Model-to-data Comparison with JETSCAPE: a Heavy Flavor Example

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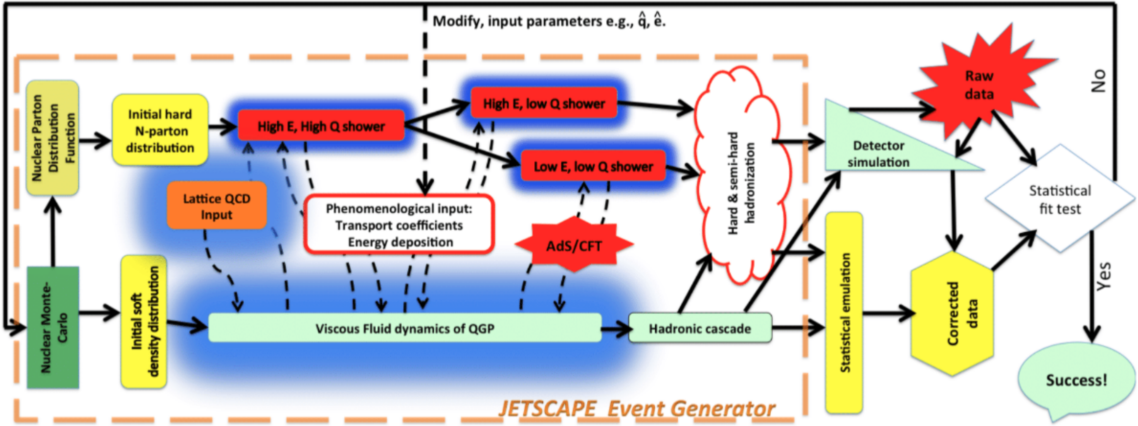
for the JETSCAPE Collaboration

UCLA 2019 Santa Fe Jets and Heavy Flavor Workshop

Programming Framework of JETSCAPE

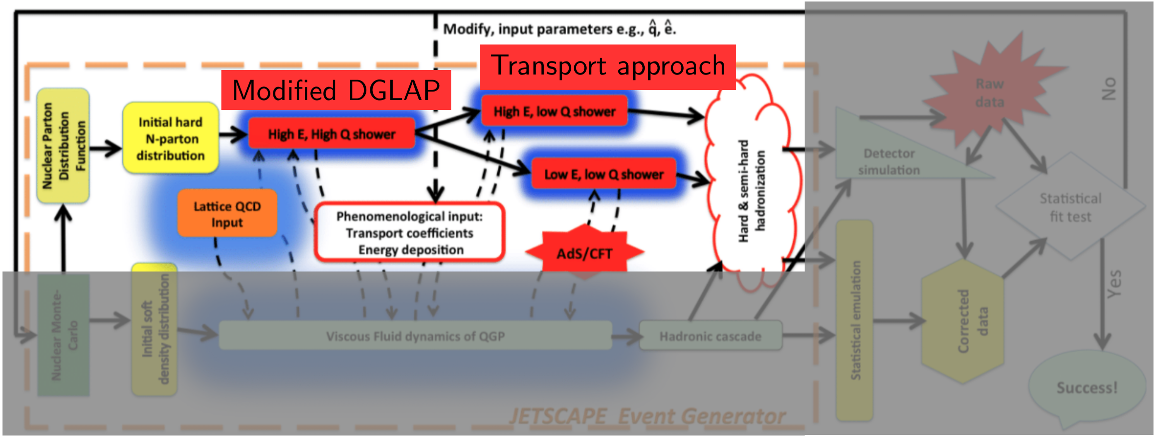
Jet Energy Loss Tomography with a Statistically and Computationally Advanced Program Envelope



Programming Framework of JETSCAPE

A multi-stage jet evolution in nuclear collisions

Jet Energy Loss Tomography with a Statistically and Computationally Advanced Program Envelope



Programming Framework of JETSCAPE

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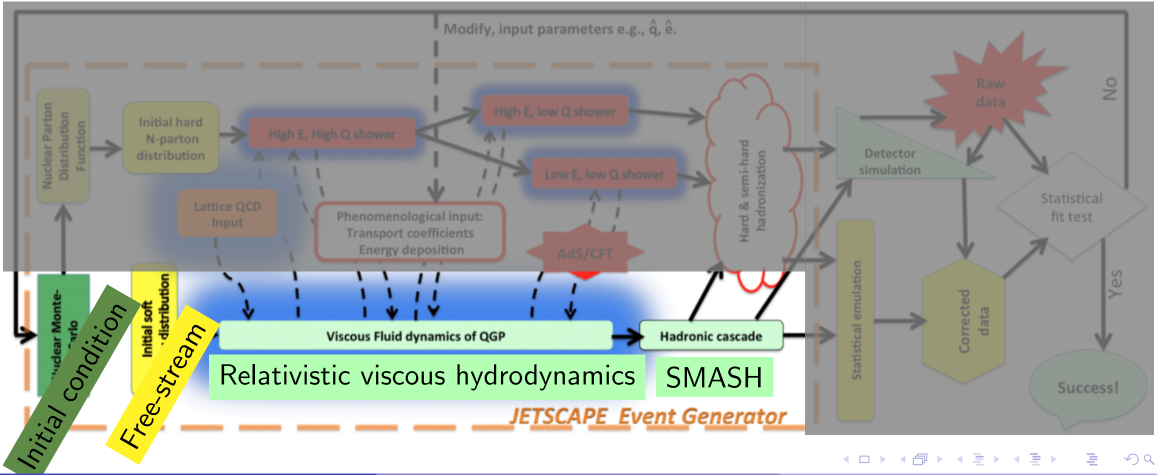
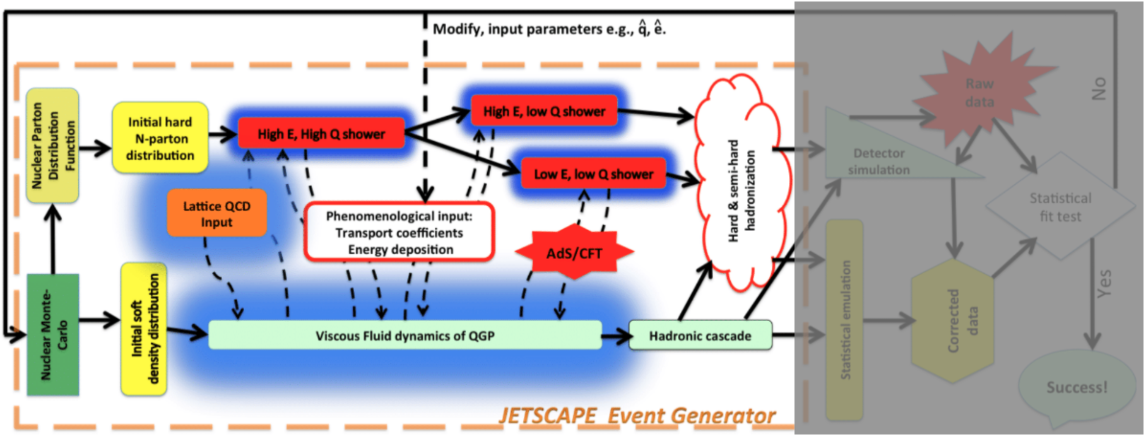
Bulk Evolution



Programming Framework of JETSCAPE

Jet Energy Loss Tomography with a Statistically and Computationally Advanced Program Envelope

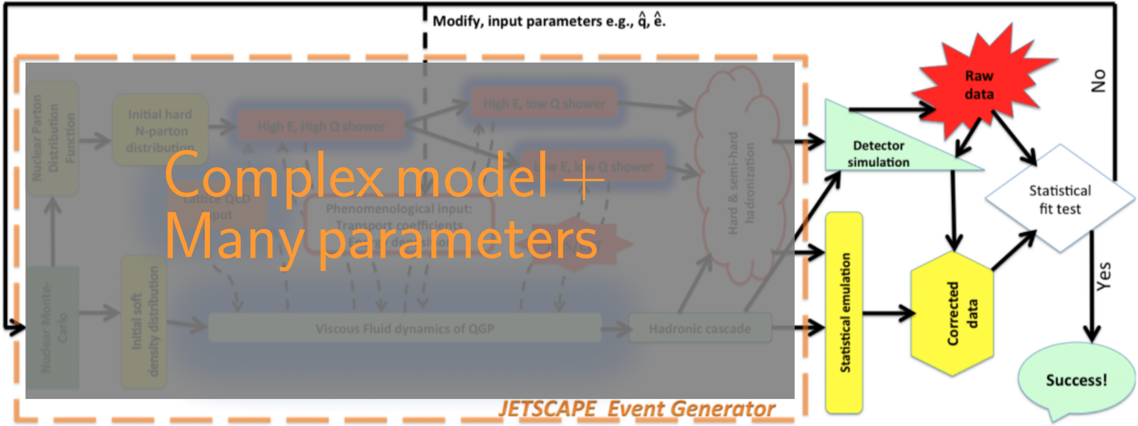
C++11 based, a modular programing model, ...



Programming Framework of JETSCAPE

A Bayesian model calibration

Jet Energy Loss Tomography with a Statistically and Computationally Advanced Program Envelope

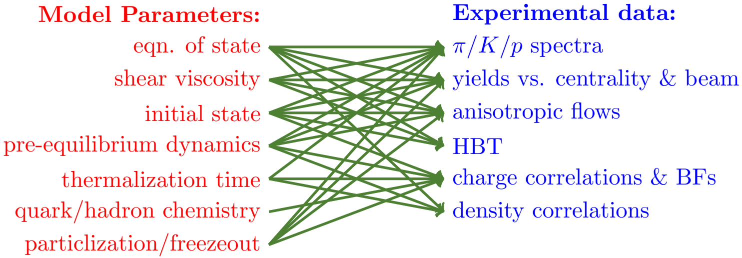


QGP/Jet-transport properties from a model-to-data comparison

Model Parameters:	**Experimental data:**
eqn. of state	$\pi/K/p$ spectra
shear viscosity	yields vs. centrality & beam
initial state	anisotropic flows
pre-equilibrium dynamics	HBT
thermalization time	charge correlations & BFs
quark/hadron chemistry	density correlations
particlization/freezeout	

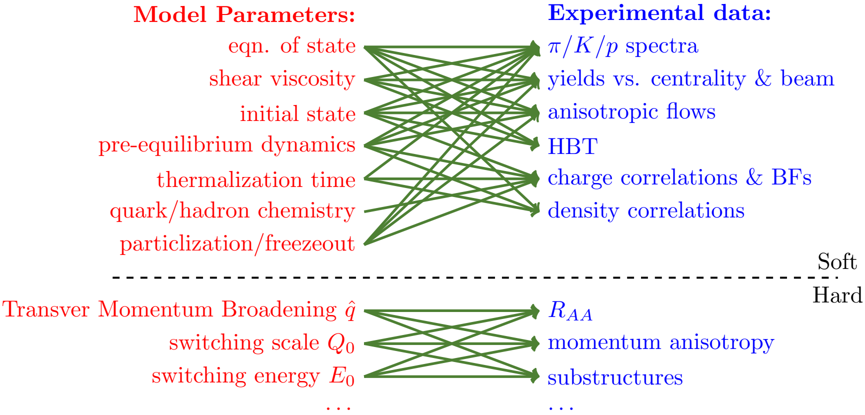
- Large number of parameters and data.

QGP/Jet-transport properties from a model-to-data comparison



- Large number of parameters and data.
- Complex and non-linear correlations.
  Bayesian statistics: infer the probability distribution of parameteres.

QGP/Jet-transport properties from a model-to-data comparison



- Large number of parameters and data.
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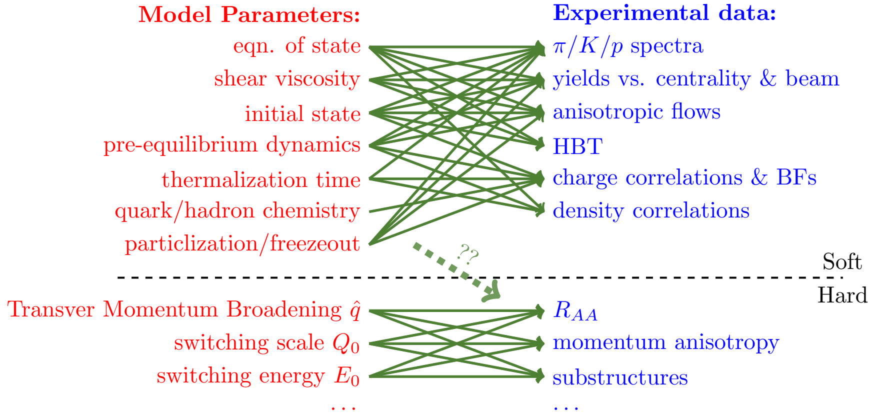
- A similar problem can be written down for hard probes.

QGP/Jet-transport properties from a model-to-data comparison



- Large number of parameters and data.
- Complex and non-linear correlations.
  Bayesian statistics: infer the probability distribution of parameteres.
- A similar problem can be written down for hard probes.
- (A simultaneous calibration of hard and soft in the future?)

JETSCAPE Statistical Package (not published yet)

Analyzing physics model and data with modern statistical tools

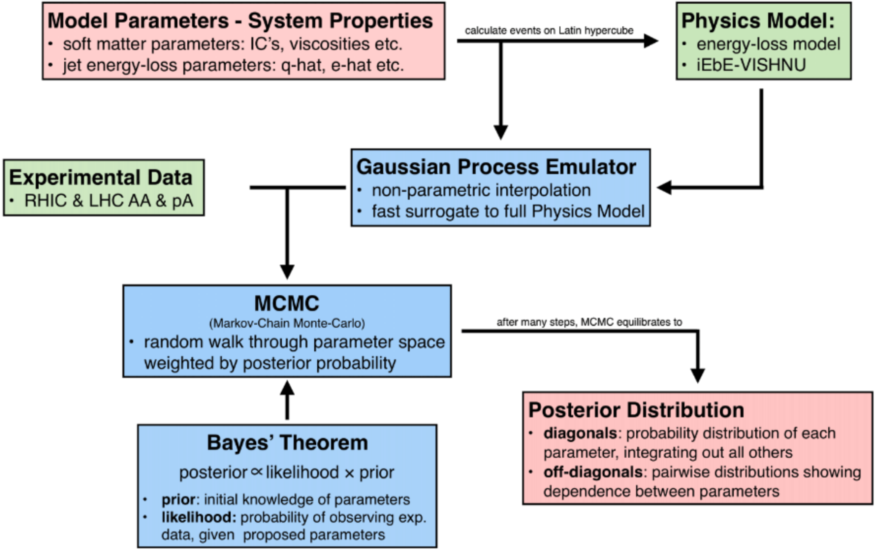


Figure from Steffen Bass

JETSCAPE Statistical Package (not published yet)

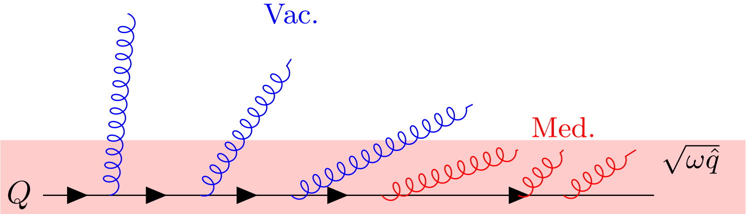
JETSCAPE has been developing the software package for this purpose.

- Python3 module, command-line based software.
- Provide a "wrap-around" of well-tested external packages and workflow control.
  - R: for parameter design.
  - scikit-learn: for data reduction, building and training model emulator.
  - emcee: python based implementation of Markov chain Monte Carlo (MCMC).
- It has been applied within the collaboration (extracting jet $\hat{q}$).
- The package is still under development for publication.

Statistical package application: charm quark $\hat{q}$ extraction

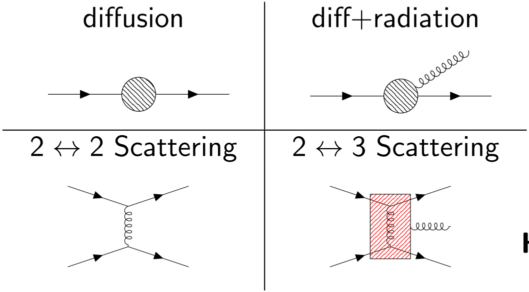
**This calculation (preliminary) is outside of JETSCAPE. Here we use the results for demonstrating the capability of the JETSCAPE statistical package.*

- Medium evolution: the hic-eventgen package (J Bernhard 1804.06469).
- Charm quark initial production: Pythia8.
- Transport model for heavy quark: LIDO (W Ke et al. PRC 98 064901 and 1810.08177) should only applies to low virtuality (Q) particles.
- Currently, to separate the treatment of high / low Q processes, we interface Pythia8 and LIDO at a $Q_0 \sim R\sqrt{\hat{q}\omega}$ (P. Caucal et al. PRL 120, 232001, see Edmond's talk Monday).
- The LIDO model will be integrated into the JETSCAPE framework, where such a separation will be between the modified DGLAP module and transport module.



Statistical package application: charm quark $\hat{q}$ extraction

1. Four incoherent processes



2. Solving Langevin+Boltzmann Eq.

W Ke, Y Xu, S Bass PRC 98 064901

3. Iterative approach for LPM effect

W Ke, Y Xu, S Bass ArXiv:1810.08177

The LIDO transport model:

- A separation between
  Small-q (momentum transfer $q < Q_{\mathrm{cut}}$): diffusion.
  Large-q ($q > Q_{\mathrm{cut}}$): scattering rate.
- Allow a flexible parametrization of $\hat{q}$.
- An interpolation between scattering and diffusion picture.

Hadronization:

- Recombination + fragmentation S. Cao et al. PRC 88, 044907.

Hadronic phase:

- Ultra-relativistic Quantum Molecular Dynamics (UrQMD) (with D-π, D-ρ cross-sections from Z. Lin et al. NPA 689, 965)

Bayesian Analysis: Identifying Tunable Parameter

- Effective coupling: $\alpha_s(Q) = \frac{2\pi}{9}\left(\ln \frac{\max\{Q, \mu\pi T\}}{\Lambda_{\rm QCD}}\right)^{-1}$, $Q^2 = |\hat{t}|, k_\perp^2$, $N_f = 3$.
- Energy loss starting time τ_i.
- Matching between vac-like and medium-induced radiation, $Q^2_{\rm sw} = R_v \Delta k_\perp^2$.
- $\hat{q}$ is separated into: $\hat{q} = \underbrace{\hat{q}_0}_{\text{perturbative part}} + \underbrace{\Delta\hat{q}}_{\text{additional part}}$

- $\hat{q}_0 = \hat{q}_S + \hat{q}_H$ has a soft and a hard contribution, switching at $Q^2_{\rm cut}$,

$$\hat{q}_S = \int_0^{Q^2_{\rm cut}} \frac{d^2\mathbf{q}}{(2\pi)^2} \frac{g^2 C_F m_D^2}{q_\perp^2 (q_\perp^2 + m_D^2)},$$

$$\hat{q}_H = \int_{t_{\rm min}}^{-Q^2_{\rm cut}} d\hat{t} \frac{dR_{22}}{d\hat{t}} q_\perp^2.$$

- $\Delta\hat{q}$ takes a parametric form, and is allowed to be anisotropic,

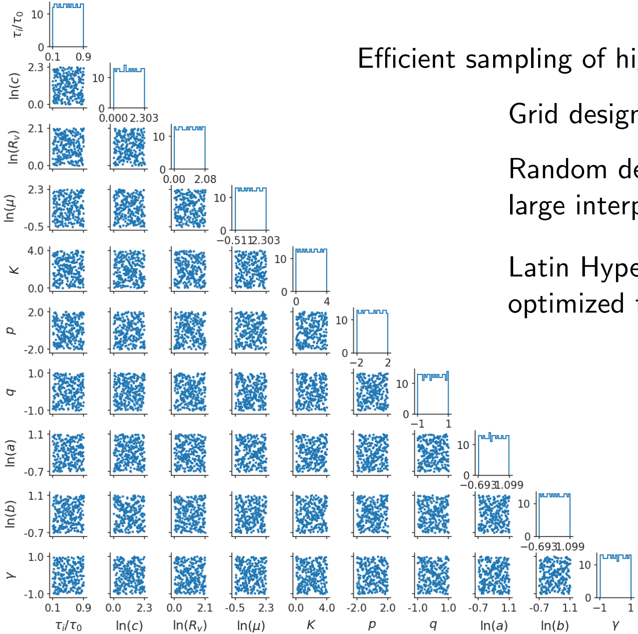
$$\Delta\hat{q} = \frac{K T^3}{\left[1 + \left(a\frac{T}{T_c}\right)^p\right]\left[1 + \left(b\frac{E}{T}\right)^q\right]},$$

$$\Delta\hat{q}_L = \frac{\Delta\hat{q}}{2}\left(\frac{E}{M}\right)^\gamma.$$

Bayesian Analysis: Parameter Design

Symbol	Description	Range
$\xi = \frac{\tau_i}{\tau_0}$	energy loss starting time	(.1, .9)
$c = \frac{Q^2_{\mathrm{cut}}}{m^2_D}$	soft/hard switching scale	$(.1, 10.)$
$R_v = \frac{Q^2_{\mathrm{sw}}}{\Delta k^2_\perp}$	vac/medium-ind. switching scale	$(0.14, \infty)$
μ	Running α_s stops at $Q = \mu\pi T$	$(.6, 10)$
K	Norm for $\Delta\hat{q}$	$(0, 20)$
p	Additional T-dep power	$(-2, 2)$
q	Additional E-dep power	$(-1, 1)$
a	Additional T-dep scale	$(-.5, 3)$
b	Additional E-dep scale	$(-.5, 3)$
γ	Relation of $\Delta\hat{q}$ and $\Delta\hat{q}_L$	(-1, 1)

Bayesian Analysis: Parameter Design

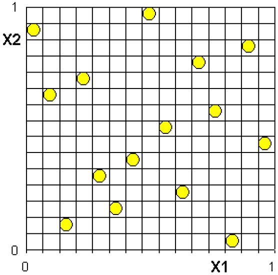


Efficient sampling of high-dimensional parameter space

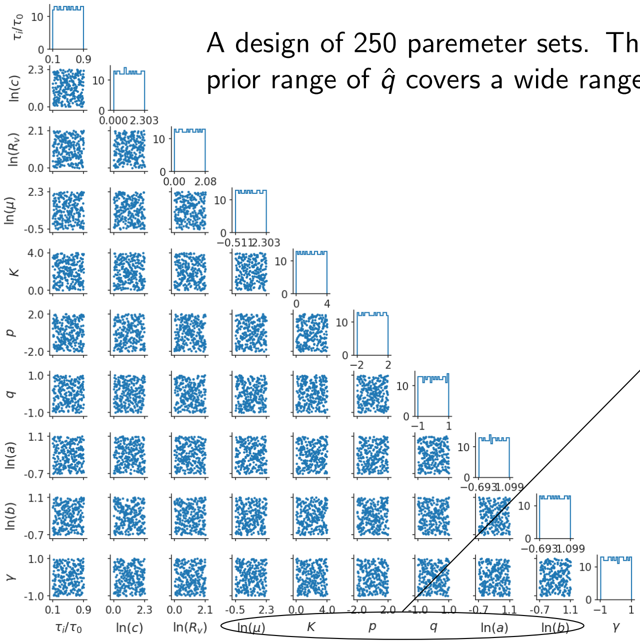
Grid design: 10^d points, not feasible.

Random design: tight clusters and large gap, large interpolation uncertainty.

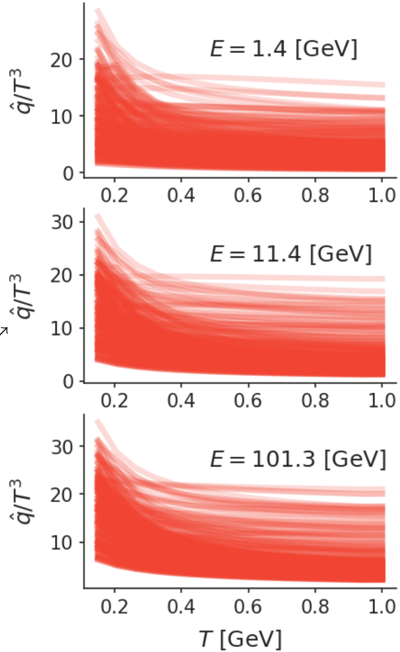
Latin Hypercube design: maginally uniform but optimized for space filling. In practice, $20 \times d$.



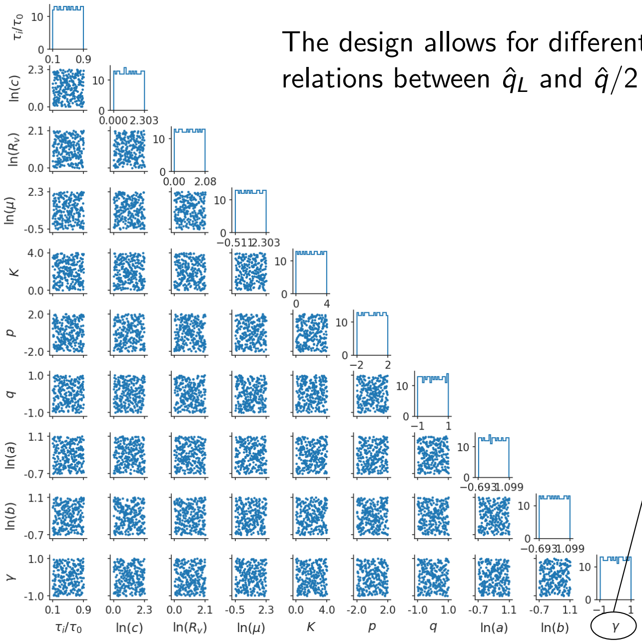
Bayesian Analysis: Parameter Design



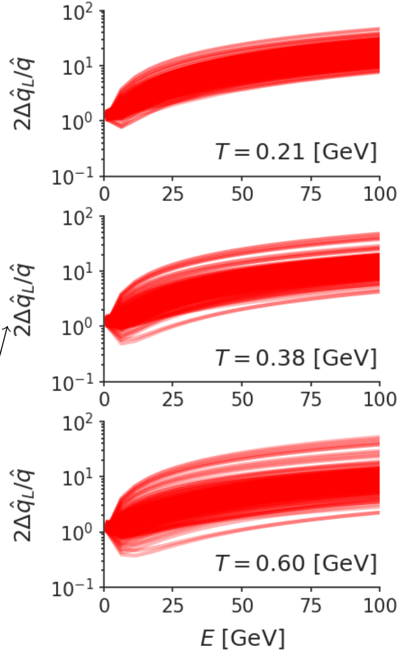
A design of 250 paremeter sets. The prior range of $\hat{q}$ covers a wide range.



Bayesian Analysis: Parameter Design

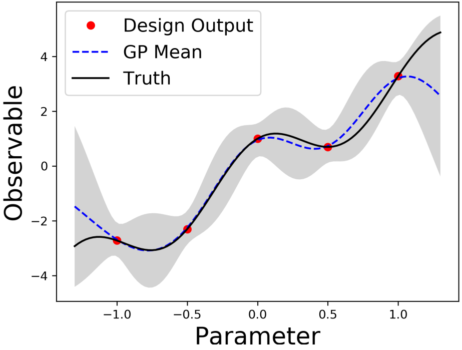


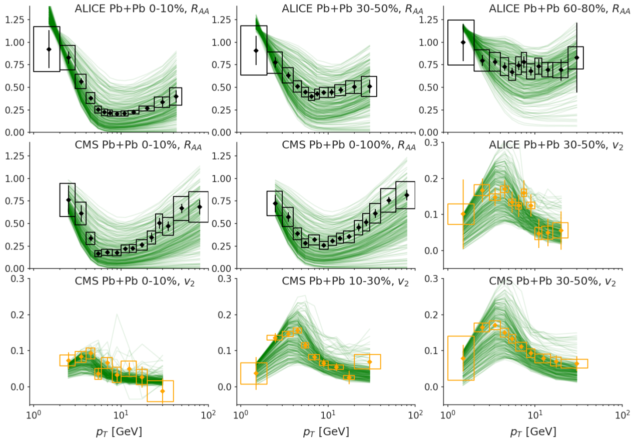
The design allows for different relations between $\hat{q}_L$ and $\hat{q}/2$



Bayesian Analysis: Surrogate Model

- Compute model at the 250 parameter sets (3×10^6 CPU hours on NERSC, the time-consuming part).
- The "mapping" from parameters to observables is "learned" by Gaussian Process Emulators (non-parametric, fast interpolators).

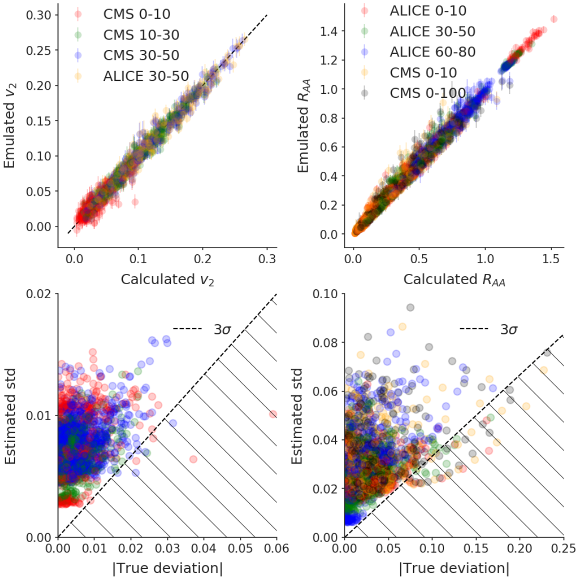




ALICE: v_n PRL 120, 102301; R_{AA} JHEP 10 (2018) 174;

CMS: v_n PRL 120, 202301; R_{AA} PLB 782, 474;

Bayesian Analysis: Surrogate Model

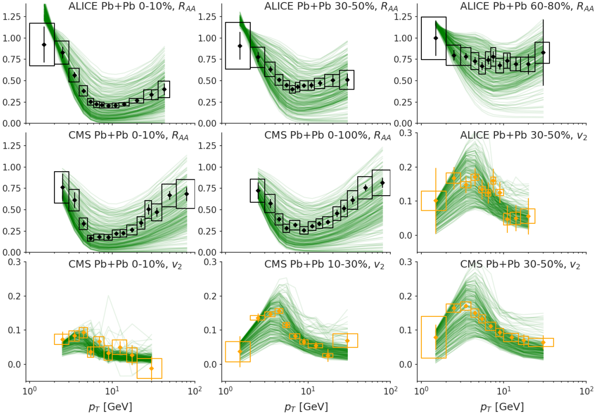


How do the emulators perform?

- Validation: compare emulator predictions to calculations at novel parameter sets (top). Emulator has uncertainty!
- Gaussian Process can quantify its own interpolation uncertainty (bottom).
- From the validation: deviation of predictions are mostly within the 3σ uncertainty band of the emulator.
- **Interpolation error is an important source of uncertainty!**

Bayesian Analysis: The Likelihood Function and Covariance Matrix

To define a closeness between data and calculation:
the likelihood function



$$P(\mathrm{Exp}|p, \mathrm{Model}) \propto \exp\left\{-\frac{1}{2}\mathbf{dy}^T\boldsymbol{\Sigma}^{-1}\mathbf{dy}\right\}$$

$$\begin{aligned}\mathbf{dy} &= \mathbf{y}_{\mathrm{model}}(p) - \mathbf{y}_{\mathrm{exp}} \\ \boldsymbol{\Sigma} &= \boldsymbol{\Sigma}_{\mathrm{emulator}} + \sigma^2_{\mathrm{stat},i}\delta_{ij} \\ &+ \sigma_{\mathrm{sys},i}\sigma_{\mathrm{sys},j} C_{ij} \exp\left\{-\frac{\ln^2 \frac{p_{T,i}}{p_{T,j}}}{2L^2_{\mathrm{corr}}}\right\}\end{aligned}$$

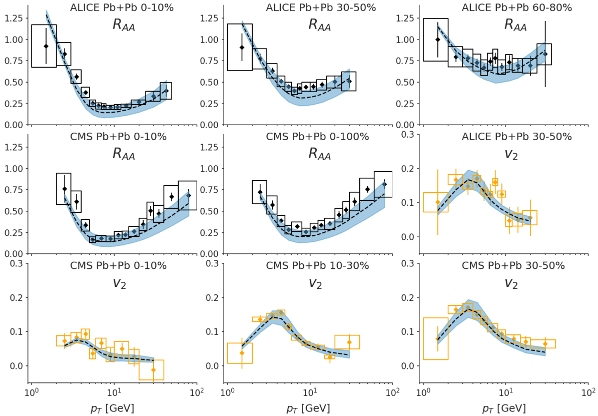
Assume σ_{sys} correlates in $\ln(p_T)$ with L_{corr}. C models correlation across centrality for R_{AA}.

Bayesian Analysis: Bayes' rule and Posterior

From Bayes' rule one obtains the posterior distribution

$$P(p|\mathrm{Exp},\mathrm{Model}) \propto P(\mathrm{Exp}|p,\mathrm{Model}) \times \mathrm{Prior}(p)$$

$L_{\mathrm{corr}} = 1$



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$$\mathbf{dy} = \mathbf{y}_{\mathrm{model}}(p) - \mathbf{y}_{\mathrm{exp}}$$

$$\mathbf{\Sigma} = \mathbf{\Sigma}_{\mathrm{emulator}} + \sigma^2_{\mathrm{stat},i}\delta_{ij} + \sigma_{\mathrm{sys},i}\sigma_{\mathrm{sys},j}C_{ij}\exp\left\{-\frac{\ln^2\frac{p_{T,i}}{p_{T,j}}}{2L^2_{\mathrm{corr}}}\right\}$$

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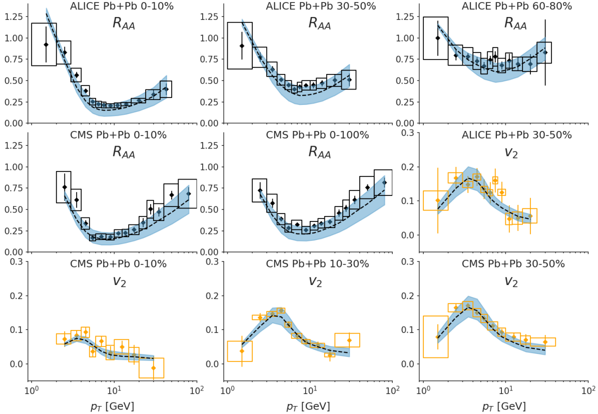
From Bayes' rule one obtains the posterior distribution

$$P(p|\mathrm{Exp}, \mathrm{Model}) \propto P(\mathrm{Exp}|p, \mathrm{Model}) \times \mathrm{Prior}(p)$$

$L_{\mathrm{corr}} = 0.5$



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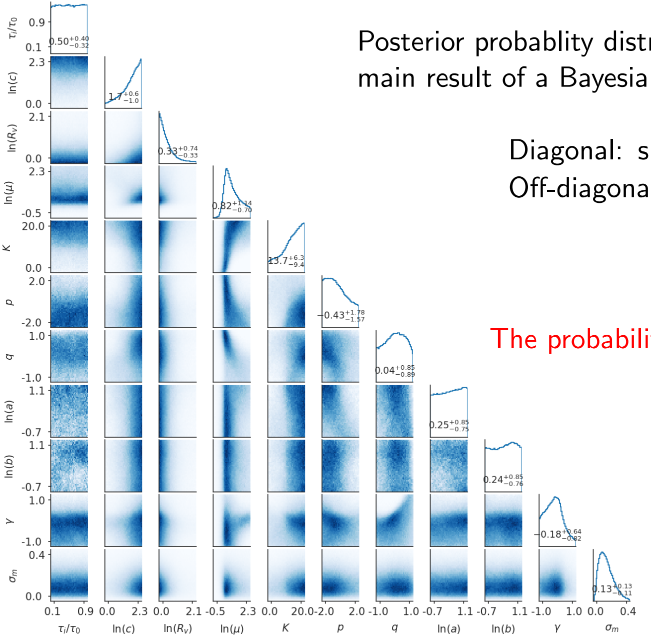
Bayesian Analysis: Posterior and Interpretation

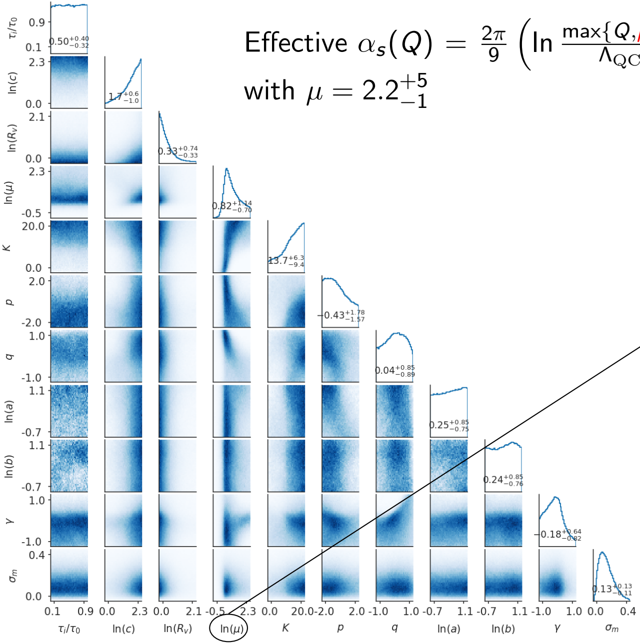


Posterior probablity distribution of model parameters is the main result of a Bayesian analysis.

Diagonal: single parameter distribution.
Off-diagonal: two-parameter joint distribution.

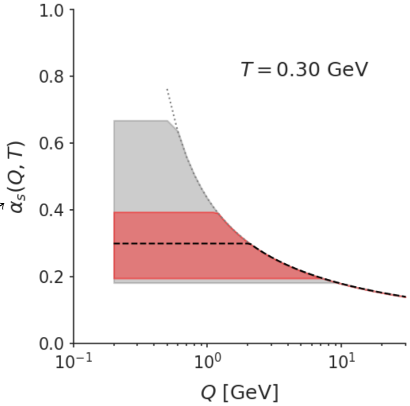
The probability of parameters given model & data

Bayesian Analysis: Posterior and Interpretation



Effective $\alpha_s(Q) = \frac{2\pi}{9}\left(\ln\frac{\max\{Q, \mu\pi T\}}{\Lambda_{\mathrm{QCD}}}\right)^{-1}$,

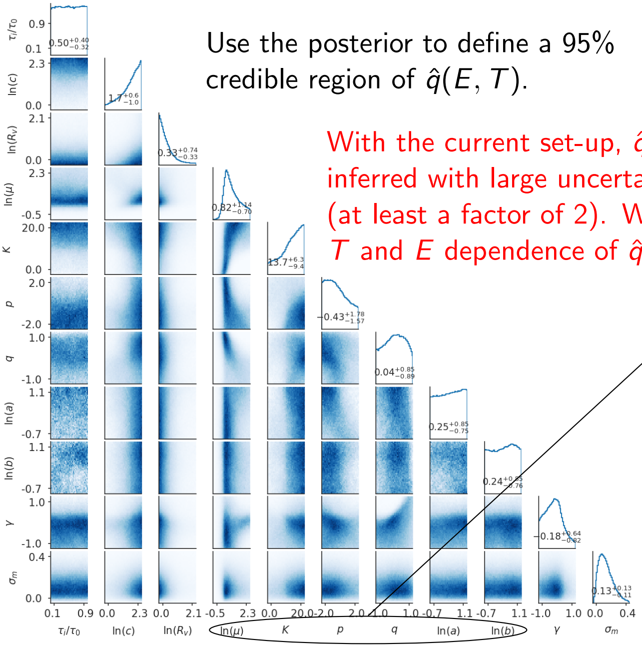
with $\mu = 2.2^{+5}_{-1}$



Effective $\alpha_s = 0.2$ - 0.4 ($g = 1.5 - 2.2$)

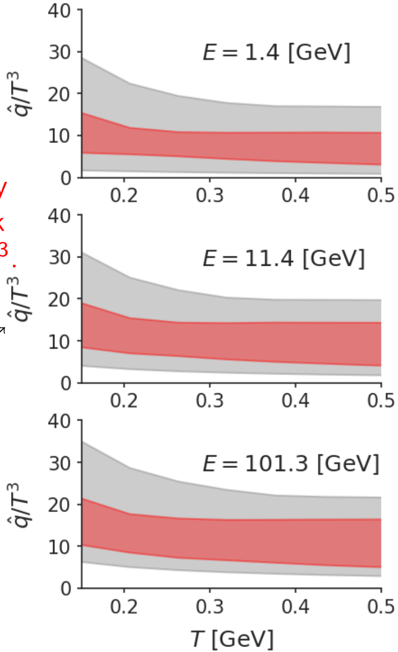
$T = 0.3$ MeV.

Bayesian Analysis: Posterior and Interpretation

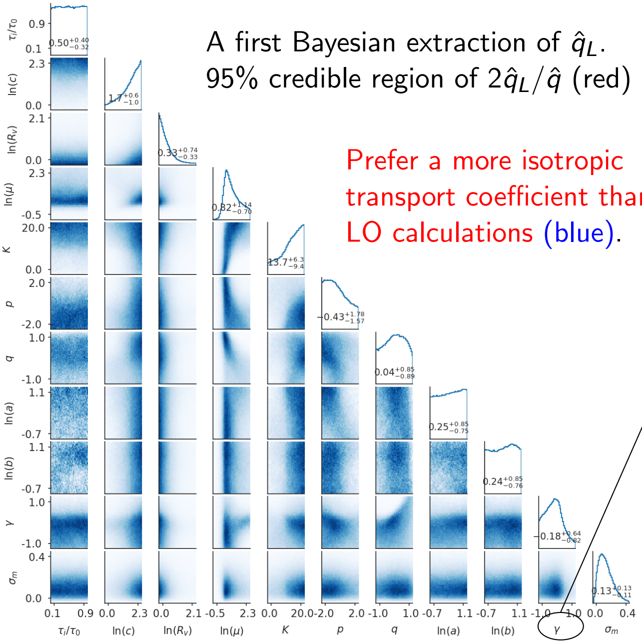


Use the posterior to define a 95% credible region of $\hat{q}(E, T)$.

With the current set-up, $\hat{q}$ is inferred with large uncertainty (at least a factor of 2). Weak T and E dependence of $\hat{q}/T^3$.

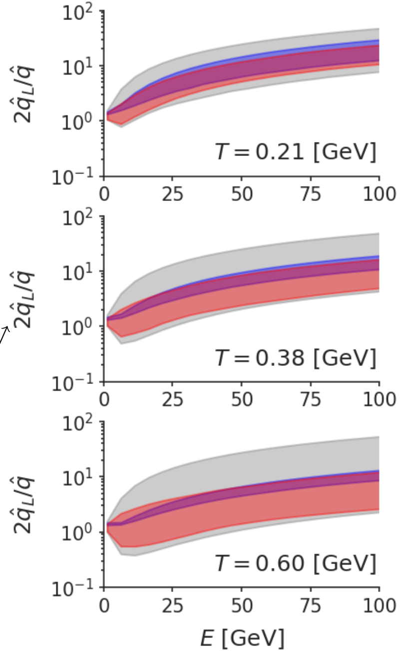


Bayesian Analysis: Posterior and Interpretation



A first Bayesian extraction of $\hat{q}_L$.
95% credible region of $2\hat{q}_L/\hat{q}$ (red)

Prefer a more isotropic transport coefficient than LO calculations (blue).

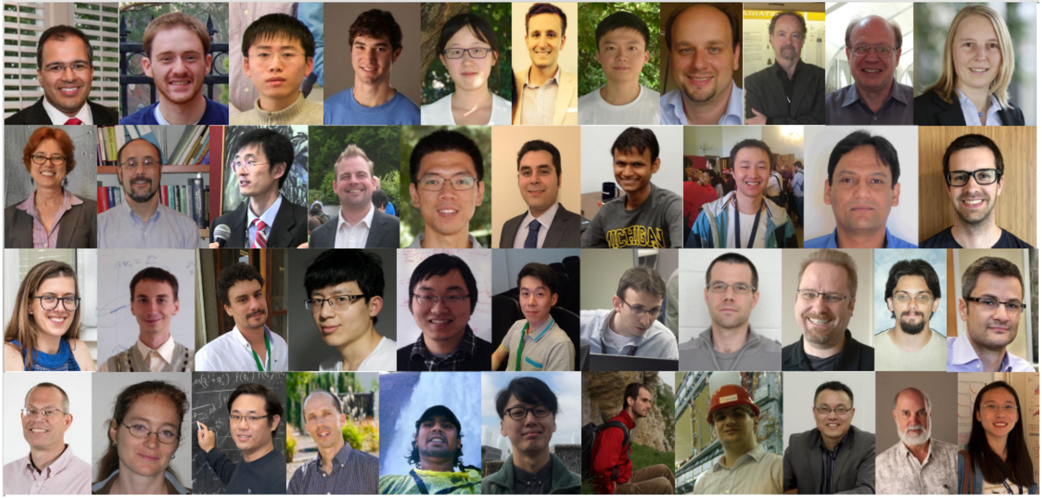


Summary

- JETSCAPE: modular framework for simulating jet+medium evolution in nuclear collisions.
- Quantifying physical properties in heavy-ion collision often requires **global comparisons**.
- The **JETSCAPE statistical package** provides modern statistical tools for computer model analysis, parameter extraction, and **uncertainty propagation**.
- Applying the statistical package, we went through a recent application to charm quark transport properties analysis using the LIDO model.
  - A large coupling evaluated at $2.2^{+5}_{-1}\pi T$.
  - Still large uncertainty in $\hat{q}$ given present model and data. What to improve next?
  - A first extraction of the longitudinal transport coefficient.

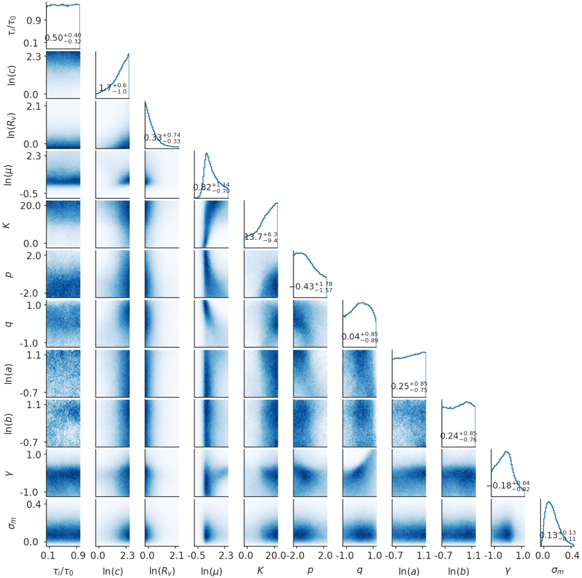
Summary

The JETSCAPE Members

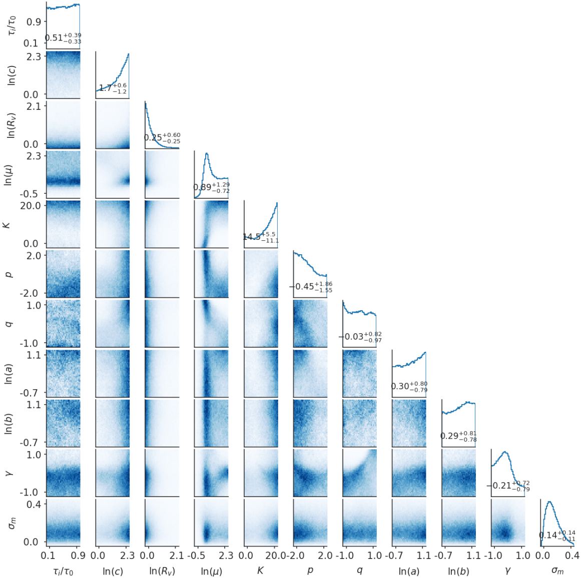


Back-up: how L_{corr} affects the calibration

Use $L_{\mathrm{corr}} = 1.0$



Use $L_{\mathrm{corr}} = 0.5$



Extrapolate the calibrated $\hat{q}$ to zero momentum