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

Oleksandr Vitiuk[1], David Blaschke[1,2,3], Benjamin Dönigus[4], Gerd Röpke[5]

[1]University of Wroclaw, Poland
[3]Center for Advanced Systems Understanding, Germany
[5]University of Rostock, Germany

[2]Helmholtz-Zentrum Dresden-Rossendorf, Germany
[4]Goethe University Frankfurt, Germany

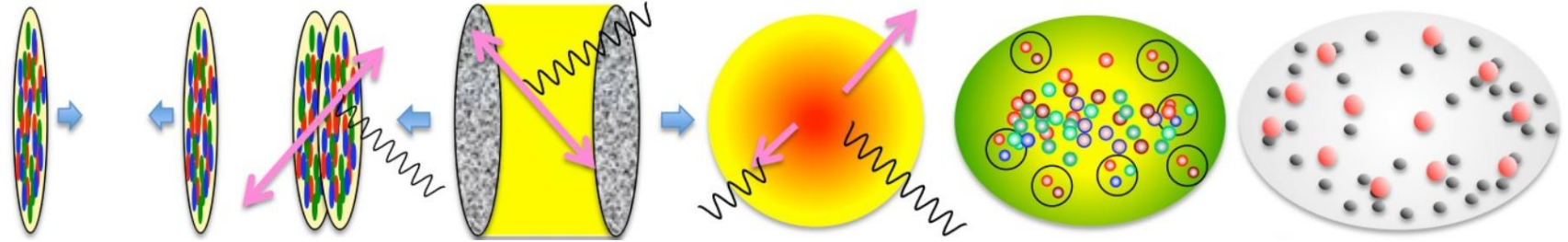XVI Polish Workshop on Relativistic Heavy-Ion Collisions
December 2nd, 2023, Kielce, Poland

Outline

- Introduction
- Theoretical background
  - Zubarev approach
  - Blast-Wave Model
- Fit to experimental data
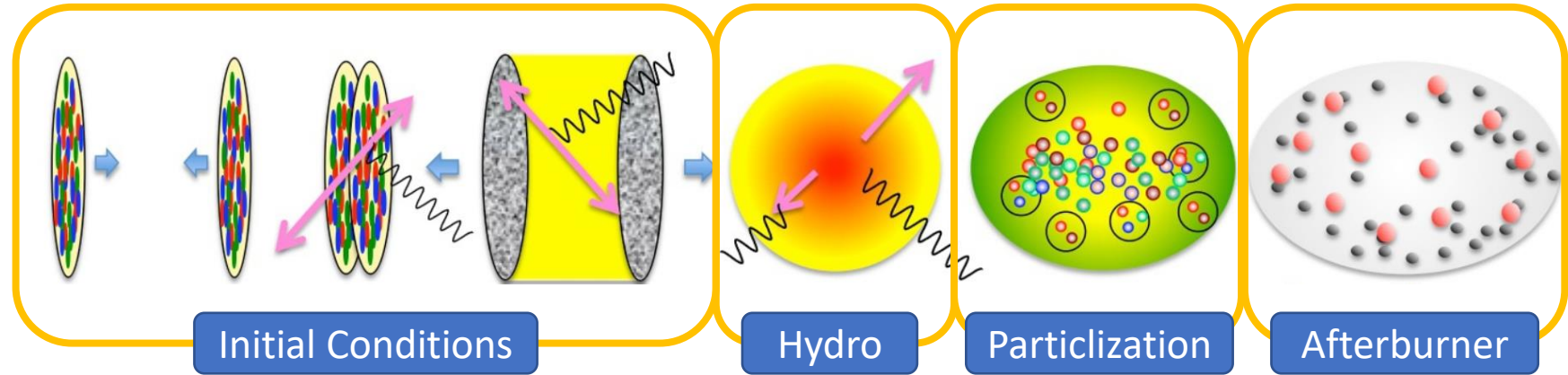 - Bayesian inference
  - Results
- Summary

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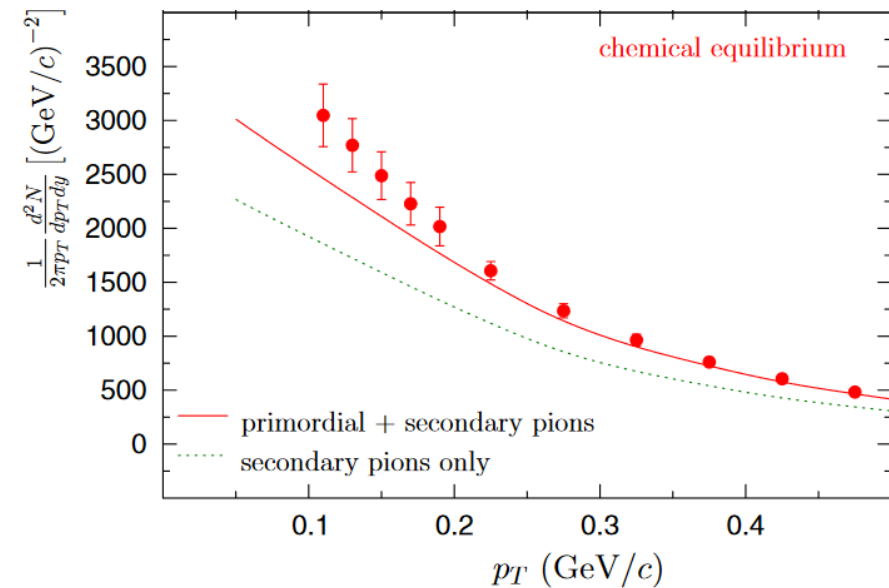
Hydro

Particlization

Afterburner

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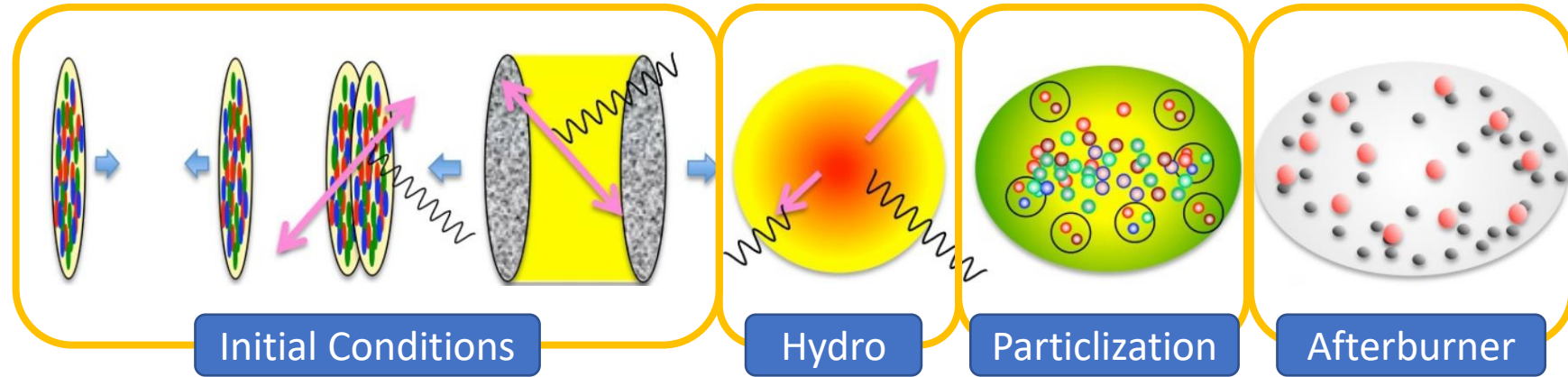[V. Begun et al., PRC 90, 014906 (2014)]

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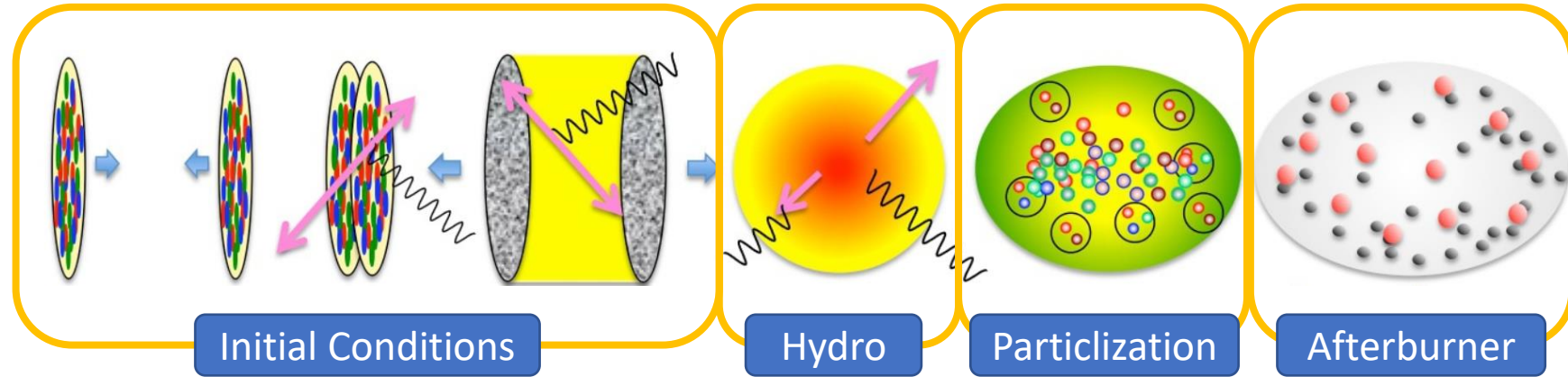
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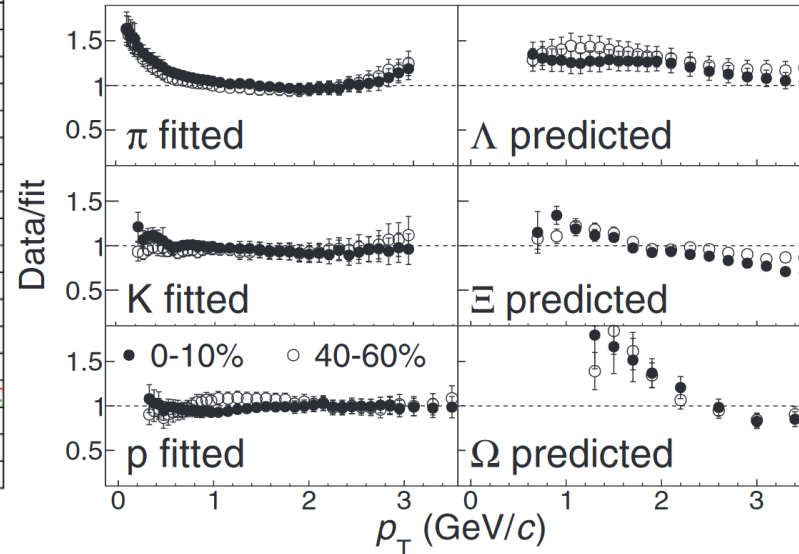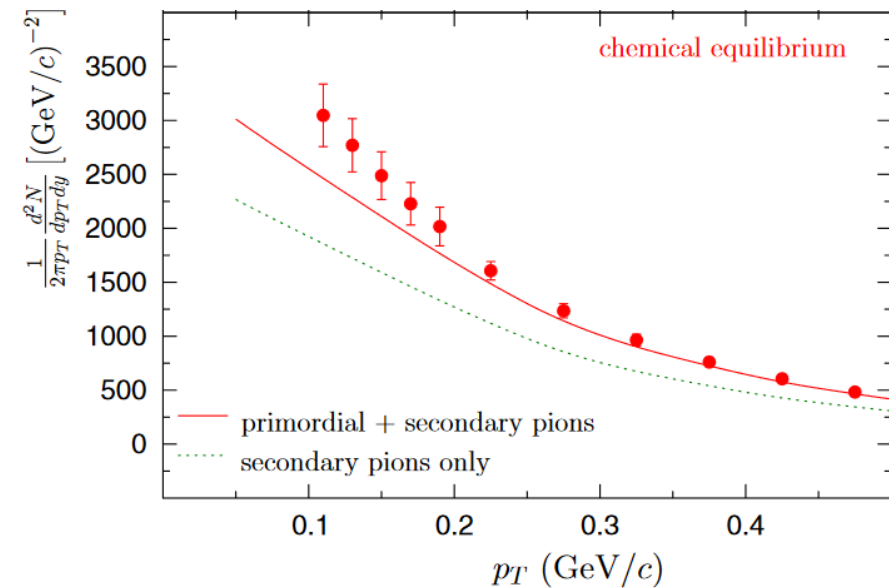Initial Conditions   Hydro   Particlization   Afterburner
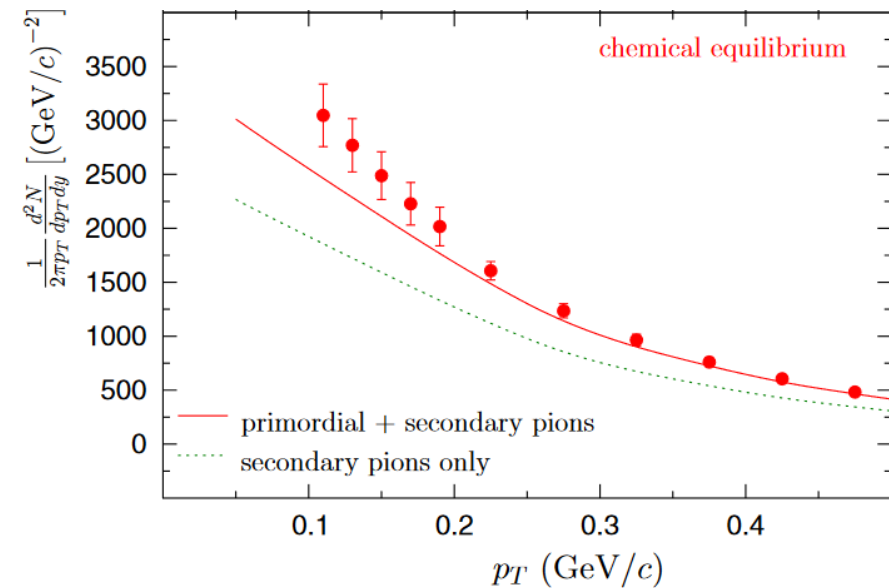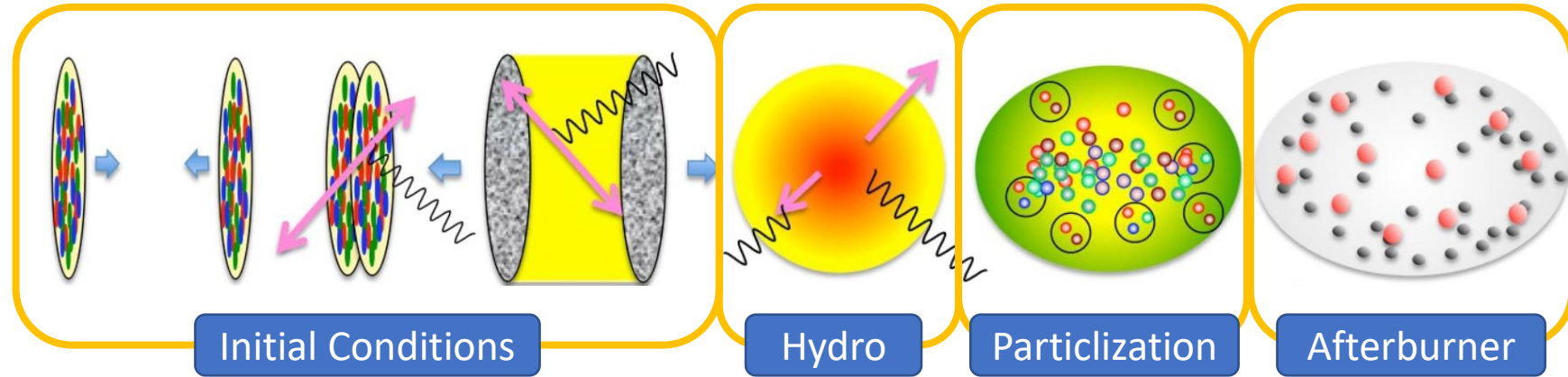
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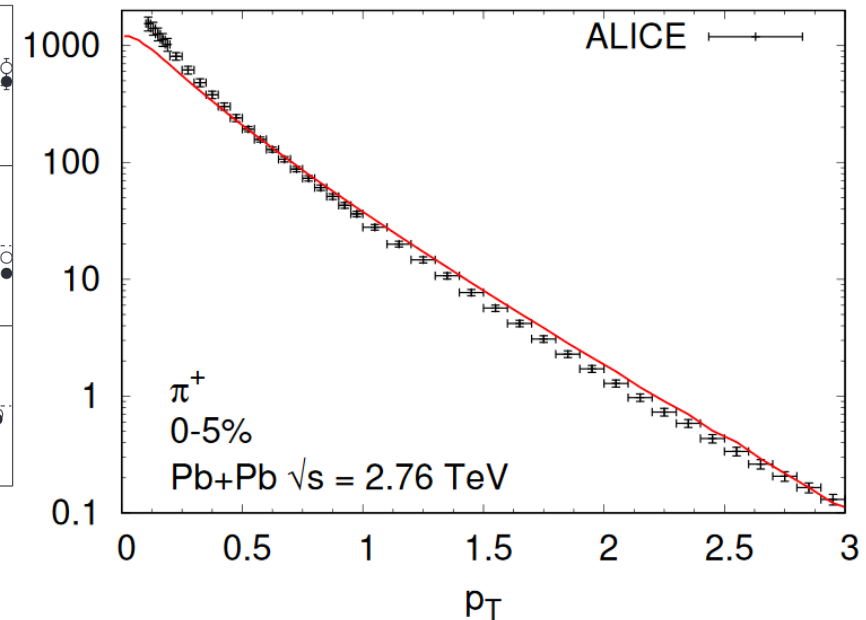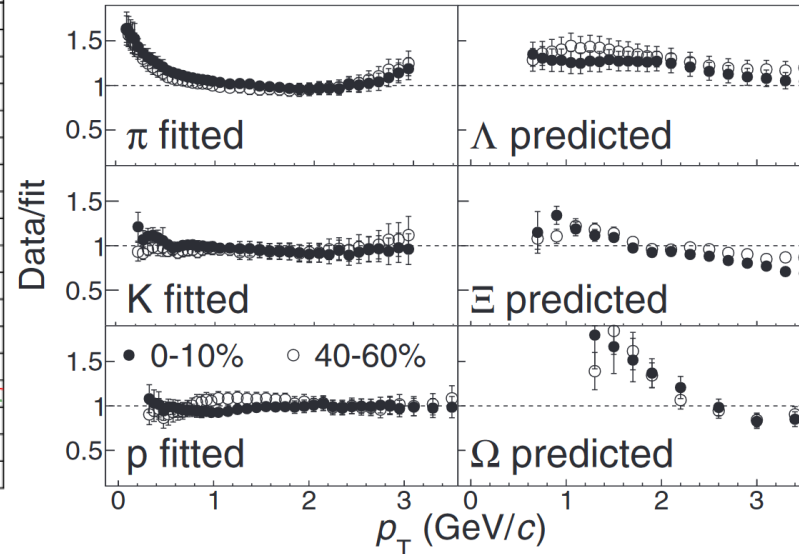

Initial Conditions

Hydro

Particlization

Afterburner

chemical equilibrium

primordial + secondary pions

secondary pions only

p fitted

Ω predicted

ALICE

π^+
0-5%
Pb+Pb $\sqrt{s}$ = 2.76 TeV
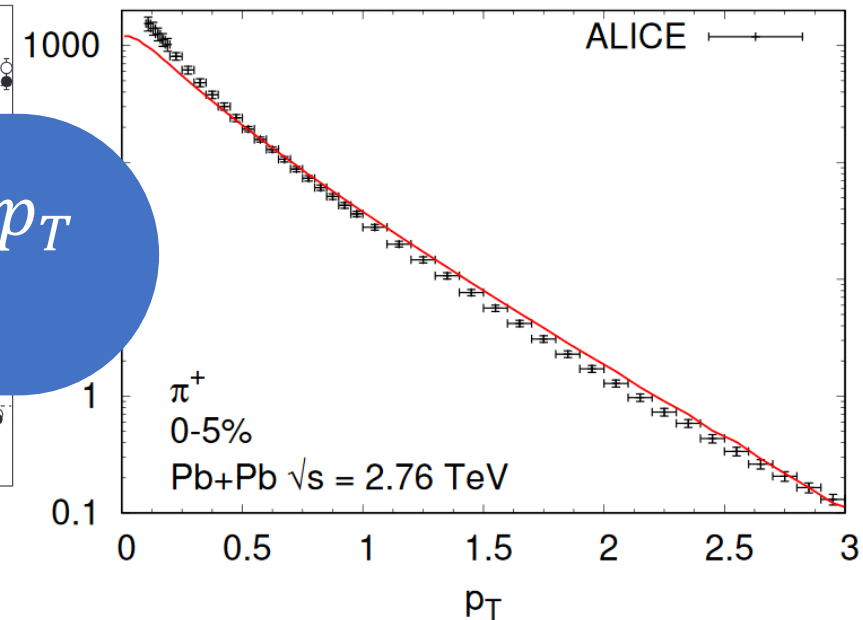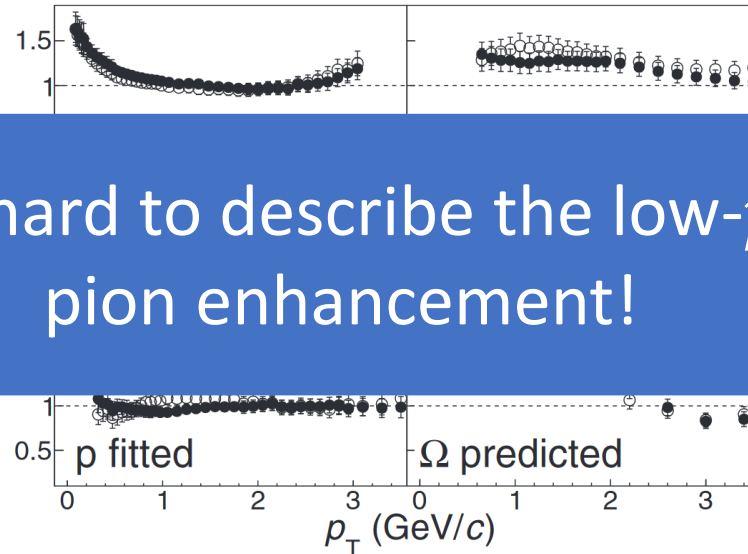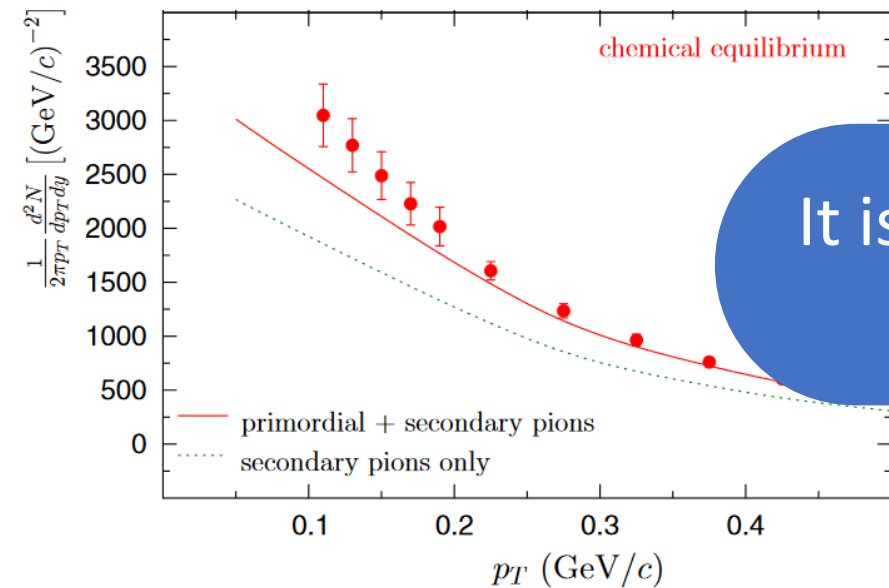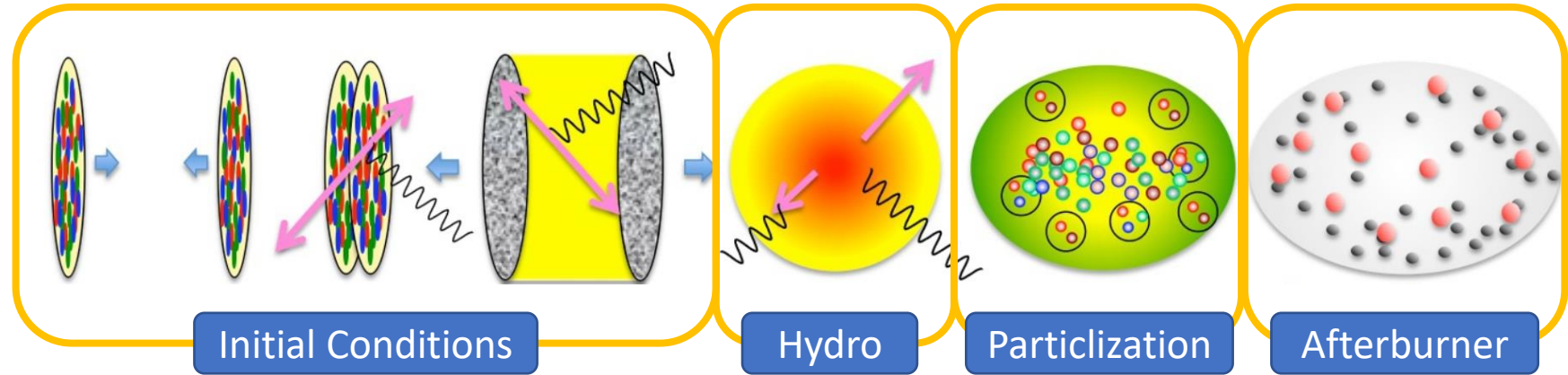
It is hard to describe the low-p_T pion enhancement!

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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 $S_{\text{inf}} = -\text{Tr}\{\rho_{rel}(t) \ln \rho_{rel}(t)\}$:

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

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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.

Zubarev approach: Model for π

Here we assume the following:

- A state overpopulated by soft pions is formed at $\tau < \tau_\pi^{CFO}$
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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
[Particles 2020, 3, 380–393]

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

Blast-Wave Model

Here we consider chemical freeze-out on the cylindrical boost-invariant hypersurface at constant freeze-out proper time

$$\Sigma^\mu = (\tau \cosh \eta, r \cos \varphi, r \sin \varphi, \tau \sinh \eta), \text{where } \tau = \sqrt{t^2 - z^2} = const. \text{ and } \eta = \frac{1}{2} \ln \frac{t+z}{t-z}$$
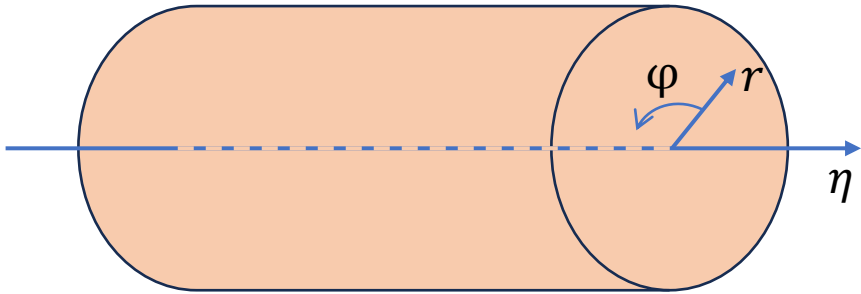
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Then with the help of the Cooper-Frye formula $E \frac{d^3 N}{d^3 \vec{p}} = \int_{\Sigma_{FO}} p^\mu d\Sigma_\mu \, f(x^\mu, p^\mu u_\mu)$ one finds

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

$$p_T = \sqrt{p_x^2 + p_y^2}, \qquad m_T = \sqrt{m_i^2 + p_T^2}, \qquad y = \frac{1}{2} \ln \frac{E + p_z}{E - p_z}$$
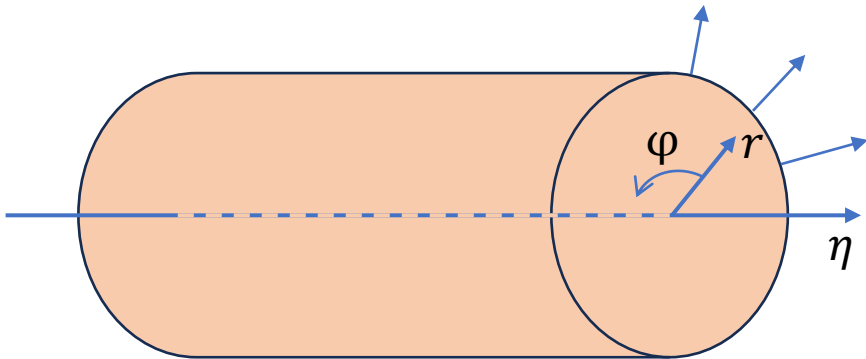
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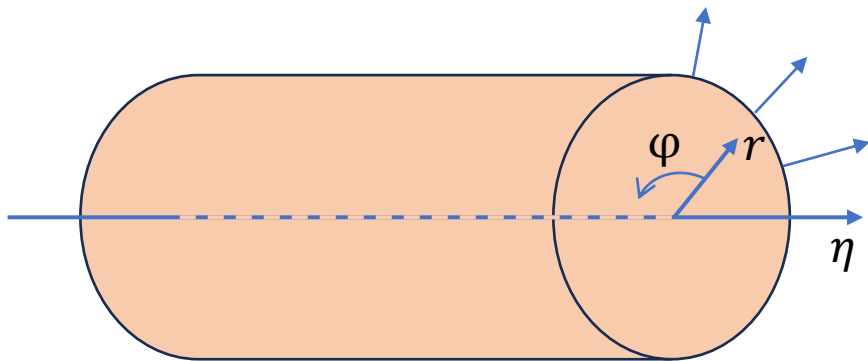
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τ, R, T, μ_π, v and n are free model parameters
In some cases, the overall normalization is defined with the combination τR^2
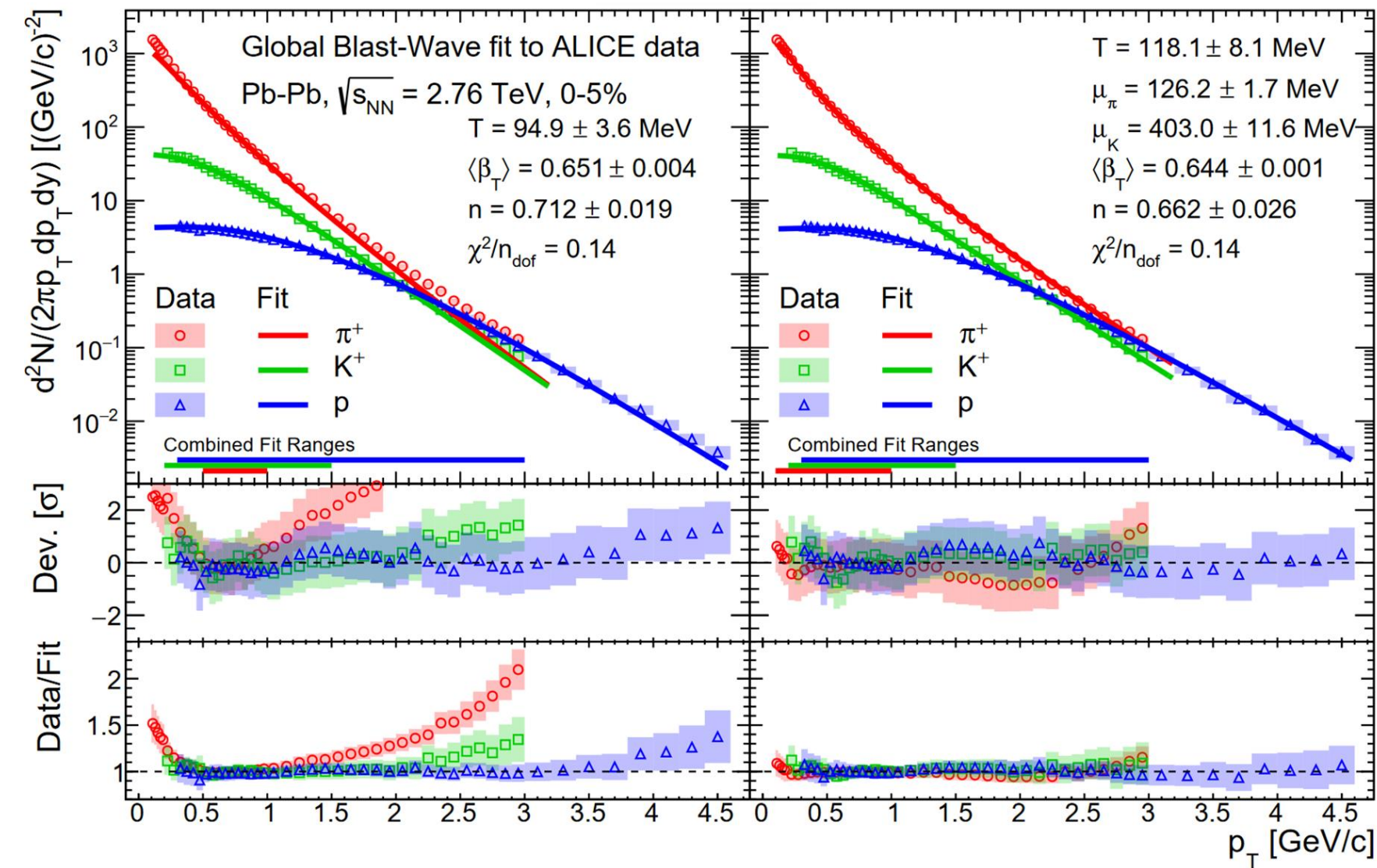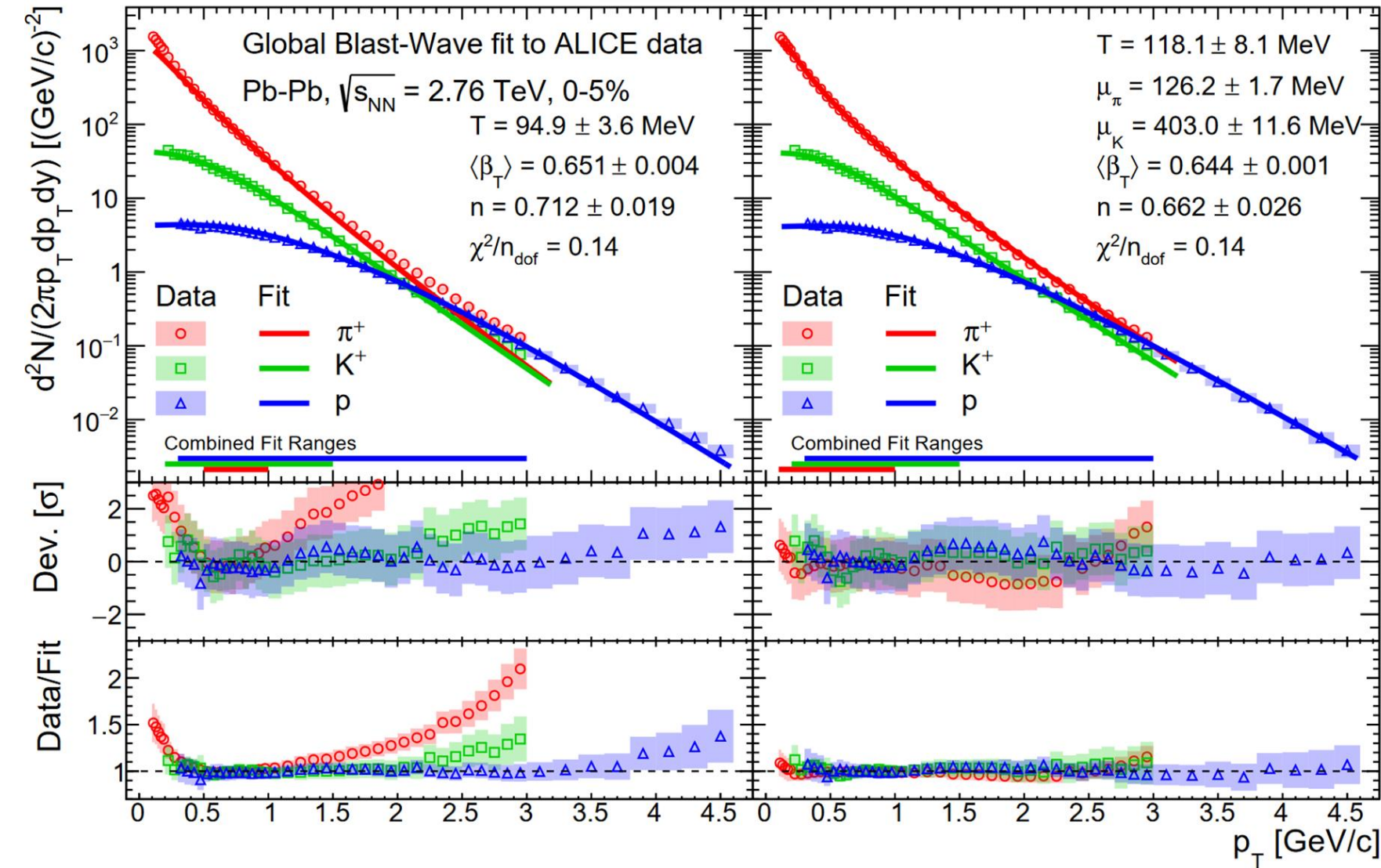
Naïve Model

Global Blast-Wave fit to ALICE data

Pb-Pb, $\sqrt{s_{NN}}$ = 2.76 TeV, 0-5%

$T = 94.9 \pm 3.6$ MeV

$\langle \beta_T \rangle = 0.651 \pm 0.004$

$n = 0.712 \pm 0.019$

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

$T = 118.1 \pm 8.1$ MeV

$\mu_\pi = 126.2 \pm 1.7$ MeV

$\mu_K = 403.0 \pm 11.6$ MeV

$\langle \beta_T \rangle = 0.644 \pm 0.001$

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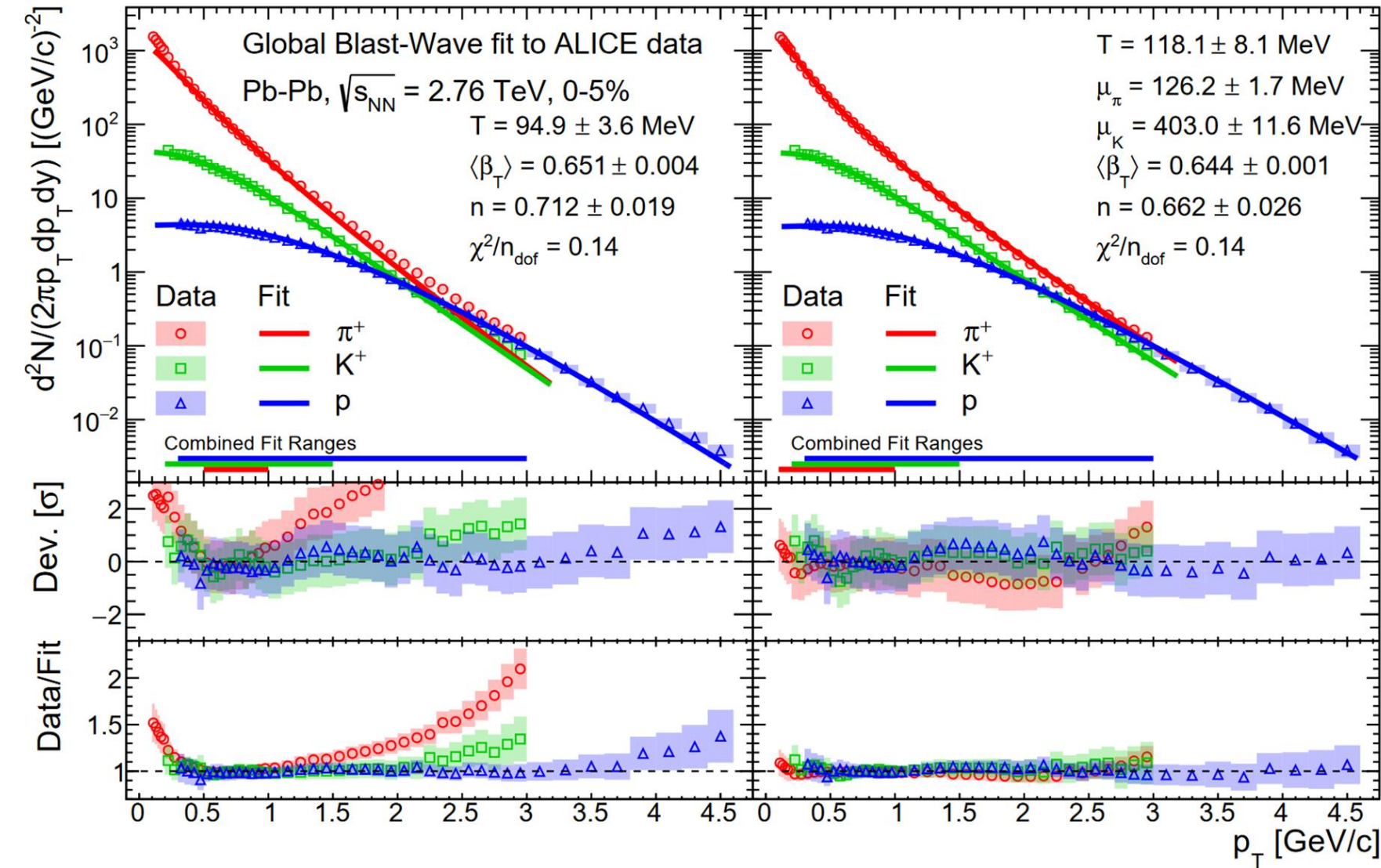$\langle \beta_T \rangle$ = 0.644 ± 0.001
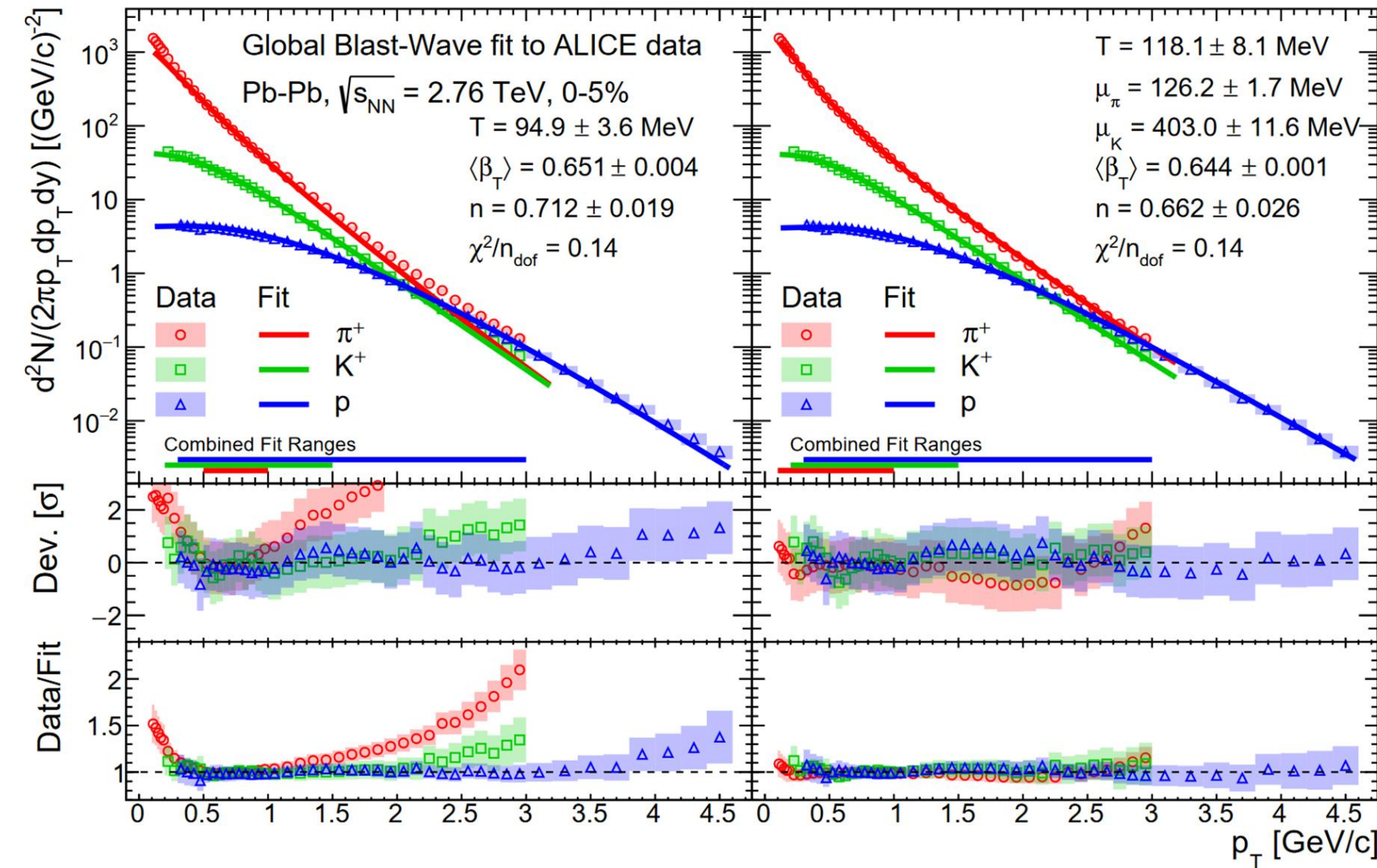n = 0.662 ± 0.026
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Thermal particle generator ➕ smash

Afterburner instead of solving generalized kinetics!

Bayesian Inference

Bayes theorem:

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

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

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

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Prior

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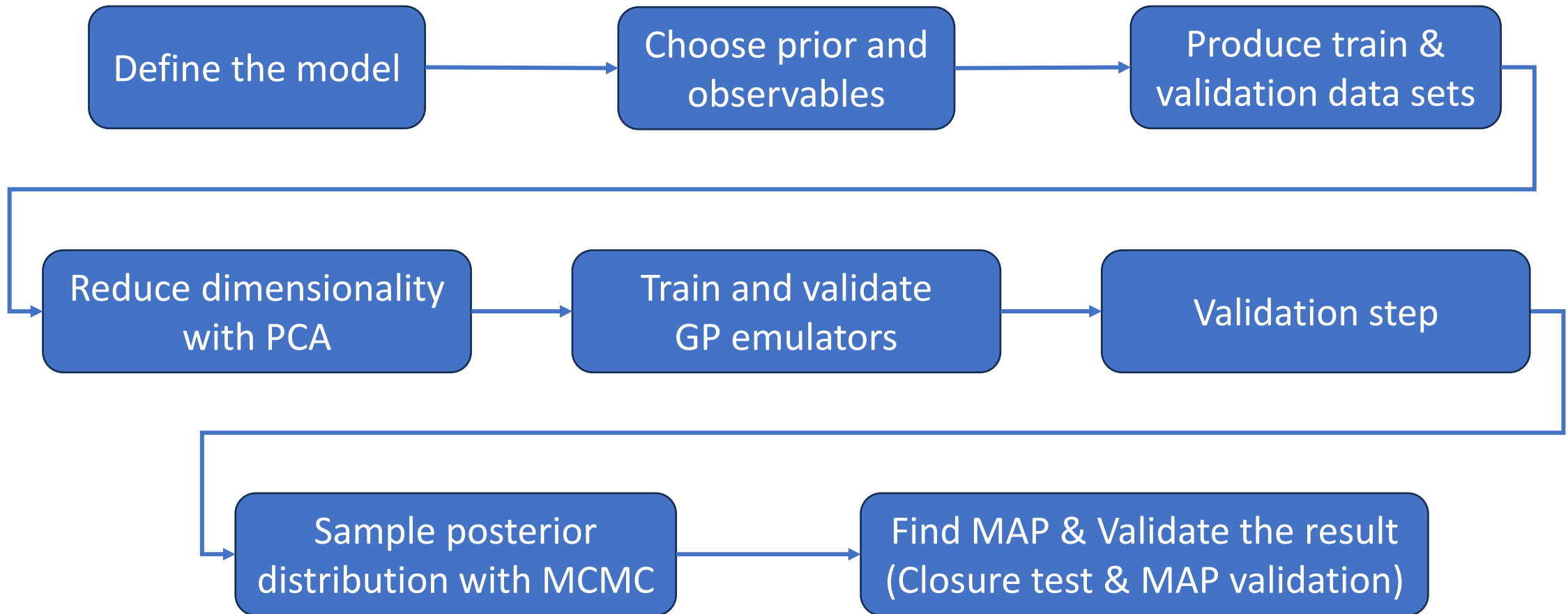$$\mathrm{P}(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

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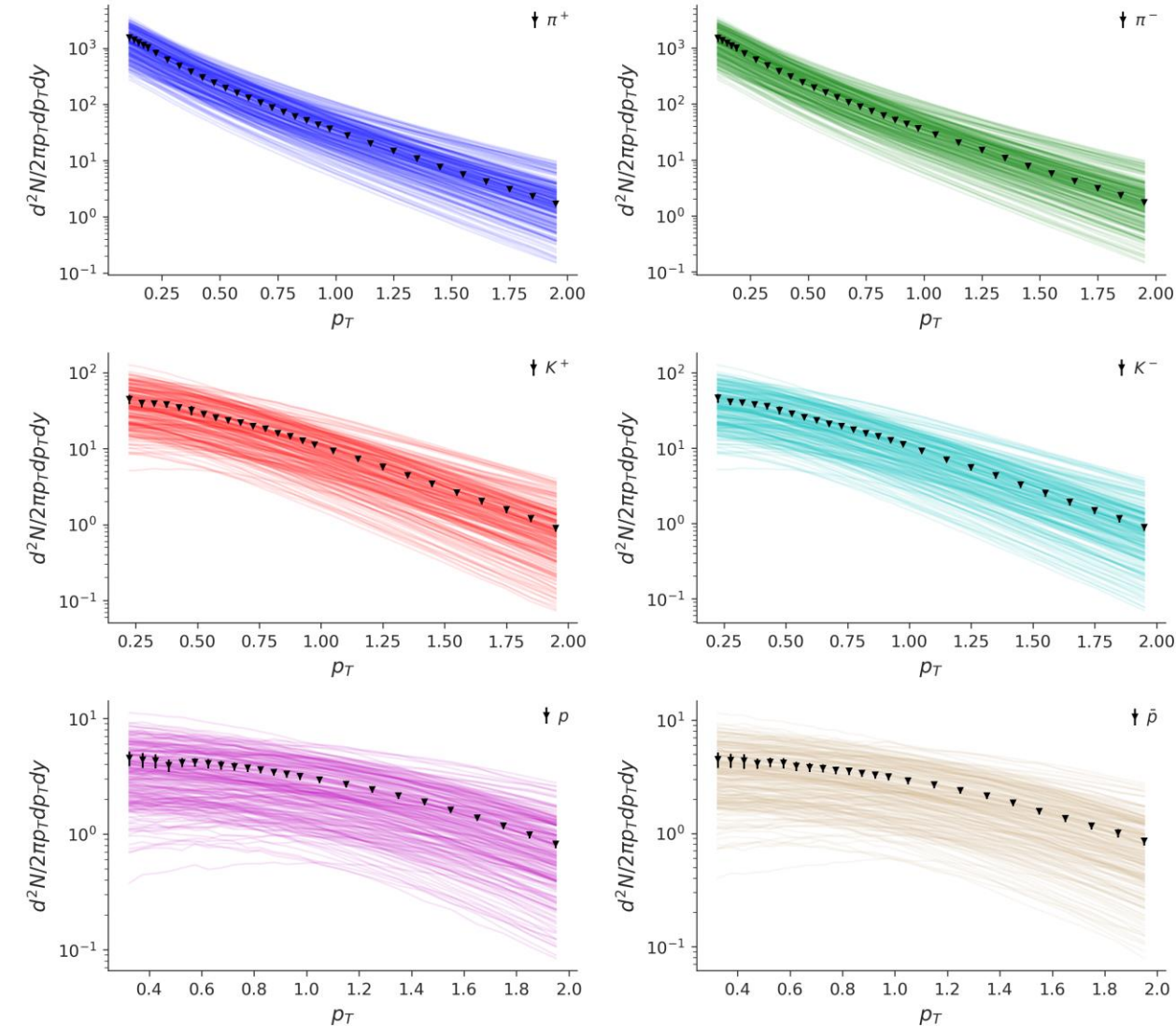
If we know mean values and variance, then the likelihood takes the form of multivariate Gaussian

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

Bayesian Inference Workflow

Define the model → Choose prior and observables → Produce train & validation data sets → Reduce dimensionality with PCA → Train and validate GP emulators → Validation step → Sample posterior distribution with MCMC → Find MAP & Validate the result (Closure test & MAP validation)
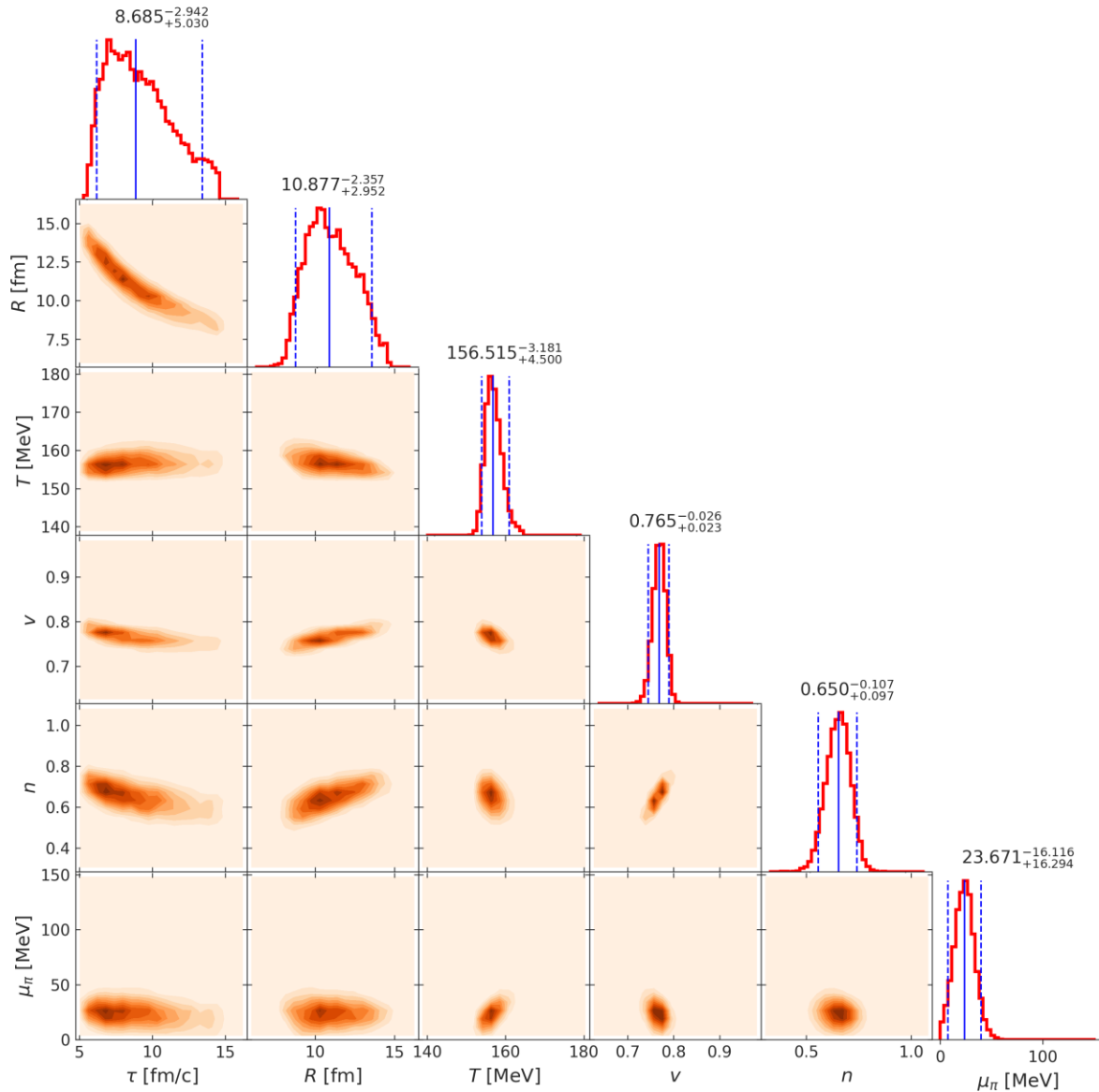
Model Setup
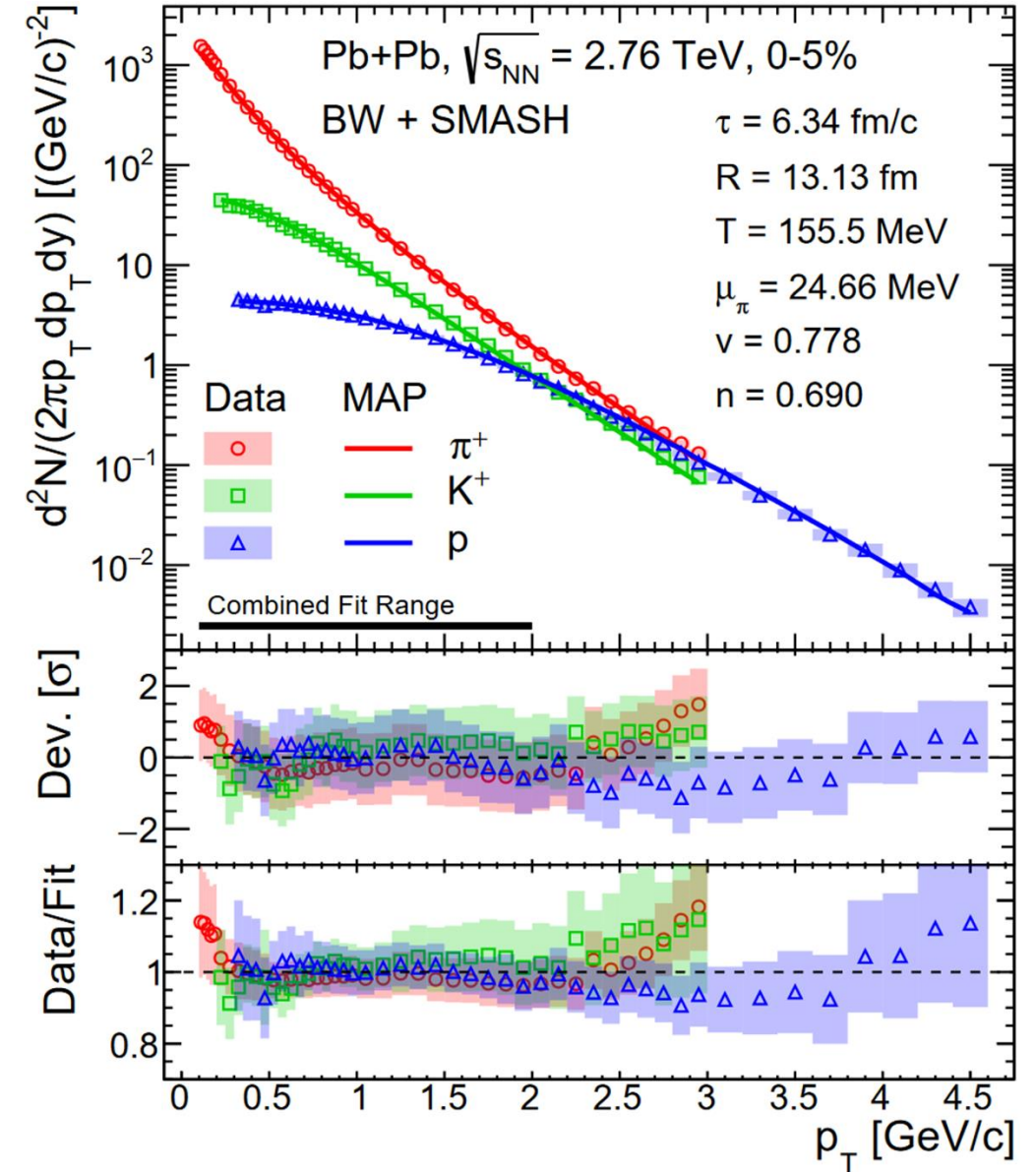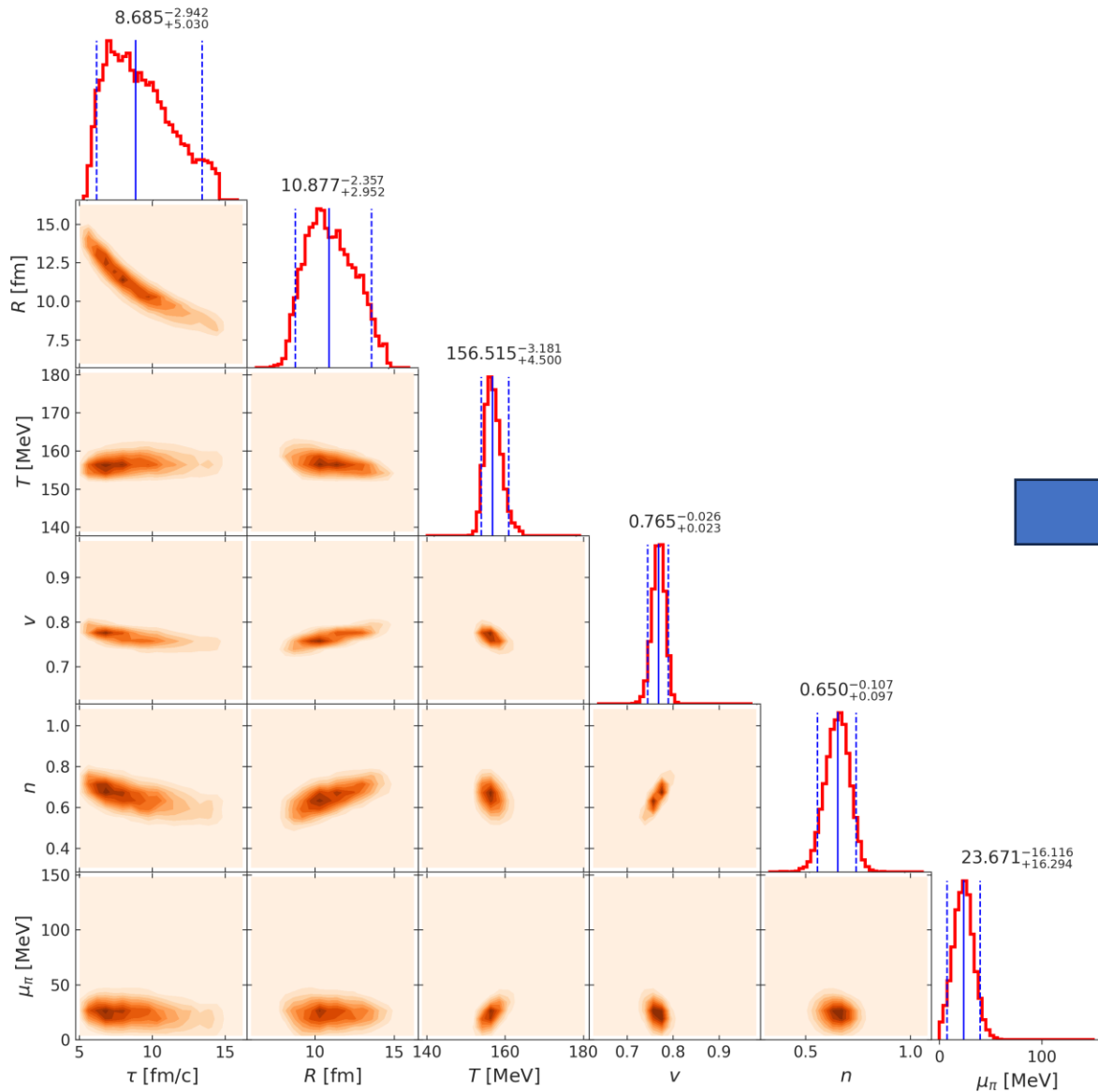

- Blast-Wave thermal particle generator model with SMASH afterburner
- Uniform prior:

$$\tau \in [5; 15] \ fm/c$$
$$R \in [6; 15] \ fm$$
$$T \in [145; 165] \ MeV$$
$$v \in [0.65; 0.9]$$
$$n \in [0.3; 1.0]$$
$$\mu_\pi \in [0; 137.9] \ MeV$$

- 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
- 200 training and 50 validation data sets
- 10 PCs

- Kernel: $\mathrm{K}(x_i, x_j) = \theta_A^2 \exp\left[-\frac{(x_i - x_j)^2}{2\theta_L^2}\right] + \theta_n \delta_{i,j}$

- 10000 MCMC samples

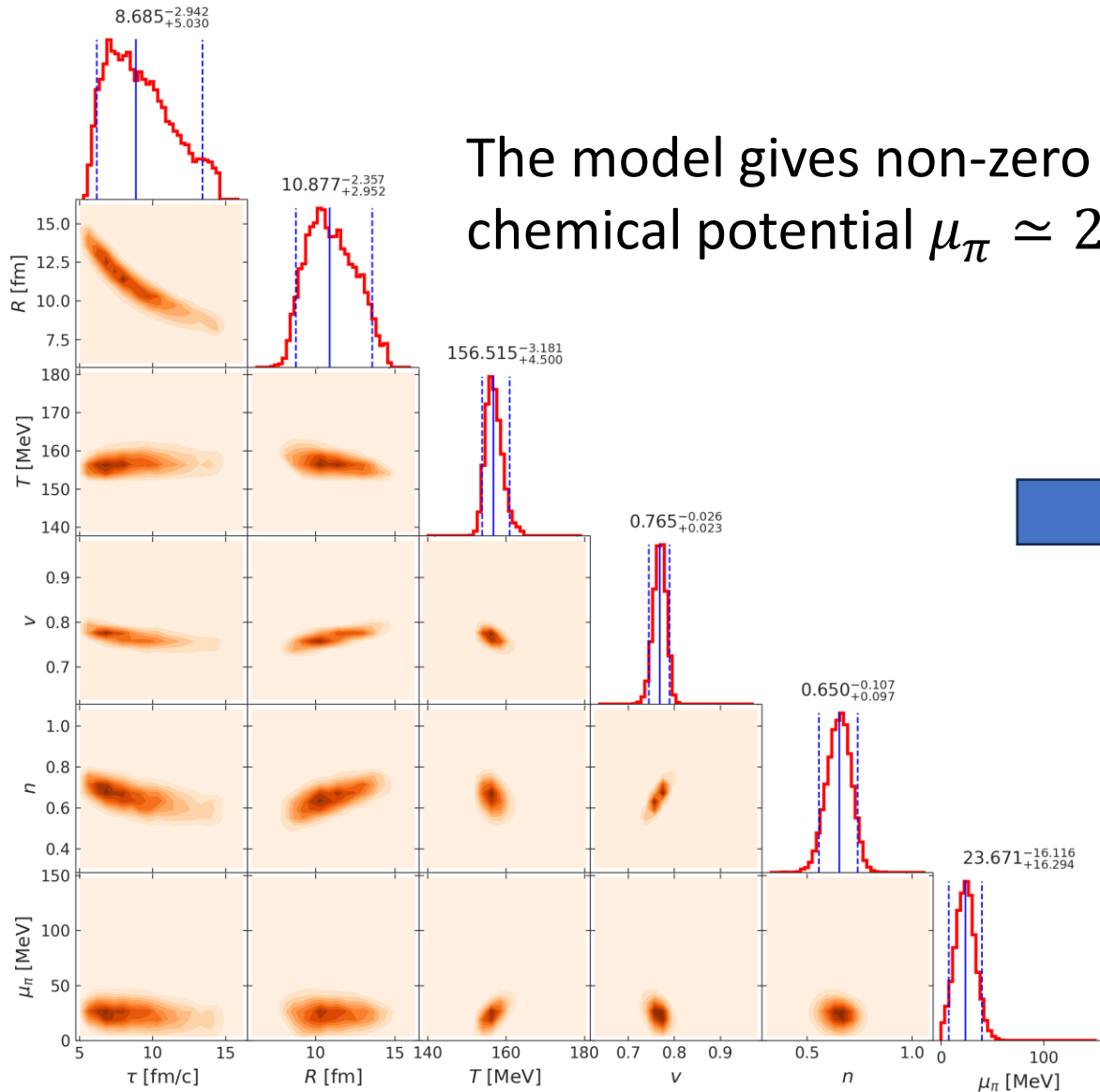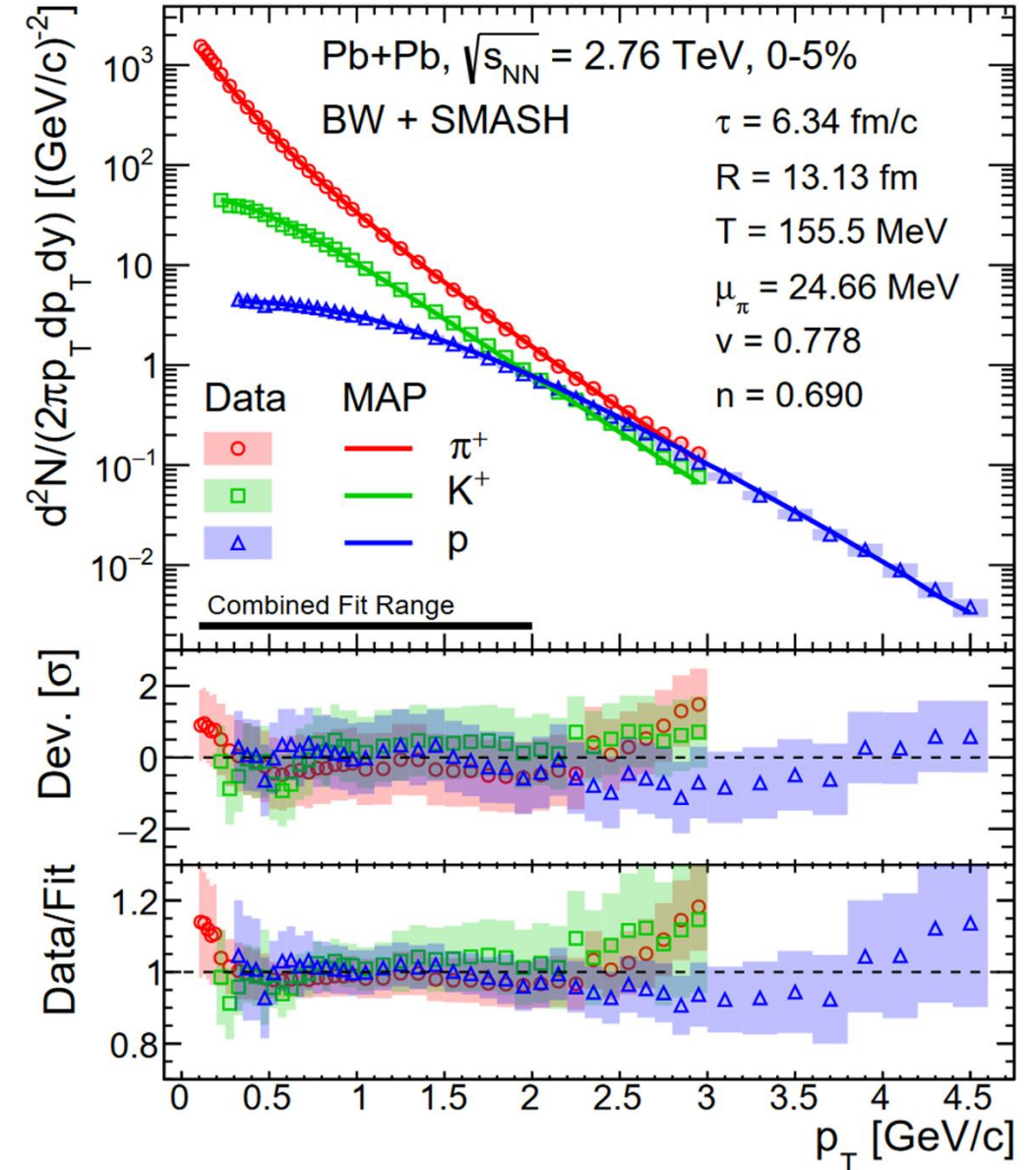# Posterior Probability Distribution

The model gives non-zero pion chemical potential $\mu_\pi \simeq 24$ MeV!

Pb+Pb, $\sqrt{s_{NN}}$ = 2.76 TeV, 0-5%

BW + SMASH

τ = 6.34 fm/c
R = 13.13 fm
T = 155.5 MeV
μ_π = 24.66 MeV
v = 0.778
n = 0.690

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
- Naïve model gives the value of effective chemical potential close to the pion mass and can describe data well, but it does not resonance decays and final state interactions
- More sophisticated model gives much smaller, but non-zero value of pion chemical potential

Standard Fit
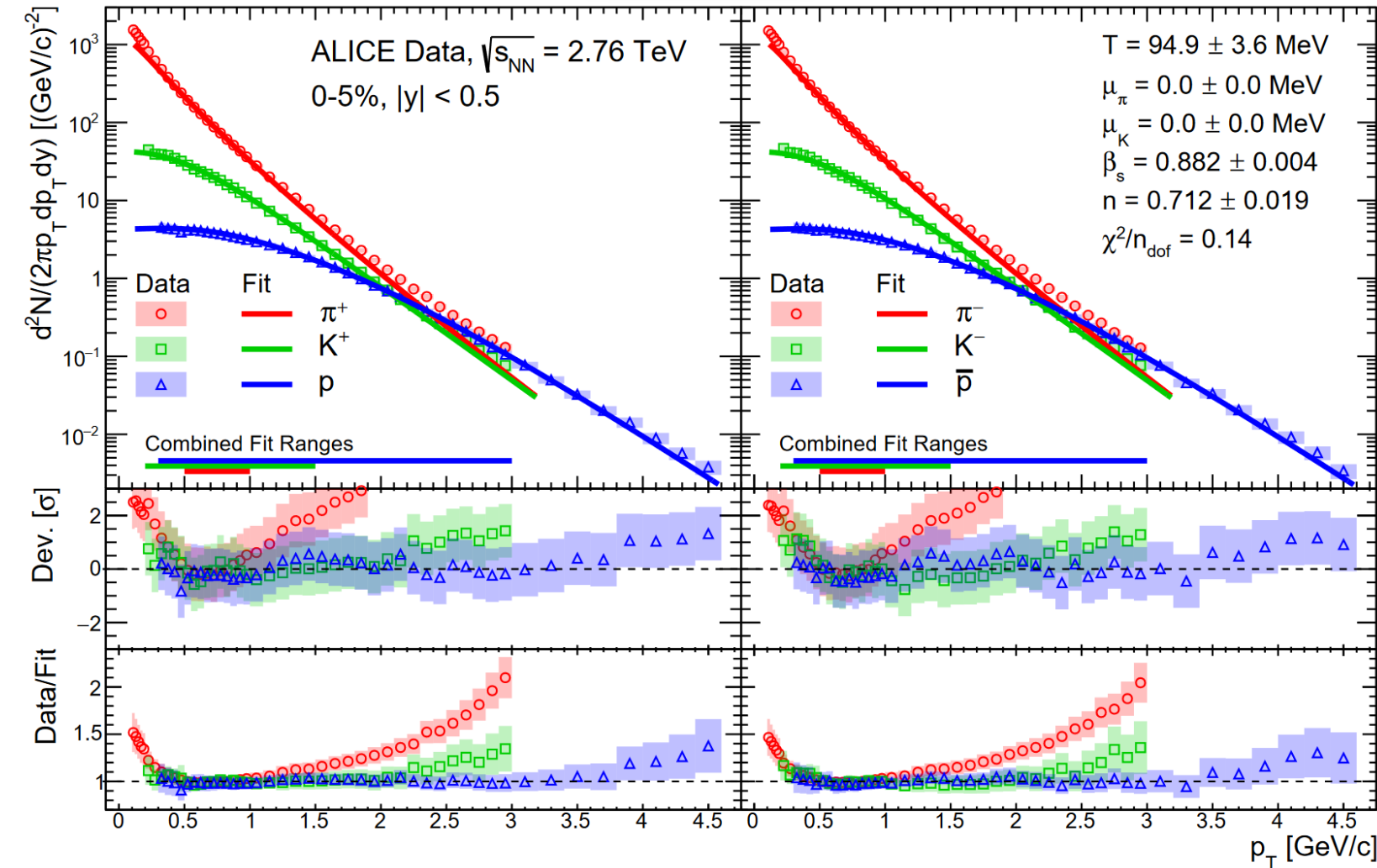
Standard fit – Blast-Wave model

$$\frac{dN}{p_T dp_T} \propto \int\limits_{0}^{R} r dr\, m_T I_0 \left(\frac{p_T \sinh\rho}{T} \right) K_1 \left(\frac{m_T \cosh\rho}{T} \right)$$

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

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

But in this model, we have less "slow" $\pi^{\pm}$ than in the data:

- Bose enhancement?
- Feed-down?

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 $A(\vec{x}_i \to \vec{x}'_{i+1}) = \min\left(1; \dfrac{\mathcal{L}(\vec{x}'_{i+1}; \vec{y}^{obs}) \times P(\vec{x}'_{i+1})}{\mathcal{L}(\vec{x}_i; \vec{y}^{obs}) \times P(\vec{x}_i)} \dfrac{Q(\vec{x}'_{i+1} \to \vec{x}_i)}{Q(\vec{x}_i \to \vec{x}'_{i+1})}\right)$
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 $A \sim N(\vec{\mu}, \Sigma)$. If $A' = TA + c$, then $A' \sim N(T\vec{\mu} + c, T\Sigma T^T)$.

$$\begin{bmatrix} f \\ Y \end{bmatrix} \sim N\left(\begin{bmatrix} \mu_f \\ \mu_Y \end{bmatrix}, \begin{bmatrix} \Sigma_{X^*,X^*} & \Sigma_{X^*,X} \\ \Sigma_{X,X^*} & \Sigma_{X,X} \end{bmatrix}\right), T = \begin{bmatrix} I & -\Sigma_{X^*,X}\Sigma_{X,X}^{-1} \\ 0 & I \end{bmatrix} \Rightarrow \begin{bmatrix} f' \\ Y' \end{bmatrix}$$

$$\sim N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \Sigma_{X^*,X^*} - \Sigma_{X^*,X}\Sigma_{X,X}^{-1}\Sigma_{X,X^*} & 0 \\ 0 & \Sigma_{X,X} \end{bmatrix}\right)$$

$$f' = f - \Sigma_{X^*,X}\Sigma_{X,X}^{-1}Y \quad \Rightarrow \quad f\Big|_{Y=y} \sim N(\Sigma_{X^*,X}\Sigma_{X,X}^{-1}y, \Sigma_{X^*,X^*} - \Sigma_{X^*,X}\Sigma_{X,X}^{-1}\Sigma_{X,X^*})$$

We need to know the covariance matrix for the given data set. It is parametrized in terms of hyperparameters $\vec{\theta}$
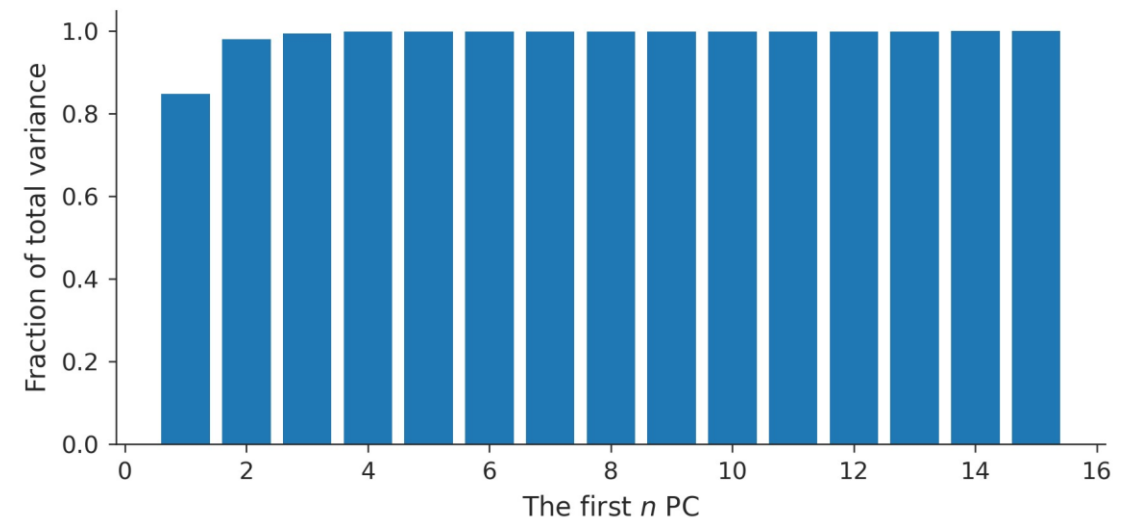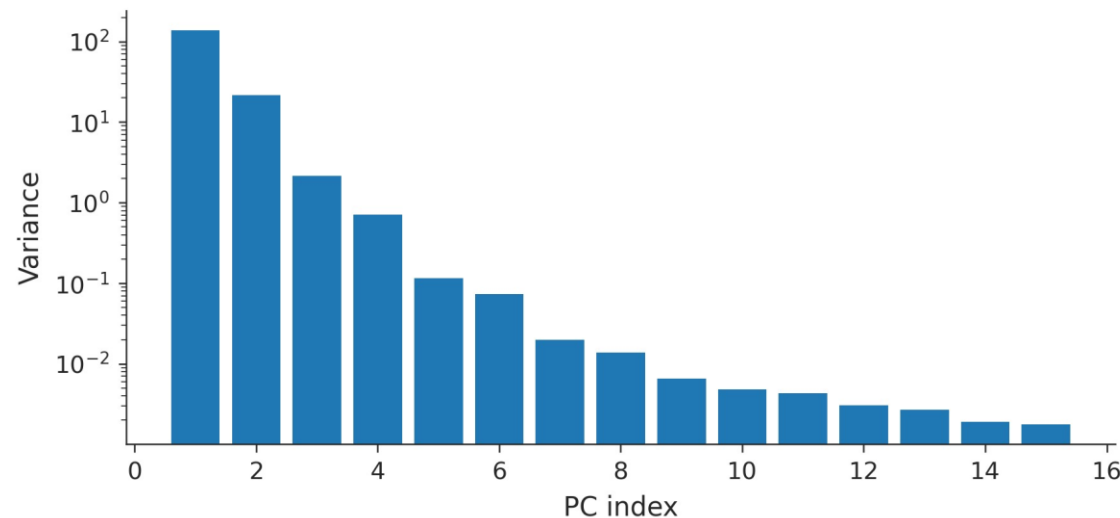
$$\Sigma_{ij} = K\left(x_i, x_j; \vec{\theta}\right) \Rightarrow \frac{d \ln P\left(Y|\vec{\theta}\right)}{d\vec{\theta}} = 0$$
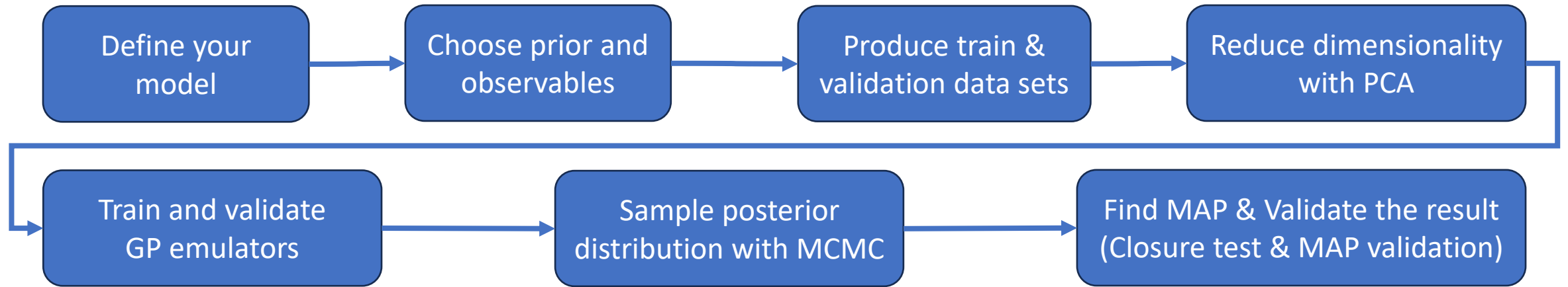
Principal Component Analysis

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. $V_p = [\vec{v}_1 \quad \dots \quad \vec{v}_p] \rightarrow \vec{z} = \vec{y} V_p, \ \vec{y} = \vec{z} V_p^T, \ \Sigma_z = V_p^T \Sigma_y V_p$

Likelihood with PCA and GP

```
┌─────────────┐   ┌─────────────┐   ┌─────────────┐   ┌──────────────────┐
│ Define your │──▶│ Choose prior │──▶│ Produce train & │──▶│ Reduce dimensionality │
│    model    │   │ and          │   │ validation data │   │     with PCA     │
│             │   │ observables  │   │     sets        │   │                  │
└─────────────┘   └─────────────┘   └─────────────┘   └──────────────────┘
```

- Define your model
- Choose prior and observables
- Produce train & validation data sets
- Reduce dimensionality with PCA
- Train and validate GP emulators
- Sample posterior distribution with MCMC
- Find MAP & Validate the result (Closure test & MAP validation)

Likelihood with GP emulators and PCA:

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

Where:

$$\vec{z}^{obs} = \vec{y}^{obs}\, V_p, \qquad \Sigma_{\exp} = V_p^T \Sigma V_p$$