Quantifying properties of hot and dense QCD matter through systematic model-to-data comparison

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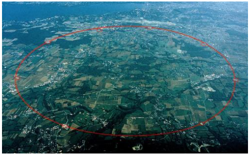
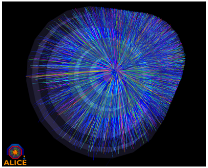
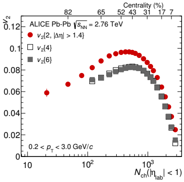
INT workshop: Correlations and fluctuations in p+A and A+A collisions
Tuesday, July 14, 2015

J. E. Bernhard, P. W. Marcy, C. E. Coleman-Smith,
S. Huzurbazar, R. L. Wolpert, and S. A. Bass,
PRC **91**, 054910 (2015), arXiv:1502.00339 [nucl-th].

Model-to-data comparison



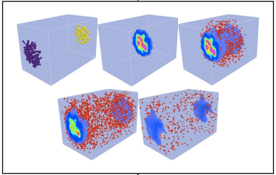


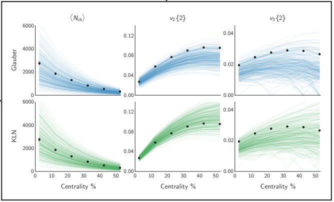


Model

Initial conditions,

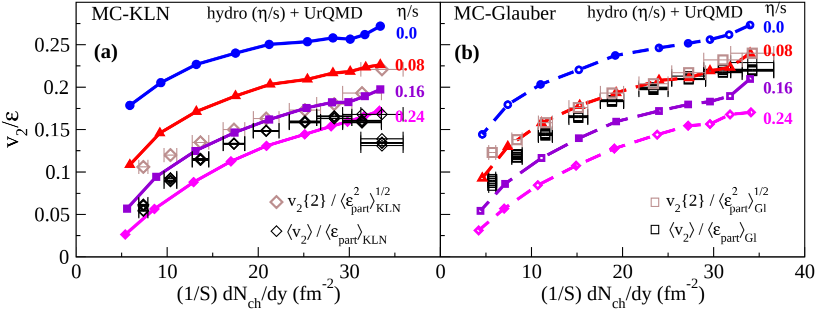
τ_0, η/s, . . .





Measuring QGP η/s

1. Observe experimental flow coefficients v_n
2. Run model with variable η/s
3. Constrain η/s by matching v_n



H. Song, S. A. Bass, U. Heinz, T. Hirano, and C. Shen, PRL **106**, 192301 (2011), arXiv:1011.2783 [nucl-th].

Extracting QGP properties

Older work

- Average calculations
- Single parameter and observable ($\eta/s \leftrightarrow v_2$)
- Several discrete values
- Qualitative constraints lacking uncertainty

$\longrightarrow$

New projects

- Event-by-event model
- Multiple parameters and observables
- Continuous parameter space
- Quantitative constraints including uncertainty

See also, e.g.:

- J. Novak, K. Novak, S. Pratt, C. Coleman-Smith, and R. Wolpert, PRC **89**, 034917 (2014), arXiv:1303.5769 [nucl-th].
- R. A. Soltz, I. Garishvili, M. Cheng, B. Abelev, A. Glenn, J. Newby, L. A. Linden Levy, and S. Pratt, PRC **87**, 044901 (2013), arXiv:1208.0897 [nucl-th].
- S. Pratt, E. Sangaline, P. Sorensen, and H. Wang, PRL **114**, 202301 (2015), arXiv:1501.04042 [nucl-th].

Strategy

1. Choose set of salient model parameters
   - physical properties
   - model nuisance parameters
2. Run model at small $\mathcal{O}(10^1\text{–}10^2)$ set of parameter points
3. Interpolate with Gaussian process emulator
   $\rightarrow$ fast stand-in for actual model
4. Systematically explore parameter space using Bayes' theorem and Markov chain Monte Carlo (MCMC)
5. Calibrate model emulator to optimally reproduce data
   $\rightarrow$ extract probability distributions for each parameter

Event-by-event model

- MC-Glauber & MC-KLN initial conditions

  H.-J. Drescher and Y. Nara, PRC **74**, 044905 (2006).

- Viscous 2+1D hydro

  H. Song and U. Heinz, PRC **77**, 064901 (2008).

- Cooper-Frye hypersurface sampler

  C. Shen, Z. Qiu, H. Song, J. Bernhard, S. Bass, and U. Heinz, arXiv:1409.8164 [nucl-th].

- UrQMD

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

Calibration parameters

Initial condition parameters:

- Overall normalization factor
- α (Glauber), λ (KLN)
  $\rightarrow$ both control centrality dependence of multiplicity

Hydro parameters:

- Thermalization time τ_0
- Specific shear viscosity η/s
- Shear relaxation time $\tau_\pi = 6k_\pi\eta/(sT)$ [vary k_π]

Computer experiment design

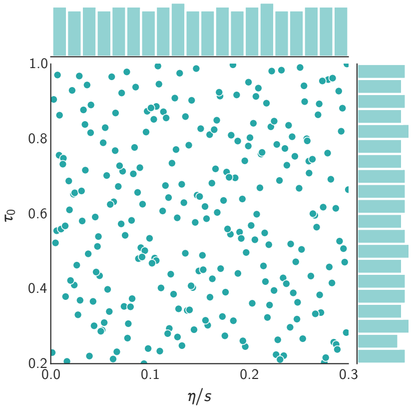
Latin-hypercube design:

- Semi-randomized, space-filling points
- Avoids large gaps and tight clusters
- All parameters varied simultaneously
- Needs only $m \gtrsim 10n$ points

This work:

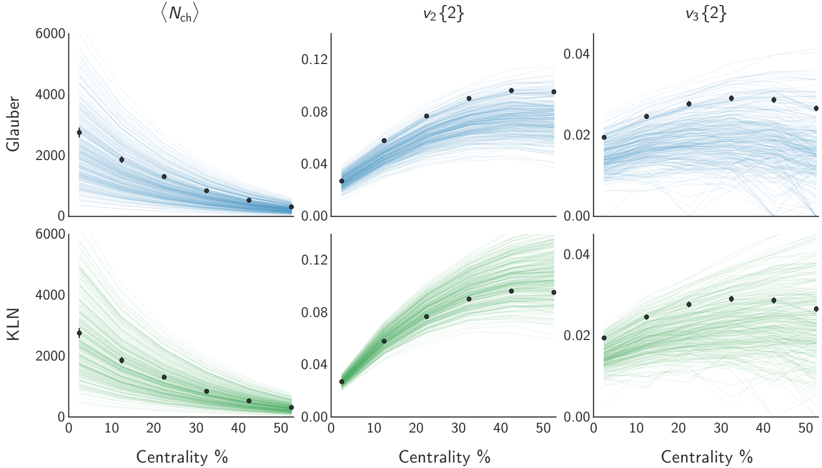
- $m = 256$ points across $n = 5$ dimensions
- $\mathcal{O}(10^4)$ events per point

Design projected into $(\tau_0, \eta/s)$ dimensions:



Training data

Model calculations at each parameter point



Data points: ALICE Collaboration, Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV
B. B. Abelev *et al.*, PRC **90**, 054901 (2014), arXiv:1406.2474 [nucl-ex].

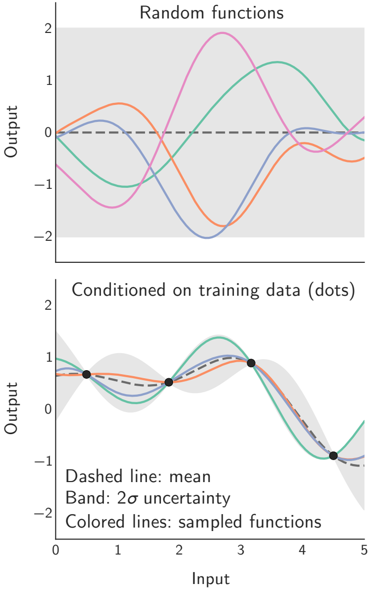
Gaussian process emulator

Gaussian process:

- Stochastic function: maps inputs to normally-distributed outputs
- Specified by mean and covariance functions

As a model emulator:

- Non-parametric interpolation
- Predicts *probability distributions*
  - Narrow near training points, wide in gaps
- Fast "surrogate" to actual model



Multivariate output

Model outputs ($N_{\mathrm{ch}}, v_2, v_3$)
$\rightarrow$ independent emulators?

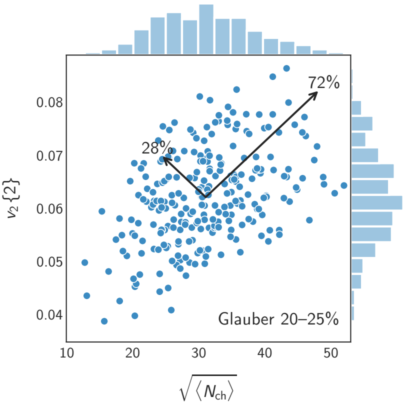
- Neglects correlations
- What if 100 outputs?

Principal components:

- Linear combinations of model output data
- Orthogonal and uncorrelated

$\rightarrow$ Emulate each PC

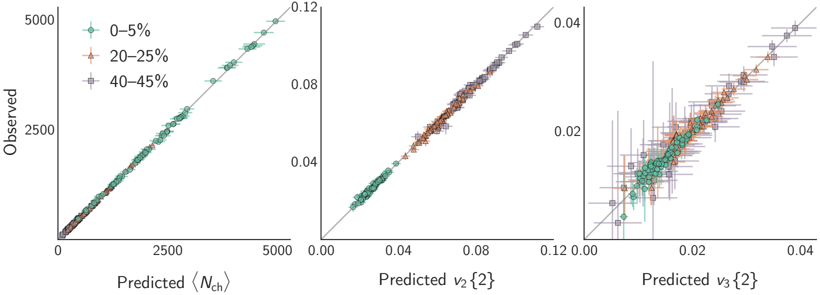
PC decomposition of N_{ch} and v_2 data in one centrality bin:



$N_{\mathrm{ch}} : v_2 : v_3$ weighted $1.2 : 1.0 : 0.6$
$\rightarrow$ encodes relative importance of describing each observable

Validation

- Independent set of validation points
- Run model and predict output with emulator at each point
- Accurate predictions fall on diagonal line



Horizontal error bars: 2σ emulator uncertainty
Vertical error bars: 2σ statistical uncertainty

Calibration

Input parameters:

$$\mathbf{x} = (\text{Norm}, \text{I.C. param}, \tau_0, \eta/s, k_\pi)$$

Assume true parameters $\mathbf{x}_\star$ exist $\rightarrow$ find probability dist. for $\mathbf{x}_\star$

Bayes' theorem:

$$P(\mathbf{x}_\star | X, Y, \mathbf{y}_{\text{exp}}) \propto P(X, Y, \mathbf{y}_{\text{exp}} | \mathbf{x}_\star) P(\mathbf{x}_\star)$$

- $P(\mathbf{x}_\star) =$ prior
  $\rightarrow$ initial knowledge of $\mathbf{x}_\star$
- $P(X, Y, \mathbf{y}_{\text{exp}} | \mathbf{x}_\star) =$ likelihood
  $\rightarrow$ prob. of observing $(X, Y, \mathbf{y}_{\text{exp}})$ given proposed $\mathbf{x}_\star$
- $P(\mathbf{x}_\star | X, Y, \mathbf{y}_{\text{exp}}) =$ posterior
  $\rightarrow$ prob. of $\mathbf{x}_\star$ given observations $(X, Y, \mathbf{y}_{\text{exp}})$

Markov chain Monte Carlo (MCMC)

- Random walk through parameter space weighted by posterior
- Large number of samples
  $\rightarrow$ chain equilibrates to posterior distribution

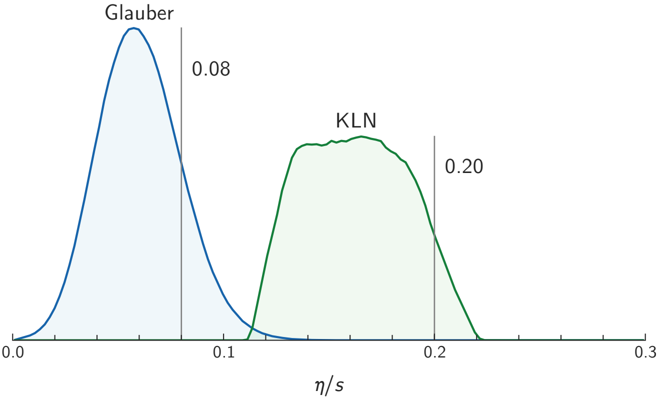
- Flat prior within design range, zero outside
- Likelihood:

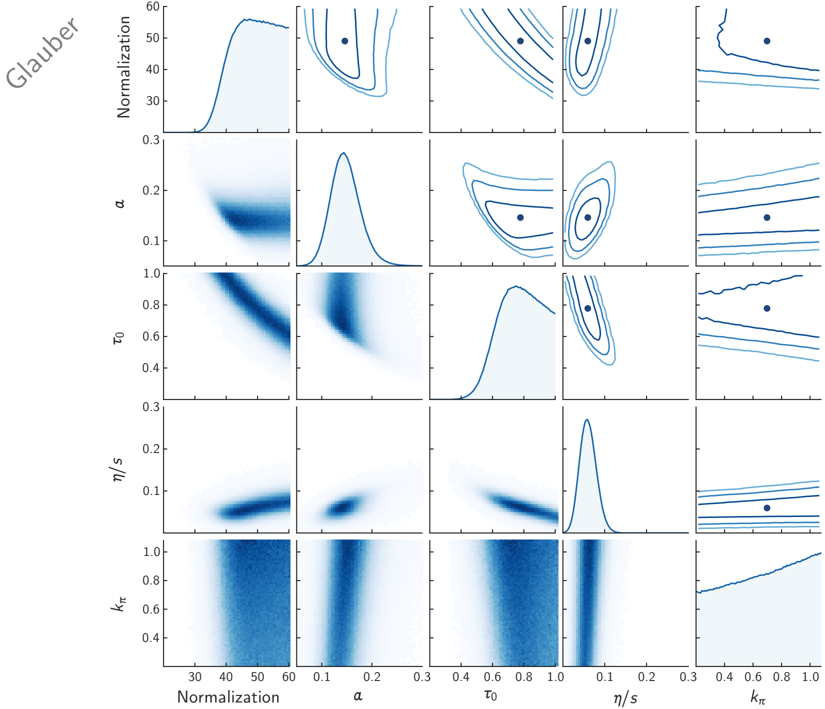
$$\log P(X, Y, \mathbf{y}_{\text{exp}} | \mathbf{x}_\star) \sim -\frac{(\mathbf{y}_\star - \mathbf{y}_{\text{exp}})^2}{2\sigma^2}$$

  $\sigma = 0.06$ on principal components (includes correlations)
- Posterior = likelihood within design range, zero outside

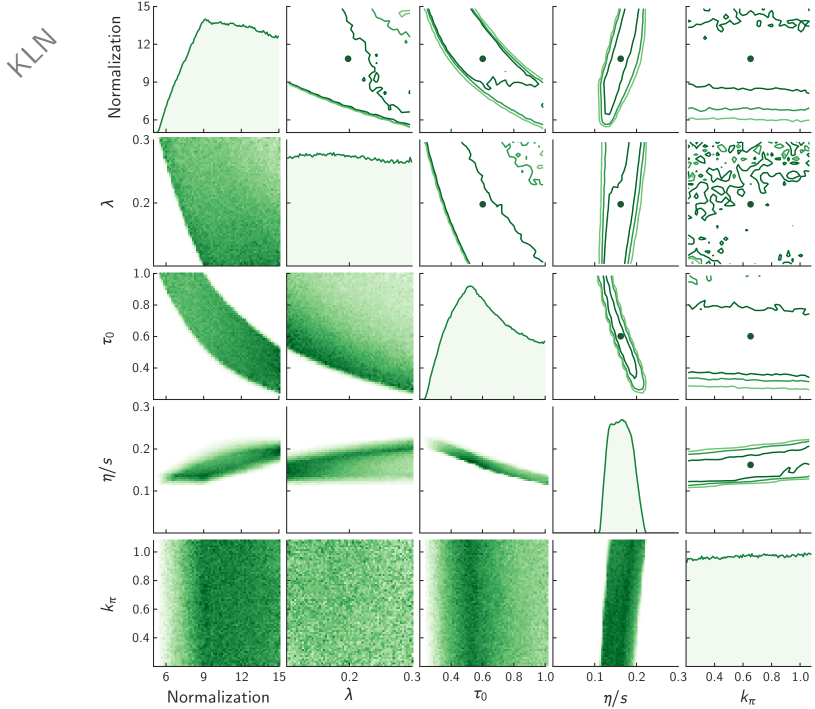
η/s posteriors

- Glauber $\eta/s \sim 0.06$, 95% C.I. $\sim$ 0.02–0.10
- KLN $\eta/s \sim 0.16$, 95% C.I. $\sim$ 0.12–0.21



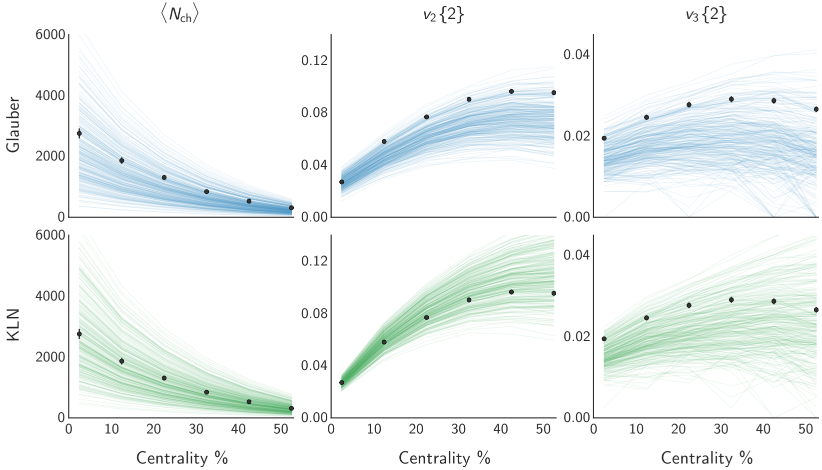


Glauber
Normalization
α
τ0
η/s
kπ


KLN
Normalization
λ
τ0
η/s
kπ
15
12
9
6
0.3
0.2
1.0
0.8
0.6
0.4
0.3
0.2
0.1
1.0
0.8
0.6
0.4
6
9
12
15
0.2
0.3
0.4
0.6
0.8
1.0
0.1
0.2
0.3
0.4
0.6
0.8
1.0
Normalization
λ
τ0
η/s
kπ

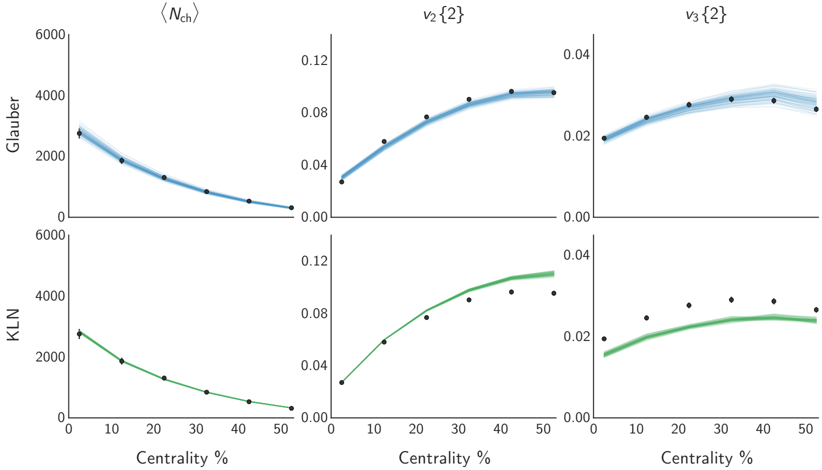
Posterior samples

Model calculations over full design space



Posterior samples

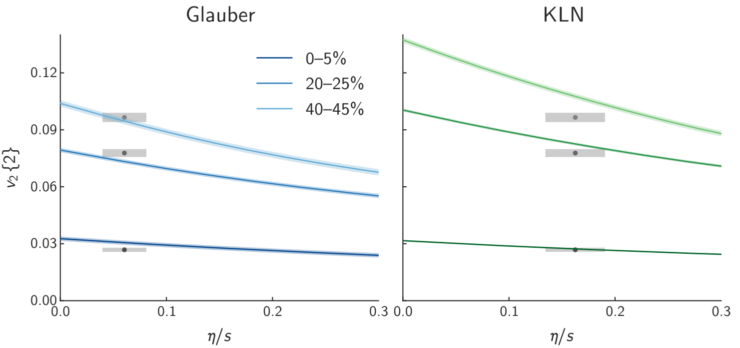
Emulator predictions from calibrated posterior



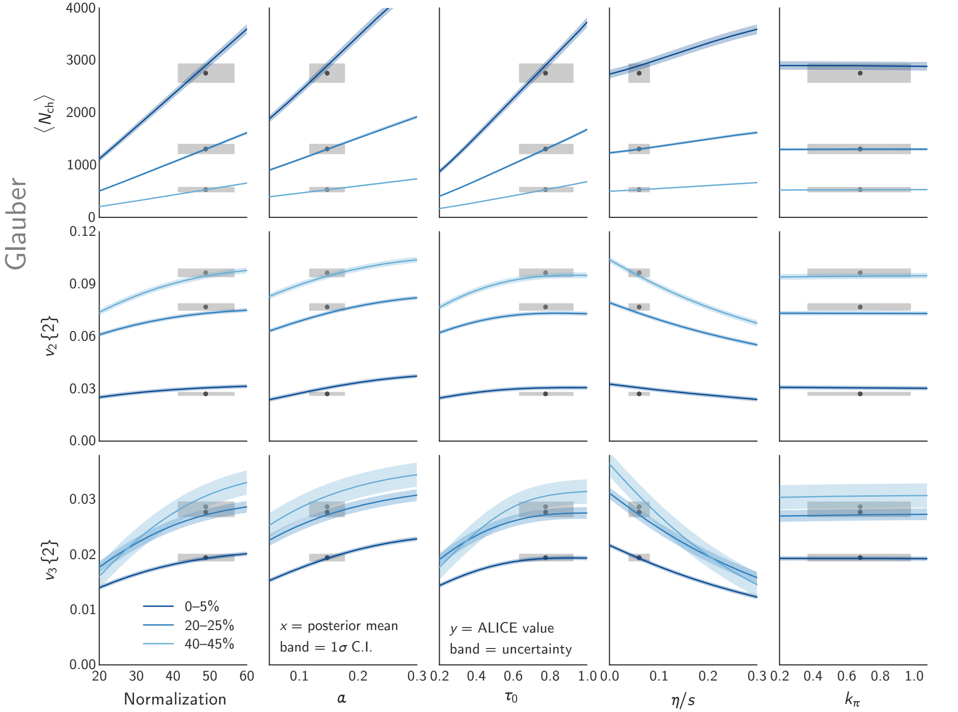
Sensitivity

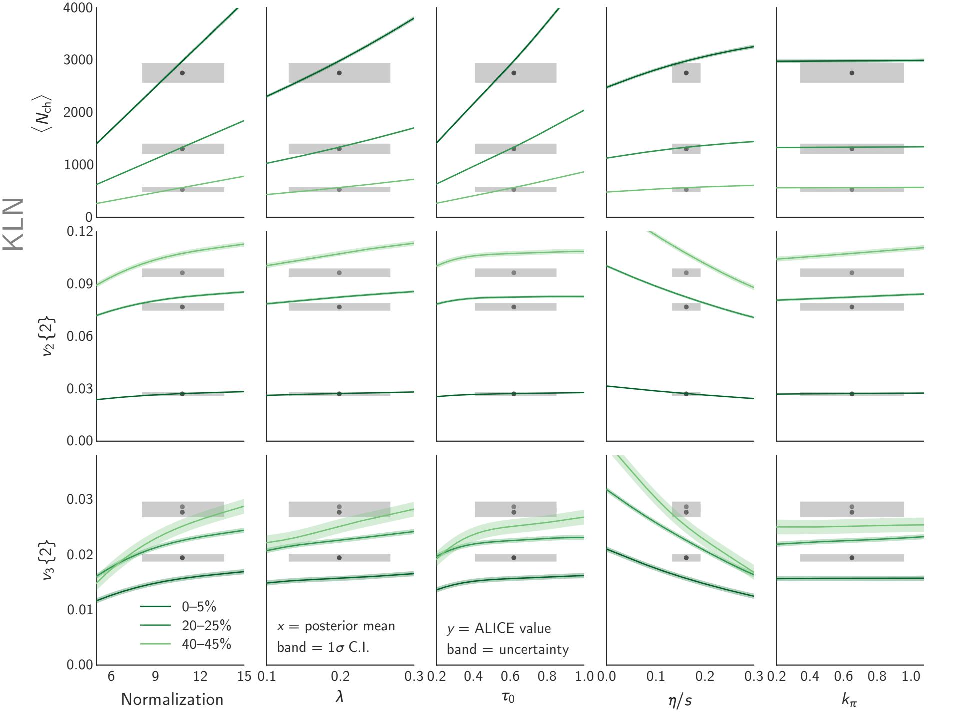
1. Go to posterior mean
2. Vary one parameter at a time; keep others fixed at mean
3. Emulate response of each observable

Effect of η/s on v_2



x point = posterior mean $\pm 1\sigma$ C.I., y point = ALICE value


Glauber
⟨N_{ch}⟩
$v_2\{2\}$
$v_3\{2\}$
0–5%
20–25%
40–45%
x = posterior mean
band = 1σ C.I.
y = ALICE value
band = uncertainty
Normalization
α
τ_0
η/s
k_π


KLN
⟨N_ch⟩
v_2{2}
v_3{2}
0–5%
20–25%
40–45%
x = posterior mean
band = 1σ C.I.
y = ALICE value
band = uncertainty
Normalization
λ
τ_0
η/s
k_π

Summary

Framework for quantitative, systematic parameter extraction and model evaluation

- Gaussian process emulator accurately predicts model output
- MCMC gives full probability distributions for all parameters
- Glauber approximately describes N_{ch}, v_2, v_3
- KLN cannot simultaneously fit v_2, v_3

Version 2.0

- Parametric initial condition models
  - TRENTo (see Scott Moreland's talk tomorrow)
  - fluctuated Glauber
- More input parameters: nucleon size, temperature-dependent η/s, bulk viscosity, hydro-to-UrQMD switching temperature
- More observables: $\langle p_T \rangle$, $v_2\{4\}$, identified particles, HBT
- RHIC and LHC
- Improve treatment of uncertainty
- Eventually: simultaneous calibration to small systems

Gaussian processes

Definition

A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.

Stochastic function: $\mathbf{x} \to y$

- $\mathbf{x} =$ n-dimensional input vector
- $y =$ normally distributed output

Specified by

- Mean function $\mu(\mathbf{x})$
- Covariance function $\sigma(\mathbf{x}, \mathbf{x}')$, e.g.:

$$\sigma(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{|\mathbf{x} - \mathbf{x}'|^2}{2\ell^2}\right)$$

Conditioning a Gaussian process

Given

- training input points X and
- observed training outputs $\mathbf{y}$ at X

the predictive distribution at arbitrary test points X_* is the multivariate-normal distribution

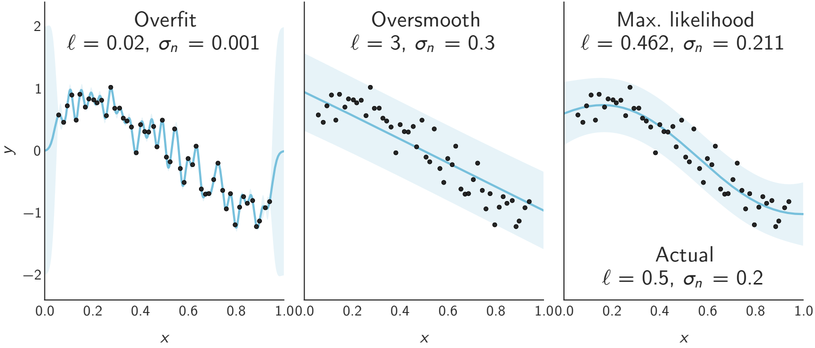
$$\begin{aligned}
\mathbf{y}_* &\sim \mathcal{N}(\boldsymbol{\mu}, \Sigma), \\
\boldsymbol{\mu} &= \sigma(X_*, X)\sigma(X, X)^{-1}\mathbf{y}, \\
\Sigma &= \sigma(X_*, X_*) - \sigma(X_*, X)\sigma(X, X)^{-1}\sigma(X, X_*).
\end{aligned}$$

Training the emulator

Covariance function:

$$\sigma(x, x') = \exp\left(-\frac{|x - x'|^2}{2\ell^2}\right) + \sigma_n^2 \delta_{xx'}$$

(ℓ, σ_n) are unknown hyperparameters



Principal component analysis

- Concatenate model output data into matrix Y where columns correspond to observables and rows to design points.
- Principal components are the eigenvectors U of the sample covariance matrix:

$$Y^\intercal Y = U \Lambda U^\intercal$$

- "Rotate" data into PC space:

$$Z = \sqrt{m}\, Y U$$

- Transform back:

$$Y' = \frac{1}{\sqrt{m}} Z' U^\intercal$$