Statistical analysis of transport+hydrodynamics hybrid model in 62.4 GeV Au+Au collisions

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Transport meeting
Frankfurt am Main
July 1, 2015

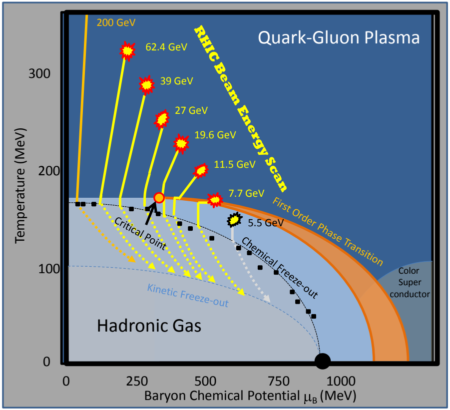
Duke
UNIVERSITY

Outline

RHIC beam energy scan

Reaching from $\sqrt{s_{NN}} = 200$ GeV down to FAIR energies $\sqrt{s_{NN}} \approx 5$ GeV.

QGP volume and lifetime decreases with decreasing $\sqrt{s_{NN}}$ ⇒ signals (jet quenching, strong collective flow, etc.) should turn off at some point



Picture taken from G. Odyniec, Acta Phys. Polon. B 43, 627 (2012).

Transport + hydrodynamics hybrid model

I. A. Karpenko *et al.* PRC91, 064901 (2015), arXiv:1502.01978

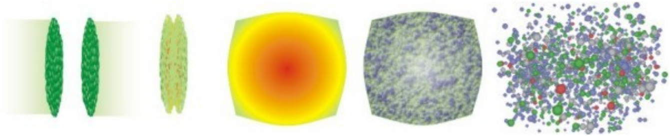


Image source: S. A. Bass

- Initial State from UrQMD[1] hadron+strings cascade
- Start the hydrodynamical evolution when nuclei have passed through each other: $\tau_0 \geq \frac{2R_{\text{nucleus}}}{\sqrt{\gamma_{CM}^2 - 1}}$
- Particle properties (energy, baryon number) to densities: 3D Gaussians with "smearing" parameters R_{trans}, R_{long} $(\equiv \sqrt{2}\sigma)$
- 3+1D viscous hydrodynamics[2] with viscosity parameter η/s
- Transition from hydro back to transport ("particlization") when energy density $\epsilon \leq \epsilon_C$

[1] S. A. Bass *et al.*, Prog. Part. Nucl. Phys. **41**, 255 (1998), M. Bleicher *et al.*, J. Phys. G **25**, 1859 (1999).

[2] Iu. Karpenko *et al.*, Comput.Phys.Commun. 185, 3016 (2014).

The modeling problem

Model parameters (input): $\vec{x} = (x_1, ..., x_n)$

$(\tau_0,\ R_{\text{trans}},\ R_{\text{long}},\ \eta/s,\ \epsilon_C)$

$\Downarrow$

Model output $\vec{y} = (y_1, ..., y_m) \Leftrightarrow$ Experimental values $\vec{y}^{\text{exp}}$

$(N_{\text{ch}},\ \langle p_T \rangle,\ v_2, ...)$

Goal: Find the "true" values of the input parameters, for which $\vec{x}^* \Rightarrow \vec{y}^{\text{exp}}$.

What is the level of uncertainty associated with the proposed values?

Bayesian analysis

- Bayes' theorem:
  Given a set $X = \{\vec{x}_k\}_{k=1}^N$ of points in parameter space and a corresponding set $Y = \{\vec{y}_k\}_{k=1}^N$ of points in observable space,

$$\boxed{P(\vec{x}^*|X,Y,\vec{y}^{\text{exp}}) \propto P(X,Y,\vec{y}^{\text{exp}}|\vec{x}^*)P(\vec{x}^*)}$$

- $P(\vec{x}^*|X,Y,\vec{y}^{\text{exp}})$ is the *posterior* probability distribution of $\vec{x}^*$ for given $(X,Y,\vec{y}^{\text{exp}})$
- $P(\vec{x}^*)$ is the *prior* probability distribution (simplest case: ranges of parameter values)
- $P(X,Y,\vec{y}^{\text{exp}}|\vec{x}^*)$ is the *likelihood* of $(X,Y,\vec{y}^{\text{exp}})$ for given $\vec{x}^*$ (to be determined with statistical analysis)

Likelihood function

$$P(X, Y, \vec{y}^{\text{exp}} | \vec{x}^*) \propto \exp\left(-\frac{1}{2}(\vec{y}^* - \vec{y}^{\text{exp}})^T \Sigma^{-1} (\vec{y}^* - \vec{y}^{\text{exp}})\right),$$

where

- $\vec{y}^*$ is model output for the input parameter point $\vec{x}^*$
- Σ is the covariance matrix. In this study $\Sigma = \text{diag}(\sigma^2)$, with $\sigma \approx 0.05$ as a global estimate of relative uncertainty associated with comparing $\vec{y}^*$ to $\vec{y}^{\text{exp}}$

⇒ Need a way to predict model output for arbitrary input parameter point
⇒ Model emulation using Gaussian processes

Gaussian process

Assumption: Set Y_a of values of observable y_a, corresponding to set X of points in parameter space, has a multivariate normal distribution:

$$Y_a \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

where $\boldsymbol{\mu} = \mu(X) = \{\mu(x_1), ..., \mu(x_N)\}$ is the mean and

$$\boldsymbol{\Sigma} = \sigma(X, X) = \begin{pmatrix} \sigma(\vec{x}_1, \vec{x}_1) & \cdots & \sigma(\vec{x}_1, \vec{x}_N) \\ \vdots & \ddots & \vdots \\ \sigma(\vec{x}_N, \vec{x}_1) & \cdots & \sigma(\vec{x}_N, \vec{x}_N) \end{pmatrix}$$

is the covariance matrix with covariance function $\sigma(\vec{x}, \vec{x}')$ (model-dependent choice; constant, linear, exponential, periodic, ...).

Gaussian process

Choice: Squared-exponential covariance function with a noise term

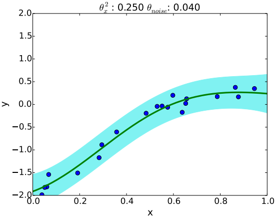
$$\sigma(\vec{x},\vec{x}') = \theta_0 \exp\left(-\sum_{i=1}^{n} \frac{(x_i - x_i')^2}{2\theta_i^2}\right) + \theta_{\text{noise}}\delta_{\vec{x}\vec{x}'}$$

The *hyperparameters* $\vec{\theta} = (\theta_0, \theta_1, ...\theta_n, \theta_{\text{noise}})$ are not known a priori and must be estimated from the given data

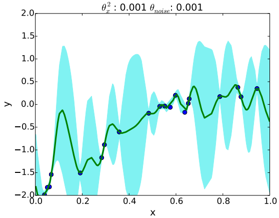
$\Rightarrow$ emulator training: Maximise the marginal likelihood (aka "evidence")

$$\log P(Y|X,\vec{\theta}) = \underbrace{-\frac{1}{2}Y^T\boldsymbol{\Sigma}^{-1}(X,\vec{\theta})Y}_{\text{data fit}} \underbrace{-\frac{1}{2}\log|\boldsymbol{\Sigma}(X,\vec{\theta})|}_{\text{complexity penalty}} \underbrace{-\frac{N}{2}\log(2\pi)}_{\text{normalization}}$$

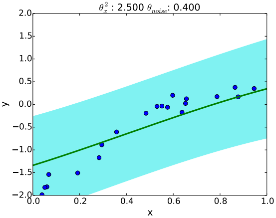
1-D example



Original: $\theta_x^2 = 0.25, \theta_n = 0.04$

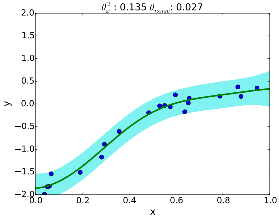


Overfit: $\theta_x^2 = 0.001, \theta_n = 0.001$



Underfit: $\theta_x^2 = 2.5, \theta_n = 0.4$

$\Downarrow$



After training: $\theta_x^2 = 0.135, \theta_n = 0.027$

Principal component analysis

m observables $\Rightarrow$ m Gaussian processes

Number of emulators can be reduced with principal component analysis:

- Construct orthogonal linear combinations of observables (= principal components) by performing an eigenvalue decomposition on the covariance matrix
- Eigenvalue λ_i represents the variance explained by principal component p_i
- Select the number of principal components which together explain desired fraction of total variance; often only a few PCs are needed to explain 99% of the variance

Principal component analysis

N simulation points, m observables $\Rightarrow$ N x m data matrix Y

- Center the data by subtracting the mean of each observable from all points
- Eigenvalue decomposition: $Y^T Y = U \Lambda U^T$; U (m x m) eigenvector matrix, $\Lambda = \text{diag}(\lambda_1 ... \lambda_m)$ eigenvalue matrix, $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_m$ $\Rightarrow$ (N x m) observable matrix in principal component space: $Z = \sqrt{N} Y U$
- Fraction of variance explained by principal component q: $V(q) = \frac{\lambda_q}{\sum_{i=1}^{m} \lambda_i}$
- $V(q) \approx 0$ starting from some $i < q < m \Rightarrow$ Reduced-dimension transformation $Z_q = \sqrt{N} Y U_q$ with minimal loss of precision

Markov Chain Monte Carlo

The posterior distribution $p(x|y)$ is sampled with Markov Chain Monte Carlo (MCMC) method

- Random walk in parameter space, where each step is accepted or rejected based on a relative likelihood
- Converges to posterior distribution as number of steps $N \to \infty$
- Common example: Metropolis-Hastings algorithm
  - Given position $x(t)$, sample proposal position x' from a transition distribution $Q(x'; x(t))$ (should be symmetric; typically Gaussian)
  - Accept the proposal with probability $\frac{p(x'|y)}{p(x(t)|y)} \frac{Q(x(t);x')}{Q(x';x(t))}$
- Acceptance fraction of steps measures the quality of random walk; should be 0.2-0.5[3]
- Autocorrelation time $=$ Number of steps between independent samples "Burn-in" takes a few autocorrelations, gathering enough samples $\sim \mathcal{O}(10)$ autocorrelations

[3] D. Foreman-Mackey *et al.*, Publ. Astron. Soc. Pacific **125**, 306 (2013), arXiv:1202.3665

Analysis procedure

Verify normal distribution of observables
(apply a transformation if necessary)

$\Downarrow$

Scale with experimental values $\Rightarrow$ Unitless quantities of the order ($\mathcal{O}(1)$)
Center the data by subtracting the mean

$\Downarrow$

Principal component analysis $\Rightarrow$ Determine required number of Gaussian processes

$\Downarrow$

Train the emulator(s)

$\Downarrow$

Calibrate on experimental data by running MCMC

Investigated parameter ranges

- Shear viscosity over entropy density η/s: 0.001 - 0.3
- Transport-to-hydro transition time τ_0: 0.4 - 2.0 fm
- Transverse Gaussian smearing of particles R_{trans}: 0.5 - 2.1 fm
- Longitudinal Gaussian smearing of particles R_{long}: 0.5 - 2.1 fm
- Hydro-to-transport transition energy density ϵ_C: 0.15 - 0.75 GeV/fm^3

Latin hypercube sampling used for sampling the simulation points; covers the parameter space in more robust way compared to pure random sampling

Investigated observables

- N_{ch} in $|\eta| < 0.5$ in (0-5)%, (10-20)% centrality

  STAR, PRC79, 034909 (2009)

- $N_{\bar{p}}$ at $y = 0$ in (0-15)%, (15-35)% centrality

  PHOBOS, PRC75, 024910 (2007)

- $dN_{\text{ch}}/d\eta$ at $\eta = 1.1$ in (0-3)%, (20-25)% centrality

  PHOBOS, PRC83, 024913 (2011)

- $\langle p_T \rangle$ for π^-, K^+ in (0-5)%, (20-30)% centrality

  STAR, PRC79, 034909 (2009)

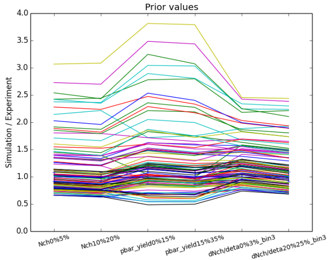
- dN/dp_T for π^-, K^+ at $p_T = 0.3, 0.5$ GeV at $y = 0.8$ in (0-15)%, (15-30)% centrality

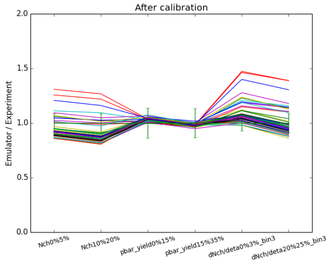
  PHOBOS, PRC75, 024910 (2007)

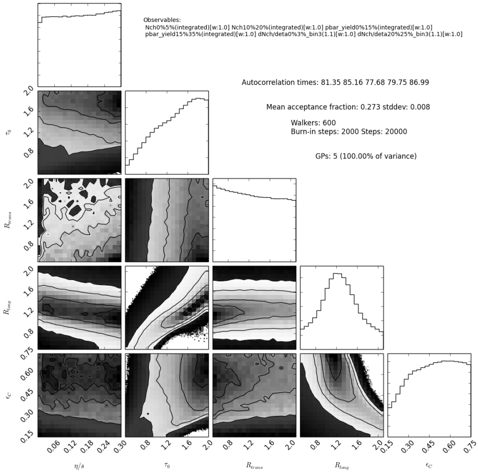
- $v_2\{\text{EP}\}$ in $|\eta| < 0.3$ in (10-40)% centrality

  STAR, PRC86, 054908 (2012)

$N_{\mathrm{ch}} + N_{\bar{p}}$

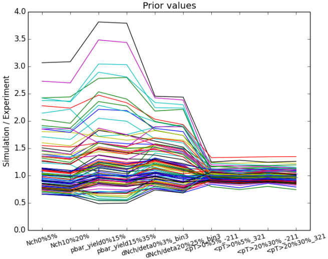


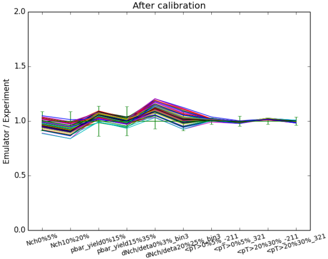


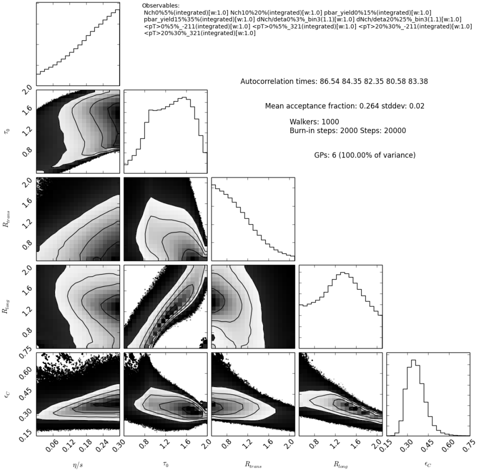


Results preliminary

$N_{\text{ch}} + N_{\bar{p}} + \langle p_T \rangle$

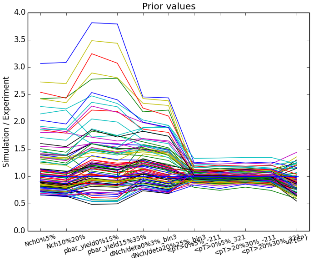


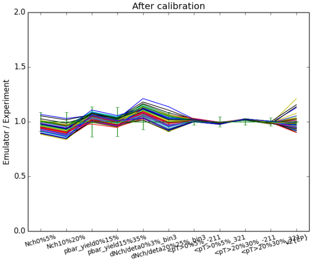


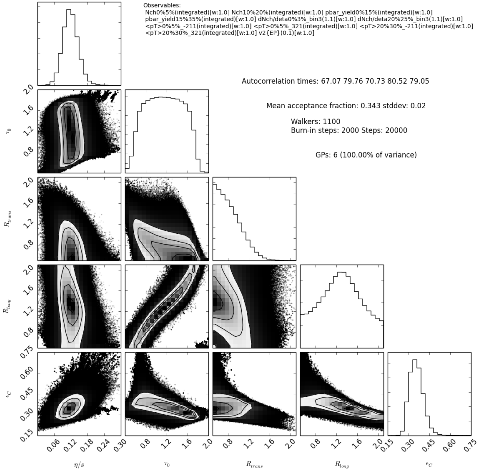


Results preliminary

$N_{\text{ch}} + N_{\bar{p}} + \langle p_T \rangle + v_2$

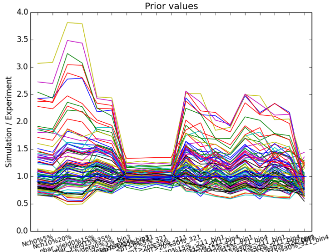


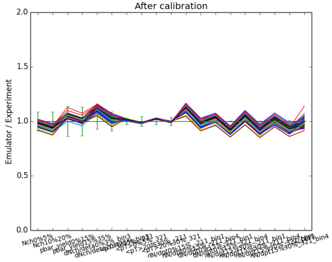


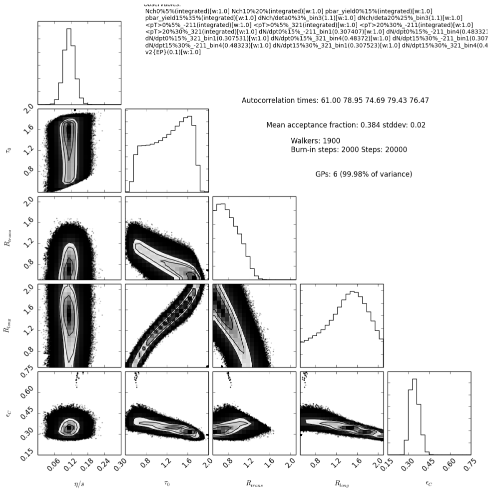


Results preliminary

$$N_{\mathrm{ch}} + N_{\bar{p}} + \langle p_T \rangle + \frac{dN}{dp_T}(\pi, K) + v_2$$







Results preliminary

Summary

- Gaussian processes allow the emulation of complex models, making it possible to investigate multidimensional parameter spaces within reasonable computational effort
- Findings from the analysis of a transport+hydro+transport hybrid model:
  - $\langle p_T \rangle$ constrains hydro-to-transport switching energy density ϵ_C to ≈ 0.35 GeV/fm^3.
  - $\langle p_T \rangle$ and v_2 together constrain η/s to ≈ 0.1.
  - dN/p_T does not seem to provide any strong additional constraints
  - Initial state parameters τ_0, R_{trans} and R_{long} remain largely unconstrained by the investigated set of observables (Investigate HBT? More baryon-related observables?).

Literature

"Gaussian Processes for Machine Learning"
Carl Edward Rasmussen and Christopher K. I. Williams
The MIT Press, 2006. ISBN 0-262-18253-X
http://www.gaussianprocess.org/gpml/

J. Novak, K. Novak, S. Pratt, J. Vredevoogd, C. Coleman-Smith and R. Wolpert,
"Determining Fundamental Properties of Matter Created in Ultrarelativistic Heavy-Ion Collisions,"
Phys. Rev. C **89**, 034917 (2014)
arXiv:1303.5769 [nucl-th]

J. E. Bernhard, P. W. Marcy, C. E. Coleman-Smith, S. Huzurbazar, R. L. Wolpert and S. A. Bass,
"Quantifying properties of hot and dense QCD matter through systematic model-to-data comparison,"
Phys. Rev. C **91**, 054910 (2015)
arXiv:1502.00339 [nucl-th]

Extra slides

Box-Cox transformation

- Gaussian process assumes normally distributed data
- However, many times data is skewed; distribution peaks at values smaller or larger than mean

⇒ Try to fix the skew with Box-Cox transformation[4] $y \to y^{(\lambda)}$:

$$y^{(\lambda)} = \begin{cases} (y^\lambda - 1)/\lambda & : \lambda \neq 0 \\ \log y & : \lambda = 0 \end{cases}$$

- Assumes $y > 0$; shift if necessary
- Normality not guaranteed: Apply normality tests on $y^{(\lambda)}$ (D'Agostino-Pearson, Shapiro-Wilk, Anderson-Darling...)

[4] G.E.P. Box and D.R. Cox, Journal of the Royal Statistical Society B, 26, 211 (1964)