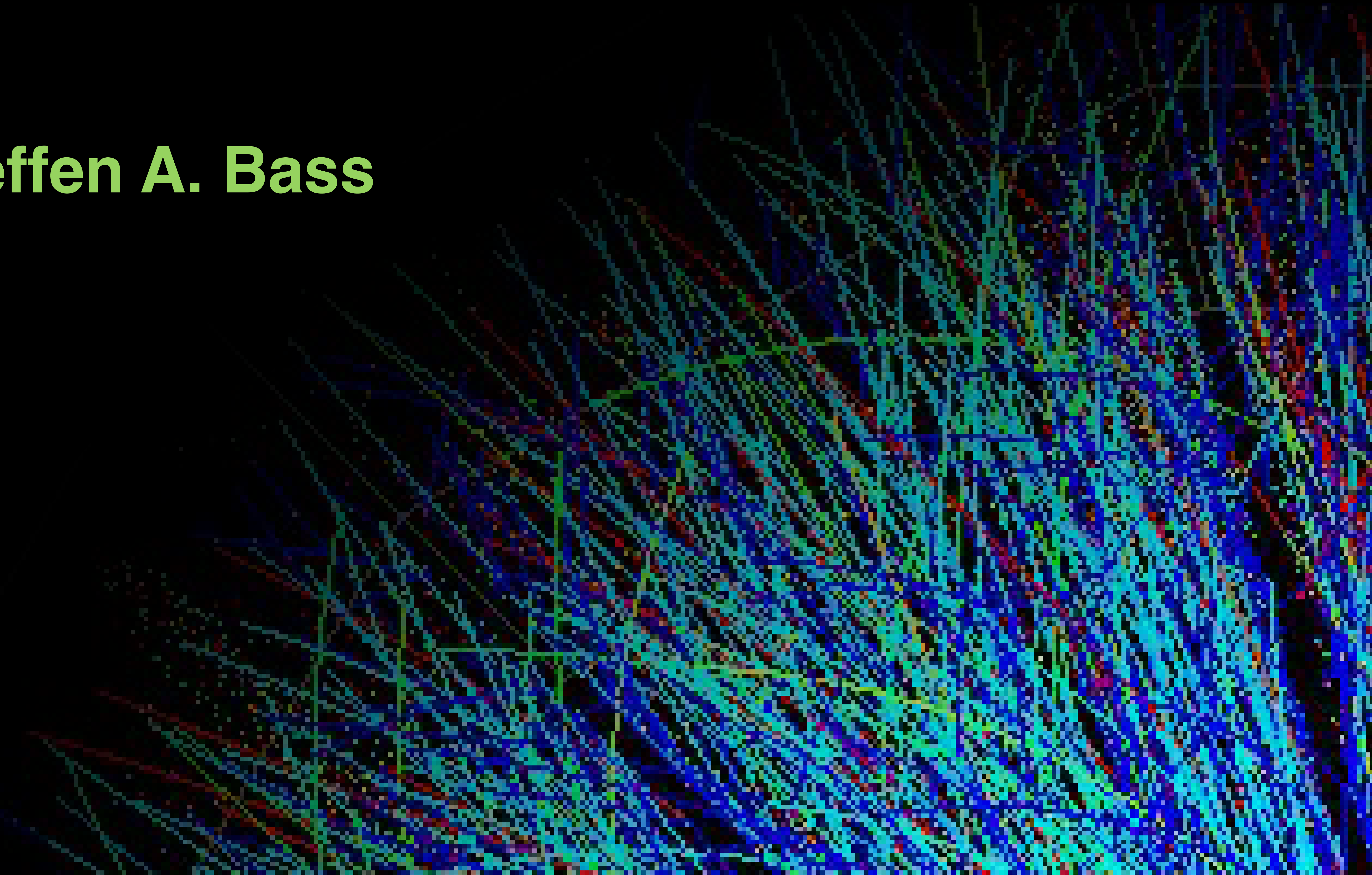
Data-driven analysis of the temperature dependence of the heavy-quark transport coefficient

Steffen A. Bass

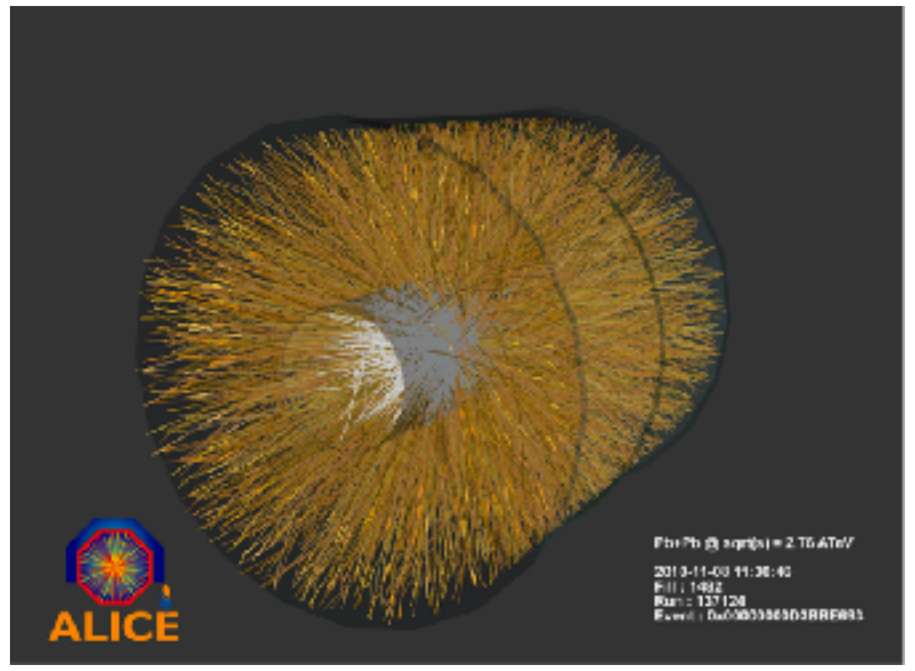
Duke University

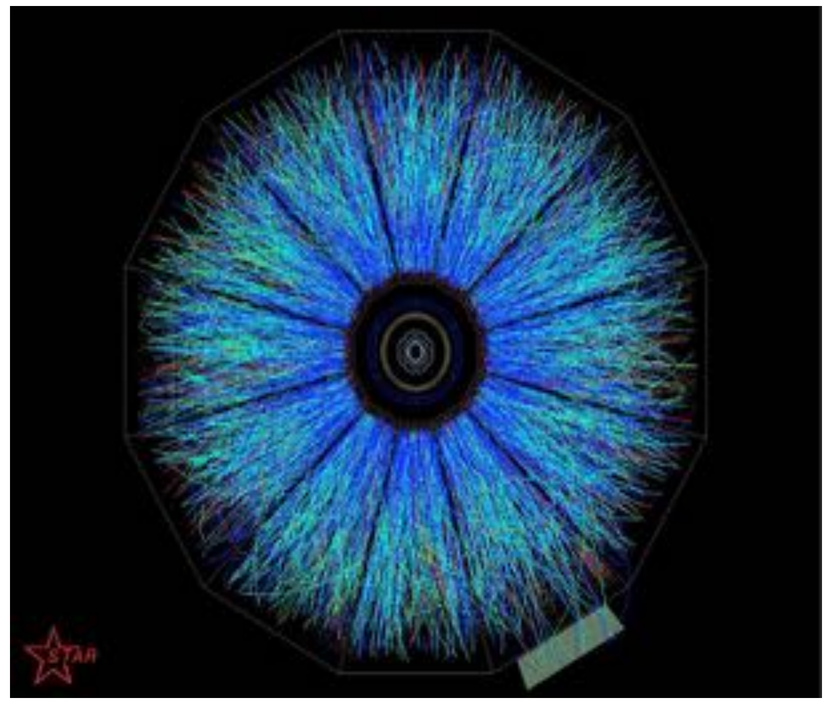


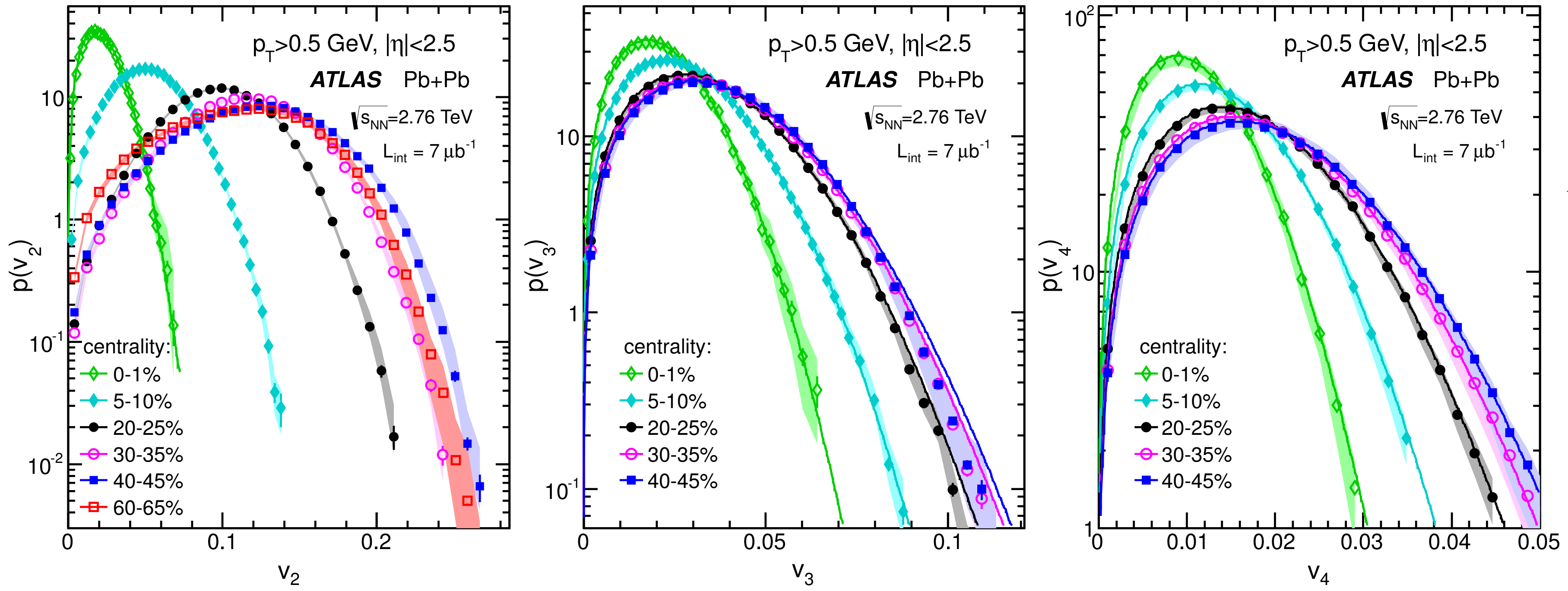
How do we learn about Heavy Quarks in a QGP Medium?

Extraction of HQ and QGP Properties from Data

Data:

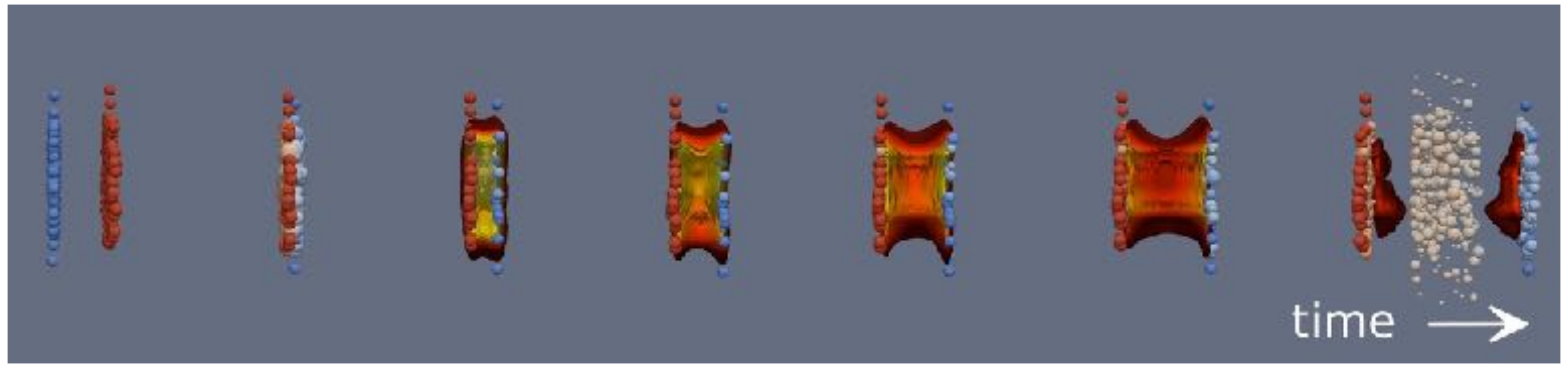


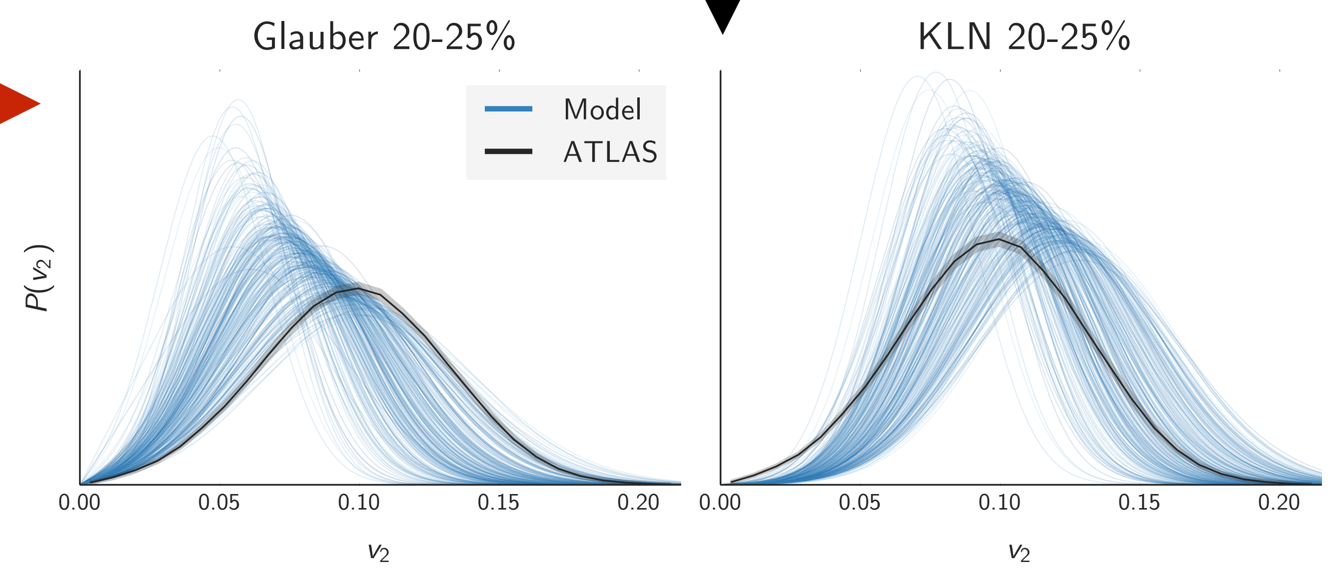




Model:

initial conditions, τ_0, η/s, ζ/s, ….





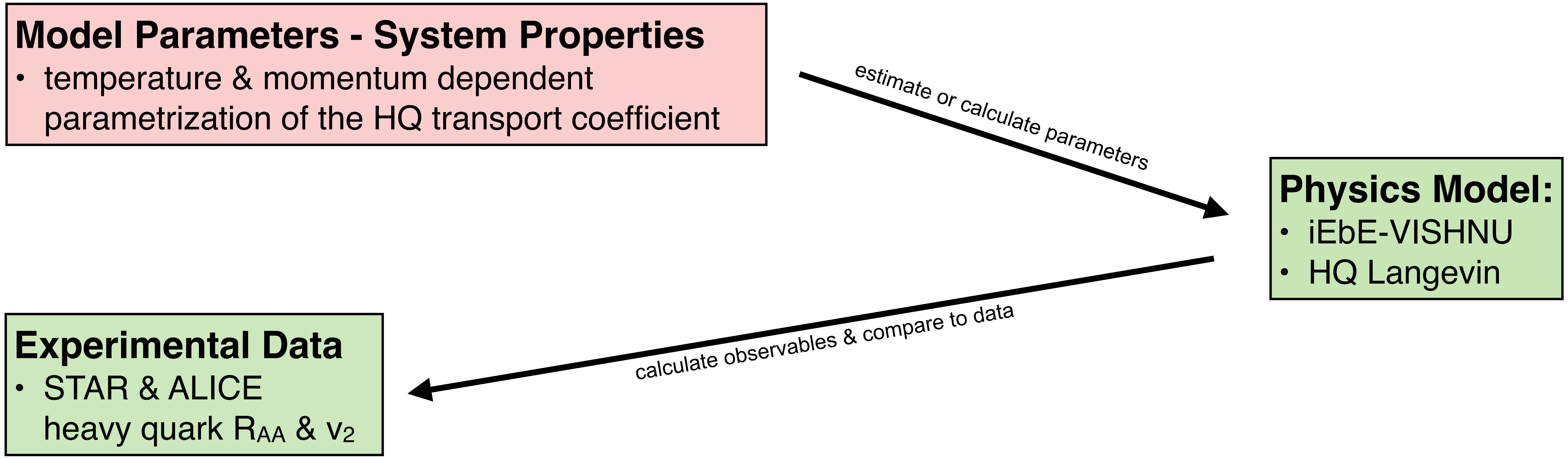
extracted QGP properties: η/s, …

Principal Challenges of Probing the QGP with Heavy-Ion Collisions:

- confinement: quarks & gluons form bound states, experiments don't observe them directly
- observables are limited to final state hadrons - we want to learn about the dynamics of the collision
- computational models are expensive: about 1 cpu-hour per simulated event

Bayesian Analysis

Each computational model relies on a set of physics parameters to describe the dynamics and properties of the system. These physics parameters act as a representation of the information we wish to extract from RHIC & LHC.



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Model Parameters - System Properties
- temperature & momentum dependent parametrization of the HQ transport coefficient

Bayesian analysis

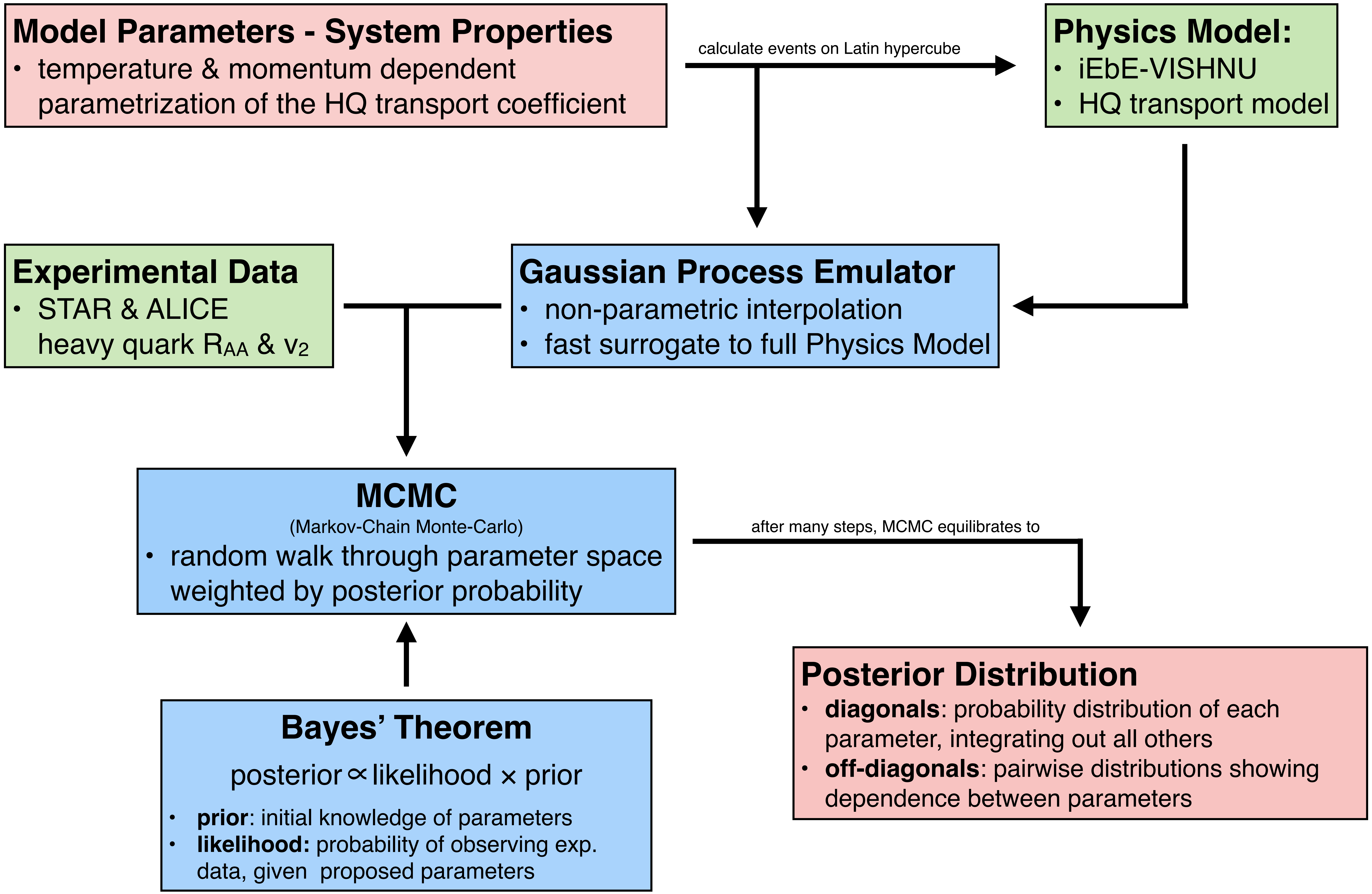
Physics Model:
- iEbE-VISHNU
- HQ Langevin

Experimental Data
- STAR & ALICE heavy quark R_{AA} & v_2

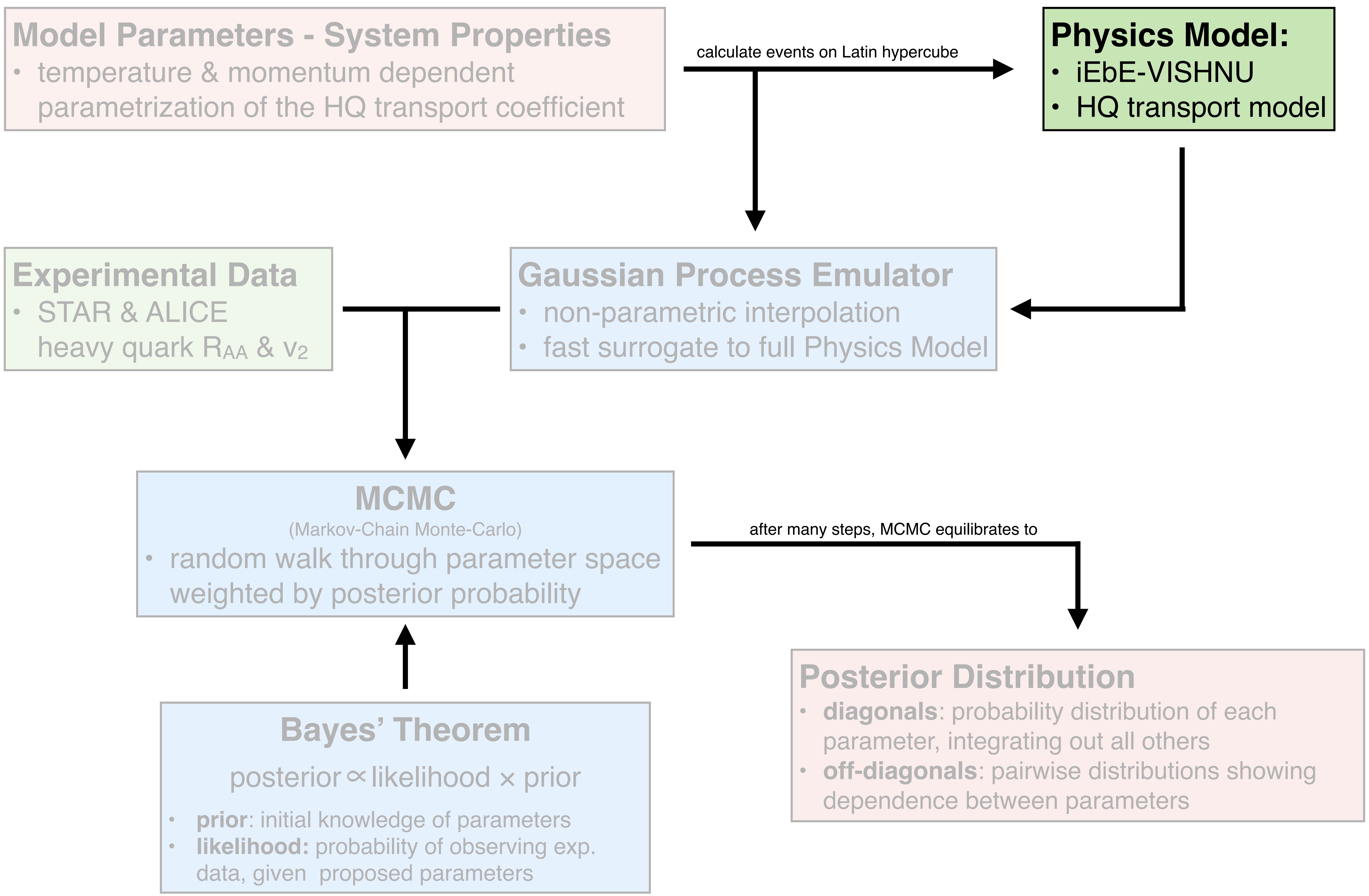
- Bayesian analysis allows us to simultaneously calibrate all model parameters via a model-to-data comparison
- determine parameter values such that the model best describes experimental observables
- extract the probability distributions of all parameters

Setup of a Bayesian Analysis

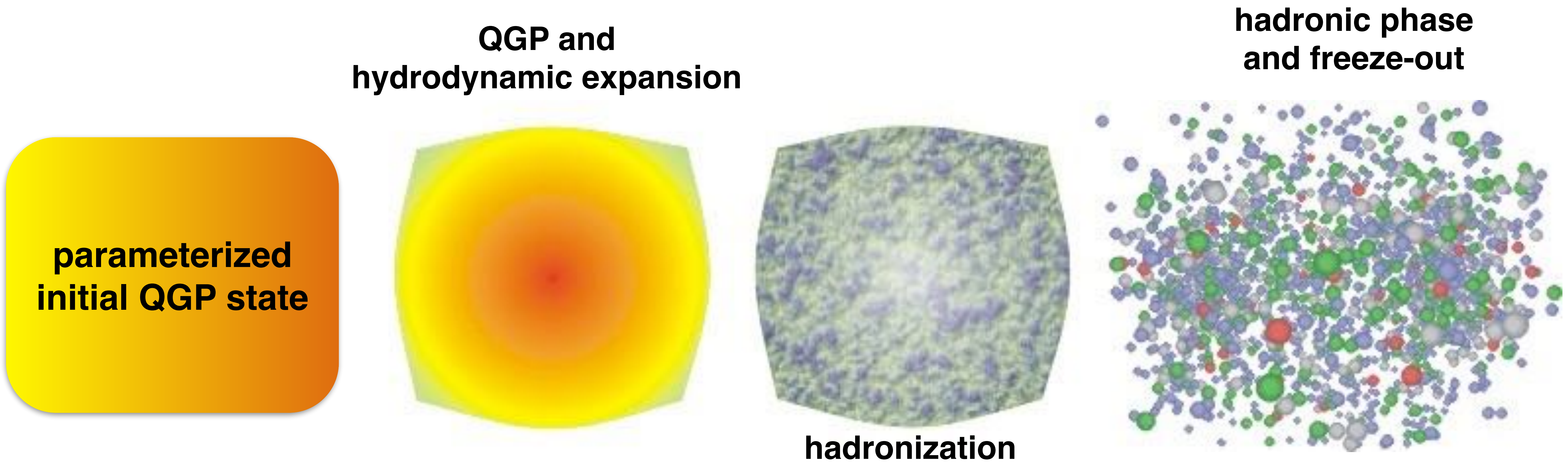
Setup of a Bayesian Statistical Analysis



Methodology



Physics Model: HQ evolution embedded in iEbE-VISHNU



Trento:

- based on simple phenomenological ideas for entropy deposition
- constrained by global model to data fit

Heavy Quarks:

- leading order pQCD with CTEQ5 & EPS09

iEbE-VISHNU (OSU):

- EbE 2+1D viscous RFD
- describes QGP dynamics & hadronization
- Lattice QCD EoS

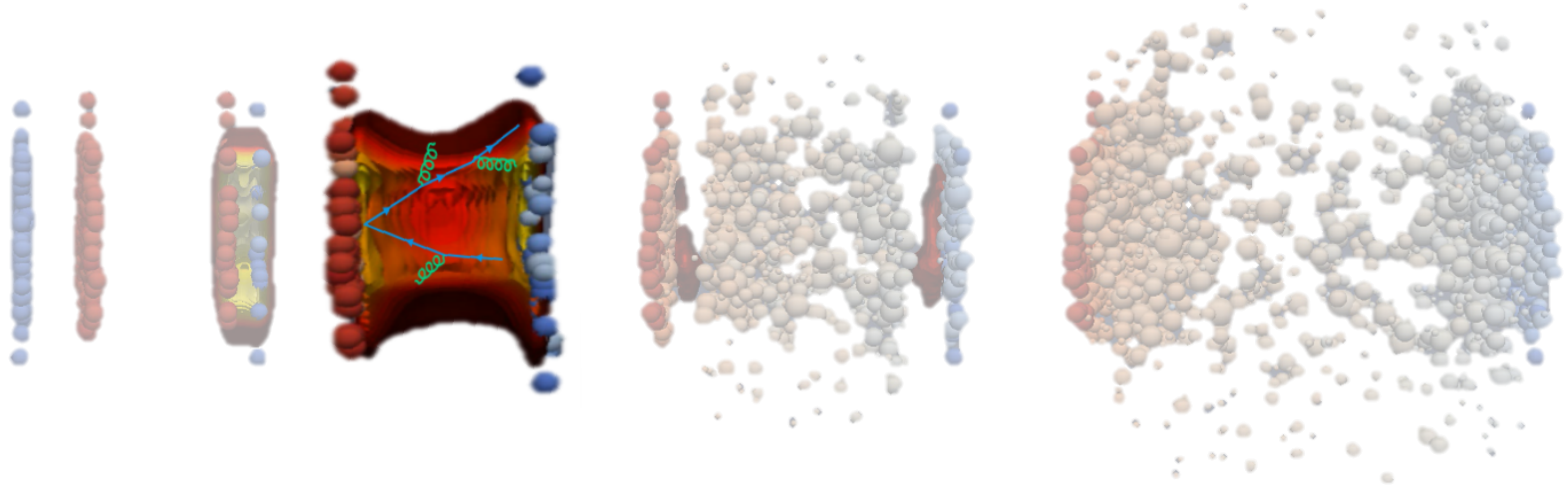
HQ transport:

1. improved Langevin w/ collisions & radiation
2. Lido: linearized Boltmann & Langevin hybrid
3. MATTER/LBT: multi-scale energy-loss

UrQMD:

- non-equilibrium evolution of an interacting hadron gas
- separation of chemical and kinetic freeze-out
- hadron gas shear & bulk viscosities are implicitly contained in calculation

Heavy Quark Transport



Langevin dynamics:

- no assumptions on medium constituents
- heavy quarks get frequent kicks from the medium → transport coefficients

Boltzmann dynamics:

- medium constituents: thermal light partons
- heavy quarks scatter with medium partons based on pQCD matrix elements

Hybrid models

- Improved Langevin (with radiative energy loss)
- Lido - **Li**nearized Boltzmann with **d**iffusion m**o**del
- MATTER/LBT: multi-scale energy-loss

Langevin with Radiative Processes

modify Langevin Eqn. with force term
due to gluon radiation:

$$\frac{d\vec{p}}{dt} = -\eta_D(p)\,\vec{p} + \vec{\xi} + \vec{f}_g$$

radiation force defined through rate of
radiated gluon momenta:

$$\vec{f}_g = \frac{d\vec{p}}{dt}$$

- same noise correlator and fluctuation-dissipation relation still hold:

$$\eta_D(p) = \frac{\kappa}{2TE} \quad \text{and} \quad \langle \xi^i(t)\,\xi^j(t')\rangle = \kappa\,\delta^{ij}\,\delta(t-t')$$

- gluon radiation calculated in Higher Twist formalism:

$$\frac{dN_g}{dx\,dk_\perp^2\,dt} = \frac{2\alpha_s(k_\perp)}{\pi} P(x)\,\frac{\hat{q}}{k_\perp^4}\,\sin^2\left(\frac{t-t_i}{2\,\tau_f}\right)\left(\frac{k_\perp^2}{k_\perp^2 + x^2 M^2}\right)^4$$

Guo & Wang: *PRL 85, 3591*
Majumder: *PRD 85, 014023*
Zhang, Wang & Wang: *PRL 93, 072301*

- relevant transport coefficients are now:

$$D = \frac{t}{M\eta_D(0)} = \frac{2T^2}{\kappa} \quad \text{and} \quad \hat{q} = 2\,\kappa\,C_A/C_F$$

Energy-Loss Transport Coefficient $\hat{q}$

- can be related to diffusion coefficient via:

$$D = \frac{t}{M\eta_D(0)} = \frac{2T^2}{\kappa} \quad \text{and} \quad \hat{q} = 2\,\kappa\, C_A/C_F$$

▸ tune either *D* or $\hat{q}$ in order to describe data

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▸ tune either *D* or $\hat{q}$ in order to describe data

alternative approach:

- calculate $\hat{q}$ using leading order pQDCD matrix elements
- integrate over thermal distribution for light parton scattering partner
- tabulate $\hat{q}$ as function of momentum and temperature for HQ

$$\hat{q}_{pQCD}(\vec{p},T) = \frac{\gamma_2}{2E_1}\int\frac{d^3p_2}{(2\pi)^3 2E_2}\int\frac{d^3p_3}{(2\pi)^3 2E_3}\int\frac{d^3p_4}{(2\pi)^3 2E_4}(\vec{p}_3 - \hat{p}_1\vec{p}_3)\times$$
$$f_2(\vec{p}_2)(2\pi)^4\delta^4(p_1+p_2-p_3-p_4)|M_{12\to34}|^2$$

▸ parmeter-free pQCD baseline that can be utilized in Langevin transport

Shanshan Cao, Tan Luo, Guang-You Qin, Xin-Nian Wang: Phys. Rev. **C94**, 014909 (2016)

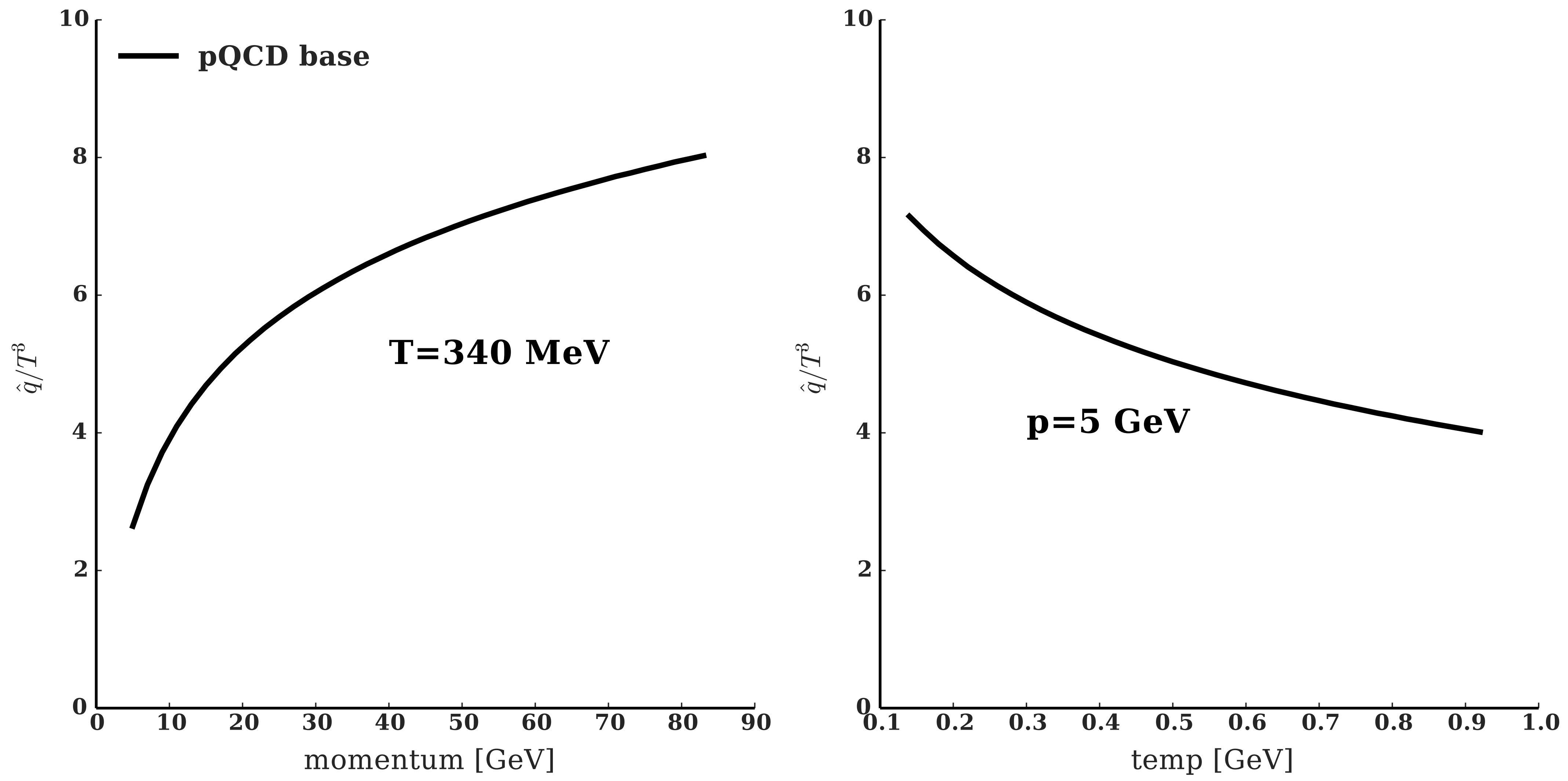
Energy-Loss Transport Coefficient $\hat{q}$

- can be related to diffusion coefficient via:

$$D \ldots \frac{t}{\ldots} \ldots \frac{2T^2}{\ldots}$$

▸ tune ei

Momentum- and Temperature Dependence of $\hat{q}$



alternati

- calcula
- integra … r
- tabulat

$$\hat{q}_{pQCD}(\vec{p}, T) \ldots \frac{\ldots}{2E_1} \int \frac{\ldots}{(2\pi)^3 2E_2} \int \frac{\ldots}{(2\pi)^3 2E_3} \int \frac{\ldots}{(2\pi)^3 2E_4} (\vec{p}_3 - \hat{p}_1 \vec{p}_3) \times$$
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Data-driven approach to D_s

- develop empirical parametrization of Ds that captures reasonable physical dependencies:

$$D_s 2\pi T(T,p) = \frac{1}{1+(\gamma^2 p)^2}(D_s 2\pi T)^{\mathrm{soft}} + \frac{(\gamma^2 p)^2}{1+(\gamma^2 p)^2}(D_s 2\pi T)^{\mathrm{pQCD}}$$

  - soft non-perturbative component with linear temperature dependence:

$$(D_s 2\pi T)^{\mathrm{soft}} = \alpha \cdot \left[1 + \beta \cdot \left(\frac{T}{T_c} - 1\right)\right]$$

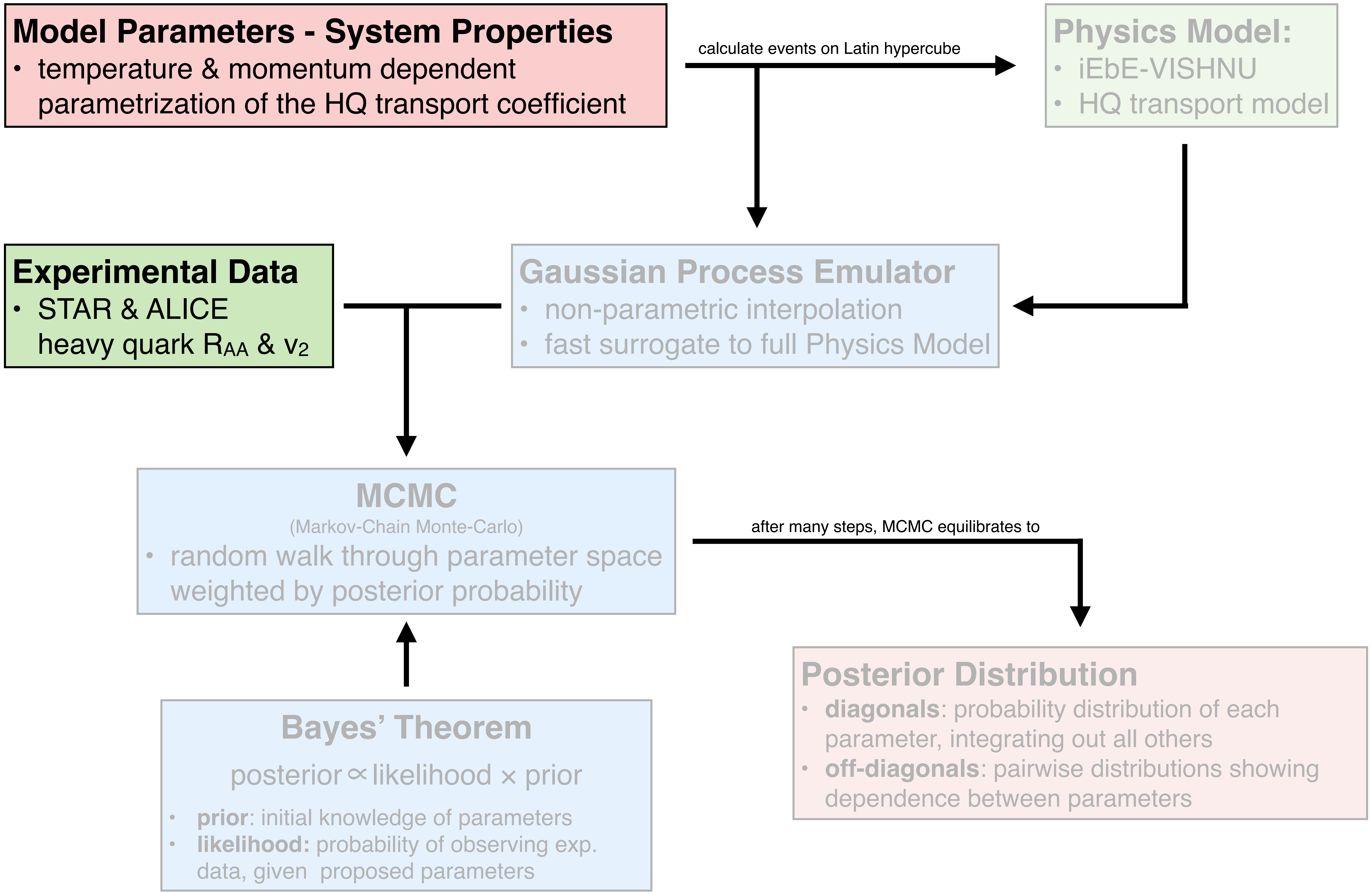
  - hard perturbative component:

$$(D_s 2\pi T)^{\mathrm{pQCD}}(\alpha_s) = 8\pi T^3 / \hat{q}^{\mathrm{pQCD}}(\alpha_s)$$

- asymptotic behavior reduces to soft/hard components in appropriate limit:
  - $p \ll 1/\gamma^2$: $D_s 2\pi T \rightarrow D_s 2\pi T^{\mathrm{soft}}$
  - $p \gg 1/\gamma^2$: $D_s 2\pi T \rightarrow D_s 2\pi T^{\mathrm{qQCD}}$

calibrate parameters $\alpha, \beta, \gamma, \alpha_s$ to data to extract functional form of of $D_s 2\pi T(T,p)$

Methodology



Calibration Parameters & Data

- the calibration parameters are the model parameters that codify the physical properties of the system that we wish to characterize with the analysis

Improved Langevin:

- functional form of temperature- and momentum dependence of $D_s\, 2\pi T$
- 4 parameters: α, β, γ, α_s

Lido: Linearized Boltzmann + Langevin

- functional form of temperature- and energy dependence of diffusion contribution to D_s: κ_D, x_D
- scale for α_s in pQCD contribution: μ

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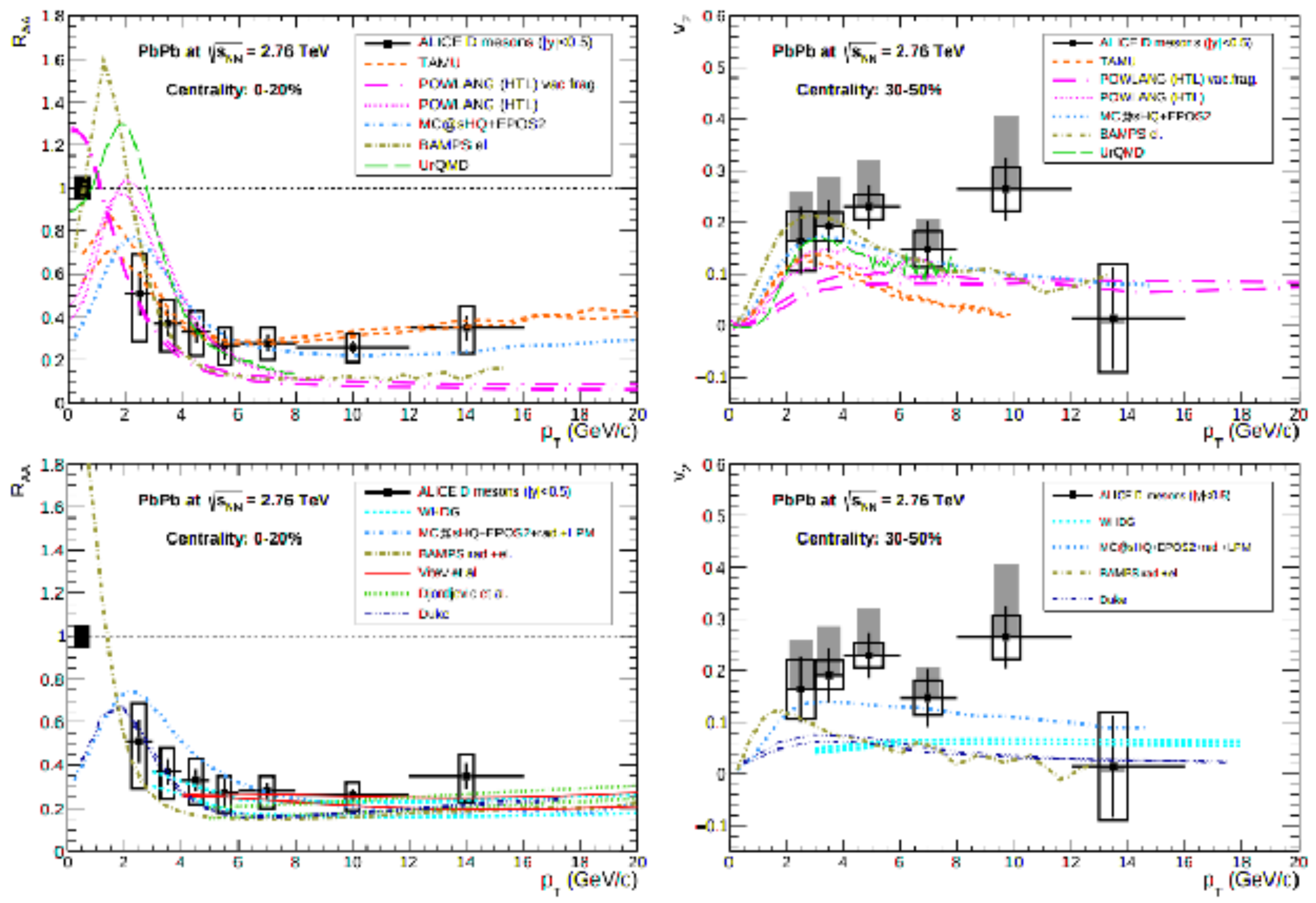
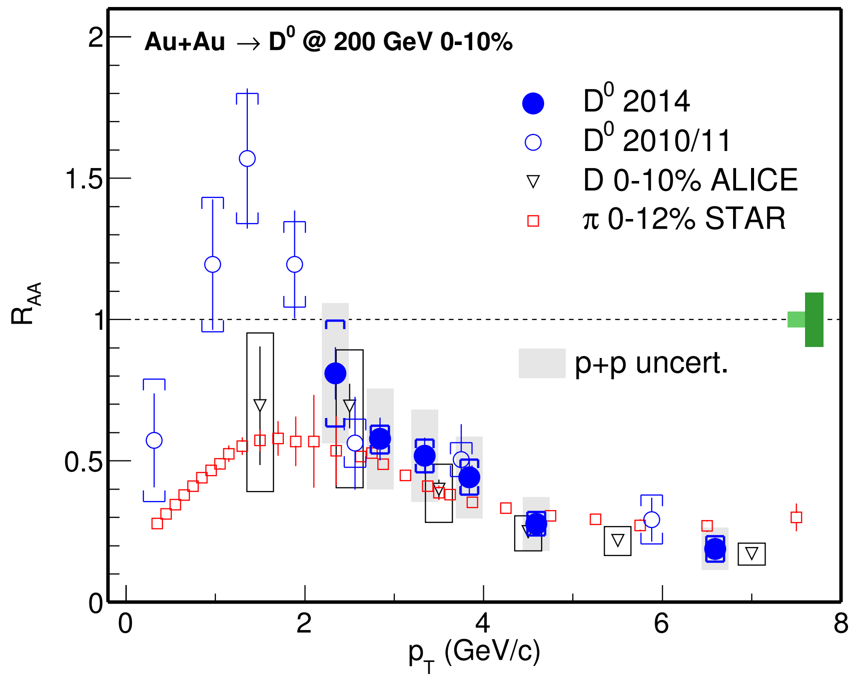
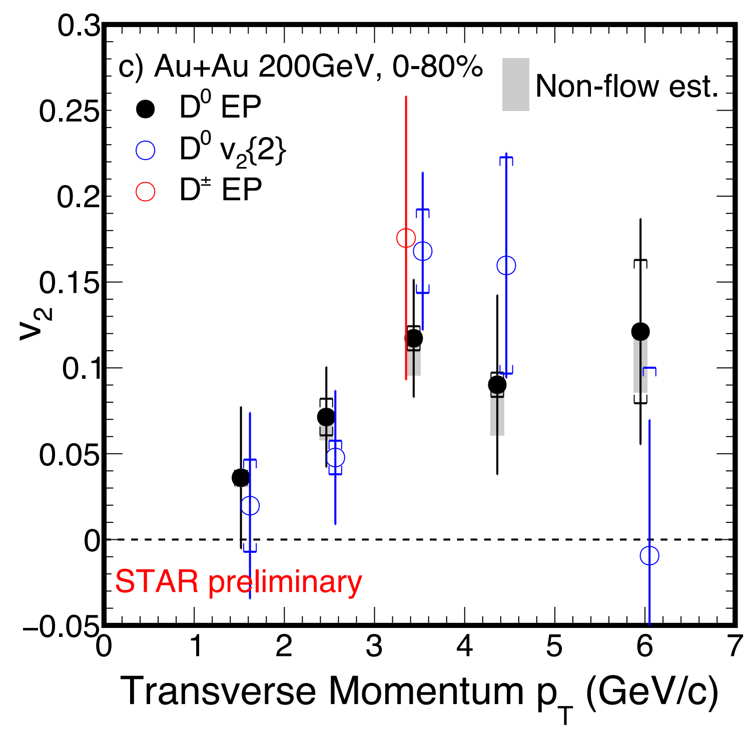
STAR and ALICE data:

- D-meson R_{AA} and v_2 for multiple centrality bins







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calculate events on Latin hypercube

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Experimental Data

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Gaussian Process Emulator

- non-parametric interpolation
- fast surrogate to full Physics Model

MCMC

(Markov-Chain Monte-Carlo)

- random walk through parameter space weighted by posterior probability

after many steps, MCMC equilibrates to

Posterior Distribution

- **diagonals**: probability distribution of each parameter, integrating out all others
- **off-diagonals**: pairwise distributions showing dependence between parameters

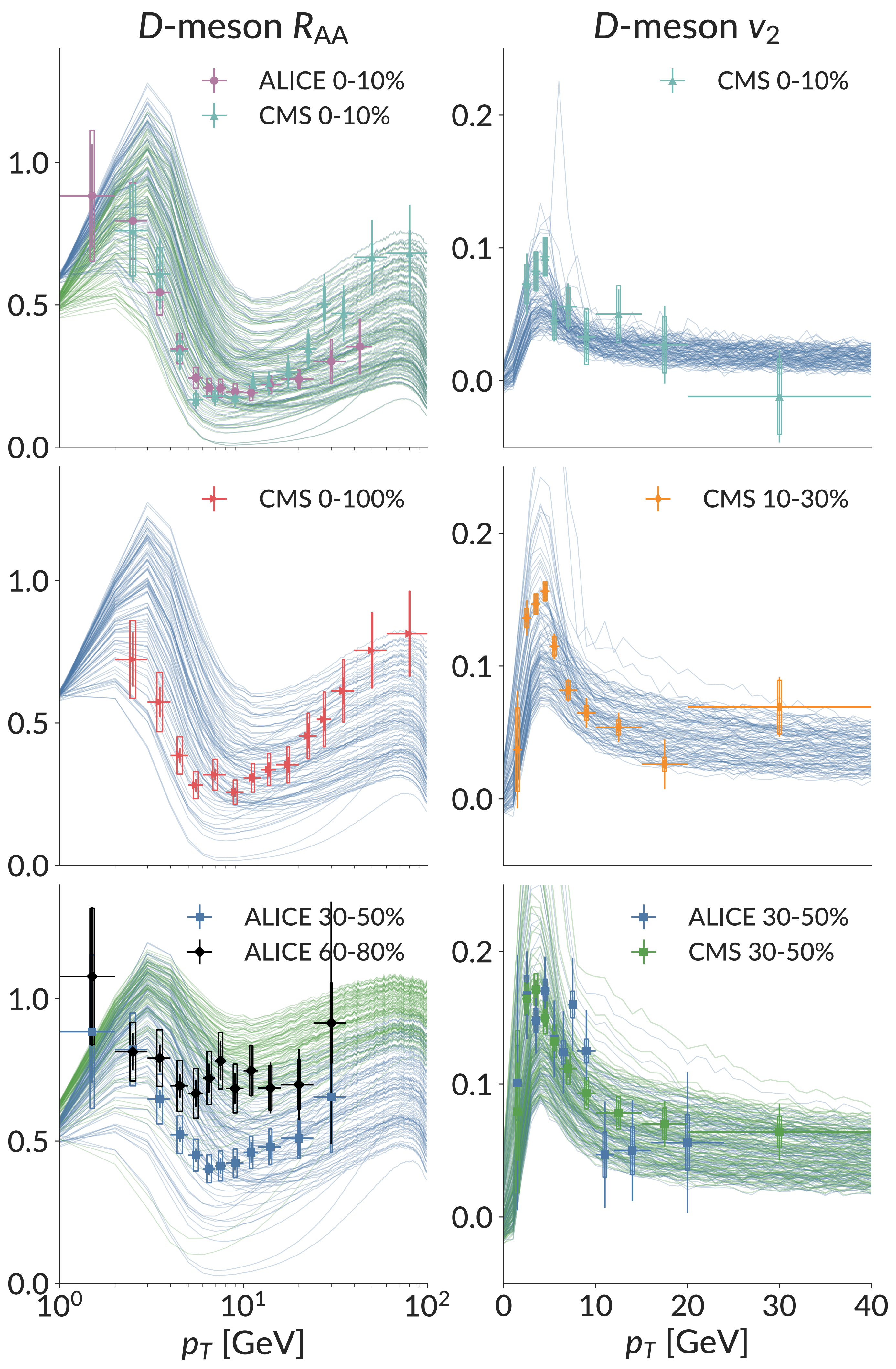
Bayes' Theorem

posterior $\propto$ likelihood $\times$ prior

- **prior**: initial knowledge of parameters
- **likelihood:** probability of observing exp. data, given proposed parameters

Langevin: Prior vs. Posterior

Prior: model calculations evenly distributed over full design space



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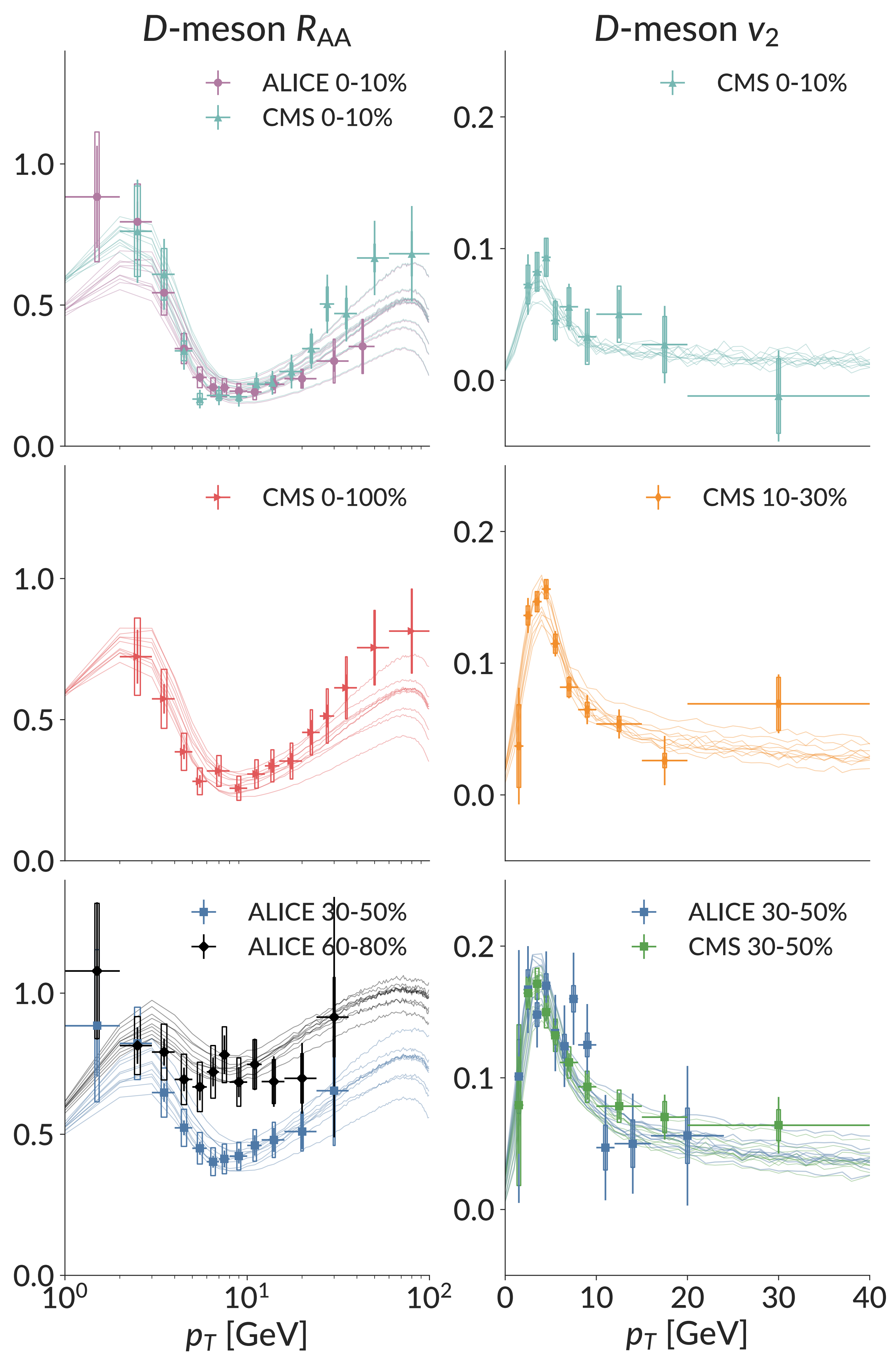

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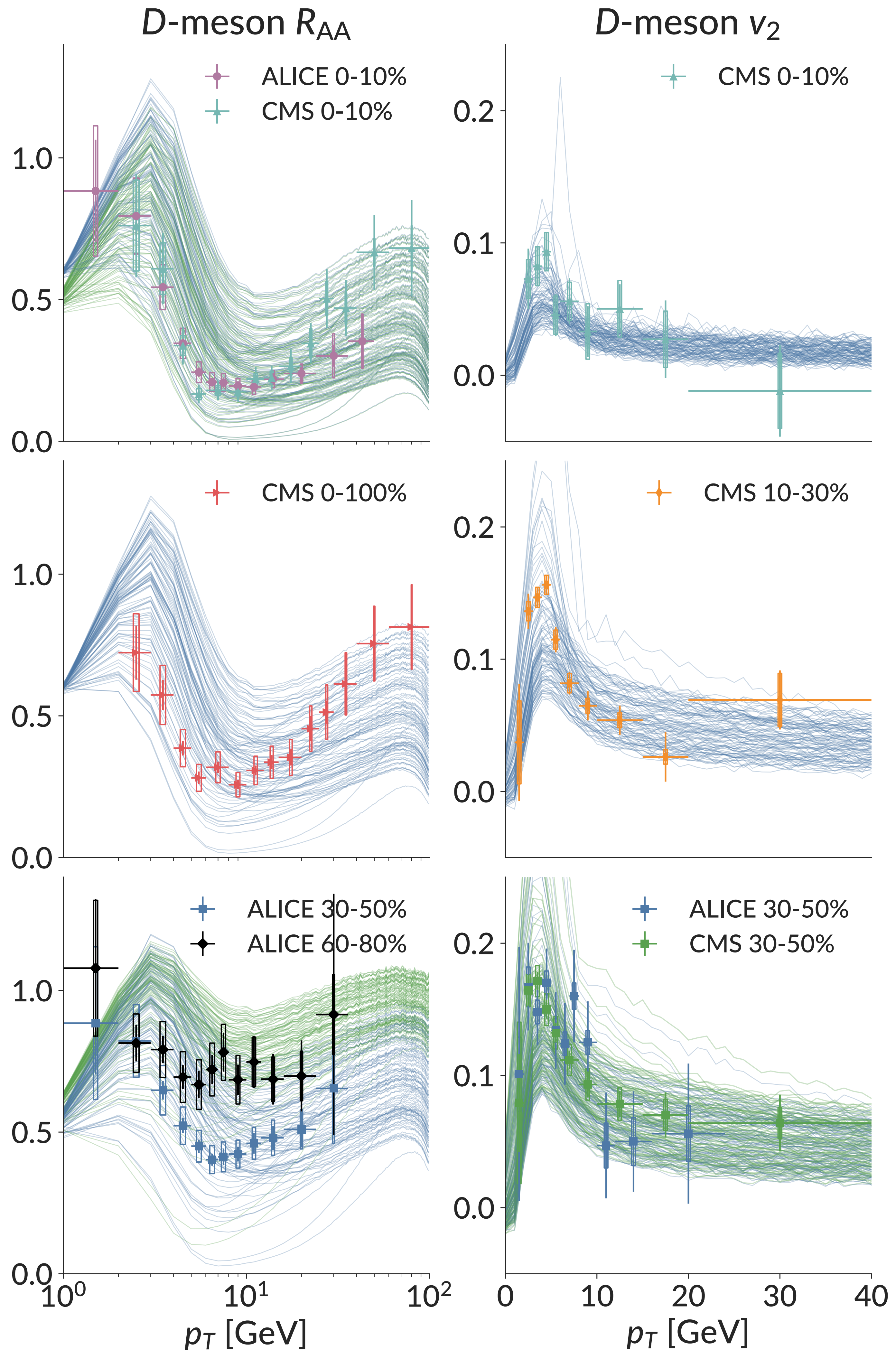

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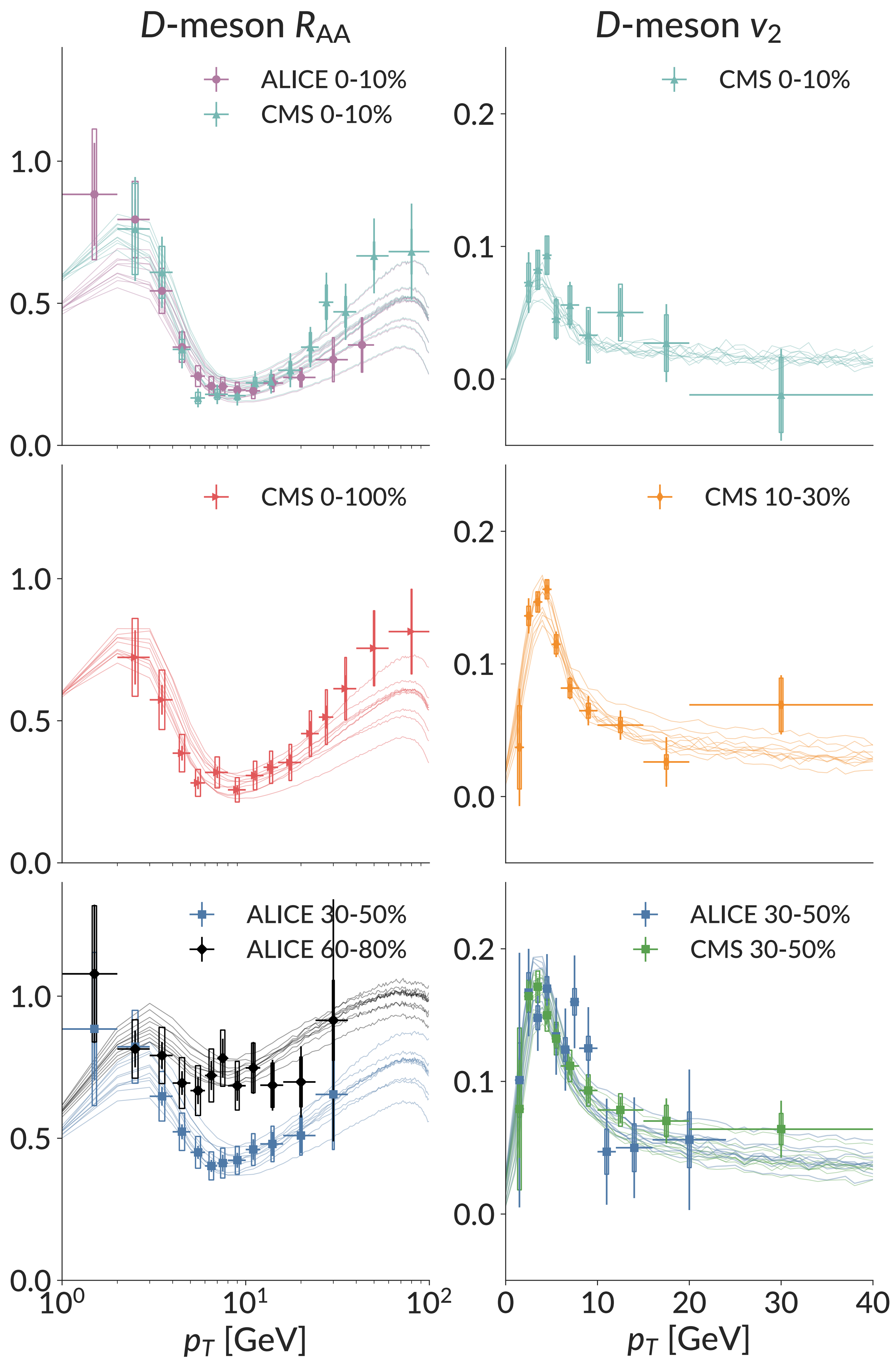

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Posterior Distribution
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Langevin: Calibrated Posterior Distribution

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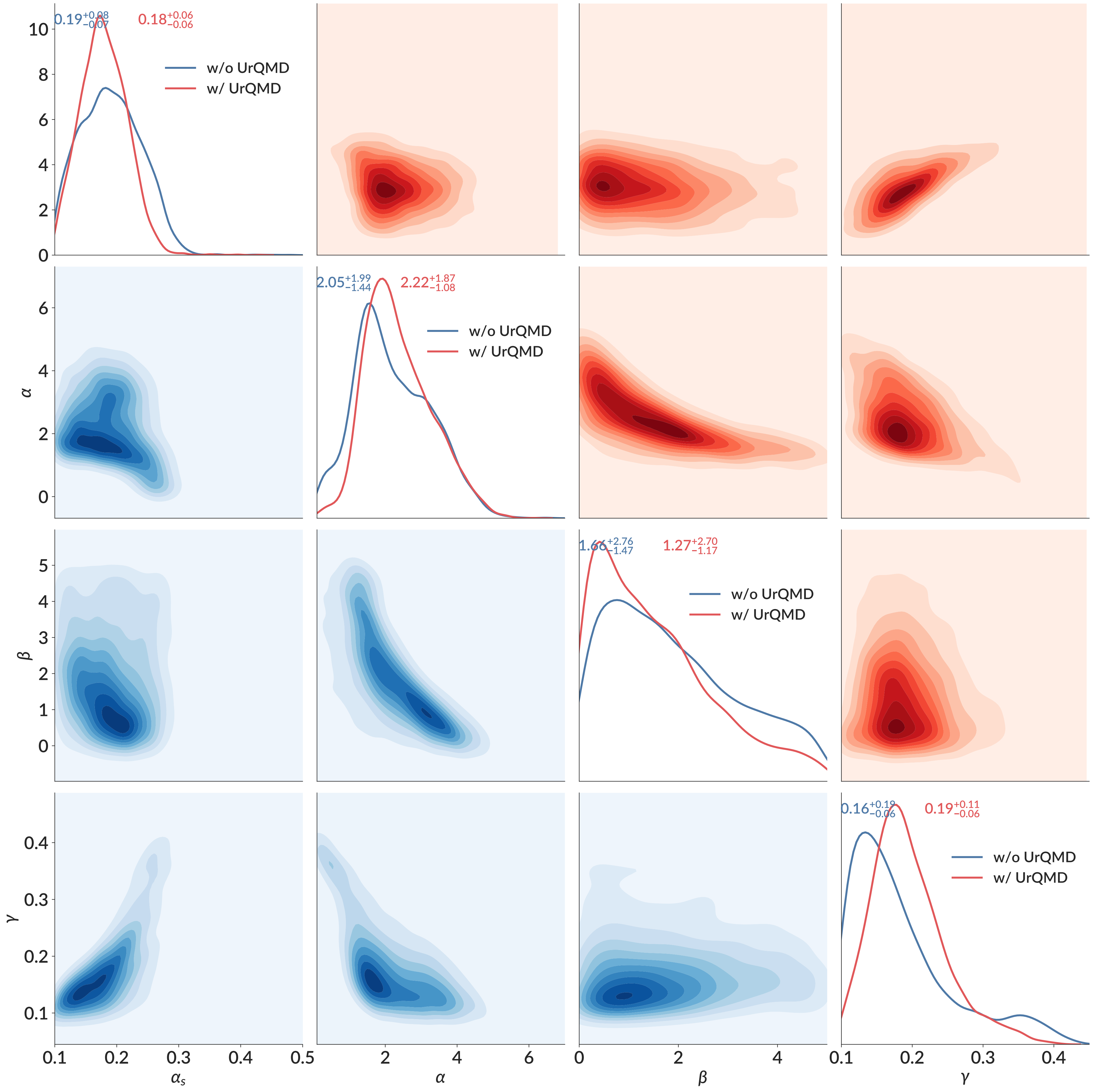
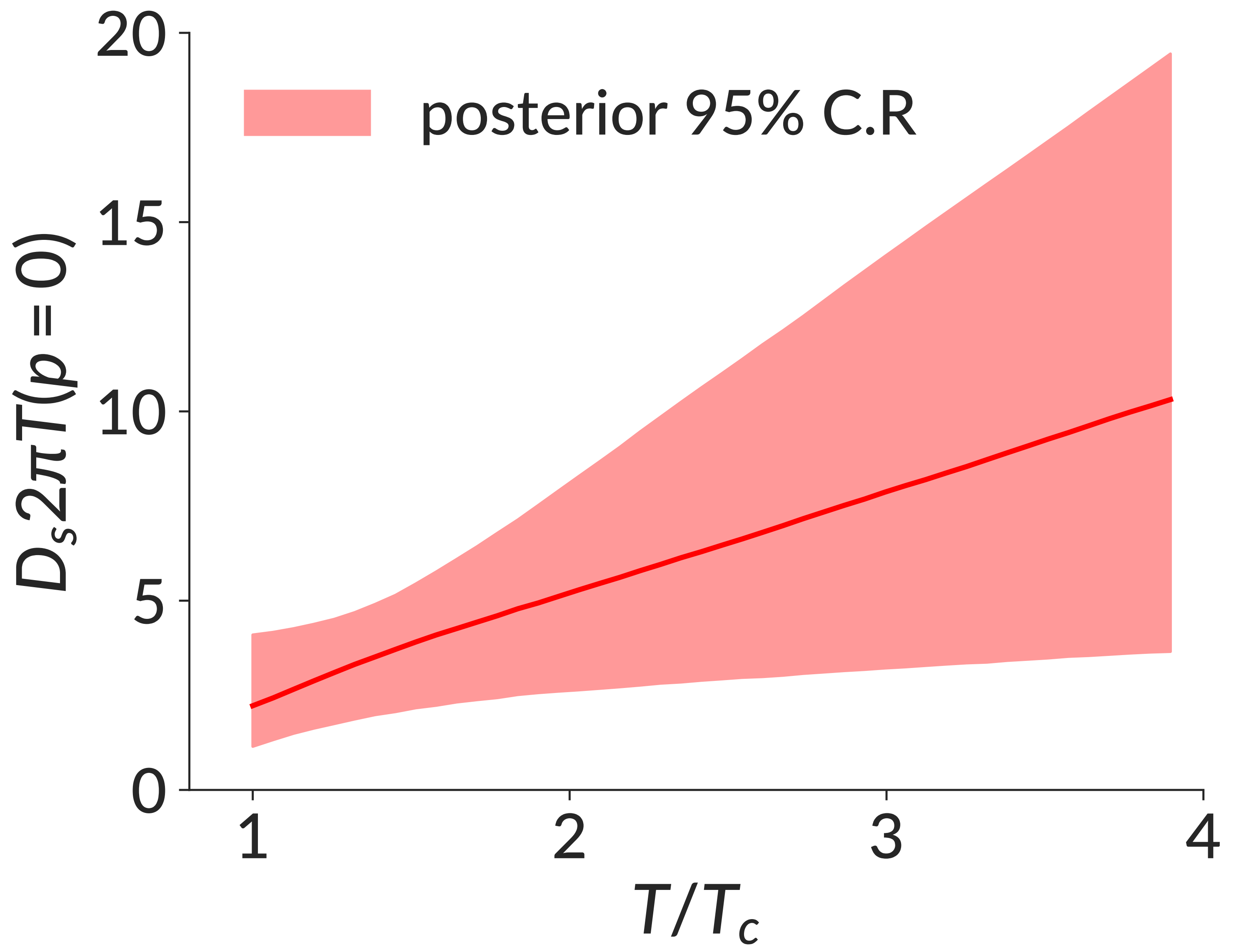
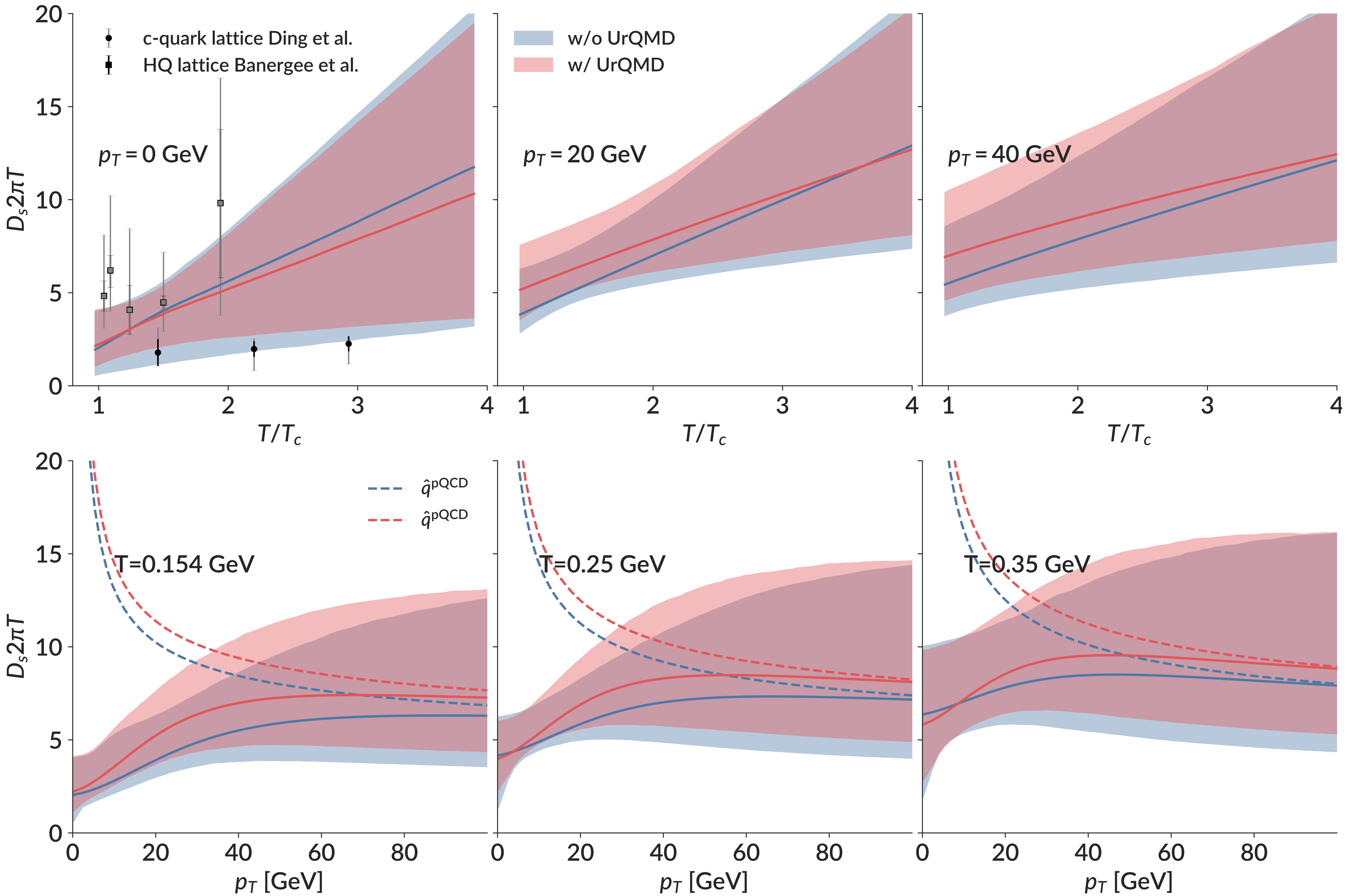


- peaks in posterior indicate that high likelihood ranges for parameters can be identified
- only weak sensitivity to hadronic rescattering
- key result: temperature-dependence of heavy-quark diffusion coefficient D_s:



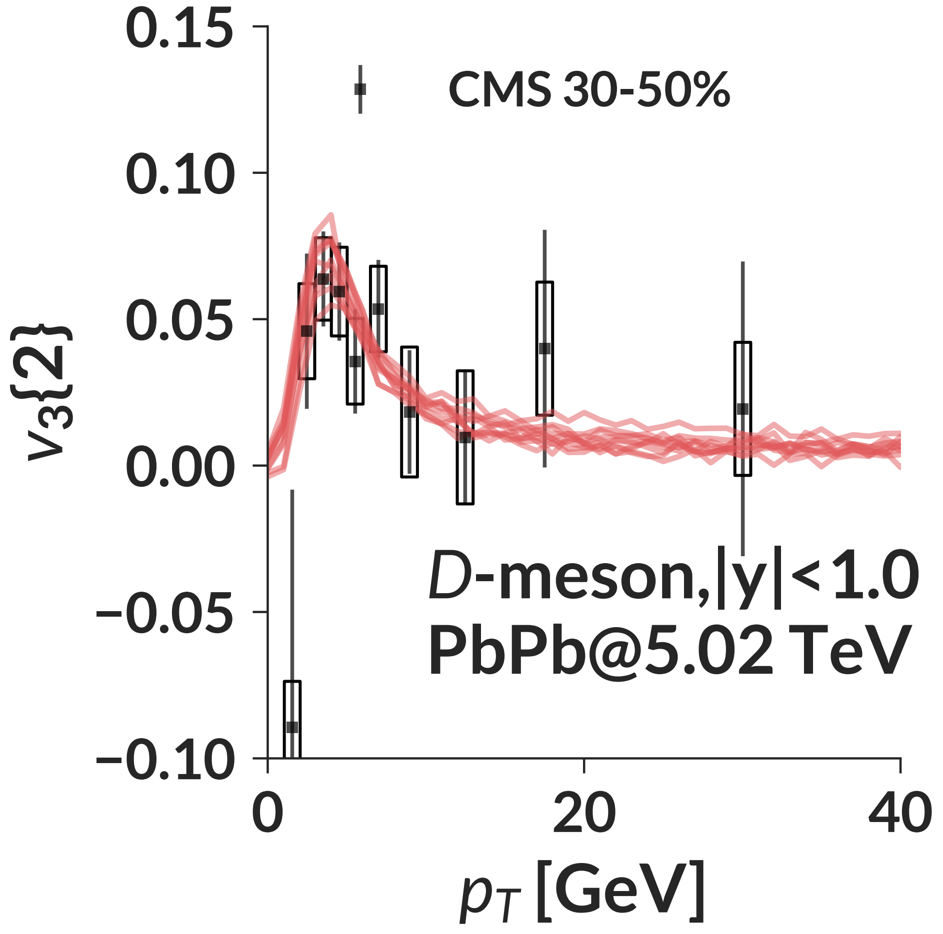
Temperature- & momentum-dependence of D_s



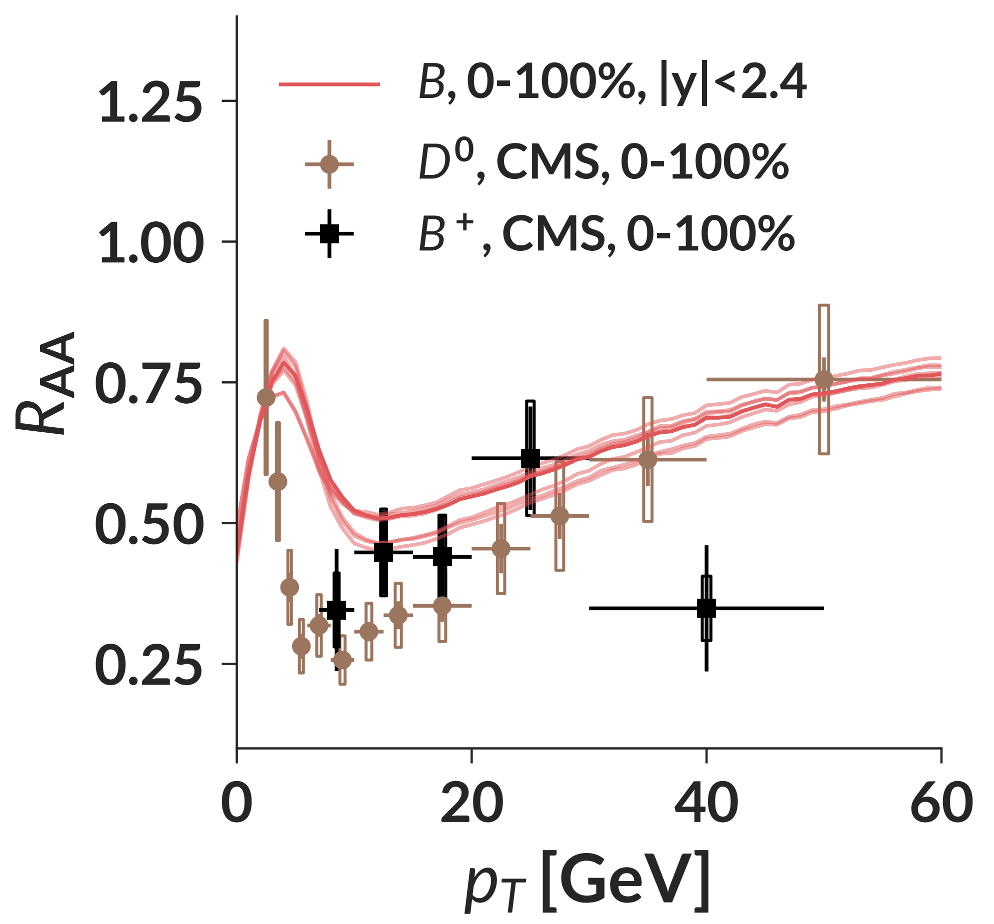
Langevin: Validation

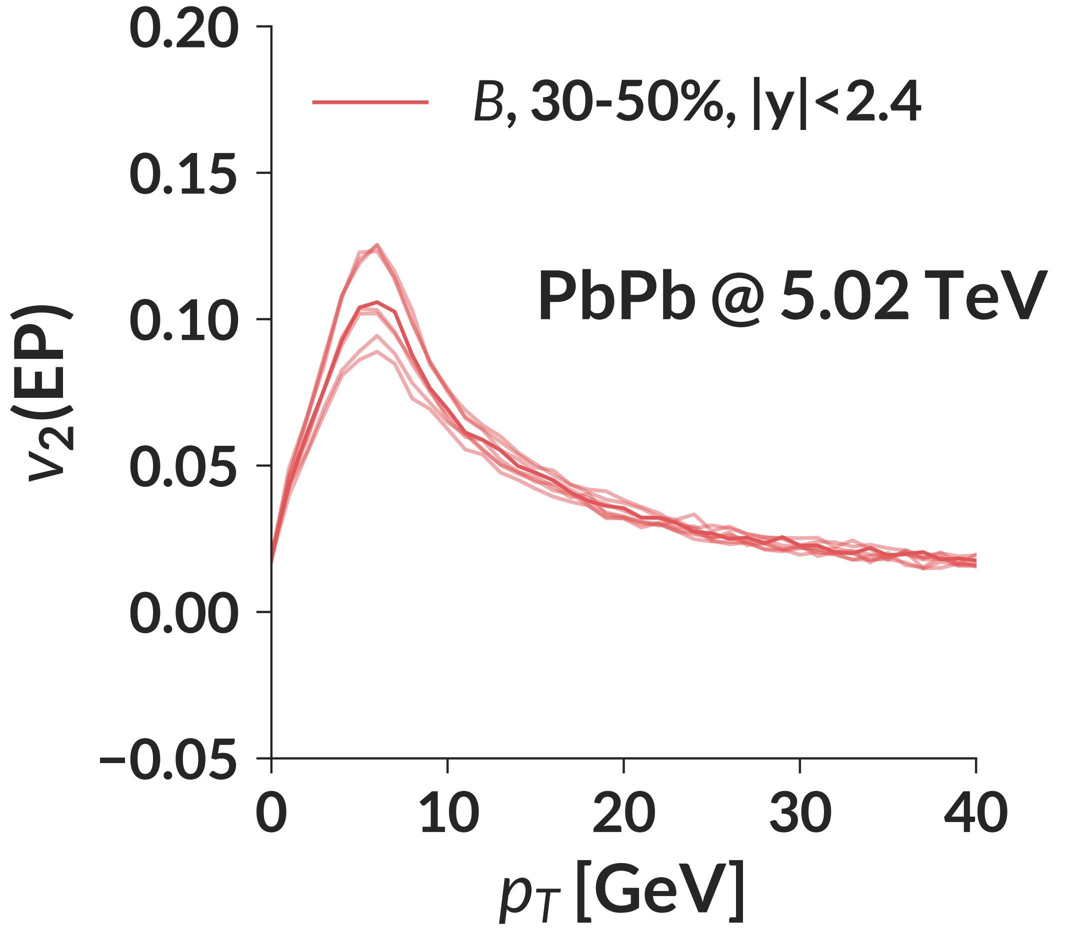
Validation: run model with parameter values sampled from posterior distribution for observables that were not included in original calibration

D-meson v_3:

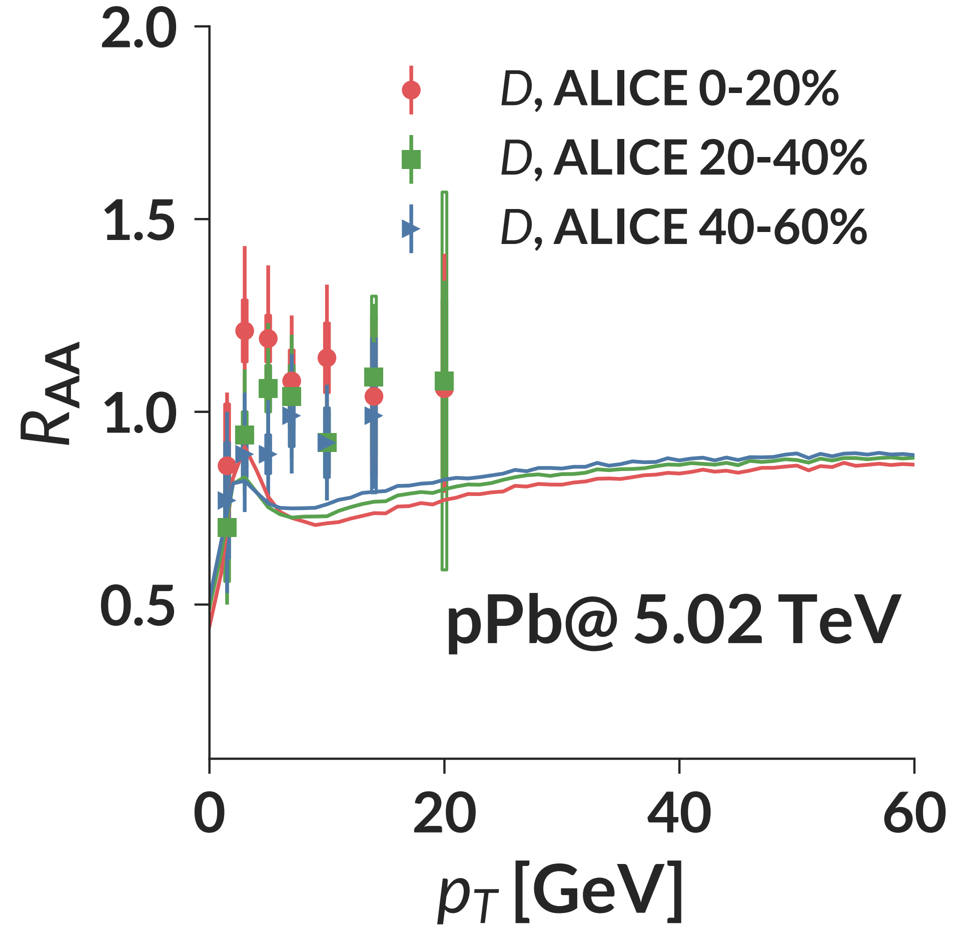


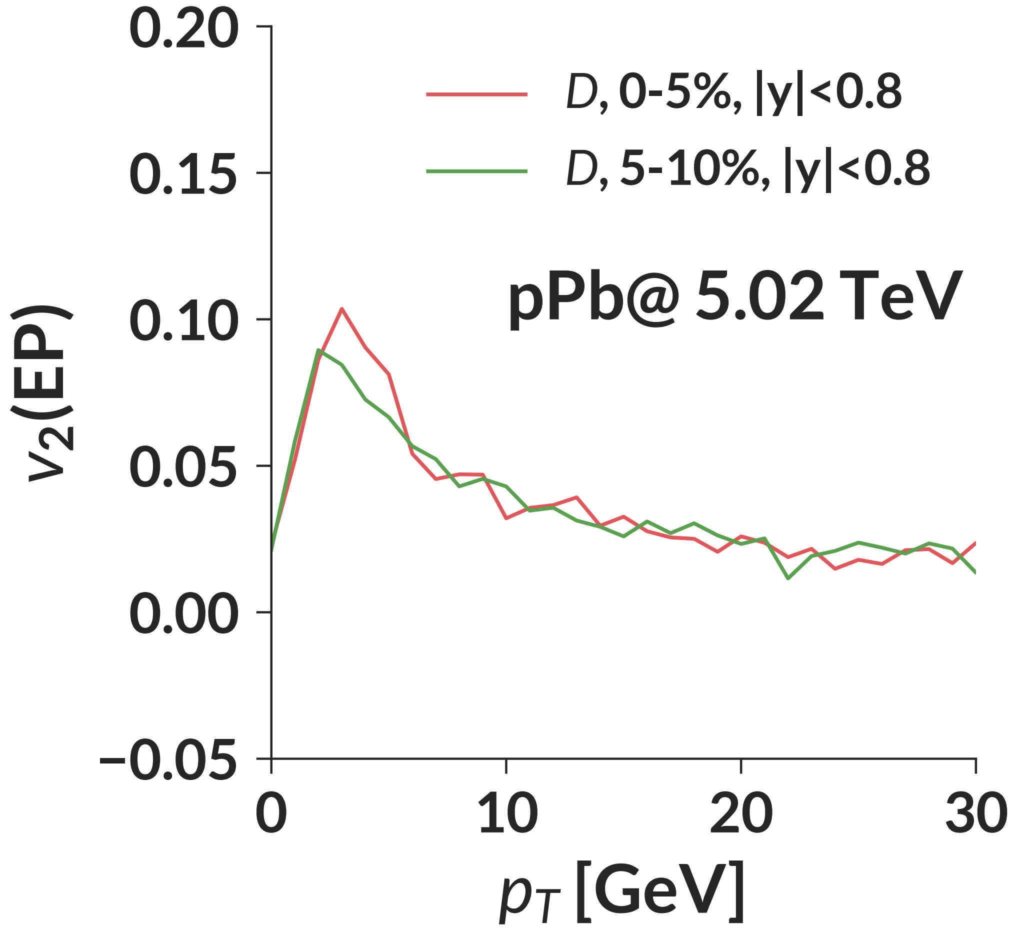
B-meson R_{AA} & v_2:





D-meson R_{AA} & v_2 in p+Pb:





- Radiation improved Langevin shows decent agreement to with validation data and allows for further predictions of new observables

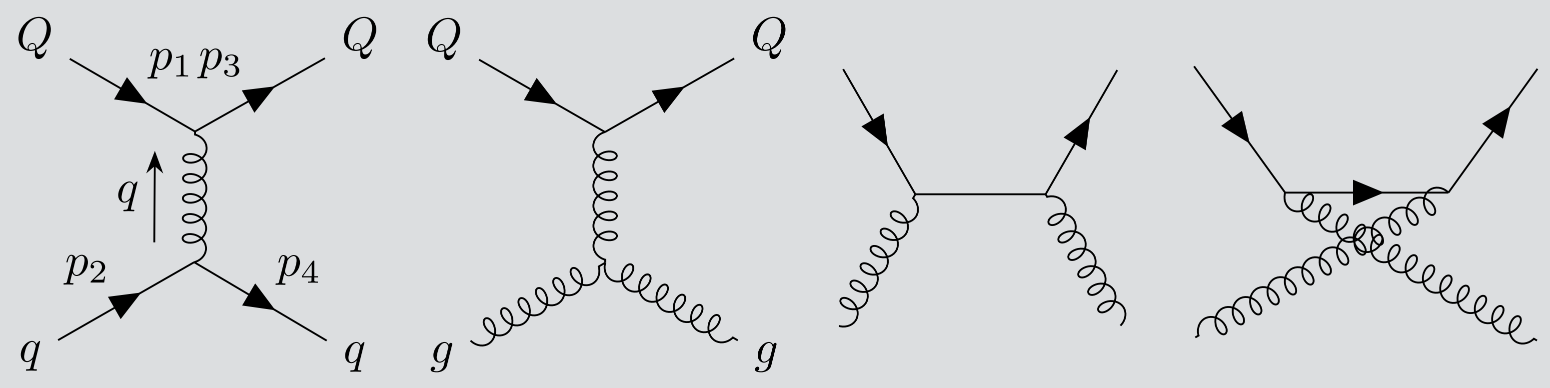
Lido: Boltzmann + Langevin Hybrid

Combine the strength of the linearized-Boltzmann and Langevin approaches:

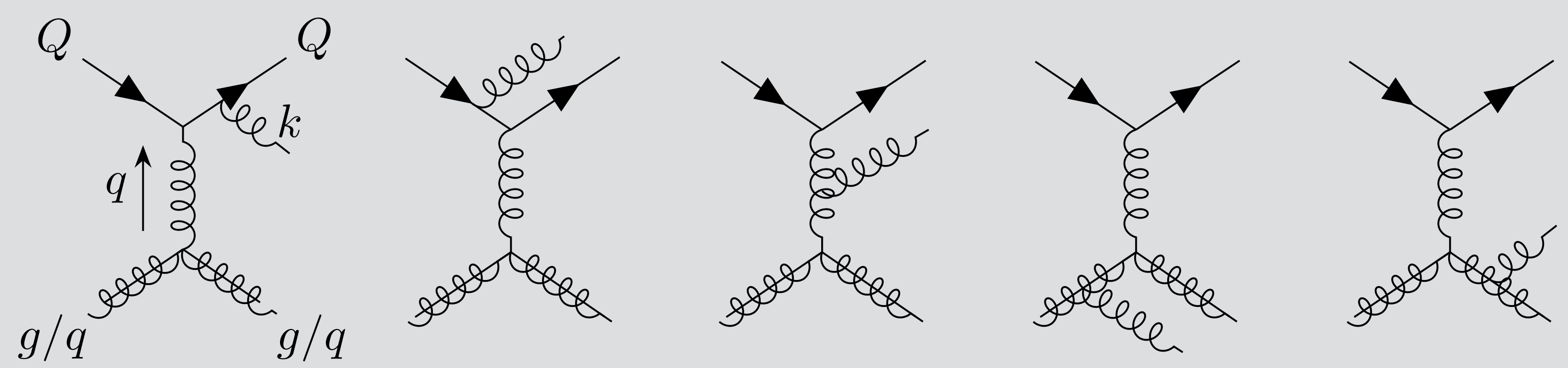
$$\frac{p \cdot \partial f_Q}{E} = \mathcal{C}[f_Q] - \frac{\partial}{\partial p_i}\left(A_i - \frac{1}{2}\frac{\partial}{\partial p_j}B_{ij}\right) f_Q = \left(\hat{\mathcal{C}} + \hat{\mathcal{D}}\right) f_Q$$

perturbative processes:

- elastic scattering:



- inelastic: improved Gunion Bertsch



Fochler et al. PRD88 014018

- gluon radiation **and** absorption implemented to conserve detailed balance

non-perturbative processes:

- treated in a Langevin equation with isotropic random force

$$\Delta \vec{x_i} = \frac{\vec{p_i}}{E}\Delta t \quad \Delta \vec{p_i} = -\eta_D\, \vec{p_i}\, \Delta t + \Delta t\, \vec{\xi_i}(t)$$

- Einstein relation connects random force to drag coefficient to ensure proper equilibrium

Calibrating D_s in Lido

- The collision integral contains pQCD scattering matrix elements - their contribution to D_s is well-defined, modulo a scale for the running coupling constant:

$$\alpha_s(Q) = \alpha_s(\max\{Q, \mu\pi T\})$$

- The diffusion component relies on a parametrization of the energy- and temperature dependence of the non-perturbative contribution to D_s:

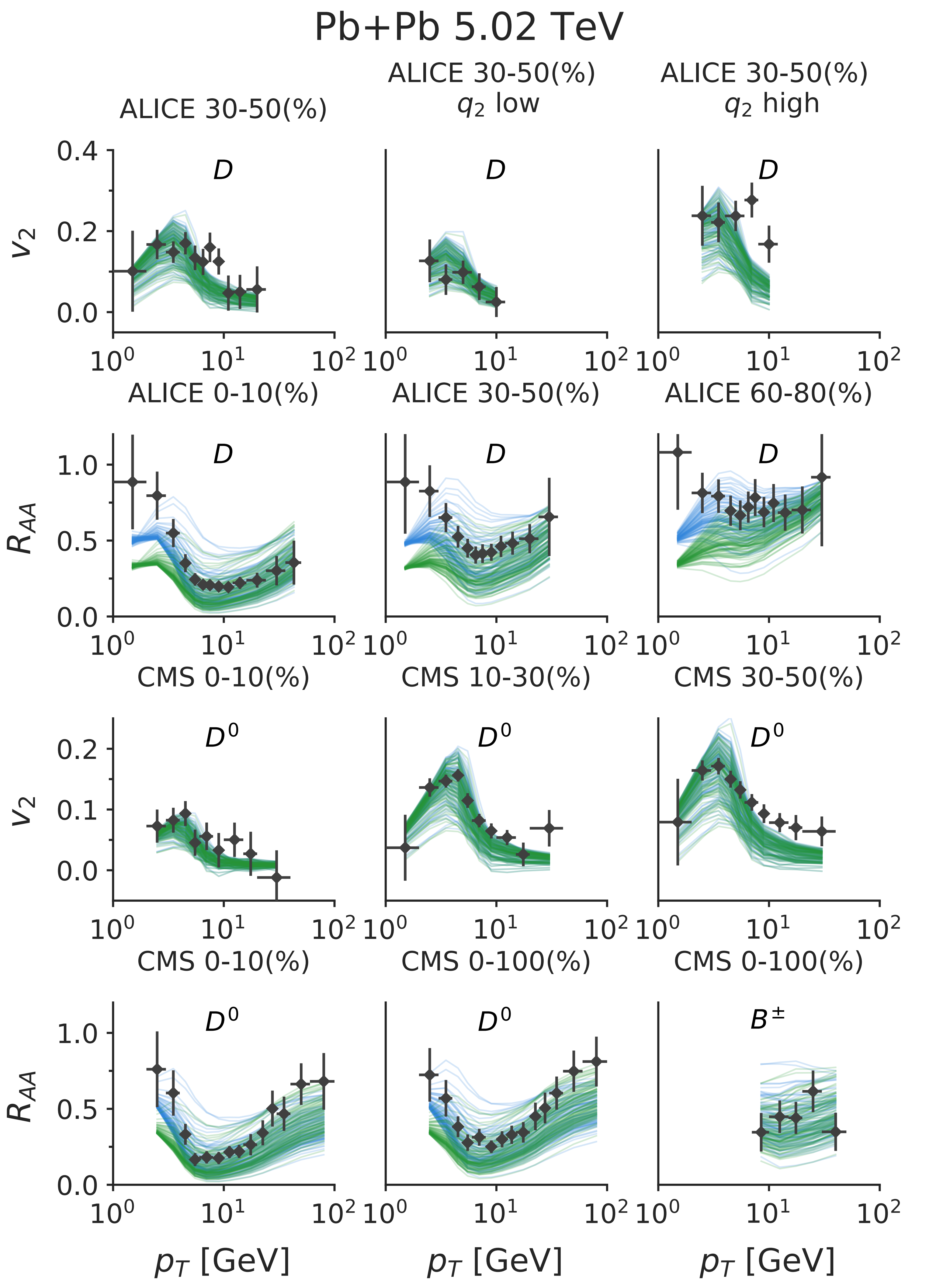
$$\hat{q}_{\text{diffusion}} = 2\,T^3\,\kappa\left(x_D + \frac{1 - x_D}{E\,T}\right)$$

- The full transport coefficient is the sum of both contributions:

$$\hat{q} = \hat{q}_{\text{pQCD}} + \hat{q}_{\text{diffusion}}\ , \qquad \hat{q} \Leftrightarrow D_s 2\pi T$$

Lido: Prior vs. Posterior

Prior: model calculations evenly distributed over full design space



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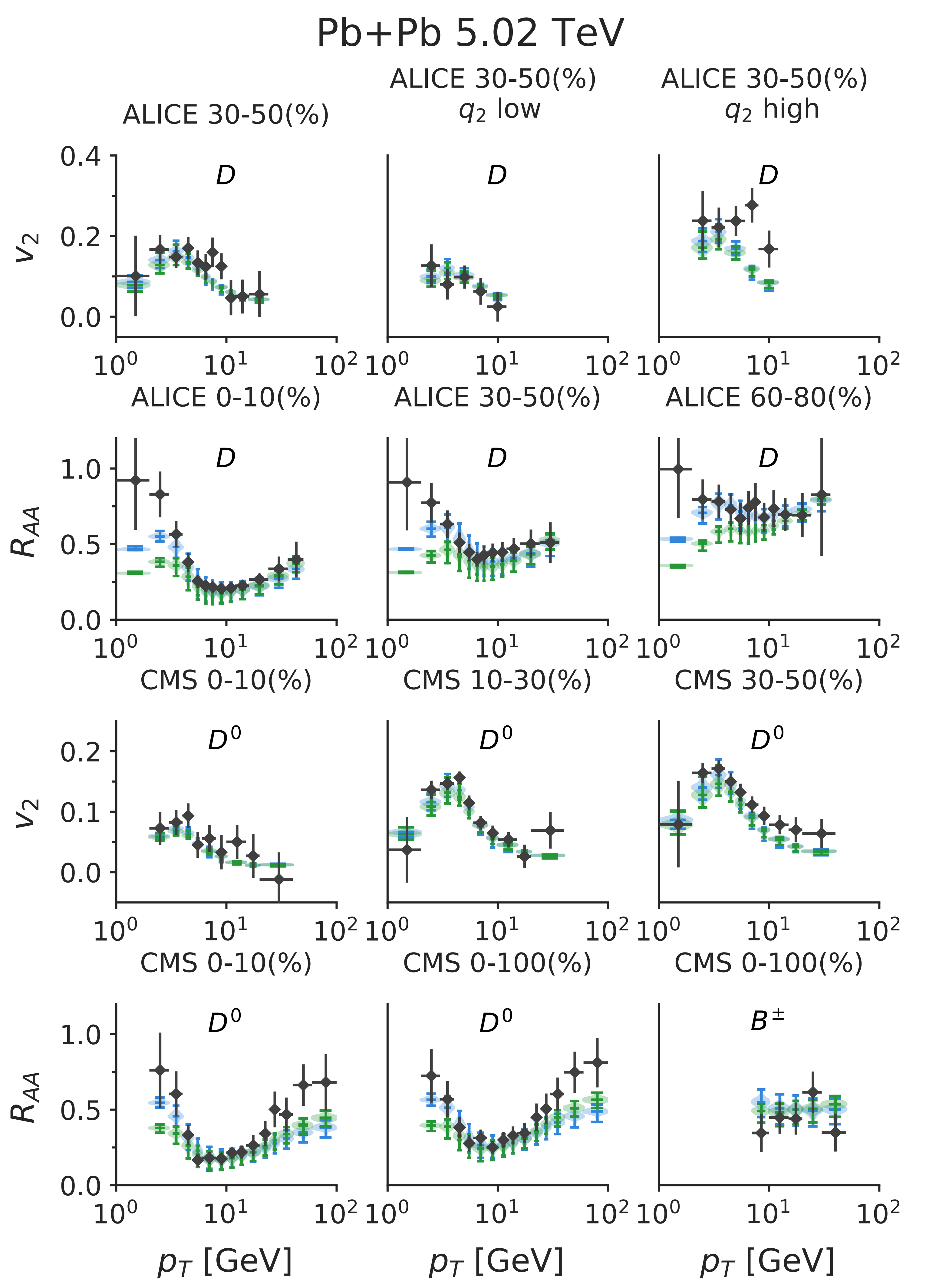

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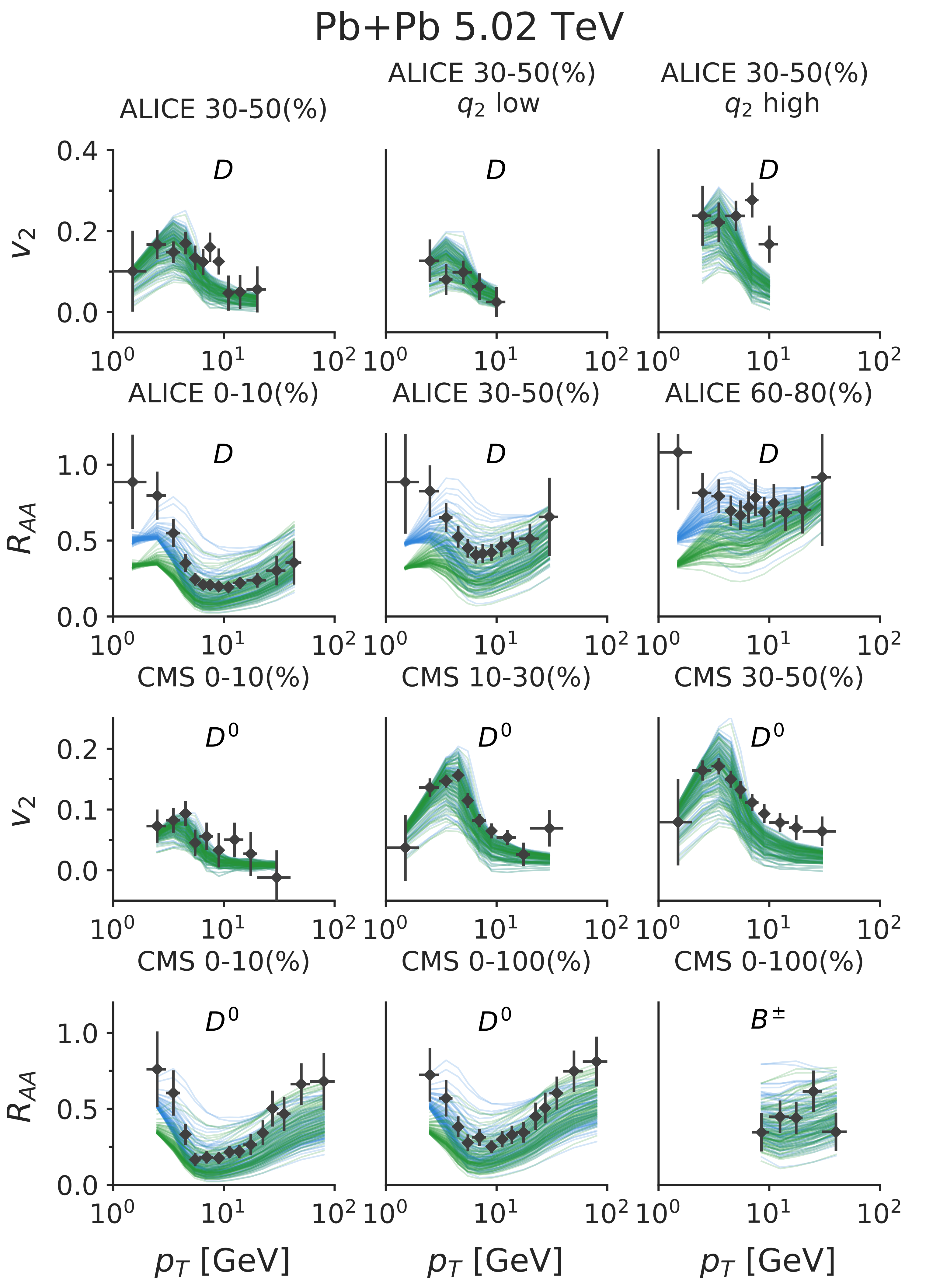

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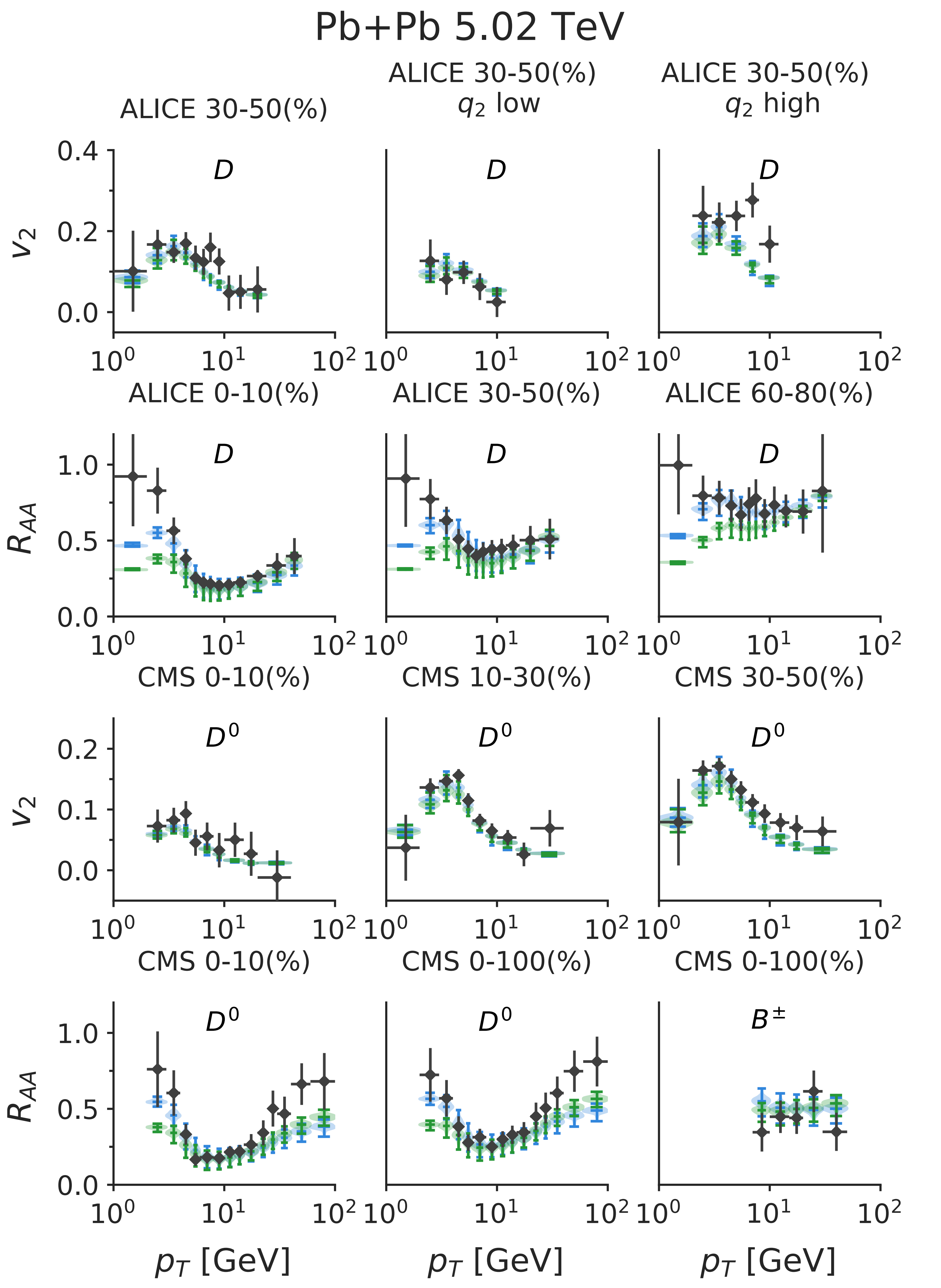
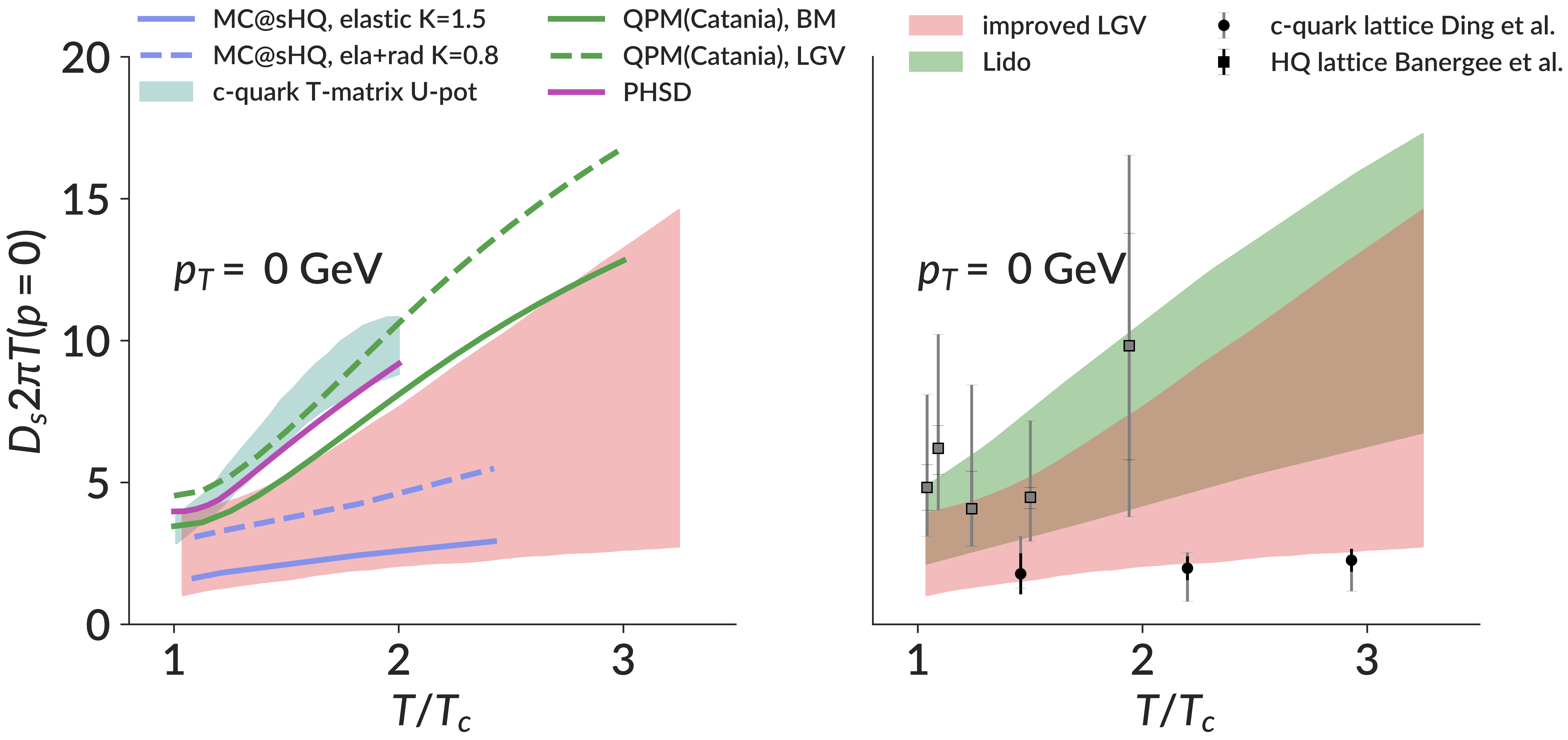


T- & p-dependent D_s: model comparison

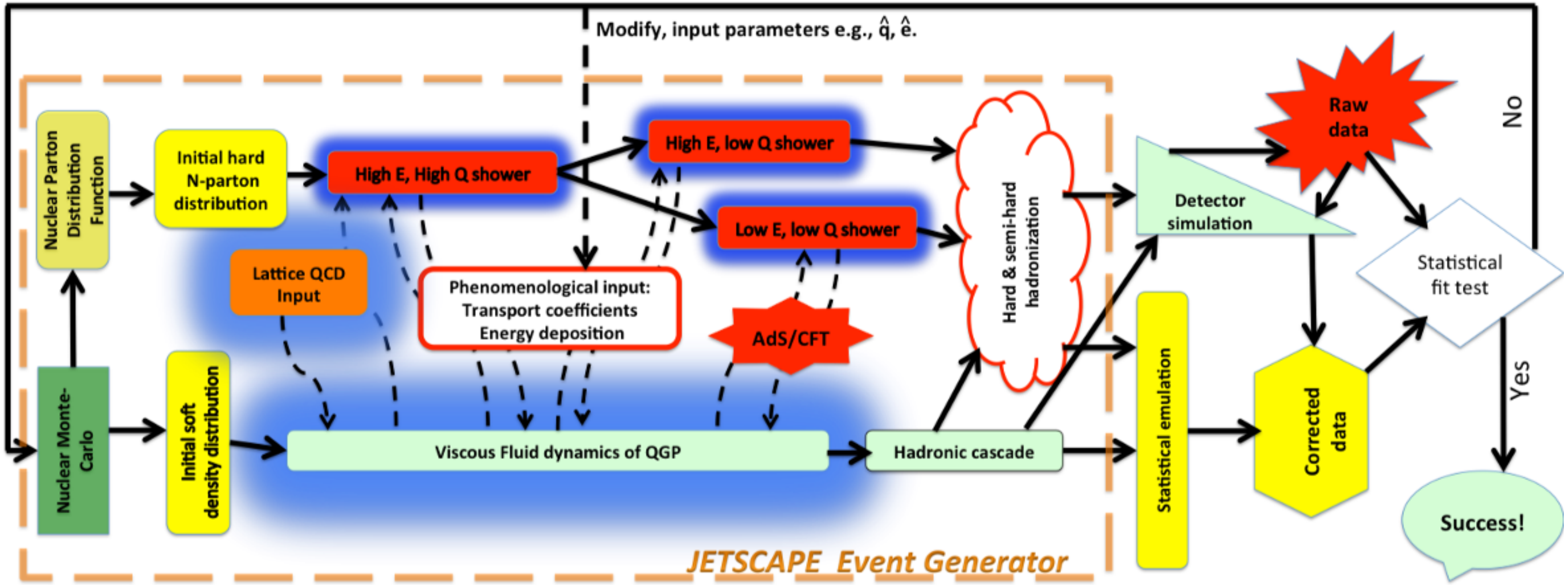


- comparison shows large variability in D_s between different heavy quark transport/ interaction models
- Lattice results favor data-driven extraction (within large uncertainties)
- Lido vs. radiation improved Langevin:
  - large overlap in extracted D_s band
  - Lido trends to larger D_s values (influence of pQCD contribution in model)

Studying energy-loss with the Jetscape framework

JETSCAPE: **J**et **E**nergy Loss **T**omography with a **S**tatistically and **C**omputationally **A**dvanced **P**rogram **E**nvolope

- provide a tool (modular software library) to study the physics of energy-loss
- large area of research, many different approaches exist, no single group or PI has the capability to do them all
- collaboration of theoretical and experimental physicists, computer scientists and statisticians



- Trento (2+1) + free Streaming
- Medium evolution:
  - MUSIC (2+1, 3+1),
  - external reader
  - brick
  - Gubser
- Pythia8 (parton gun, string fragmentation)
- MATTER
- Martini
- AdS/CFT
- LBT
- Cooper Frye
- SMASH
- Custom and HepMC output

- JETSCAPE package interfaces with leading community tools that are publicly available and well-tested
- additional functions and codes can be linked as external modules (e.g. Lido) or utilize the framework for their own energy-loss kernel (e.g. Tequila)

Energy-Loss in Matter/LBT

- high virtuality **in medium** parton showering is solved by the Matter model which employs the Higher Twist formalism. It generates a virtuality ordered shower with splittings above $Q \gg Q_0$

- virtuality dependent q is parametrized:

$$\hat{q}(Q) = \hat{q}^{HTL} \frac{c_0}{1 + c_1 \ln^2 Q^2 + c_2 \ln^4 Q^2}$$

with: $c_0 = 1 + c_1 \ln^2 Q_0^2 + c_2 \ln^4 Q_0^2$

- low virtuality parton showering is solved via a Linearized Boltzmann Transport (LBT model):

$$p_1^\mu \partial_\mu f_1(x_1, p_1) = \mathcal{C}_{\text{el}}[f_1] + \mathcal{C}_{\text{inel}} f_1$$

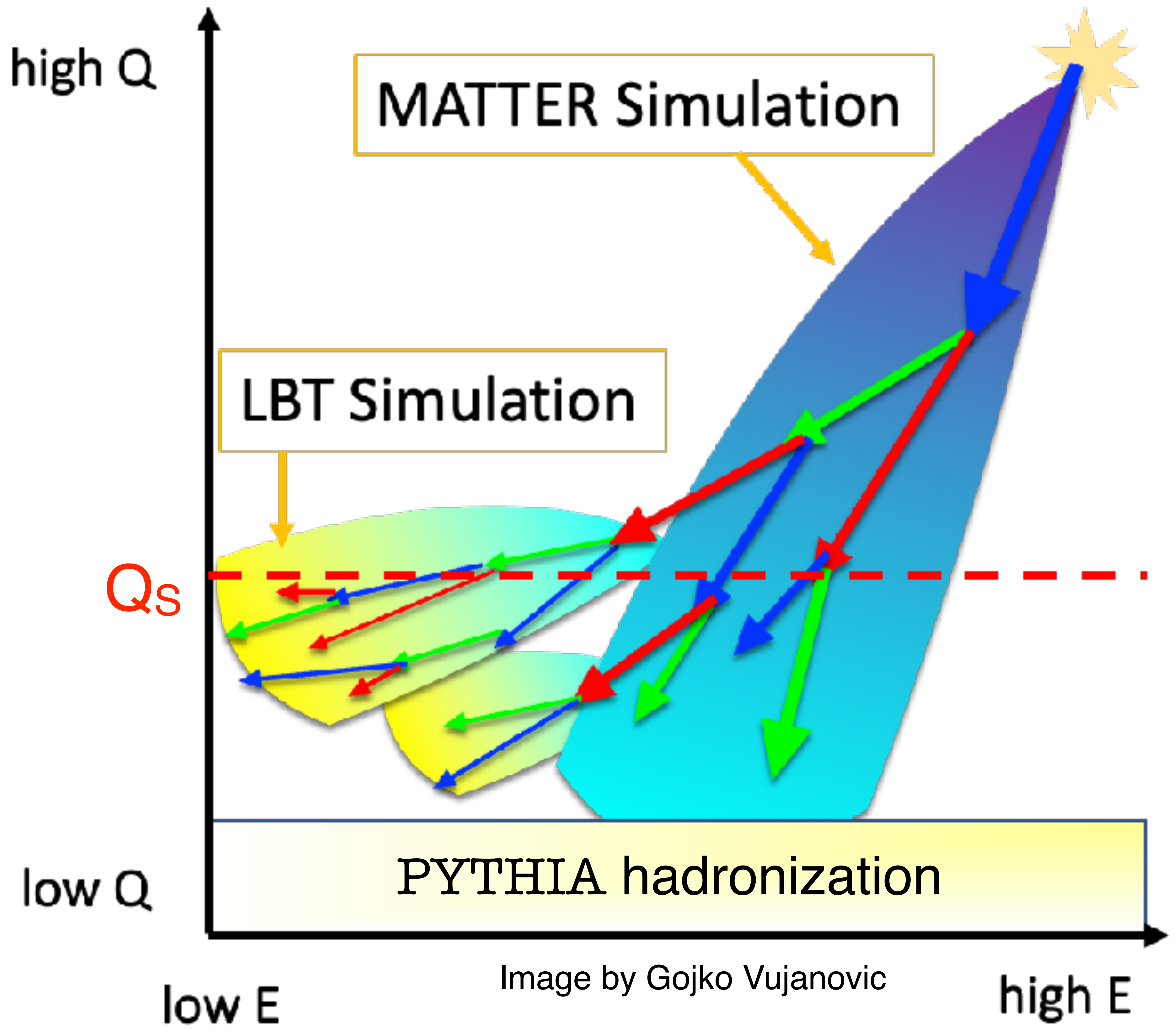
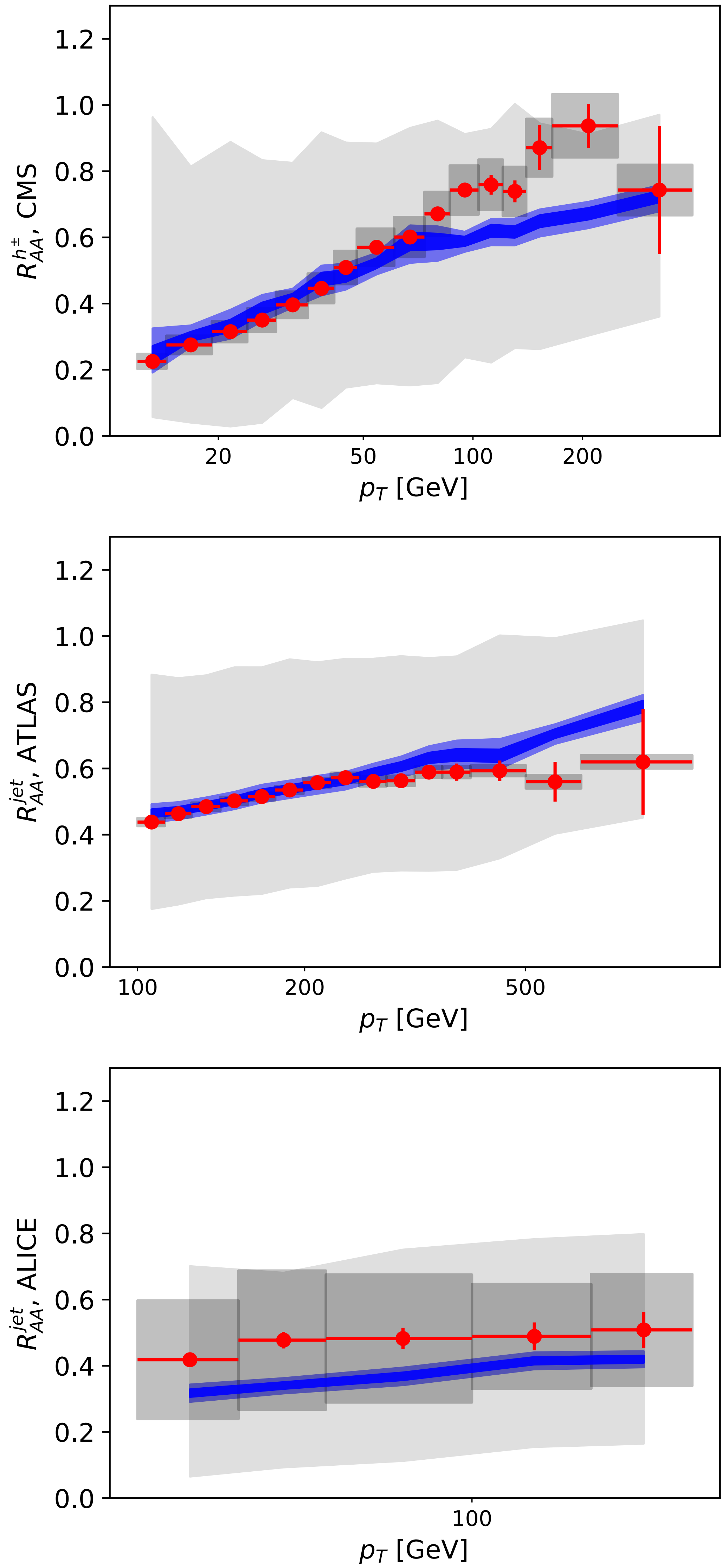


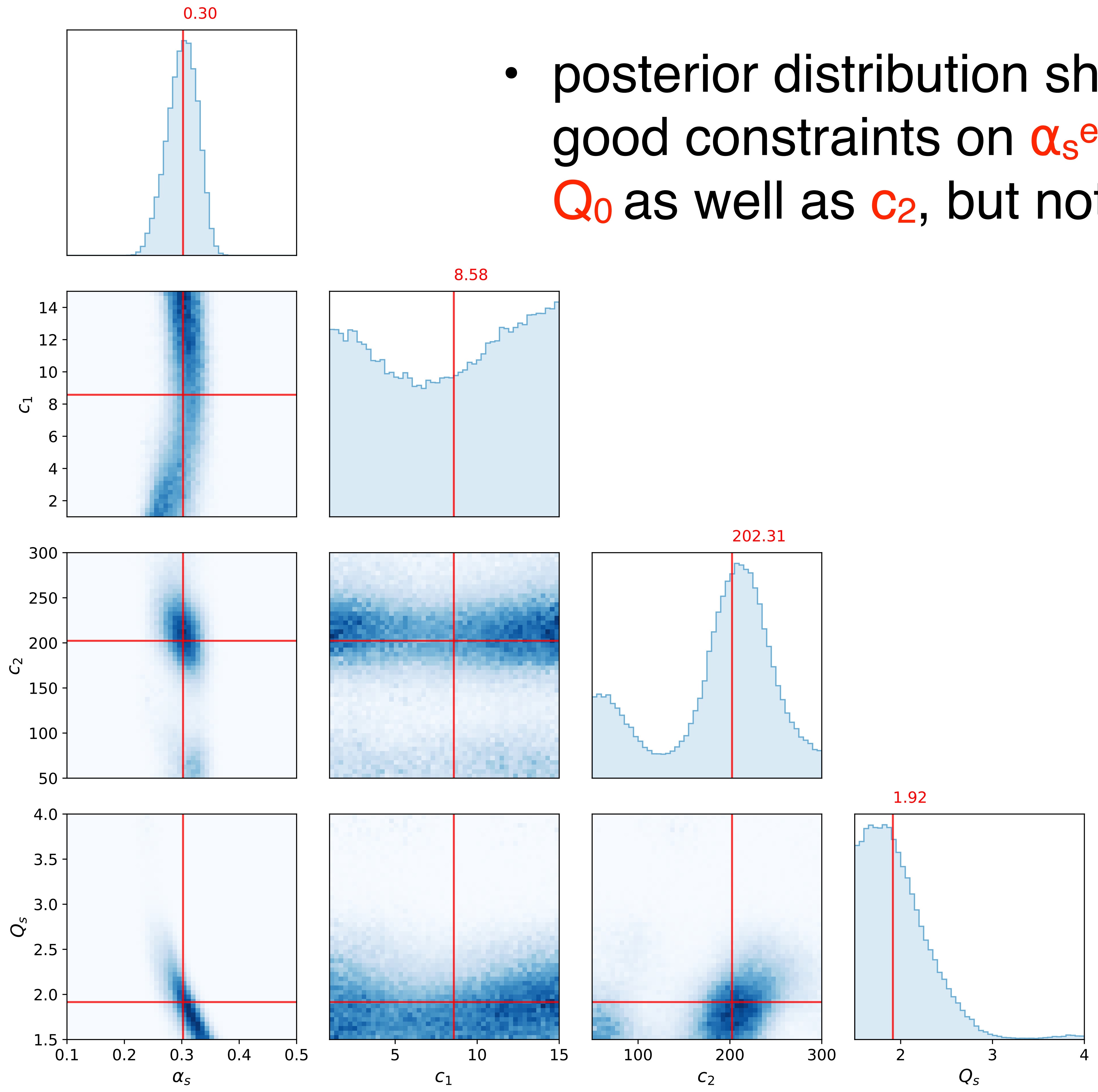
Image by Gojko Vujanovic

calibration on 4 parameters:
- energy-loss coefficient parameters c_1 and c_2
- switching virtuality Q_S
- effective coupling constant α_s^{eff}

Wenkai Fan: e-Print: 2208.00983 [nucl-th]

Matter/LBT **Calibration Results**



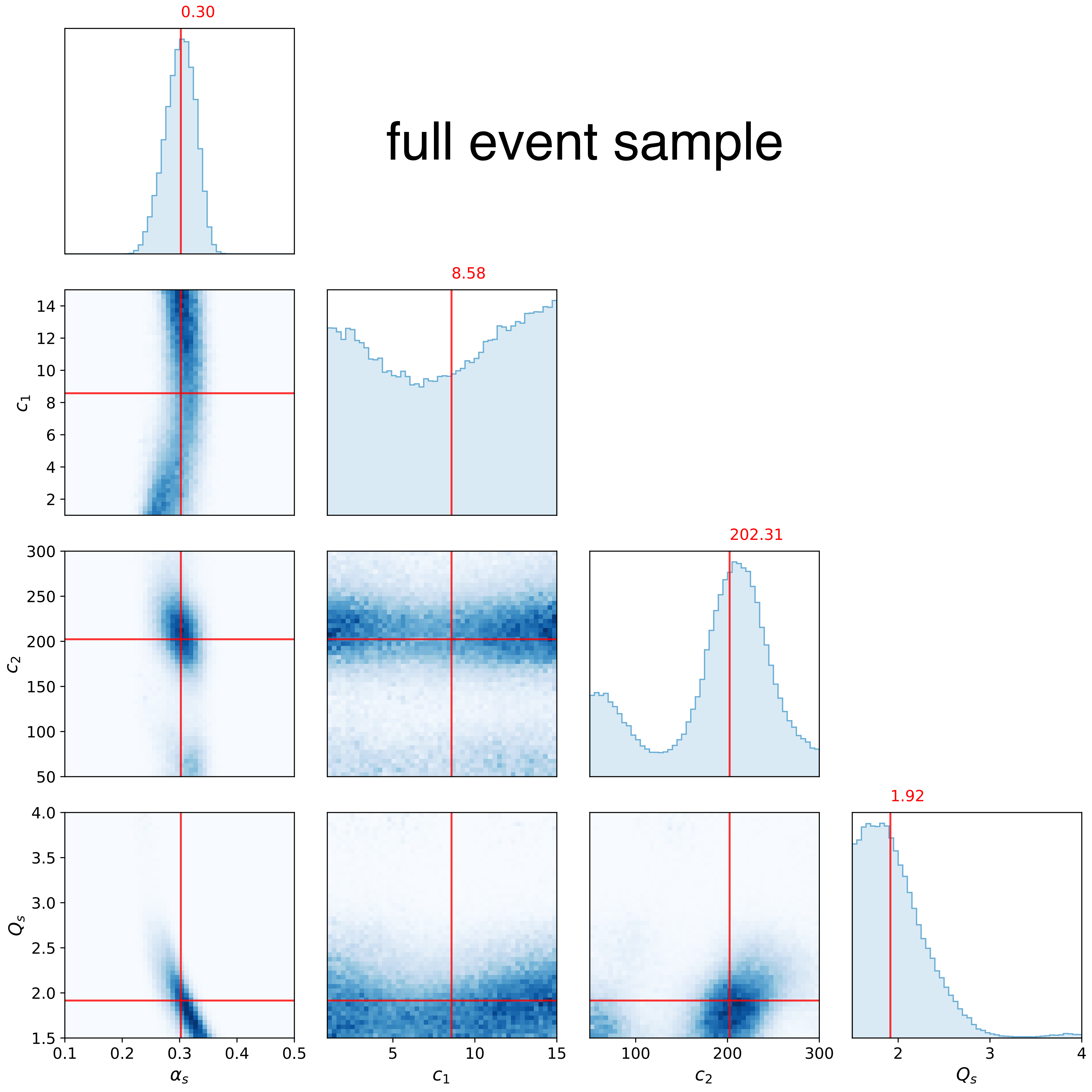


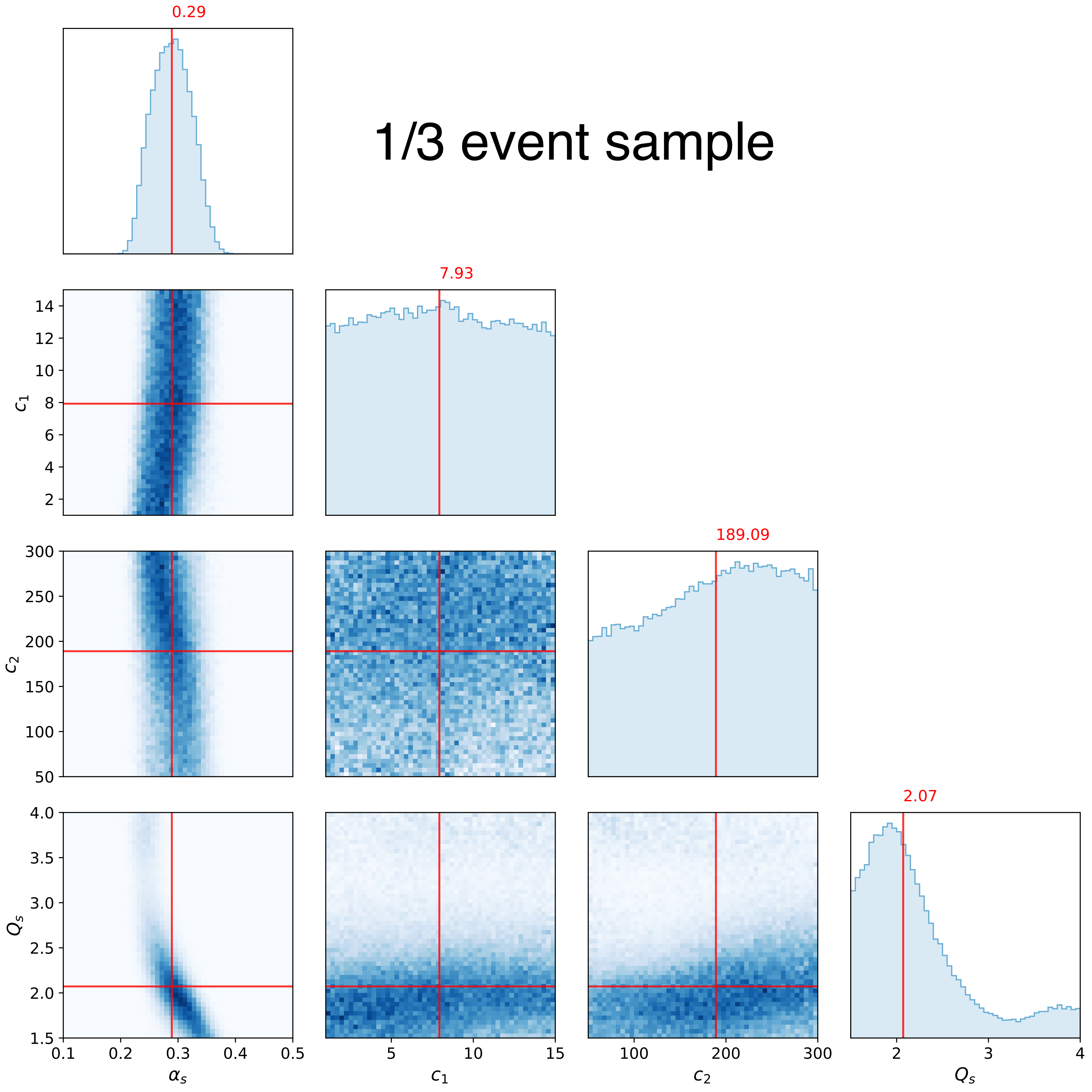
- posterior distribution shows good constraints on α_s^{eff} and Q_0 as well as c_2, but not c_1

- calibration provides good description of charged hadron, D-meson and jet R_{AA} simultaneously

Wenkai Fan: PhD thesis and to be published

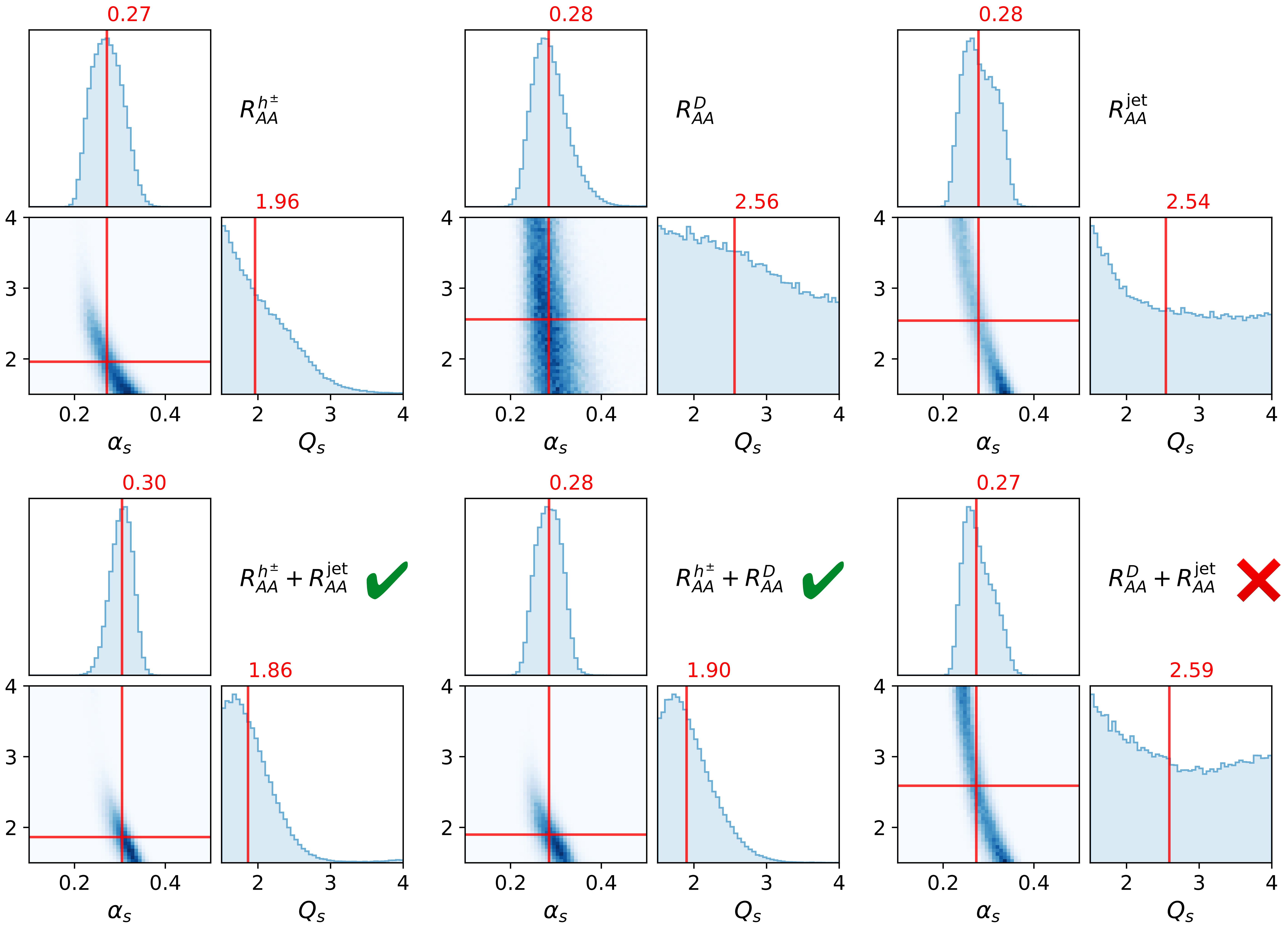
Matter/LBT: number of events in analysis





- increasing the event count provides better constraining power on c_1 and c_2
- additional events may even improve resolution of c_1 and c_2 further…

Matter/LBT **Sensitivity to Observables**



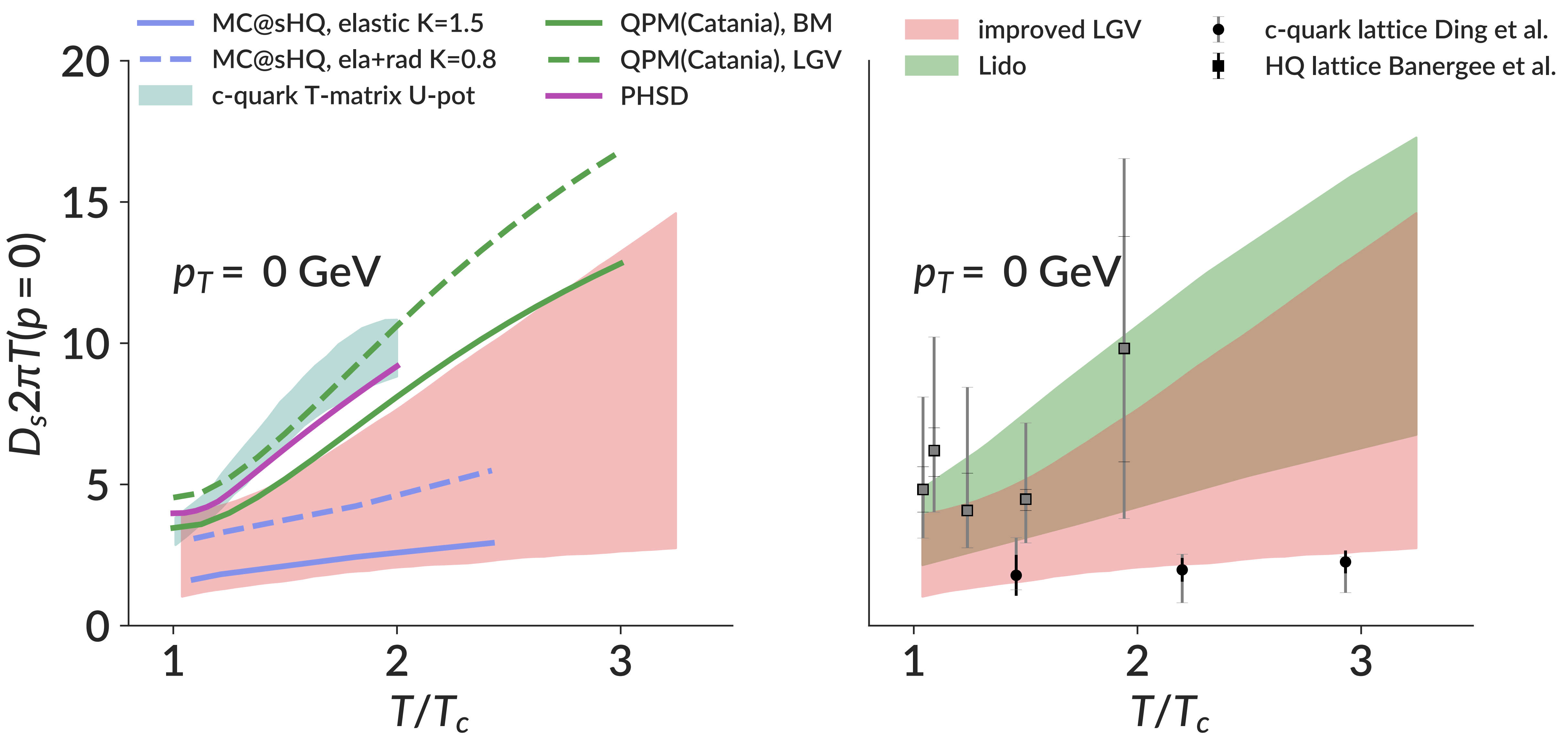
- each of the individual measurements can provide guidance on α_s^{eff} but not Q_0
- charged hadron R_{AA} plus either D-meson R_{AA} or jet R_{AA} is needed to constrain both
- the combination of jet and D-meson R_{AA} is insufficient without the information from charged hadron R_{AA}
- hierarchy of information: why is charged hadron R_{AA} more important than the other two?

Outlook and Future Studies

Summary & Outlook

first data-driven extraction of temperature & momentum dependence of D_s

- D_s significantly smaller than pQCD baseline at temperatures that can be probed at RHIC & LHC ($T<4T_C$)
- extracted D_s compatible with Lattice QCD within (large) uncertainties
- Lido prefers slightly larger D_s values than Langevin



caveats:
- need better data to reduce experimental uncertainties (& uncertainty-band)
- need additional observables to better constrain D_s

outlook:
- add more observables to analysis
- run analysis on different physics- and medium models to test robustness of D_s extraction

The End

HQ Interactions with the QCD Medium

- Djordjevic & Gyulassy
- Buzatti & Gyulassy
- Sharma & Vitev
- Armesto, Cacciari, Dainese, Salgado & Wiedemann
- Nahrgang, Gossiaux & Aichelin
- Cao & Bass
- Majumder, Bhattacharyya, Alam & Das
- Ke, Xu & Bass
- Uphoff, Fochler, Xu & Greiner
- Huang, Kang & Vitev
- Chatterjee, Srivastava & Bass
- …

perturbative QCD

astic scatterin

- Teaney & Moore
- Gossiaux & Aichelin
- Uphoff, Fochler, Xu & Greiner
- Meistrenko, Uphoff, Greiner & Peshier
- Young, Schenke & Gale
- …

radiative processes

- Abir, Jamil, Mustafa & Srivastava
- …

resonance scattering

- v. Hees, Greco & Rapp
- He, Fries & Rapp
- Lang, v. Hees & Bleicher
- …

- Horowitz & Gyulassy
- Chesler, Lekaveckas & Rajagopal
- …

AdS/CFT

visualization adapted from talks by C. Greiner & J. Uphoff

Initial Conditions

QGP medium: Trento

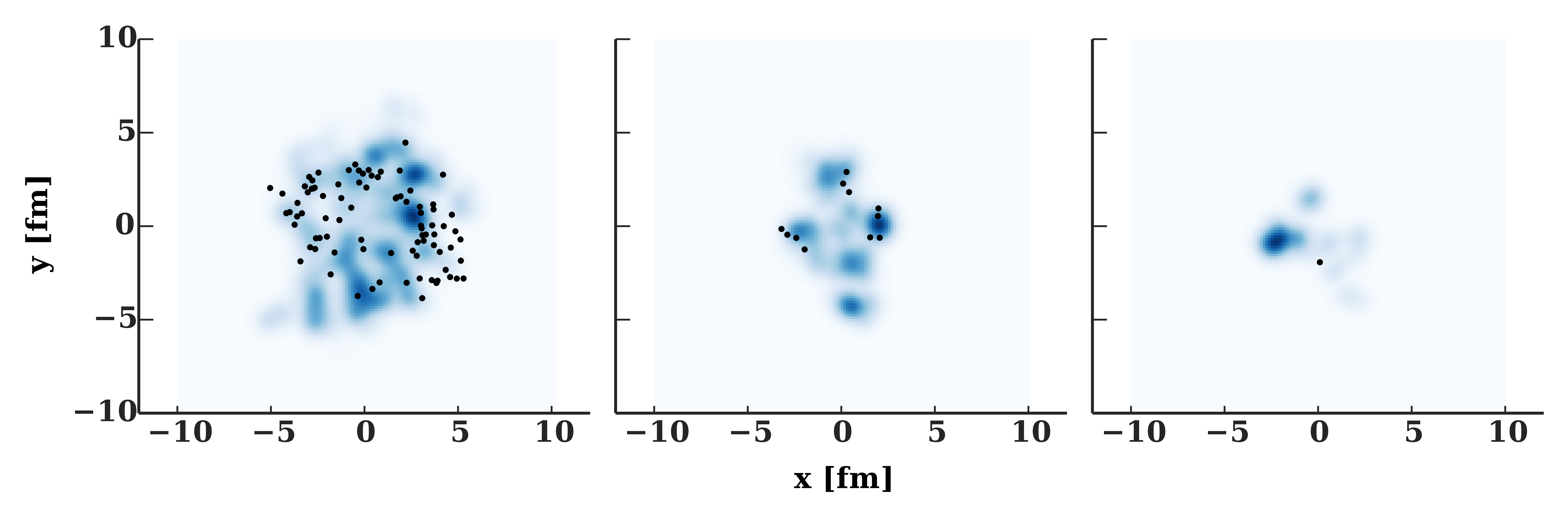
- effective, parametric, description of entropy production prior to thermalization
- entropy deposition *dS/dy* parmeterized in terms of T_A, T_B:

$$dS/dy\,|_{\tau=\tau_0} \propto T_R(p; T_A, T_B) \equiv \left(\frac{T_A^p + T_B^p}{2}\right)^{1/p}$$

- choose p=0: EKRT & IP-Glasma scaling

Heavy Quarks:

- initial spatial production probability: $\propto T_A T_B$, consistent with soft QGP medium
- momentum space: leading order pQCD
  - parton distribution function: CTEQ5
  - nuclear shadowing: EPS09



Calibration of QGP Medium at the LHC

Data:
- ALICE v_2, v_3 & v_4 flow cumulants
- identified particle spectra
- identified particle mean p_T

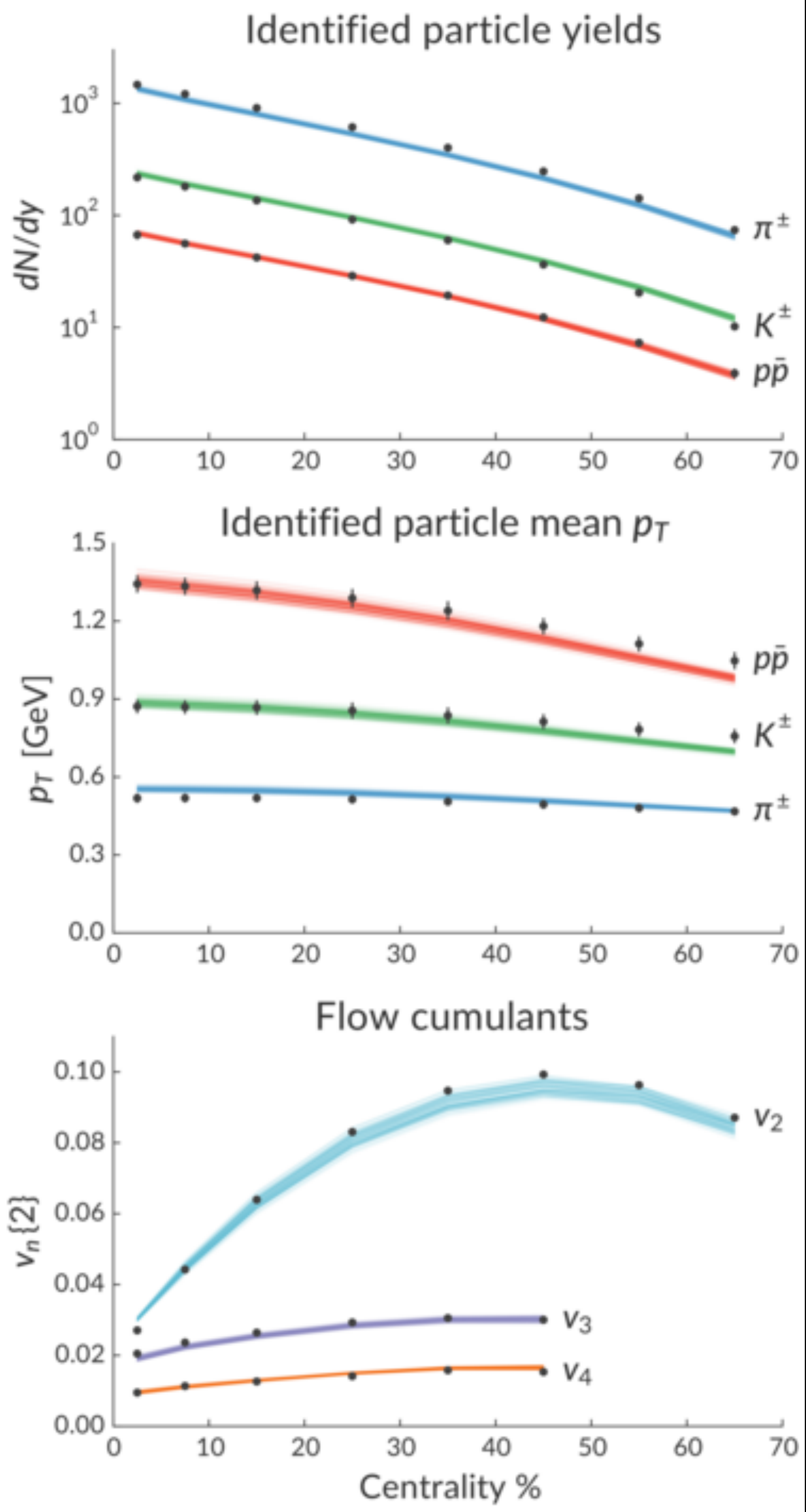
Model:
- Trento & EbE VISHNU

Parameter Space:
- Trento initial condition:
  - p: entropy deposition
  - k: nucleon fluctuation
  - w: Gaussian nucleon width
- specific shear viscosity η/s slope and intercept at T_C
- normalization scale for ζ/s
- hydro to micro switching temperature T_{sw}

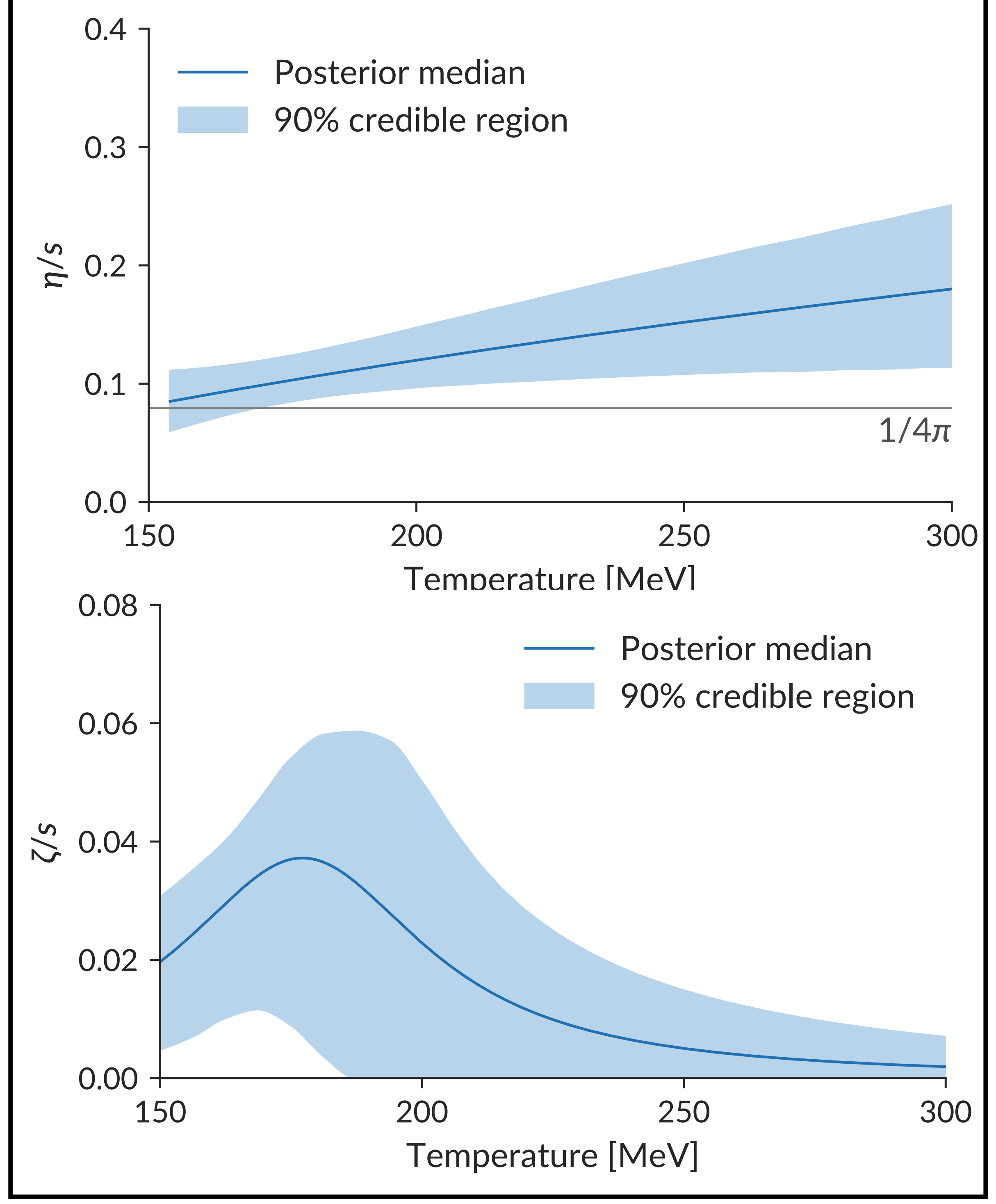
Analysis Design:
- 6 centrality bins
- 300 point Latin Hypercube
- total of 10,000,000 events
- Gaussian Process Emulators for interpolation between LH points

use MCMC for analysis

Posterior: emulator predictions for highest likelihood parameter values



Key Results:
- excellent agreement with data, simultaneous description of v_2, v_3 and v_4 data
- initial condition favors scaling properties of EKRT, IP-Glasma
- non-zero bulk viscosity
- temperature dependence of η/s requires data at several beam energies to pin down



Recombination+Fragmentation Model

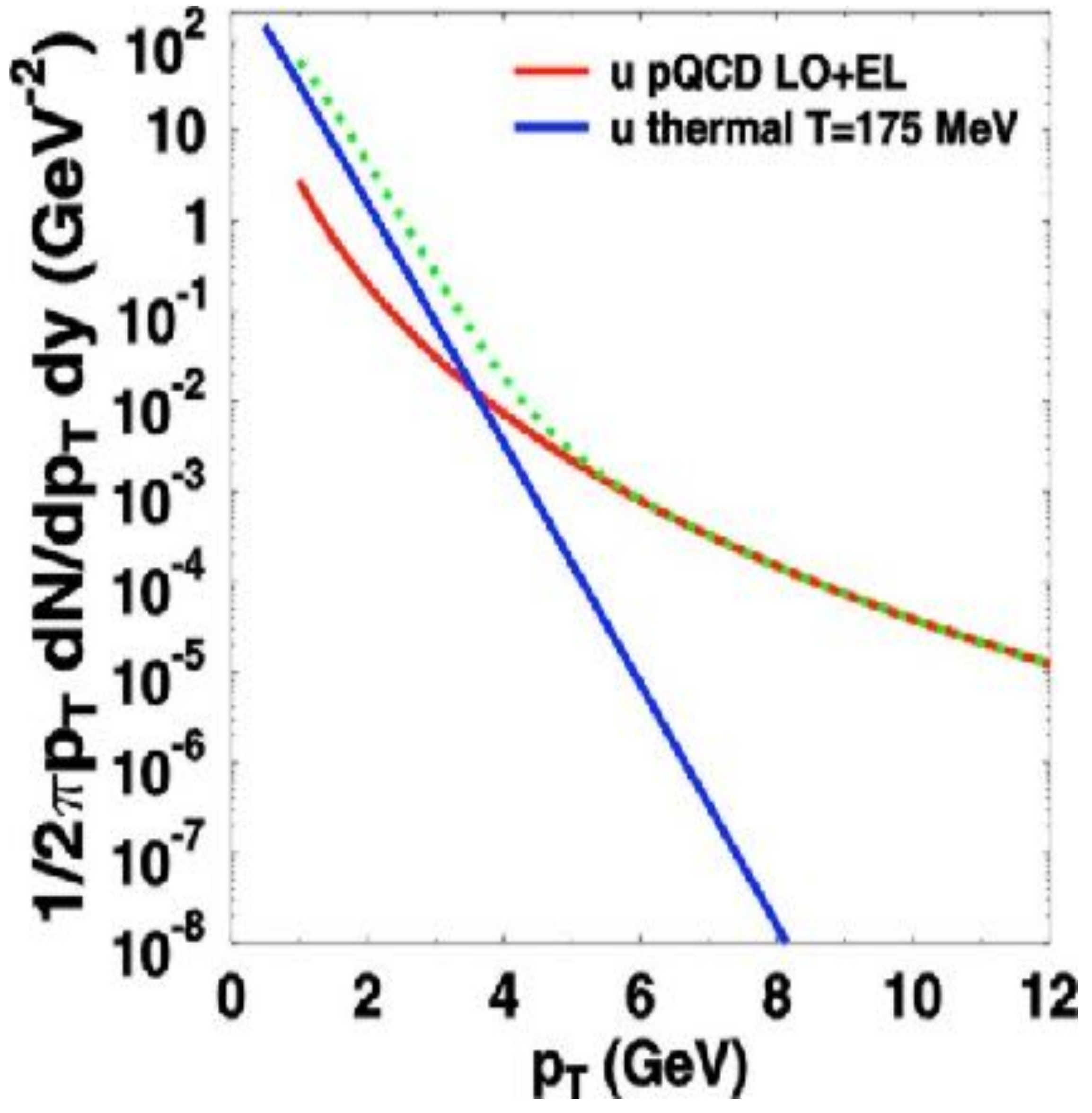
basic assumptions:

- at low p_t, the parton spectrum is thermal and HQs recombine with light quarks into hadrons locally “at an instant”:

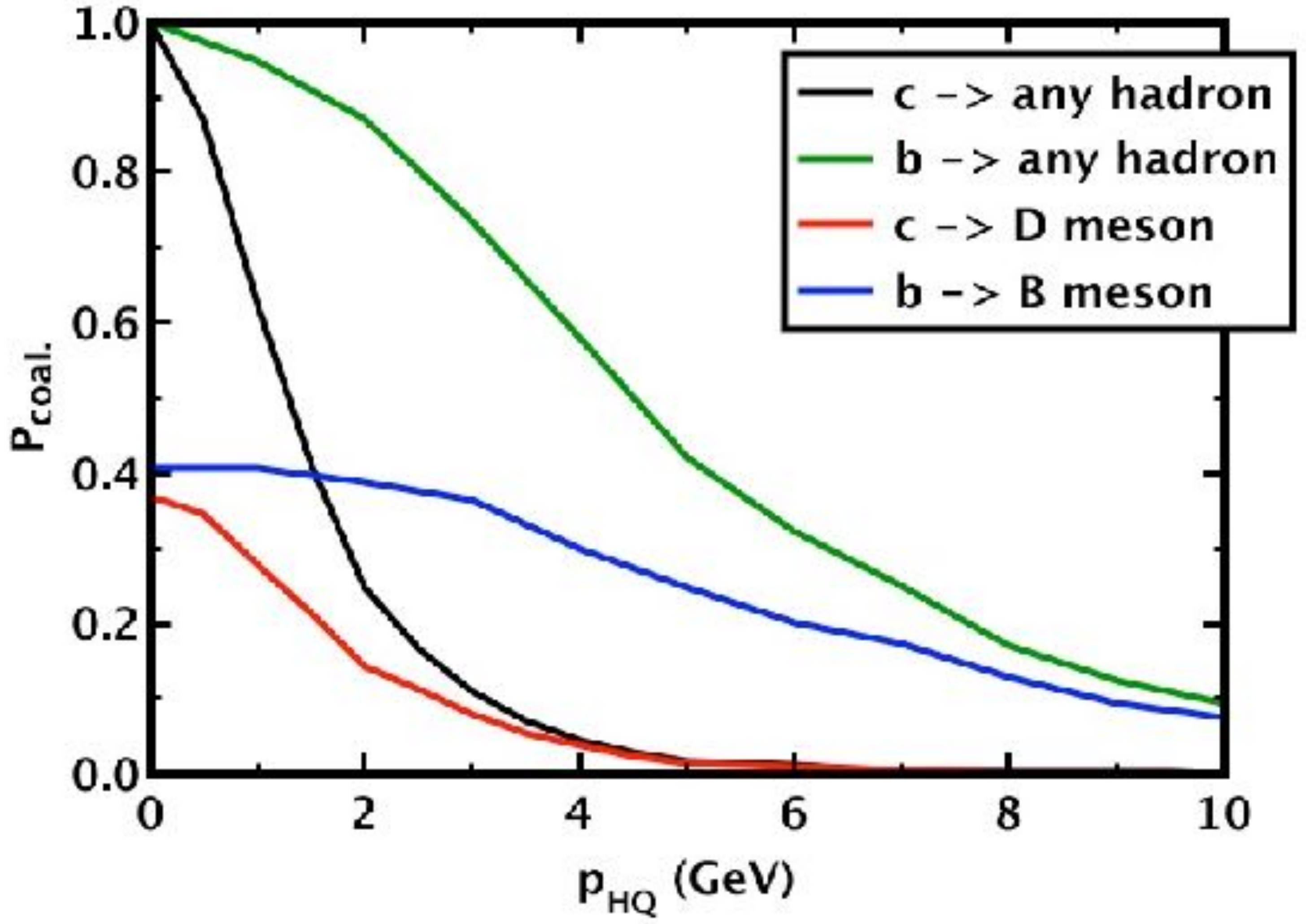
$$\frac{dN_M}{d^3P} = C_M \frac{V}{(2\pi)^3}\int \frac{d^3q}{(2\pi)^3} w\left(\tfrac{1}{2}P-q\right) w\left(\tfrac{1}{2}P+q\right)\left|\hat{\varphi}_M(q)\right|^2$$

- at high p_t, the parton spectrum is given by a pQCD power law, HQs suffer radiative energy loss and hadrons are formed via fragmentation of HQs:

$$E\frac{dN_h}{d^3P} = \int d\Sigma \frac{P\cdot u}{(2\pi)^3}\int_0^1 \frac{dz}{z^2}\sum_\alpha w_\alpha(R,\tfrac{1}{z}P) D_{\alpha\to h}(z)$$



- shape of spectrum determines if reco or fragmentation is more effective:
  - for thermal distribution recombination yield dominates fragmentation yield
  - vice versa for pQCD power law distribution



Hadronic Rescattering for HQs

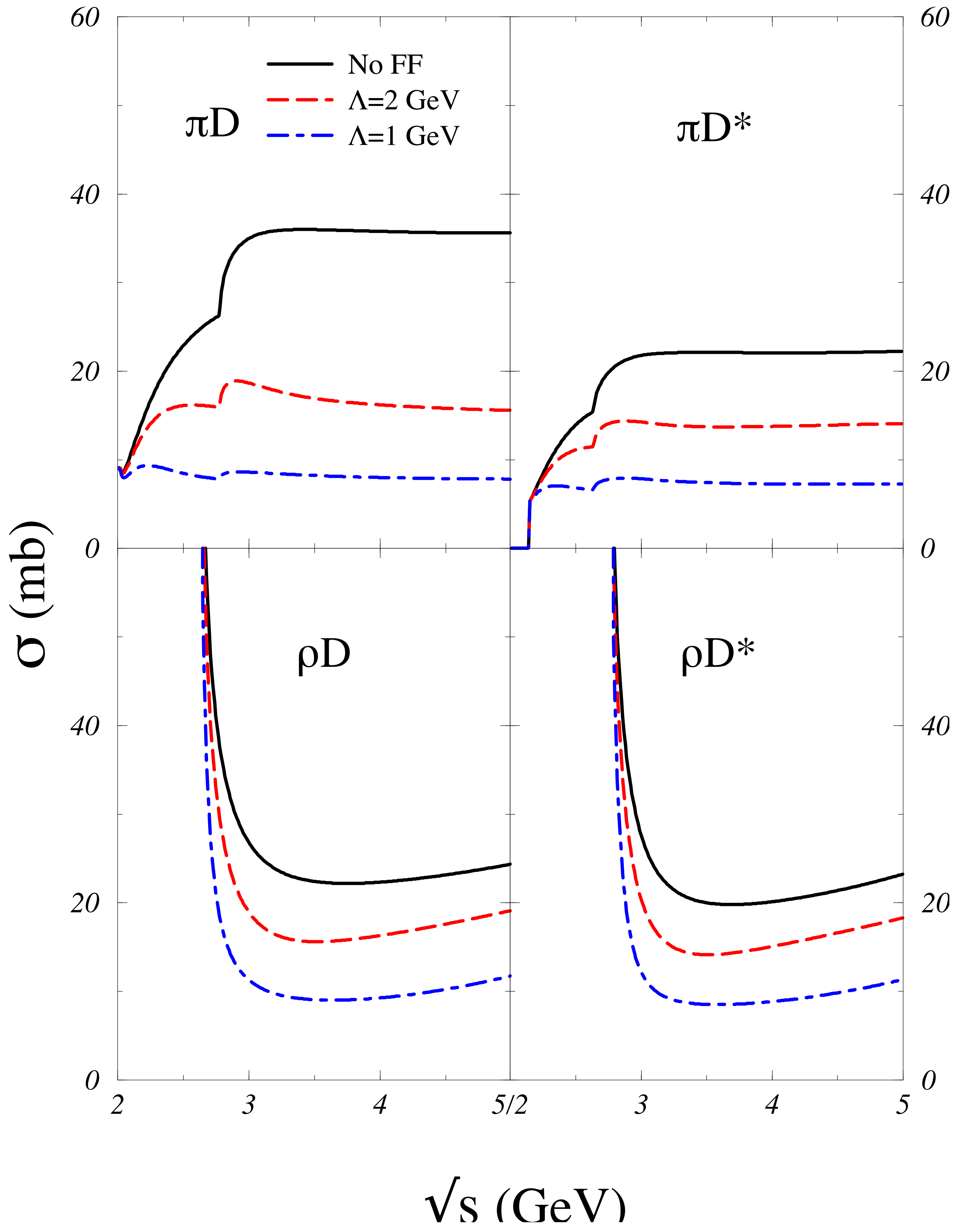
soft hadrons from QGP

heavy mesons from heavy quarks

UrQMD

scattering cross sections for heavy mesons:

- Ziwei Lin, T.G. Di & C.M. Ko: Nucl. Phys. **A689** (2001), 965
- consider scattering of D and D* with π and ρ mesons
- Λ: cutoff parameter in hadron form factors



future plans:

- resonant scattering via D* formation (see e.g. He, Fries & Rapp: PLB701 (2011), 445

Scanning a high-dimensional parameter space

Latin hypercube:

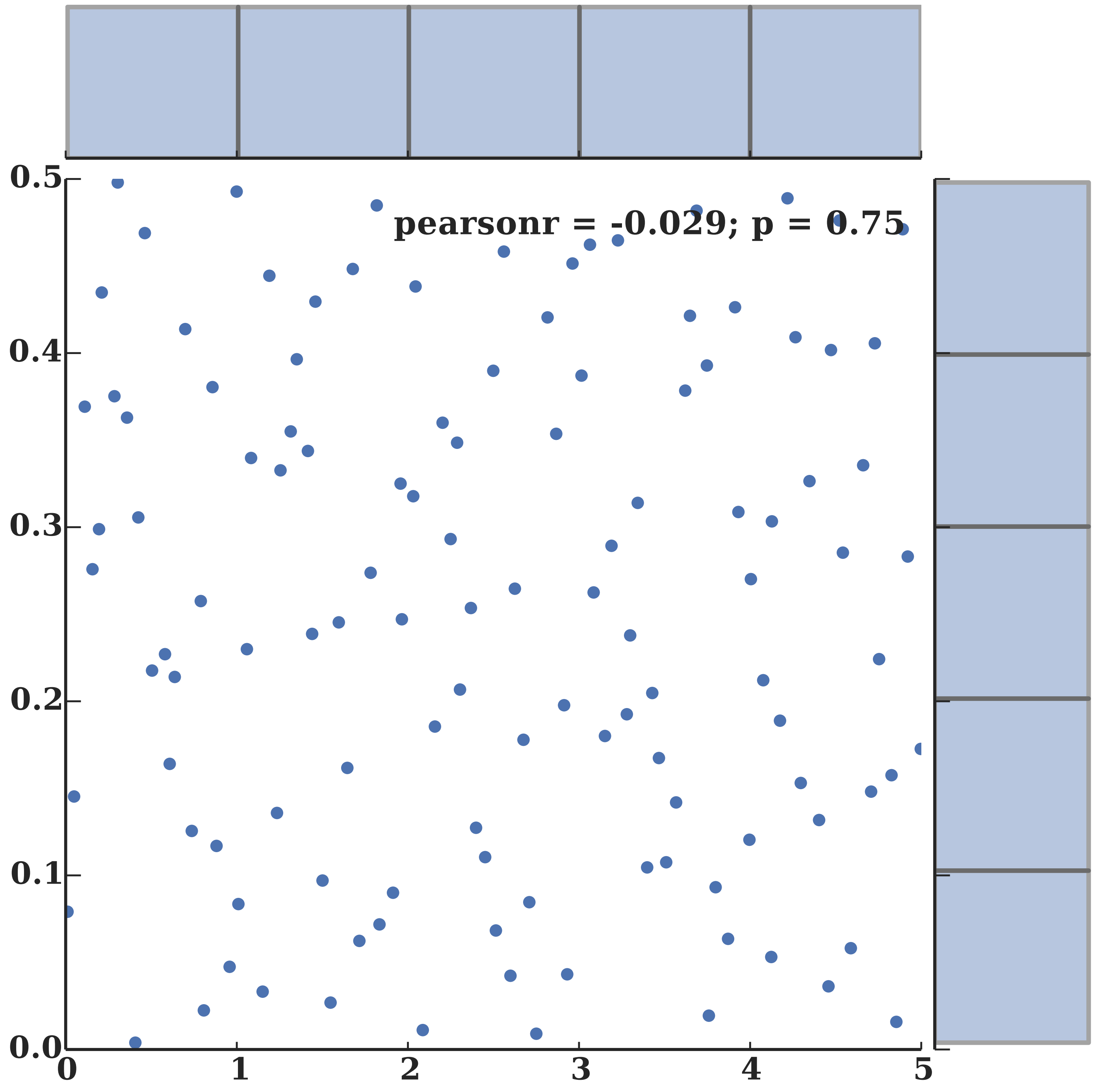
- algorithm for generating semi-randomized, space-filling points
- avoids large gaps and tight clusters
- all parameters varied simultaneously
- needs only *m≥10n* points, with n: number of model parameters

this analysis:

- n=3-4 model parameters
- 2 beam energies, 2 centralities
- Latin hypercube with m=120 points
- $\mathcal{O}(10^4)$ events per point, for a total of approx. 1,200,000 events
- use Gaussian Process Emulators to interpolate between points

Example:

- Latin-hypercube projection for the β_T - σ_T parameter subspace



- CPU expenditure for 1,200,000 events was 240,000 hours on the Open Science Grid

Gaussian Process Emulator

Exploring the high dimensional calibration parameter space at high resolution would require running the physics model at so many points in parameter space that it becomes computationally unfeasible: use **Gaussian Process Emulators** to interpolate between physics model calculations.

Gaussian Process Emulator

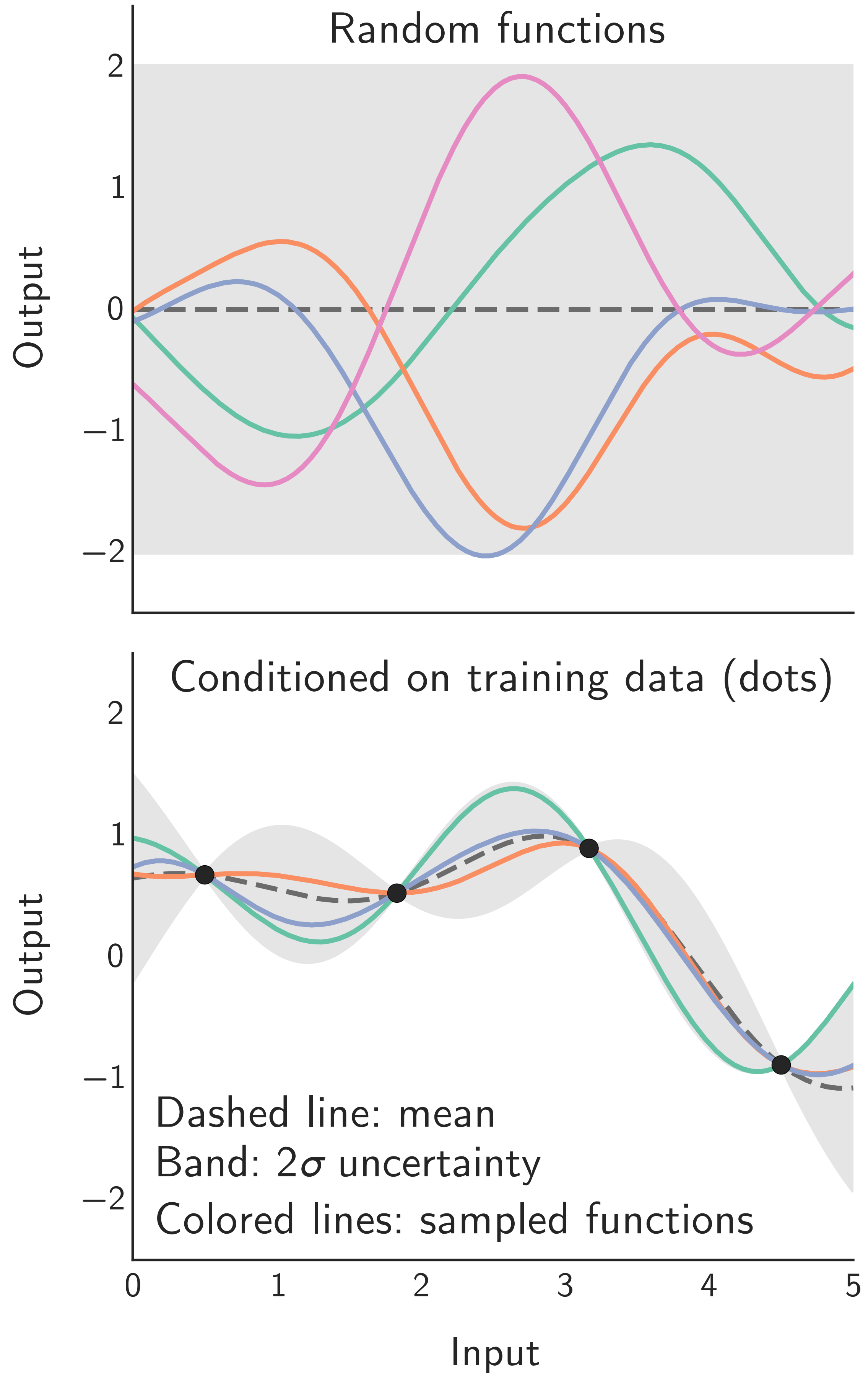
Exploring the high dimensional calibration parameter space at high resolution would require running the physics model at so many points in parameter space that it becomes computationally unfeasible: use **Gaussian Process Emulators** to interpolate between physics model calculations.

Gaussian process:

- stochastic function:
  maps inputs to normally distributed outputs
- specified by mean and covariance functions

GP as a model emulator:

- non-parametric interpolation of physics model
- predicts probability distributions for model output at any given input value
  - narrow near training points, wide in gaps
- needs to be conditioned on training data (Latin hypercube points)
- fast *surrogate* to actual model



Calibration

Vector of input parameters: $\mathbf{x}=[p,k,w,(\eta/s)_{min},(\eta/s)_{slope},(\zeta/s)_{norm},T_{sw}]$

- assume true parameters $\mathbf{x}_\star$ exist ⇒ find probability distribution for $\mathbf{x}_\star$

Bayes' Theorem: $P(\mathbf{x}_\star | X,Y,\mathbf{y}_{exp}) \propto P(X,Y,\mathbf{y}_{exp} | \mathbf{x}_\star)P(\mathbf{x}_\star)$

- X: training data design points
- Y: model output on X
- $P(\mathbf{x}_\star)$ = prior
  ⇒ initial knowledge of $\mathbf{x}_\star$
- $P(X,Y,\mathbf{y}_{exp} | \mathbf{x}_\star)$ = likelihood
  ⇒ probability of observing $(X,Y,\mathbf{y}_{exp})$ given proposed $\mathbf{x}_\star$
- $P(\mathbf{x}_\star | X,Y,\mathbf{y}_{exp})$ = posterior
  ⇒ probability of $\mathbf{x}_\star$ given observations $(X,Y,\mathbf{y}_{exp})$

Calibration

Vector of input parameters: $\mathbf{x}$=[p,k,w,$(\eta/s)_{min}$,$(\eta/s)_{slope}$,$(\zeta/s)_{norm}$,T_{sw}]

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- $P(\mathbf{x}_\star | X,Y,\mathbf{y}_{exp})$ = posterior
  ⇒ probability of $\mathbf{x}_\star$ given observations $(X,Y,\mathbf{y}_{exp})$

Markov-Chain Monte-Carlo:

- random walk through parameter space weighted by posterior
- large number of samples ⇒ chain equilibrates to posterior distribution

- flat prior within design range, zero outside
- likelihood: $\log[P(X,Y,\mathbf{y}_{exp} | \mathbf{x}_\star)] \sim -(\mathbf{y}(\mathbf{x}_\star) - \mathbf{y}_{exp})^2/(2\sigma^2)$
  - σ=0.1 on principal components (includes correlations)
- posterior ~ likelihood within design range, zero outside