Multi-parameter analysis of a transport+hydrodynamics model of heavy ion collisions using Bayesian statistics and Gaussian emulators

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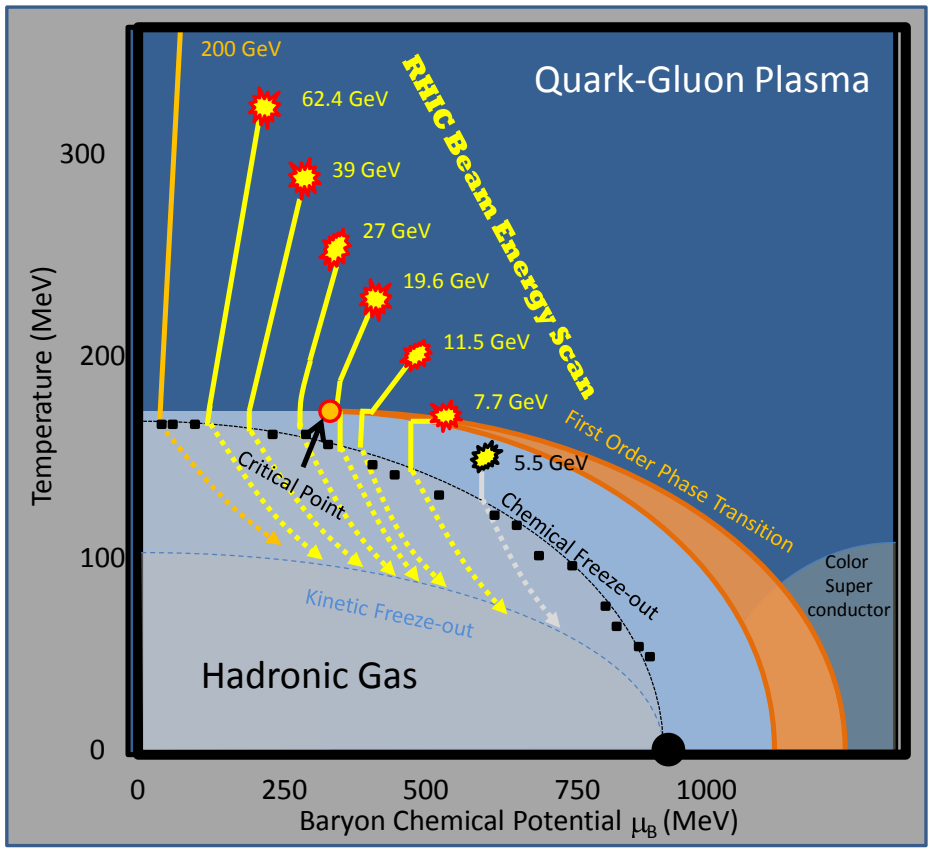
RHIC beam energy scan

- Different collision energies probe different areas of the phase diagram of nuclear matter
- Baryochemical potential μ_B, related to the conservation of net-baryon number, becomes increasingly important at lower energies (nuclear stopping)
- $\mu_B \approx 0$ at 200 GeV and above; good for investigating temperature dependence of physical properties of the formed medium, such as viscosity



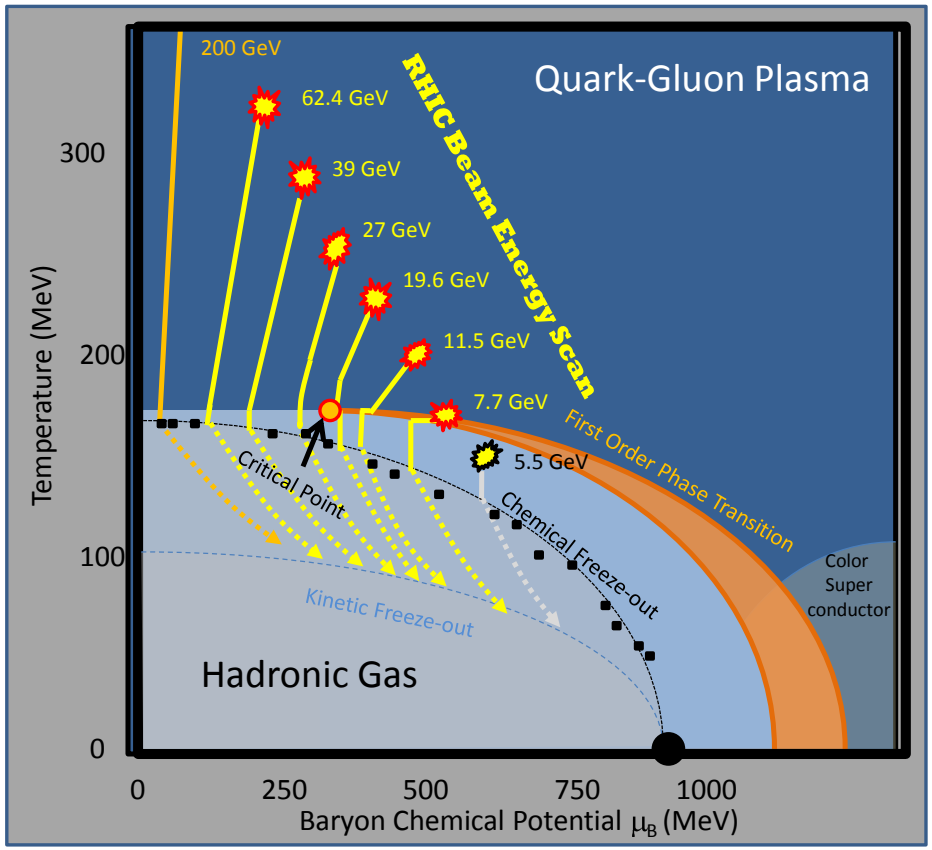
Picture: G. Odyniec, Acta Phys. Polon. B 43, 627 (2012).

RHIC beam energy scan

- Collision energy dependence of the physical parameters of the model $\Rightarrow$ μ_B dependence
- Phase A: Find best-fitting model parameters for several collision energies independently
- If energy dependence observed in the best-fit parameters

$\Downarrow$

Phase B: parametrize the dependence and find the best fit over all collision energies simultaneously



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

Hybrid model

Transport + hydrodynamics hybrid model

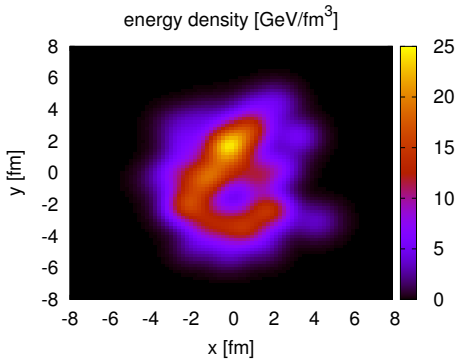
Karpenko, Huovinen, Petersen, Bleicher, Phys.Rev.C, 91, 064901 (2015)

Initial state described by UrQMD[1] hadron transport

- Start the hydrodynamical evolution at time τ_0 when the two nuclei have passed through each other
- Convert energy, momentum and baryon number of each particle into 3D Gaussian distributions:

$$\Delta P^i = CP \exp\left(-\frac{\Delta x^2+\Delta y^2}{{R_{\text{trans}}}^2} - \frac{\Delta\tilde{\eta}^2}{{R_{\text{long}}}^2}\gamma_{\tilde{\eta}}^2{\tau_0}^2\right)$$

$$\Delta N_B = CN_B \exp\left(-\frac{\Delta x^2+\Delta y^2}{{R_{\text{trans}}}^2} - \frac{\Delta\tilde{\eta}^2}{{R_{\text{long}}}^2}\gamma_{\tilde{\eta}}^2{\tau_0}^2\right)$$

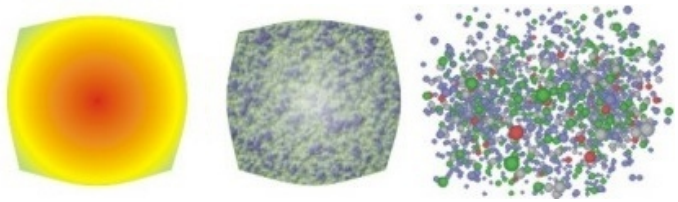


Karpenko et al., PRC91, 064901

- Add all Gaussians and map the resulting densities onto the hydro grid

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

Transport + hydrodynamics hybrid model



- (3+1)D viscous hydrodynamics with constant ratio of shear viscosity over entropy density η/s (bulk viscosity ignored)

  Karpenko et al., Comput. Phys. Commun. 185, 3016 (2014)

- Transition from hydro to transport ("particlization") when energy density ϵ is smaller than critical value ϵ_C
- Construct 4-dimensional hypersurface σ with constant ϵ

  "Cornelius" hypersurface finder, P. Huovinen and H. Petersen, arXiv:1206.3371.

- Particle distributions sampled according to the Cooper-Frye formula

$$p^0 \frac{N_i(x)}{d^3p} = d\sigma_\mu p^\mu f_i(p \cdot u(x), T(x), \mu_i(x))$$

- Rescatterings and final decays calculated in hadron transport (UrQMD)

Bayesian analysis

Calibrating model to experimental data

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 $\vec{x}^* \Rightarrow \vec{y}^{\text{exp}}$.
Determine the level of uncertainty associated with the proposed values

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)

Bayesian analysis

Likelihood function:

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

where

- Σ is the covariance matrix
- $\vec{y}^*$ is model output for the input parameter point $\vec{x}^*$

The posterior distribution can be sampled with Markov chain Monte Carlo (MCMC) random walk in parameter space (defined by prior), where each step is accepted or rejected based on the likelihood.

However: 1 hybrid simulation run requires $\approx$ 5 hours, 50 events produced
$\approx$ 100 000 events needed $\Rightarrow$ 2 000 runs
$\Rightarrow \mathcal{O}(10^4)$ CPU hours for one evaluation of $\vec{y}^*$!
$\Rightarrow$ Need a way to predict model output for arbitrary input parameter point
$\Rightarrow$ Model emulation using Gaussian processes

Gaussian process

http://dan.iel.fm/george

Set Y of values corresponding to set X of points in parameter space, has a multivariate normal distribution if

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

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, ...
- Restrictions: Needs to be symmetric and positive semidefinite

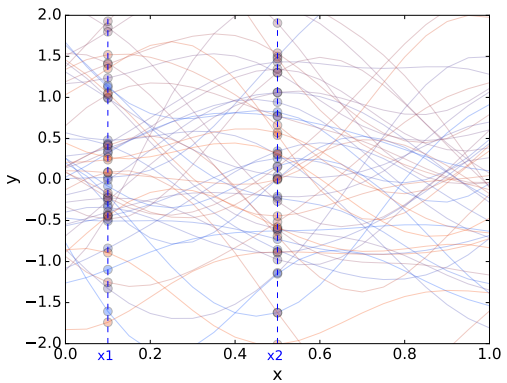
Gaussian process

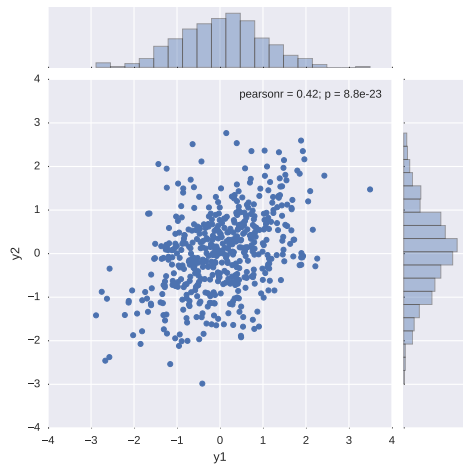
Stochastic process: A parameterized collection of random variables $\{r_t\}_{t\in T}$ (T possibly infinite). E.g. random walk over time.

Gaussian process: A stochastic process, in which every finite set $\{r_t\}$ is a multivariate Gaussian random variable.

$\mu(X) \equiv 0 \Rightarrow$ GP fully defined by the covariance function $\sigma(\vec{x}, \vec{x}')$. Choice: Gaussian with noise

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



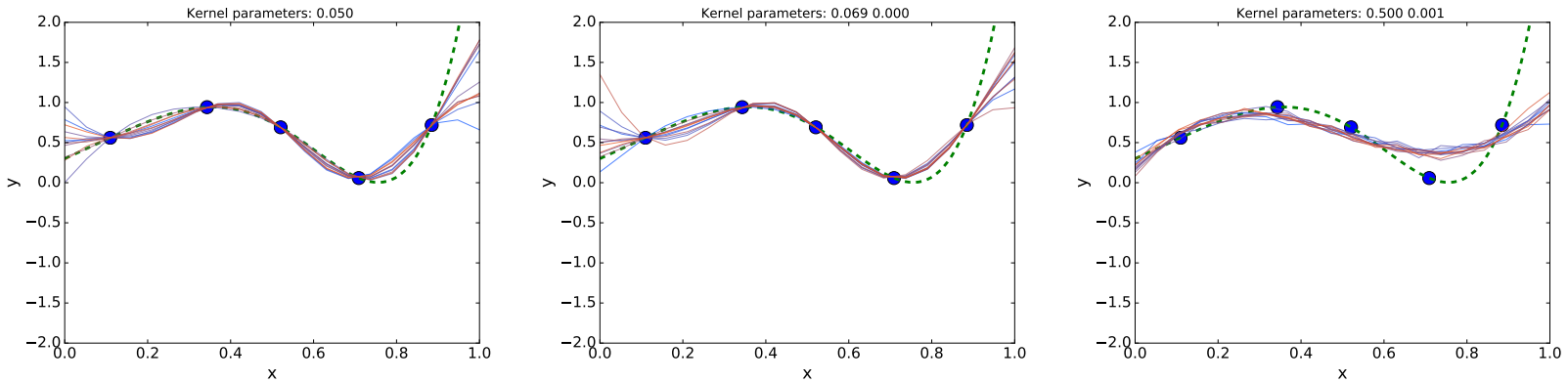


Gaussian process

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 ("empirical Bayes")

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

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



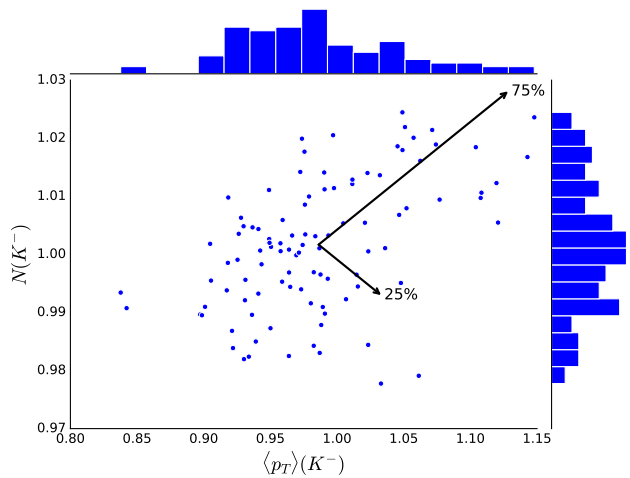
Principal component analysis

m observables $\Rightarrow$ m Gaussian processes

However, m can be up to $\mathcal{O}(100)$ at top RHIC energies and at the LHC!
Number of emulators can be reduced with principal component analysis:

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

- Goal: Find orthonormal matrix P such that the covariance matrix $S = \frac{1}{N} Z^T Z$ is diagonalized for $Z = YP$
- Solution: Columns of P (principal components) are eigenvectors of $Y^T Y$ (directions of maximal variance)



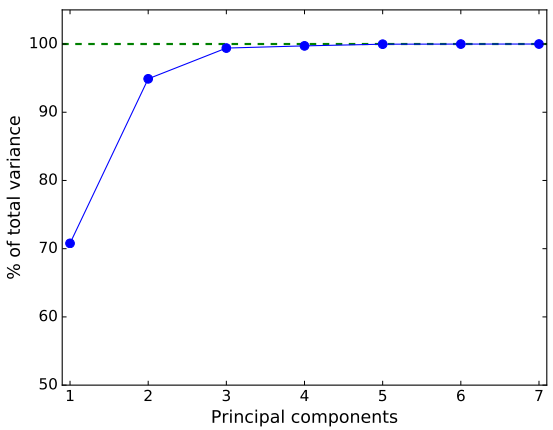
PCA and dimensional reduction

Fraction of variance explained by principal component p_q: $\mathrm{Var}(p_q) = \frac{\lambda_q}{\sum_{i=1}^{m} \lambda_i}$

- $\lambda_1 > \lambda_2 > ... > \lambda_q > ... > \lambda_m$
  $\Rightarrow \mathrm{Var}(p_q) \approx 0$ starting from some $i < q < m$
  $\Rightarrow$ Reduced-dimension transformation

$$Z_q = \sqrt{N} Y V_q$$

- 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



Likelihood function

The likelihood function used in MCMC:

$$\exp\left(-\frac{1}{2}\sum_{i=1}^{q}\lambda_i\frac{(z_i^*-z_i^{\text{exp}})^2}{(\sigma z_i^{\text{exp}})^2+\Sigma_i^*}\right)$$

- λ_i is the variance explained by ith principal component
- z_i^* is the emulator prediction for ith principal component at the input parameter point $\vec{x}^*$
- $\vec{z}^{\text{exp}}$ is the experimental data transformed to principal component space
- Σ_i^* is the predictive variance (emulator uncertainty)
- $\sigma = 0.1$ is global estimate for all other uncertainties (experimental sys and stat errors etc.)

Analysis procedure

Scale with experimental values $\Rightarrow$ Unitless quantities of the order ($\mathcal{O}(1)$)

$\Downarrow$

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

$\Downarrow$

Apply weights
Center the data

$\Downarrow$

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

$\Downarrow$

Train the emulator(s)

$\Downarrow$

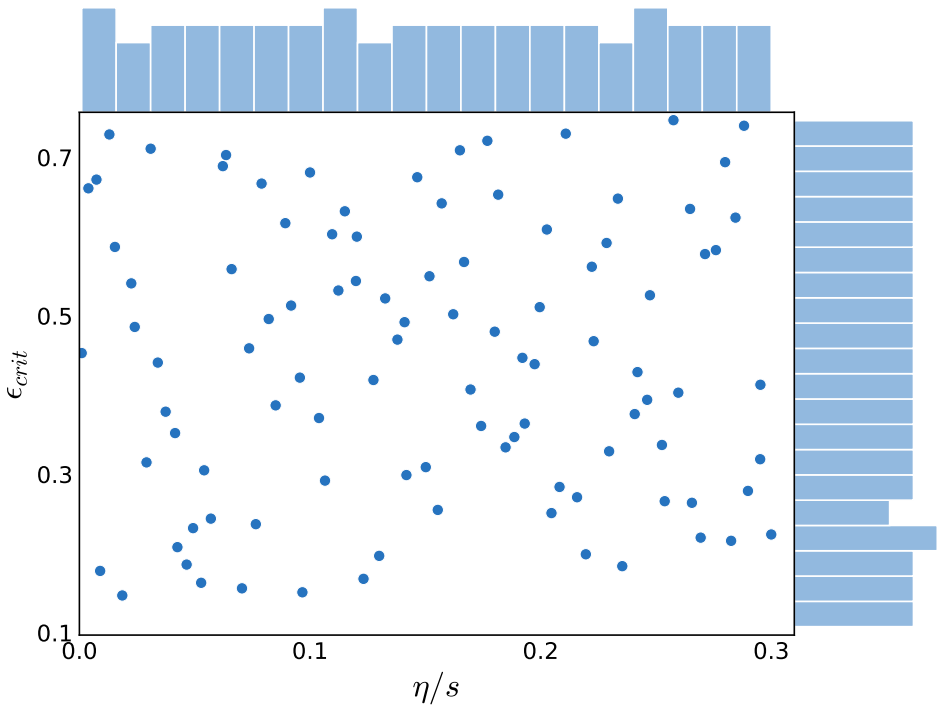
Calibrate on experimental data by running MCMC

Model results

Investigated parameter ranges

Sample points evenly over whole parameter space using Latin hypercube method

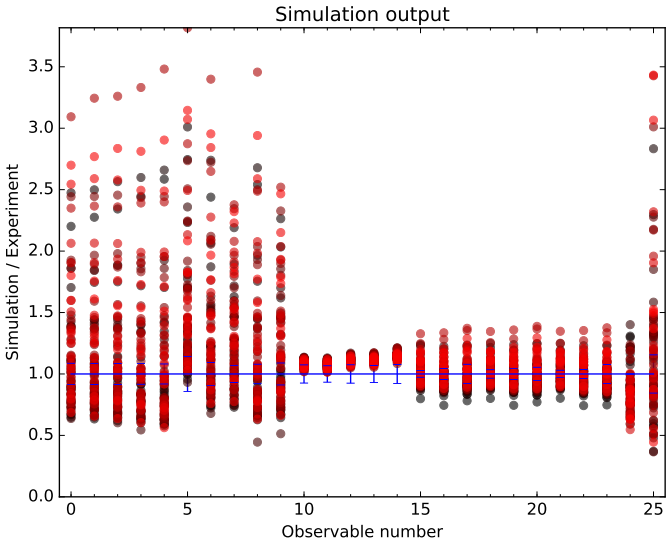
- Shear viscosity over entropy density η/s: 0.001 - 0.4
- Transport-to-hydro transition time τ_0: 0.4 - 3.1 fm
- Transverse Gaussian smearing of particles R_{trans}: 0.2 - 2.2 fm
- Longitudinal Gaussian smearing of particles R_{long}: 0.2 - 2.2 fm
- Hydro-to-transport transition energy density ϵ_C: 0.15 - 0.75 GeV/fm^3

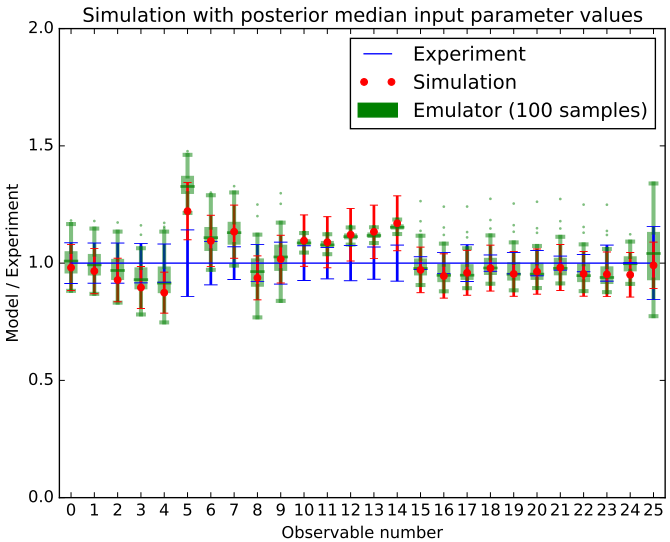


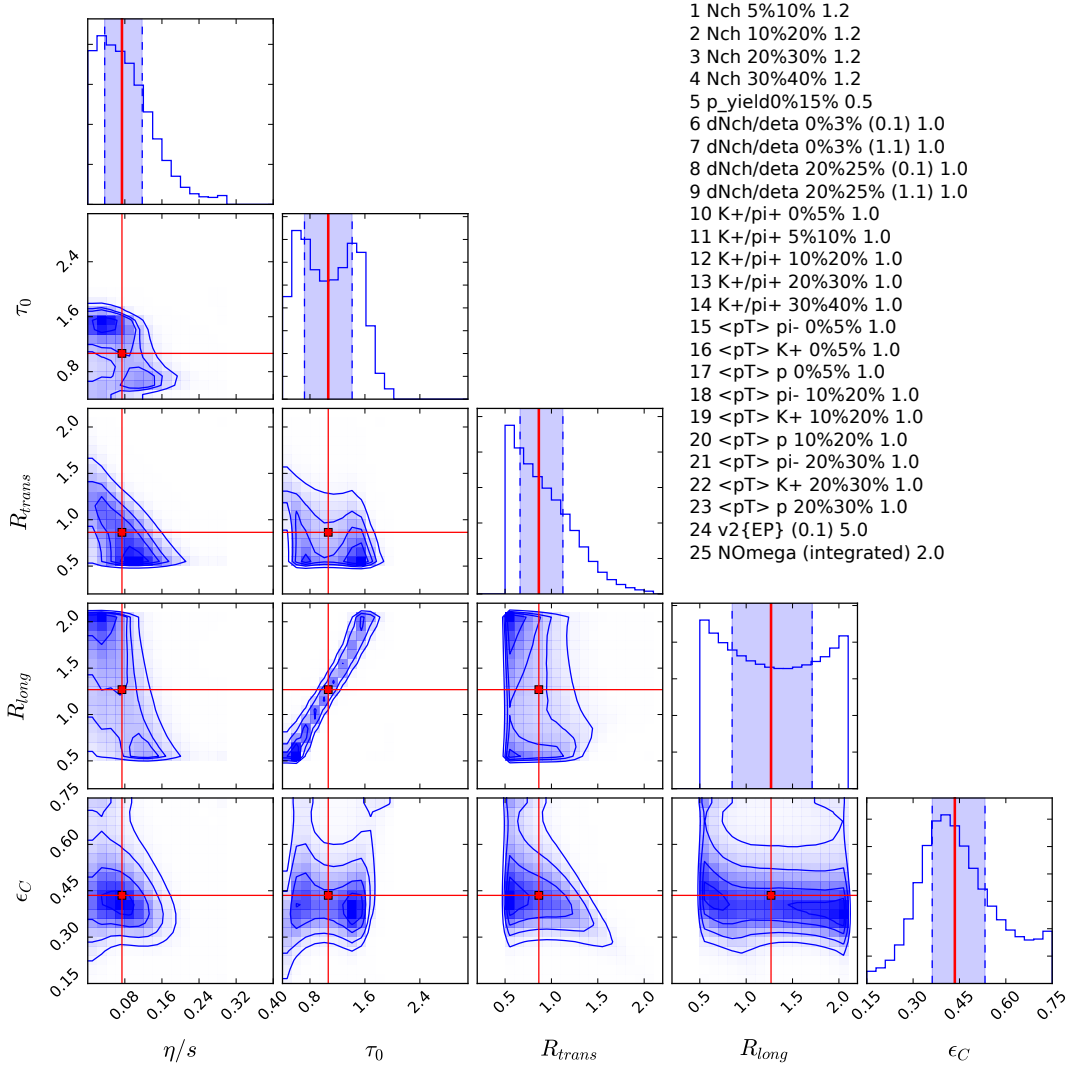
Investigated observables

- Charged particles at midrapidity N_{ch}
- Charged particle pseudorapidity distribution $dN_{\text{ch}}/d\eta$
- Number of π, K, p, Ω at midrapidity
- Mean transverse momentum $\langle p_T \rangle$ for π, K, p
- Lowest p_T bin of dN/dp_T for Ω (when $N(\Omega)$ not available)
- Charged particle elliptic flow $v_2\{\text{EP}\}$ or $v_2\{2\}$

Results at 62.4 GeV







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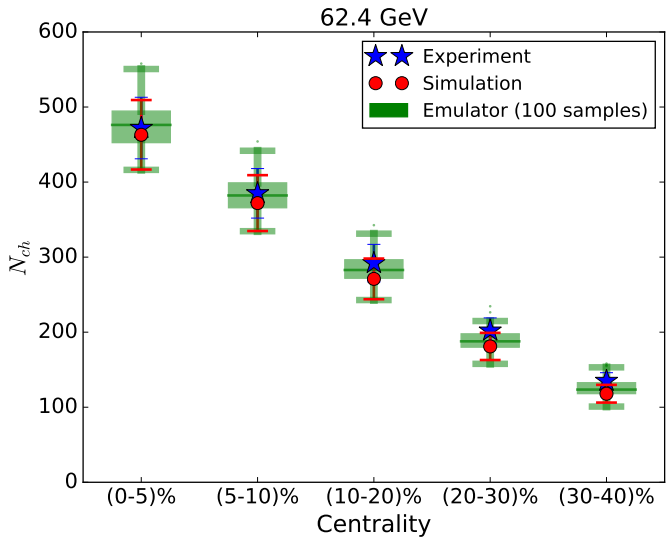

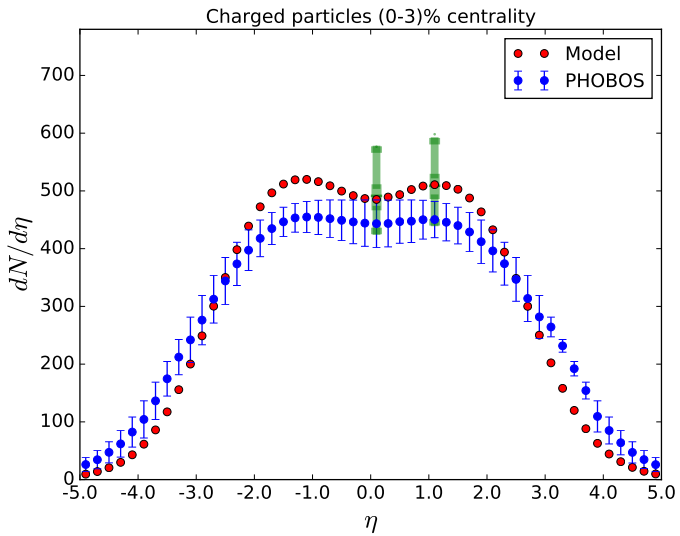

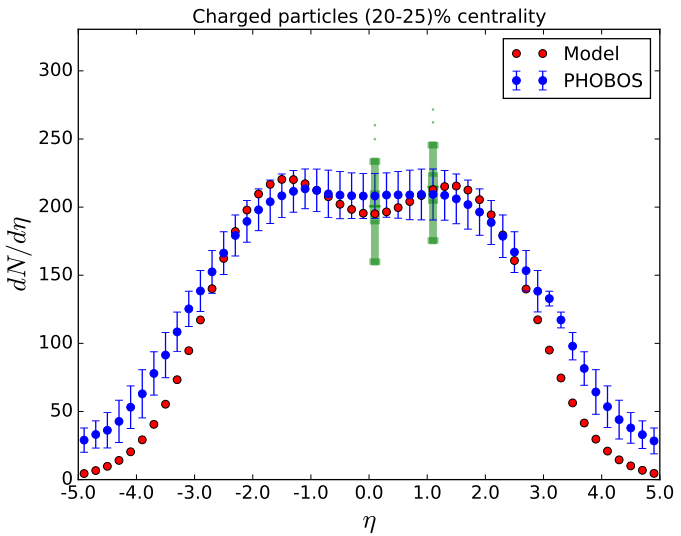

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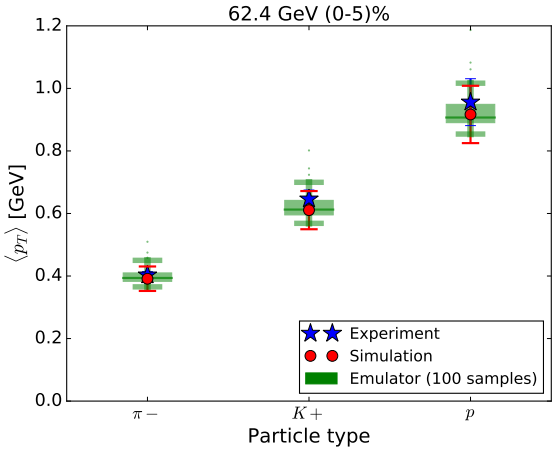
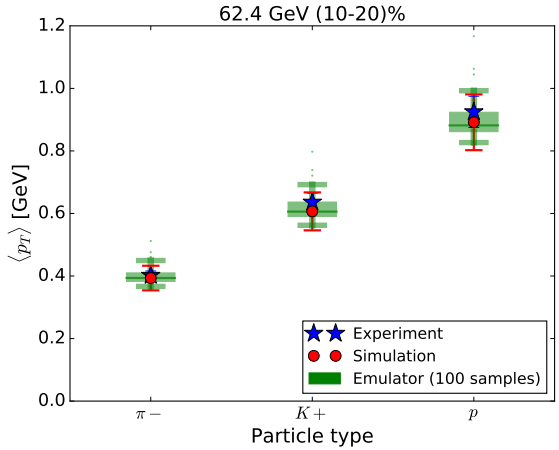
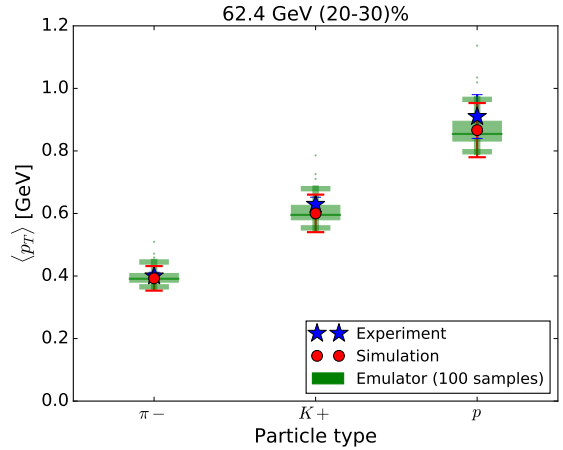
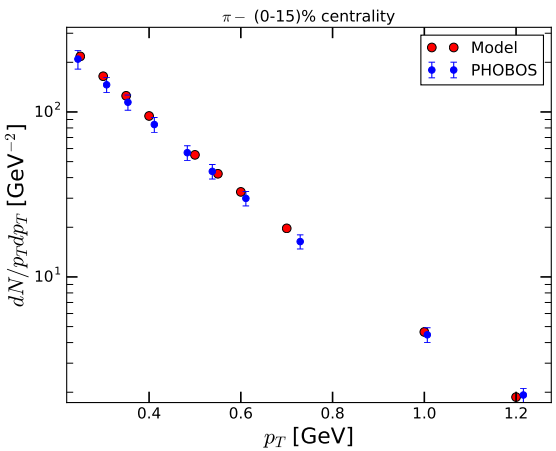
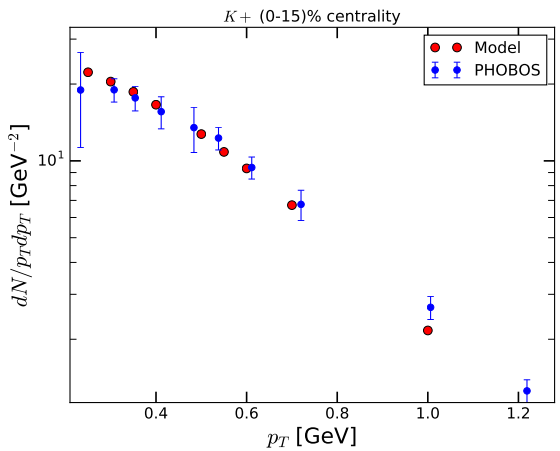
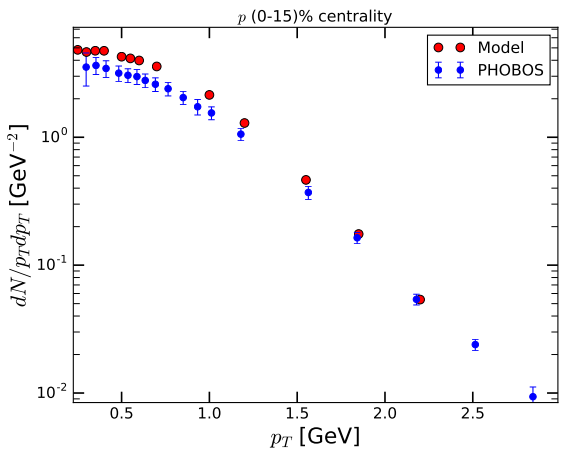




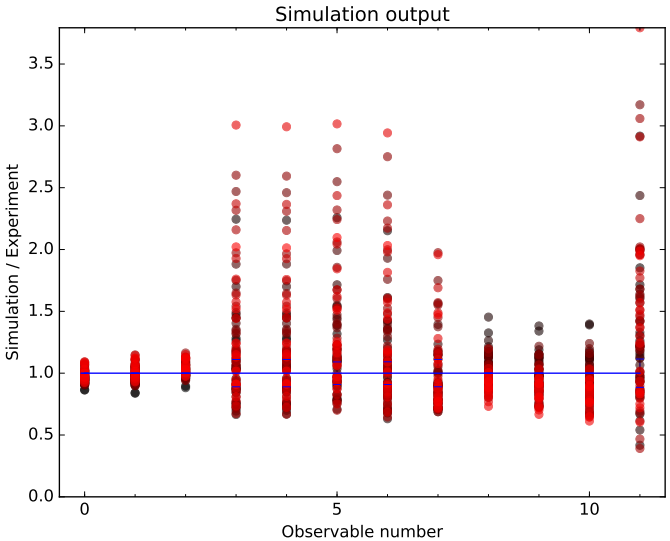


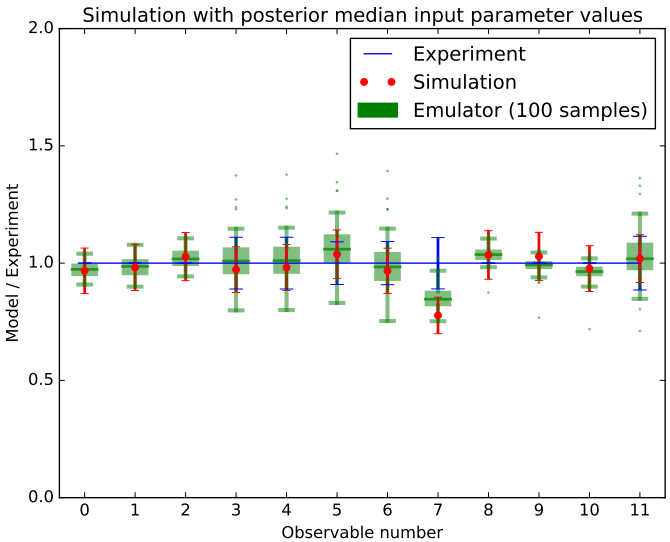


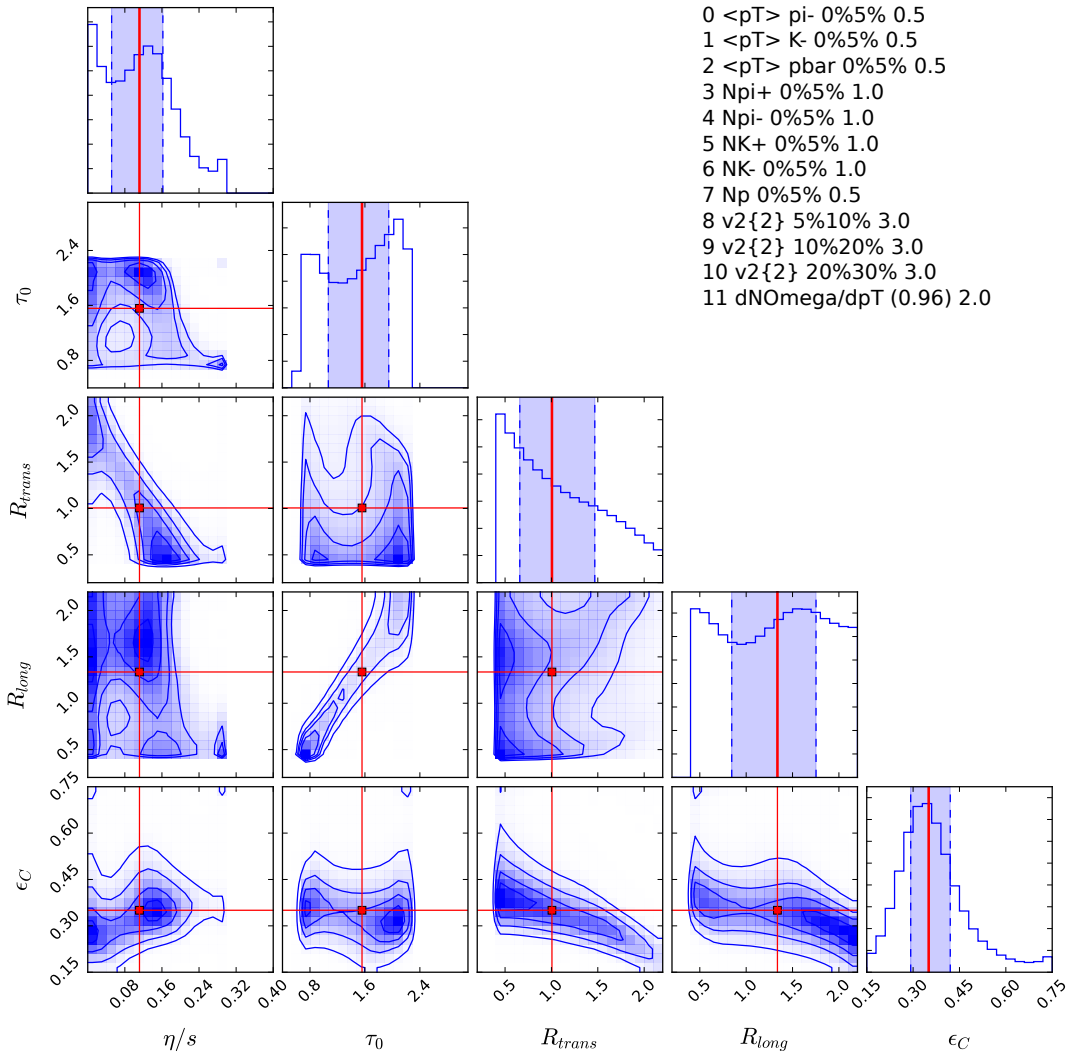




Results at 39 GeV







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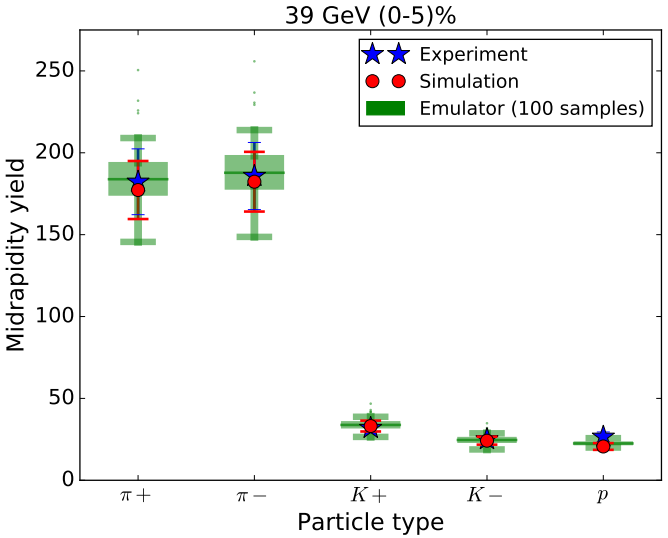
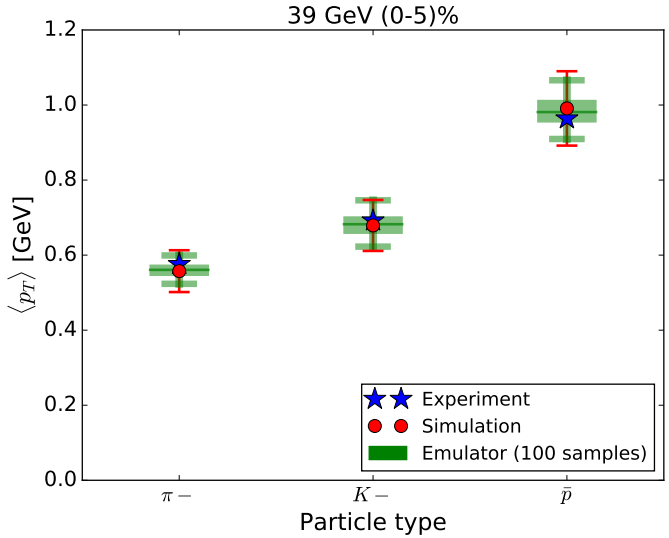
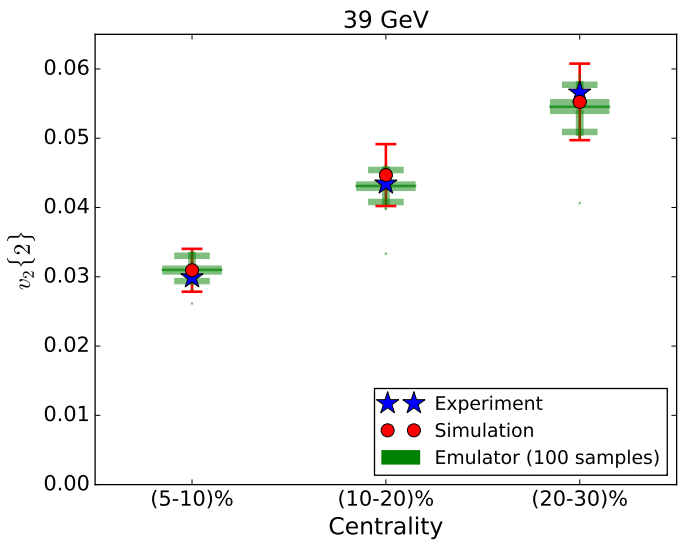
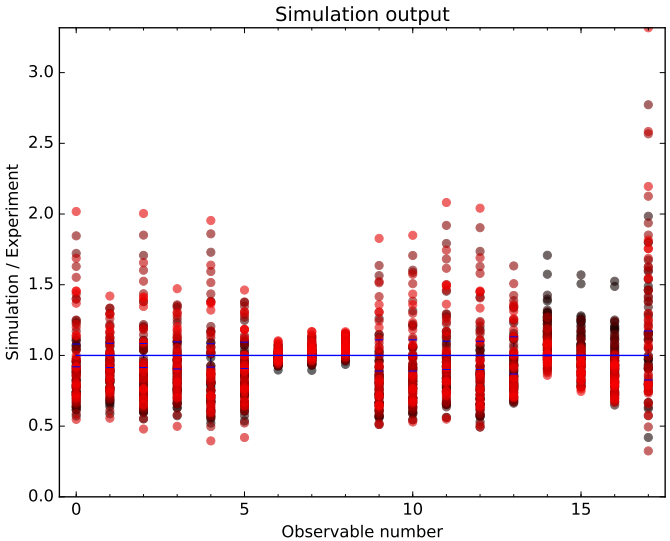
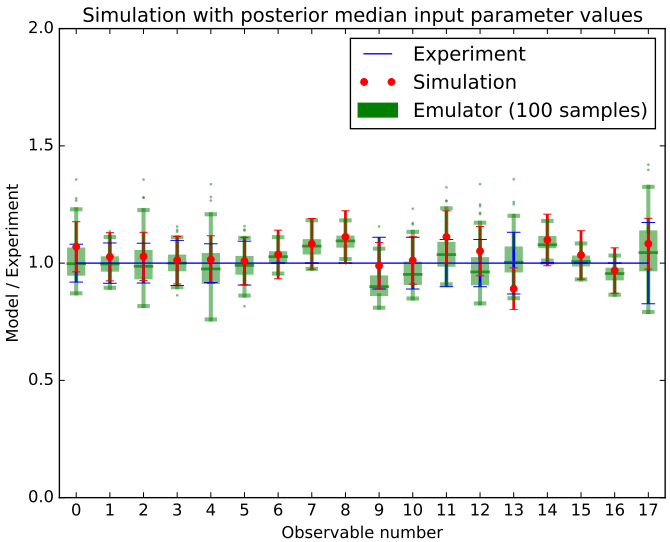


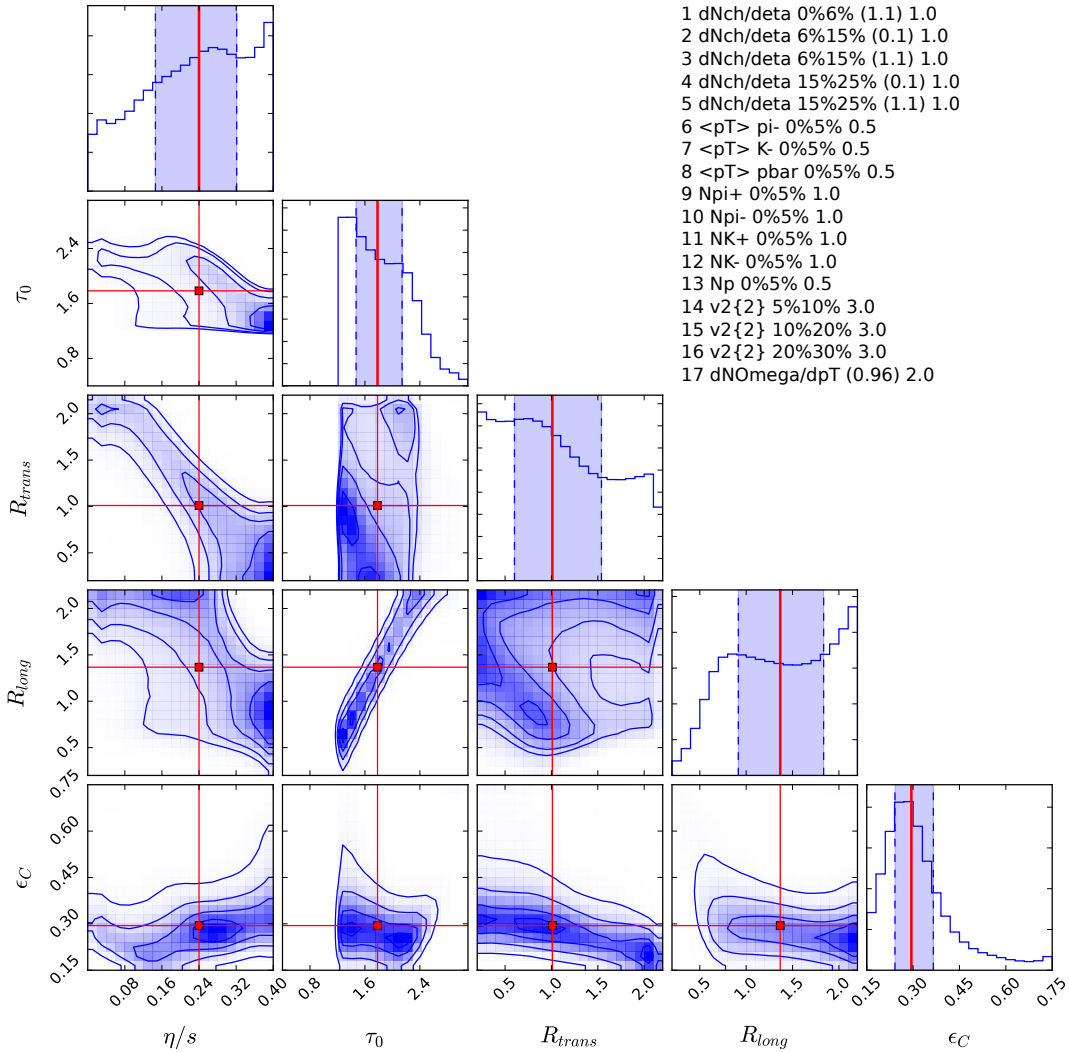




Results at 19.6 GeV







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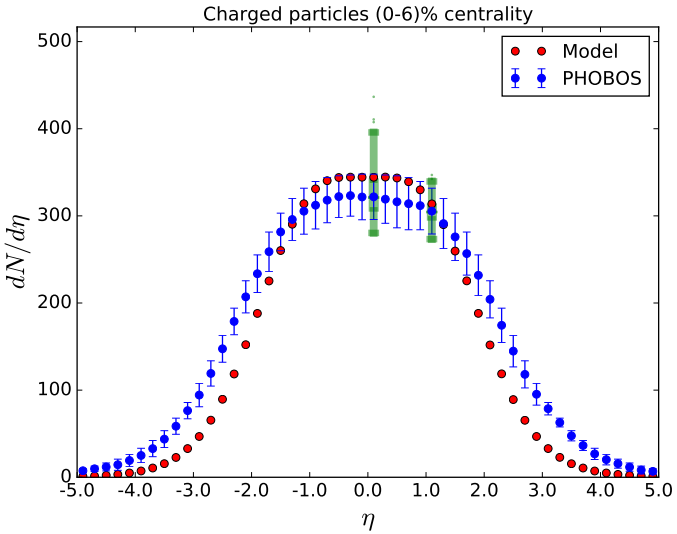
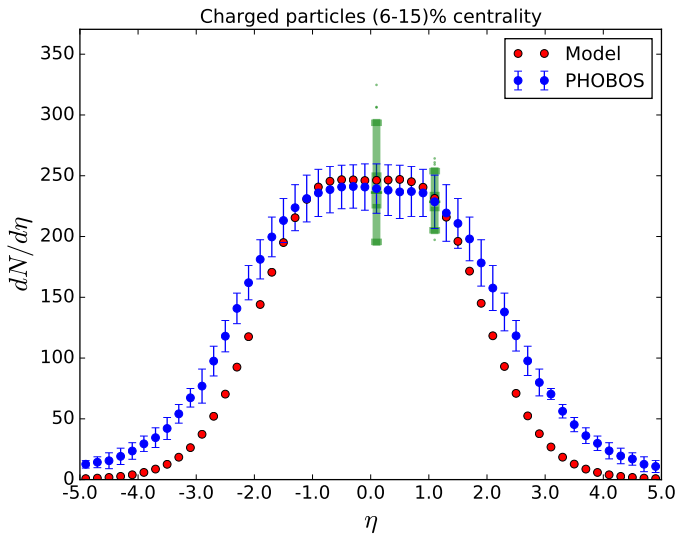
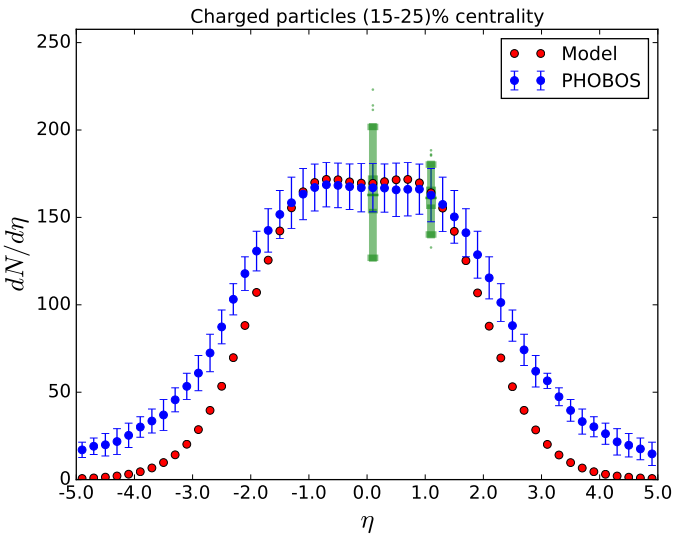
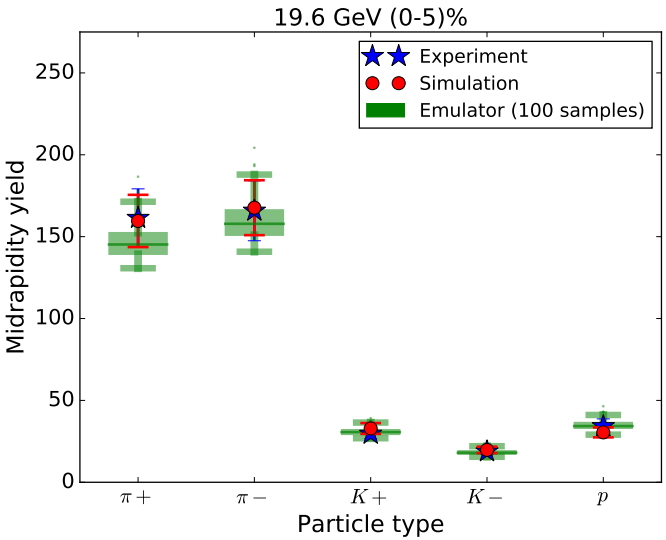
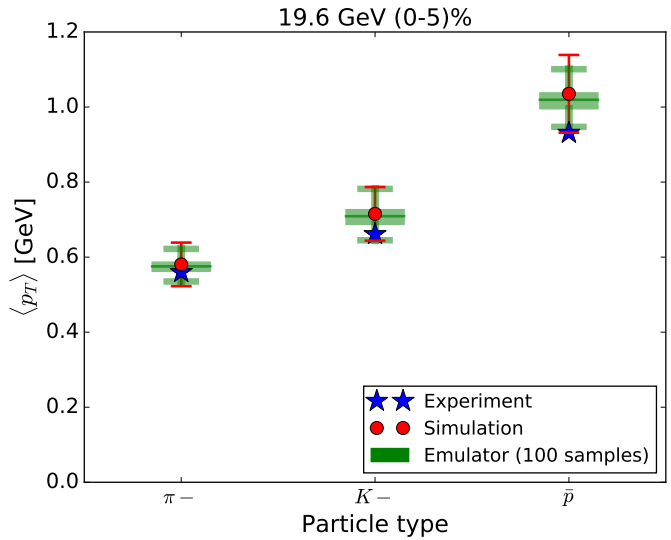


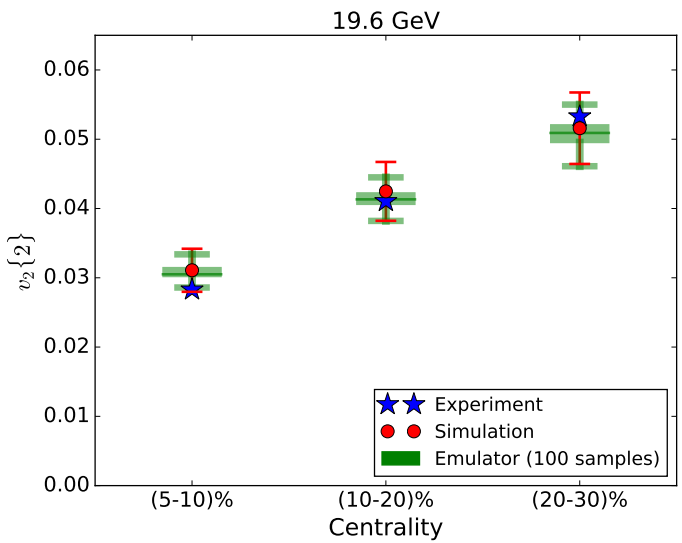




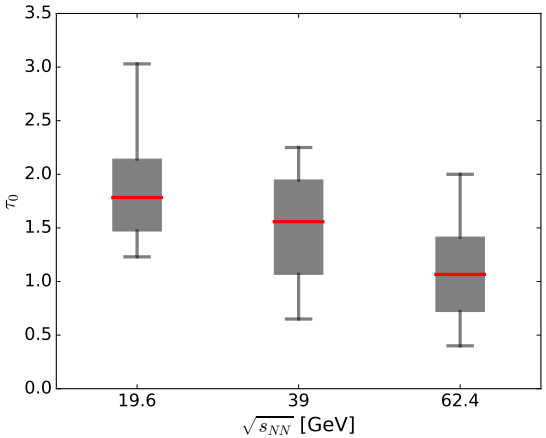
Results at 19.6 GeV

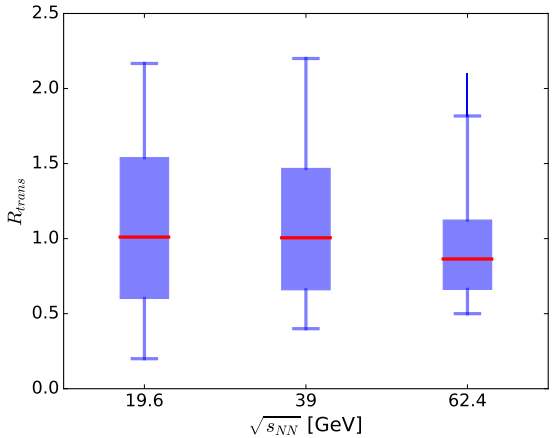


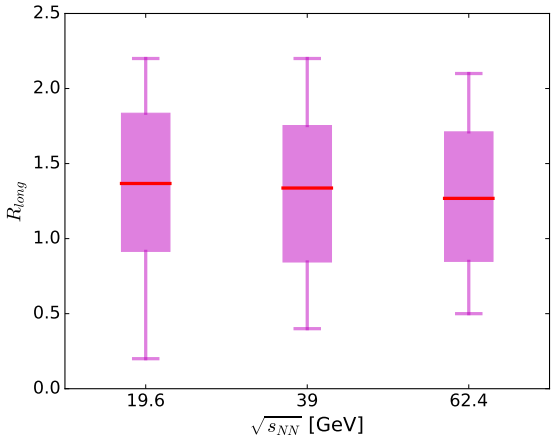


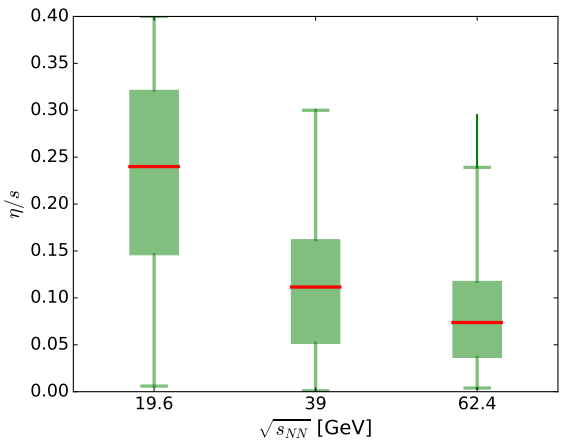


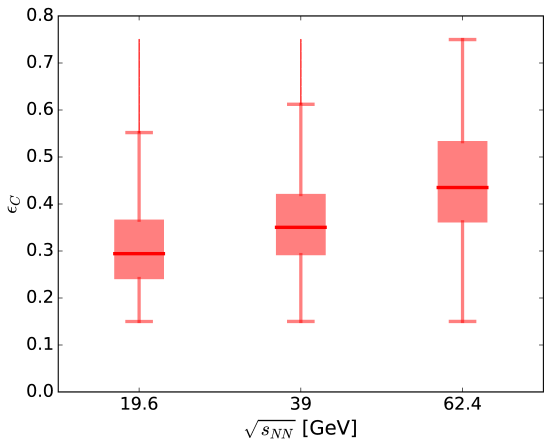
Parameter dependence on collision energy



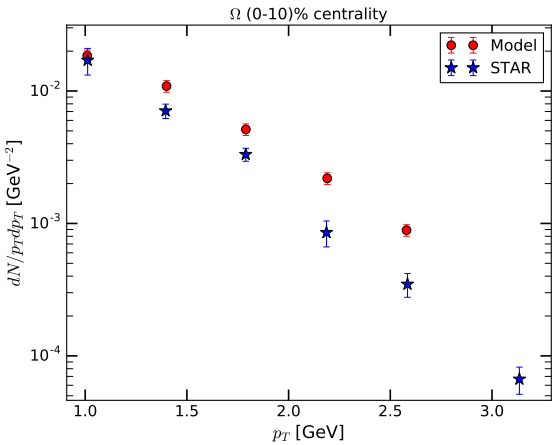


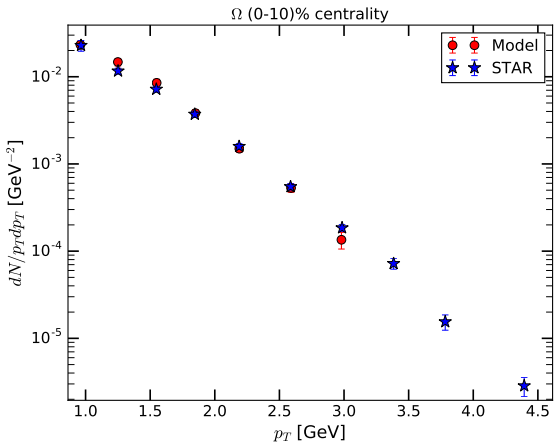


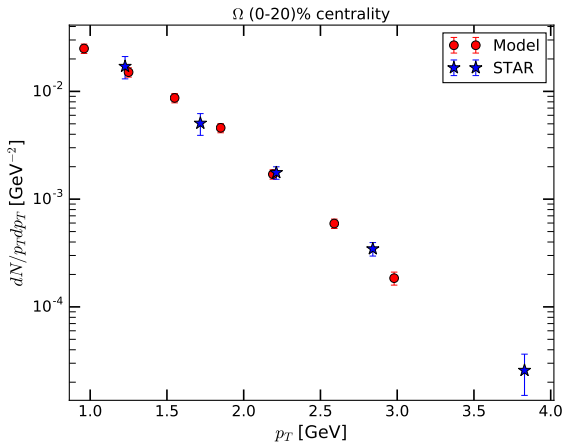


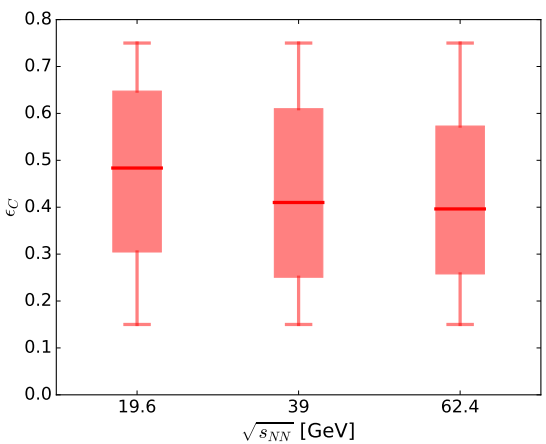


Effect of Ω yields on ϵ_C

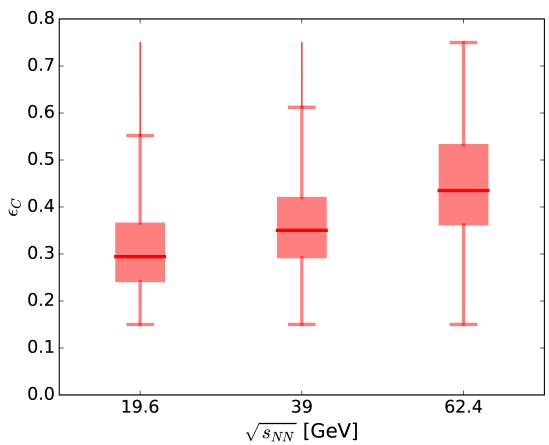








Without Ω yields



With Ω yields

Summary

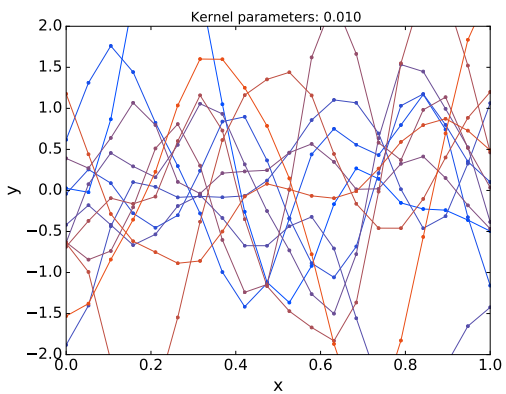
- Bayesian analysis provides a rigorous method for simultaneous estimation of both the best-fit values and the associated uncertainties for the parameters of heavy ion collision models
- Using posterior median values for the hybrid model gives good agreement with experimental data
- Ω yields provide important constraints on switching energy density ϵ_C
- Posterior distributions still rather wide
  - Initial state needs stronger constraints (use higher η bins in $dN_{\mathrm{ch}}/d\eta$?)
  - Refine uncertainty estimates in likelihood function; use reported error estimates from experiments for each observable:
    $(\sigma z_i^{\mathrm{exp}})^2 + \Sigma_i^* \rightarrow \Sigma_i^{\mathrm{exp}} + \Sigma_i^*$
    Correlated uncertainties between different observables (non-diagonal elements in Σ^{exp})?

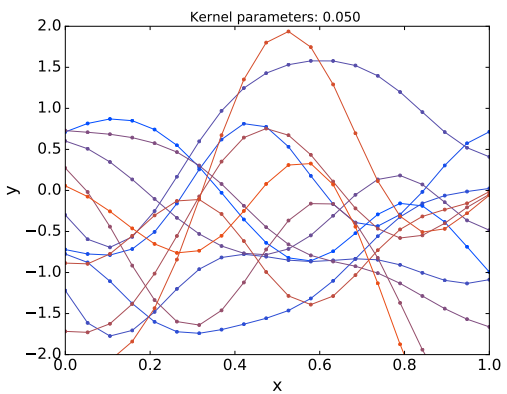
Extra slides

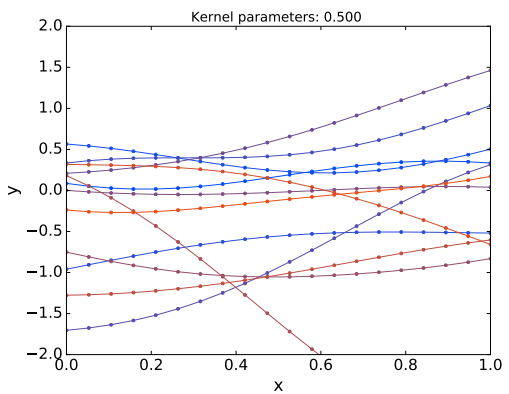
Gaussian process

Drawing samples from a Gaussian process:

- Define a vector of N points, $\vec{x} = (x_1, ..., x_N)$, on which to evaluate the GP
- Compute covariance matrix $\Sigma_{ij} = \sigma(x_i, x_j)$
- Compute Cholesky decomposition $\Sigma = SS^T$
- The vector $\vec{y} = \mu(\vec{x}) + S\vec{u}$, $u_i \sim N(0, 1)$, defines a GP sample







Gaussian process

The joint distribution of k observations $Y_o = (y(x_{o1}), ..., y(x_{ok}))$ and q predictions $Y_p = (y(x_{p1}), ..., y(x_{pq}))$ is

$$\begin{pmatrix} Y_p \\ Y_o \end{pmatrix} = \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \Sigma_{p,p} & \Sigma_{p,o} \\ \Sigma_{o,p} & \Sigma_{o,o} \end{pmatrix} \right),$$

resulting to a conditional probability distribution $p(Y_p|Y_o) \sim \mathcal{N}(\bar{\mu}, \bar{\Sigma})$ with posterior mean (prediction based on known values)

$$\bar{\mu}(X_p) = \Sigma_{p,o}\Sigma_{o,o}^{-1}Y_o$$

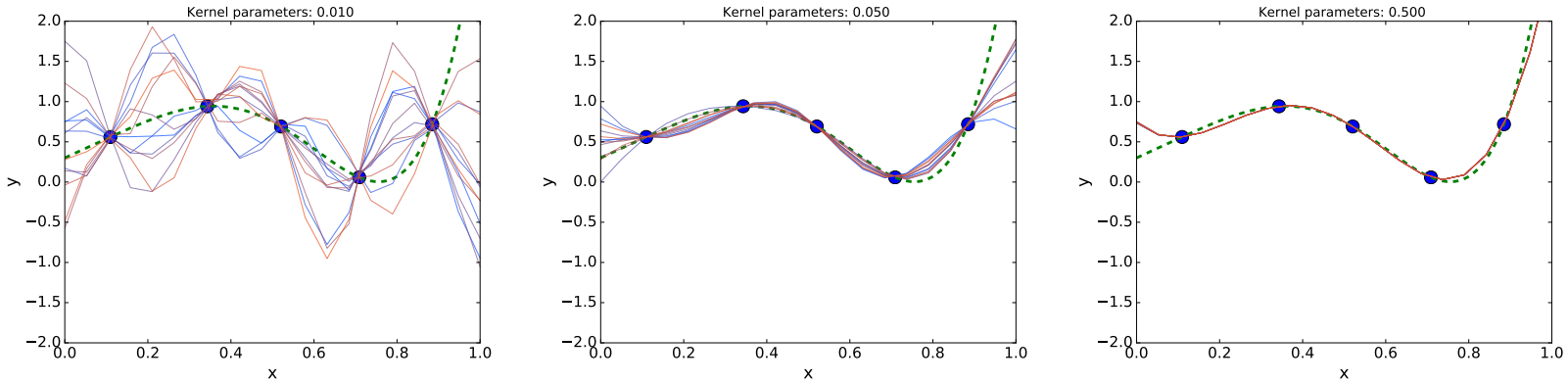
and posterior variance $\bar{\Sigma} = \Sigma_{p,p} - \Sigma_{p,o}\Sigma_{o,o}^{-1}\Sigma_{o,p}$.

For an observation point $x_o \in X_o$:

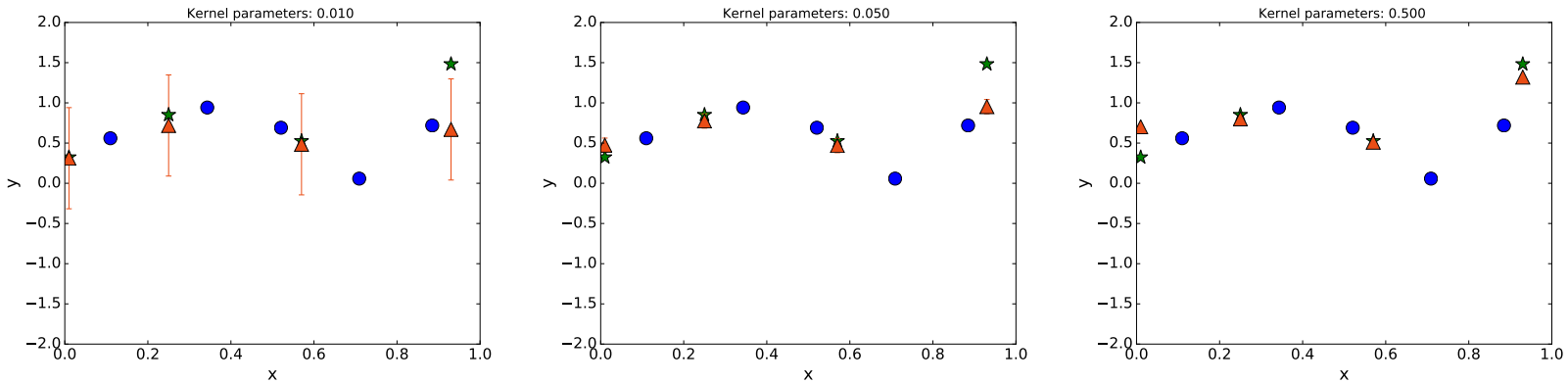
- posterior mean $\bar{\mu}(x_o) = y_o$
- posterior variance $\bar{\Sigma} = 0$

Gaussian process

GP conditioned on known values:



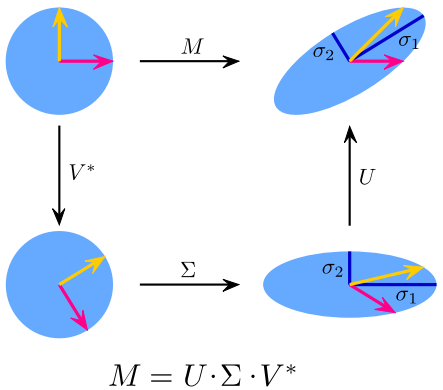
Conditioned GP predictions:



Singular value decomposition

Singular value decomposition: $Y = U\Sigma V^T$

- Σ is a diagonal matrix containing the singular values
- U and V^T are orthogonal matrices containing the left- and right-singular vectors, respectively



Wikipedia

- Eigenvalue decomposition of Y^TY becomes

$$Y^TY = V\Sigma^2V^T$$

  - Singular values in Σ are square roots of eigenvalues λ_i of Y^TY
  - Right singular vectors in V^T are eigenvectors of Y^TY
  - $V^TY^TYV = \Sigma^2 = \frac{1}{N}Z^TZ \Rightarrow Z = \sqrt{N}YV$

Box-Cox transformation

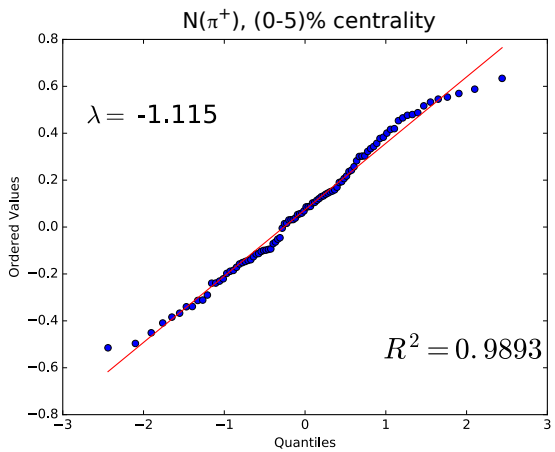
PCA assumes that mean and variance are sufficient statistics to describe the distribution of model output
Many times data is skewed, which reduces the quality of principal component analysis

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

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

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

- y dimensionless $\Rightarrow$ Scale with experimental values y^{exp} first
- Assumes $y > 0$; shift if necessary
- Check against normal distribution after transformation (probability plot, QQ plot)



Markov chain Monte Carlo

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

The posterior distribution 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 (calculated in terms of principal components)
- Converges to posterior distribution as number of steps $N \to \infty$
- Acceptance fraction a_f of steps measures the quality of random walk
  - $a_f \sim 0 \Rightarrow$ walker "stuck"
  - $a_f \sim 1 \Rightarrow$ purely random walk
  - aim for 0.2-0.5
- Autocorrelation time = Number of steps between independent samples
  "Burn-in" takes a few autocorrelations,
  gathering enough samples $\sim \mathcal{O}(10)$ autocorrelations