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

Oleksandr Vitiuk¹, David Blaschke^{1,2,3}, Benjamin Dönigus⁴, Gerd Röpke⁵

¹University of Wroclaw, Poland

³Center for Advanced Systems Understanding, Germany

²Helmholtz-Zentrum Dresden-Rossendorf, Germany

⁴Goethe University Frankfurt, Germany

The 42nd International Conference on High Energy Physics 18-24 July 2024, Prague, Czech Republic



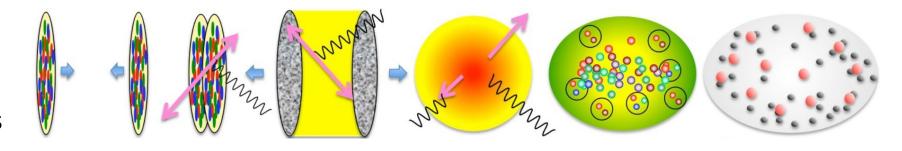


⁵University of Rostock, Germany

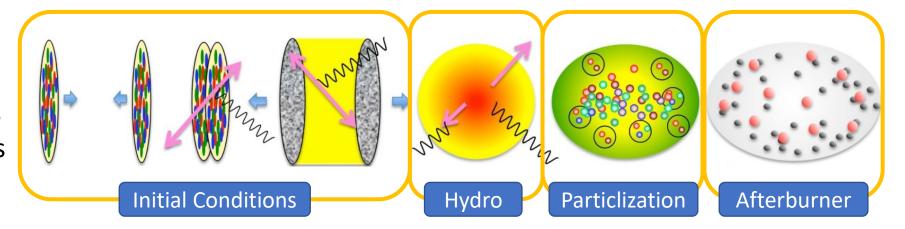
Outline

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

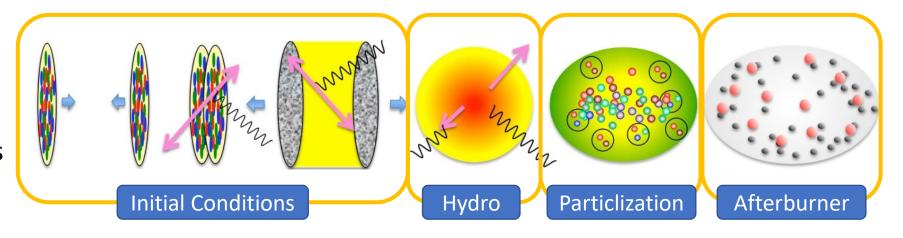
Various phenomena occur during the system evolution. We use different assumptions and models to describe stages of heavy-ion collisions.

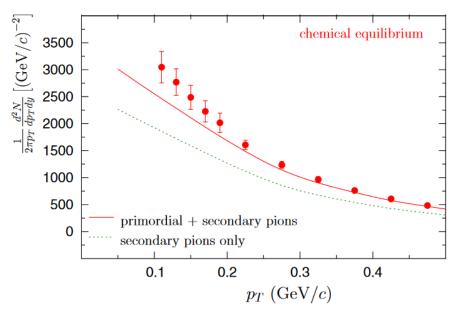


Various phenomena occur during the system evolution. We use different assumptions and models to describe stages of heavy-ion collisions.



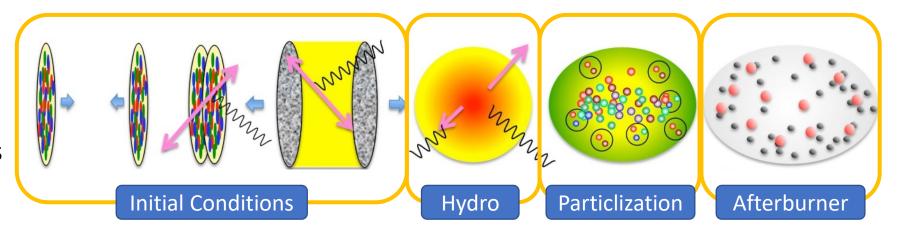
Various phenomena occur during the system evolution. We use different assumptions and models to describe stages of heavy-ion collisions.

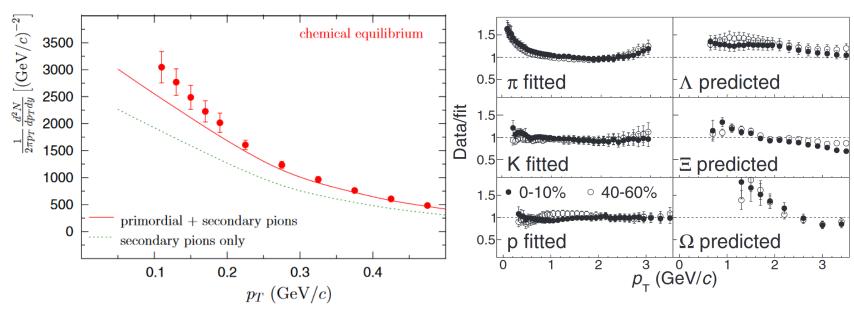




[V. Begun et al., PRC 90, 014906 (2014)]

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

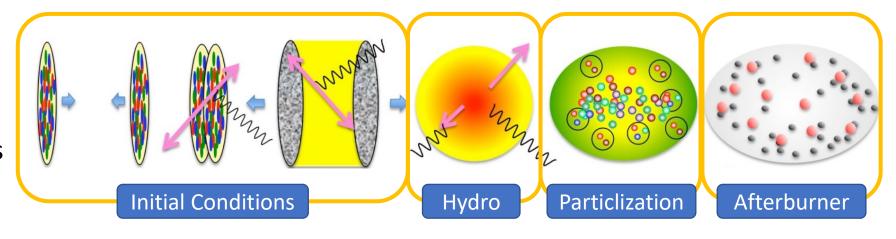


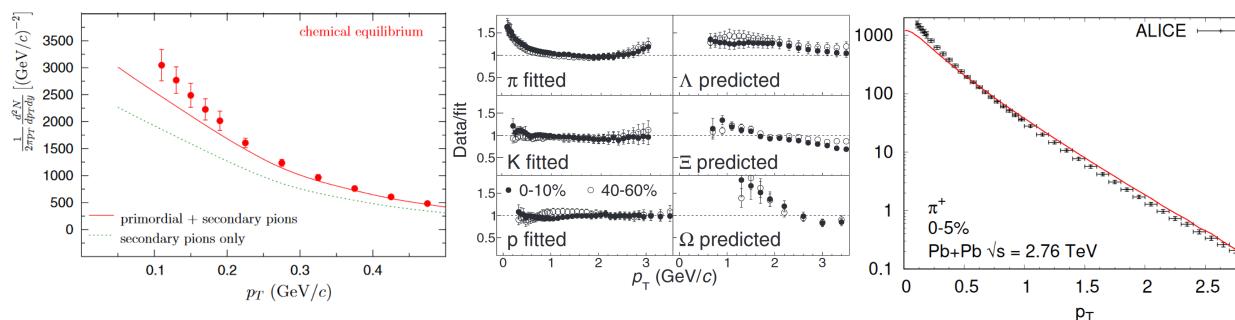


[V. Begun et al., PRC 90, 014906 (2014)]

[A. Mazeliuskas PRC 101, 014910 (2020)]

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

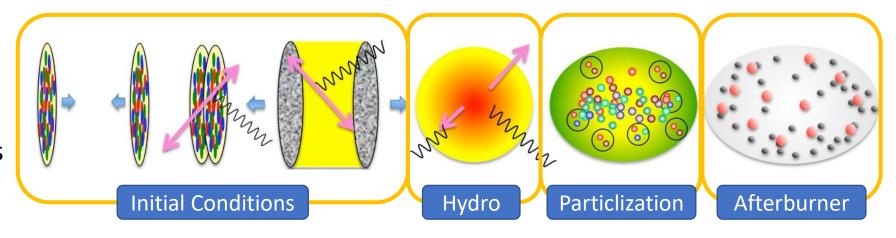


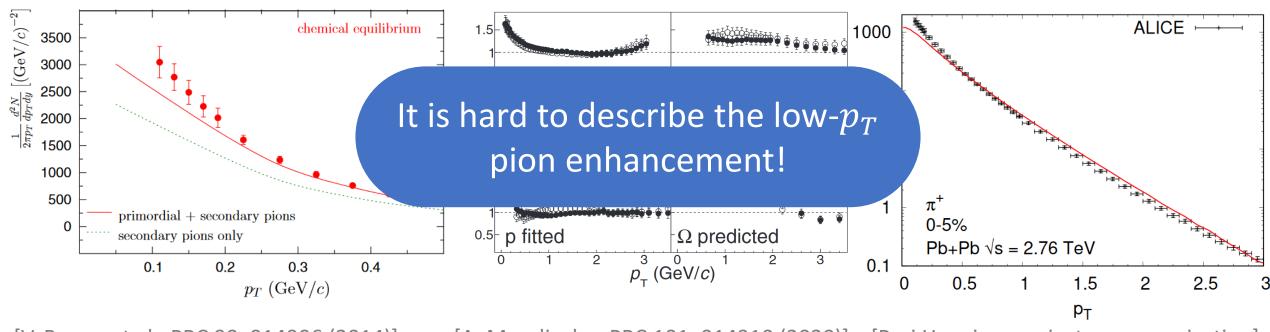


[V. Begun et al., PRC 90, 014906 (2014)]

[A. Mazeliuskas PRC 101, 014910 (2020)] [Pasi Huovinen, private communication]

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





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

[A. Mazeliuskas PRC 101, 014910 (2020)]

[Pasi Huovinen, private communication]

Here we assume the following:

- A state overpopulated by soft pions is formed at $au < au_{\pi}^{CFO}$
- For $\tau_{\pi}^{FO} < \tau < \tau_{\pi}^{CFO}$ the collisions conserve the particle number, but evolve the distribution function to a thermal equilibrium distribution (dominance of elastic collisions over inelastic ones)

Here we assume the following:

- A state overpopulated by soft pions is formed at $au < au_{\pi}^{CFO}$
- For $\tau_{\pi}^{FO} < \tau < \tau_{\pi}^{CFO}$ the collisions conserve the particle number, but evolve the distribution function to a thermal equilibrium distribution (dominance of elastic collisions over inelastic ones)



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

$$\rho_{rel}(t) = \frac{1}{Z_{rel}(t)} e^{-\sum_{n} F_n(t)B_n}, \qquad Z_{rel}(t) = \text{Tr}\{e^{-\sum_{n} F_n(t)B_n}\},$$

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

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

Here we assume the following:

- A state overpopulated by soft pions is formed at $au < au_{\pi}^{CFO}$
- For $\tau_{\pi}^{FO} < \tau < \tau_{\pi}^{CFO}$ the collisions conserve the particle number, but evolve the distribution function to a thermal equilibrium distribution (dominance of elastic collisions over inelastic ones)

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

$$\langle N_{\pi} \rangle_{rel}^t = \langle N_{\pi} \rangle^t$$

Here we assume the following:

- A state overpopulated by soft pions is formed at $au < au_{\pi}^{CFO}$
- For $\tau_{\pi}^{FO} < \tau < \tau_{\pi}^{CFO}$ the collisions conserve the particle number, but evolve the distribution function to a thermal equilibrium distribution (dominance of elastic collisions over inelastic ones)

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

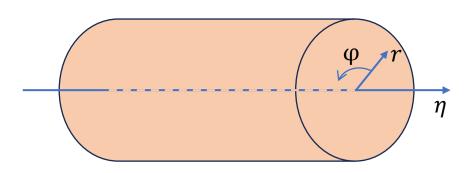
$$\langle N_{\pi} \rangle_{rel}^{t} = \langle N_{\pi} \rangle^{t}$$

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]

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

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

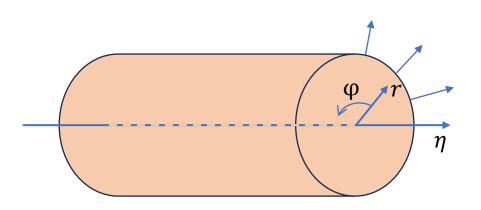
$$\Sigma^{\mu}=(\tau\cosh\eta\,,r\cos\varphi\,,r\sin\varphi\,,\tau\sinh\eta)$$
, where $\tau=\sqrt{t^2-z^2}=const.$ and $\eta=\frac{1}{2}\ln\frac{t+z}{t-z}$



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

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

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



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

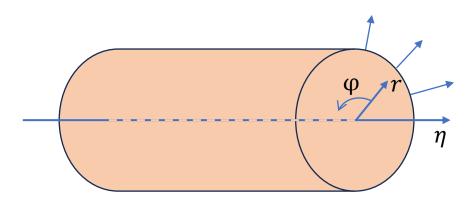
 $\Sigma^{\mu} = (\tau \cosh \eta, r \cos \varphi, r \sin \varphi, \tau \sinh \eta), \text{ where } \tau = \sqrt{t^2 - z^2} = const. \text{ and } \eta = \frac{1}{2} \ln \frac{t + z}{t - z}$

with the following velocity profile

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

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

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



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

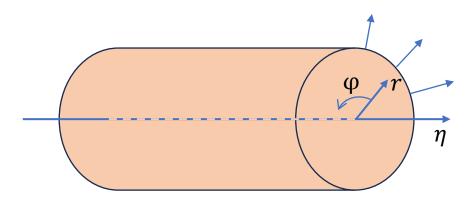
Here we consider chemical freeze-out on the cylindrical boost-invariant hypersurface at constant freeze-out proper time

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

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

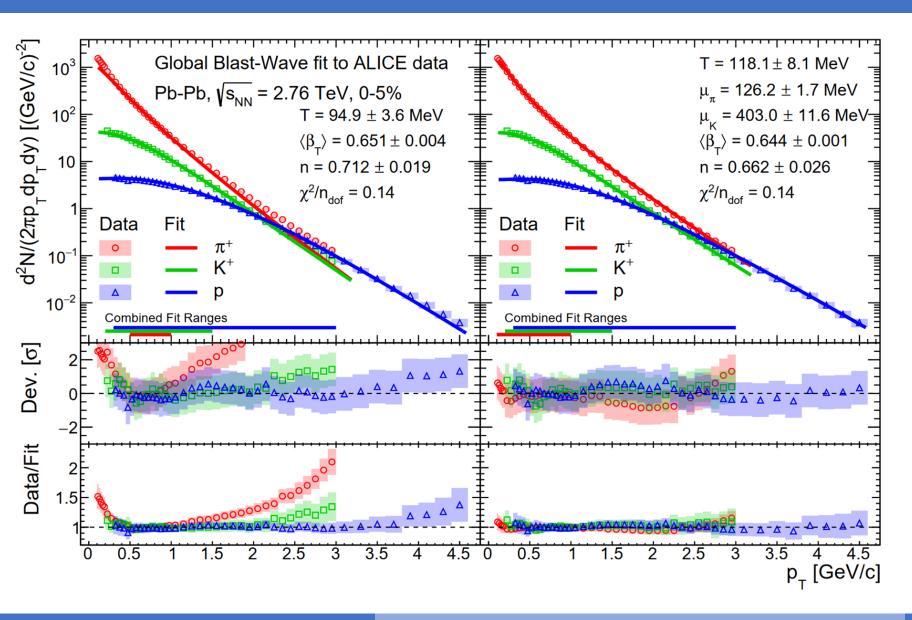
Then with the help of the Cooper-Frye formula $E \frac{d^3N}{d^3\vec{p}} = \int_{\Sigma_{FO}} p^\mu d\Sigma_\mu f(x^\mu, p^\mu u_\mu)$ one finds

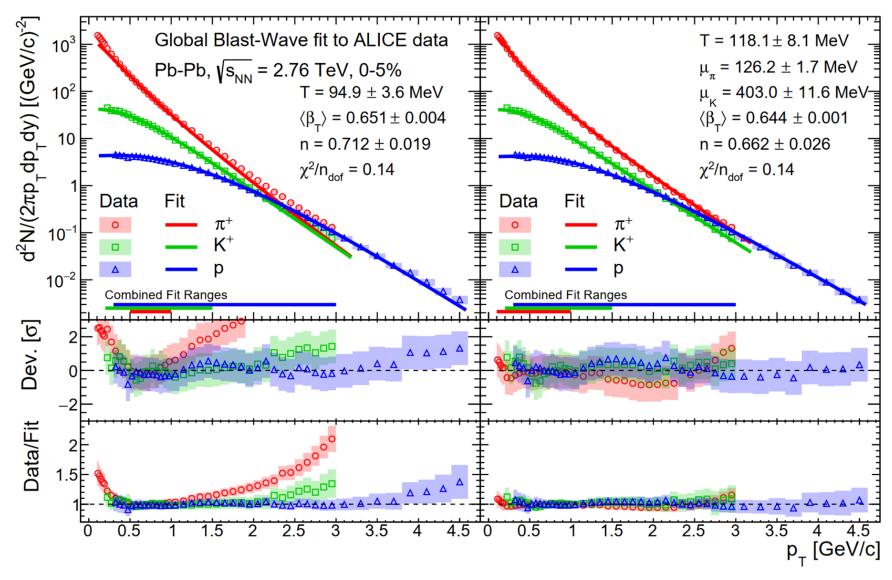
$$\frac{d^6N_i}{dp_Tdyd\psi drd\eta d\varphi} \propto \tau r p_T m_T \cosh(y-\eta) \left(\exp\left[\frac{m_T \cosh\rho \cosh(y-\eta) - p_T \sinh\rho \cos(\varphi-\psi) - \mu_i}{T}\right] \pm 1 \right)^{-1}$$



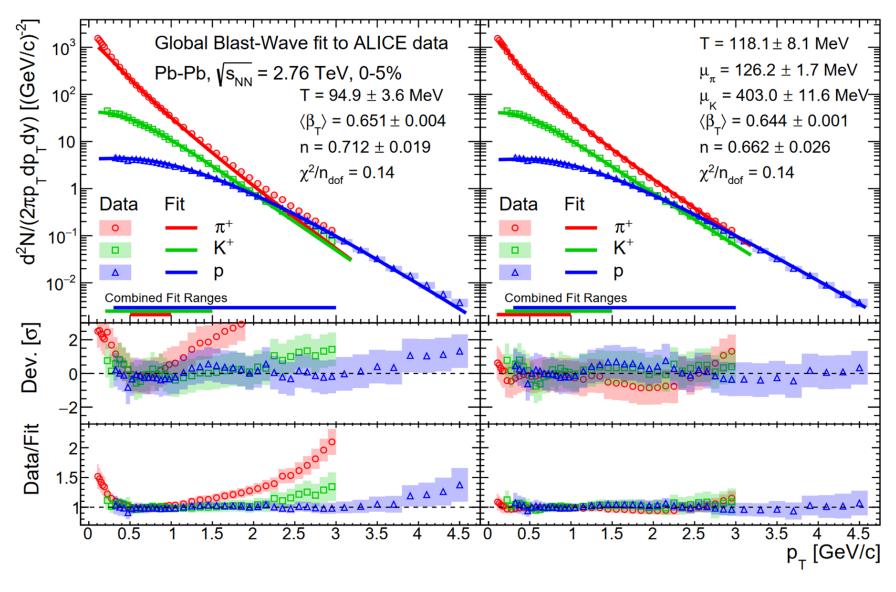
$$p_T = \sqrt{p_x^2 + p_y^2}$$
, $m_T = \sqrt{m_i^2 + p_T^2}$, $y = \frac{1}{2} \ln \frac{E + p_z}{E - p_z}$

 au,R,T,μ_π,v and n are free model parameters In some cases, the overall normalization is defined with the combination $au R^2$

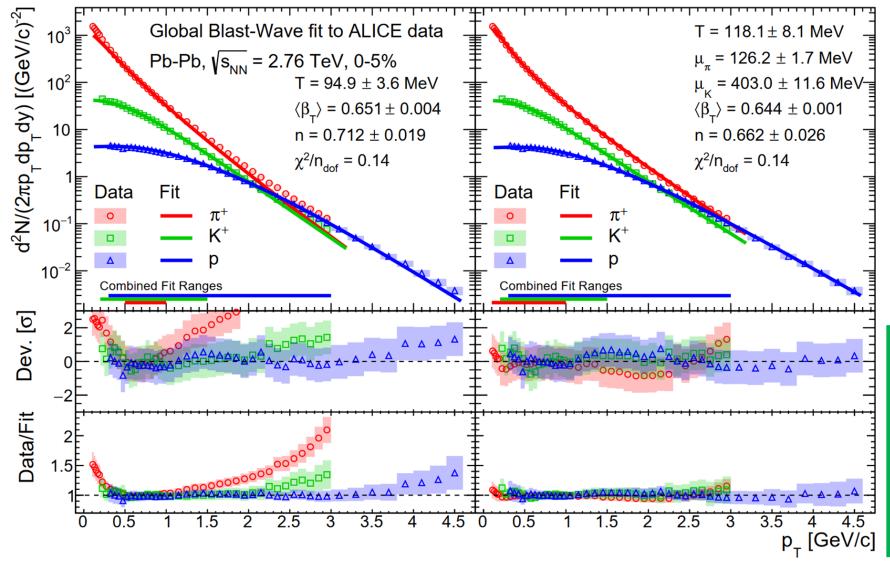




✓ Using two additional free parameters μ_{π} and μ_{K} one can achieve much better agreement between model and experimental data



- ✓ Using two additional free parameters μ_{π} and μ_{K} one can achieve much better agreement between model and experimental data
- *But feed-down and collisions are not in the model



- ✓ Using two additional free parameters μ_{π} and μ_{K} one can achieve much better agreement between model and experimental data
- ➤But feed-down and collisions are not in the model

Thermal particle generator smash

Afterburner instead of solving generalized kinetics!

Blast-Wave Based Particle Generator

Distribution function:

$$f \propto \tau r p_T m_T \cosh(y - \eta) \left(\exp\left[\frac{m_T \cosh \rho \cosh(y - \eta) - p_T \sinh \rho \cos(\varphi - \psi) - \mu_i}{T} \right] \pm 1 \right)^{-1}$$

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:

$$P(N_i = N) = \frac{\langle N_i \rangle^N}{N!} e^{-\langle N_i \rangle}$$

- 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 as an afterburner

Bayes theorem:

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

Bayes theorem:

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

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

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

Bayes theorem:

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

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

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

Bayes theorem:

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

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

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

Bayes theorem:

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

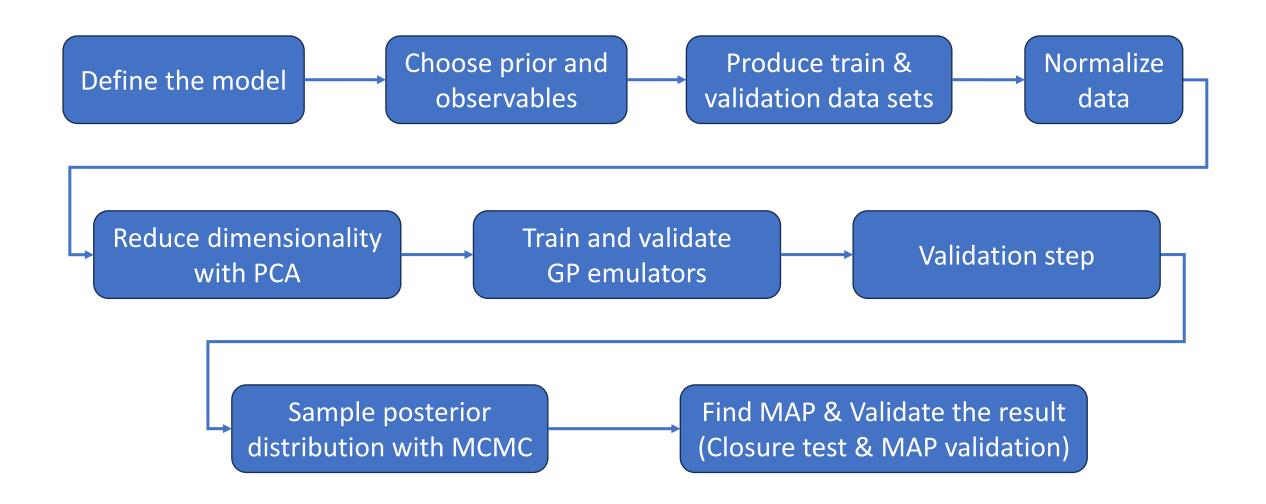
Suppose we have a model which for an input parameter vector $\vec{x} = (x_1, ..., x_n)$ gives an output $\vec{y} = \vec{y}(\vec{x}) = (y_1, ..., y_m)$. We want to find the "optimal" value of \vec{x} to describe the experimental data \vec{y}^{obs}

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

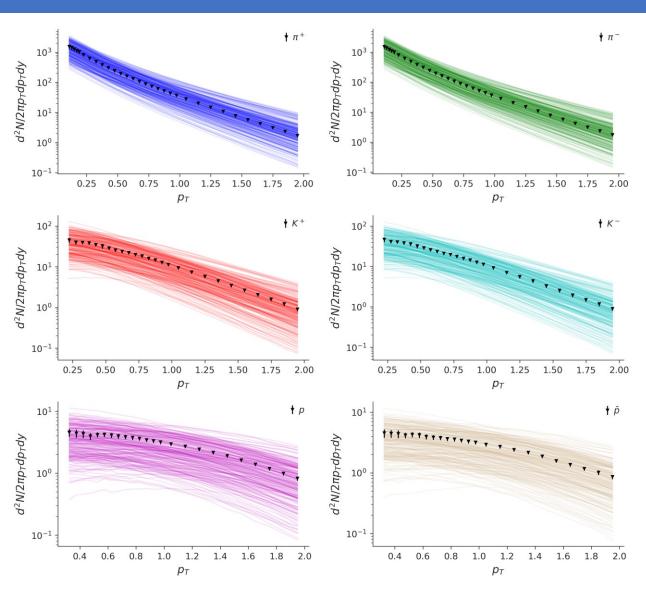
If we know mean values and variance, then the likelihood takes the form of multivariate Gaussian

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

Bayesian Inference Workflow



Model Setup



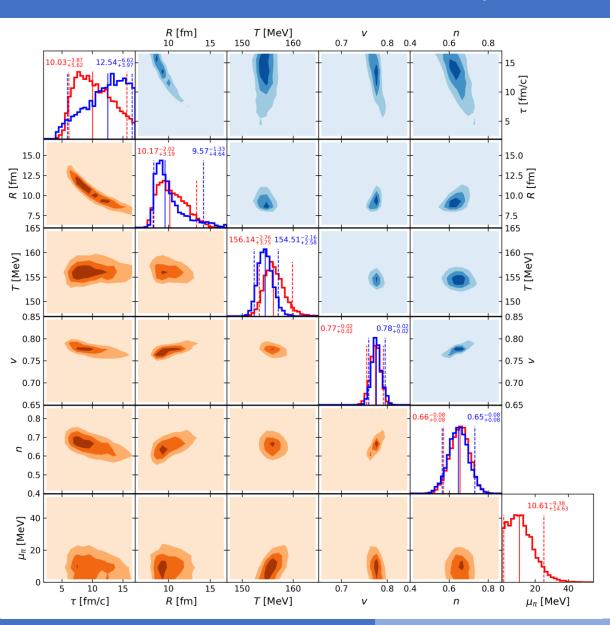
- Blast-Wave thermal particle generator model with SMASH afterburner
- Uniform prior:

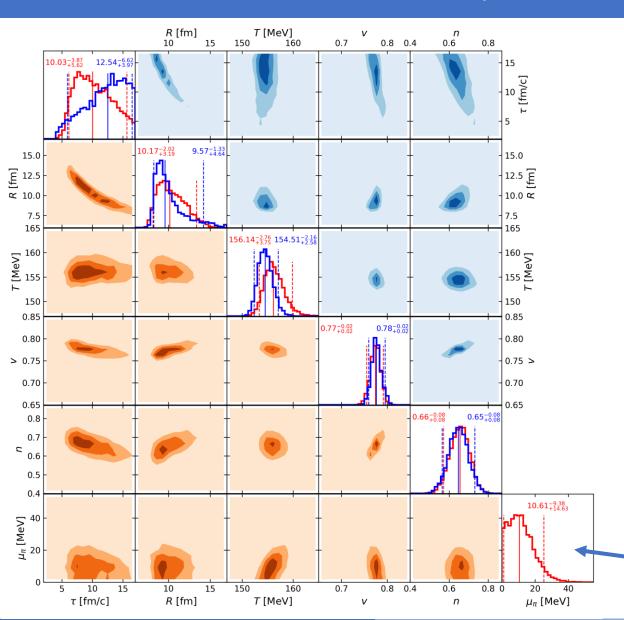
$$\tau \in [2; 17] \ fm/c$$
 $R \in [6; 17] \ fm$
 $T \in [145; 165] \ MeV$
 $v \in [0.65; 0.85]$
 $n \in [0.4; 0.85]$
 $\mu_{\pi} \in [0; 100] \ MeV \ or \ \mu_{\pi} = 0$

- 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

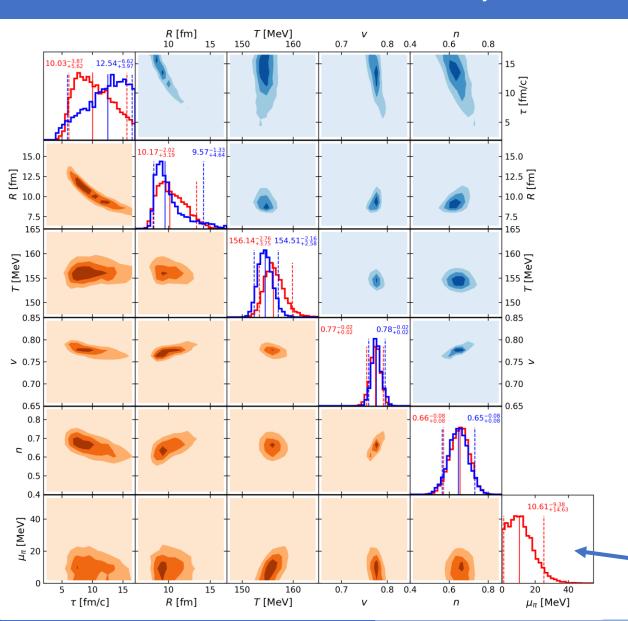
• Kernel:
$$K(x_i, x_j) = \theta_A^2 \exp\left[-\frac{(x_i - x_j)^2}{2\theta_L^2}\right] + \theta_n \delta_{i,j}$$

100000 MCMC samples



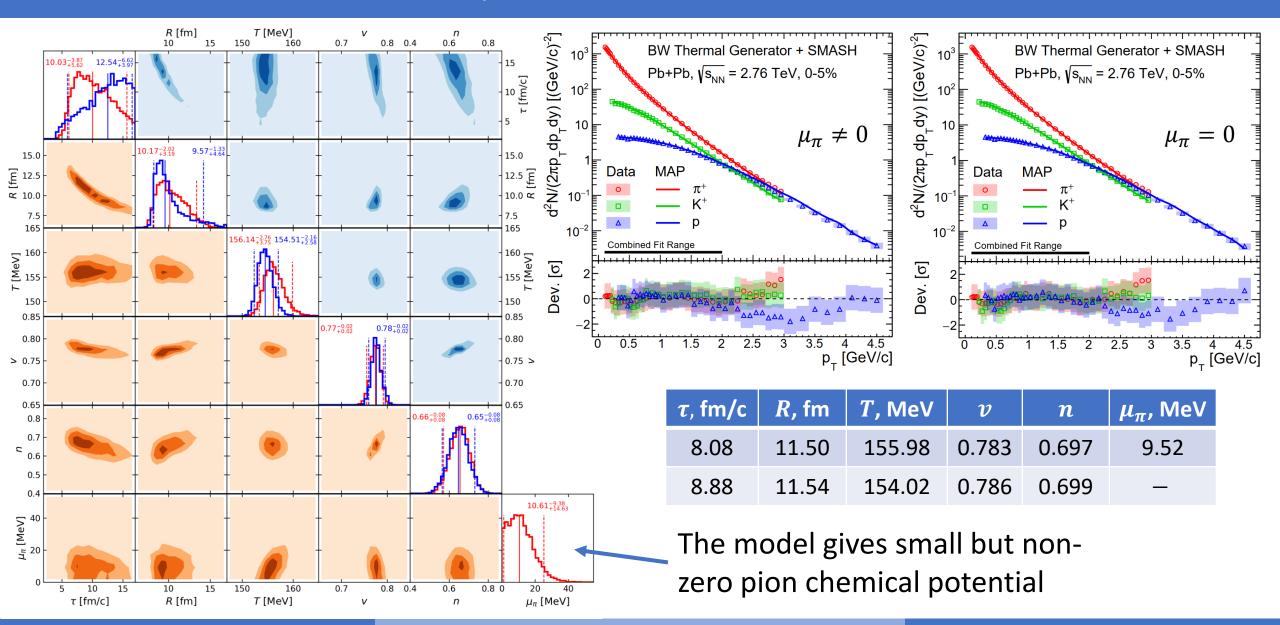


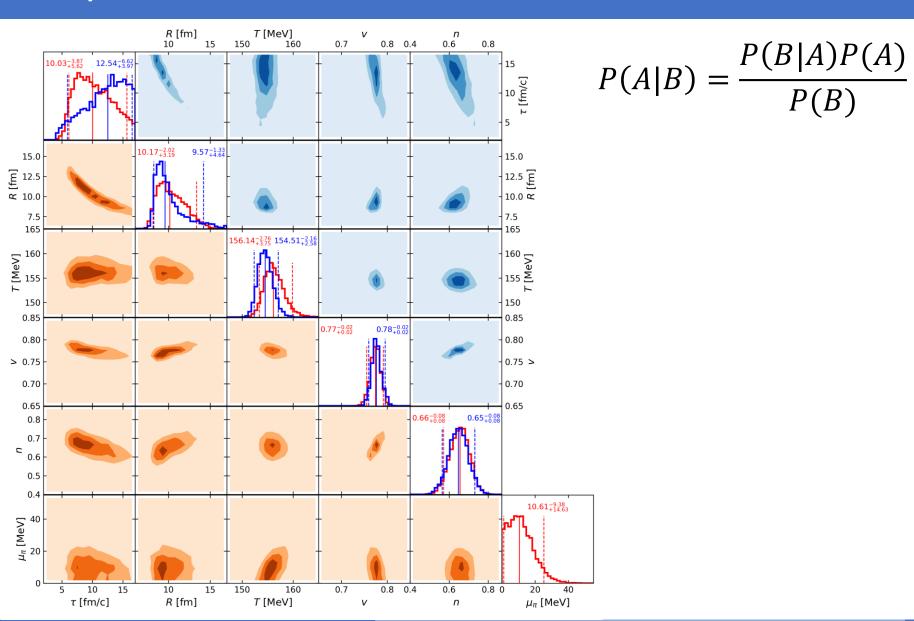
The model gives small but non-zero pion chemical potential

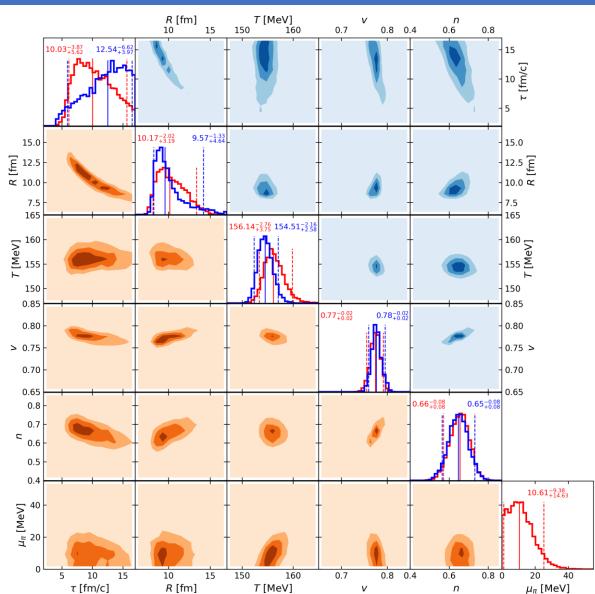


τ, fm/c	R, fm	T, MeV	v	n	μ_π , MeV
8.08	11.50	155.98	0.783	0.697	9.52
8.88	11.54	154.02	0.786	0.699	_

The model gives small but non-zero pion chemical potential



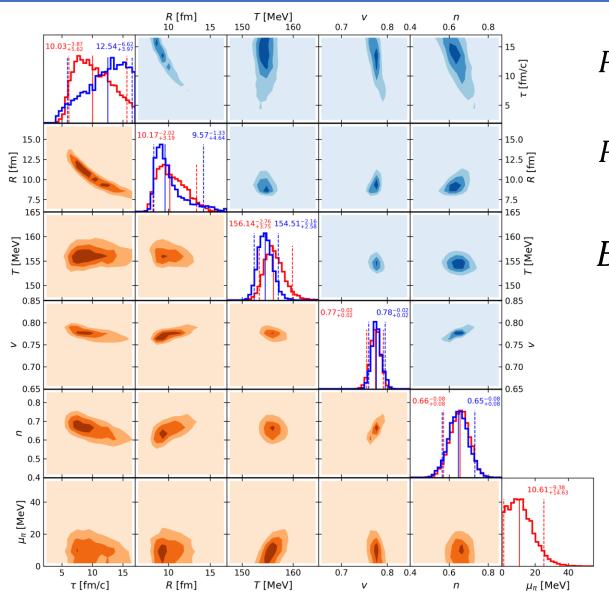




$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

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

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



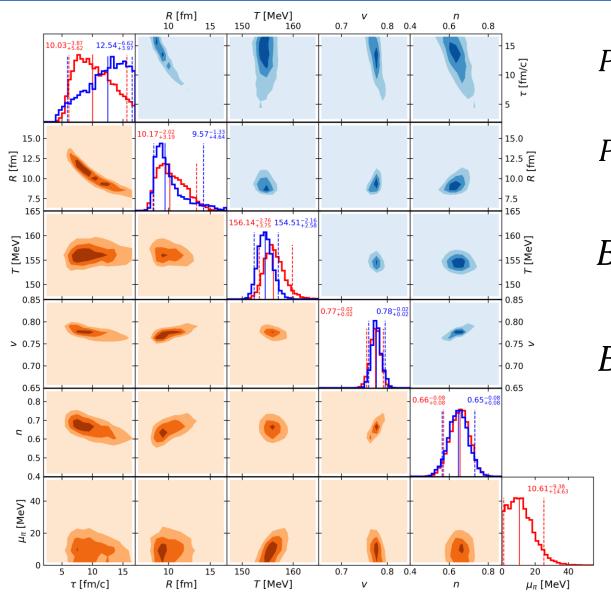
$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

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

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

$$B_2^1 = \frac{P(B|M_1)}{P(B|M_2)} = \frac{\int P(B|A,M_1)P(A|M_1) dA}{\int P(B|A,M_2)P(A|M_2) dA}$$

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



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

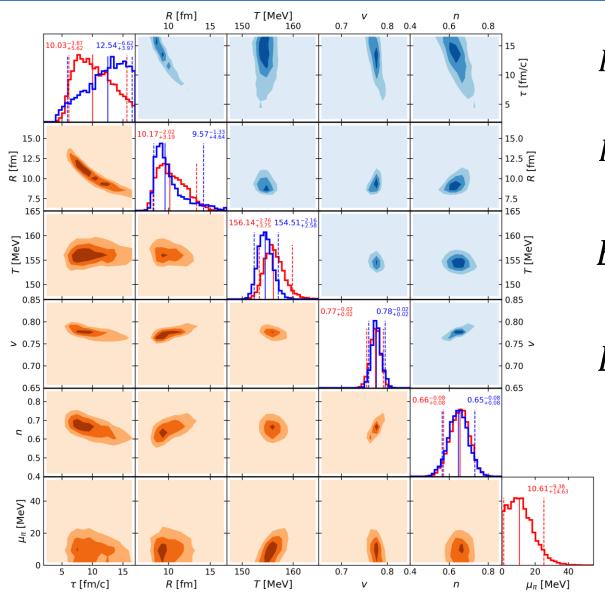
$$P(B|M) = \int P(B|A,M)P(A|M)dA$$

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

$$B_2^1 = \frac{P(B|M_1)}{P(B|M_2)} = \frac{\int P(B|A,M_1)P(A|M_1) dA}{\int P(B|A,M_2)P(A|M_2) dA}$$

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

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



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

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

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

$$B_2^1 = \frac{P(B|M_1)}{P(B|M_2)} = \frac{\int P(B|A,M_1)P(A|M_1) dA}{\int P(B|A,M_2)P(A|M_2) dA}$$

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



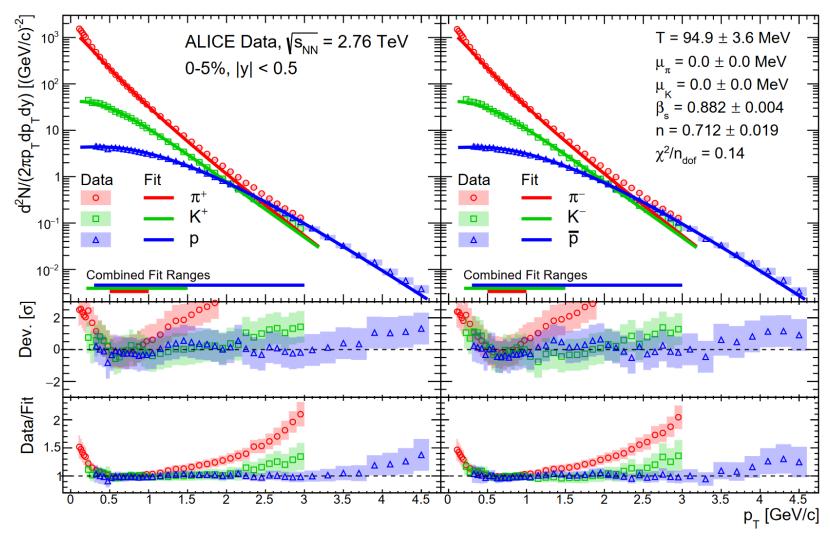
No evidence for the non-equilibrium hadronization

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

Summary

- The non-equilibrium process of pion production within the Zubarev approach of the non-equilibrium statistical operator leads to the appearance of a nonequilibrium 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
- Two model give very similar parameters and quality of the data description
- More sophisticated model gives much smaller, but non-zero value of pion chemical potential
- No evidence for the non-equilibrium hadronization, but this scenario cannot be excluded

Standard Fit



Standard fit – Blast-Wave model

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

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

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

$$\sim N \begin{pmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \Sigma_{X^*,X^*} - \Sigma_{X^*,X} \Sigma_{X,X}^{-1} \Sigma_{X,X^*} & 0 \\ 0 & \Sigma_{X,X} \end{bmatrix} \end{pmatrix}$$

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

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

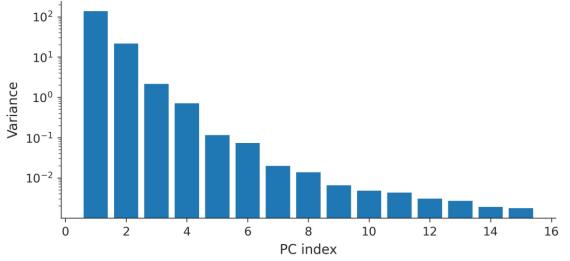
Principal Component Analysis

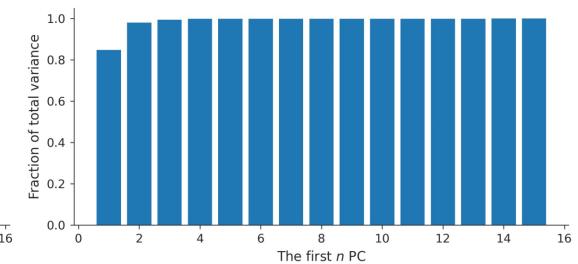
Problem: GP can take a multidimensional input, but the output is always a scalar. M observables = M GP emulators. Typical order is O(100) observables.

Solution: Dimension reduction via Principal Component Analysis

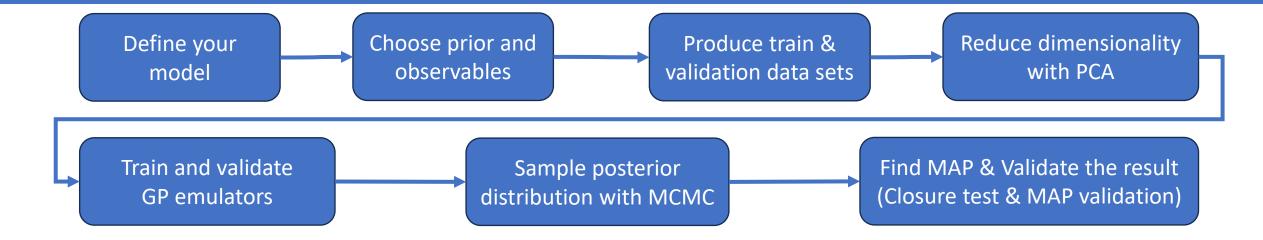
- 1. Let us define the matrix $M_{ij} = \frac{y_i(x_j) \langle y_i \rangle}{\sigma_i} \to C = M^T M m \times m$ covariance matrix
- 2. Sort eigenvalues λ_i and eigenvectors \vec{v}_i of matrix C in descending order of λ_i
- 3. Keep p first components which together explain the desired fraction of total variance

4.
$$V_p = [\vec{v}_1 \quad ... \quad \vec{v}_p] \rightarrow \vec{z} = \vec{y} V_p, \ \vec{y} = \vec{z} V_p^T, \ \Sigma_z = V_p^T \Sigma_y V_p$$





Likelihood with PCA and GP



Likelihood with GP emulators and PCA:

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

Where:

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

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

$$\rho_{rel}(t) = \frac{1}{Z_{rel}(t)} e^{-\sum_{n} F_{n}(t)B_{n}}, \qquad Z_{rel}(t) = \text{Tr}\{e^{-\sum_{n} F_{n}(t)B_{n}}\},$$

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

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

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

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

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.