Nonequilibrium Phenomenology of Identified Particle Spectra in Heavy-Ion Collisions at LHC Energies

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Uniwersytet Wrocławski

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- Introduction
- Blast-Wave Model
- Naïve Model
- Naïve Model II
- Blast-Wave Based Particle Generator
- Bayesian Inference
- Results
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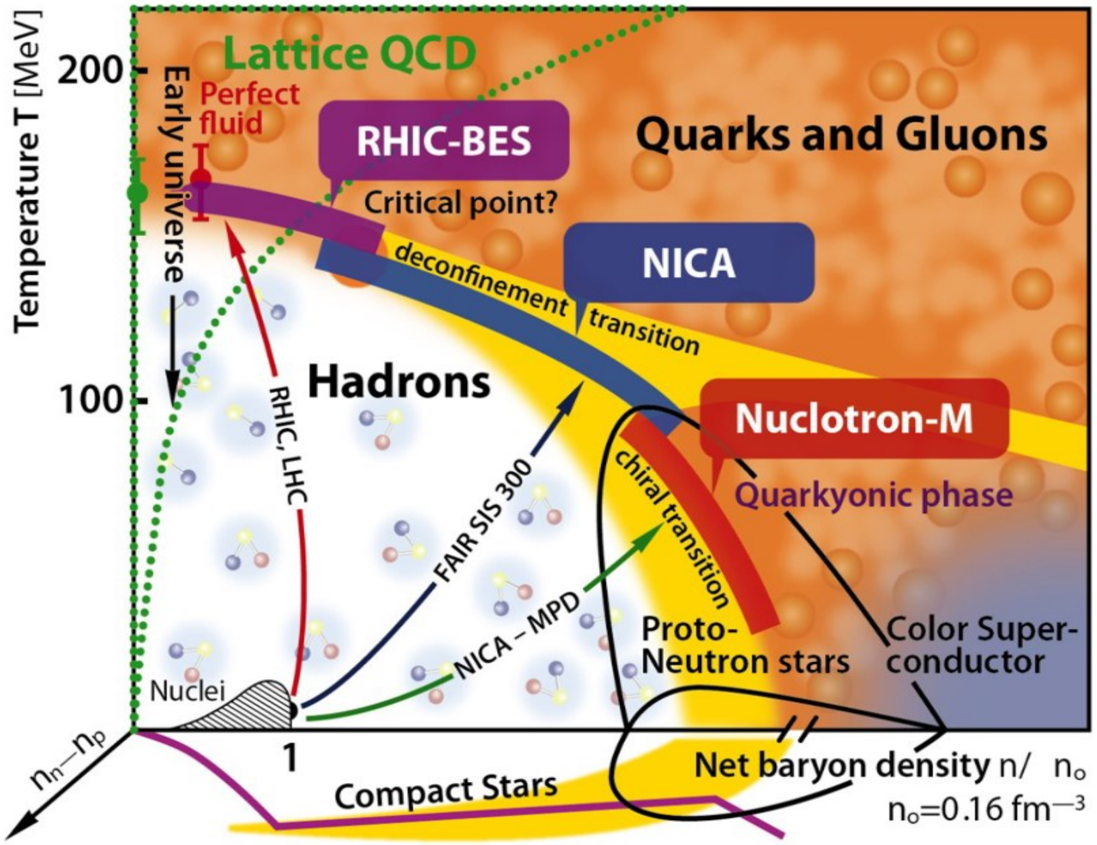
Introduction



The main goal of heavy-ion collisions experiments is to gain a better understanding of the theory of strong interactions – QCD, by detecting critical phenomena.

Exploring of the QCD phase diagram:

- Detect signals of deconfinement PT
- Detect signals of (partial) chiral symmetry restoration
- Locate (tri)critical endpoint(s) if such exists

[Credit: NICA White paper]

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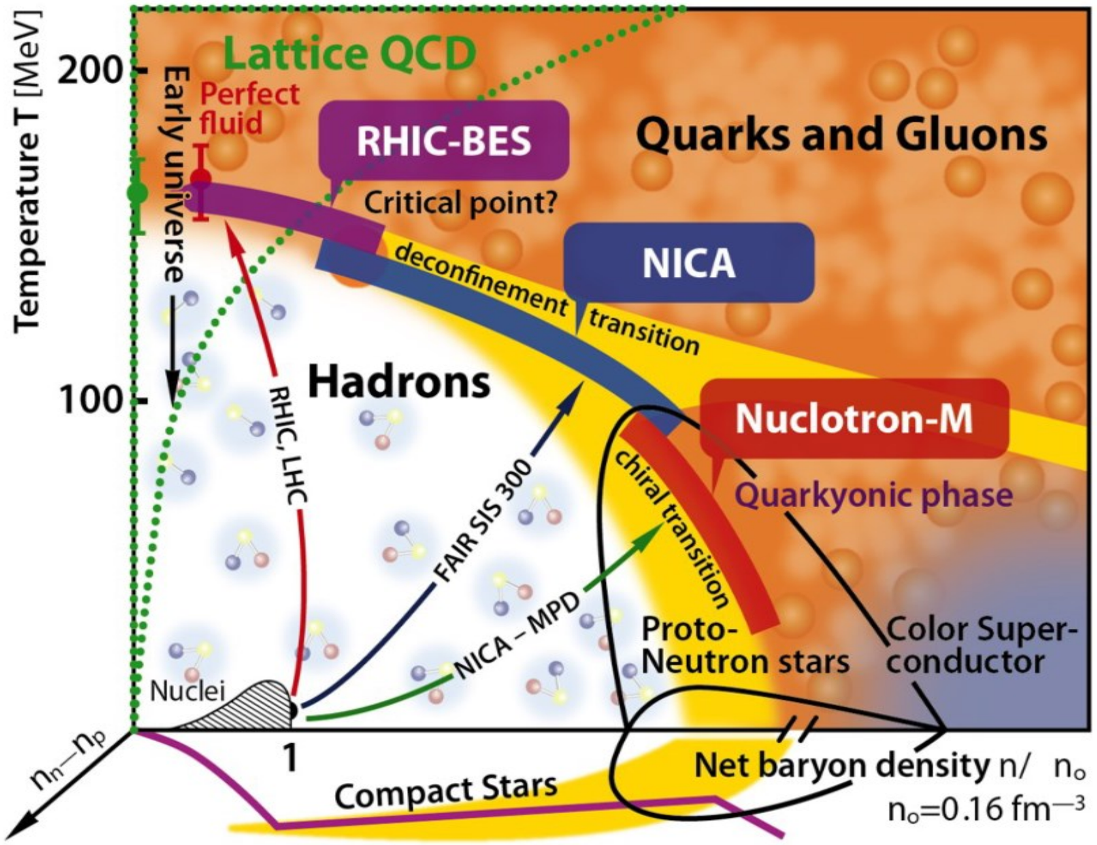

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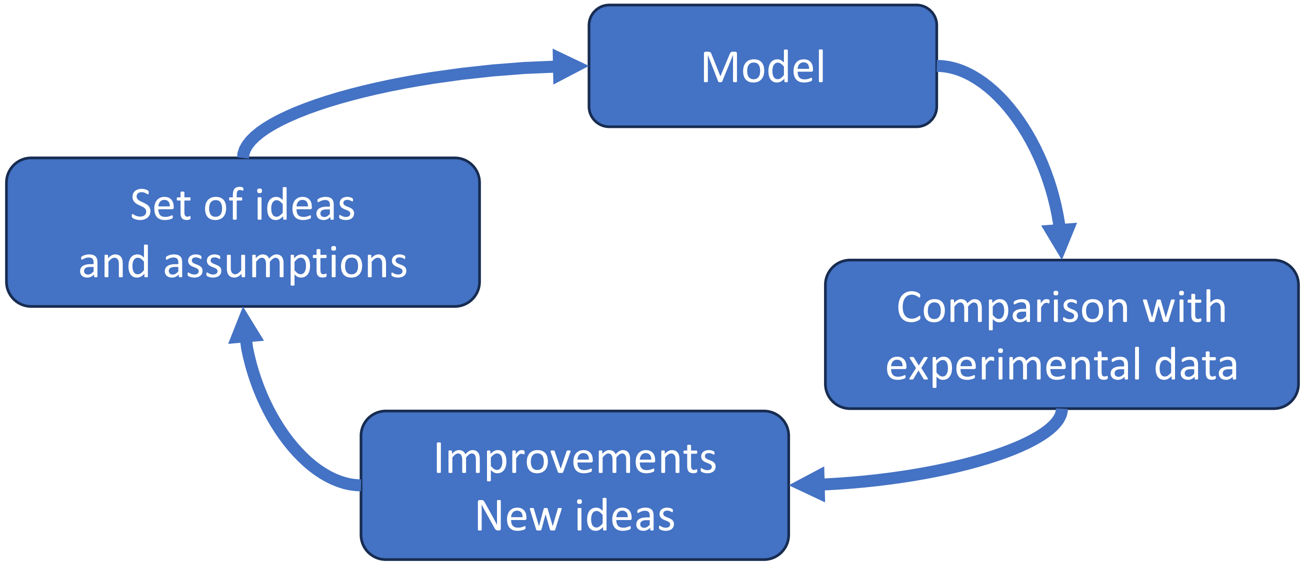

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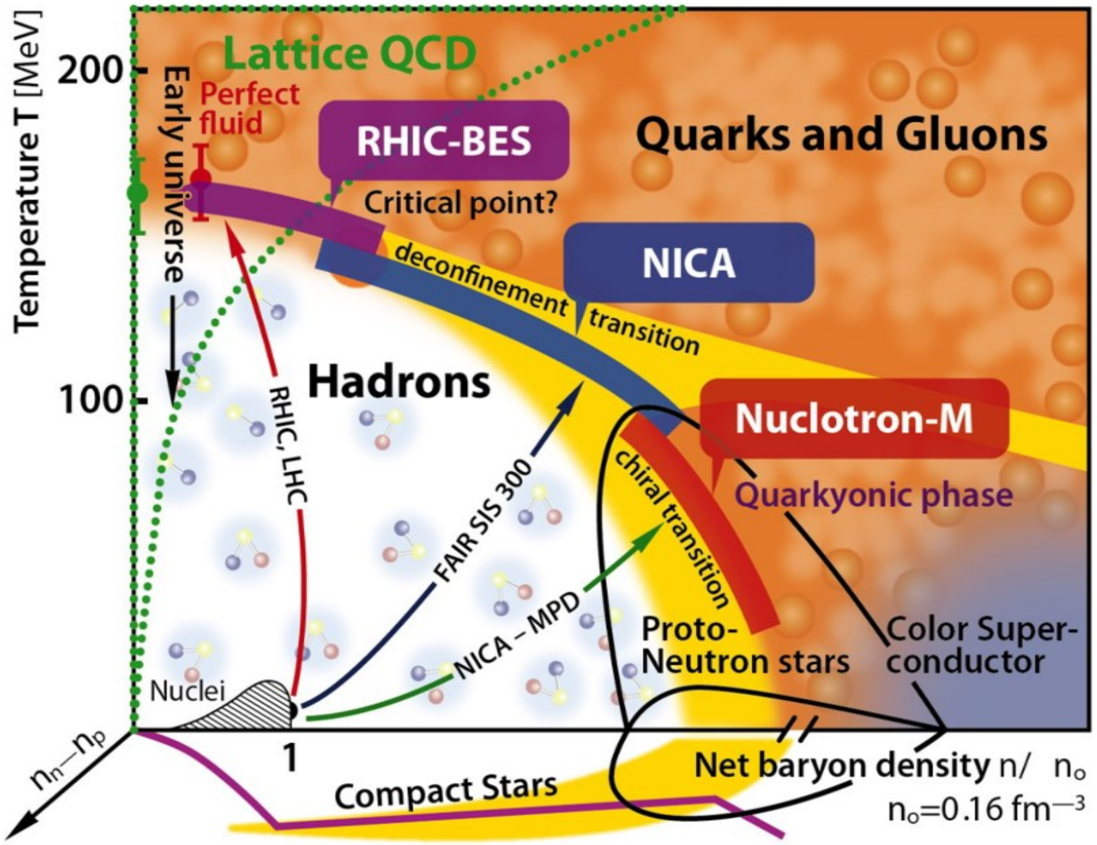

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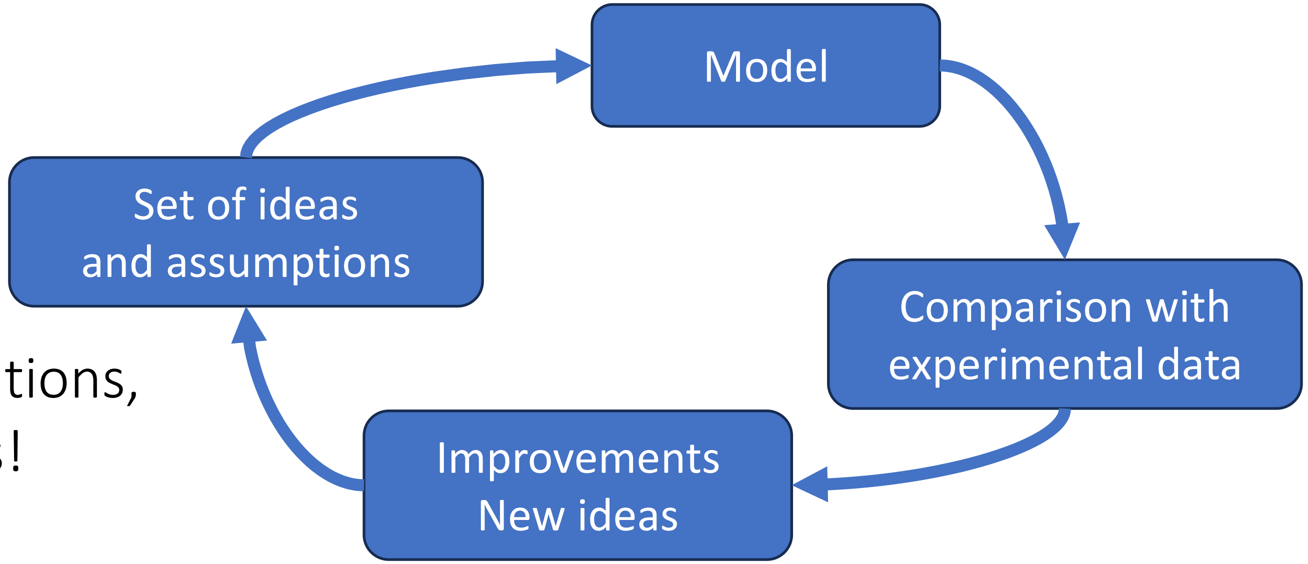

We need different models and tools for simulations, comparison with experimental data and analysis!

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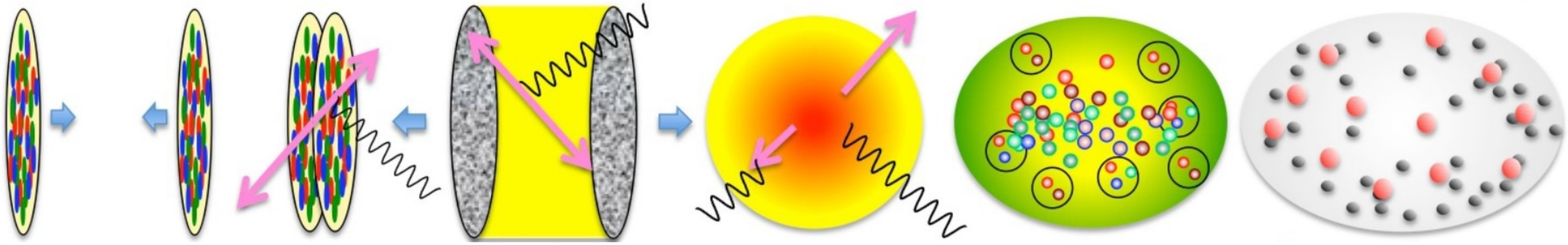
Various phenomena occur during the system evolution. We use different assumptions and models to describe stages of heavy-ion collisions.



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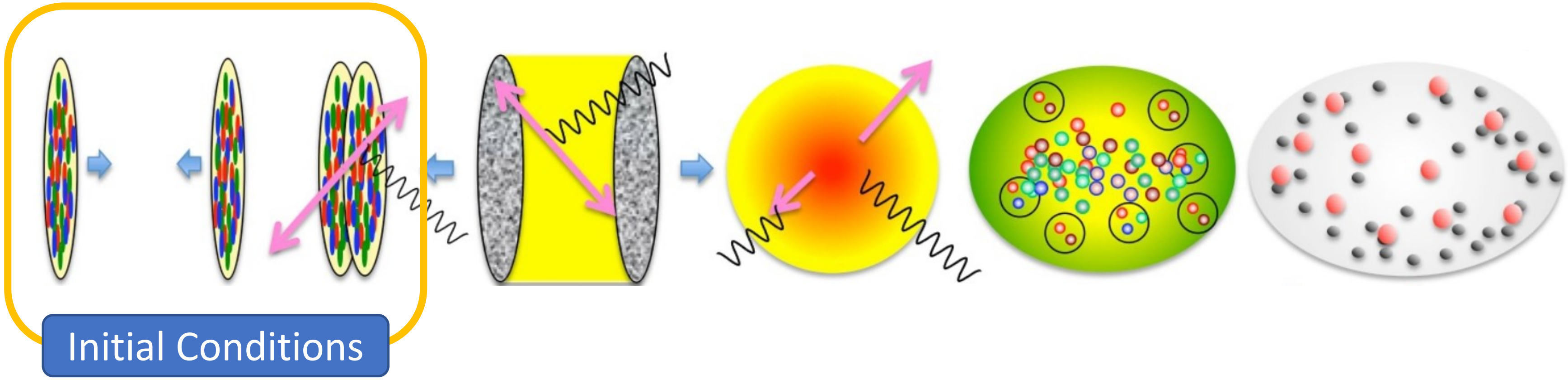

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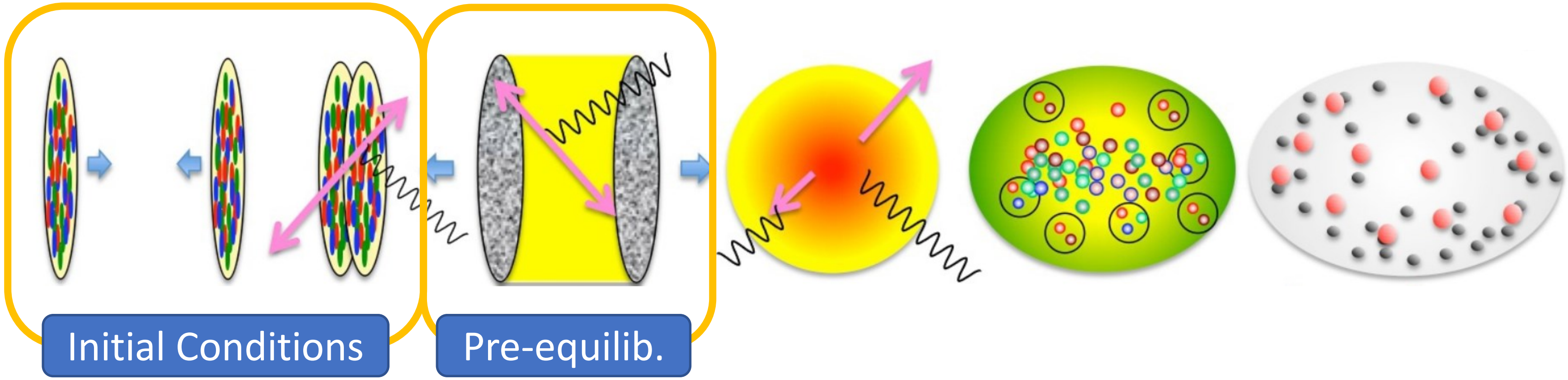

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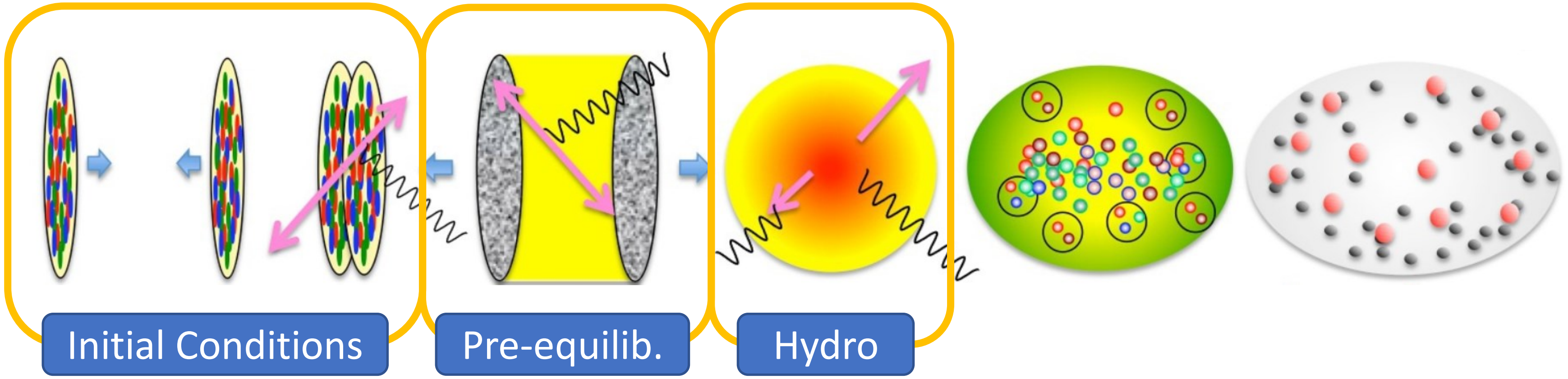

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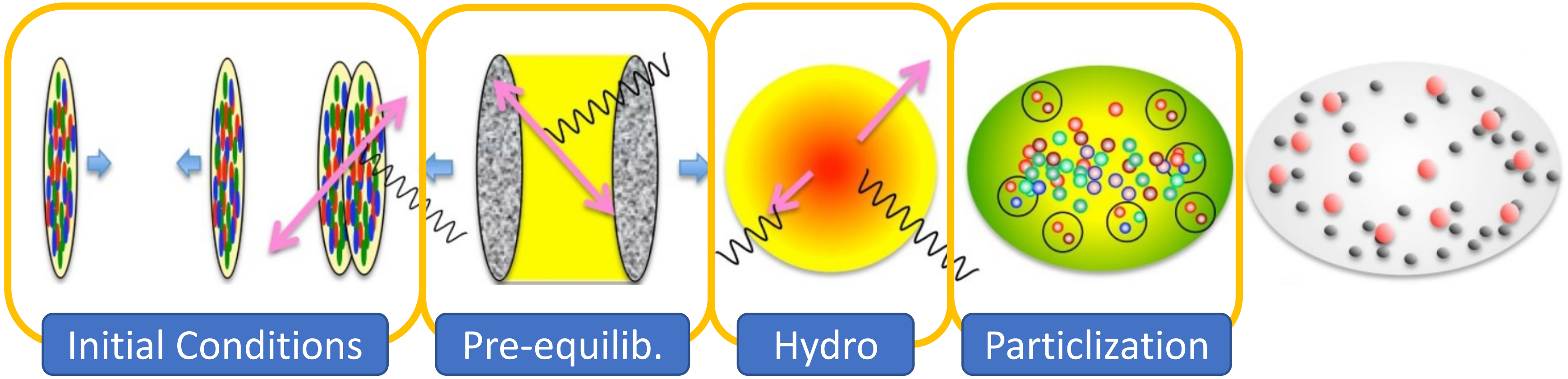

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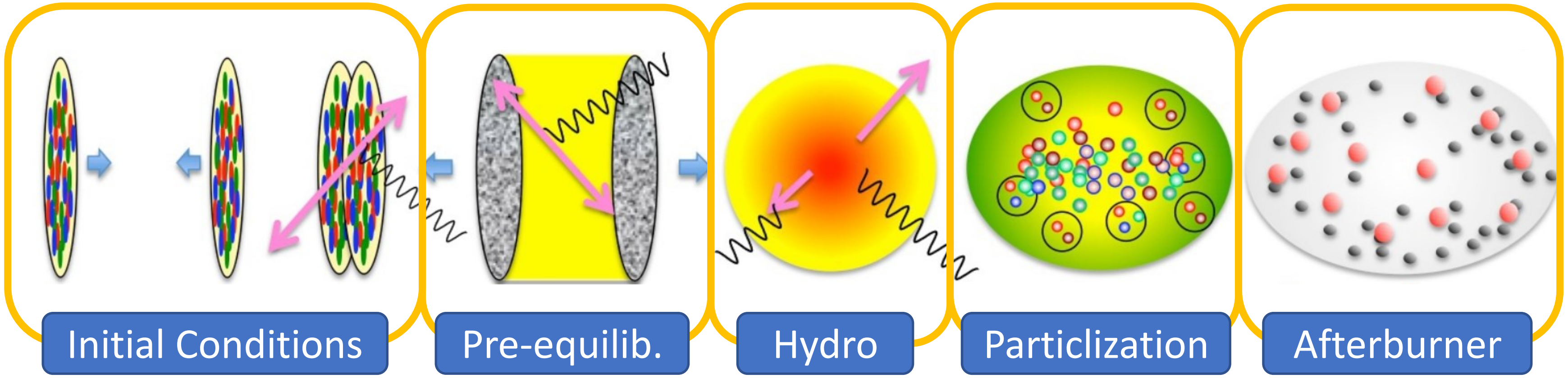

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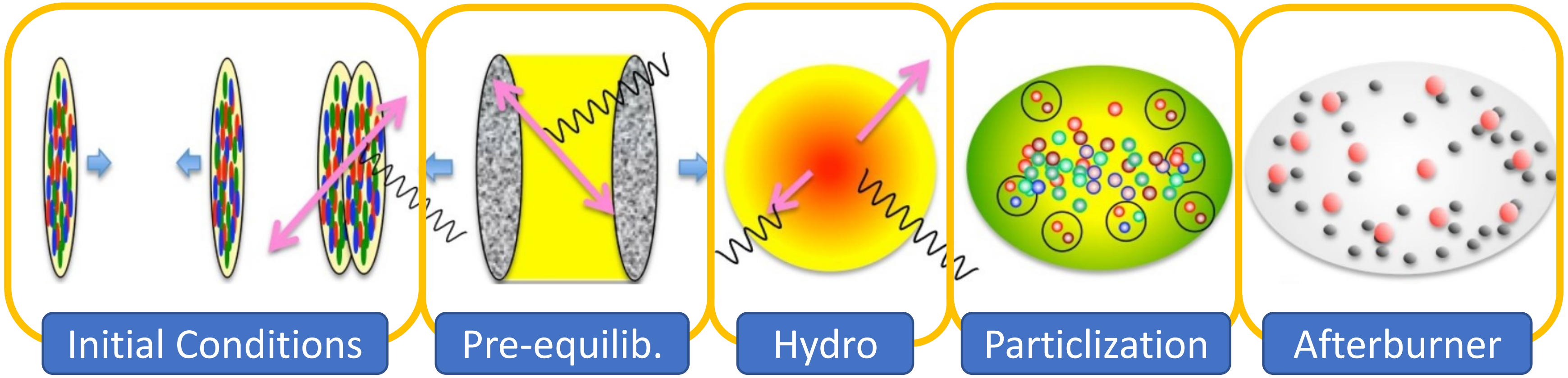

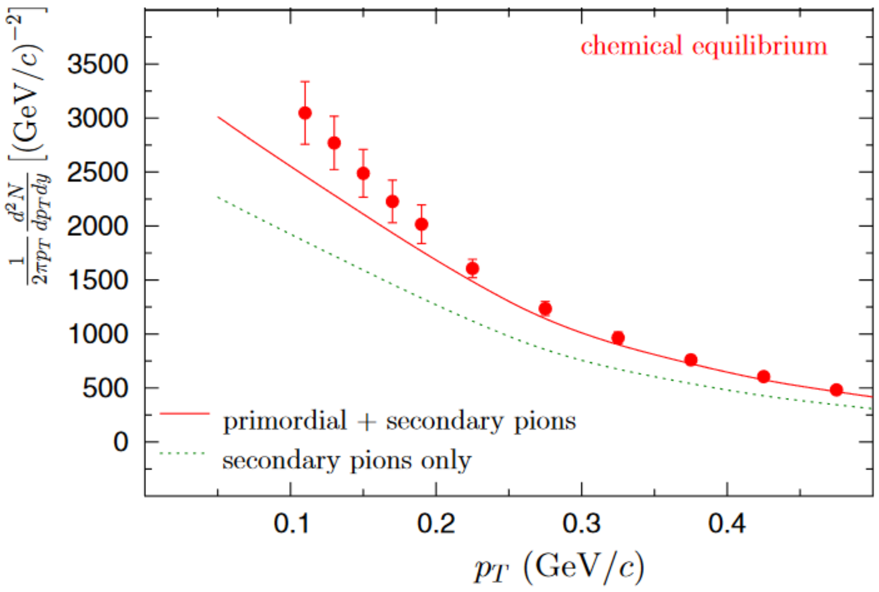

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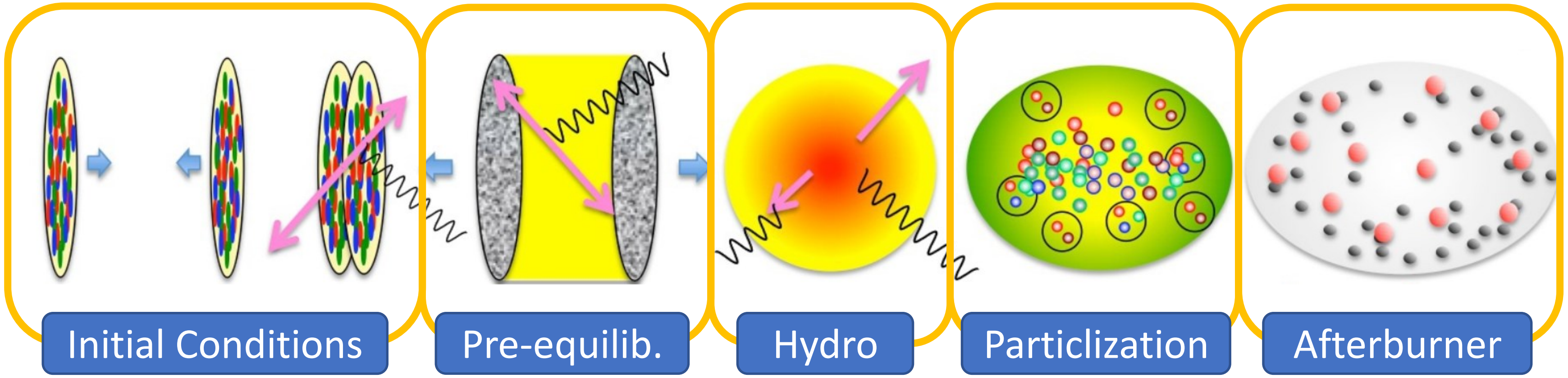

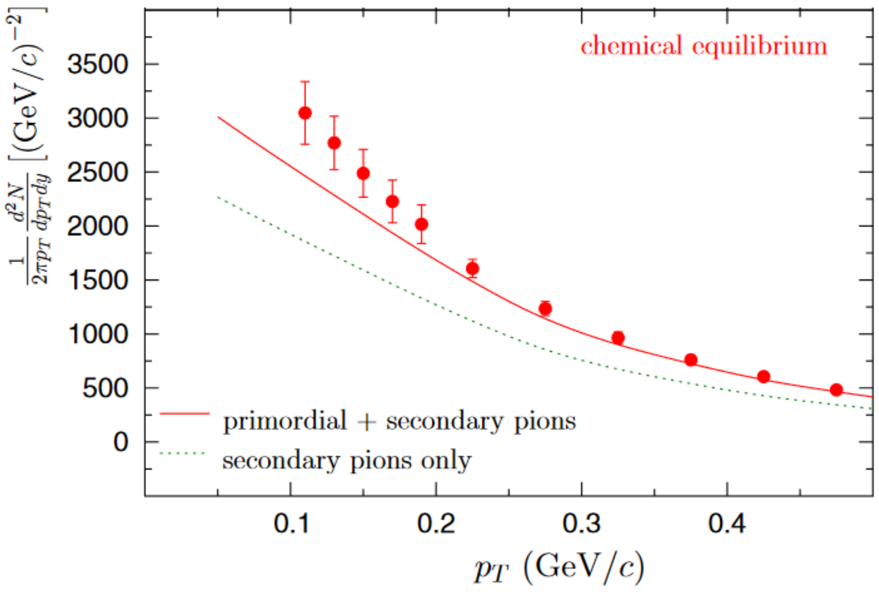

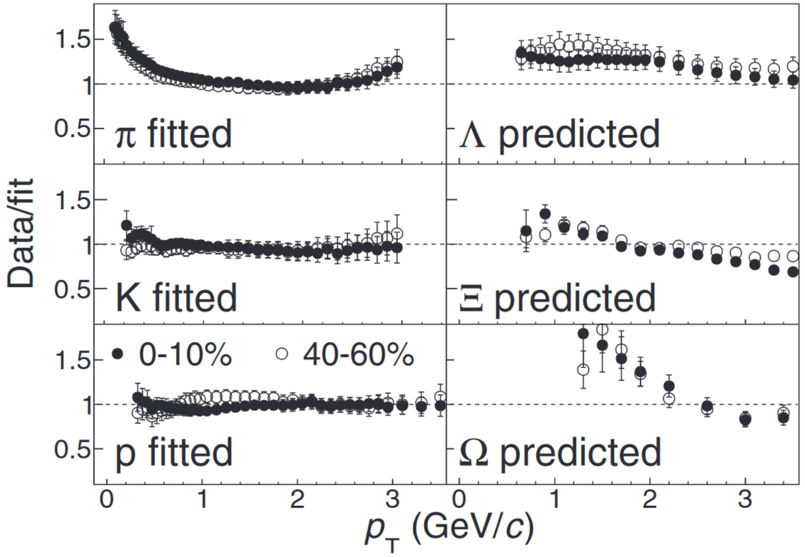

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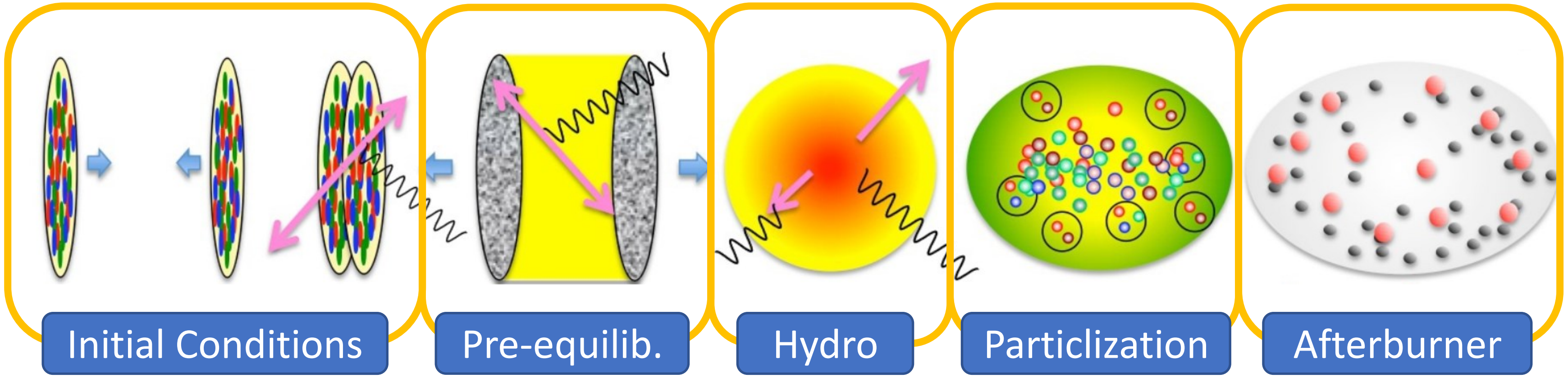

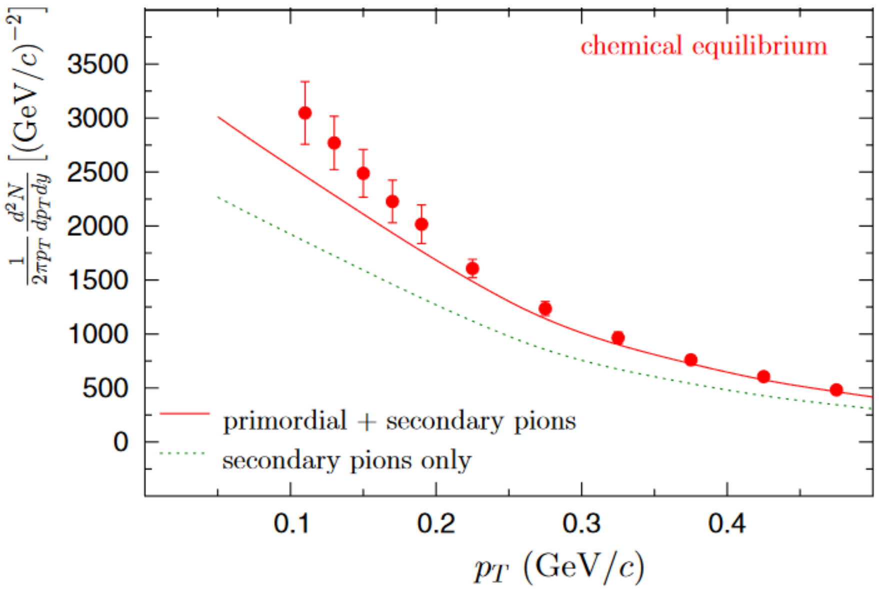

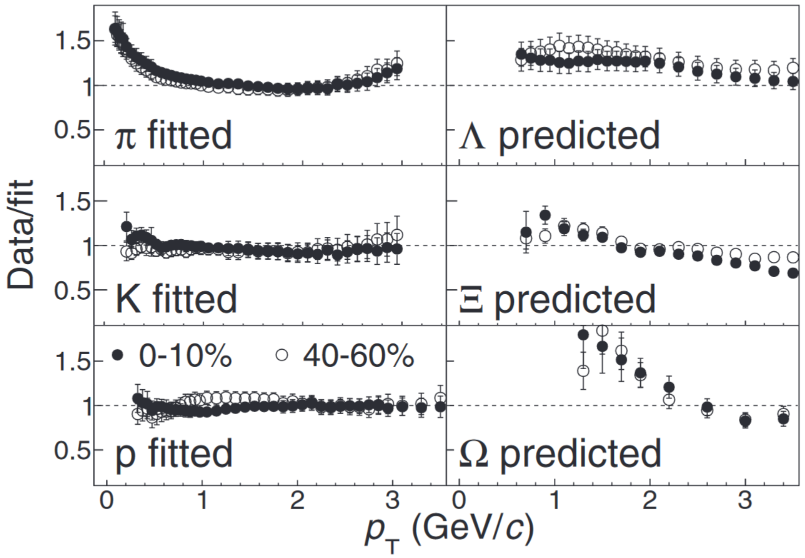

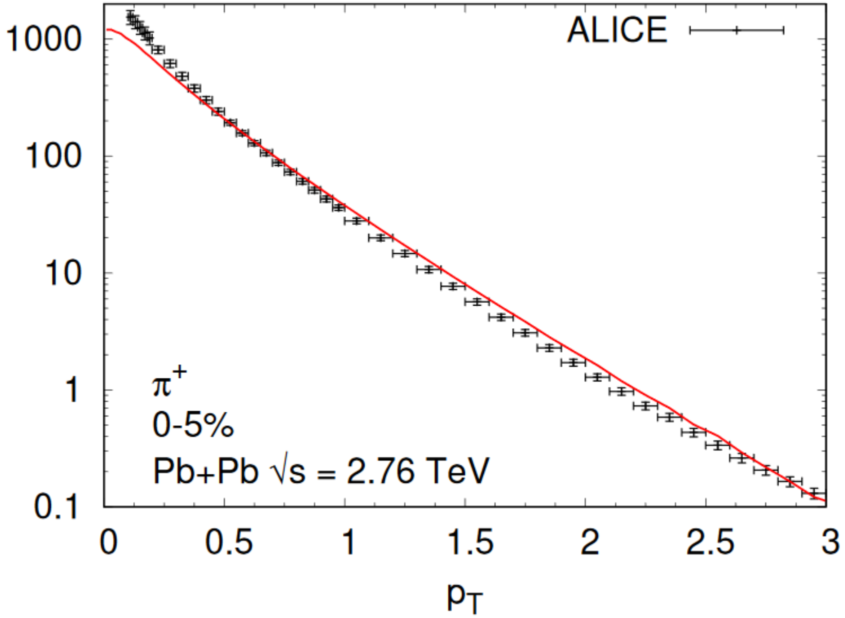

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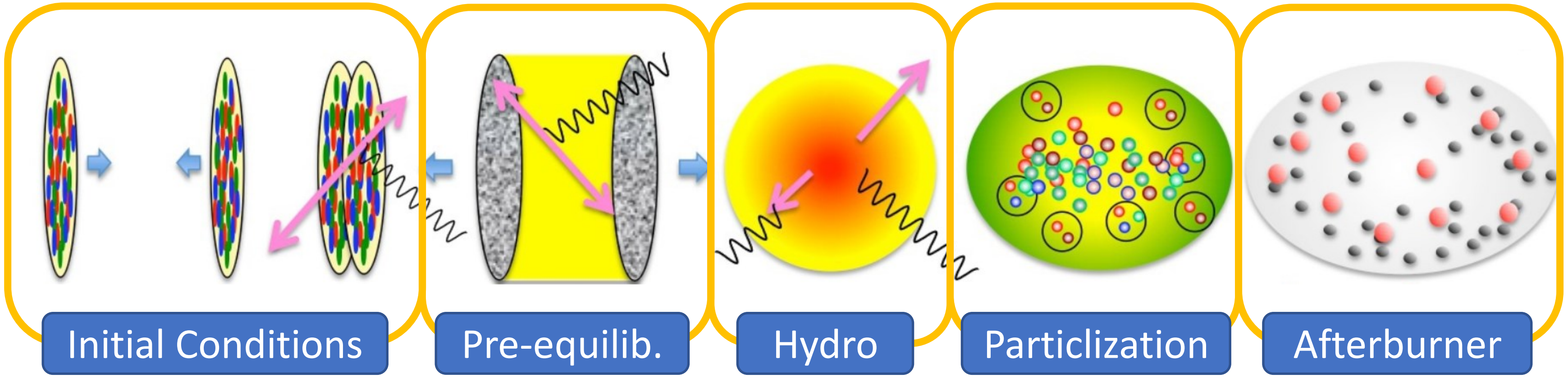

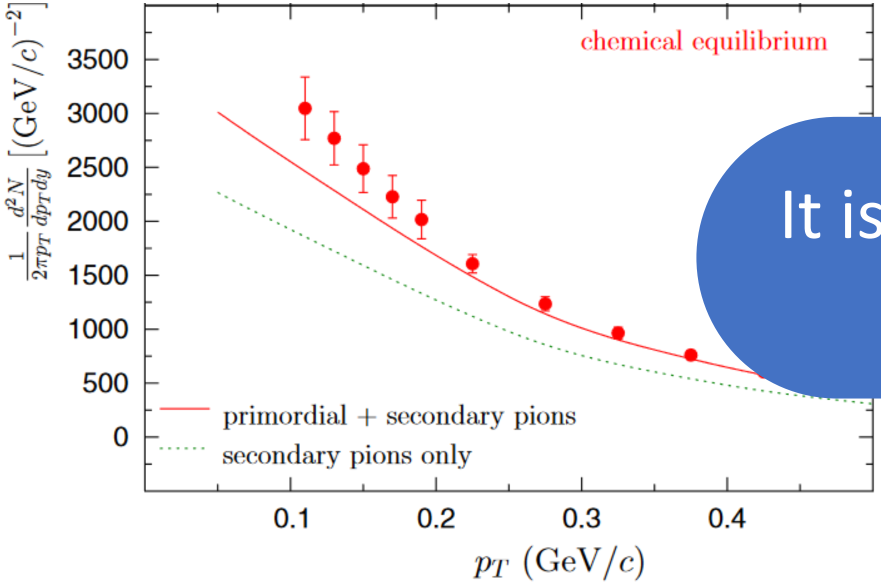

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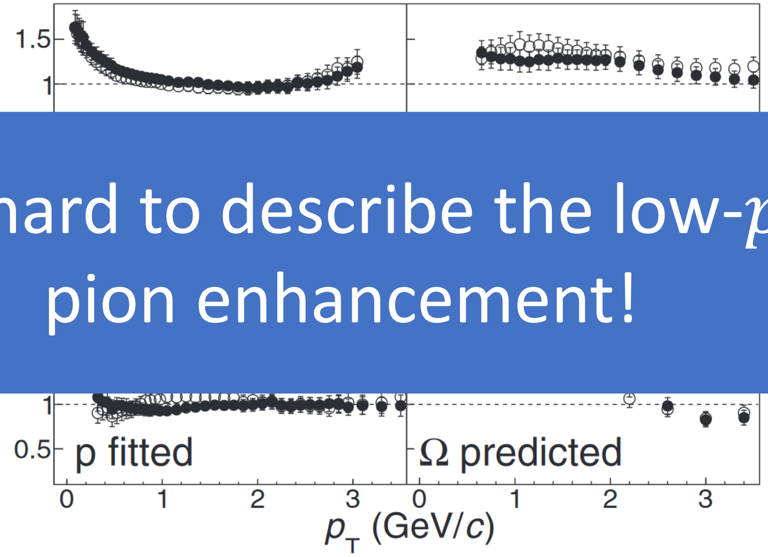

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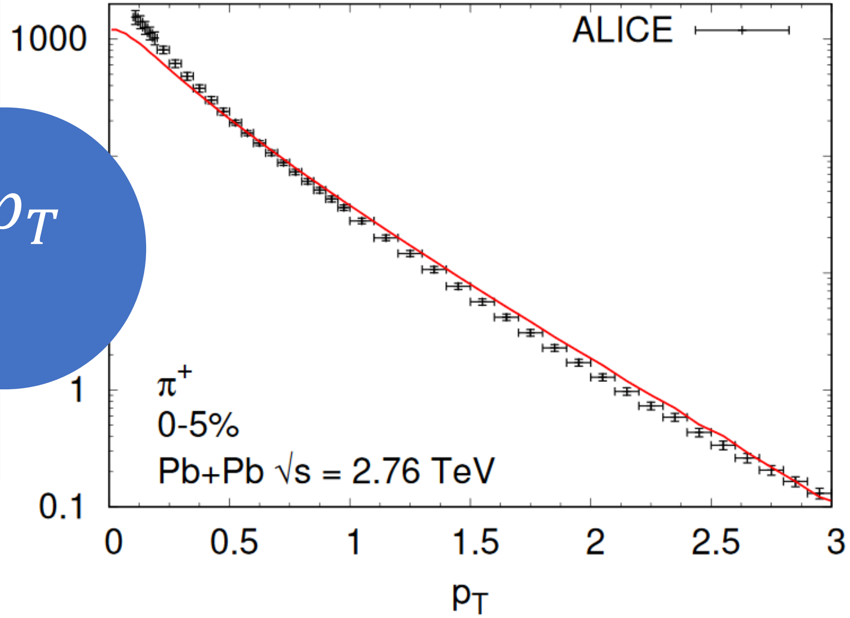

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It is hard to describe the low-p_T pion enhancement!

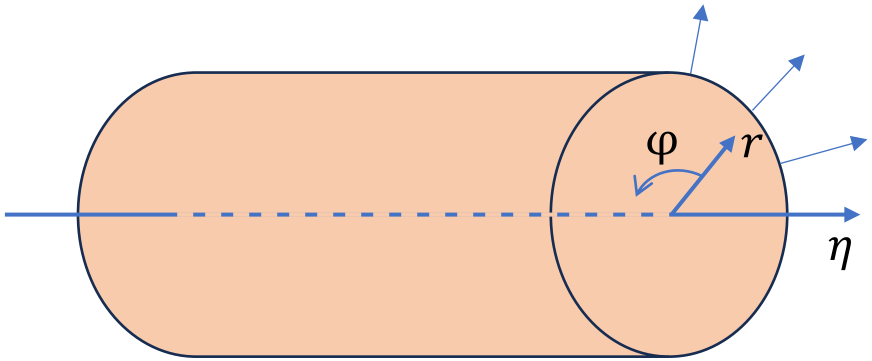
Blast-Wave Model

Let's consider particle emission from the expanding thermal source which can be parametrized by the cylindrical boost-invariant hypersurface with proper time:

$$\Sigma^{\mu} = (\tau \cosh \eta \, , r \, cos\, \varphi \, , r \sin \varphi \, , \tau \sinh \eta), \text{where } \tau = \sqrt{t^2 - z^2} = const. \text{ and } \eta = \frac{1}{2} \ln \frac{t+z}{t-z}$$

with the following velocity profile

$$u^{\mu} = (\cosh \rho \cosh \eta \, , \sinh \rho \, cos\, \varphi \, , \sinh \rho \sin \varphi \, , \cosh \rho \sinh \eta), \text{where } \rho = \text{atanh}[v(r/R)^n]$$



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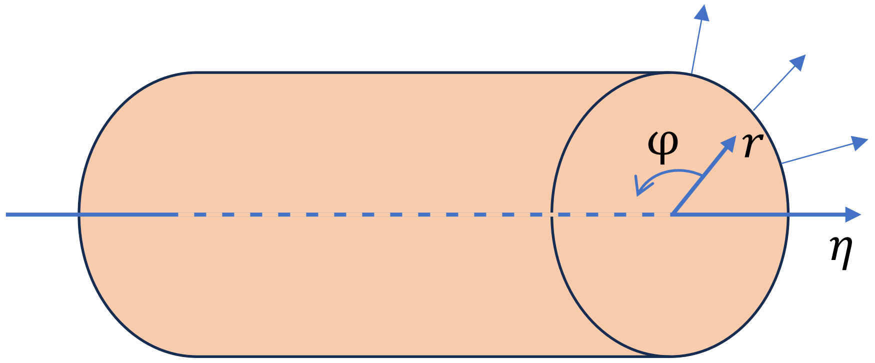
Then with the help of the Cooper-Frye formula $E\frac{d^3N}{d^3\vec{p}} = \int_{\Sigma_{FO}} p^\mu d\Sigma_\mu\, f(x^\mu, p^\mu u_\mu)$ one finds

$$\frac{d^6N_i}{dp_T dy d\psi dr d\eta d\varphi} = \frac{g_i \tau r p_T m_T}{(2\pi\hbar)^3}\cosh(y-\eta)\left(\exp\left[\frac{m_T\cosh\rho\cosh(y-\eta) - p_T\sinh\rho\cos(\varphi-\psi) - \mu_i}{T}\right] \pm 1\right)^{-1}$$



$$p_T = \sqrt{p_x^2 + p_y^2}\,, \qquad m_T = \sqrt{m_i^2 + p_T^2}, \qquad y = \frac{1}{2}\ln\frac{E+p_z}{E-p_z}$$

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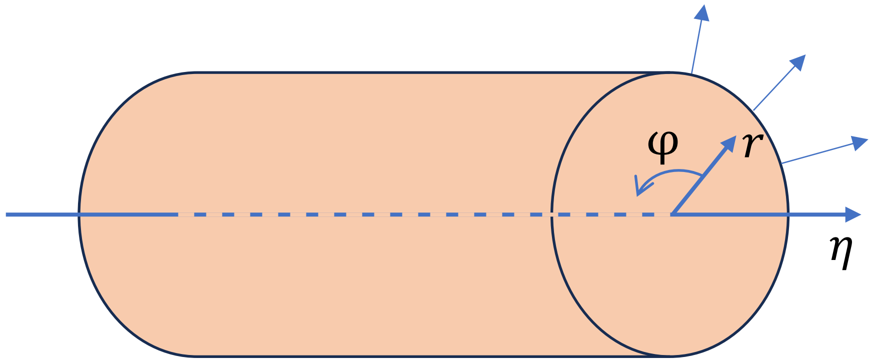

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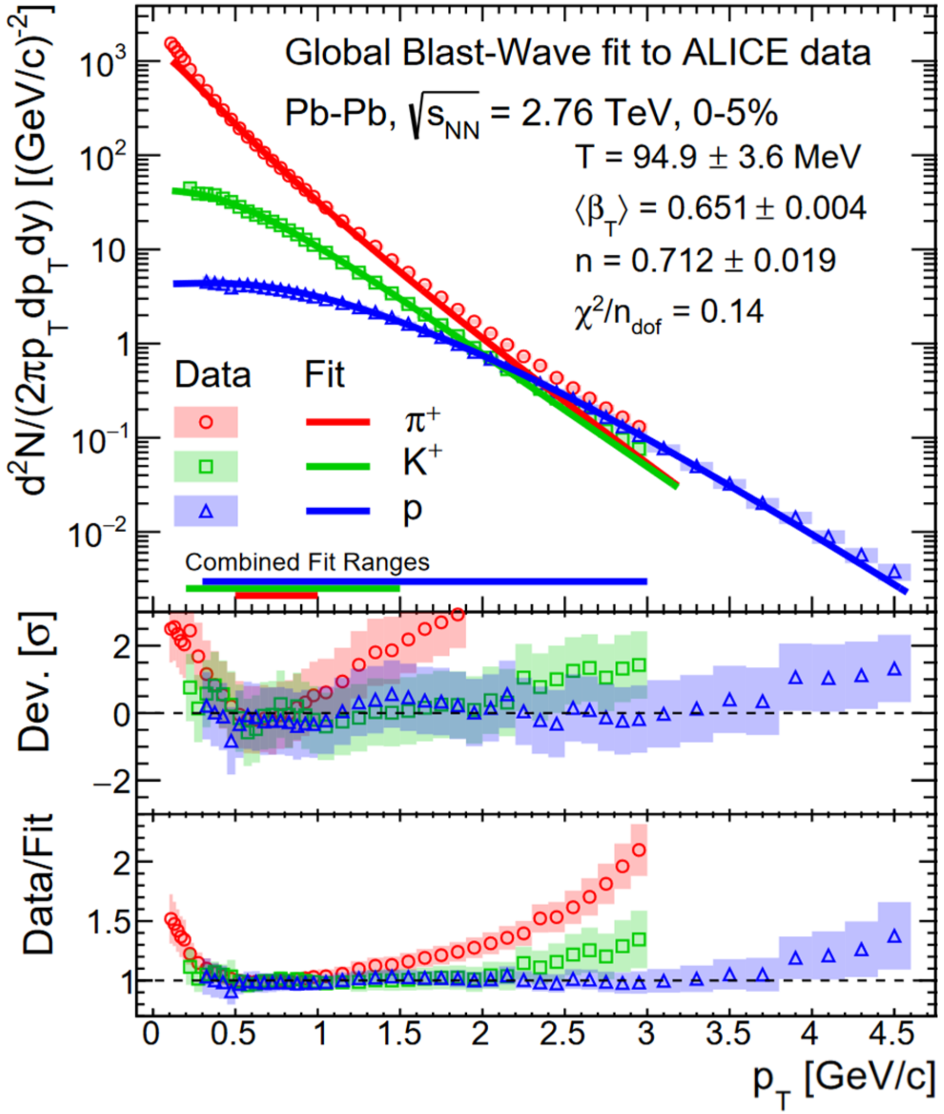
τ, R, T, μ_i, v and n are free model parameters

In some cases, the overall normalization is defined with the combination τR^2

Naïve Model



In Boltzmann approximation Blast-Wave function can be simplified to:

$$\frac{dN}{p_T dp_T} \propto \int_0^R rdr\, m_T I_0\left(\frac{p_T \sinh\rho}{T}\right) K_1\left(\frac{m_T \cosh\rho}{T}\right)$$

Result is consistent with the ALICE [PRC 88, 044910 (2013)]:

$$T = 95 \pm 4 \pm 10 \text{ MeV}$$
$$\langle\beta_T\rangle = 0.651 \pm 0.004 \pm 0.02$$
$$n = 0.712 \pm 0.019 \pm 0.086$$
$$\chi^2/n_{dof} = 0.15$$

But in this model, we have less “slow” $\pi^\pm(K^\pm)$ than in the data. Possible solutions:

- Bose enhancement?
- Feed-down by resonance decays?

Zubarev approach: Model for π

We see more $\pi^{\pm}(K^{\pm})$ in the data than in the model. To improve the model, let's assume the following:

- A state overpopulated by soft $\pi^{\pm}(K^{\pm})$ is formed at $\tau < \tau^{FO}$
- During the system evolution collisions conserve the particle number, but evolve the distribution function to a thermal equilibrium distribution, i.e. dominance of elastic collisions over inelastic ones

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Zubarev approach of the non-equilibrium statistical operator!

Zubarev approach: Overview

The non-equilibrium state of the system is characterized by relevant observables $\{B_n\}$ in addition to the standard set of conserved ones. We look for the distribution which maximizes the information entropy $\mathrm{S_{inf}} = -\mathrm{Tr}\{\rho_{rel}(t)\ln\rho_{rel}(t)\}$:

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The non-equilibrium statistical operator (NSO), i. e. solution of the Liouville-von Neumann equation at given boundary conditions is then given by

$$\rho(t) = \lim_{\varepsilon \to +0} \varepsilon \int_{-\infty}^{t} dt' \, e^{\varepsilon(t'-t)} e^{iH(t'-t)/\hbar} \rho_{rel}(t) e^{iH(t-t')/\hbar}$$

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Here we assume that the memory of the system is short. Then $\rho(t)$ can be replaced by $\rho_{rel}(t)$.

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Under these assumptions the pion number is quasi-conserved and can be chosen as a relevant observable. Then, the new self-consistency condition is:

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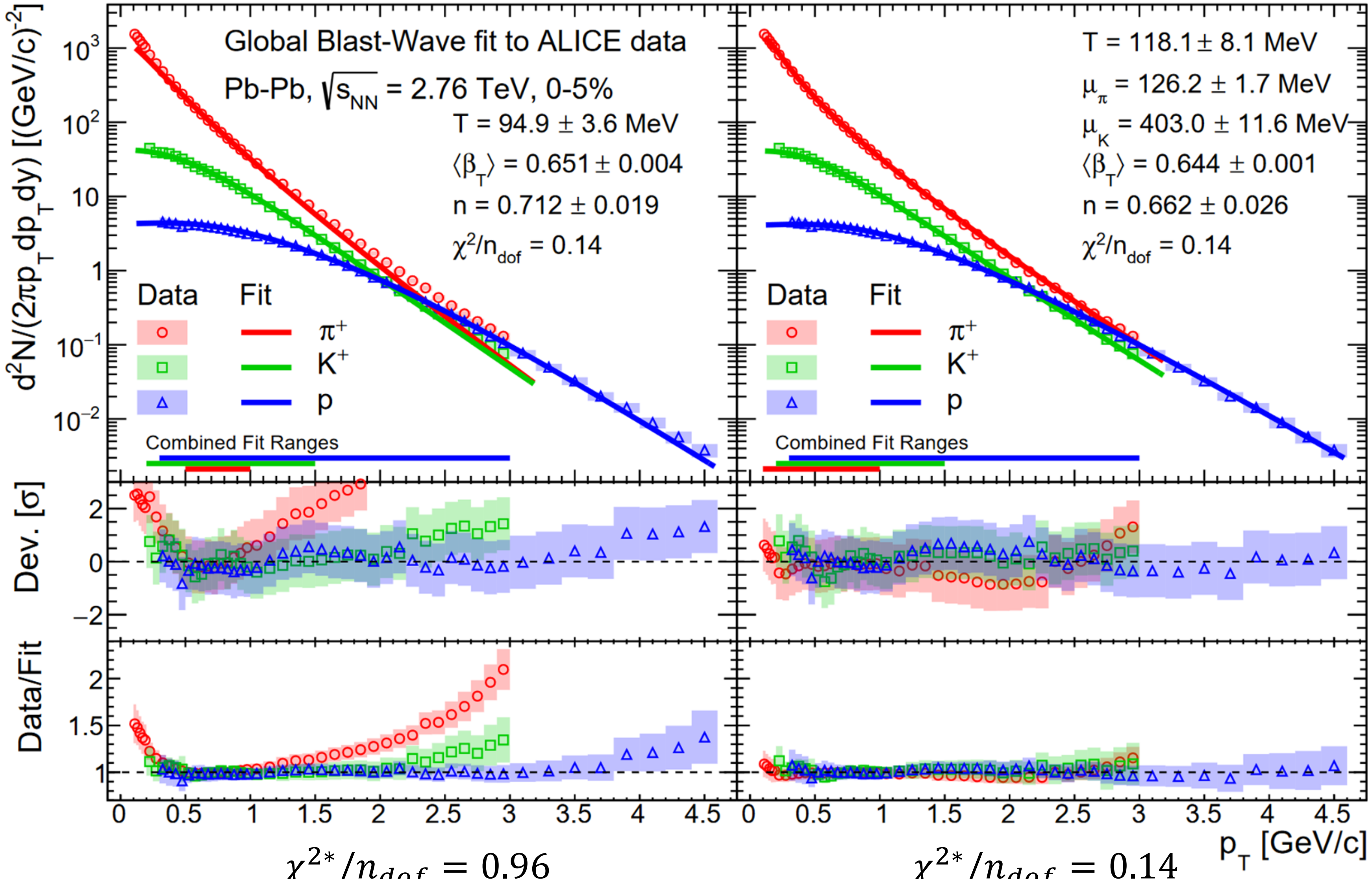
The non-equilibrium process of pion production within the Zubarev NSO approach leads to the appearance of a non-equilibrium pion chemical potential [Particles 2020, 3, 380–393]

$$f_\pi = \left(\exp\left[\frac{E}{T}\right] - 1 \right)^{-1} \quad \rightarrow \quad f_\pi = \left(\exp\left[\frac{E - \mu_\pi}{T}\right] - 1 \right)^{-1}$$

Naïve Model II



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$\chi^{2*}/n_{dof} = 0.14$

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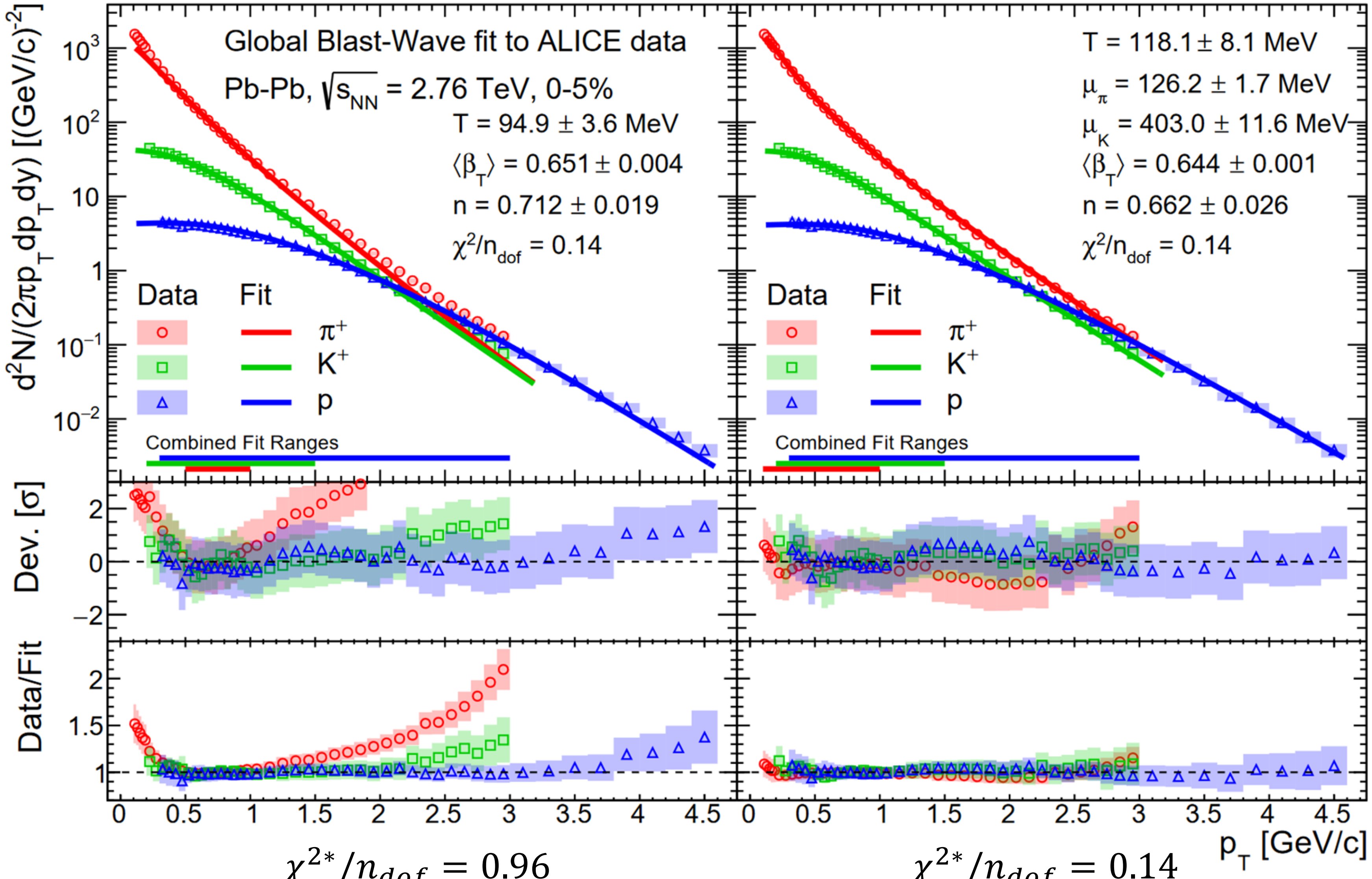

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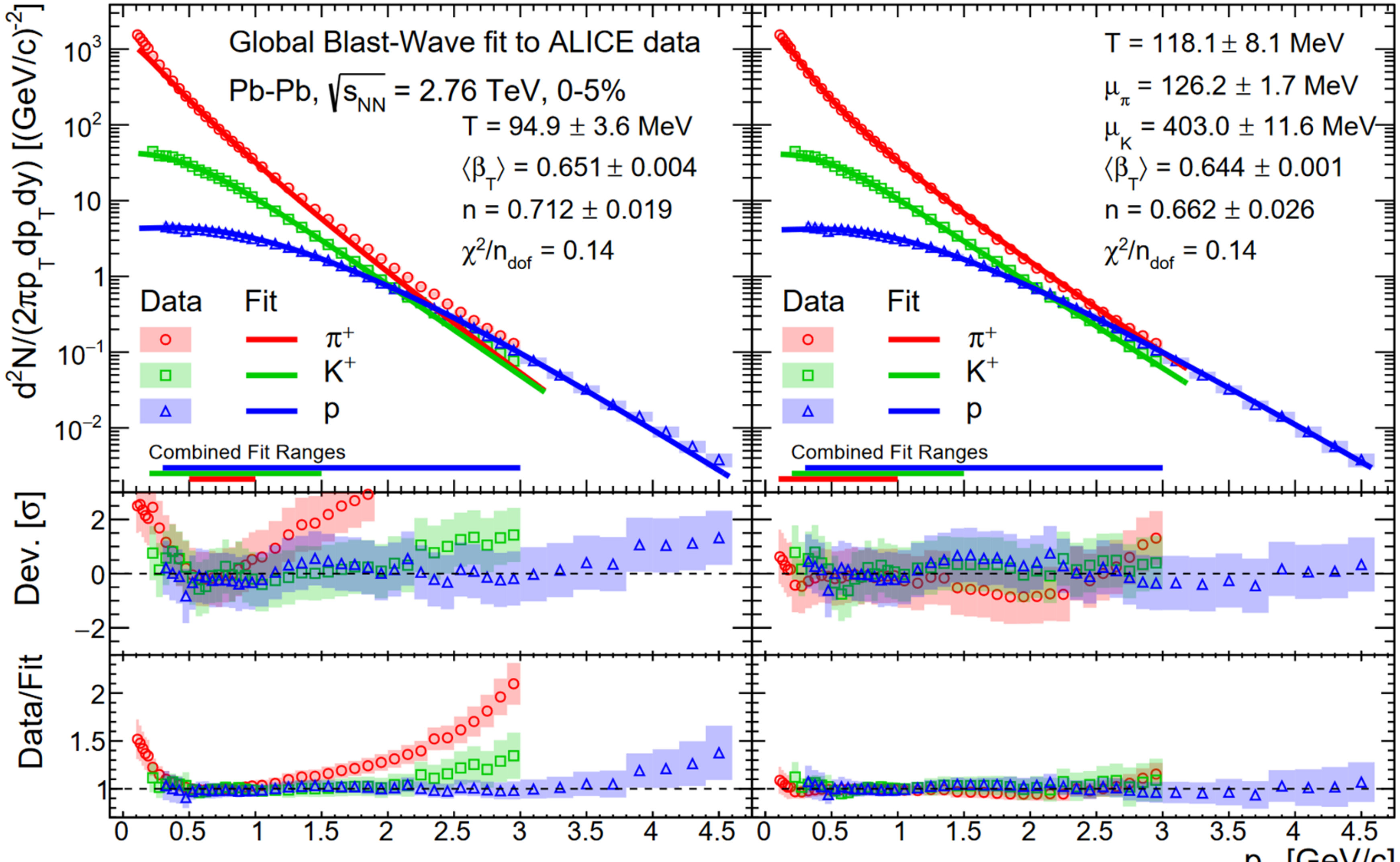

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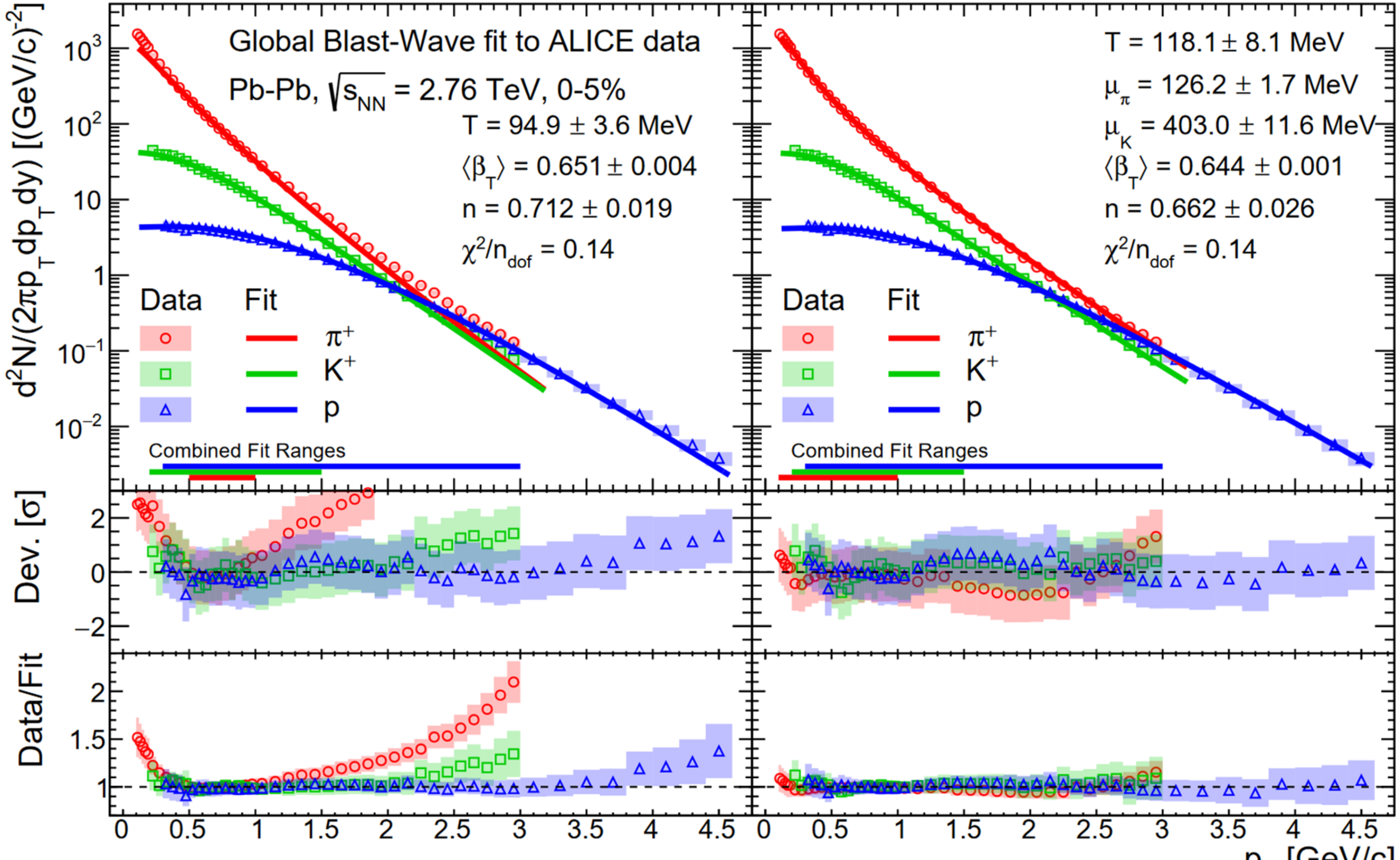

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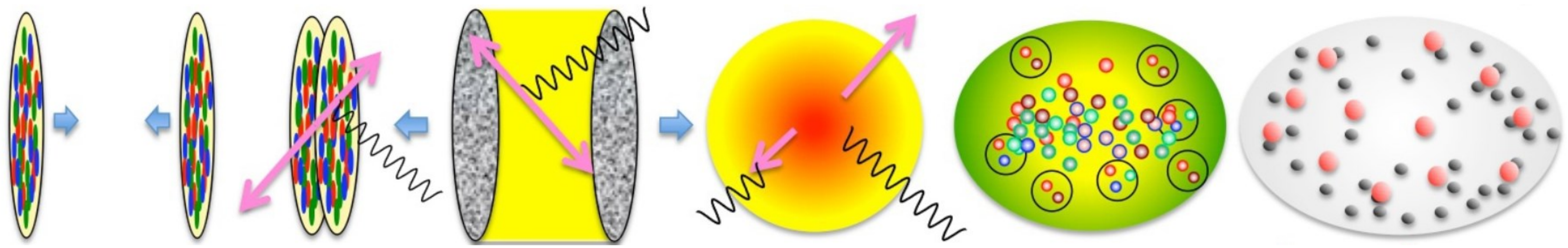

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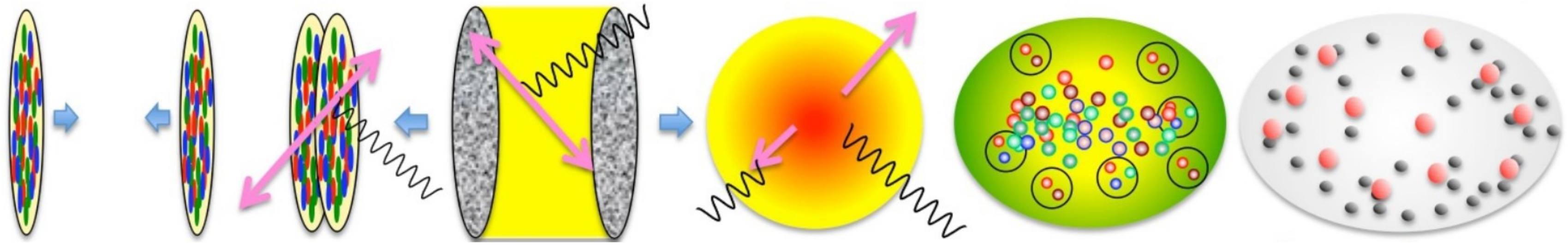
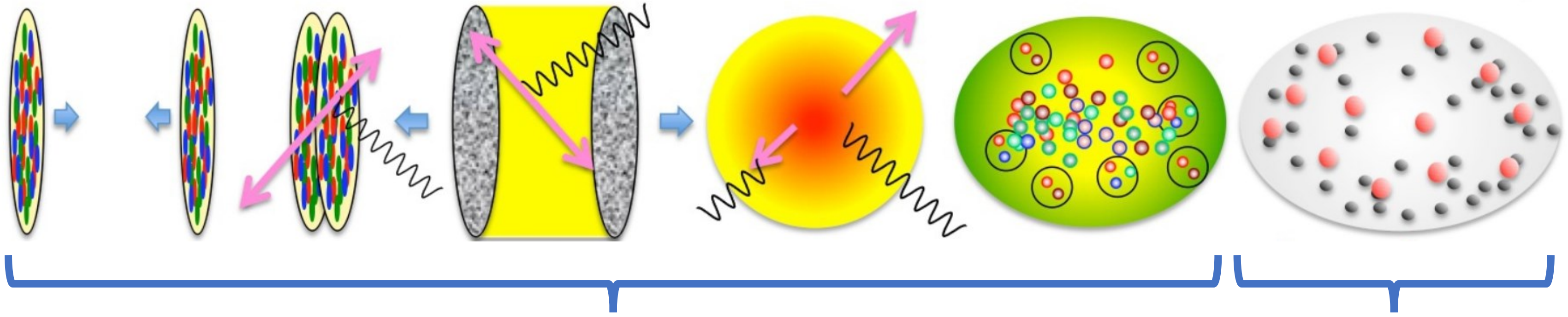


Thermal source

Blast-Wave Based Particle Generator

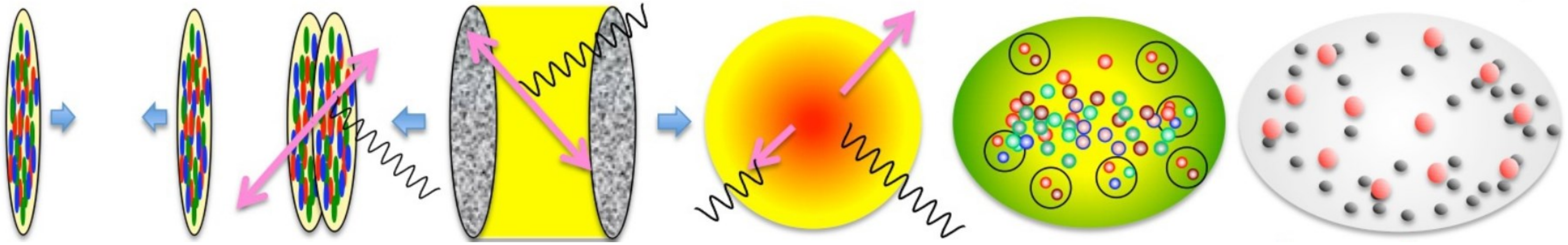


Thermal source

Afterburner

Afterburner instead of solving generalized kinetics!

Blast-Wave Based Particle Generator



Thermal source

Afterburner

Afterburner instead of solving generalized kinetics!

Two competing models

Statistical hadronization

Model with extra pions

Blast-Wave Based Particle Generator

Distribution function:

$$f_i = \frac{g_i \tau r p_T m_T}{(2\pi\hbar)^3} \cosh(y-\eta) \left(\exp\left[\frac{m_T \cosh\rho \cosh(y-\eta) - p_T \sinh\rho \cos(\varphi - \psi) - \mu_i}{T} \right] \pm 1 \right)^{-1}$$

Breit-Wigner mass attenuation for resonances:

$$f \to \tilde{f} = \frac{1}{N} \frac{f}{(m-m_0)^2 + \Gamma^2/4}$$

Multiplicity in a single event is a Poisson random variable:

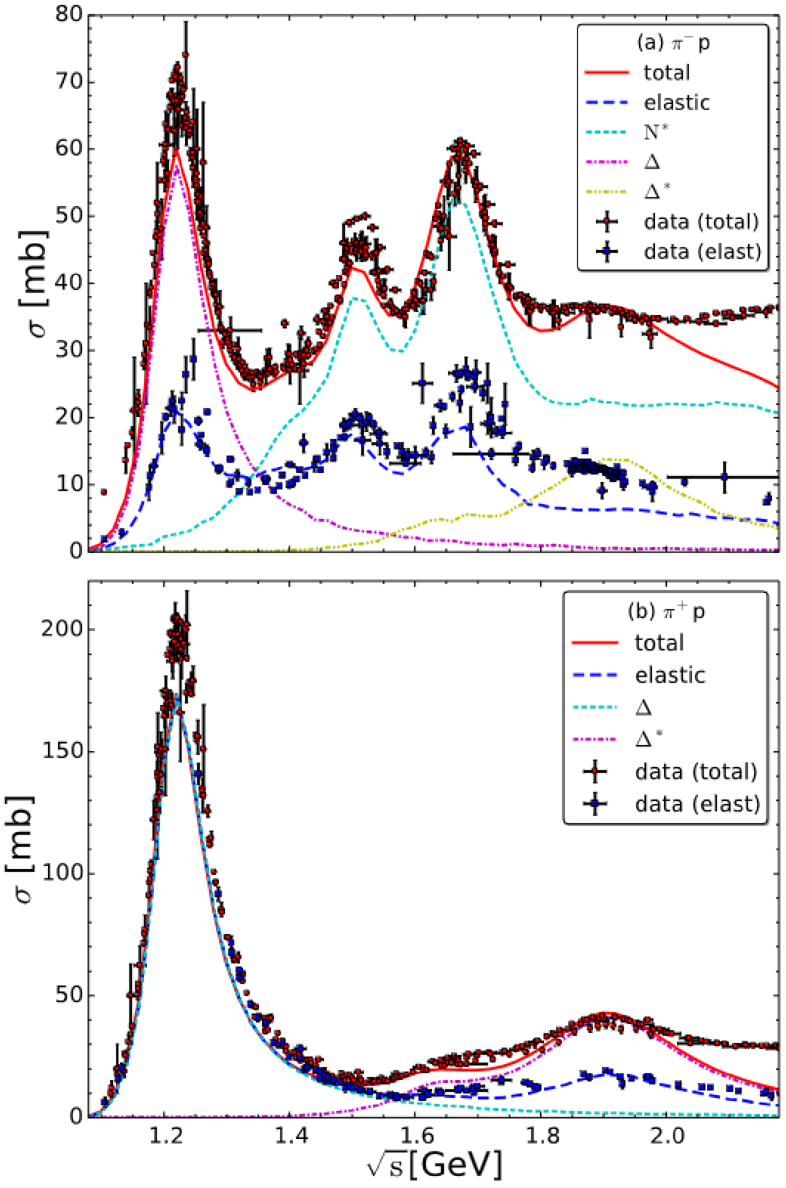
$$P(N_i = N) = \frac{< N_i >^N}{N!} e^{-<N_i>}$$

1. Set model parameters, evaluate $< N_i >$
2. For every event generate yield of particles of i^{th} type N_i
3. Generate N_i particles of i^{th} type from f
4. Feed all generated particles into SMASH

Afterburner: SMASH

SMASH: Simulating Many Accelerated Strongly interacting Hadrons
[Phys. Rev. C 94, 054905 (2016)]:

- Hadronic transport approach: particles propagate, collide, decay
- Ideologically based on relativistic Boltzmann equation
- BUU type Monte-Carlo solver which uses testparticles method
- Degrees of freedom:
  - most of established hadrons from PDG up to mass 2.5 GeV
  - strings: do not propagate, only form and decay to hadrons
  - leptons and photons production, decoupled from hadronic evolution
- Geometrical and stochastic collision criterion criteria
- C++ code, public on GitHub



Bayesian Inference

Bayes theorem:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

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Suppose we have a model which for an input parameter vector $\vec{x} = (x_1, \dots, x_n)$ gives an output $\vec{y} = \vec{y}(\vec{x}) = (y_1, \dots, y_m)$. We want to find the “optimal” value of $\vec{x}$ to describe the experimental data $\vec{y}^{obs}$

$$\mathrm{P}\left(\vec{x}|\vec{y}^{obs}\right) = \frac{\mathcal{L}\left(\vec{x}; \vec{y}^{obs}\right) P(\vec{x})}{P\left(\vec{y}^{obs}\right)} \propto \mathcal{L}\left(\vec{x}; \vec{y}^{obs}\right) \times P(\vec{x})$$

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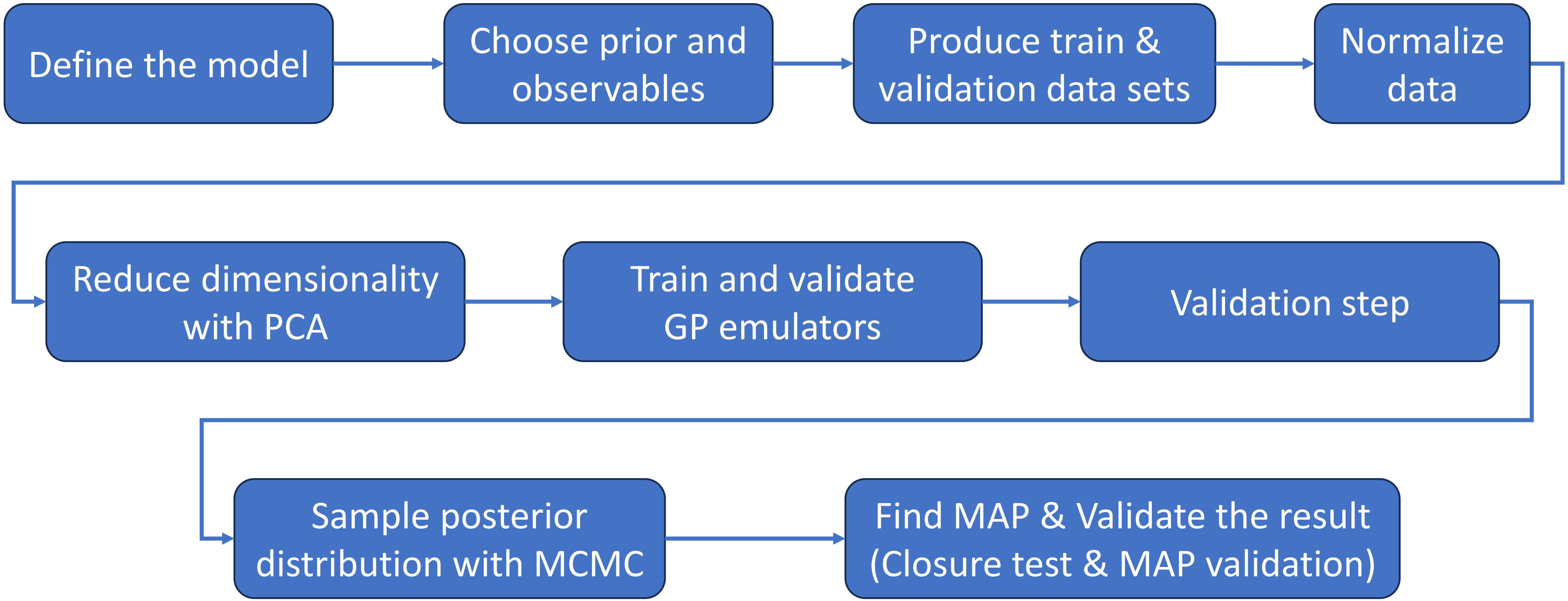
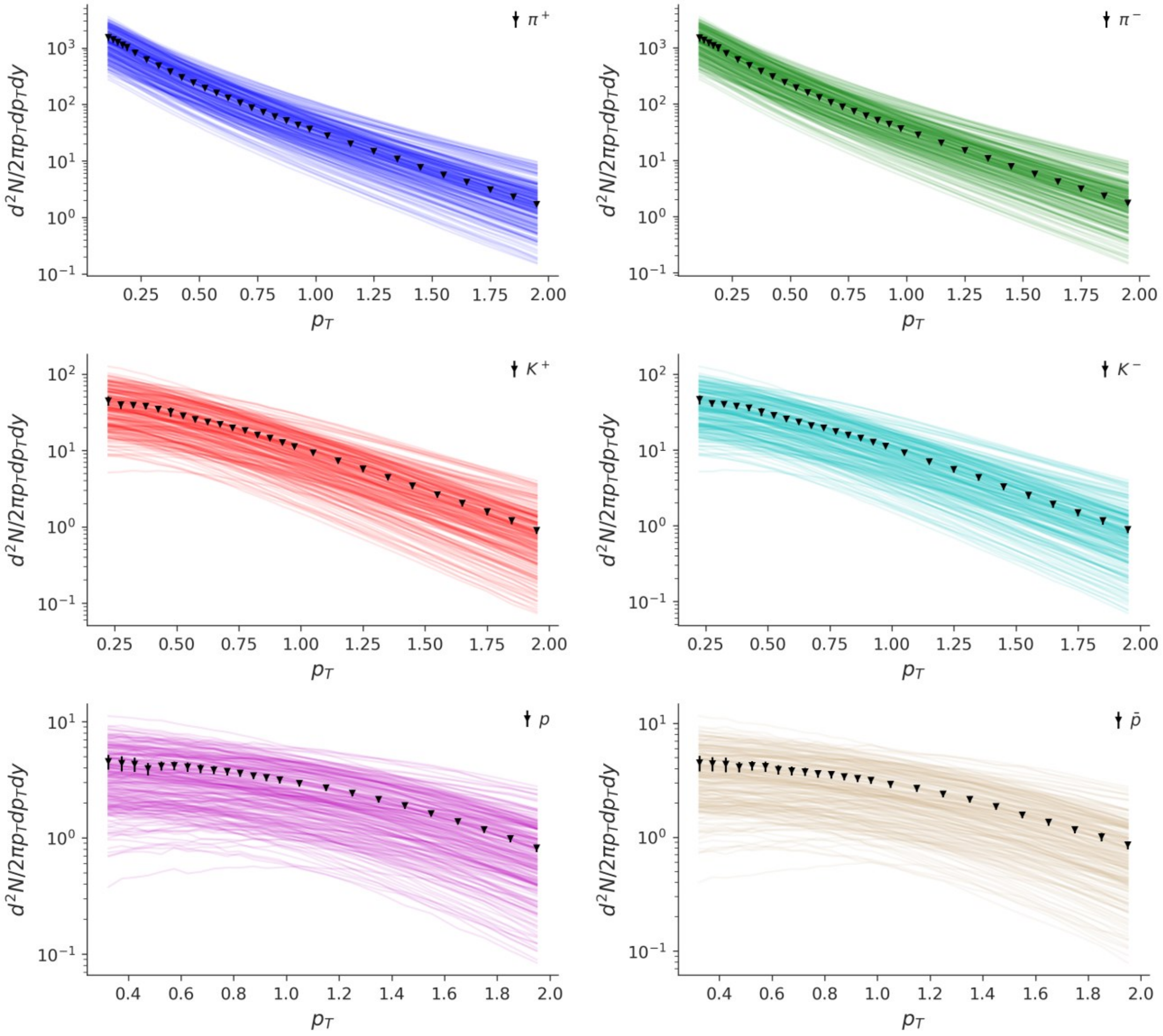
If we know mean values and variance, then the likelihood takes the form of multivariate Gaussian

$$\mathcal{L}(\vec{x};\vec{y}^{obs}) = \frac{1}{\sqrt{|2\pi\Sigma|}} \exp\left(-\frac{1}{2}\left(\vec{y}^{obs} - \vec{y}(\vec{x})\right)^T \Sigma^{-1} \left(\vec{y}^{obs} - \vec{y}(\vec{x})\right)\right)$$

Bayesian Inference Workflow



Model Setup

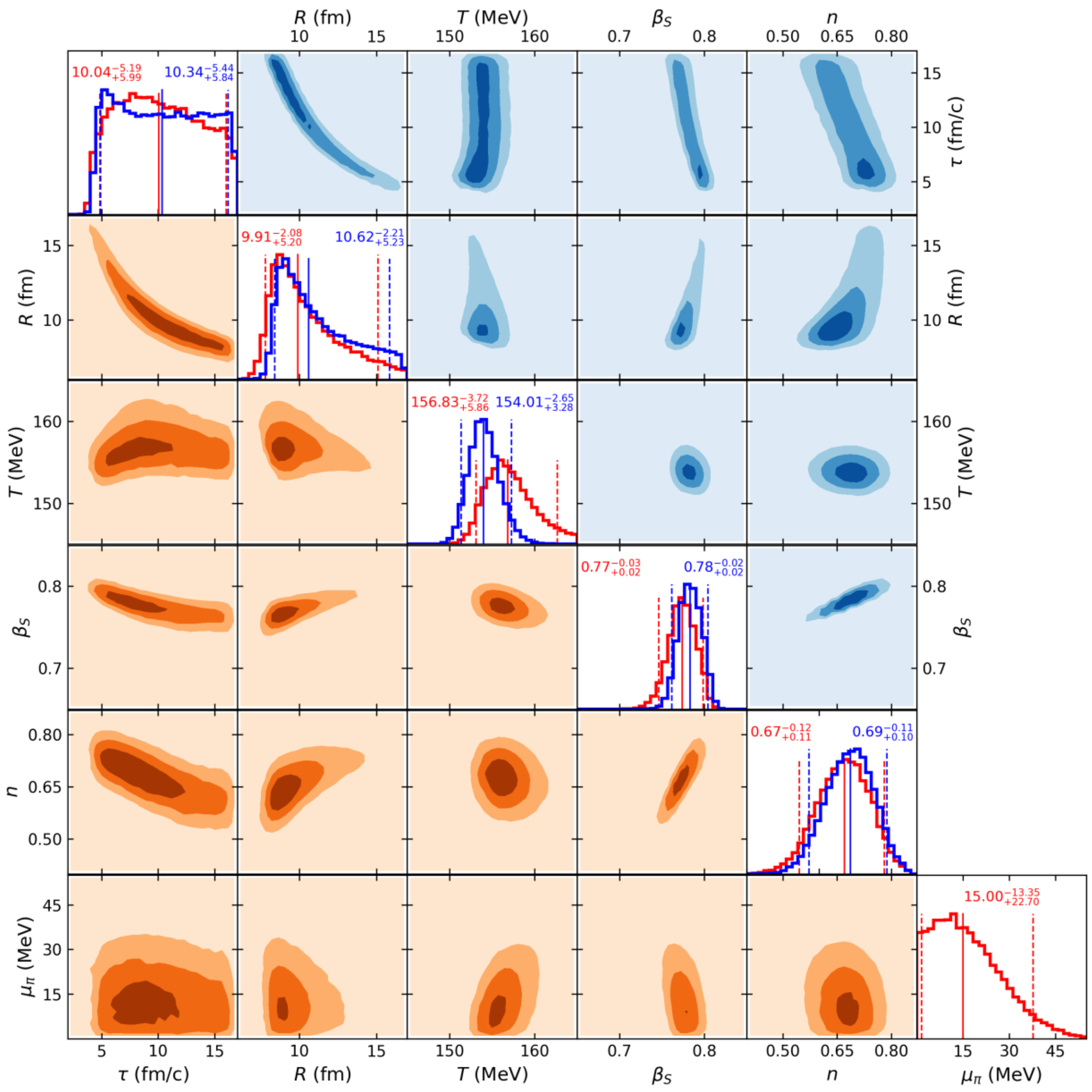


- Blast-Wave thermal particle generator model with SMASH afterburner
- Uniform prior:

$$\tau \in [2; 17]\ fm/c$$
$$R \in [6; 17]\ fm$$
$$T \in [145; 165]\ MeV$$
$$v \in [0.65; 0.85]$$
$$n \in [0.4; 0.85]$$
$$\mu_\pi \in [0; 100]\ MeV \text{ or } \mu_\pi = 0$$

- Observables: $p, \bar{p}, \pi^+, \pi^-, K^+, K^-$ spectra in 0-5% Pb-Pb@2.76 TeV collisions for $p_T \leq 2$ GeV/c
- 160 training and 40 validation data sets
- 5 PCs
- Kernel: $\mathrm{K}(x_i, x_j) = \theta_A^2 \exp\left[-\frac{(x_i - x_j)^2}{2\theta_L^2}\right] + \theta_n \delta_{i,j}$
- 100000 MCMC samples

Posterior Probability Distribution



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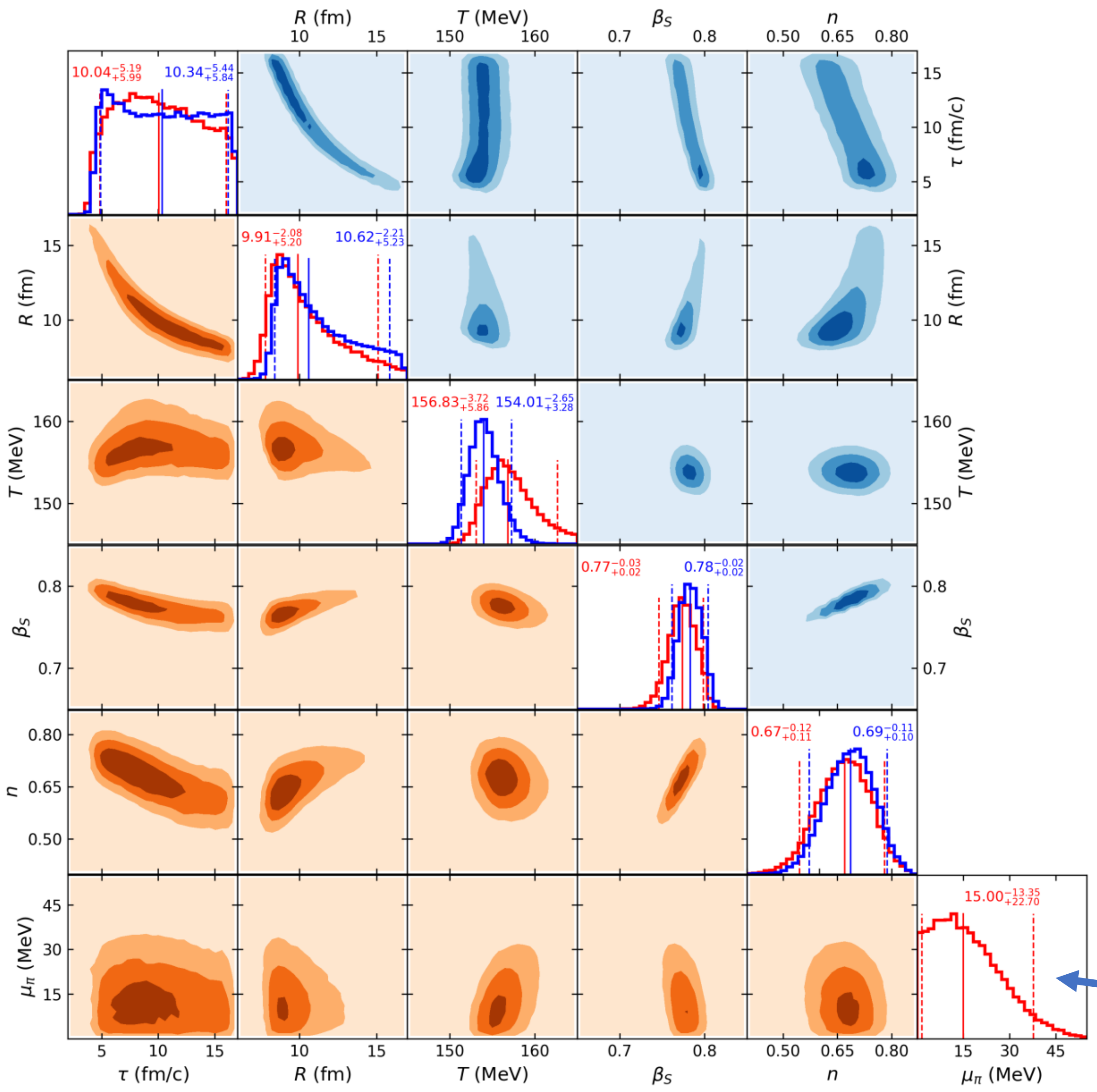
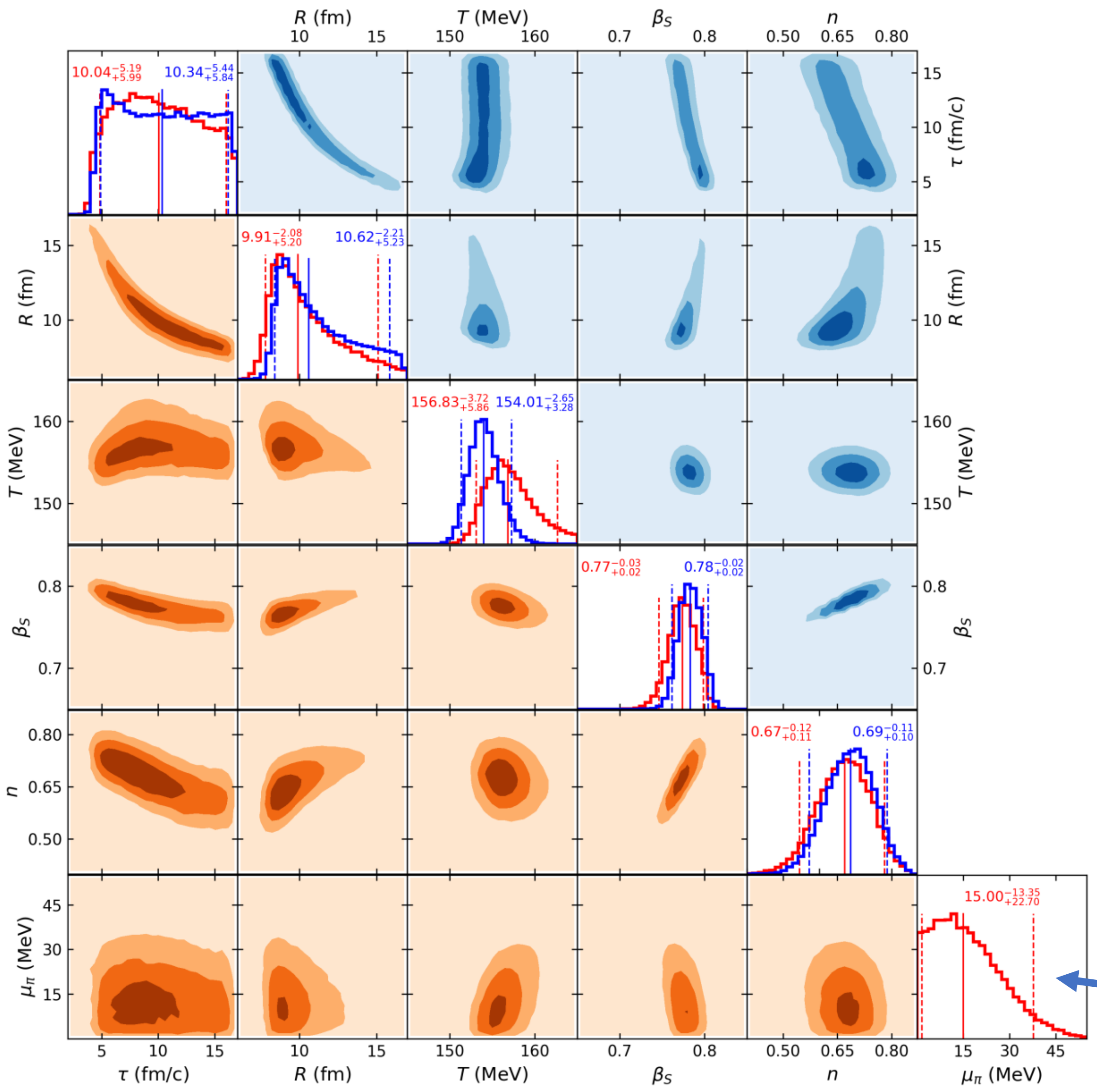


The model gives small but non-zero pion chemical potential

Posterior Probability Distribution



τ, fm/c	R, fm	T, MeV	v	n	μ_π, MeV
8.08	11.50	155.98	0.783	0.697	9.52
8.88	11.54	154.02	0.786	0.699	–

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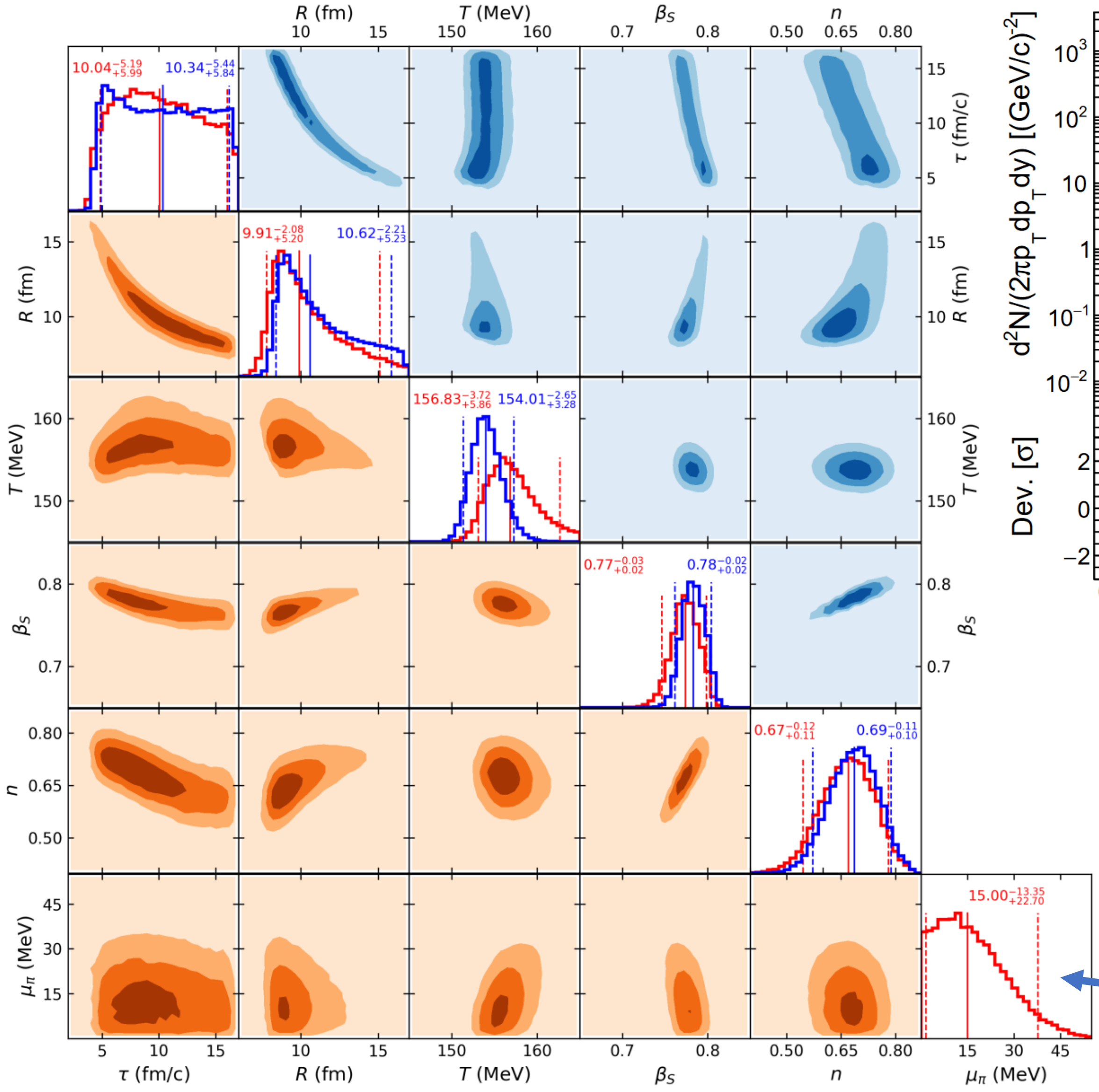

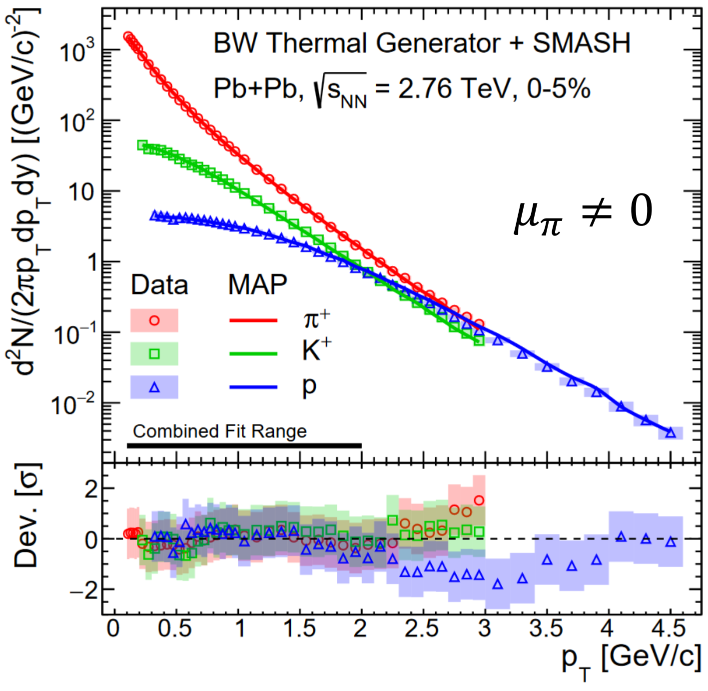

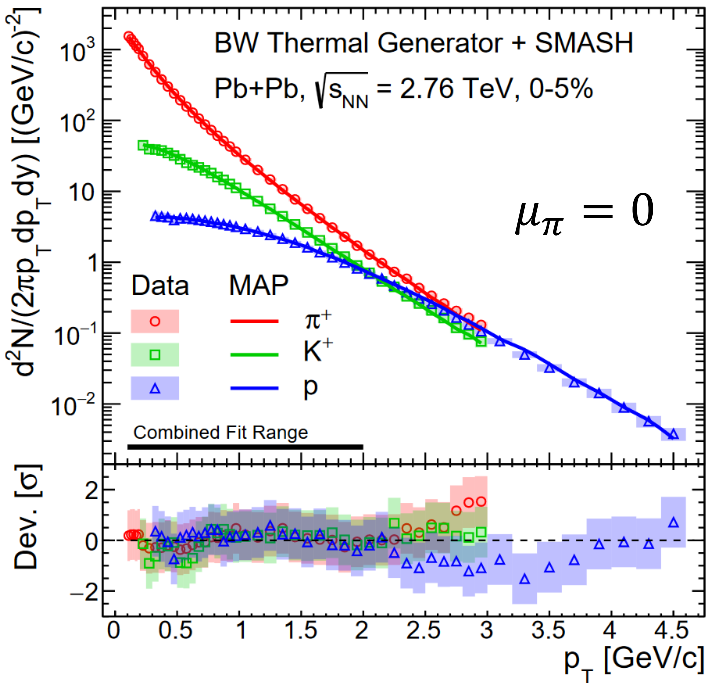

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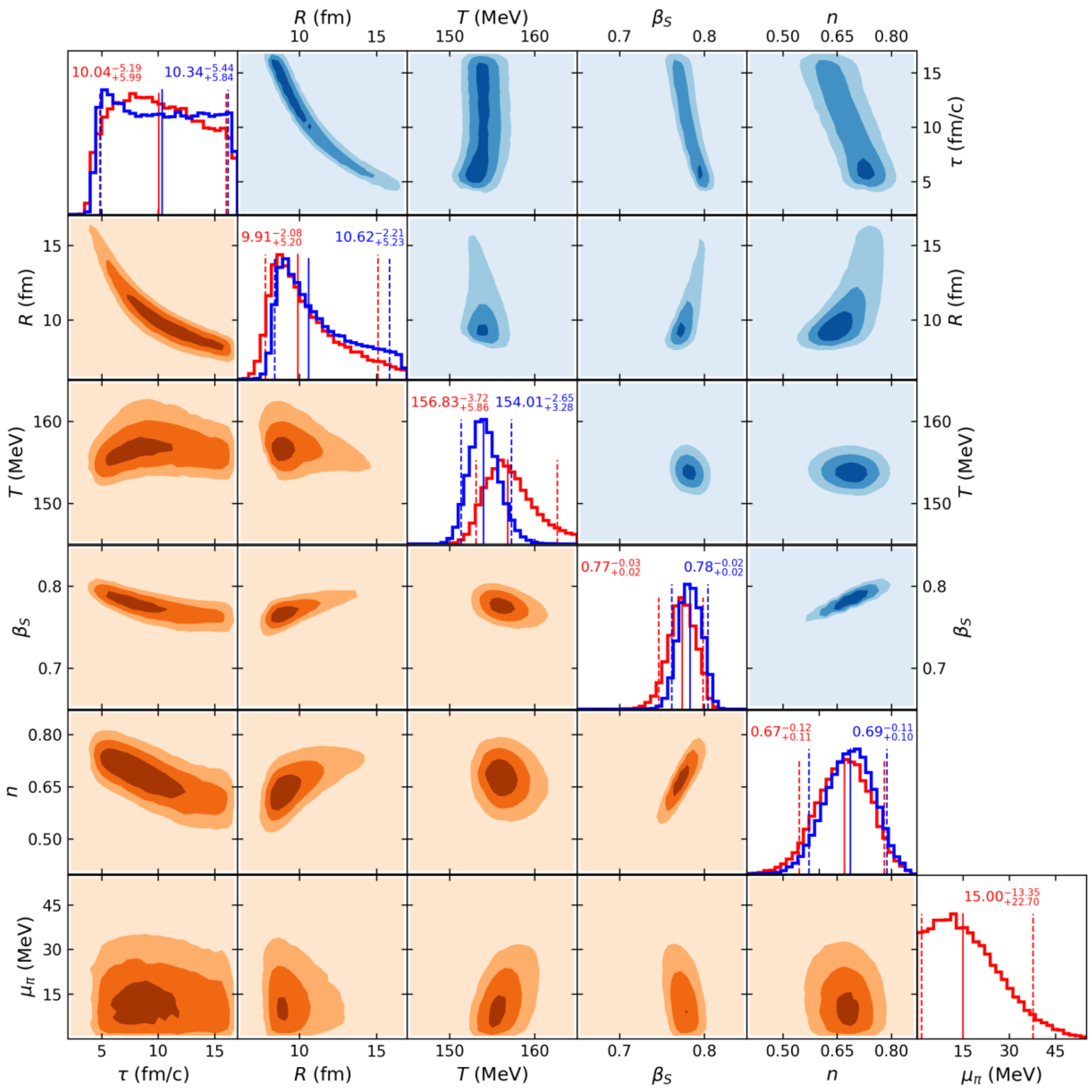
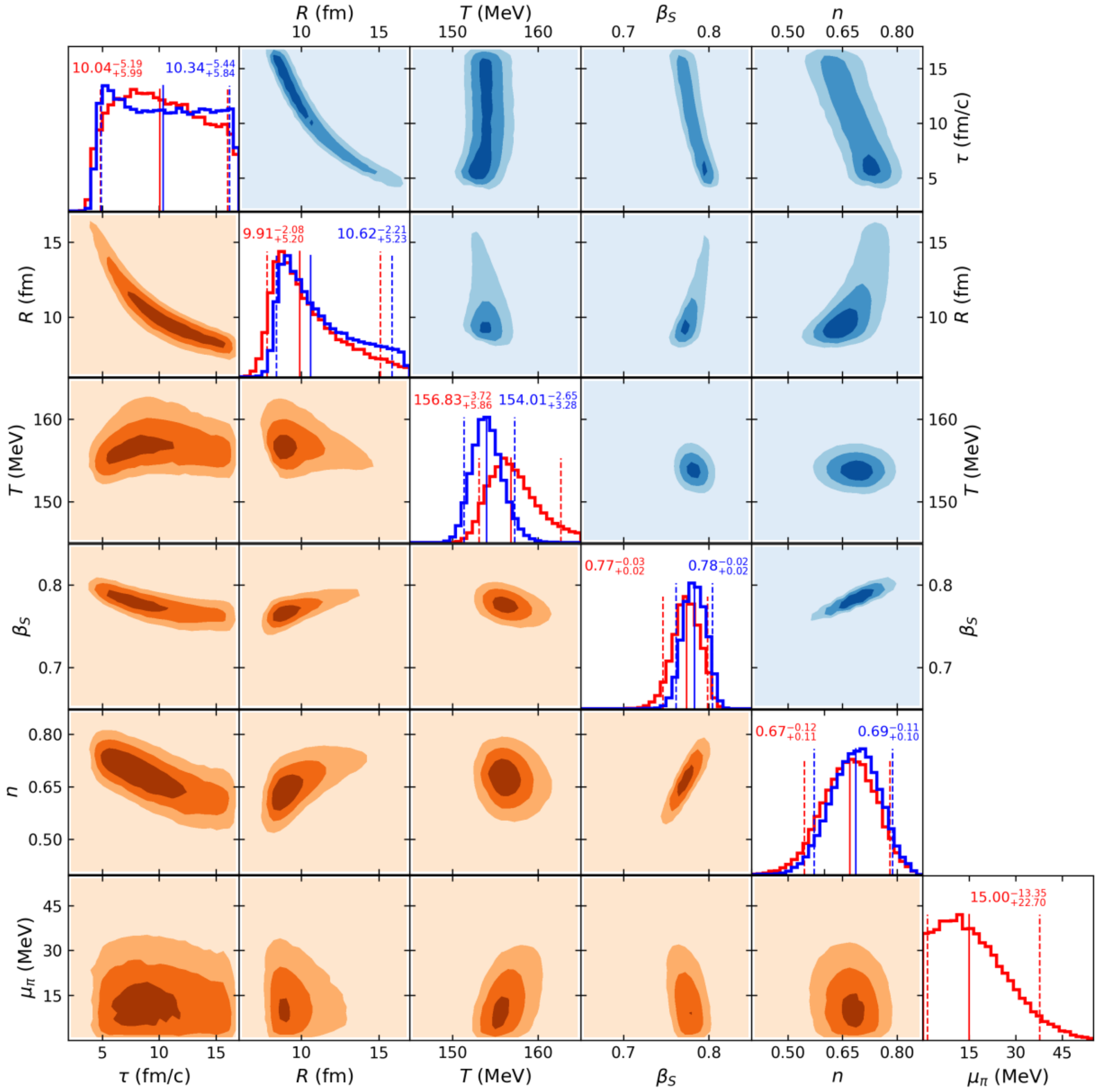
Bayes Factor



$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

According to Jeffreys classification

Bayes Factor



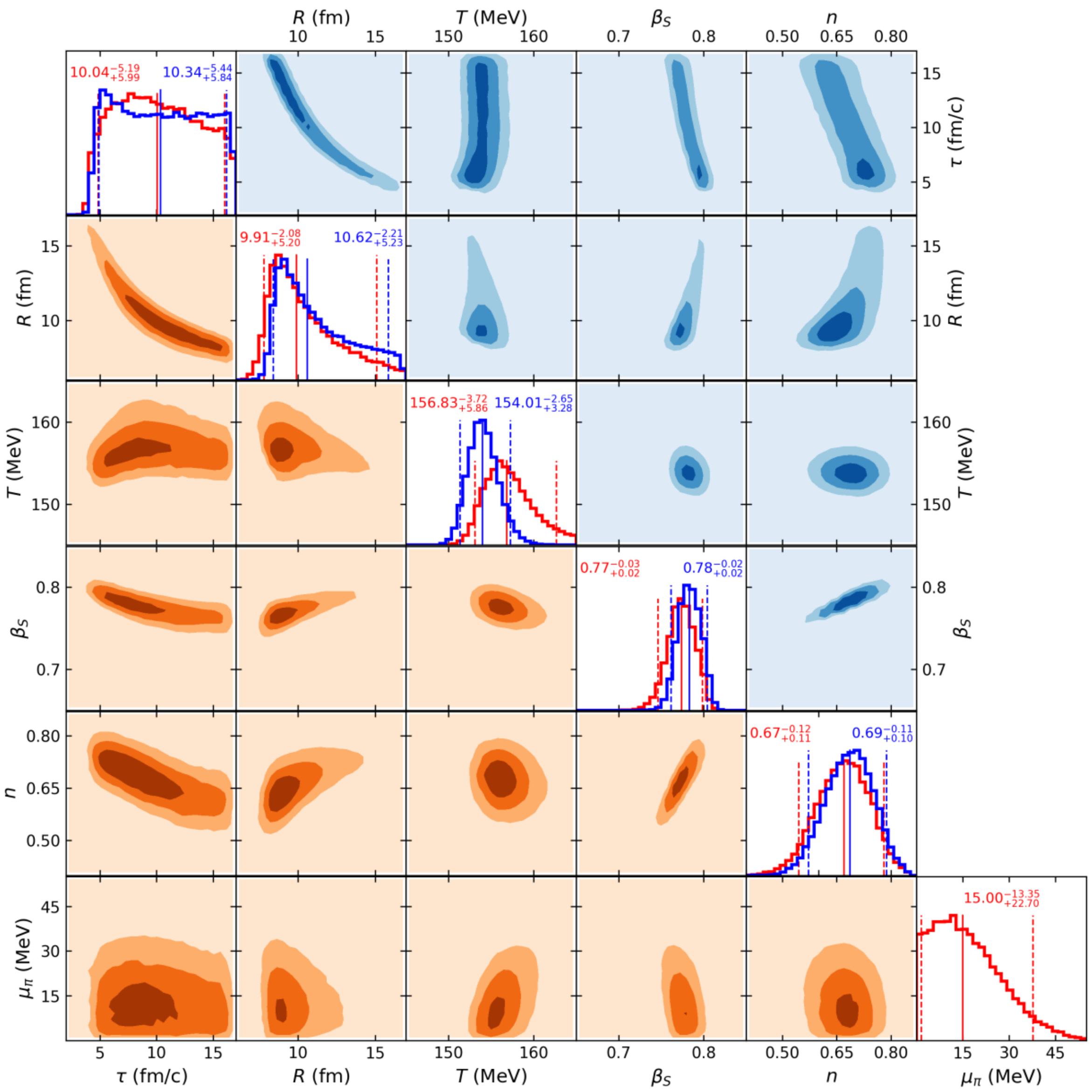
$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

$$P(B|M) = \int P(B|A,M)P(A|M)dA$$

probability that B is produced under the assumption of the model M

According to Jeffreys classification

Bayes Factor



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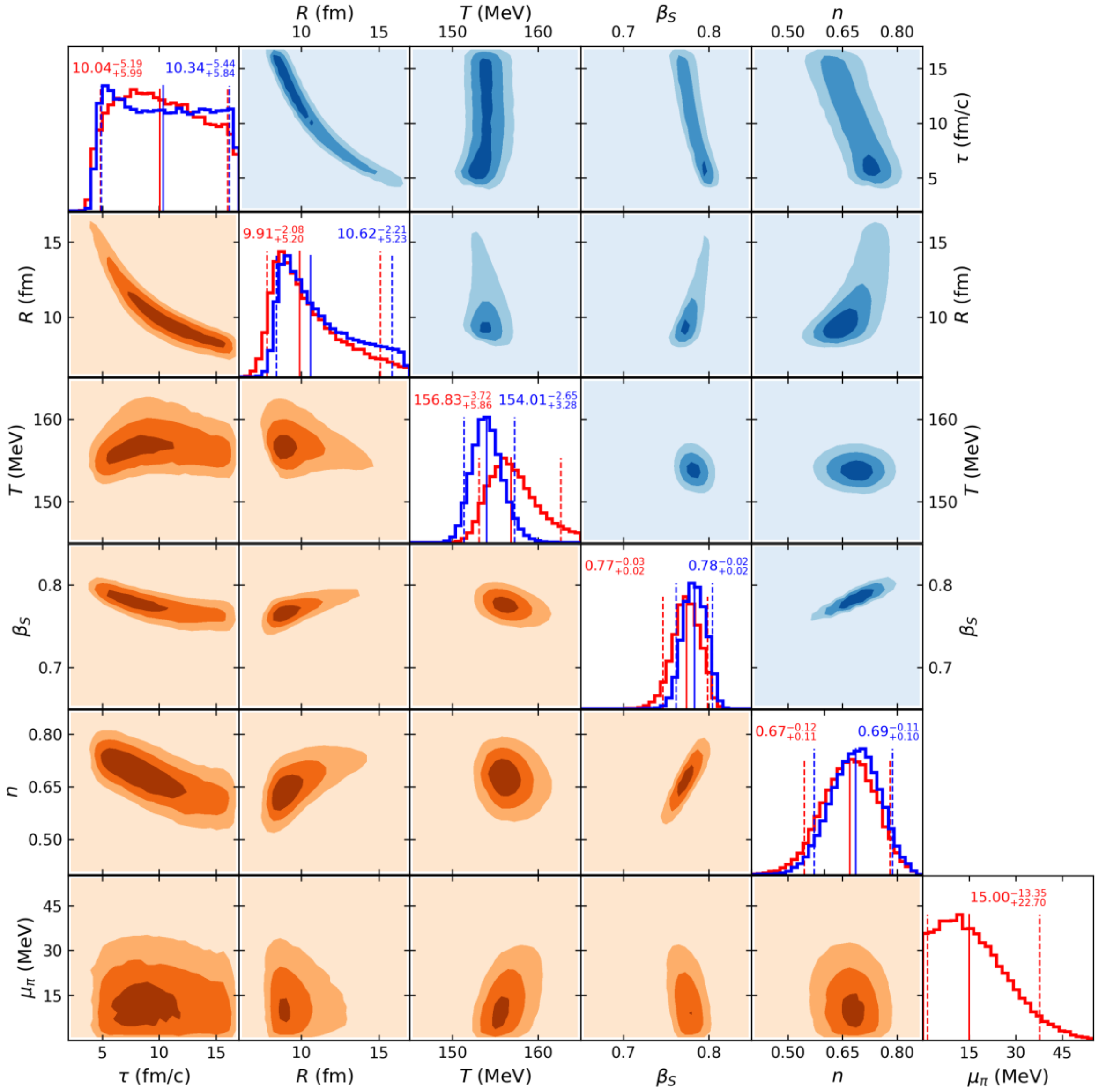
B_{12}	Evidence for M_1
1	Zero
$1-3$	Weak
$3-10$	Moderate
$10-30$	Strong
$30-100$	Very strong
> 100	Extreme

According to Jeffreys classification

Bayes Factor



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$$B_{\mu_\pi=0}^{\mu_\pi\neq 0} = 0.434$$

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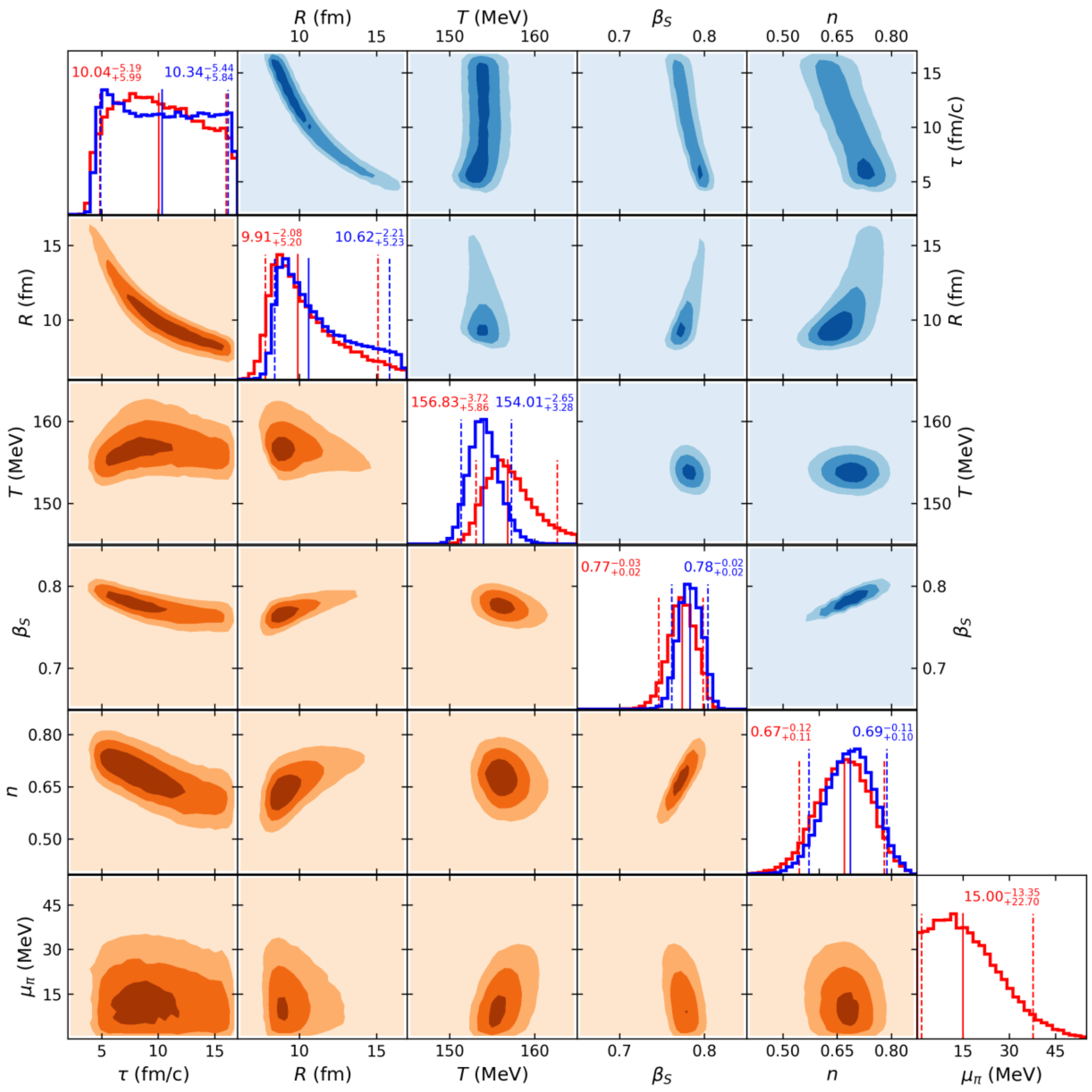

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No evidence for the non-equilibrium hadronization

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Summary

- The non-equilibrium process of pion production within the Zubarev approach of the non-equilibrium statistical operator leads to the appearance of a non-equilibrium pion chemical potential
- NSO method can be used as a powerful tool to fit experimental data
- Naïve model gives the value of effective chemical potential close to the pion mass and can describe data well, but it does not include resonance decays and final state interactions ⇒ Simple receipt for experimentalists to fit the spectra
- Two models of hadronization give very similar parameters and quality of the data description
- Model with extra pions gives small, but non-zero value of pion chemical potential
- No evidence for the non-equilibrium hadronization

Extreme QCD 2025

- **Dates:** July 2 – 4, 2025
- **Venue**: University of Wroclaw,
  Wroclaw, Poland
- **Student support:** fee, travel,
  accommodation
- **Web:** INDICO
  INSPIRE

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XQCD 2025

Uniwersytet Wrocławski

Zubarev approach: Overview

The non-equilibrium state of the system is characterized by relevant observables $\{B_n\}$ in addition to the standard set of conserved ones. We look for the distribution which maximizes the information entropy $\mathrm{S_{inf}} = -\mathrm{Tr}\{\rho_{rel}(t) \ln \rho_{rel}(t)\}$:

$$\rho_{rel}(t) = \frac{1}{Z_{rel}(t)} e^{-\sum_n F_n(t) B_n}, \qquad Z_{rel}(t) = \mathrm{Tr}\left\{e^{-\sum_n F_n(t) B_n}\right\},$$

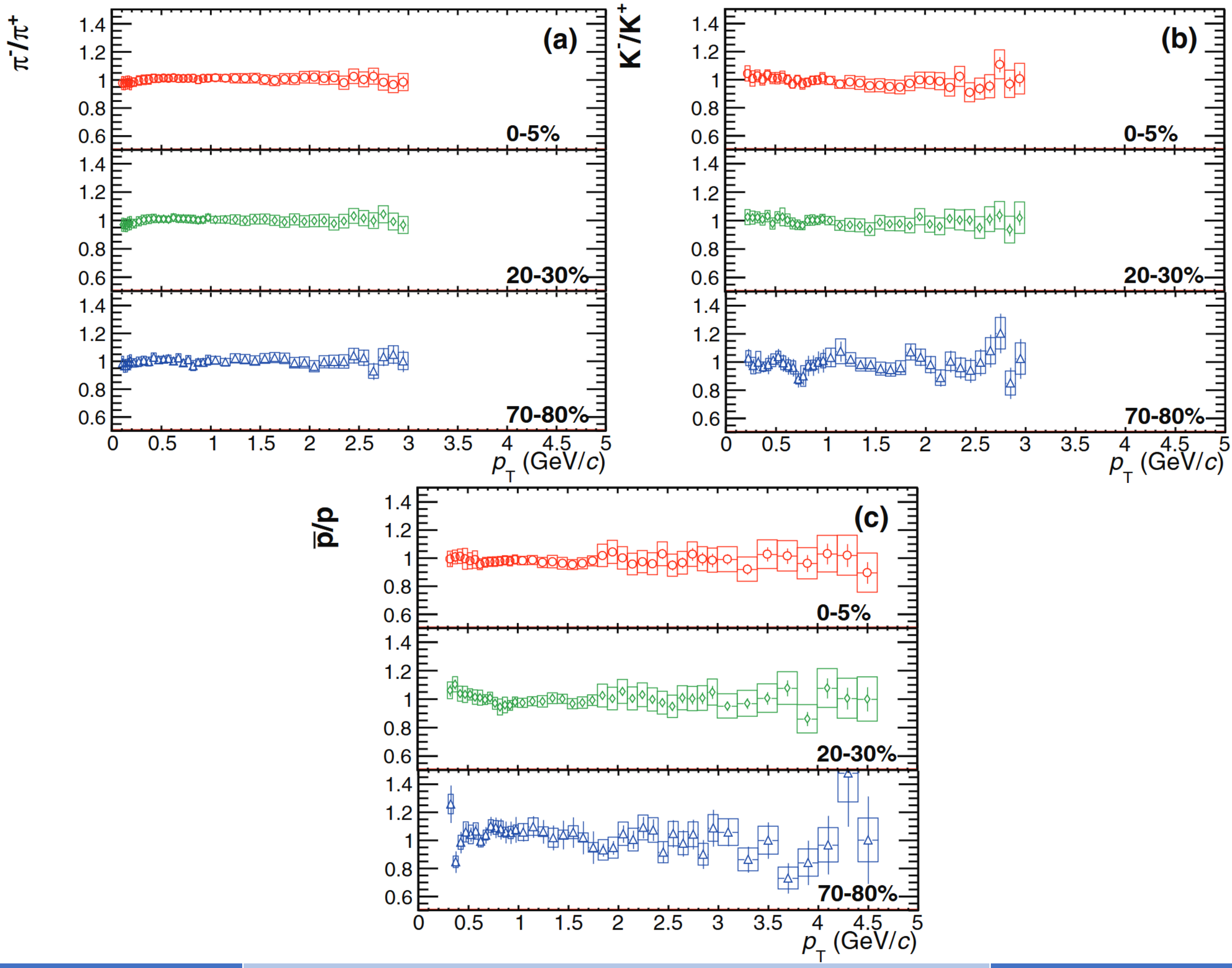
where Lagrange multipliers $F_n(t)$ are determined by the self-consistency conditions

$$\langle B_n \rangle^t = \langle B_n \rangle^t_{rel} = \mathrm{Tr}\{\rho_{rel}(t) B_n\}$$

According to the NSO method, the equations of evolution are given by

$$\frac{d}{dt}\langle B_n \rangle^t = \lim_{\varepsilon \to +0} \frac{i\varepsilon}{\hbar} \int_{-\infty}^{t} dt'\, e^{\varepsilon(t'-t)} \mathrm{Tr}\left\{\rho_{rel}(t) e^{iH(t'-t)/\hbar} [H, B_n] e^{iH(t-t')/\hbar}\right\}$$

There is no unique way to choose the relevant observables. In principle, all choices for the set of relevant observables should give the same result, but in practice it is not the case.



π^-/π^+
(a)
0-5%
20-30%
70-80%
K^-/K^+
(b)
0-5%
20-30%
70-80%
$\bar{p}/p$
(c)
0-5%
20-30%
70-80%
p_T (GeV/c)

MCMC

Problem: We don't have an analytic form of $\vec{y}(\vec{x}) \Rightarrow$ we don't have an analytic expression for $\mathcal{L}(\vec{x}; \vec{y}^{obs})$

Solution: Markov Chain Monte-Carlo Sampling

Example: Metropolis-Hastings algorithm

1. Draw a proposal for $\vec{x}_i \to \vec{x}'_{i+1}$ from the proposal distribution Q
2. Compute acceptance probability $A(\vec{x}_i \to \vec{x}'_{i+1}) = \min\left(1; \frac{\mathcal{L}(\vec{x}'_{i+1}; \vec{y}^{obs}) \times P(\vec{x}'_{i+1})}{\mathcal{L}(\vec{x}_i; \vec{y}^{obs}) \times P(\vec{x}_i)} \frac{Q(\vec{x}'_{i+1} \to \vec{x}_i)}{Q(\vec{x}_i \to \vec{x}'_{i+1})}\right)$
3. Pick a random number r from uniform range [0, 1]
4. If $A(\vec{x}_i \to \vec{x}'_{i+1}) > r$, accept the proposed move and set $\vec{x}_{i+1} = \vec{x}'_{i+1}$. Otherwise set $\vec{x}_{i+1} = \vec{x}_i$
5. Set $i = i + 1$ and repeat the process

Gaussian Processes

Problem: MCMC requires many model evaluations to reconstruct the likelihood function.

Solution: Emulate model using Gaussian processes

Gaussian process - a stochastic process, in which every finite set $\{Y_i\}_{i=1}^{m}$ is a multivariate Gaussian random variable $N(\vec{\mu}, \Sigma)$. Approach based on the important property of multivariate normal distribution:

Let $\mathrm{A} \sim N(\vec{\mu}, \Sigma)$. If $\mathrm{A}' = \mathrm{TA} + \mathrm{c}$, then $\mathrm{A}' \sim N(T\vec{\mu} + c, T\Sigma\mathrm{T}^{\mathrm{T}})$.

$$J = \begin{bmatrix} A \\ B \end{bmatrix} \sim N\left(\begin{bmatrix} \mu_A \\ \mu_B \end{bmatrix}, \begin{bmatrix} \Sigma_A & \Sigma_{AB} \\ \Sigma_{AB} & \Sigma_B \end{bmatrix}\right), T = \begin{bmatrix} I & -\Sigma_{AB}\Sigma_B^{-1} \\ 0 & I \end{bmatrix}, J' = T(J - \mu_J) = \begin{bmatrix} A' \\ B' \end{bmatrix} \sim N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \Sigma_A - \Sigma_{AB}\,\Sigma_B^{-1}\Sigma_{BA} & 0 \\ 0 & \Sigma_B \end{bmatrix}\right)$$

$$A'\Big|_{B=b_0} \sim N(0, \Sigma_A - \Sigma_{AB}\,\Sigma_B^{-1}\Sigma_{BA}) \Rightarrow A\Big|_{B=b_0} \sim N(\mu_A + \Sigma_{AB}\Sigma_B^{-1}(b_0 - \mu_B), \Sigma_A - \Sigma_{AB}\,\Sigma_B^{-1}\Sigma_{BA})$$

We need to know the covariance matrix for the given data set. It is parametrized in terms of hyperparameters $\vec{\theta}$

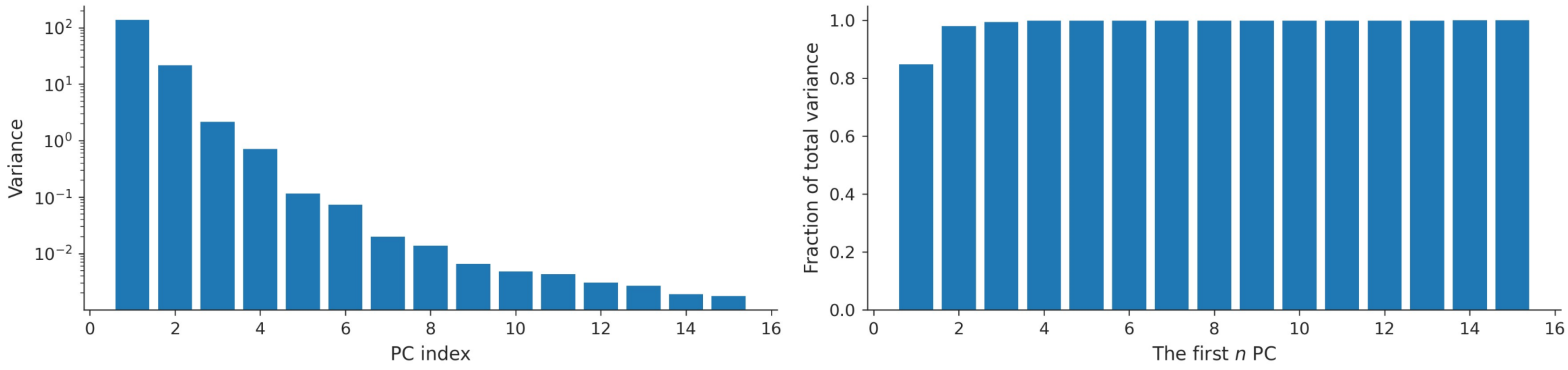
$$\Sigma_{\mathrm{ij}} = \mathrm{K}(x_i, x_j; \vec{\theta}) \Rightarrow \frac{d \ln P\left(Y|\vec{\theta}\right)}{d\vec{\theta}} = 0$$

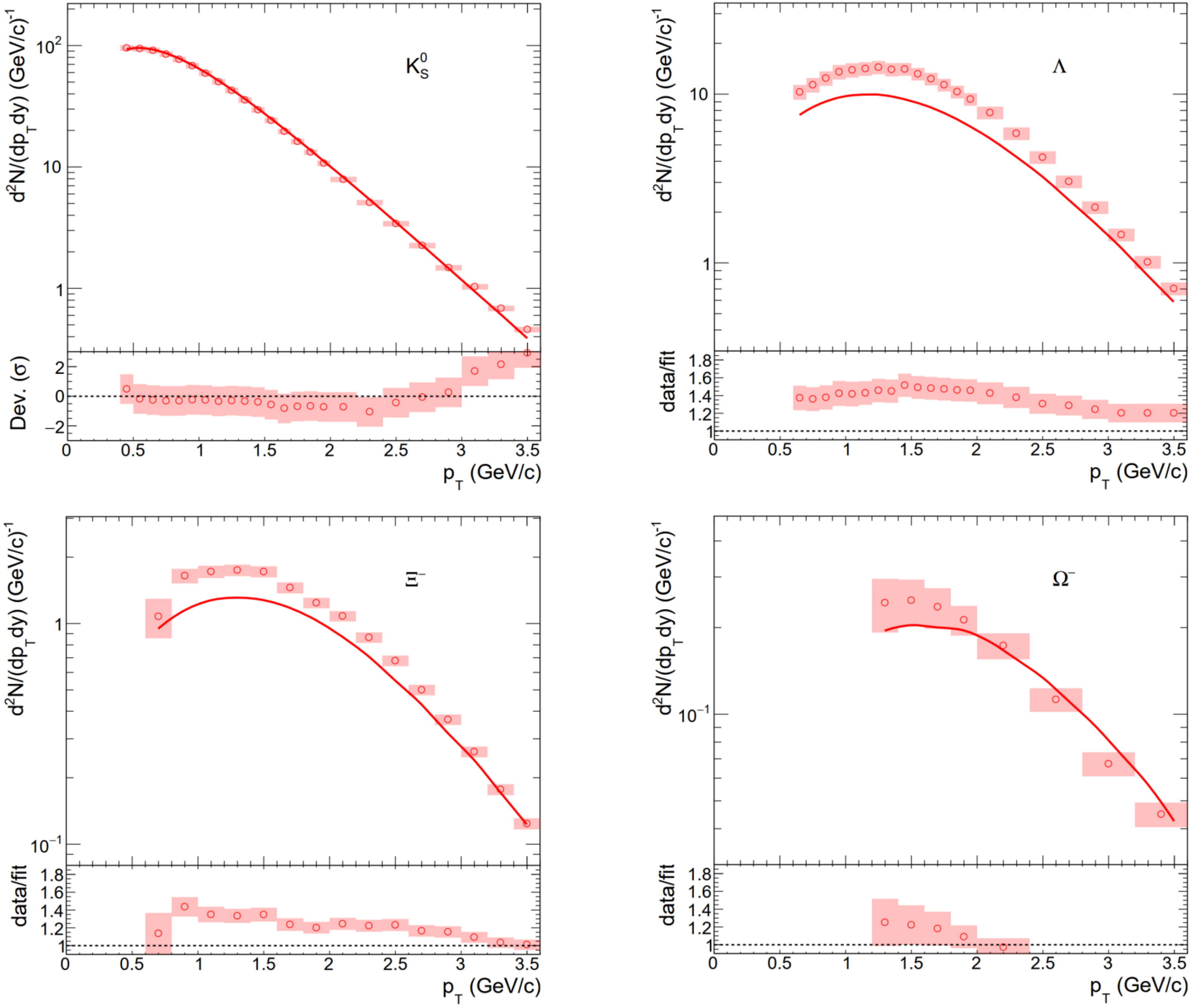
Principal Component Analysis

Problem: GP can take a multidimensional input, but the output is always a scalar.
M observables $= M$ GP emulators. Typical order is $O(100)$ observables.

Solution: Dimension reduction via Principal Component Analysis

1. Let us define the matrix $M_{ij} = \frac{y_i(x_j) - \langle y_i \rangle}{\sigma_i} \rightarrow C = M^T M - m \times m$ covariance matrix
2. Sort eigenvalues λ_i and eigenvectors $\vec{v}_i$ of matrix C in descending order of λ_i
3. Keep p first components which together explain the desired fraction of total variance
4. $V_p = [\vec{v}_1 \quad \dots \quad \vec{v}_p] \rightarrow \vec{z} = \vec{y}\, V_p,\ \vec{y} = \vec{z}\, V_p^T,\ \Sigma_z = V_p^T \Sigma_y V_p$





K^0_S
Λ
Ξ^-
Ω^-
$d^2N/(dp_T dy)$ (GeV/c)$^{-1}$
Dev. (σ)
data/fit
p_T (GeV/c)