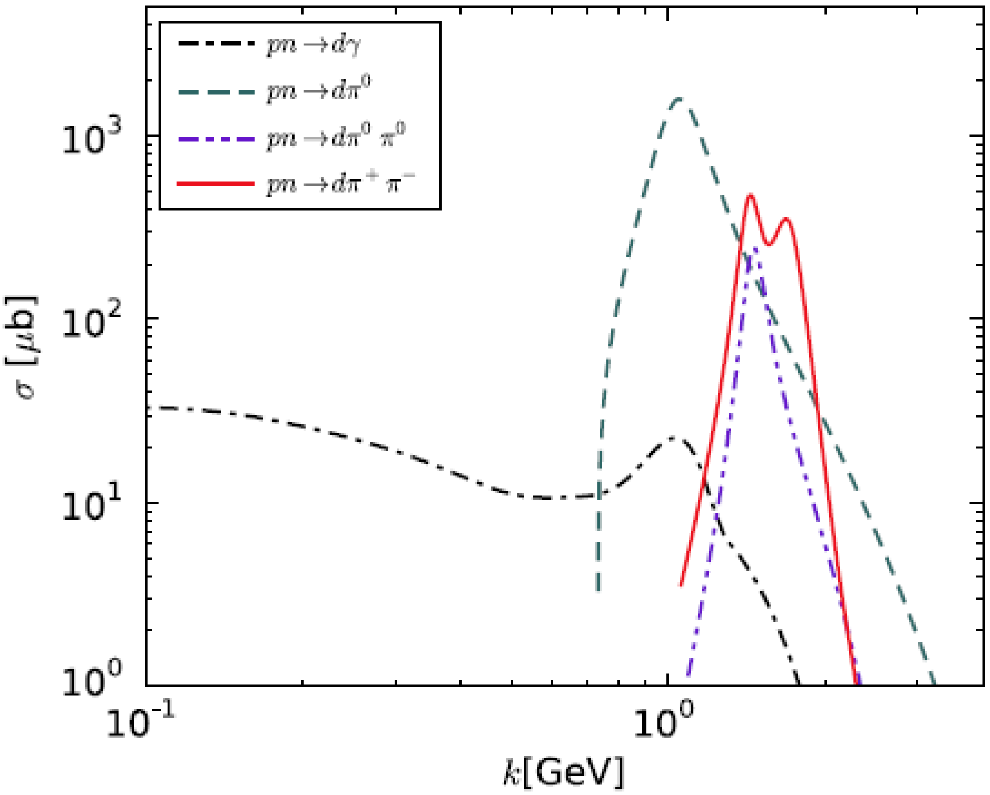
$$p_d = \sqrt{\left(\frac{s + m_d^2 - m_{d\pi}^2}{2\sqrt{s}}\right) - m_d^2}$$

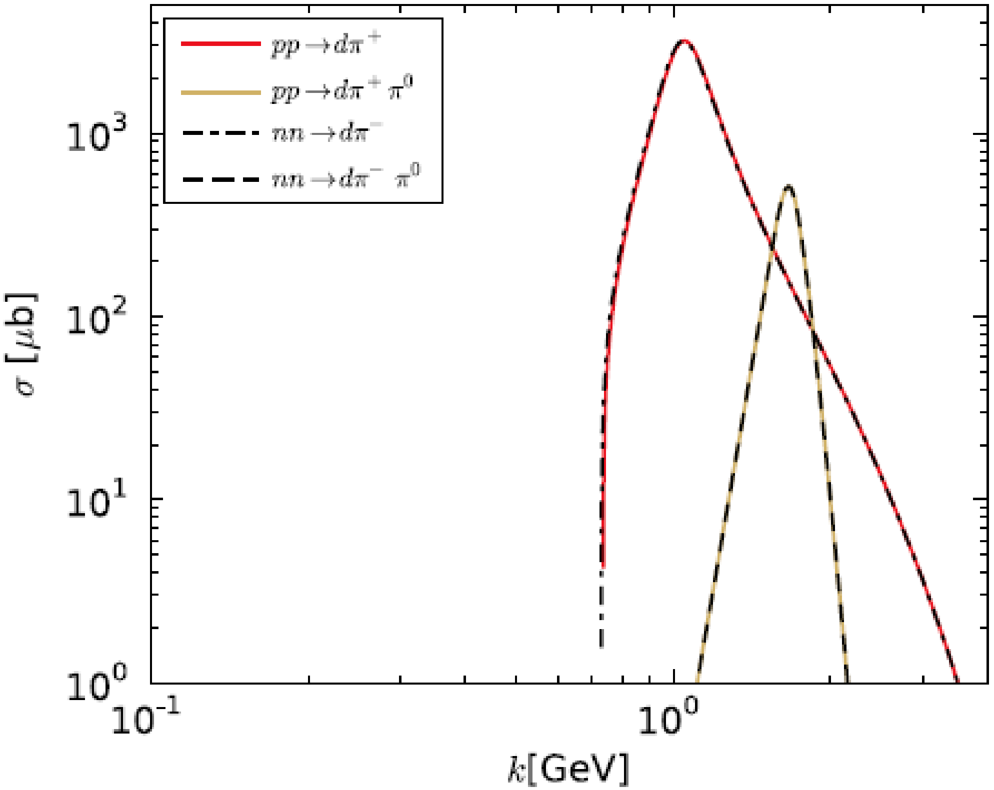


- The direction is takes from an isotropic distribution in the c.m. frame

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

Total fit parametrization



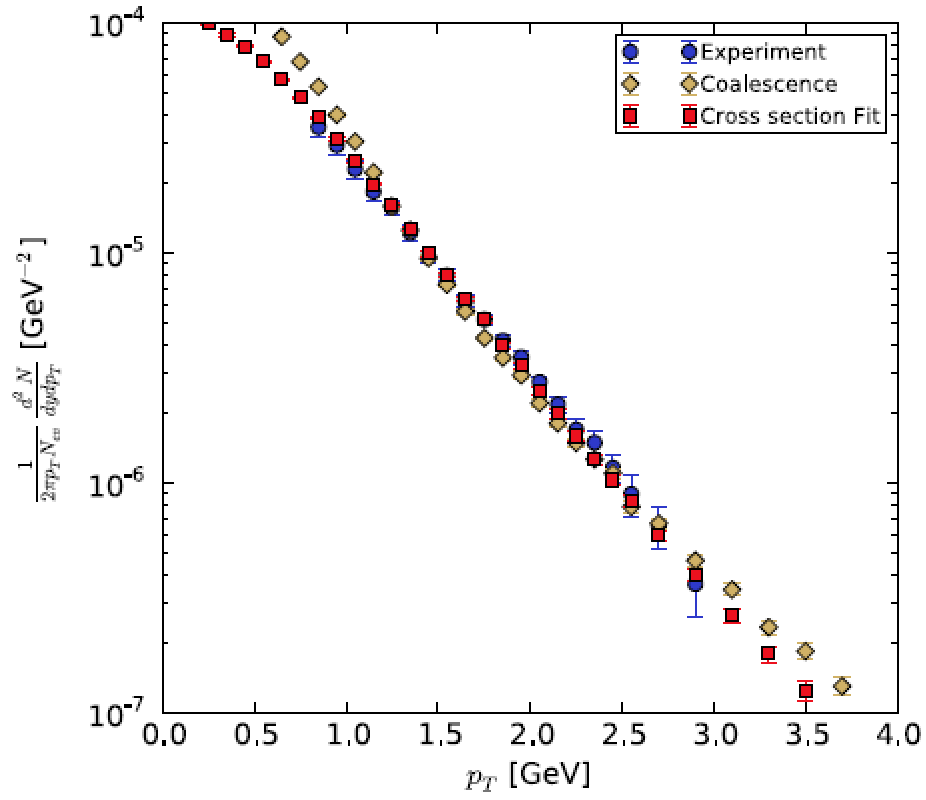


The majority of deuterons are produced at *k* values corresponding to the Δ resonance

L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

Reaction vs Coalescence – ALICE comparison

- Both the coalescence model and the reaction-based one have a free parameter to be tuned against experimental data
- Different results are available – as an example the comparison with pp collisions at 7 TeV collected by ALICE is reported using PYTHIA 8.1 simulations and applying the coalescence and the reaction-based approach
- The shape of the spectrum in the coalescence model does not match the experimental data.
- The cross section based model reproduces the shape of the spectrum better, but an overshoot a low p_T and a undershoot at high p_T are present



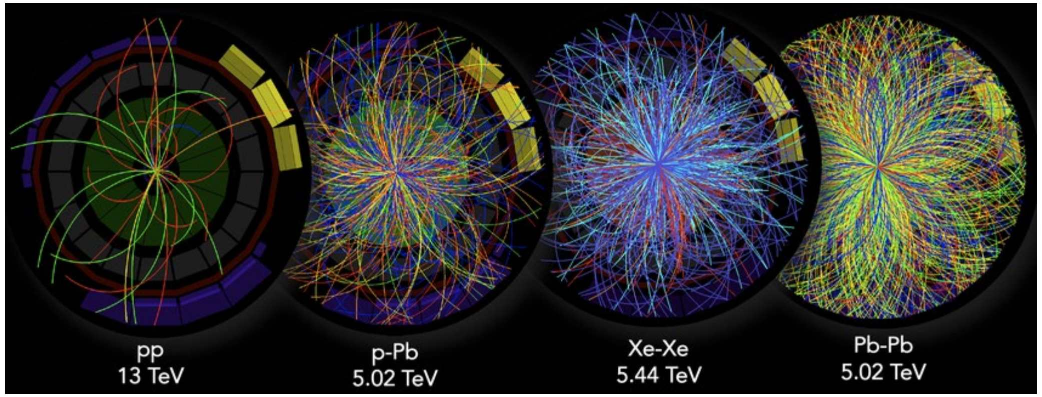
L. A. Dal and A. R. Raklev, *Phys. Rev. D 91(12), 123536 (2015)*

Comparison with data

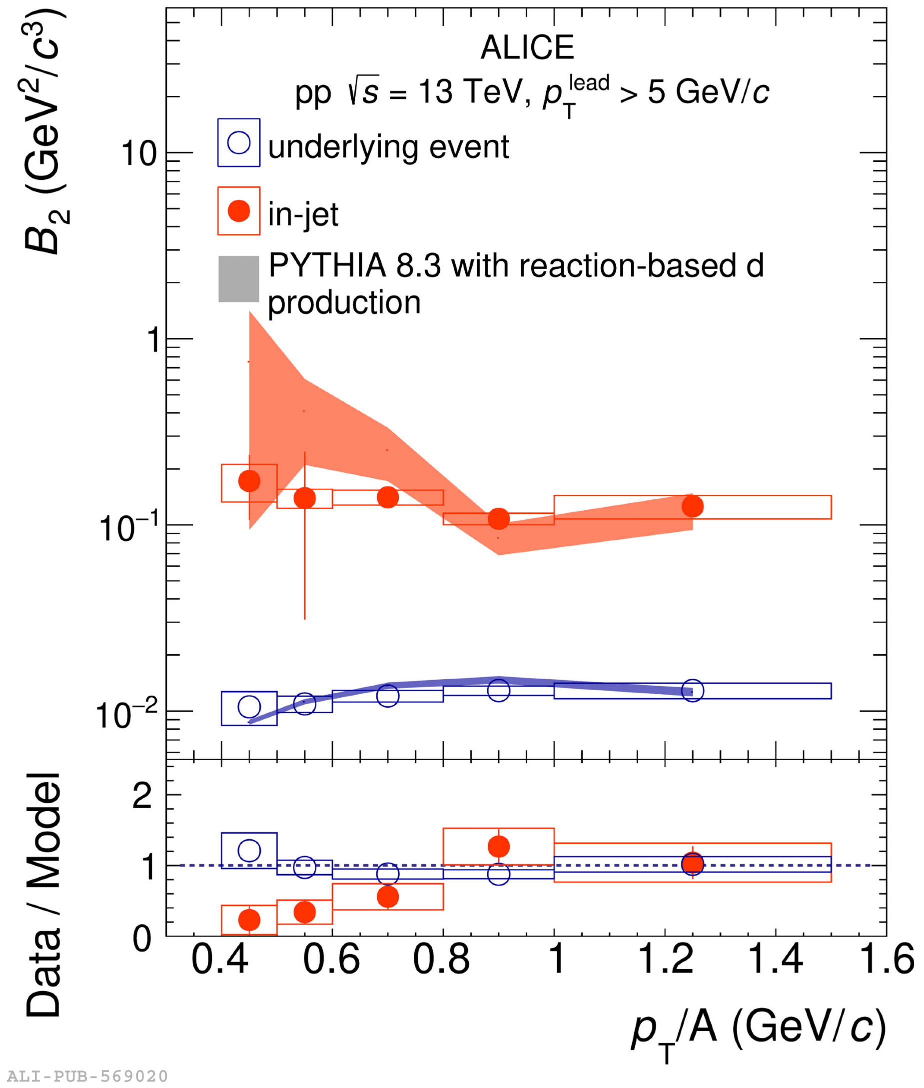
- Most of the current prediction of light (anti)nuclei production uses or thermal models (e.g. Thermal FIST, THERMUS etc) or advanced coalescence predictions implemented with afterburners using the Wigner formalism

- Still, a couple of recent results employ the «pure» PYTHIA 8.3 nuclei production without any afterburner

- Is the model capable of reproduce these experimental results?



Data vs Model – (Anti)deuteron in and out of jets

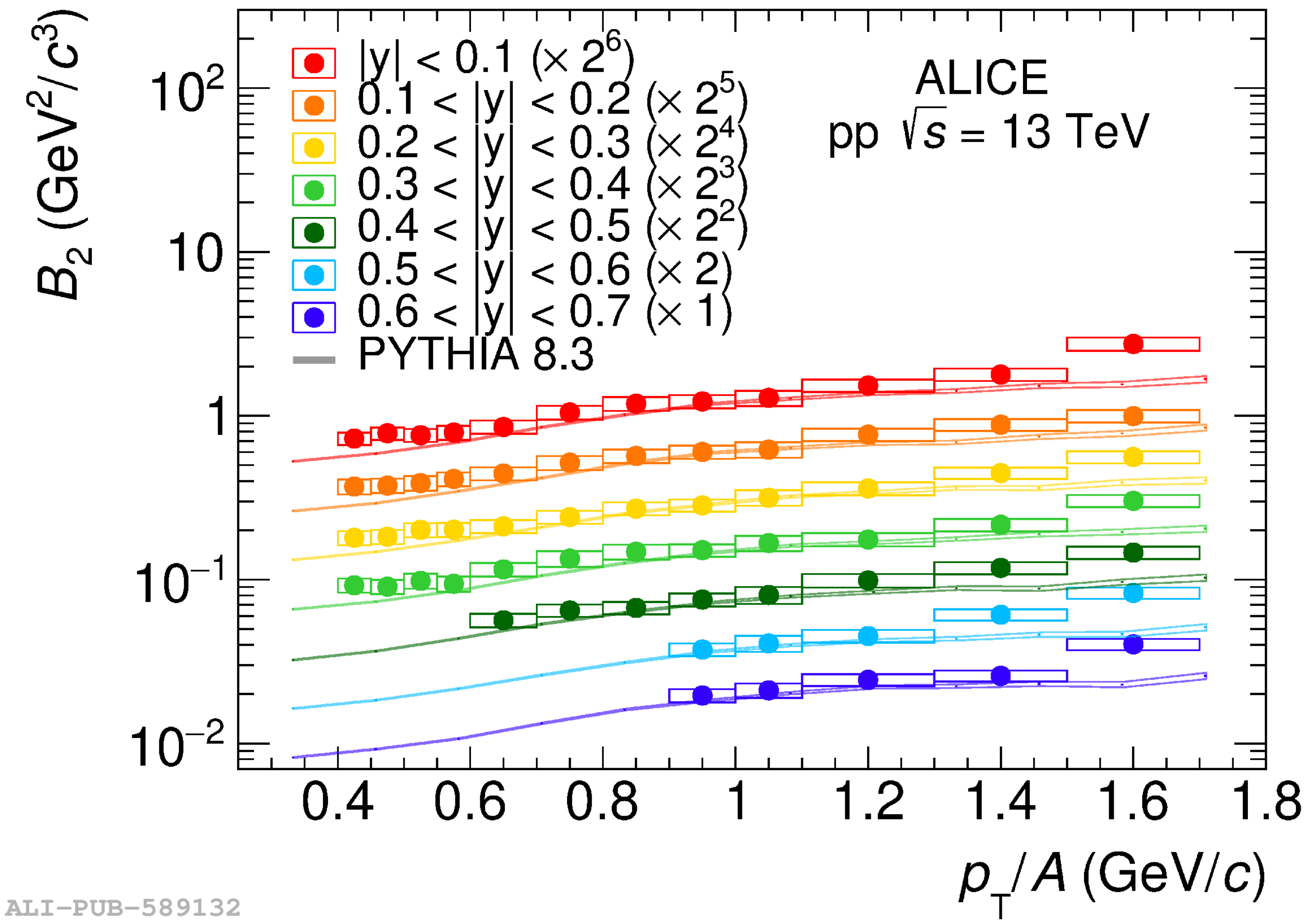


See Chiara's talk for more details!

- The model is able to reproduce the large gap between the jet and the underlying event
- Good agreement vs p_T/A in the underlying event
- The model overestimates the deuteron coalescence parameter at low p_T/A

ALICE Collaboration, *Phys. Rev. Lett.* 131 (2023) 042301

Data vs Model – Antideuteron rapidity dependence

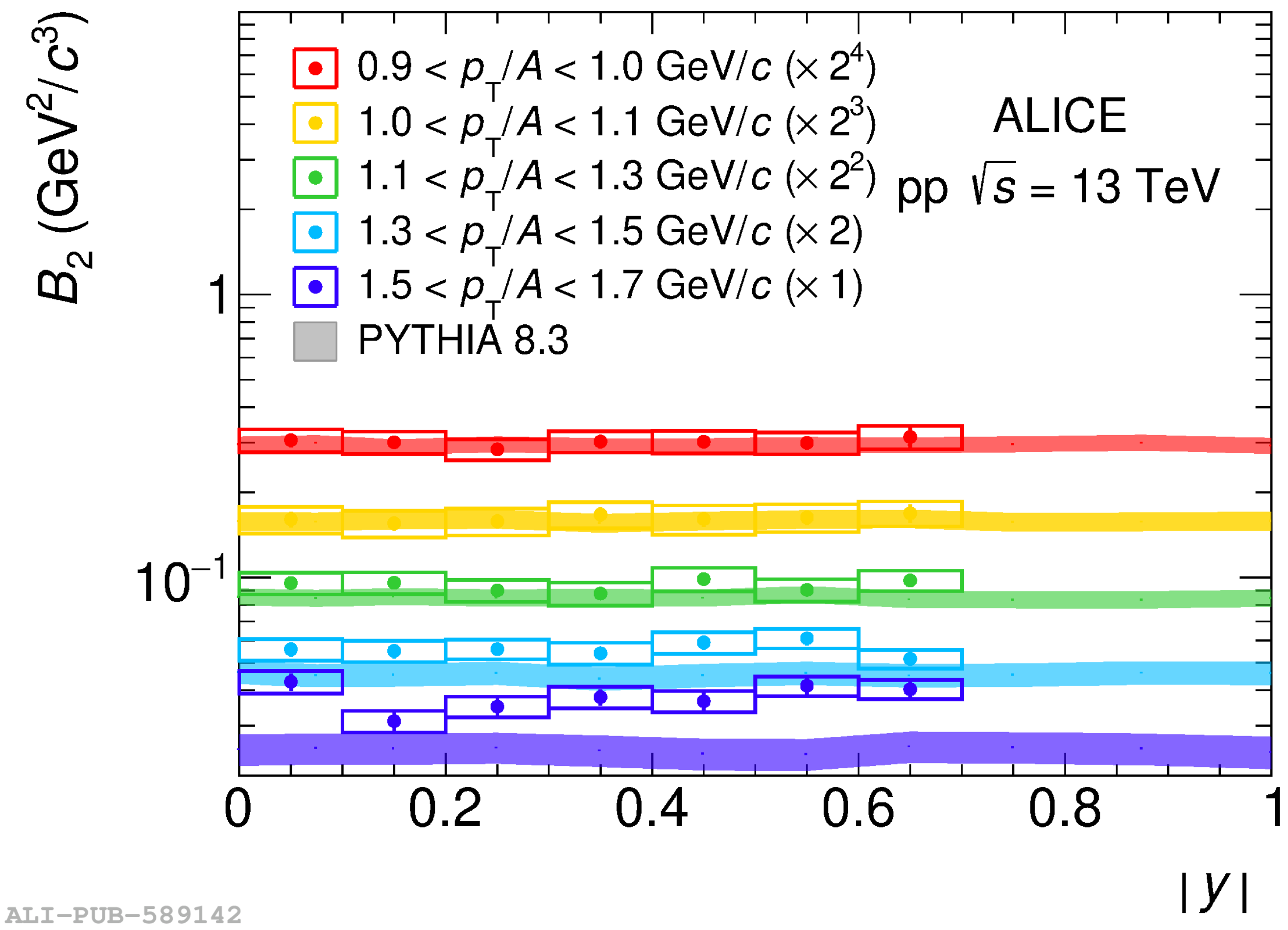


See Mario's talk for more details!

- The rising trend of the coalescence parameter as a function of p_T/A is reproduced by the model

ALICE Collaboration, *Phys. Lett. B 860 (2025) 139191*

Data vs Model – Antideuteron rapidity dependence



ALICE Collaboration, *Phys. Lett. B 860 (2025) 139191*

See Mario's talk for more details!

- The rising trend of the coalescence parameter as a function of p_T/A is reproduced by the model
- For selected intervals of p_T/A the coalescence parameter is studied as a function of rapidity.
- The model reproduce the measured trend, mostly with an agreement within 2σ.
- Some deviations beyond the 2σ level are present at high p_T/A (> 1.5 GeV/c)

Model predictions – deuteron balance function

- Not only comparison with data, but prediction of new observables are investigated using PYTHIA 8.3

- Balance function are a sensitive probe for the hadronization:
  - They probe the quantum number balance
  - At LHC B ≈ 0, hence a deuteron (B = 2) must be balanced by B = -2 baryons
  - If the deuteron is produced by coalescence, its balance is equal to the one of proton and neutron
  - If the deuteron is produced directly in the collision the baryon number must be conserved globally

- Is then possible to study the balance function of the deuteron with proton, Λ and pions:

$$B_{d\overline{X}}(\Delta y, \Delta\varphi) = Y_{d\overline{X}}(\Delta y, \Delta\varphi) - Y_{dX}(\Delta y, \Delta\varphi)$$

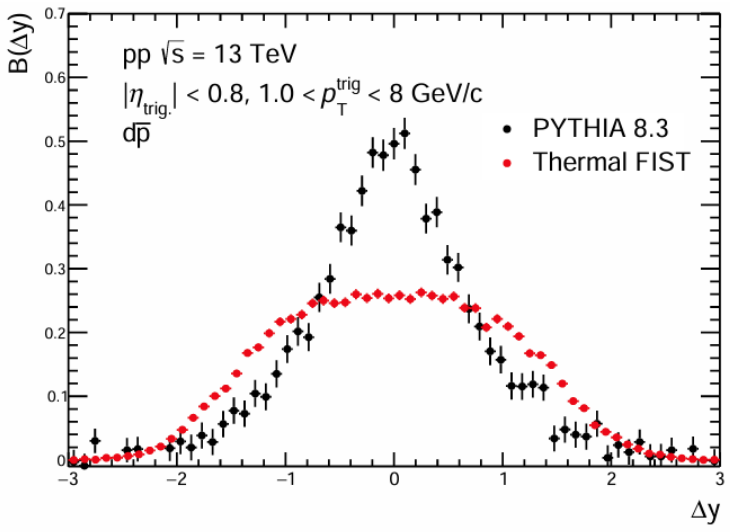
$$Y(\Delta y, \Delta\varphi) = \frac{1}{N_{trig}} \frac{d^2 N_{pairs}}{d\Delta y \, d\Delta\varphi}$$

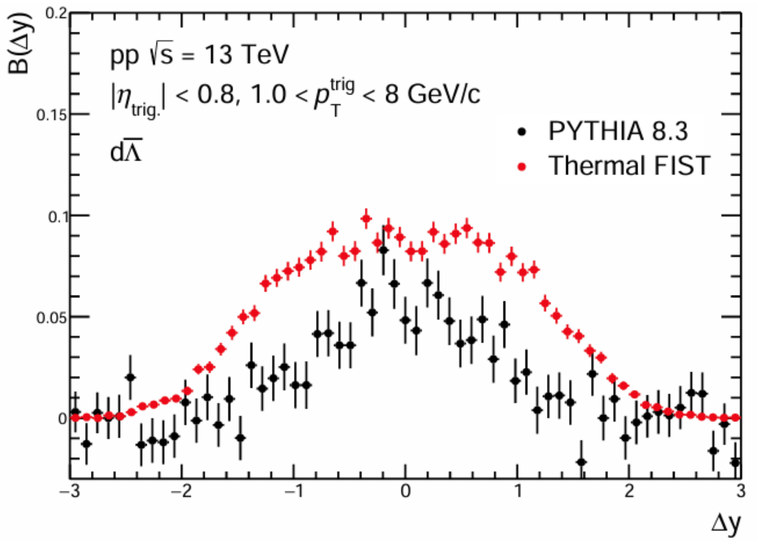
$$\Delta y = y_{assoc} - y_{trig} \qquad \Delta\varphi = \varphi_{assoc} - \varphi_{trig}$$

S. Tripathy, P. Christiansen, *arXiv:2509.03195 [hep-ph]*

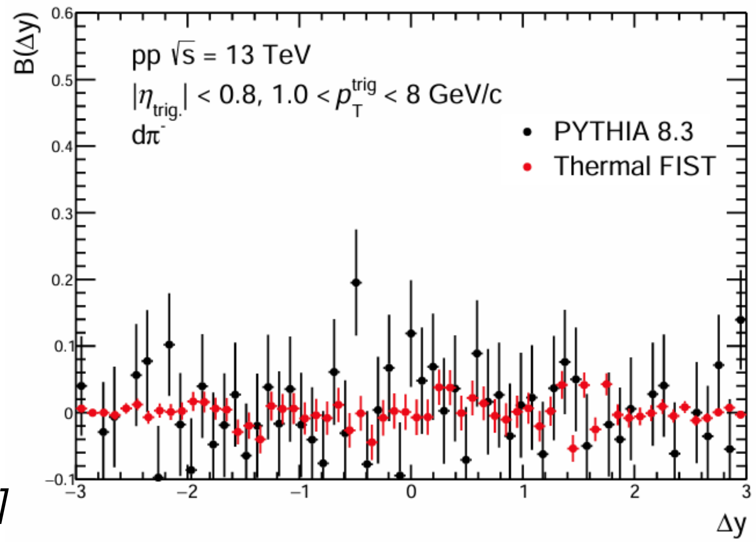
Model predictions – deuteron balance function

- Is it possible to estimate the balance function for all the cases
- Different shape for the one predicted by PYTHIA and THERMAL FIST due to the instrinsic differences of the models





- More observations can be made comparing these balance functions with the one triggered by protons
- But still, no experimental data available for these observables



S. Tripathy, P. Christiansen, *arXiv:2509.03195 [hep-ph]*

Not a summary, but a starting point for discussion...

- The reaction-based nuclear production implemented in PYTHIA is a valid alternative of the coalescence afterburners?

- What improvement can be done?
  - More precise measurement of the cross sections?
  - New data to fit for the missing channel that are approximated?
  - Consider all the possible corrections (Coulomb, isospin breaking, etc..)?

- Only (anti)deuteron production is implemented:
  - Heavier nuclei to consider?
  - ^{3}He to be considered as a two body (d + p) or a three body (p + p + n) case?
  - Which are the dominant processes?

- Relatively few comparison with the experimental data: does this model work properly for different physical cases? What observable can we use to «stress» the model?


Thank you for your attention!