Canonical ensemble simulations with multi-body interactions

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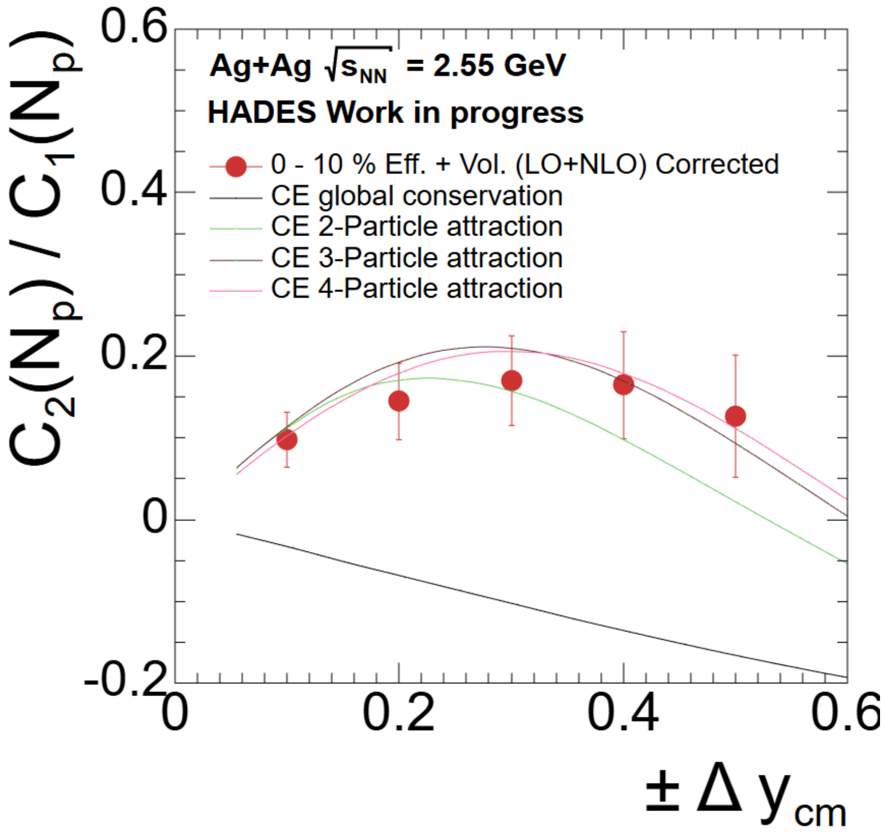
Implementation details and experimental input

Marvin Nabroth and Anar Rustamov

Outline

- Motivation - CE baselines
- Implementing attractive interactions using metropolis algo.
- Incorporating multi-body interactions
- Factorial cumulants as a function of rapidity window and particle-cluster size in the CE model
- Fit to experimental data



Motivation

Hadron Resonance Gas model

$$\ln \mathcal{Z}(T,V,\mu_B) = \sum_i \pm \frac{g_i V}{(2\pi)^3} \int d^3p \, \ln\left(1 \pm e^{-(E_i-\mu_i)/T}\right)$$

$$\kappa_n(N_q) = \frac{\partial^n \ln \mathcal{Z}(T,V,\mu_B)}{\partial(\mu_q/T)^n}$$

Boltzmann limit

$$\kappa_n(N_q) = \langle N_q \rangle,$$

$$\kappa_n(N_q - N_{\bar{q}}) = \langle N_q \rangle + (-1)^n \langle N_{\bar{q}} \rangle$$

→ Poisson, Skellam fluctuations as for a classical ideal gas

- We want to compare our data with thermal baseline

  Minimal baseline: **HRG Gas model**
  - ➢ Ideal gas of relativistic **non-interacting** multiple **particle species and resonant states**
- What statistical ensemble to chose?
  - Naive approach: Grand Canonical Ensemble (T, V, μ_B) → N fluctuates, conserved in average via μ_B
  - …But **baryon-number is strictly conserved in the full phase space** → induces correlations the wider the rapidity acceptance window → modifies cumulants

The model should be done in Canonical ensemble for the full phase space, and the fluctuations should be studied in the subset of the phase space.

CE baseline for ideal gas

P. Braun-Munzinger, B. Friman, K. Redlich, A.Rustamov, J. Stachel, NPA 1008 (2021) 122141

- Calculate in **the full phase space** with **Canonical Ensemble** where the particle number is fixed (T,V,N)
- Evaluate fluctuations in sub-set of phase space

$$\alpha(\Delta y) = \frac{\kappa_1(\Delta y)}{< N_{part} >}$$

$\kappa_1(\Delta y)$ $\quad$ *from expiermental data*

$< N_{part} >$ $\quad$ *from MC Glauber*

$$Z_B = \sum_{N_B=0}^{\infty} \sum_{N_{\bar{B}}=0}^{\infty} \frac{(\lambda_B z_B)^{N_B}}{N_B!} \frac{(\lambda_{\bar{B}} z_{\bar{B}})^{N_{\bar{B}}}}{N_{\bar{B}}!} \delta(N_B - N_{\bar{B}} - B)$$

For lower energy, if $N_{\bar{B}} = 0$

Proton are a subset of all baryons
→ Binomial selection

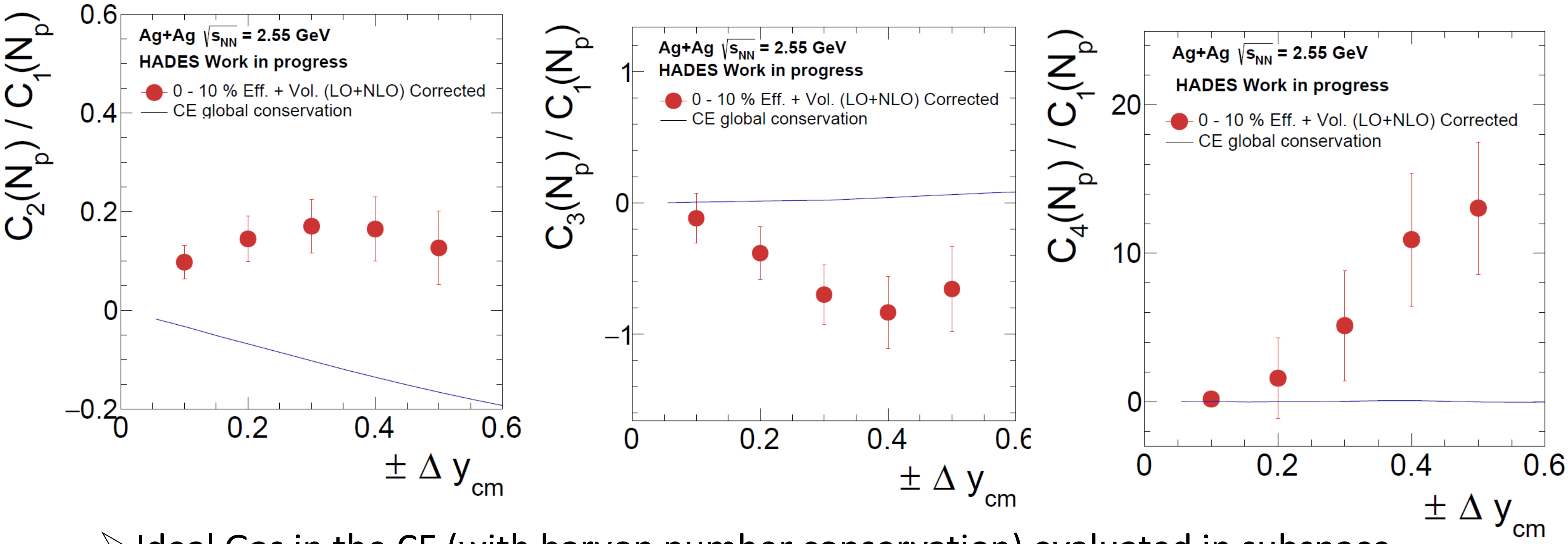
$$P(N_{prot,sub} | N_{part}) = \binom{N_{part}}{N_{prot,sub}} \alpha^{N_{prot,sub}} \alpha^{N_{part} - N_{prot,sub}}$$

$$\frac{\boldsymbol{\kappa_2}}{\boldsymbol{\kappa_1}} = \mathbf{1 - \boldsymbol{\alpha}} \qquad \frac{\boldsymbol{C_2}}{\boldsymbol{C_1}} = -\boldsymbol{\alpha}$$

$$\frac{\boldsymbol{\kappa_3}}{\boldsymbol{\kappa_2}} = \mathbf{1 - 2\boldsymbol{\alpha}} \qquad \frac{\boldsymbol{C_3}}{\boldsymbol{C_1}} = \mathbf{2}\boldsymbol{\alpha}^{\mathbf{2}}$$

$$\frac{\boldsymbol{\kappa_4}}{\boldsymbol{\kappa_2}} = \mathbf{1 - 6\boldsymbol{\alpha}(1 - \boldsymbol{\alpha})} \qquad \frac{\boldsymbol{C_4}}{\boldsymbol{C_1}} = -\mathbf{6}\boldsymbol{\alpha}^{\mathbf{3}}$$

CE baseline for ideal gas



- Ideal Gas in the CE (with baryon number conservation) evaluated in subspace does not describe data, different signs!

Implementing interaction to rapidity space

B. Friman, K. Redlich and A. Rustamov arXiv:2508.18879v1

Attractive Interaction

- Attractive interaction lead to correlations in the rapidity space
- → Use Metropolis algo. to minimize with respect to desired correlation coefficient
- Alternative approach (more physics motivated): attraction encoded in energy function E

$$\rho \equiv \frac{\mathrm{Cov}(y_1, y_2)}{\sigma_{y_1}\sigma_{y_2}}$$

$$P_n = e^{-\Delta_n/\mathbb{T}}$$

<=>

$$P(y_1, y_1) = \frac{e^{-E(y_1,y_2)}}{Z}$$

Attractive potential

$$E_a(y_1, y_2) = \alpha_a |y_1 - y_2|^{\beta_a}$$

α_a ≔ *Strength of interaction*

β ≔ *Stepness of potential*

Repulsive

- Repulsive can not be implemented by just a negative correlation coefficient! (The cumulants would be the same as for positive coefficient in the subspace)
- Use approach of energy function

Repulsive potential

$$E_r(y_1, y_2) = \alpha_r e^{-|y_1 - y_2|/\rho_r}$$

α_r ≔ *Strength of repulsion*

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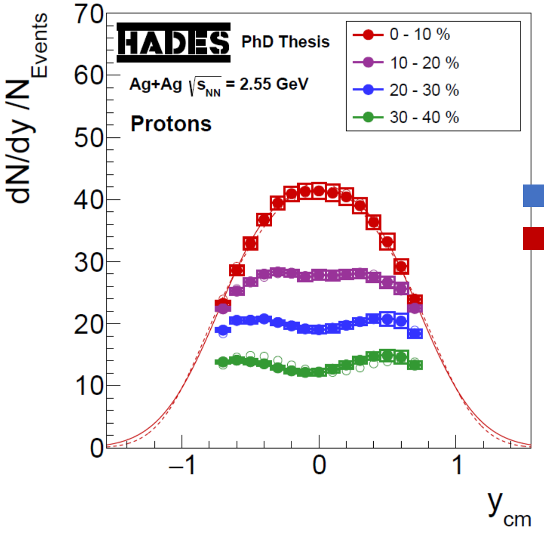
Metropolis algorithm

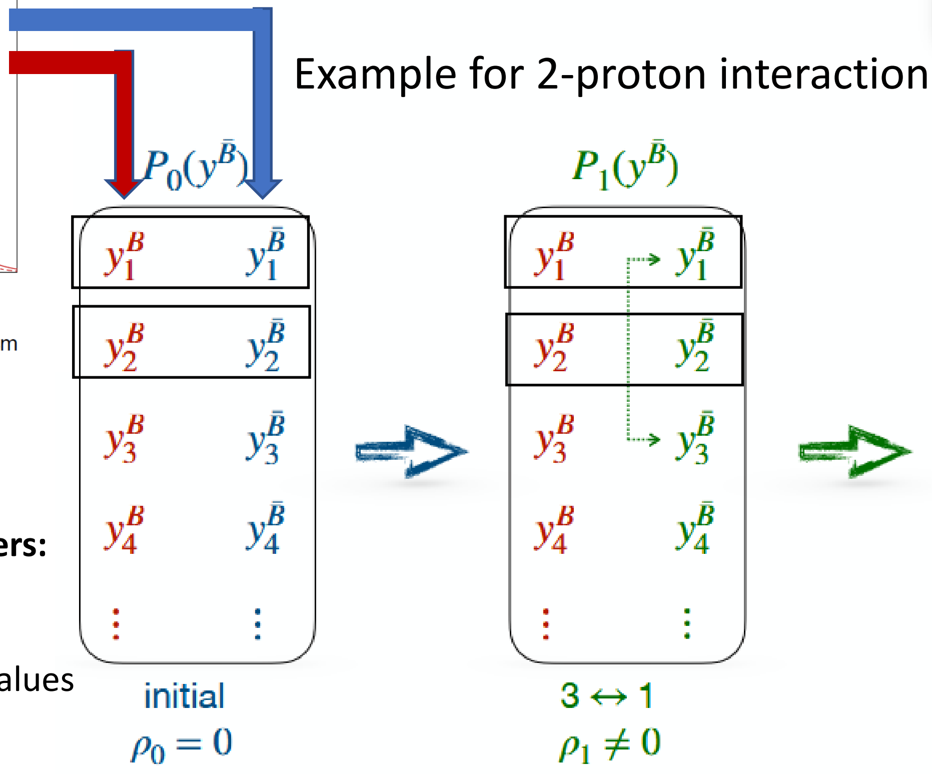
$$\rho = \frac{\langle y_1 y_2 \rangle - \langle y_1 \rangle \langle y_2 \rangle}{\sigma_{y_1} \sigma_{y_2}}$$

$$\Delta_n = |\rho_n - \rho| - |\rho_{n-1} - \rho|$$



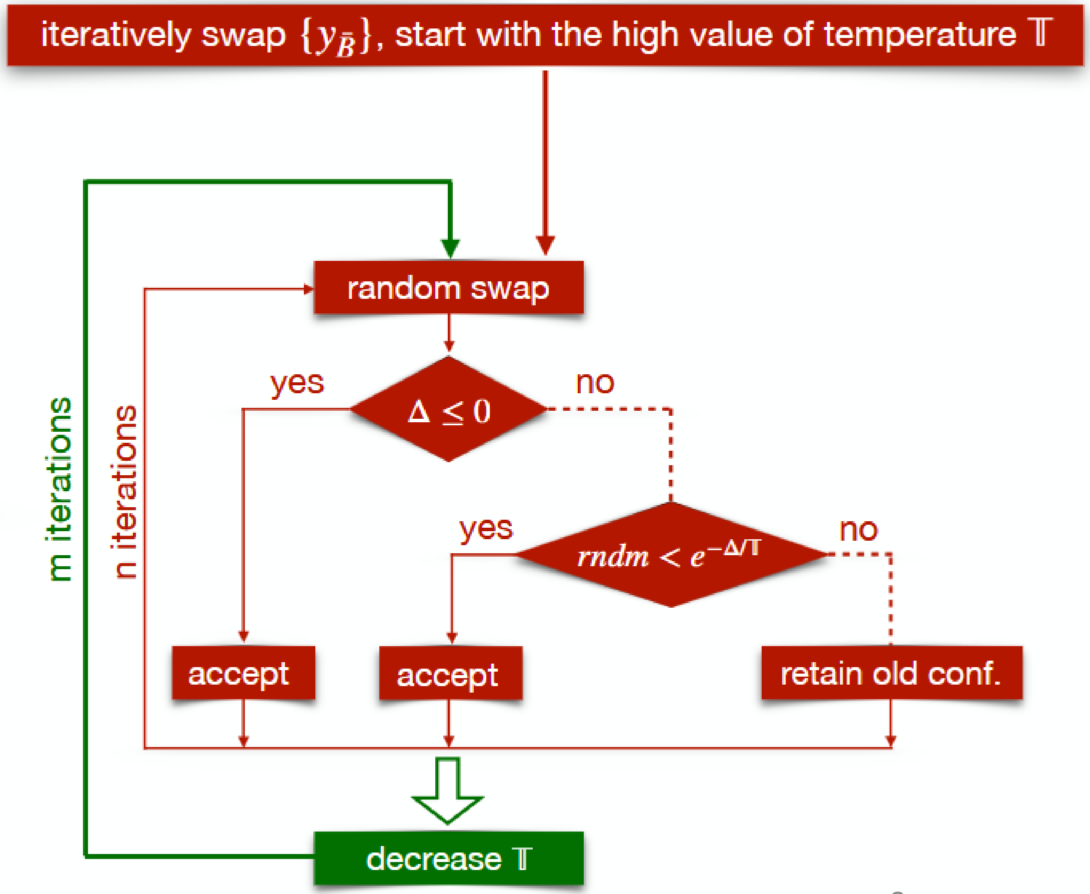
Sample independent random y values from proton dN/dy distribution (use Double-Gaussian Fit for extrapolation)

Example for 2-proton interaction



$\rho :=$ *Desired correlation coefficient*

$\rho_n :=$ *Correlation coefficient of nth iteration*



Metropolis algo. hyperparameters:

T_{init} = 0.01
Decay factor = 0.85
n_{iter}, max = 5 x No. rapidity values
$AccFrac_{\min}$ = 0.001

P.Braun-Munzinger, K.Redlich, A.Rustamov and J.Stachel, JHEP 08 (2024) 113, e-Print: 2312.15534 [nucl-th]

First Step – Generating multi-baryon y correlations → mimic attractive interaction between free baryons (protons as proxy)

Generate clusters of correlated y values
Input: Rapidity distribution
Output: Instances of m correlated random y numbers

1. Draw N times per "event" m random y values from rapidity distribution → m vectors of size N

2. Run metropolis over of m vectors each filled with y values, keep one vector fixed, apply random swapping to other m-1 vectors
→ Induce for each row (rapidity values for one entry over all vector) correlated rapidity values

Run on batch farm, store random numbers in tree

m-cluster correlations

Aim: Introduce for each possible pair out of m particles the same correlation

$$\rho \equiv \frac{\mathrm{Cov}(y_1, y_2)}{\sigma_{y_1}\sigma_{y_2}} = \frac{\langle y_1 y_2\rangle - \langle y_1\rangle\langle y_2\rangle}{\sigma_{y_1}\sigma_{y_2}}$$

Combine correlation coeff. of all pairs quadratically
→ Cost function of metropolis algo.

$$\Delta_n^{\mathrm{cluster}} = \sqrt{\sum_{1\le i<j\le m} (\rho_n^{i,j} - \rho)^2} - \sqrt{\sum_{1\le i<j\le m} (\rho_{n-1}^{i,j} - \rho)^2},$$

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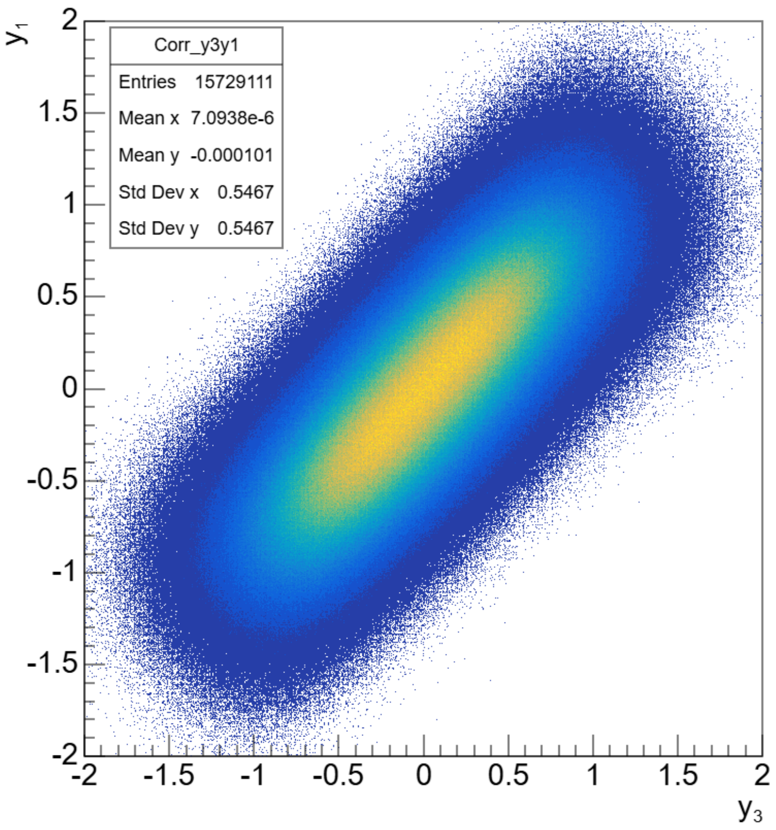
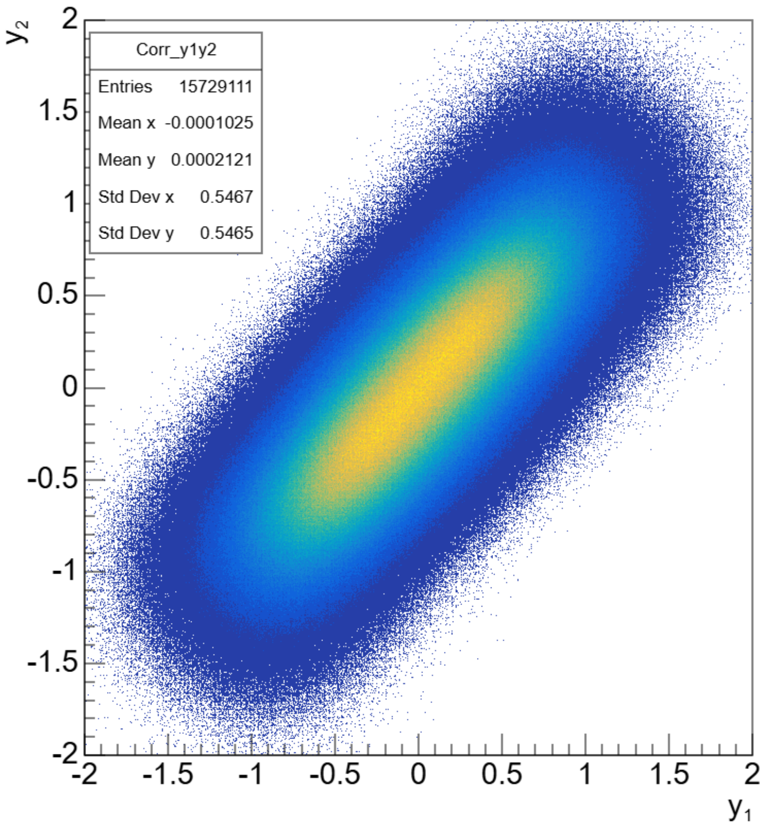
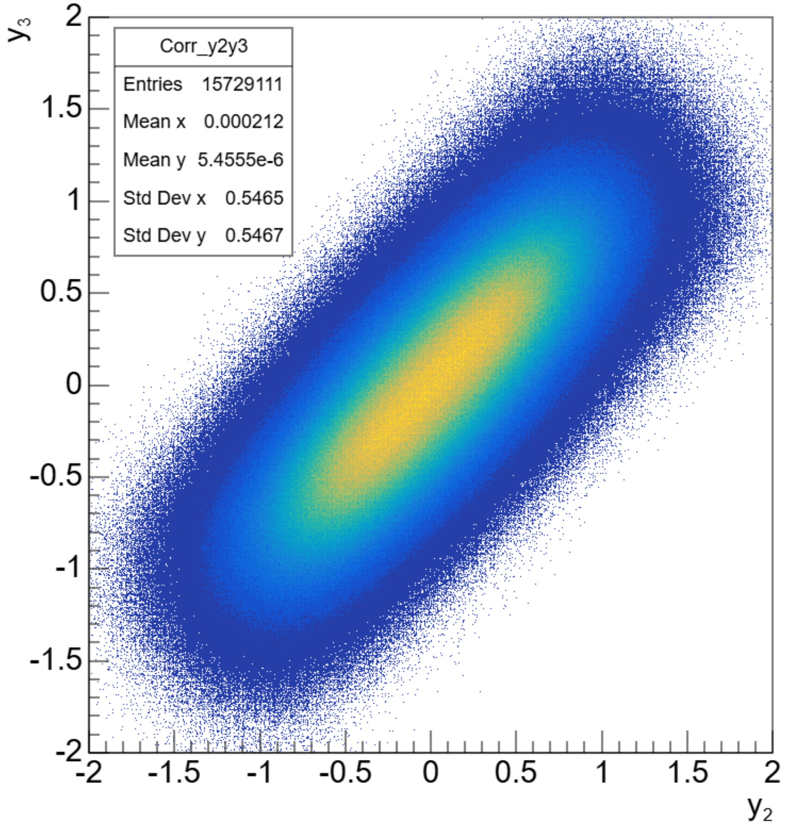
Metropolis output – Example for rho=0.8
3-particle interactions



y1 vs. y3



y2 vs. y1



y3 vs. y2

- Rapidity distribution over the full scope as before, but fluctuations change if the counting is performed subspace

Second step, CE simulation

Input for step (2):

- Set of correlates random y numbers from step (1)
- α = Proton to <Npart> ratio

Per event:

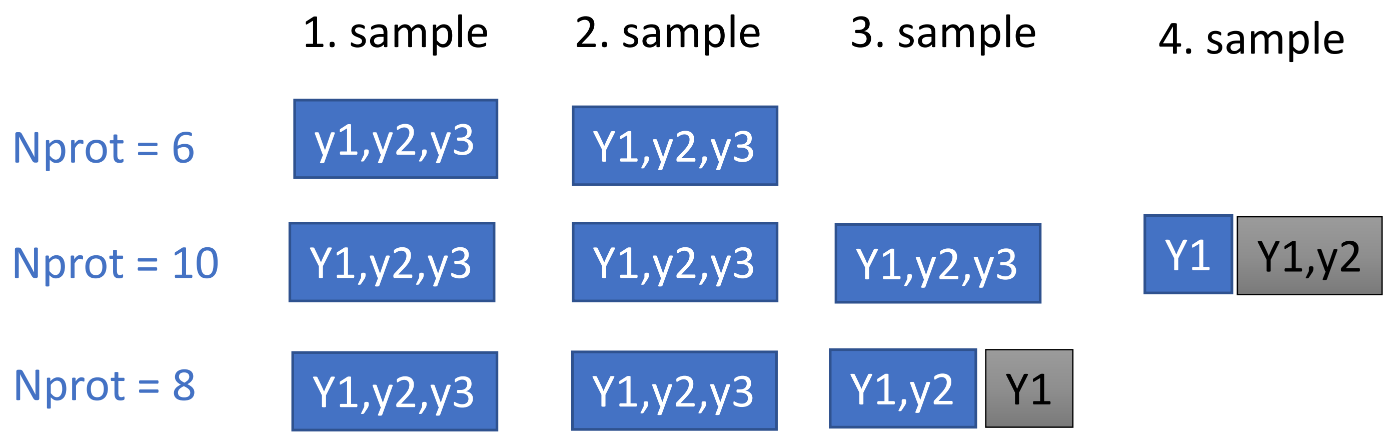
1. Nprot from Binomal(<Npart> , α) (CE of ideal Gas)
2. **Fill list with m-clusters of correlated y numbers until entries correspond to Nprot**
3. **Count rapidity numbers falling into specific rapidity window** $\rightarrow N_{proton,sub}(\Delta y)$

Over all events: calculate cumulants and factorial cumulants of $N_{proton,sub}(\Delta y)$

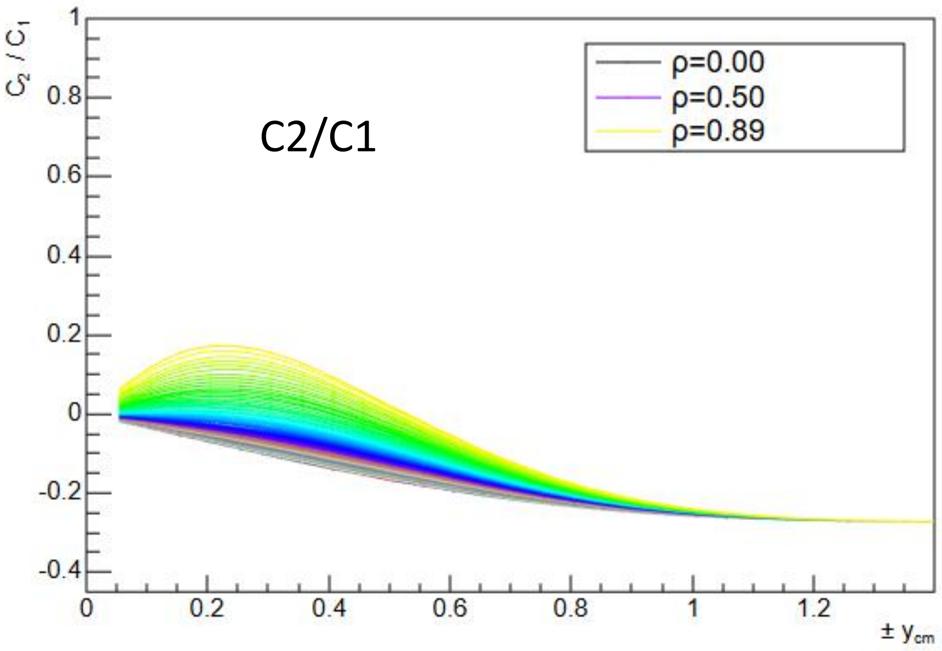
- ➢ Count m-clusters of y values
- ➢ If “remainder” is smaller than m add m-1 cluster

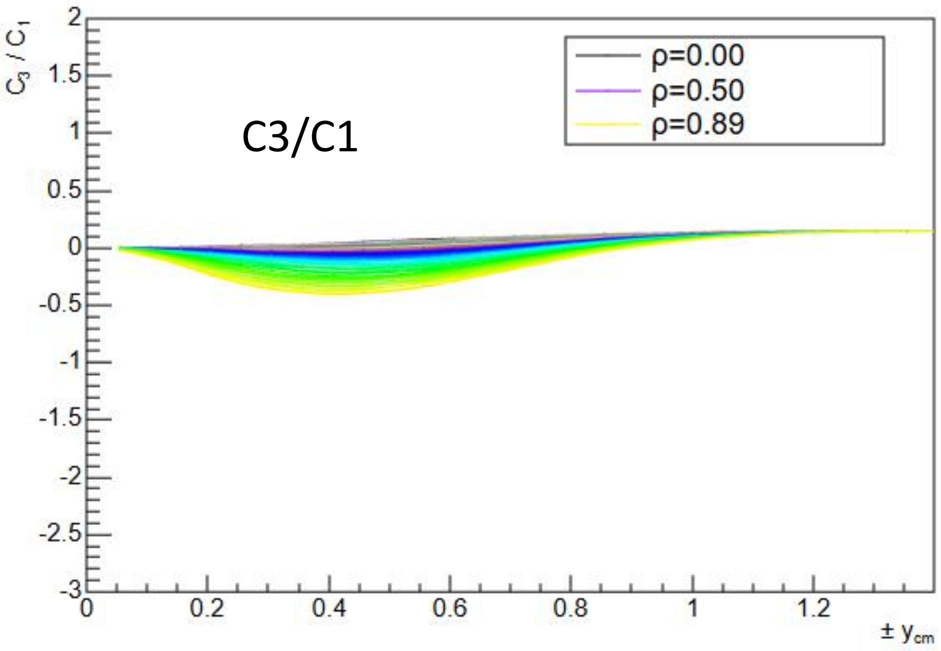
Cluster counting - Example for 3 body-interaction

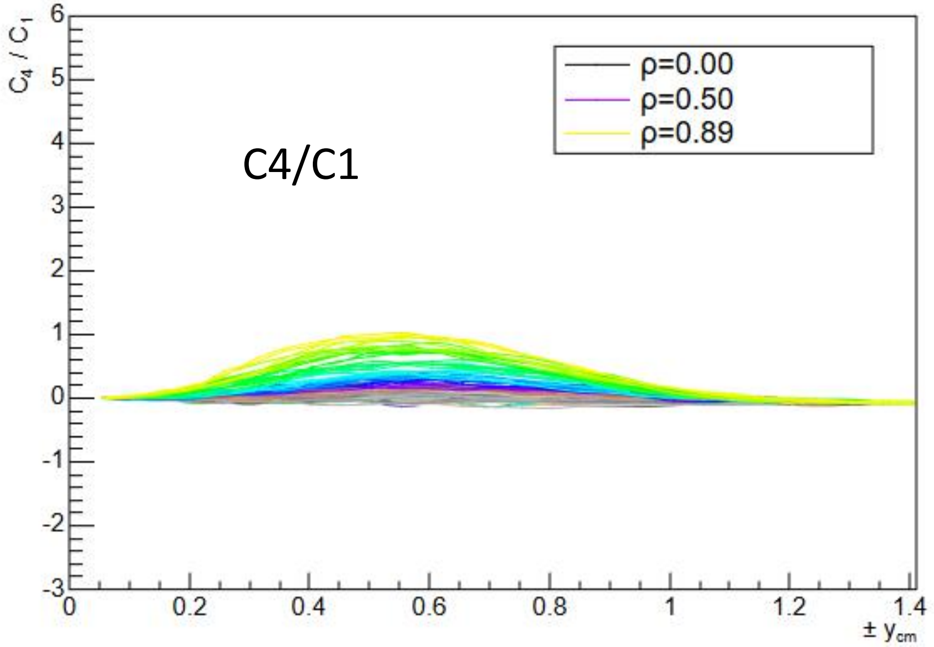
y1,y2,y3 ~ Retrieved from tree filled with instances of y1,y2,y3 correlated rapidity numbers, prepared in step (1)



$$\Delta y \coloneqq [\pm 0.1, \pm 0.2 \pm 0.3, \pm 0.4, \pm 0.5]$$



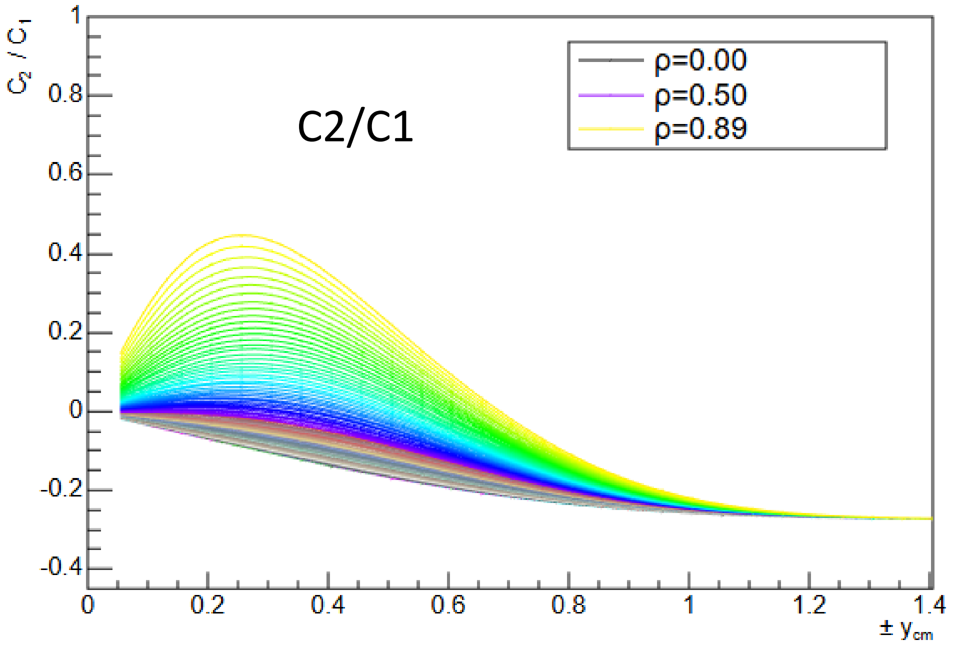


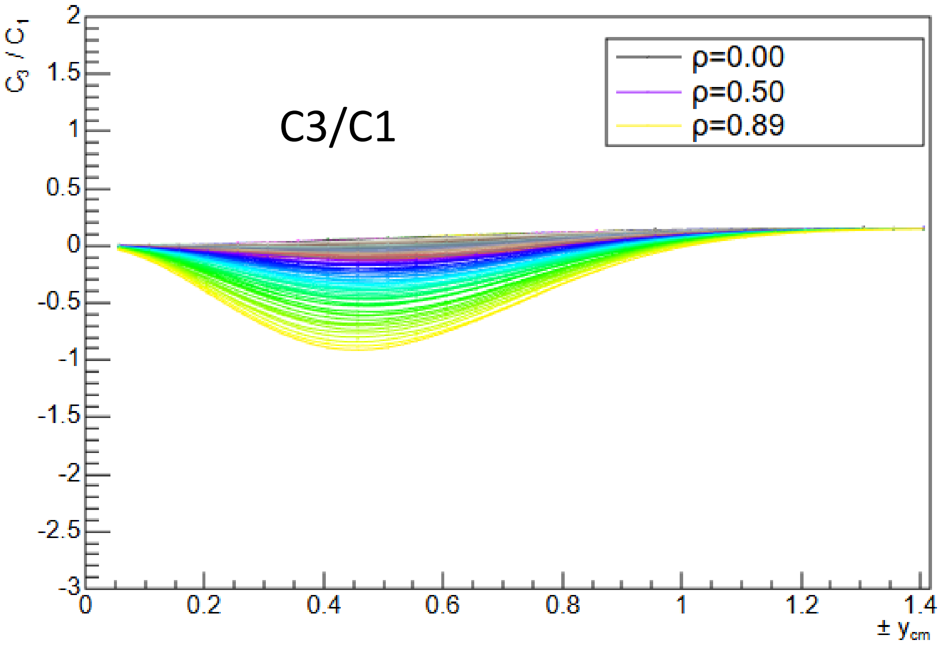


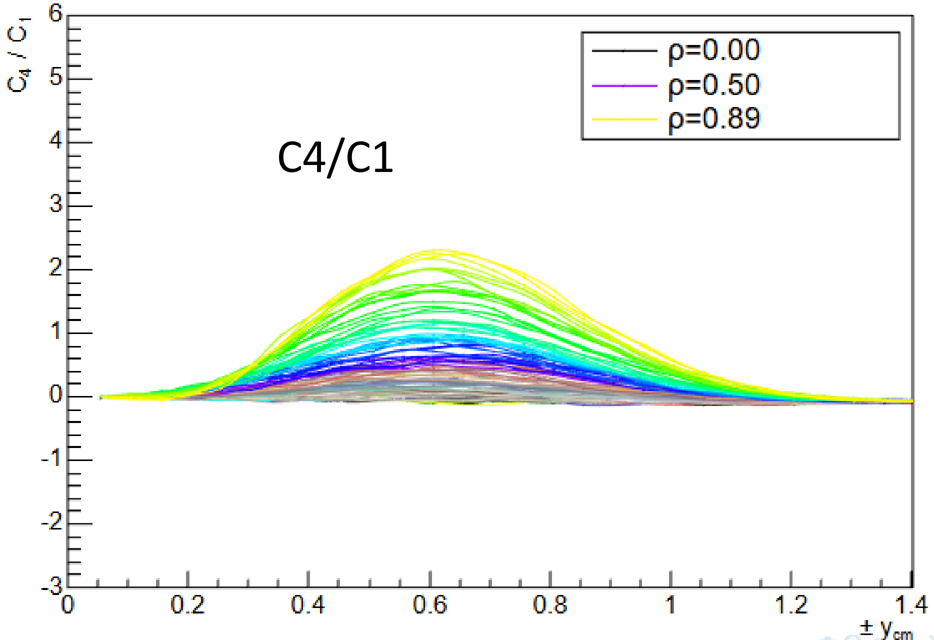
Attractive potential

2-Particle clusters

Generated for rho=0 to rho=0.9 with step-size 0.01







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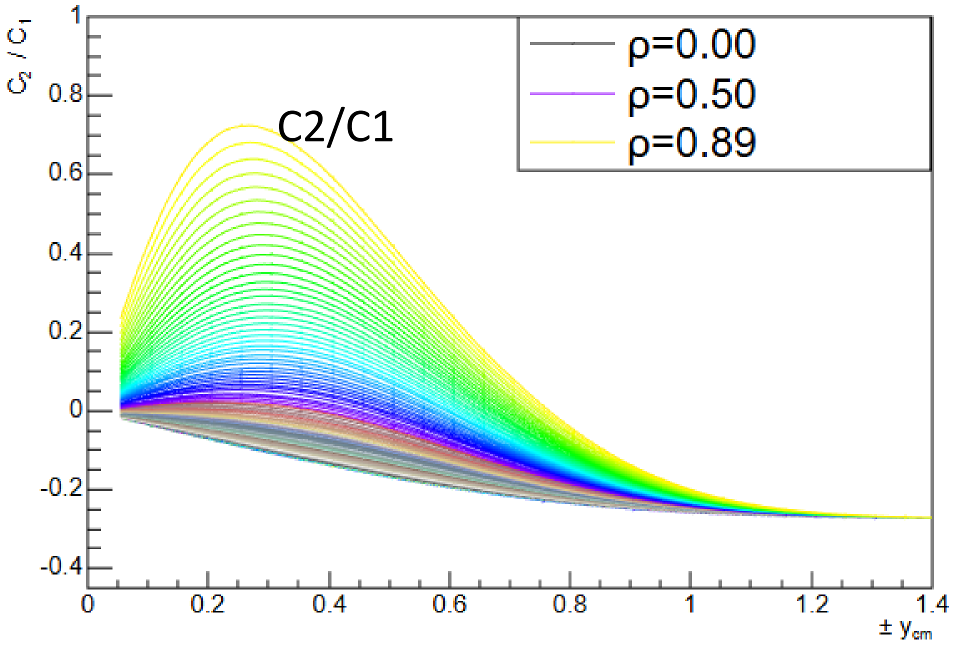
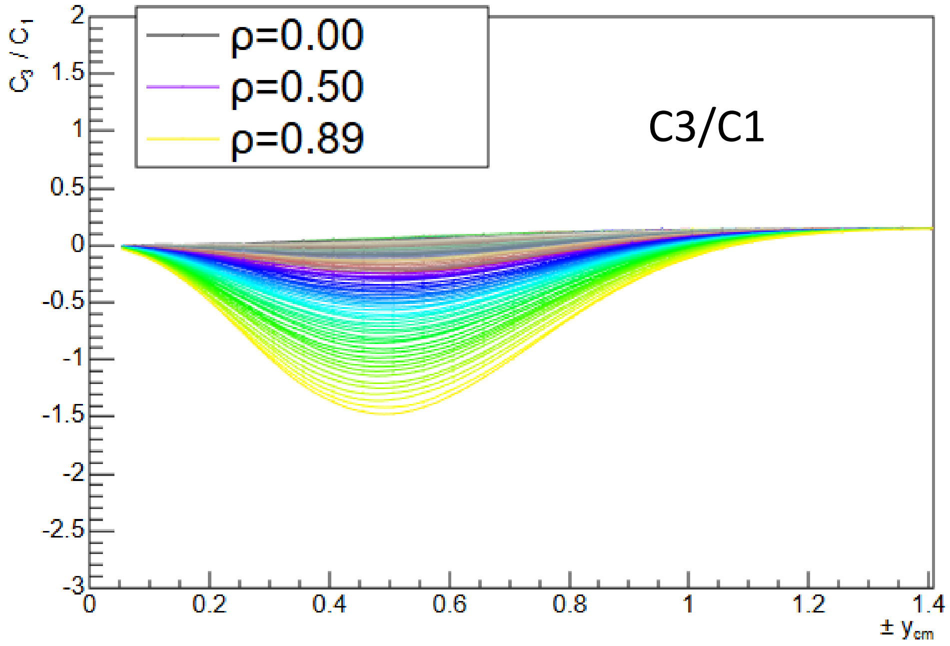
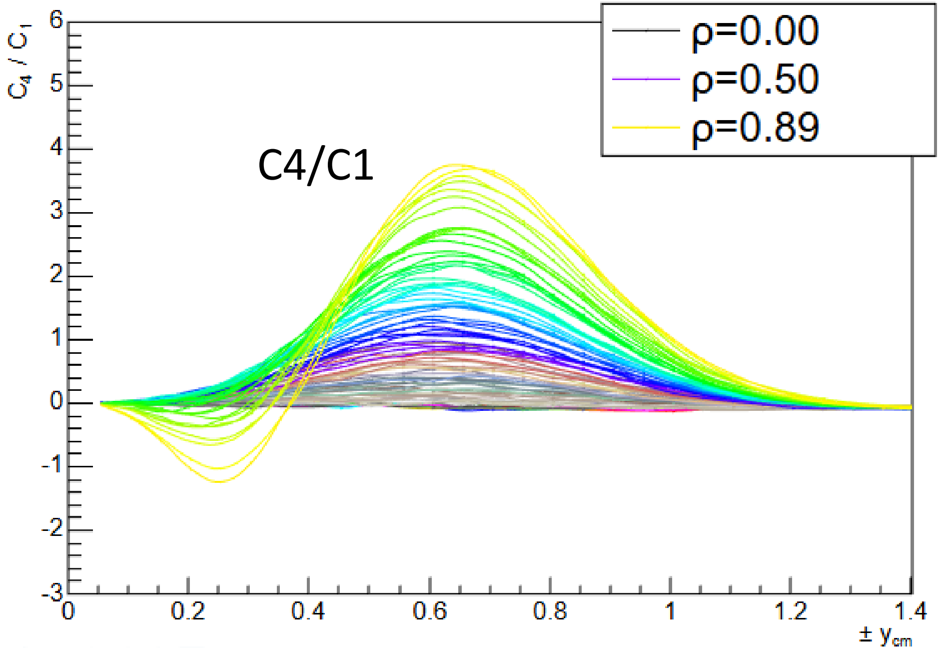






Attractive potential

4-Particle clusters

Generated for rho=0 to rho=0.9 with step-size 0.01

Experimental input

Experimental Input:

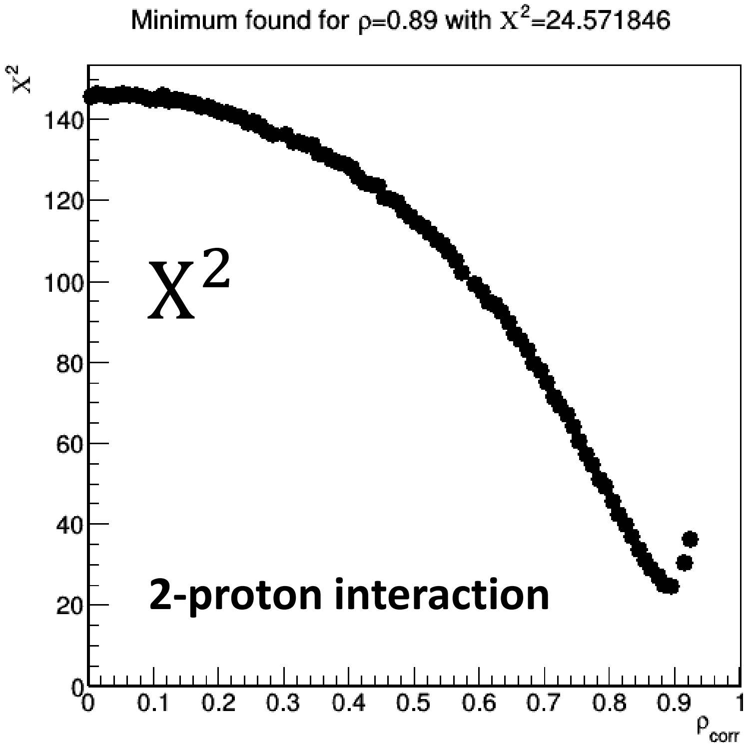
- Random y numbers drawn independently from proton **dN/dy distribution**
- **Proton to Npart ratio**

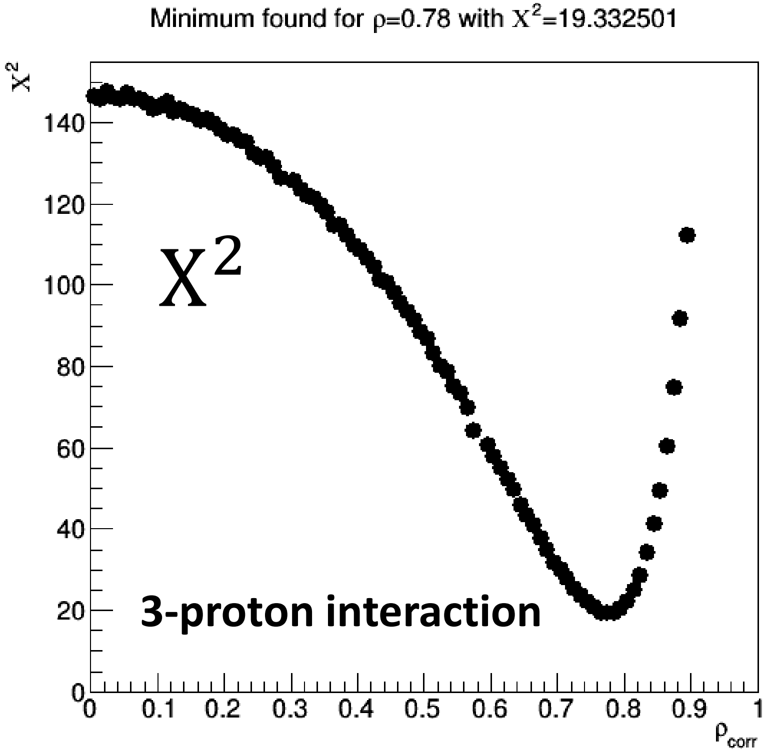
Free model parameter:

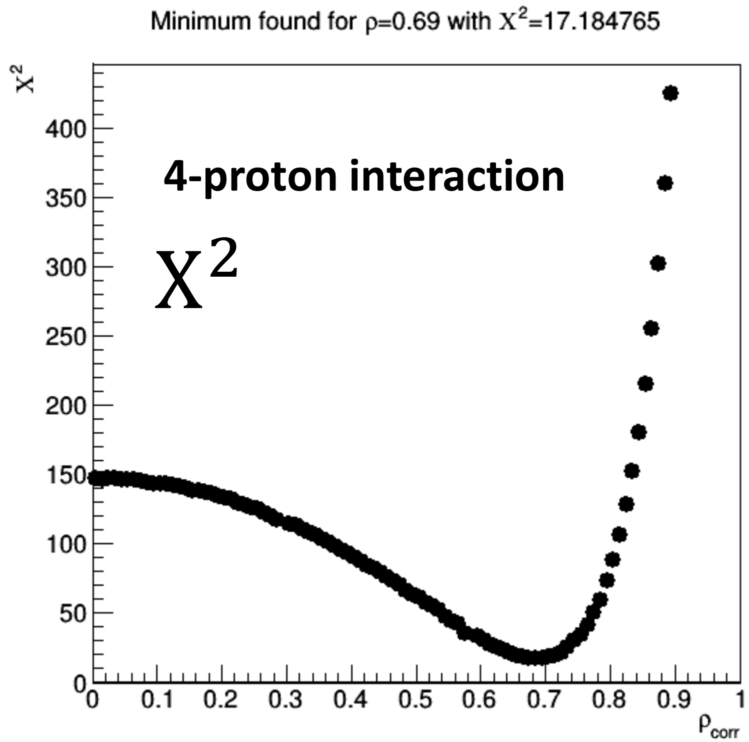
- Interaction strength := correlation coefficient rho between rapidity values
- Cluster-size m

- Rho and cluster size determined by chi2 scan to **experimental trend of factorial cumulant ratios** as **a function of rapidity acceptance** over all order.

Fit of CE model to **NLO** vol. corr. data







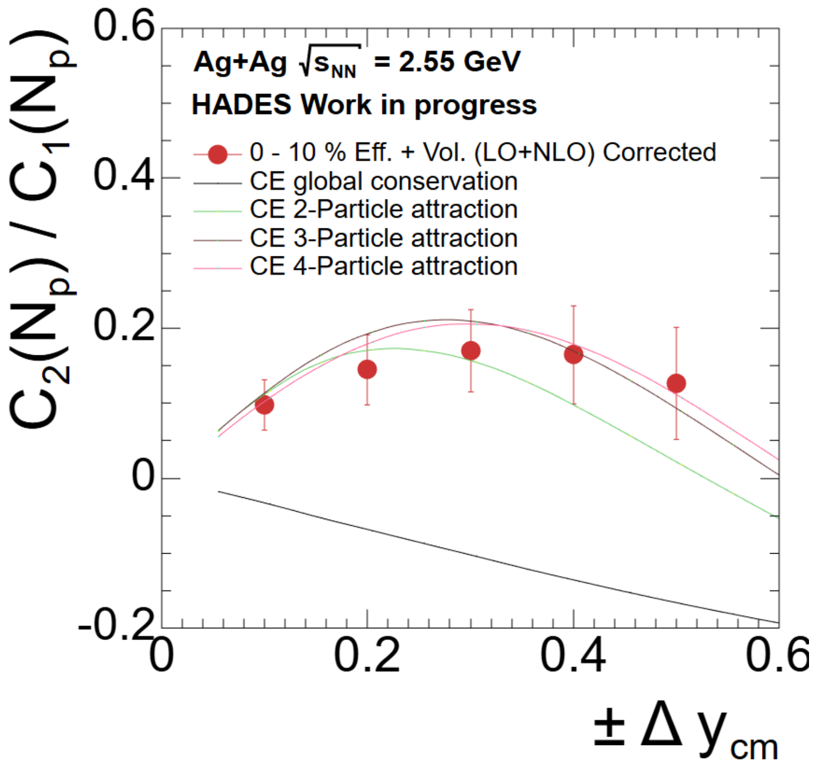
- Multi-order fit for over all rapidity intervals on factorial cumulant ratios

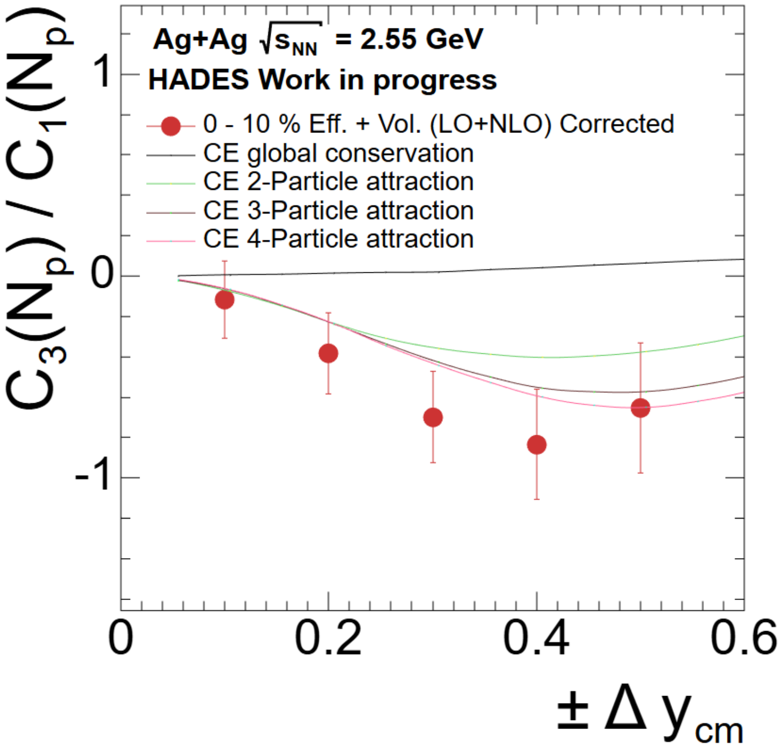
$$\chi^2=\sum_{m=1}^{m=4}\sum_{i=0}^{N_{y_{bins}}}\frac{\left(C_{m,i}(CE_{model})-C_{m,i}(Data)\right)^2}{\Delta C_{m,i}(Data)^2}$$

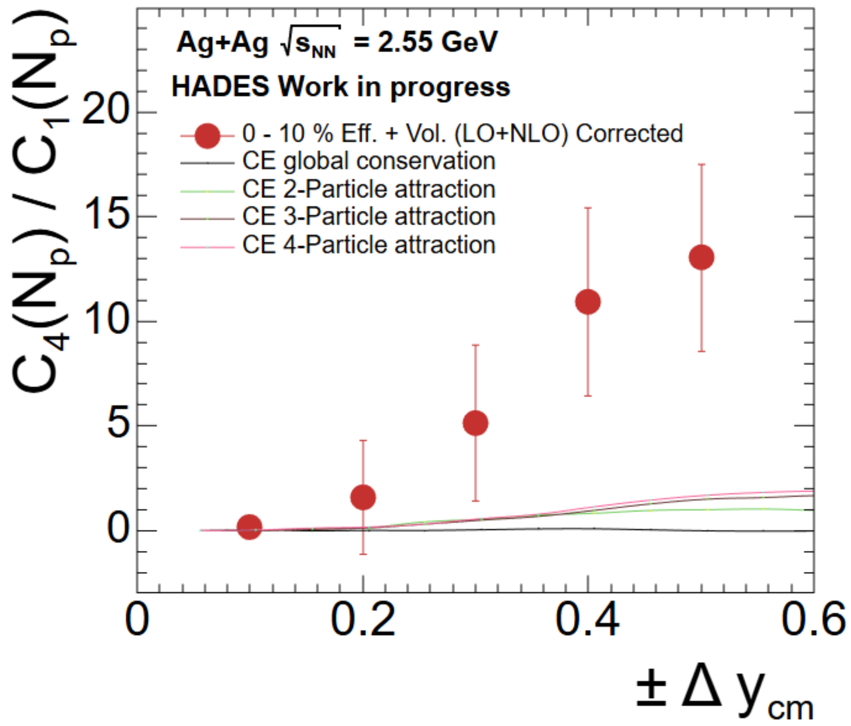
- Chi2 scan

Volume correction - LO+NLO

$\mathbf{Ag + Ag} \sqrt{s_{NN}} = \mathbf{2.55\ GeV}$







- ❑ CE baseline considering baryon number conservation only can not describe data, different sign

- ❑ 2-Particle correlations does not match the maximum of C2/C1 trend

- ❑ **Multi-particle interactions necessary to describe data within CE framework**

2-Particle corr. : $\rho_{corr} = 0.89$
3-Particle corr. : $\rho_{corr} = 0.78$
4-Particle corr. : $\rho_{corr} = 0.69$

B. Friman, K. Redlich and A. Rustamov arXiv:2508.18879v1

Summary

- Canonical ensemble in full phase space to take into account baryon number conservation
- Interaction are incorporated by correlating the rapidity values drawn from the proton dN/dy distribution, implemented using Metropolis algorithm
- CE simulation then draws full proton number from Binomial, counting of multi-cluster rapidity values
- Counting sa function of rapidity window
- Over all events: Cumulants, factorial cumulants

➢ Experimental input: Rapidity distribution, proton to Npart ratio

➢ Free parameter of model: Interaction strength, cluster size of multi-body interaction

In conclusion:

A CE based **thermal model** taking into account **interactions** manifested in rapidity space can explain the measured trend of factorial \ cumulant ratios as function of dy from 1th to 3th (4^{th}) order.

The same is seen for START data 3.3 GeV (attractive interaction) with shift to repulsive interaction for > 7 GeV

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