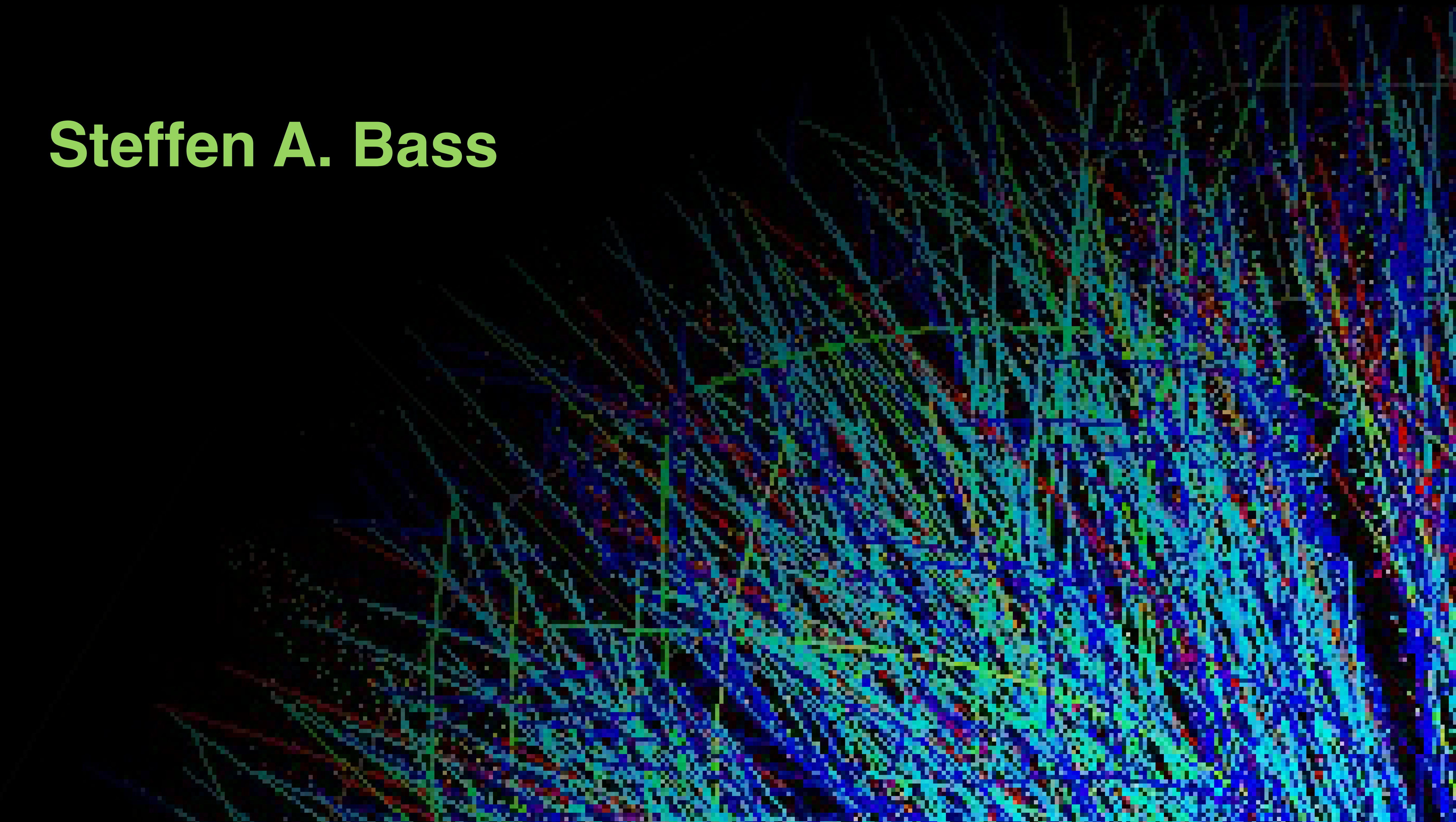
Duke UNIVERSITY

A data-driven approach to quantifying the shear viscosity of nature’s most ideal liquid

Steffen A. Bass



http://www.facebook.com/DukeQCD

@Steffen_Bass

Probing the QGP in Relativistic Heavy-Ion Collisions

Probing the QGP in Relativistic Heavy-Ion Collisions

1x 10^{-23} s

10 x 10^{-23} s

30 x 10^{-23} s

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nuclei at 99.99% speed of light

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hadronic final state interactions

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non-equilibrium early time dynamics → viscous fluid dynamics → hadronic transport

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non-equilibrium early time dynamics → viscous fluid dynamics → hadronic transport

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

- time-scale of the collision process: 10^{-24} seconds! [too short to resolve]
- characteristic length scale: 10^{-15} meters! [too small to resolve]
- confinement: quarks & gluons form bound states, experiments don't observe them directly

‣ **computational models are need to connect the experiments to QGP properties!**

Properties of QCD: Transport Coefficients

shear and bulk viscosity are defined as the coefficients in the expansion of the stress tensor in terms of the velocity fields:

$$T_{ik} = \varepsilon u_i u_k + P\left(\delta_{ik} + u_i u_k\right) - \eta\left(\nabla_i u_k + \nabla_k u_i - \frac{2}{3}\delta_{ik}\nabla\cdot u\right) + \varsigma\,\delta_{ik}\nabla\cdot u$$

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η/s from Lattice QCD:

The confines of the Euklidian Formulation:

- extracting η/s formally requires taking the zero momentum limit in an infinite spatial volume, which is numerically not possible…

- preliminary estimates:

T	1.58 T_C	2.32 T_C
η/s	0.2-0.25	0.25-0.5

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The determination of the QCD transport coefficients is one of the key goals of the global relativistic heavy-ion effort!

QGP Shear-Viscosity: 2006 vs. today

PRL **97,** 152303 (2006) PHYSICAL REVIEW LETTERS week ending 13 OCTOBER 2006

Strongly Interacting Low-Viscosity Matter Created in Relativistic Nuclear Collisions

Laszlo P. Csernai,[1,2] Joseph I. Kapusta,[3] and Larry D. McLerran[4]

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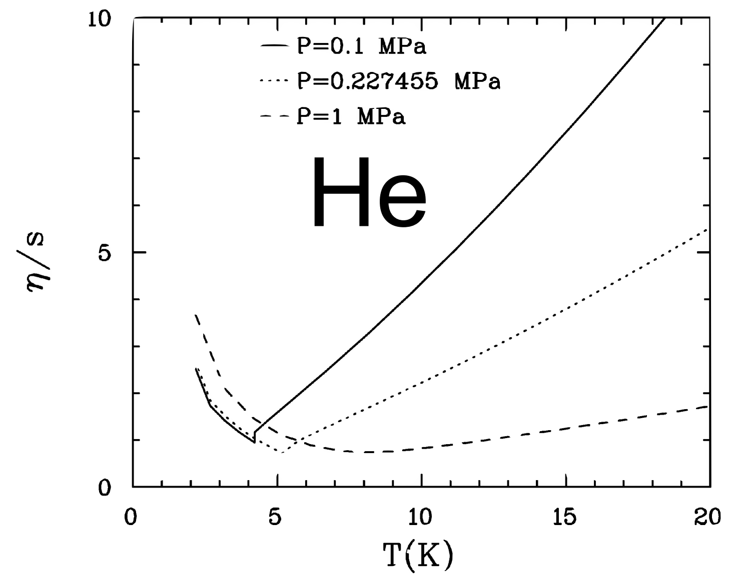
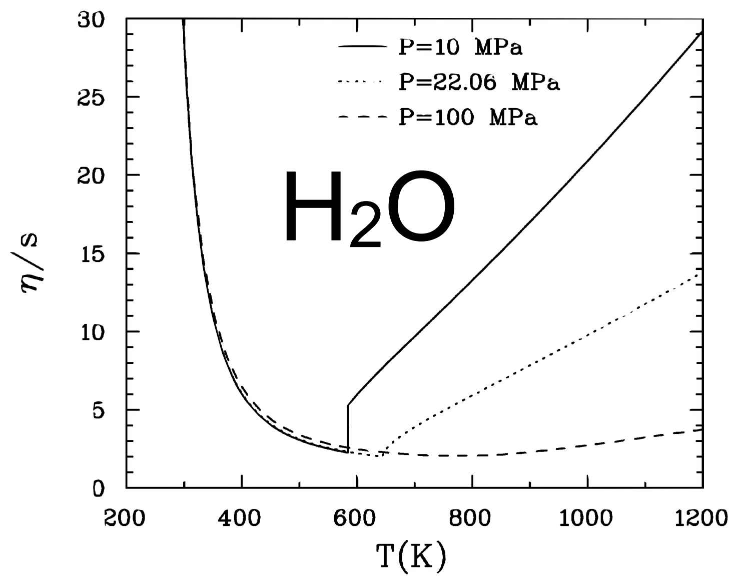
[2]*MTA-KFKI, Research Institute of Particle and Nuclear Physics, 1525 Budapest 114, P. O. Box 49, Hungary*
[3]*School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA*
[4]*Nuclear Theory Group and Riken Brookhaven Center, Brookhaven National Laboratory, Bldg. 510A, Upton, New York 11973, USA*

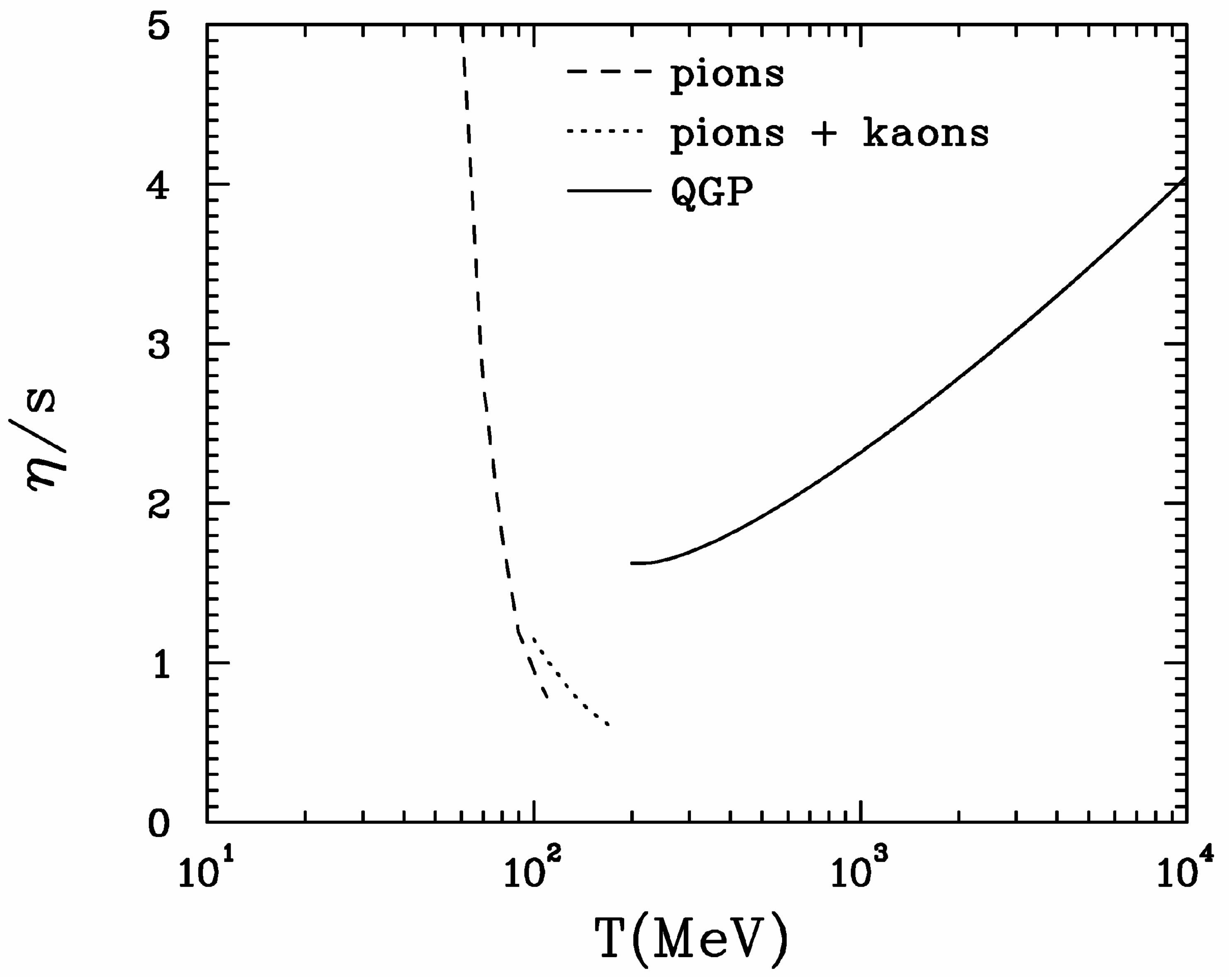
(Received 12 April 2006; published 12 October 2006)

Substantial collective flow is observed in collisions between large nuclei at BNL RHIC (Relativistic Heavy Ion Collider) as evidenced by single-particle transverse momentum distributions and by azimuthal correlations among the produced particles. The data are well reproduced by perfect fluid dynamics. A calculation of the dimensionless ratio of shear viscosity η to entropy density s by Kovtun, Son, and Starinets within anti-de Sitter space/conformal field theory yields $\eta/s = \hbar/4\pi k_B$, which has been conjectured to be a lower bound for any physical system. Motivated by these results, we show that the transition from hadrons to quarks and gluons has behavior similar to helium, nitrogen, and water at and near their phase transitions in the ratio η/s. We suggest that experimental measurements can pinpoint the location of this transition or rapid crossover in QCD.

DOI: 10.1103/PhysRevLett.97.152303 PACS numbers: 12.38.Mh, 24.10.Nz, 25.75.Nq, 51.20.+d







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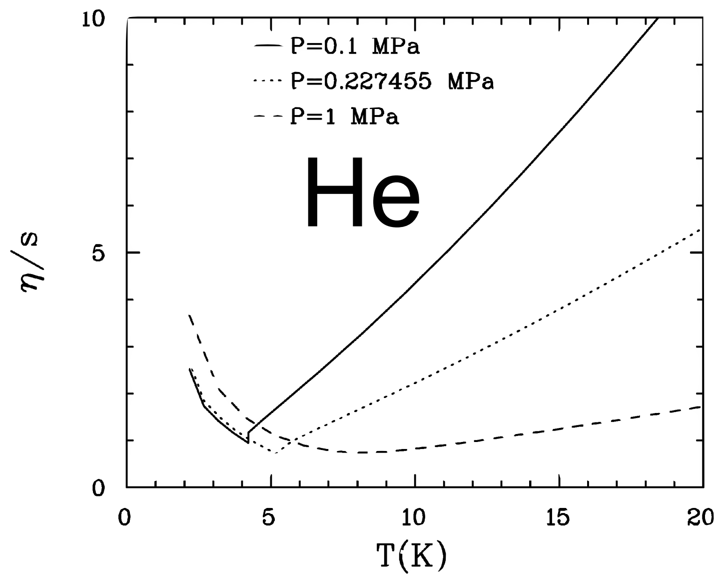
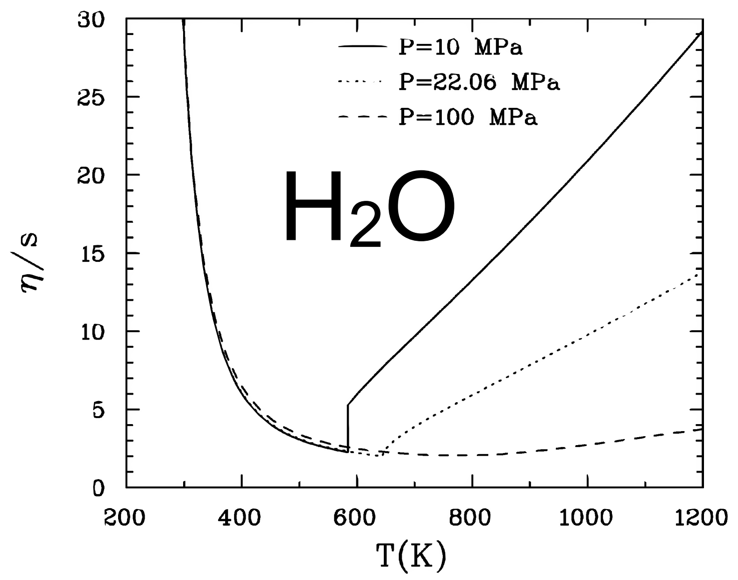
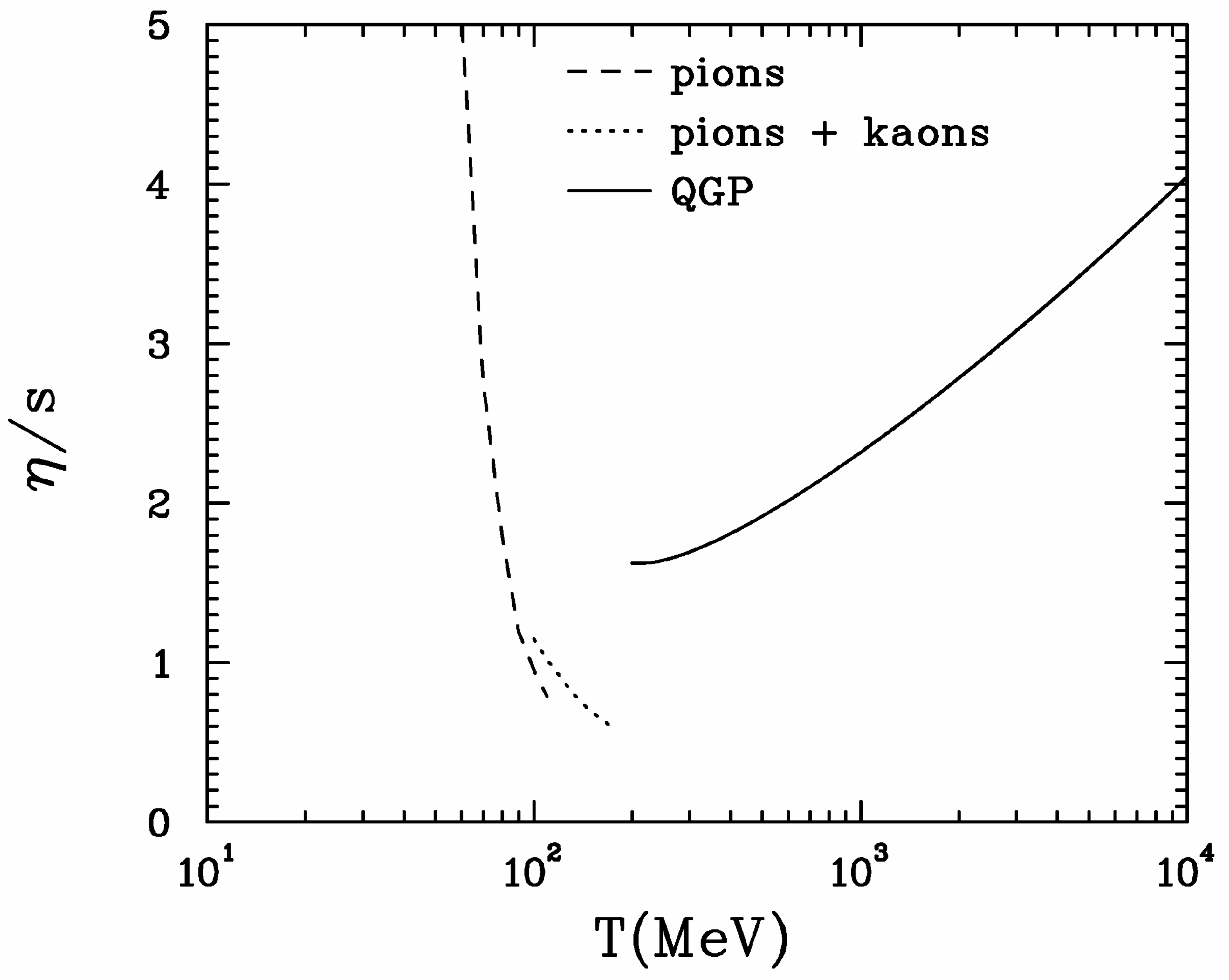
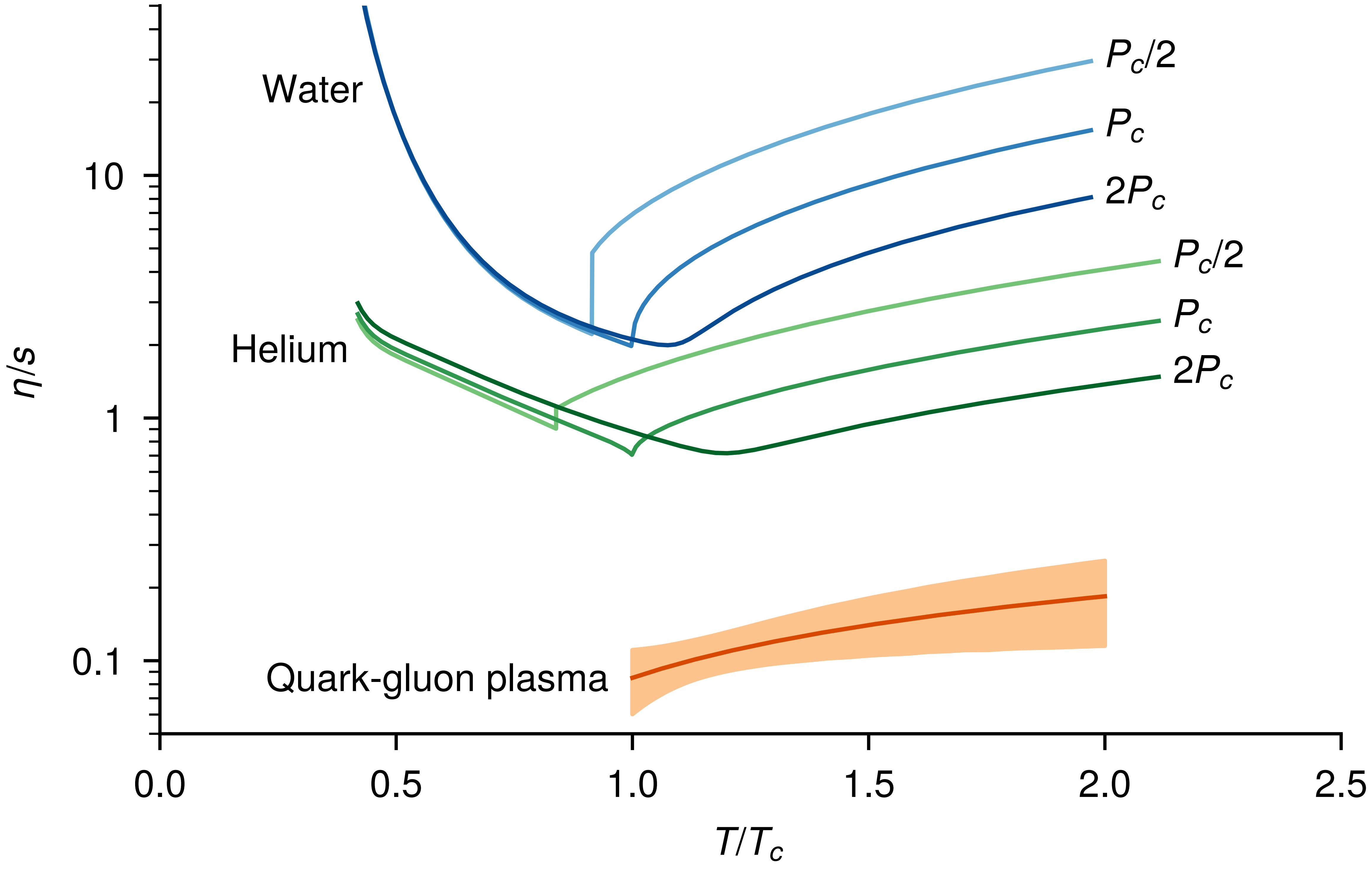






Jonah E. Bernhard, J. Scott Moreland & Steffen A. Bass,
Nature Physics **15** (2019) 11, 1113-1117



- more than a decade of hard work by multiple research groups
- cooperation between theory & experiment
- significant investment by the funding agencies

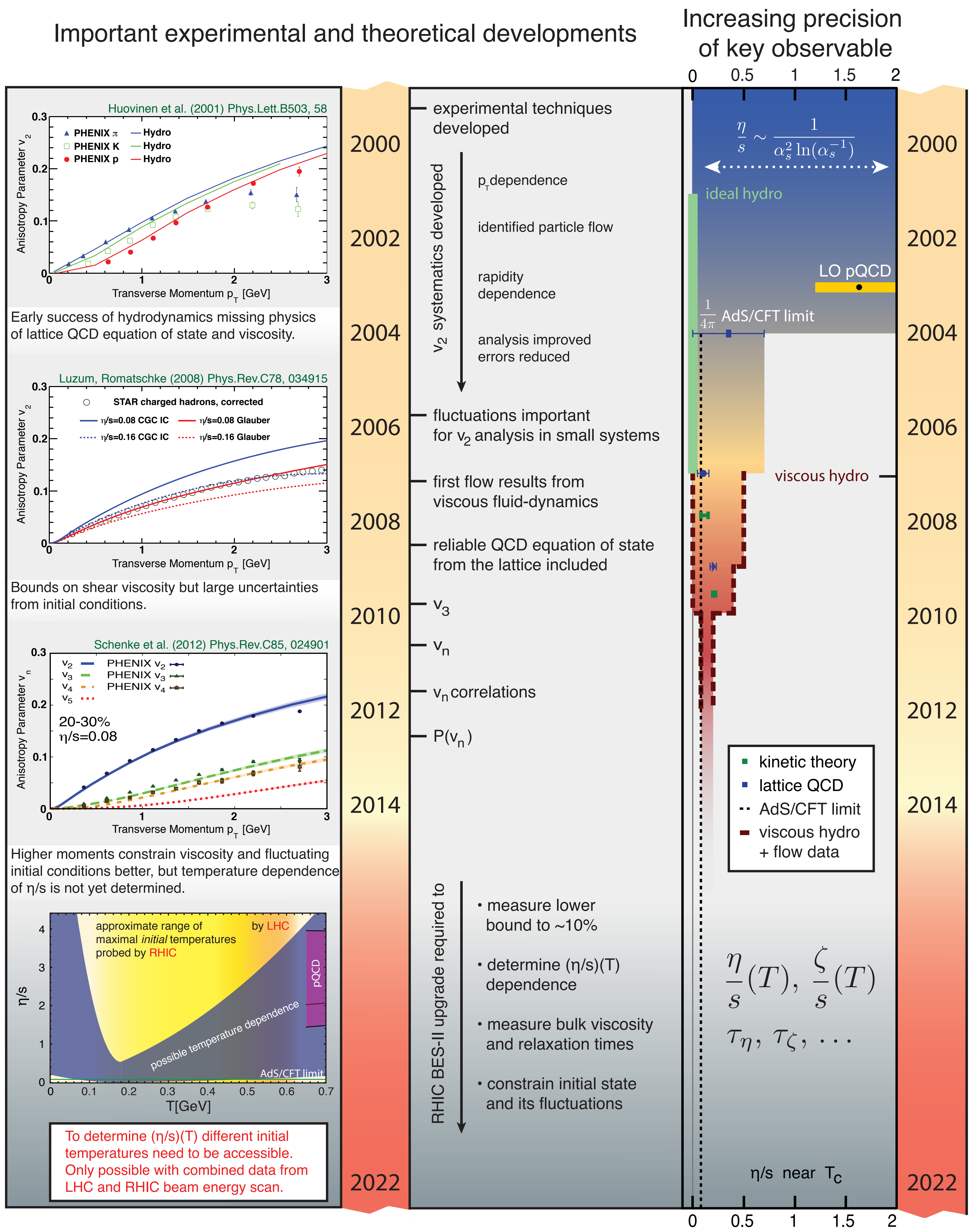
An Effort by the Heavy-Ion Community

2012 response of the US relativistic heavy-ion community to the request for comments by the NSAC subcommittee, that was tasked to recommend *optimizations* to the US Nuclear Science Program over the following five years.

2012 RHIC community White Paper identified key developments and laid out milestones for the determination of QGP properties:

Goal: by 2022 determine the temperature dependence of η/s and ζ/s as well as relaxation times and other QGP transport coefficients of interest (e.g. q-hat and e-hat)

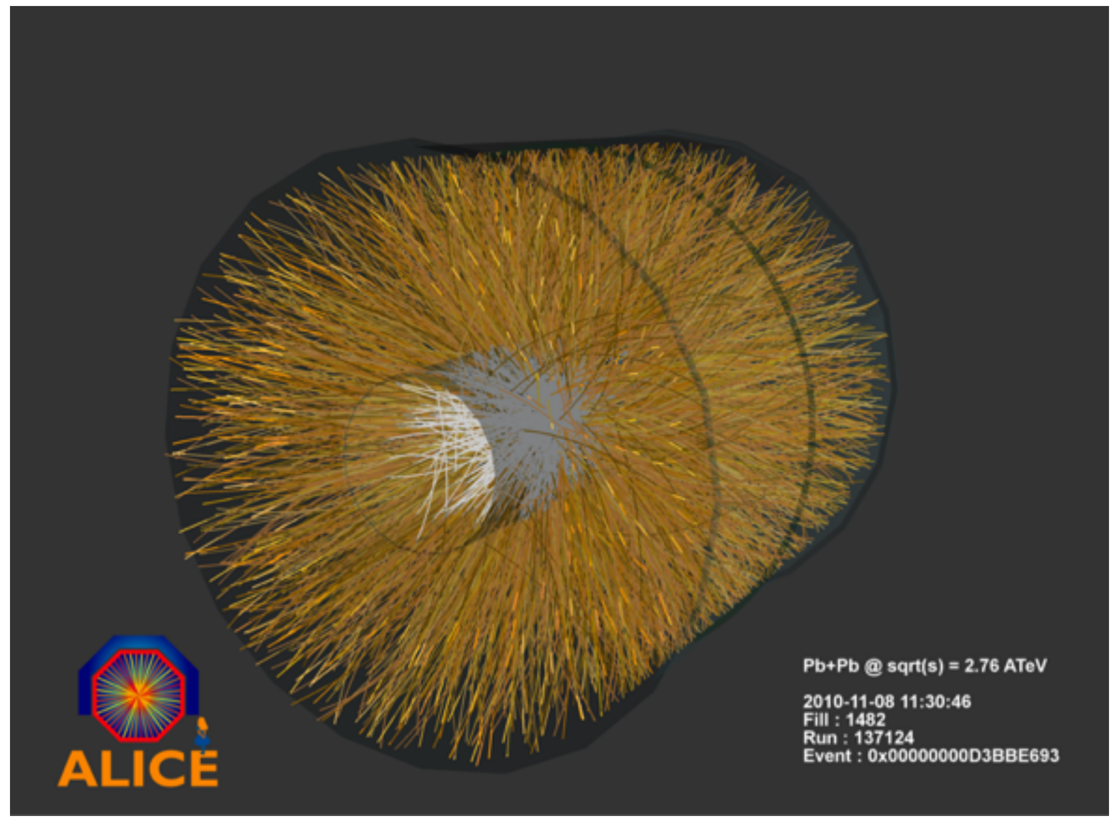
We are well on our way deliver on these goals!

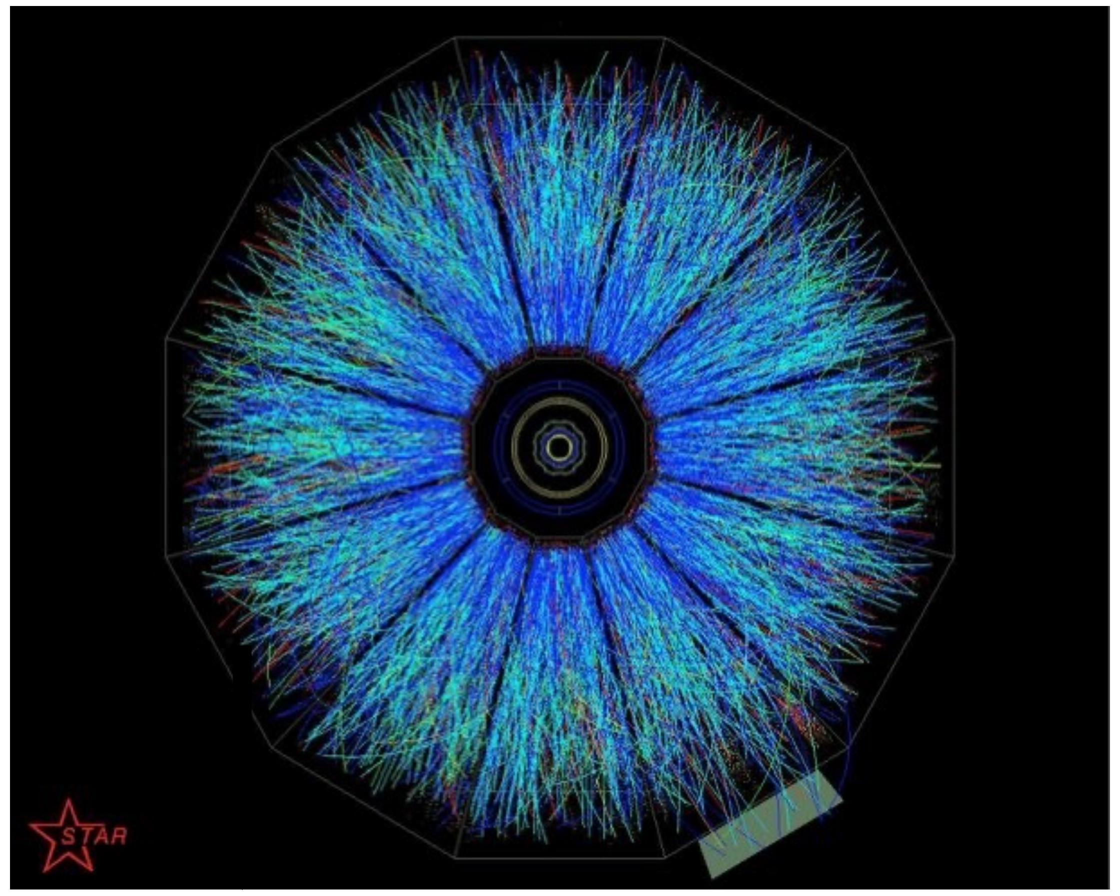


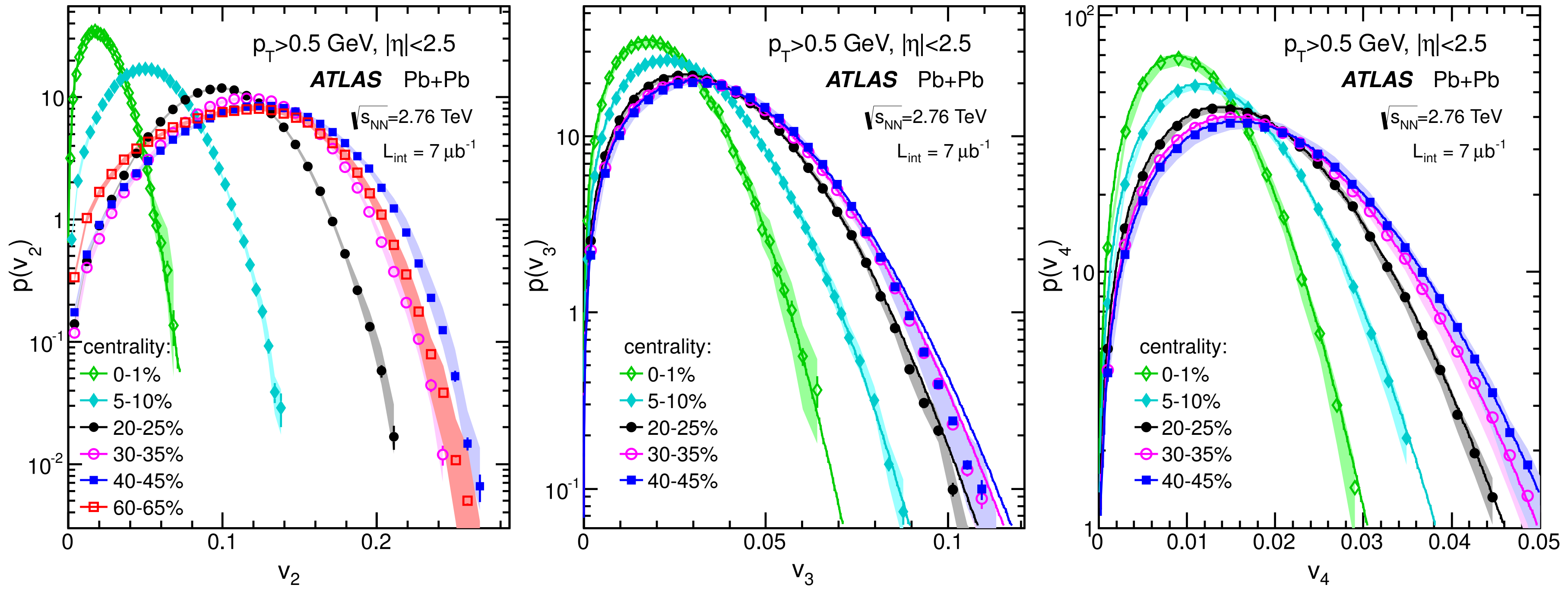
Knowledge Extraction from Relativistic Heavy-Ion Collisions

Probing QCD in Heavy-Ion Collisions

Data:

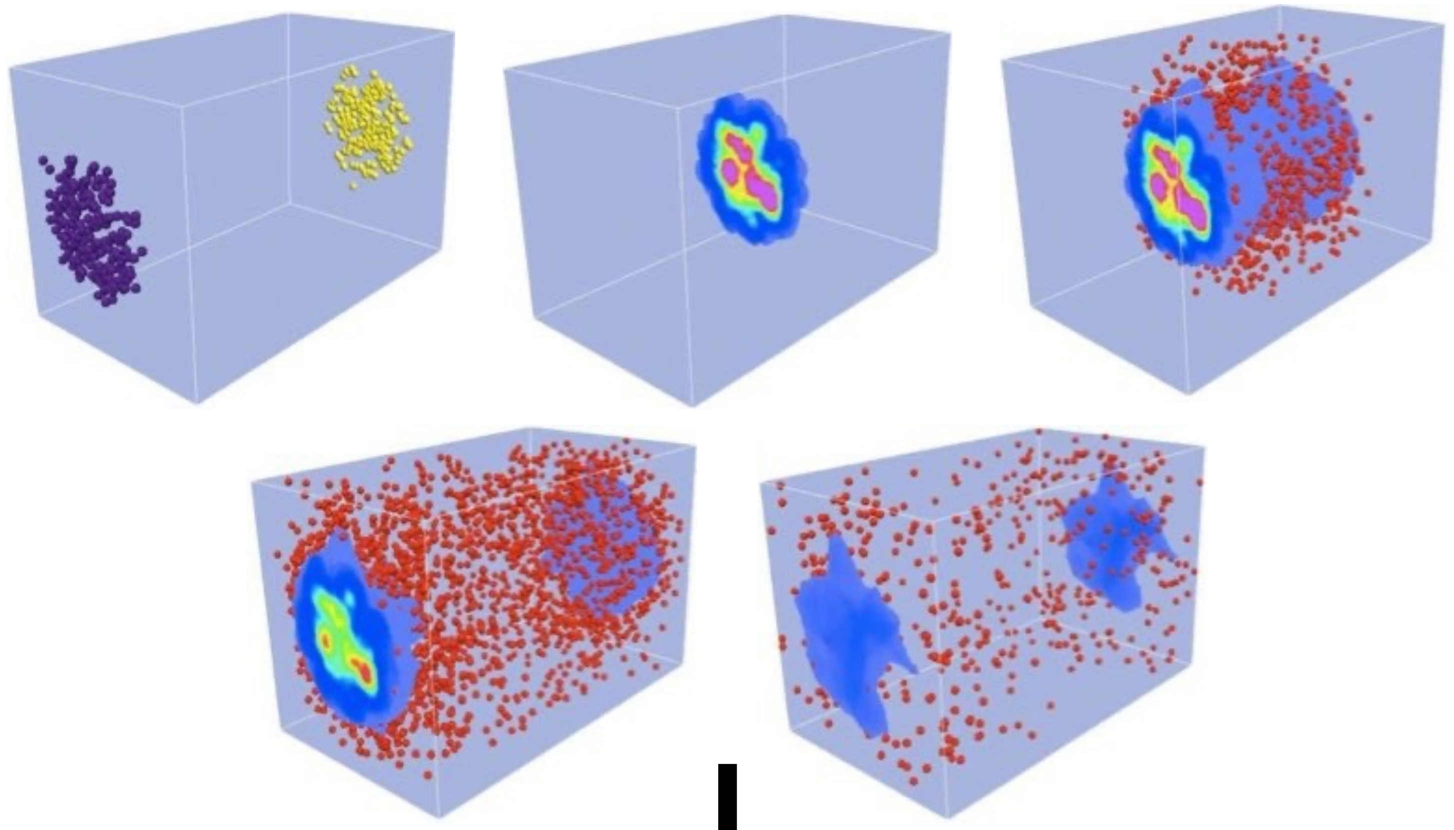


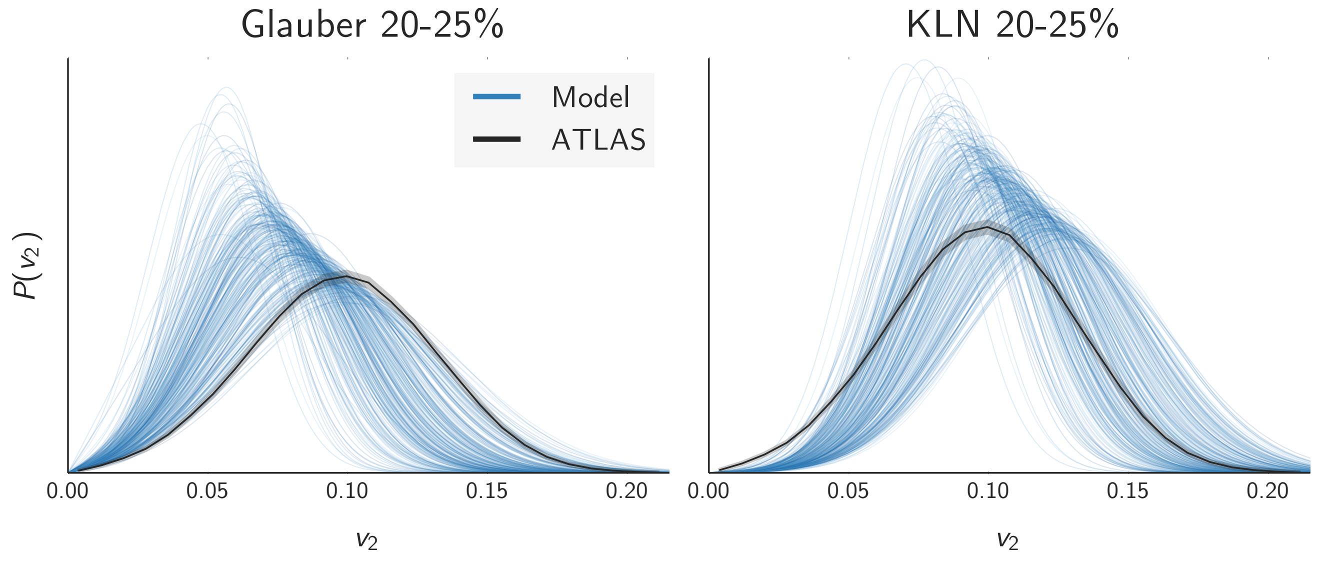




Model:

initial conditions, τ_0, η/s, ζ/s, ….





extracted QGP properties: η/s, …

Determining the QGP Properties via a Model to Data Comparison

Model Parameter:

eqn. of state

shear viscosity

initial state

pre-equilibrium dynamics

thermalization time

quark/hadron chemistry

particlization/freeze-out

experimental data:

π/K/P spectra

yields vs. centrality & beam

elliptic flow

HBT

charge correlations & BFs

density correlations

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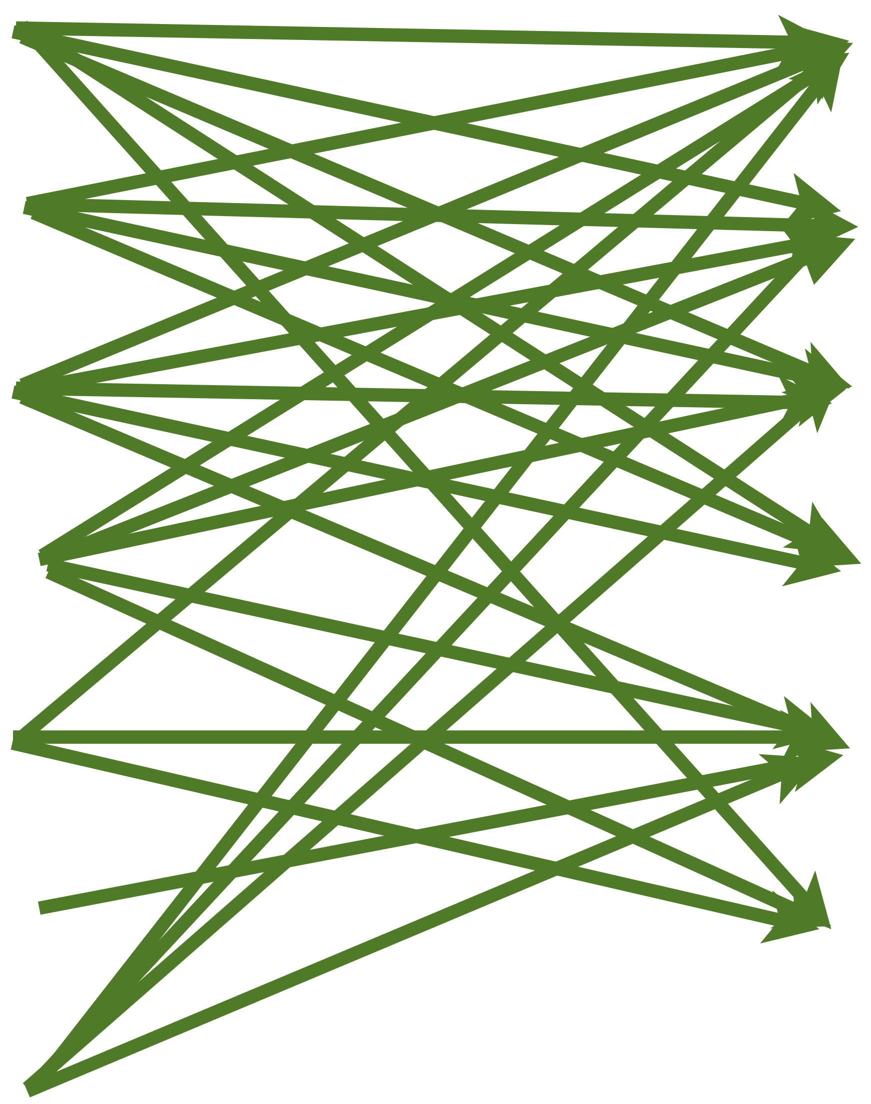

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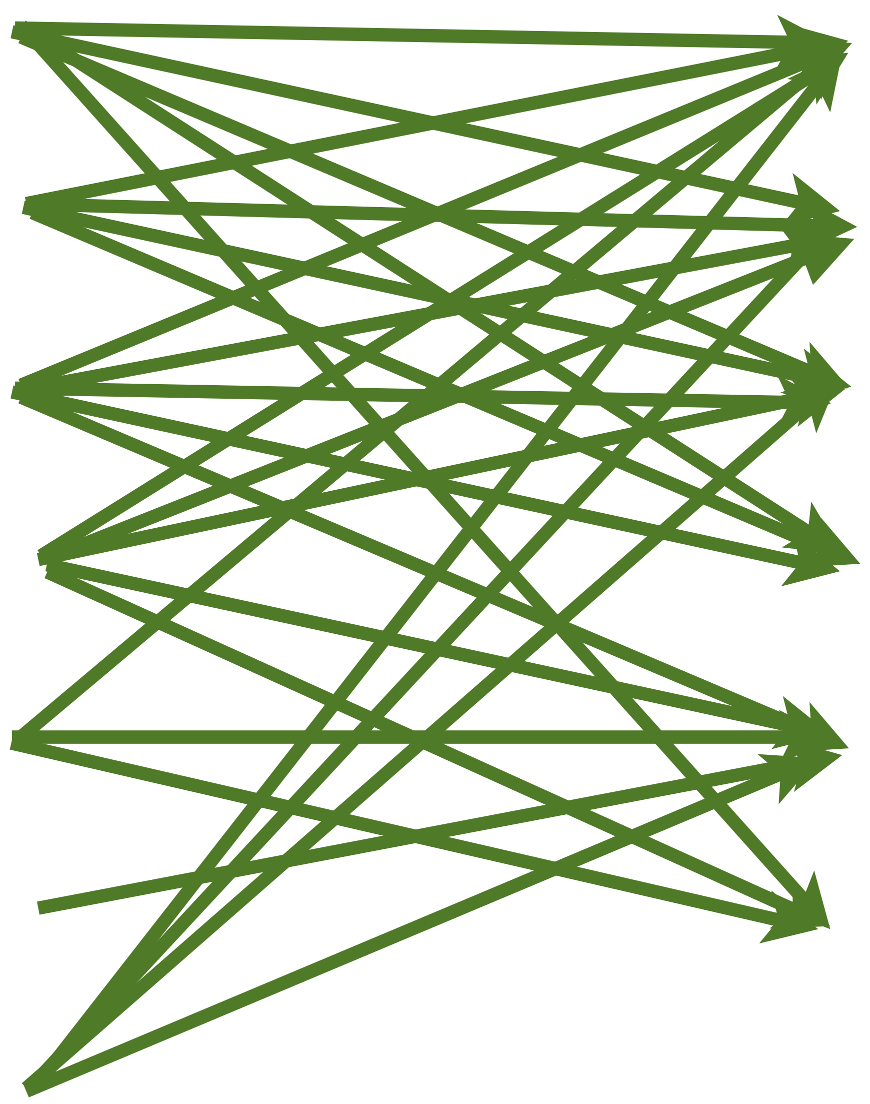

experimental data:

π/K/P spectra
yields vs. centrality & beam
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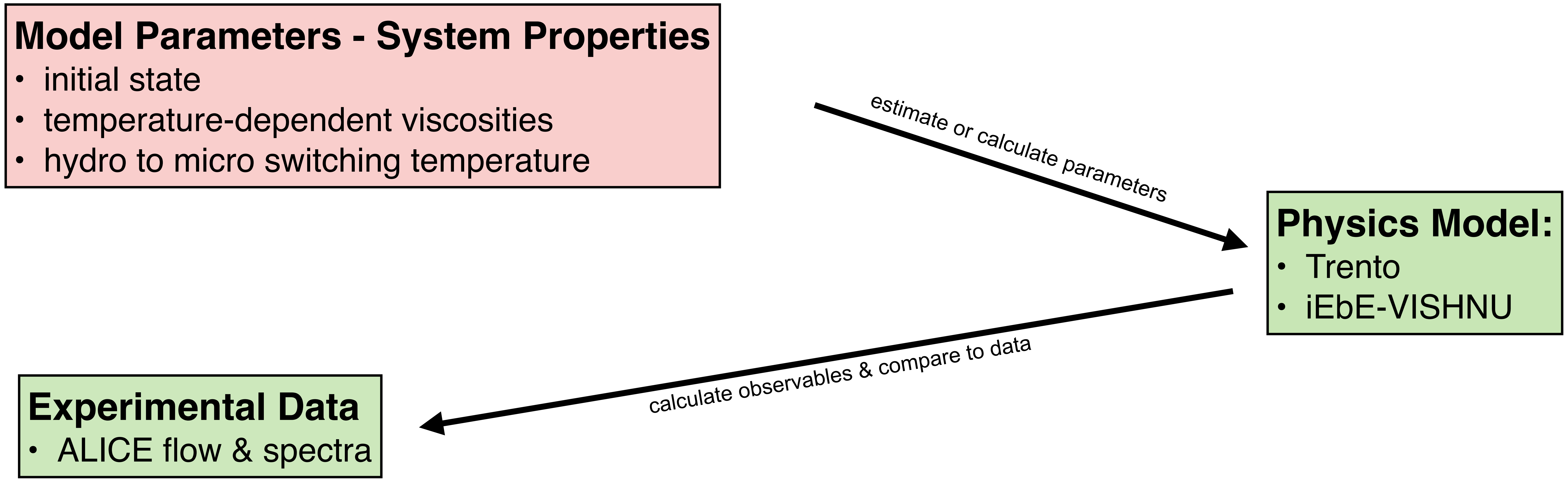
density correlations

- large number of interconnected parameters w/ non-factorizable data dependencies
- data have correlated uncertainties
- develop novel optimization techniques: Bayesian Statistics and MCMC methods
- transport models require too much CPU: need new techniques based on emulators
- general problem, not restricted to RHIC Physics → **collaboration with Statistical Sciences**

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 comparison to data.



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Model Parameters - System Properties

- initial state
- temperature-dependent viscosities
- hydro to micro switching temperature

Bayesian analysis

Physics Model:

- Trento
- iEbE-VISHNU

Experimental Data

- ALICE flow & spectra

Bayesian Analysis

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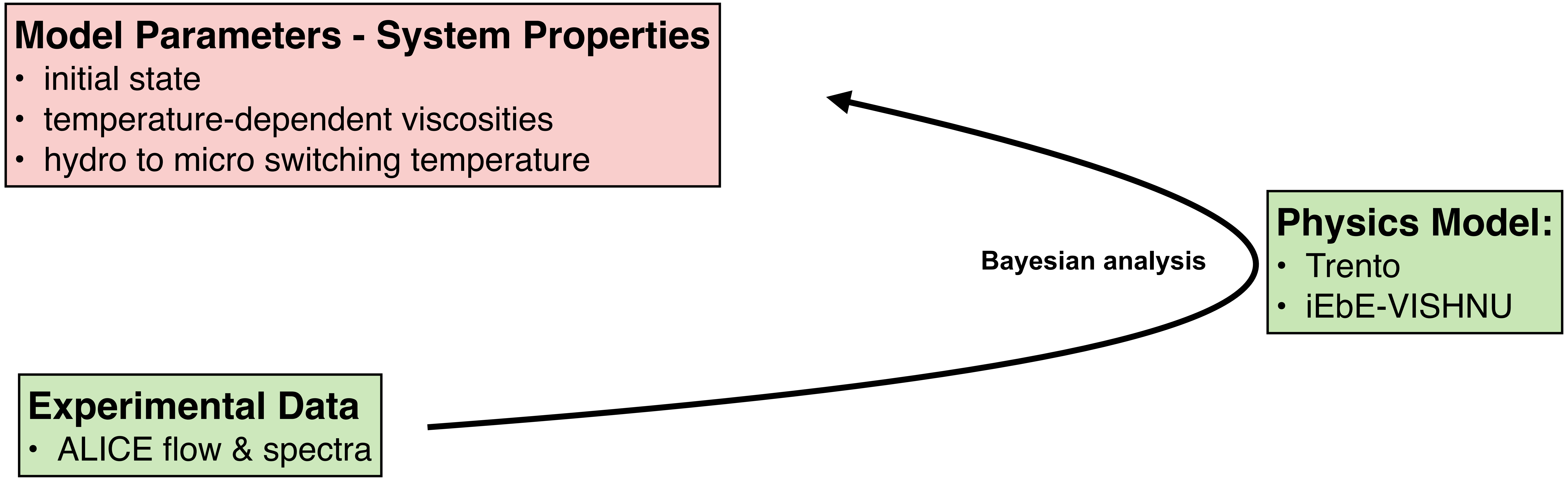
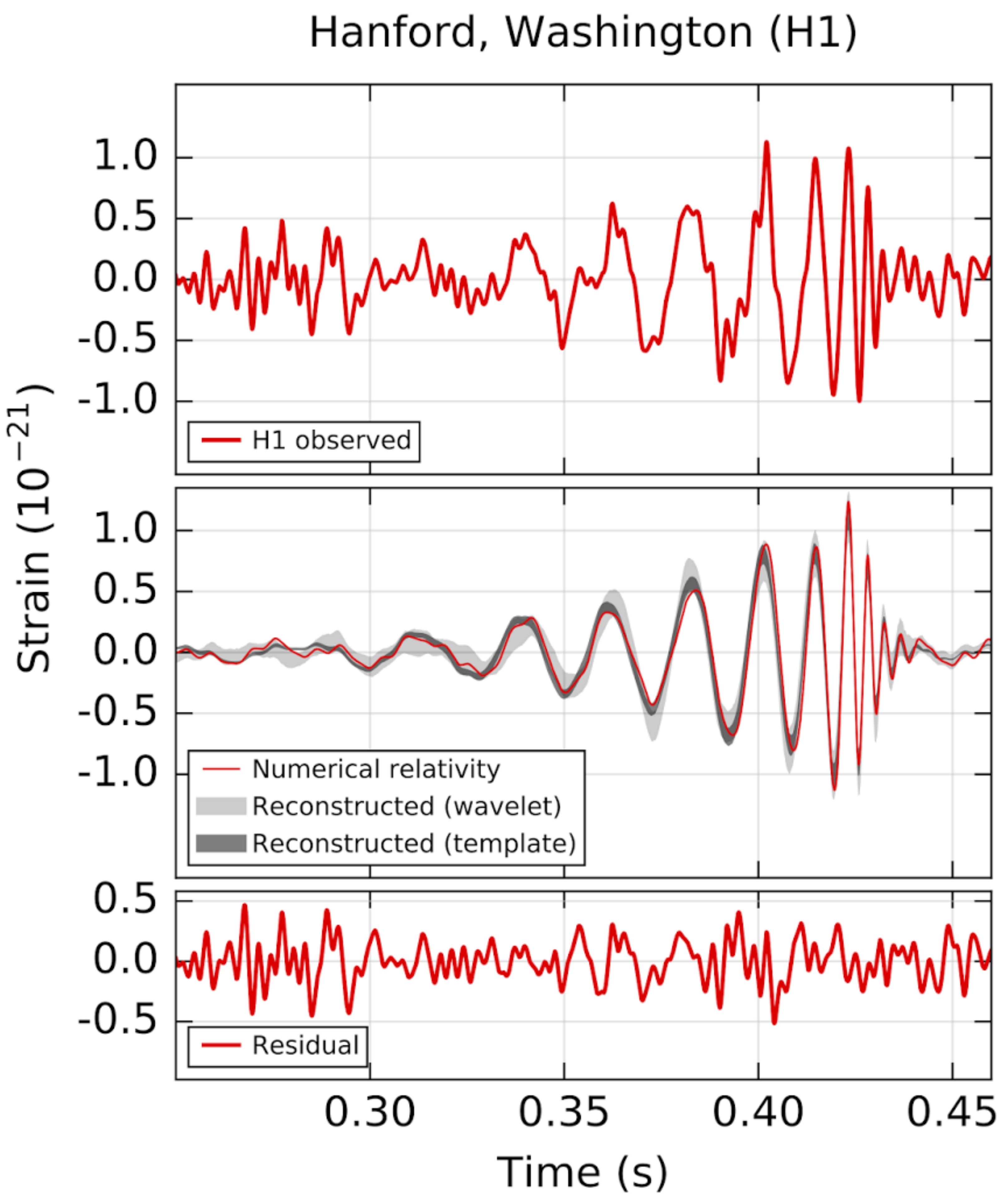


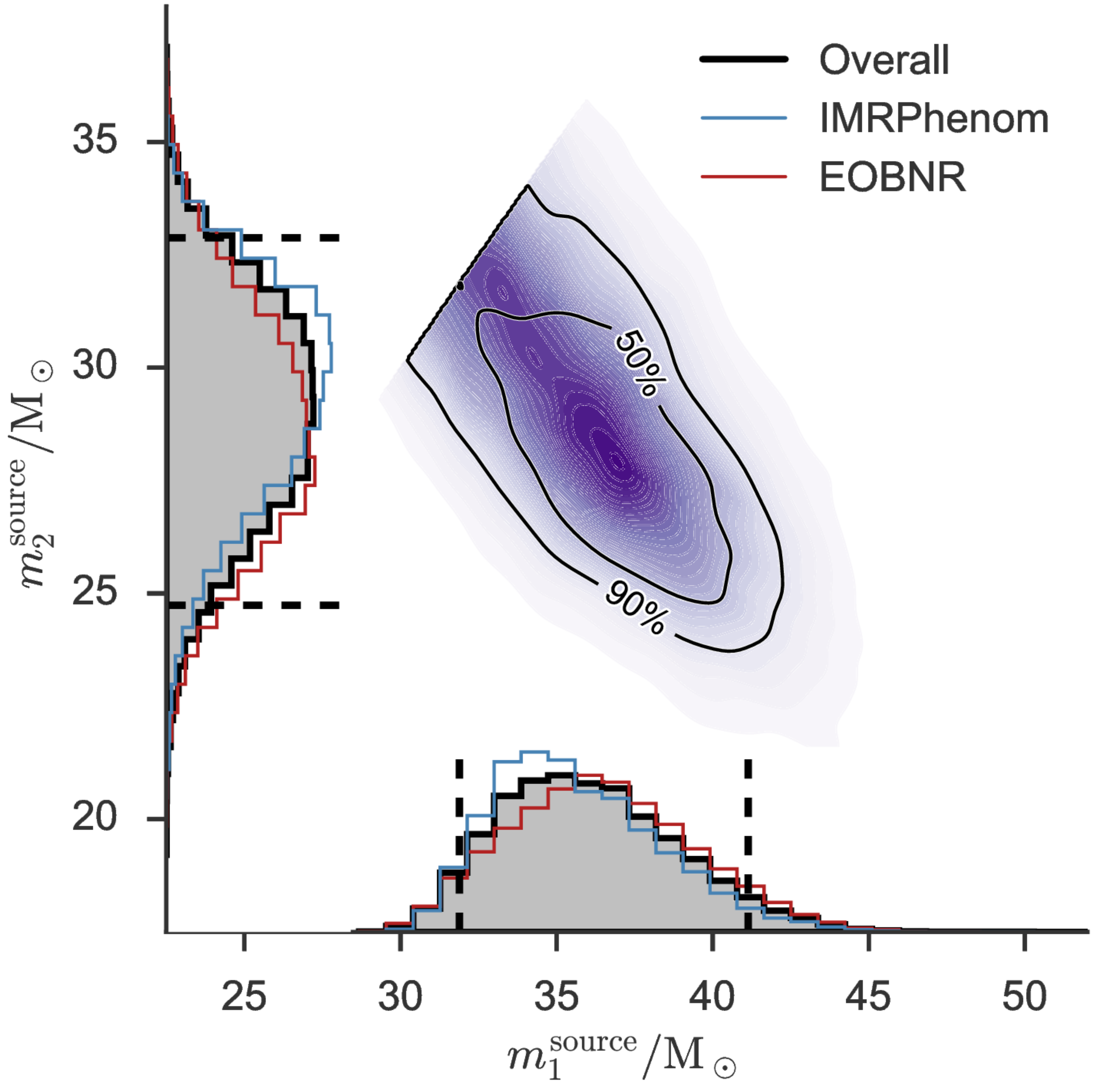
- Bayesian analysis allows us to simultaneously calibrate all model parameters via a model-to-data comparison
- determine parameter values such that the model best describes experimental observables
- extract the probability distributions of all parameters

Example: Gravitational Waves

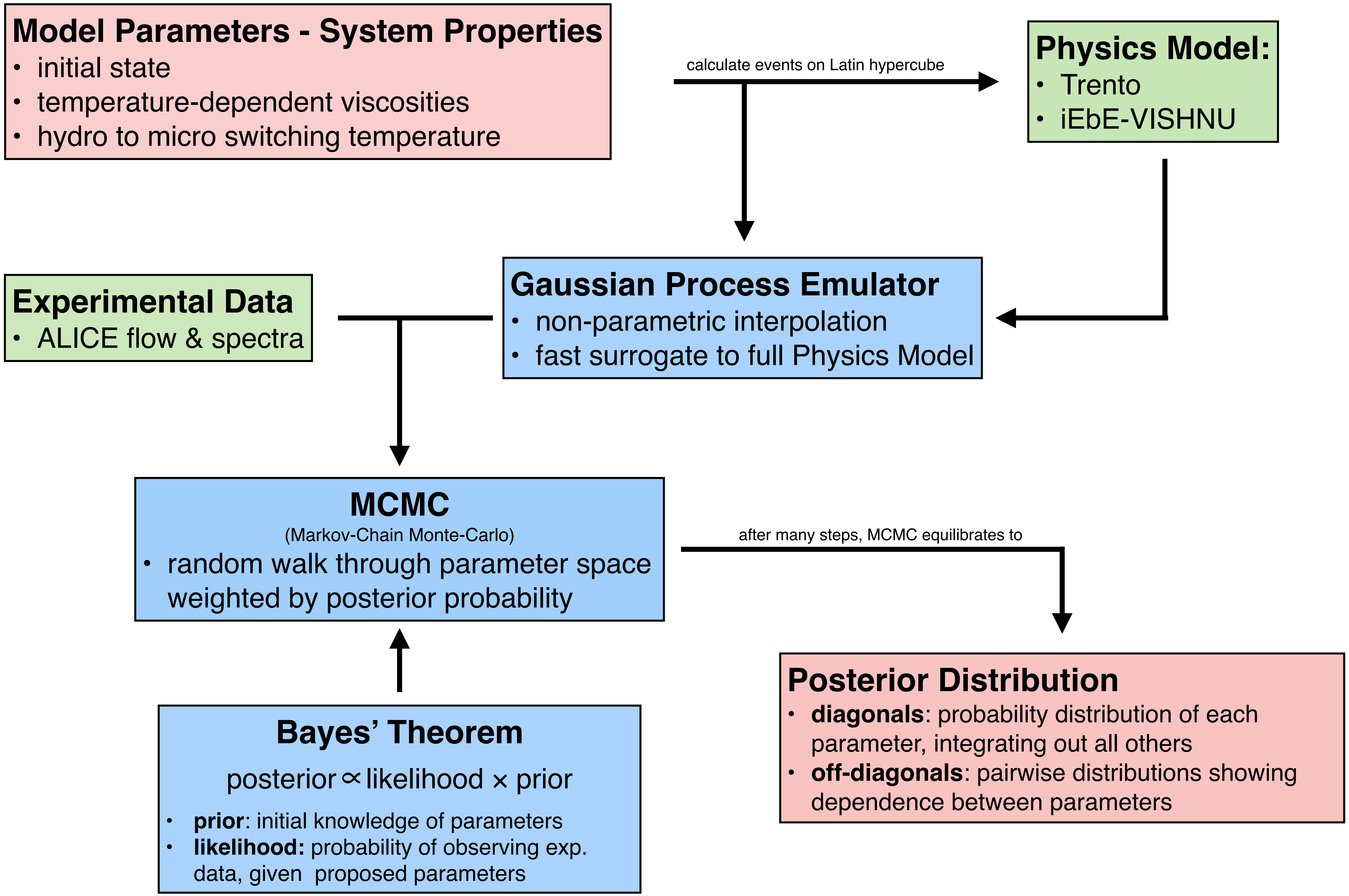
LIGO gravitational wave signal:



Bayesian analysis of GR model of merging black holes of masses m_1 and m_2 that is capable of reproducing LIGO data:



Setup of a Bayesian Statistical Analysis



Components of the Bayesian Analysis

Methodology

Model Parameters - System Properties
- initial state
- temperature-dependent viscosities
- hydro to micro switching temperature

calculate events on Latin hypercube

Physics Model:
- Trento
- iEbE-VISHNU

Experimental Data
- ALICE flow & spectra

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

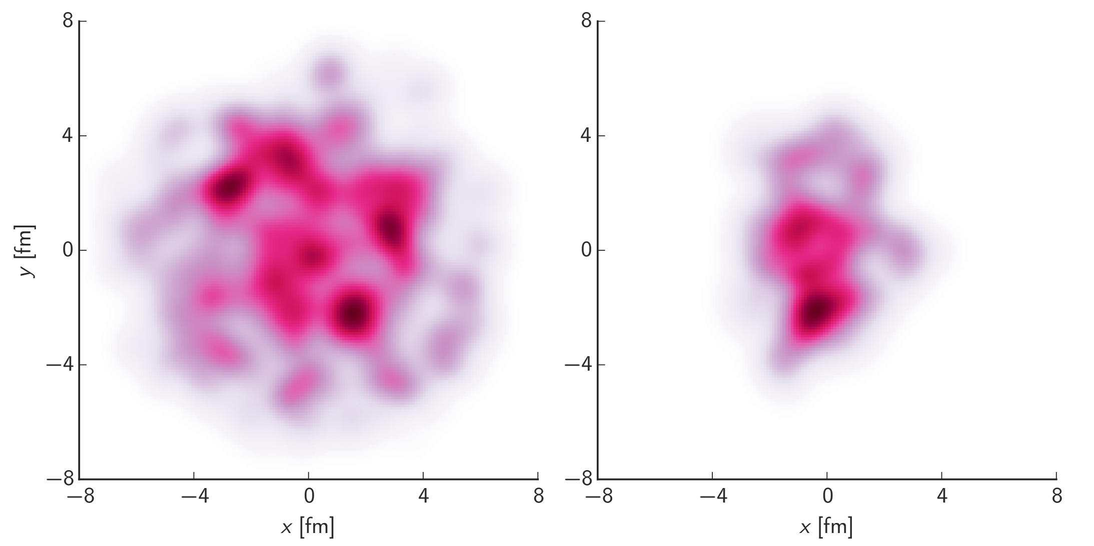
posterior ∝ likelihood × prior

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

Physics Model: Trento + iEbE-VISHNU

Trento:

- parameterized initial condition model based on phenomenological concepts for entropy deposition to a QGP



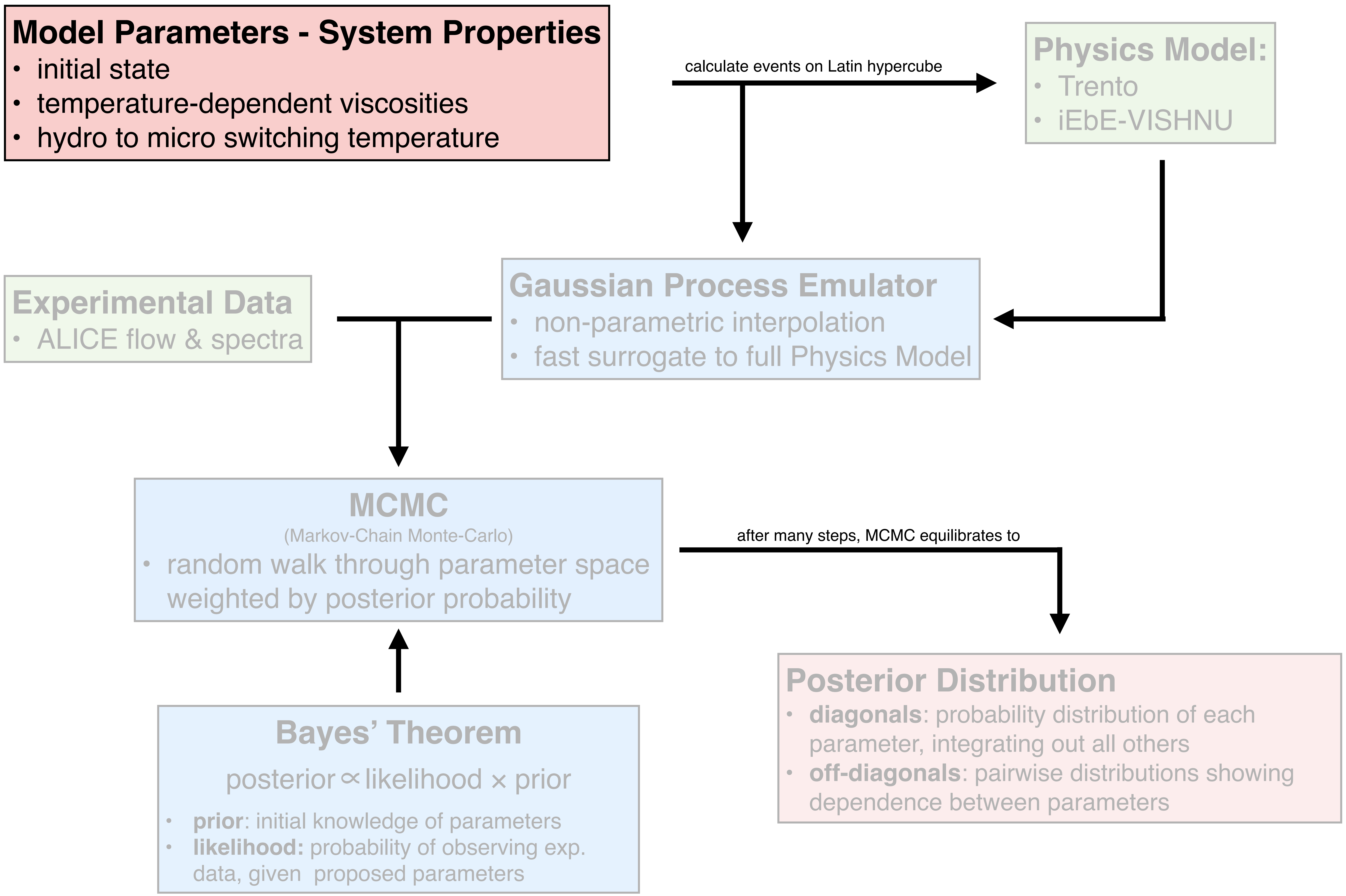
iEbE-VISHNU:

- EbE 2+1D viscous RFD
- describes QGP dynamics & hadronization
- EoS from Lattice QCD
- temperature-dependent shear and bulk viscosity as input

UrQMD:

- Microscopic transport model based on Boltzmann Eqn.
- non-equilibrium evolution of an interacting hadron gas
- hadron gas shear & bulk viscosities are implicitly contained in calculation

Methodology



Calibration Parameters

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

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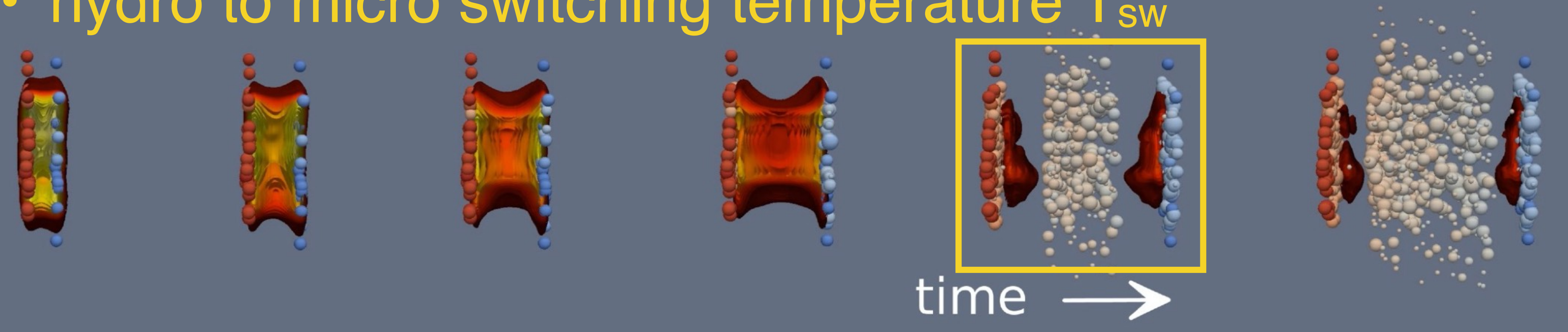

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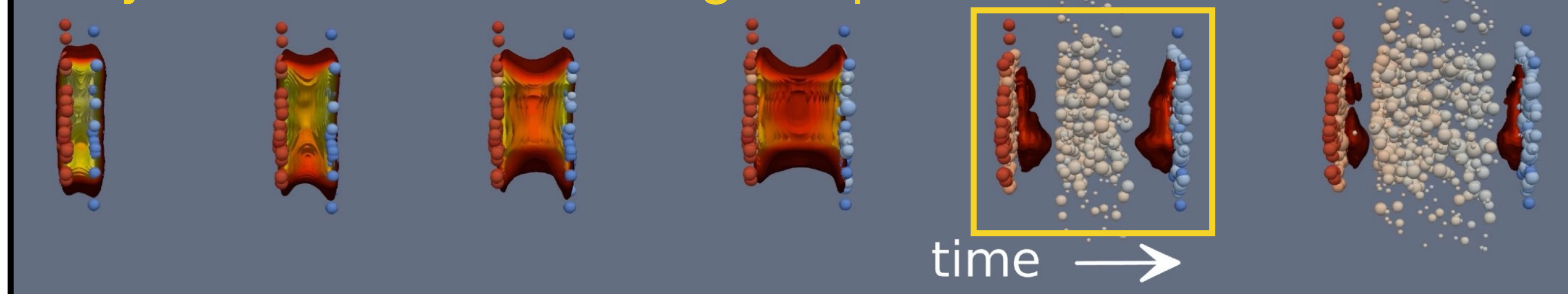
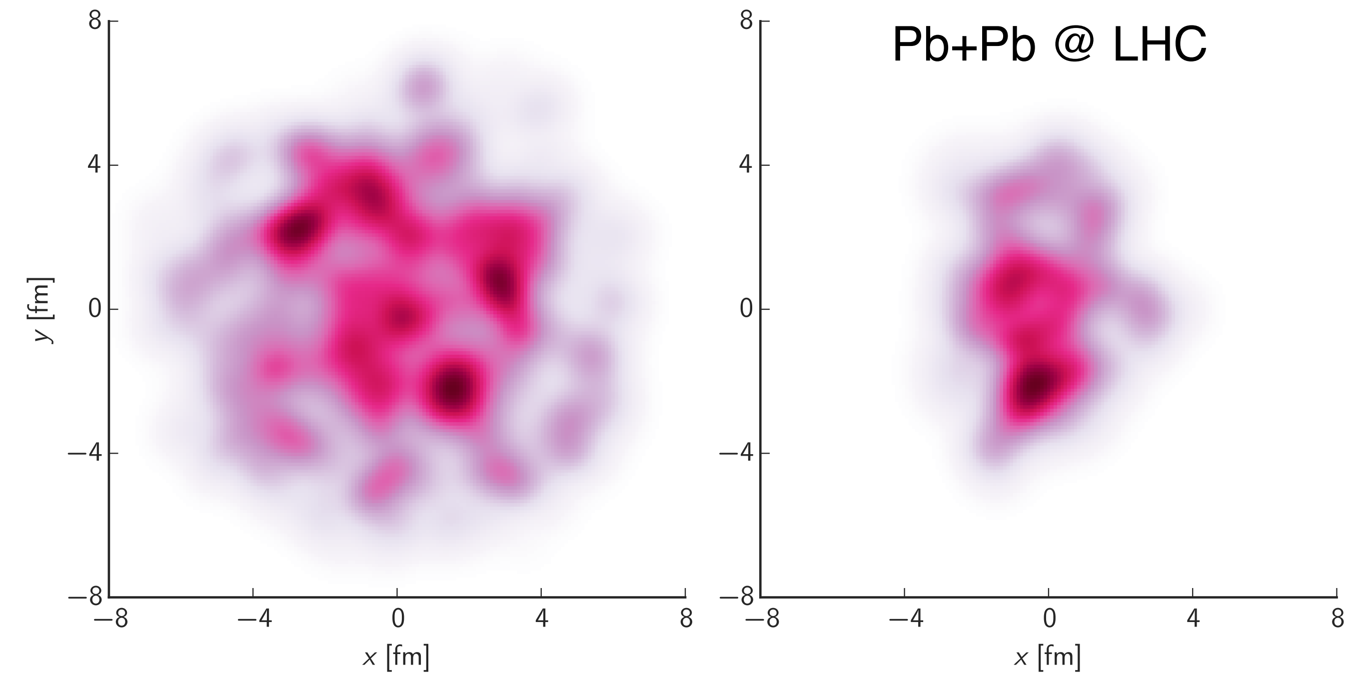


Trento initial condition:

- p: attenuation parameter - entropy deposition
- k: governs fluctuation in nuclear thickness
- w: Gaussian nucleon width



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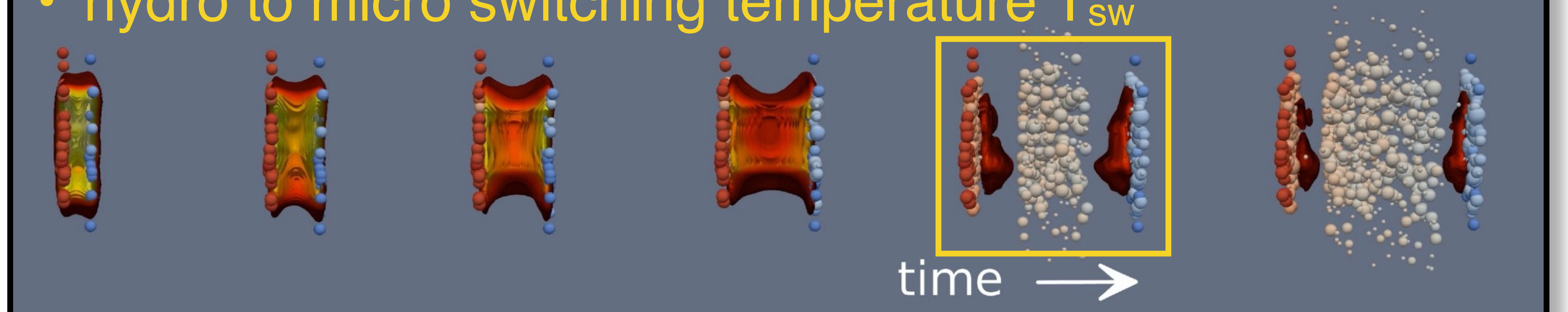

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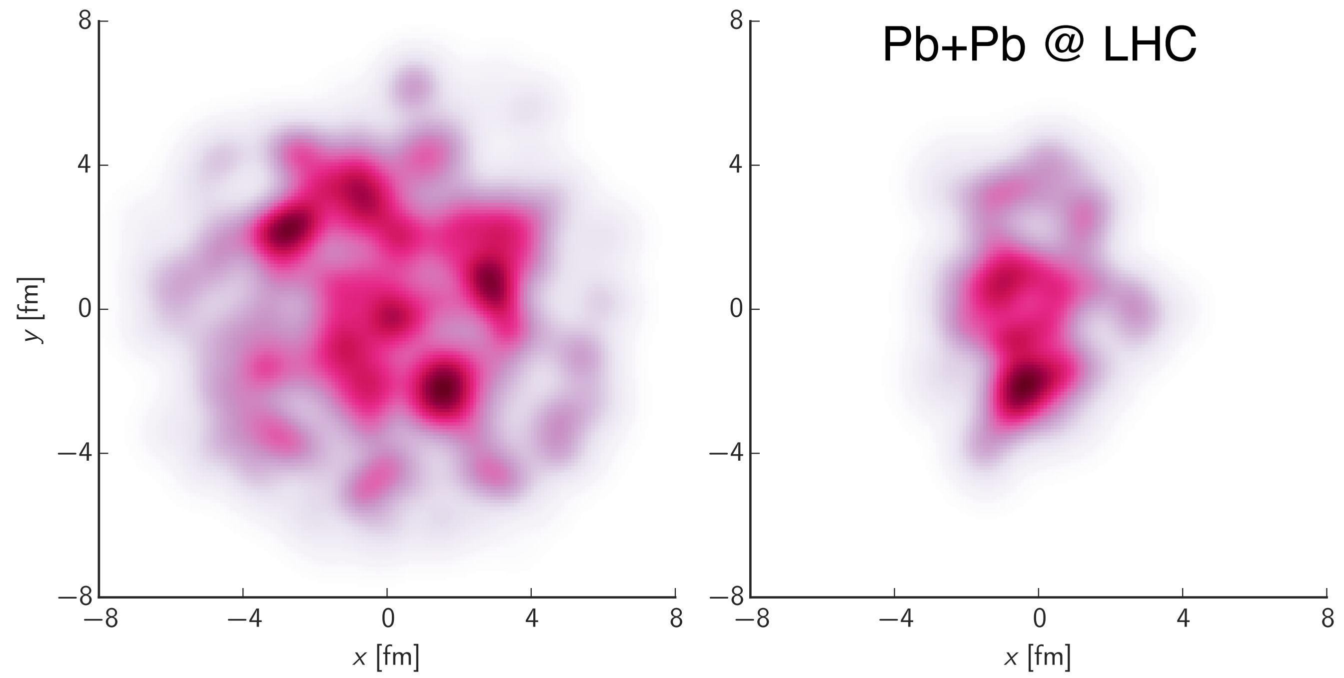
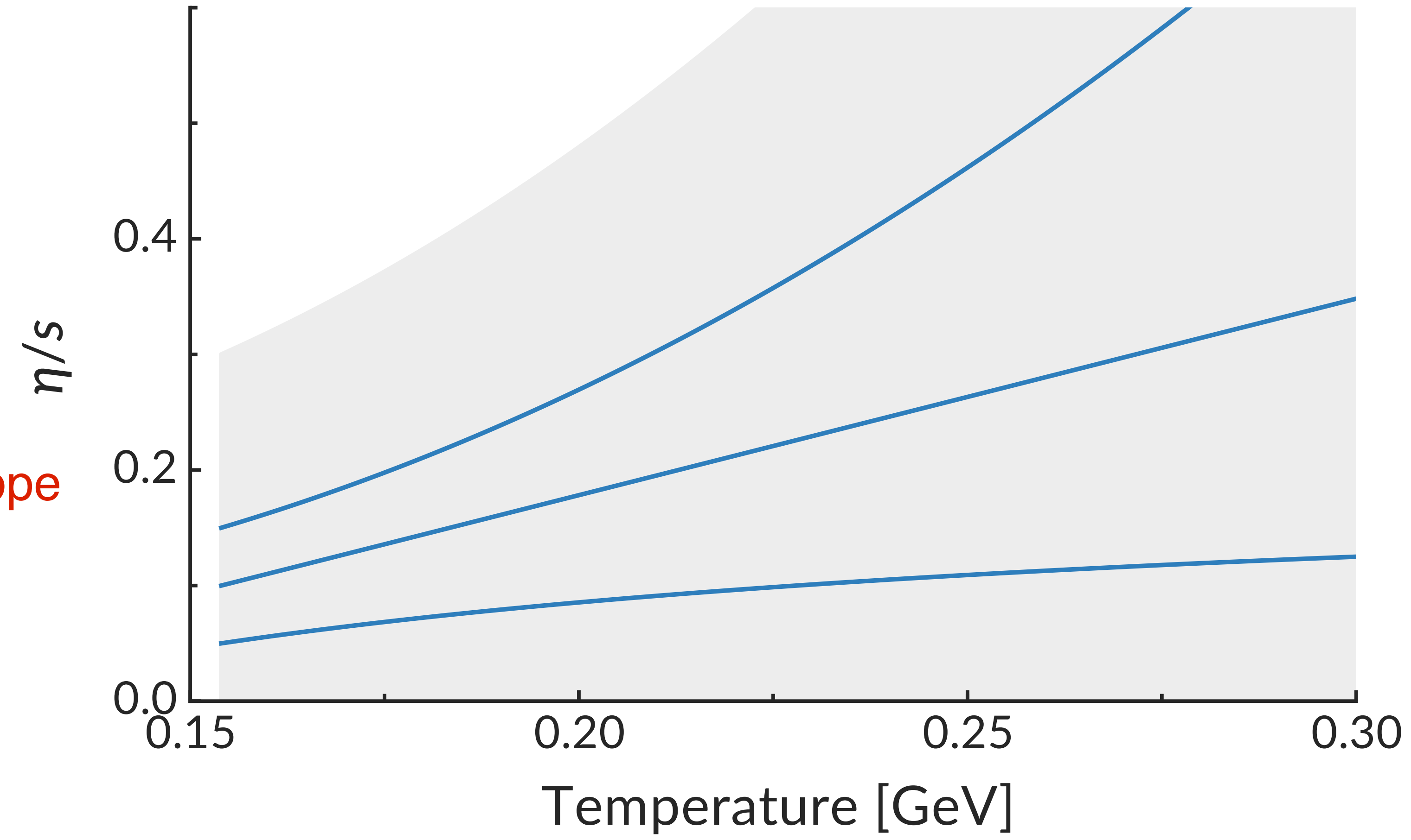


temperature dependent shear viscosity:

$$\eta/s(T) = (\eta/s)_{min} + (\eta/s)_{slope} \times (T-T_C)\times(T/T_C)^{\beta}$$

parameters:

- intercept: $(\eta/s)_{min}$ at T_C
- slope: $(\eta/s)_{slope}$
- curvature: β



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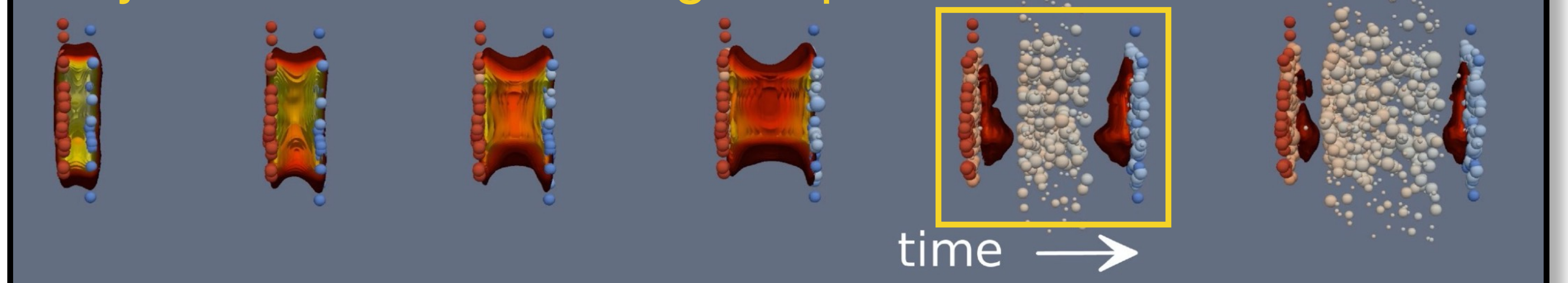

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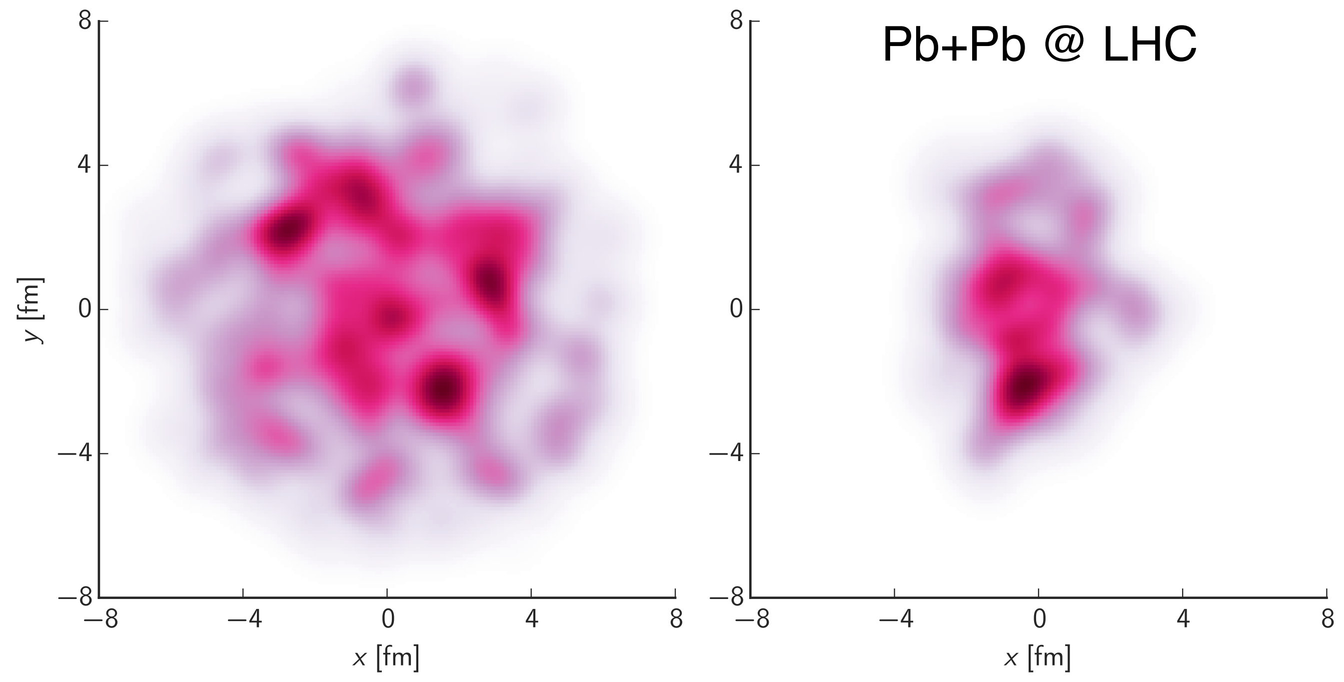

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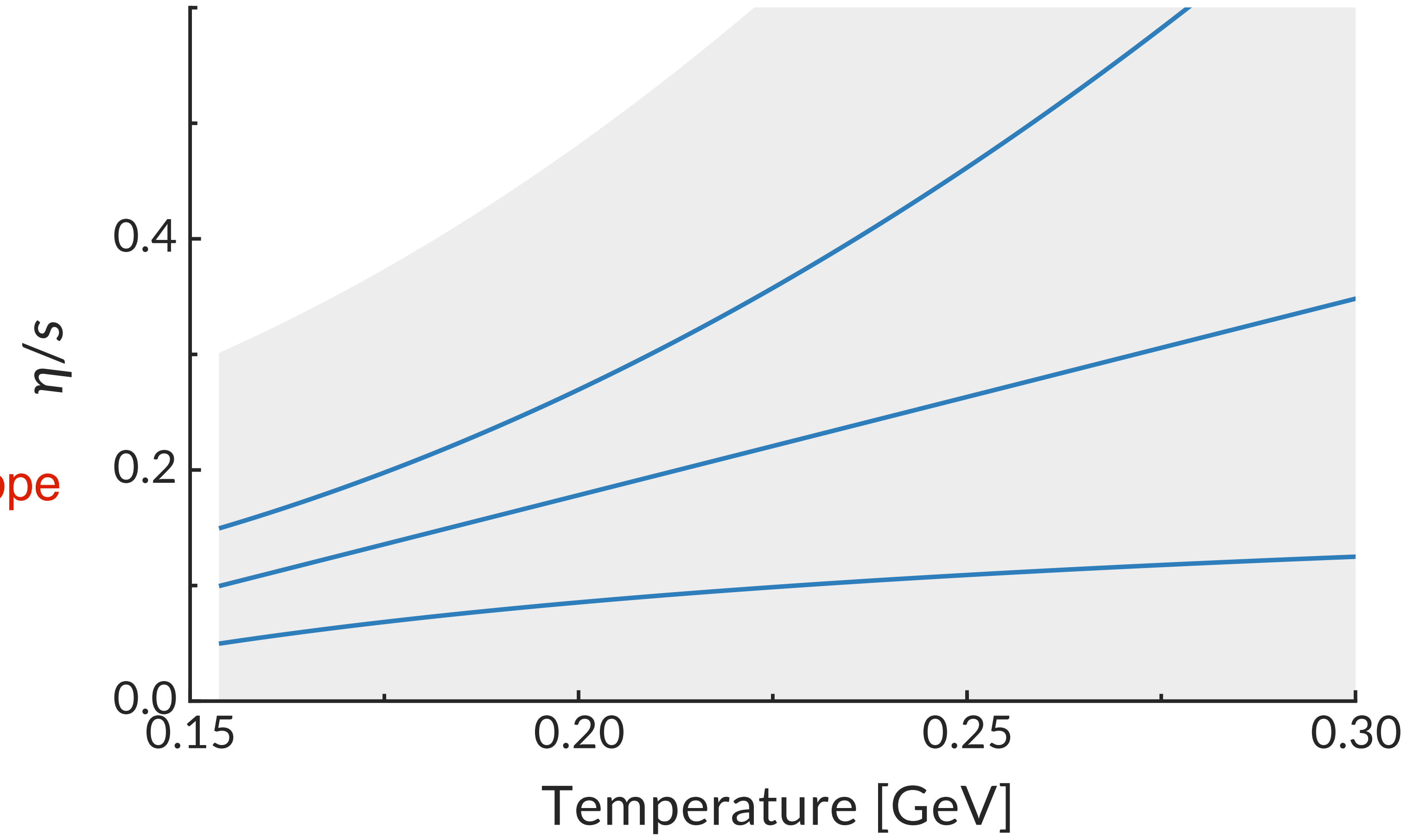
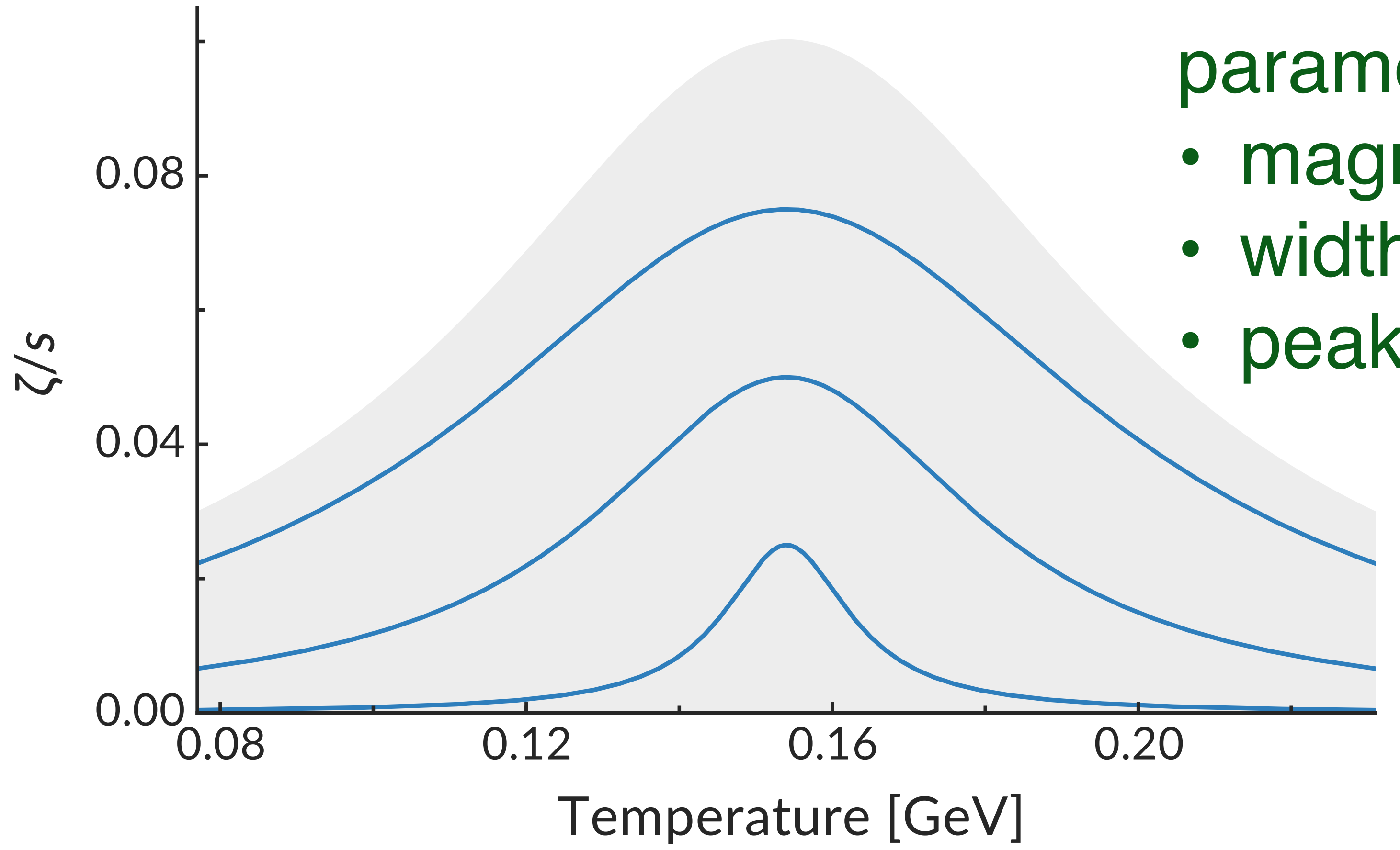


temperature dependent bulk viscosity:

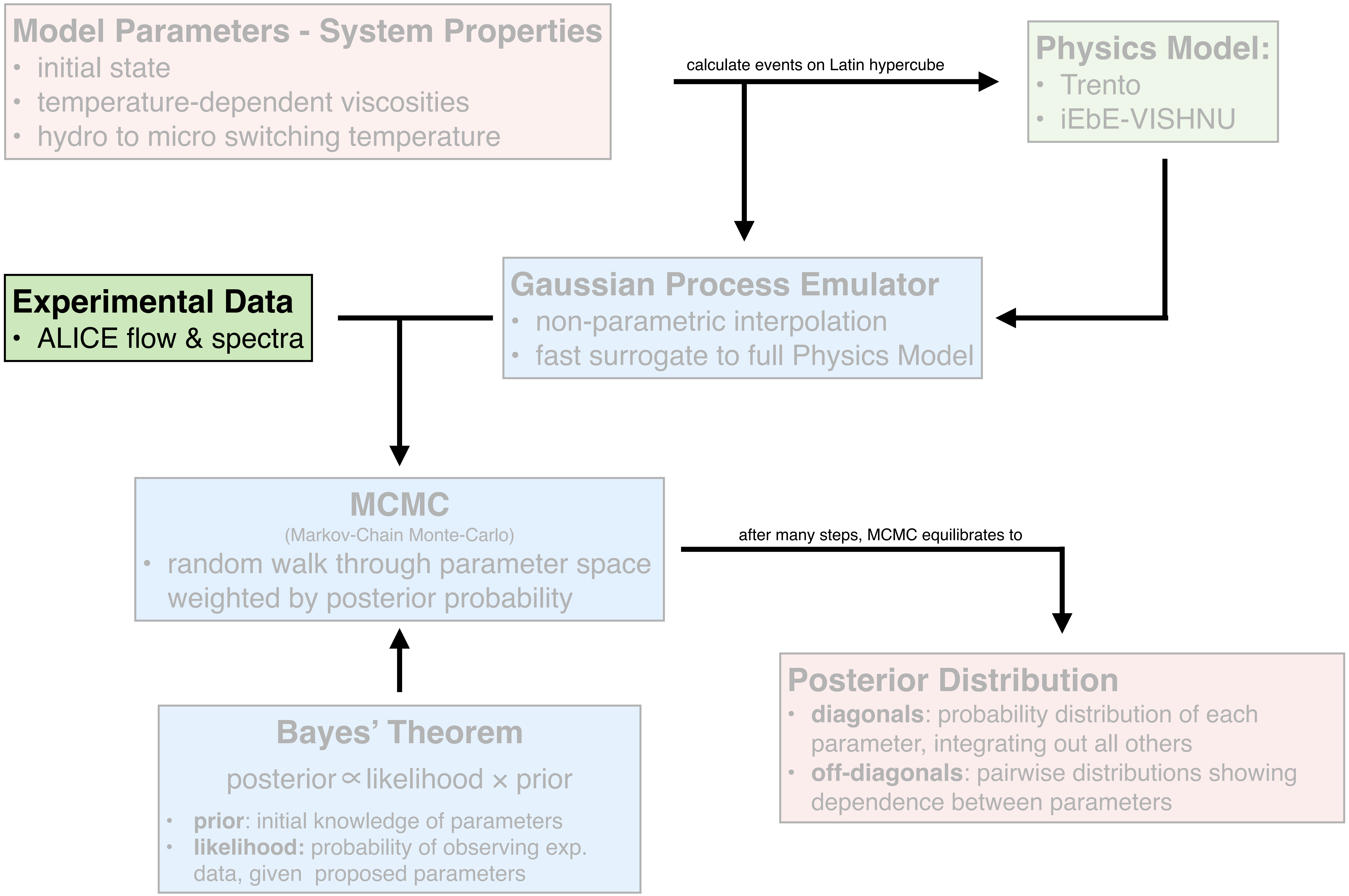
$$\zeta/s(T)=(\zeta/s)_{max} / [1+(T-(\zeta/s)_{peak})^2/\Gamma^2]$$



parameters:

- magnitude $(\zeta/s)_{max}$
- width: Γ
- peak position: $(\zeta/s)_{peak}$

Methodology

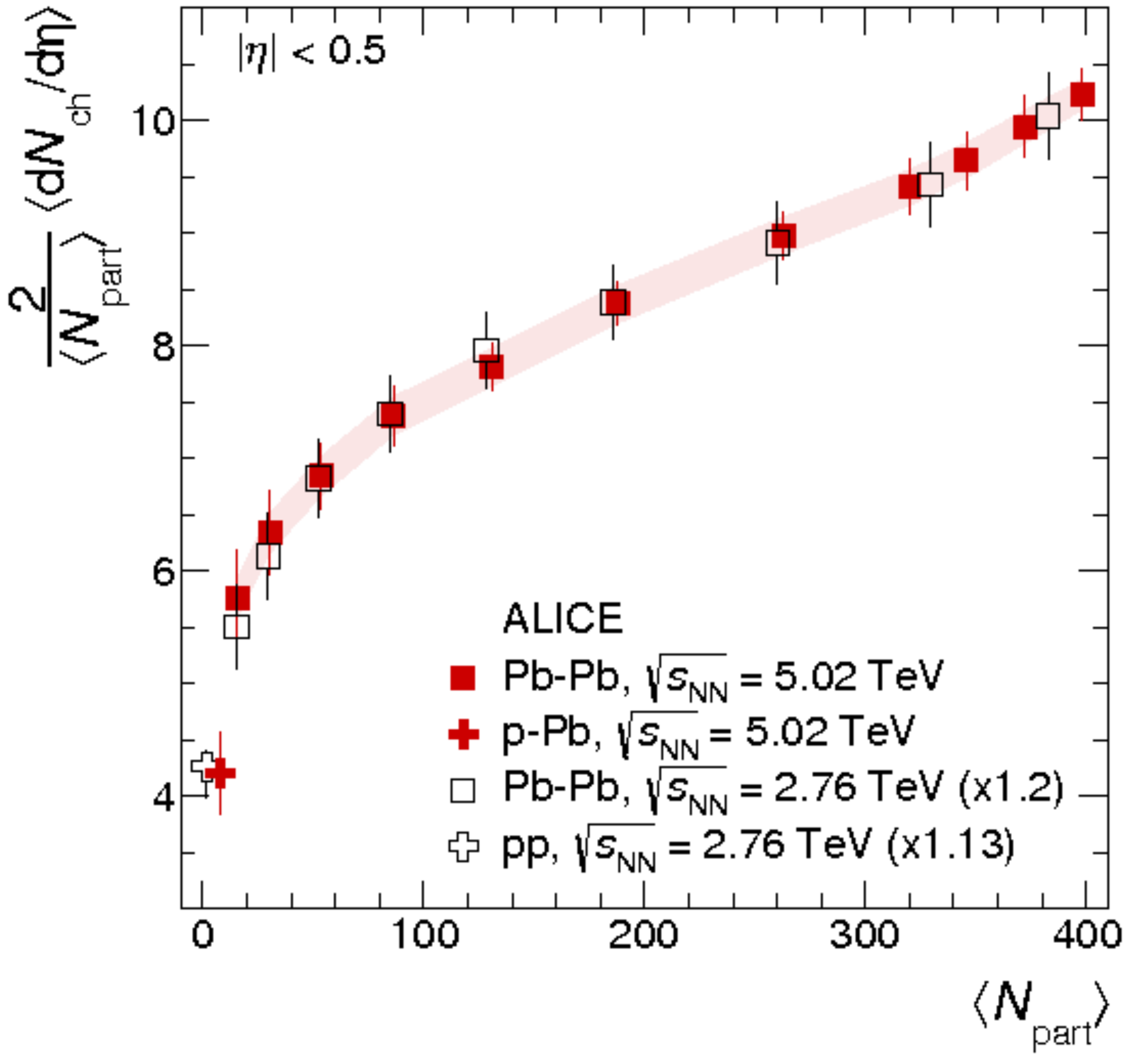


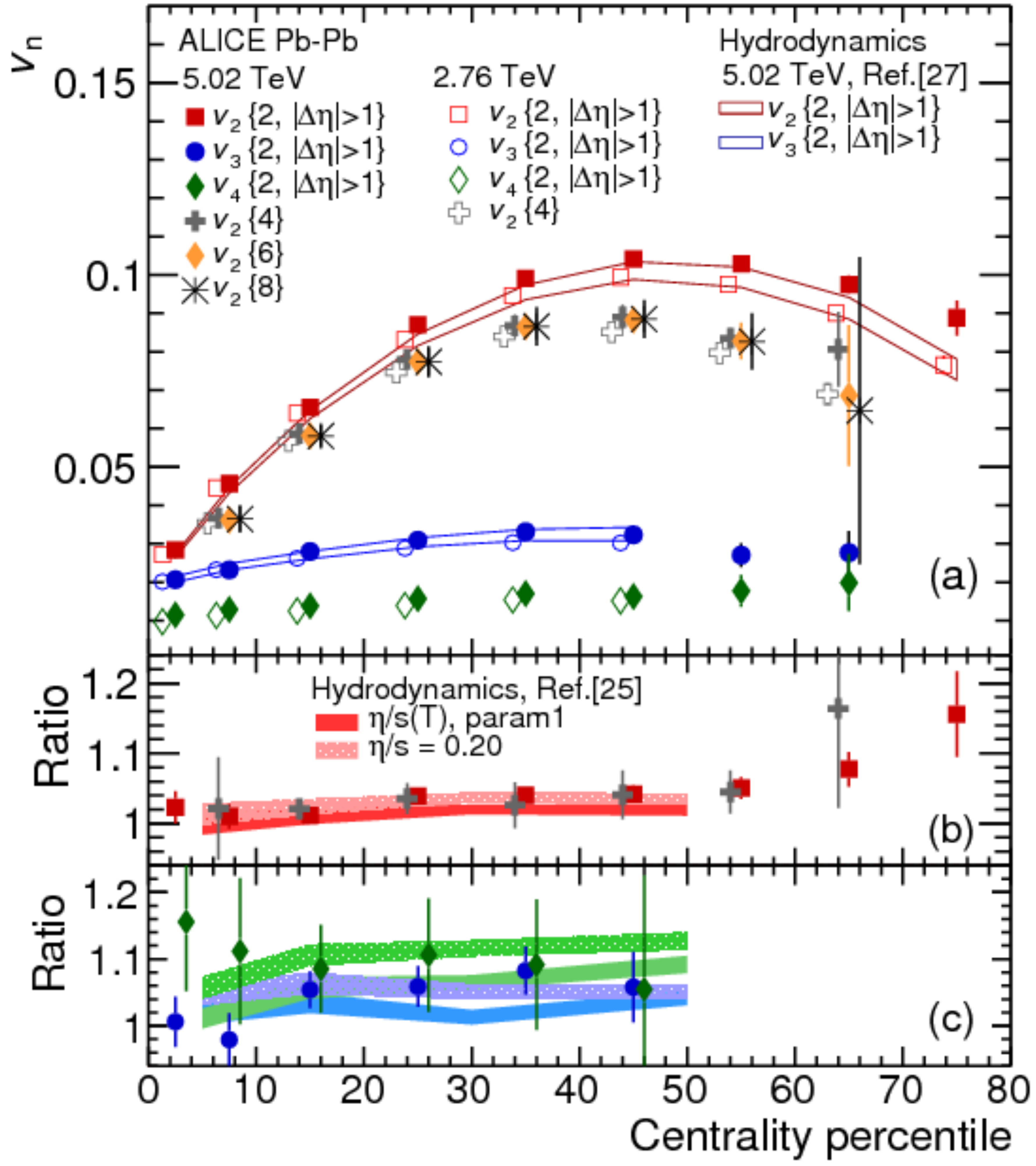
Training Data

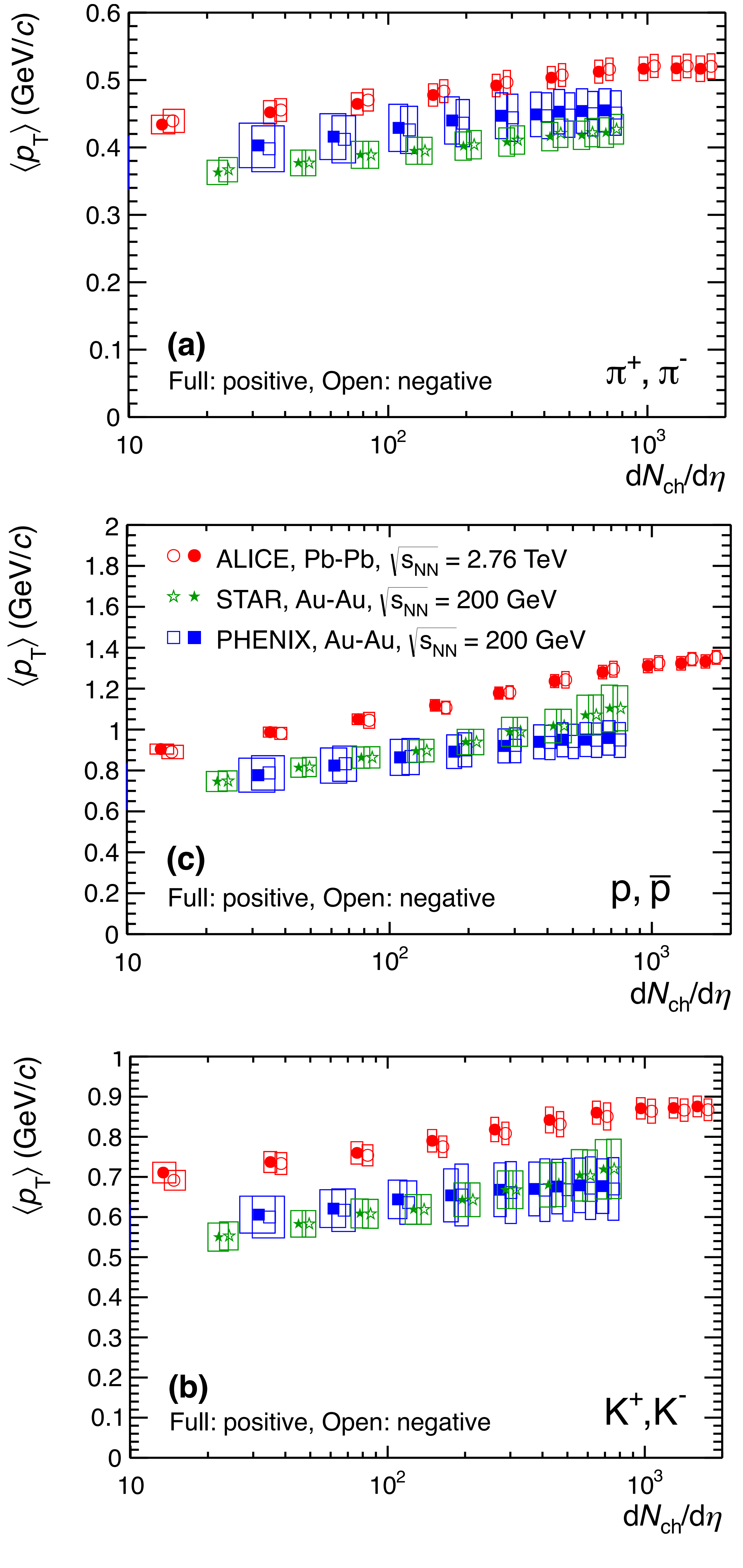
Data:

- ALICE v_2, v_3 & v_4 flow cumulants
- identified & charged particle yields
- identified particle mean p_T
- 2 beam energies:
  2.76 & 5.02 TeV

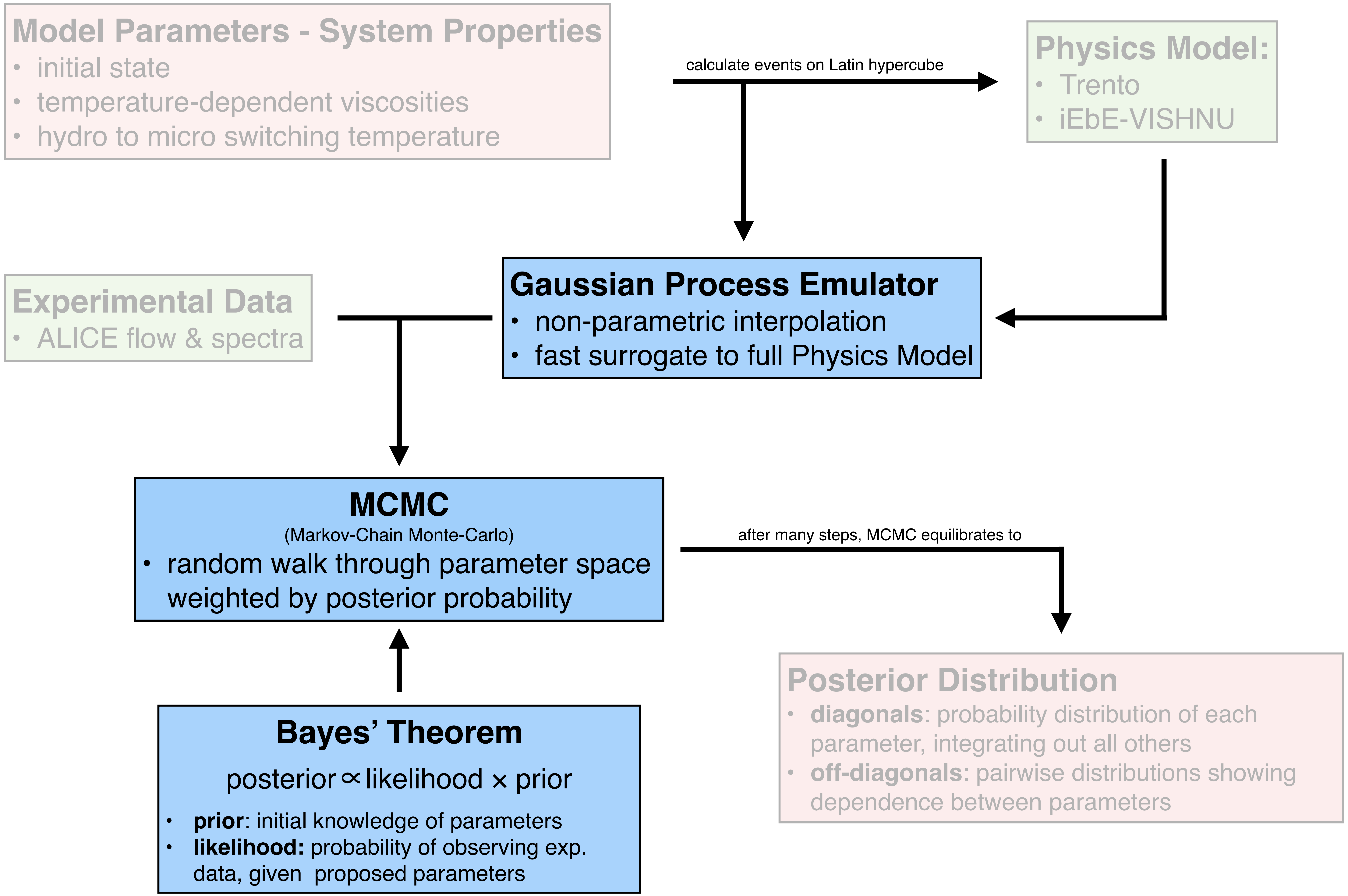
the entire success of the analysis depends on the quality of the exp. data!







Methodology



Exploring the Model Parameter-Space

Exploring the Model Parameter-Space

brute force analysis:

- 14 model parameters
- 9 centrality bins
- 20 bins per parameter
- need to evaluate model at 9×20^{14} points
- fluctuating initial conditions: $\mathcal{O}(10^4)$ events per point $\rightarrow 10^{18}$ events
- assume 1 cpu hour per event: 10^{18} cpu-hours!
- **2 billion years 100% use of TITAN @ ORNL (Cray XK7 w/ 560,640 cores)**
- then start MCMC to find point that optimally describes data…

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Need to find techniques that cut down the cpu needed by at least a factor of 10^{10}: **Gaussian Process Emulators**

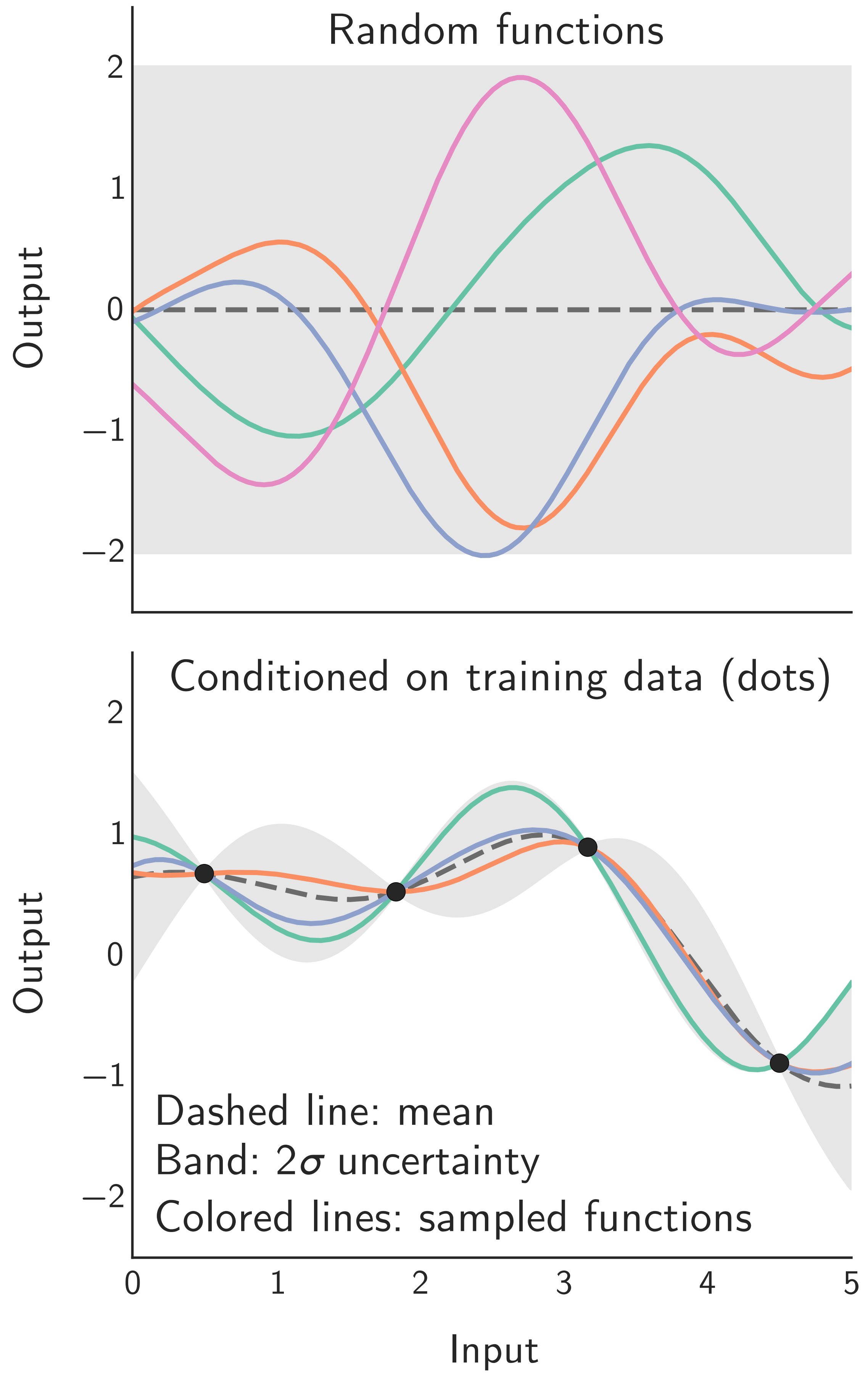
Exploring the Model Parameter-Space

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



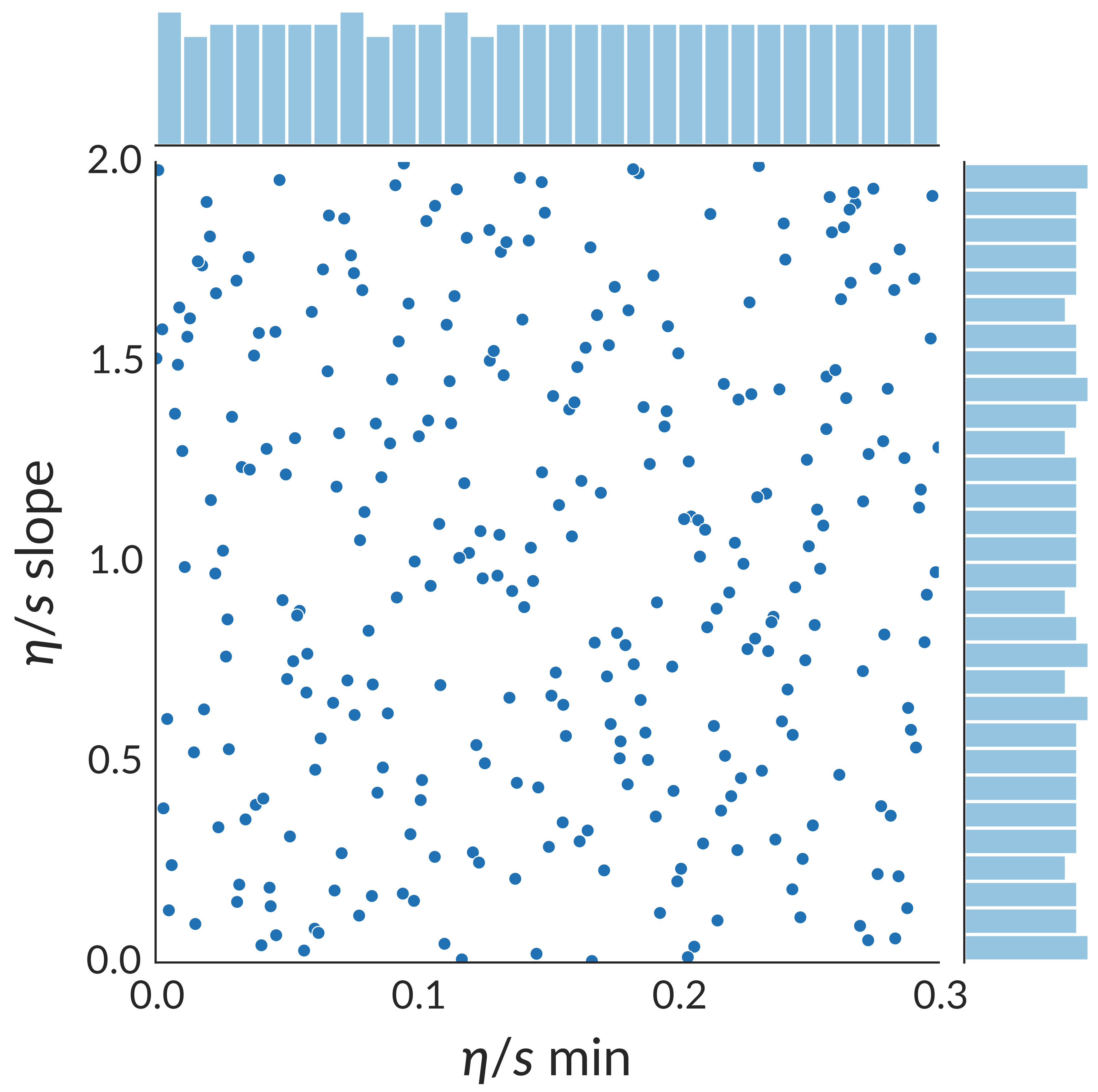
Computer Experiment Design

Latin hypercube:

- algorithm for generating semi-randomized, space-filling points (here: maximin Latin hypercube)
- avoids large gaps and tight clusters
- all parameters varied simultaneously
- needs only $m \geq 10n$ points, with n: number of model parameters

Example:

- Latin-hypercube projection for η/s parameters



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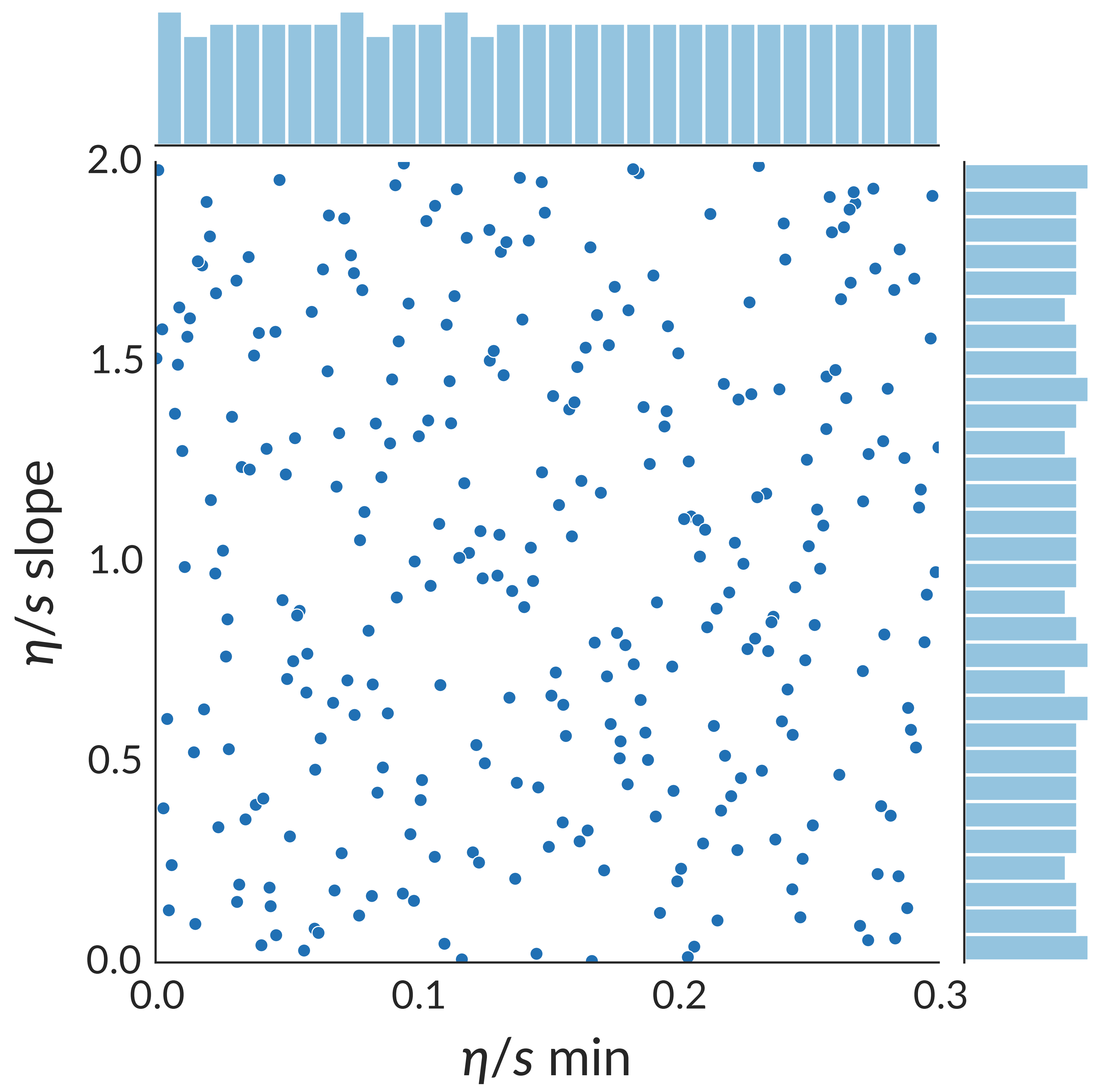
- all parameters varied simultaneously
- needs only $m \geq 10n$ points, with n: number of model parameters

this design:

- n=15 model parameters
- 9 centrality bins, 2 energies
- Latin hypercube with m=500 points
- $\mathcal{O}(10^4)$ events per point, for a total of approx. 35,000,000 events
- use Gaussian Process Emulators to interpolate between points

Example:

- Latin-hypercube projection for η/s parameters



Computer Experiment Execution

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Edison @ NERSC:
- Cray XC30: 5586 nodes w/ 24 cores each
- 2 hyperthreads per core
- 2.57 Petaflops/s

Duke QCD workflow:
- 1000 nodes per job: running on 48K cores simultaneously
- entire model design with 30M events can be computed in 1 day

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NOW COMPUTING

A small sample of massively parallel scientific computing jobs running right now at NERSC.

PROJECT	MACHINE	NODES	NERSC HOURS USED
NERSC Staff Accounts PI: Sudip S. Dosanjh, Lawrence Berkeley National Lab - NERSC	Cori KNL	1,008	115,874.8
NERSC Staff Accounts PI: Sudip S. Dosanjh, Lawrence Berkeley National Lab - NERSC	Cori KNL	1,008	77,866.5
Extraction of QCD transport coefficients from ultra-relativistic heavy-ion collisions through a Bayesian model to data analysis PI: Steffen A. Bass, Duke University	Edison	1,000	443,890.9
Extraction of QCD transport coefficients from ultra-relativistic heavy-ion collisions through a Bayesian model to data analysis PI: Steffen A. Bass, Duke University	Edison	1,000	399,224.3
Extraction of QCD transport coefficients from ultra-relativistic heavy-ion collisions through a Bayesian model to data analysis PI: Steffen A. Bass, Duke University	Edison	750	229,928.2
NERSC Staff Accounts PI: Sudip S. Dosanjh, Lawrence Berkeley National Lab - NERSC	Cori KNL	512	282,594.2

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 $\mathbf{x}_\star$

- X: training data design points
- Y: model output on X

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

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

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
- posterior ~ likelihood within design range, zero outside

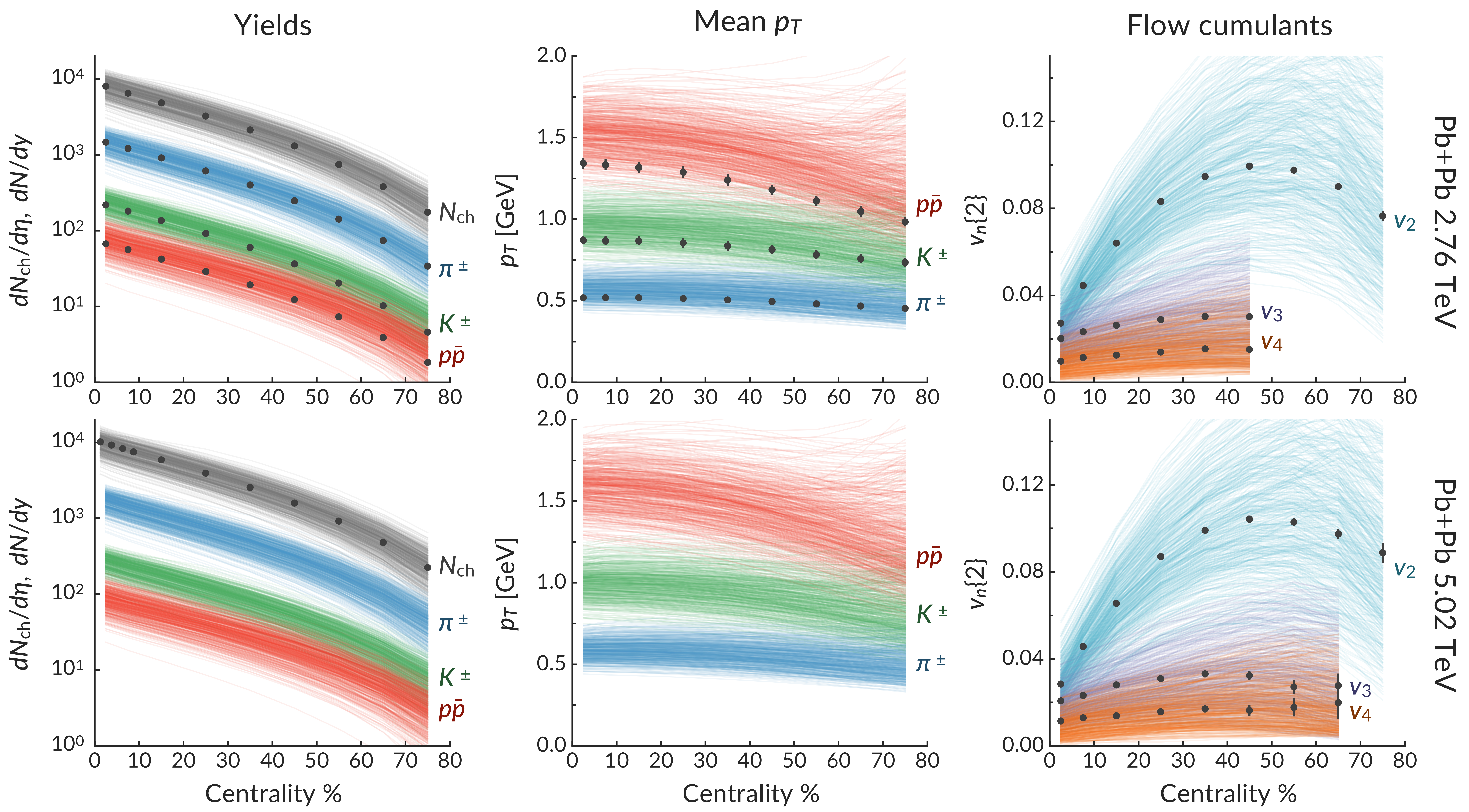
Likelihood and Uncertainty Quantification:

Likelihood $\propto \exp[-1/2\, (\mathbf{y}-\mathbf{y}_{exp})^{T} \boldsymbol{\Sigma}^{-1} (\mathbf{y}-\mathbf{y}_{exp})]$

- covariance matrix $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}_{experiment} + \boldsymbol{\Sigma}_{model}$
- $\boldsymbol{\Sigma}_{experiment}$=stat(diagonal) + sys(non-diagonal)
- $\boldsymbol{\Sigma}_{model}$ conservatively estimated as 5%

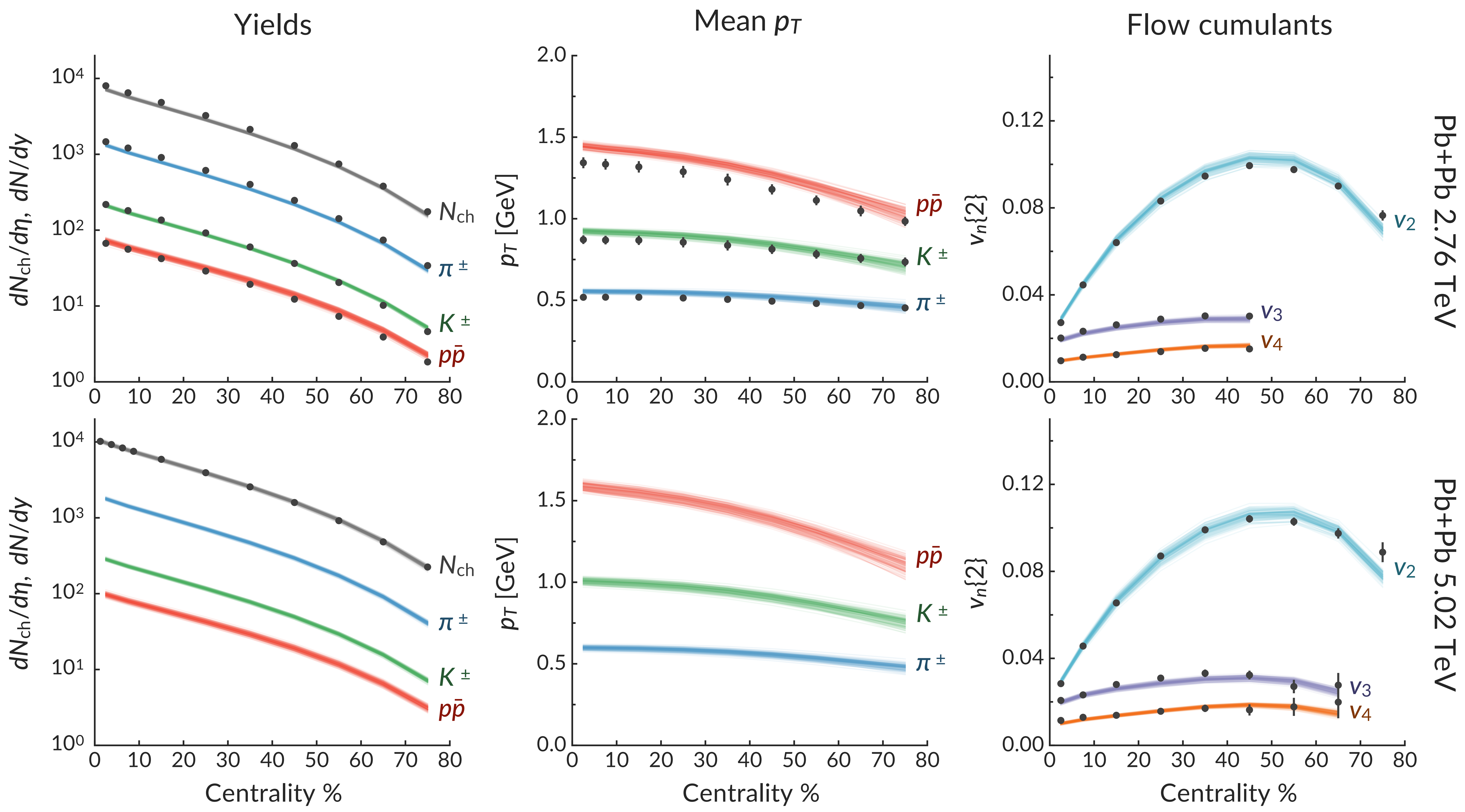
Prior vs. Posterior

Prior: model calculations evenly distributed over full design space



Prior vs. Posterior

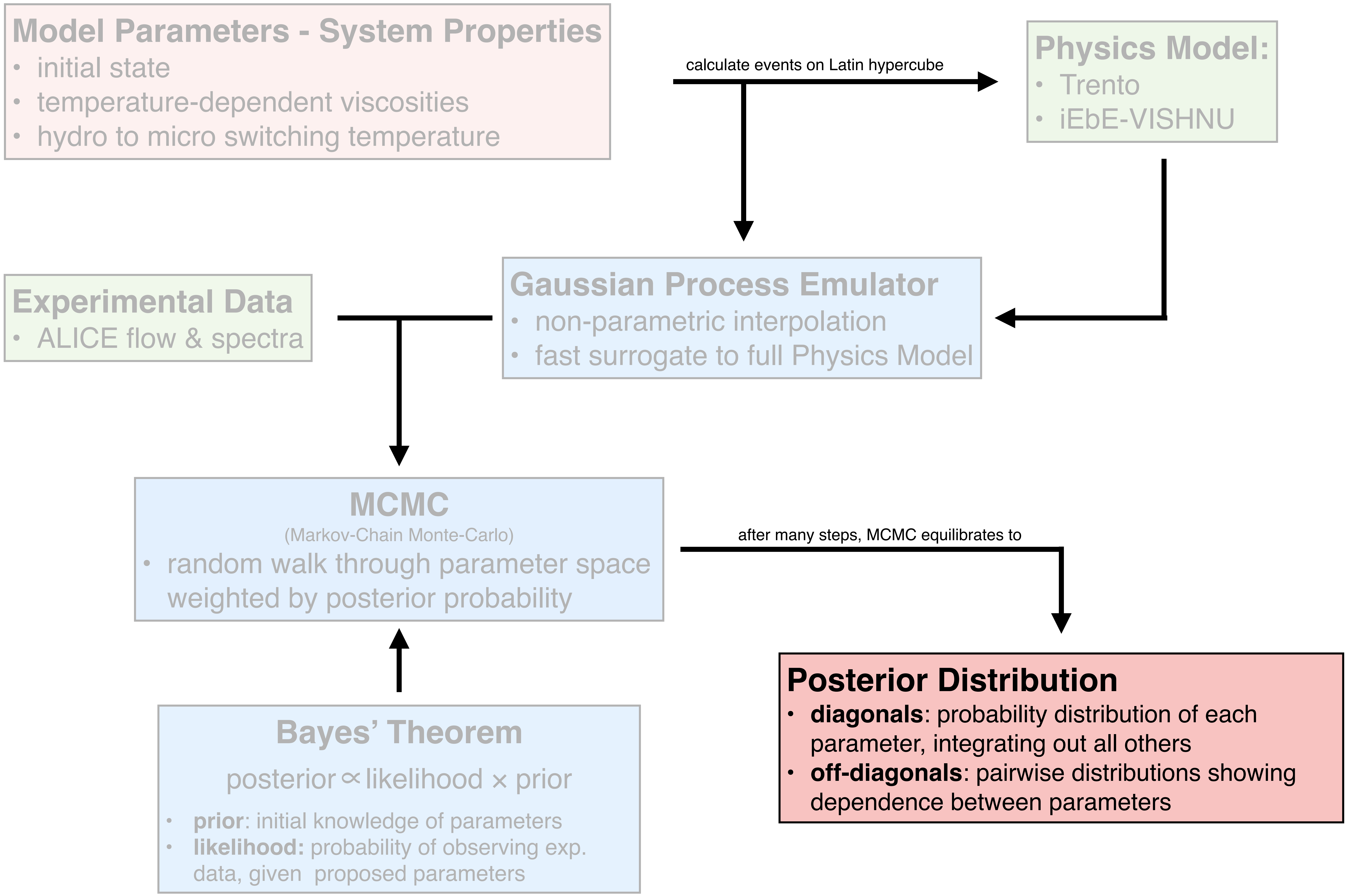
Posterior: emulator predictions for highest likelihood parameter values



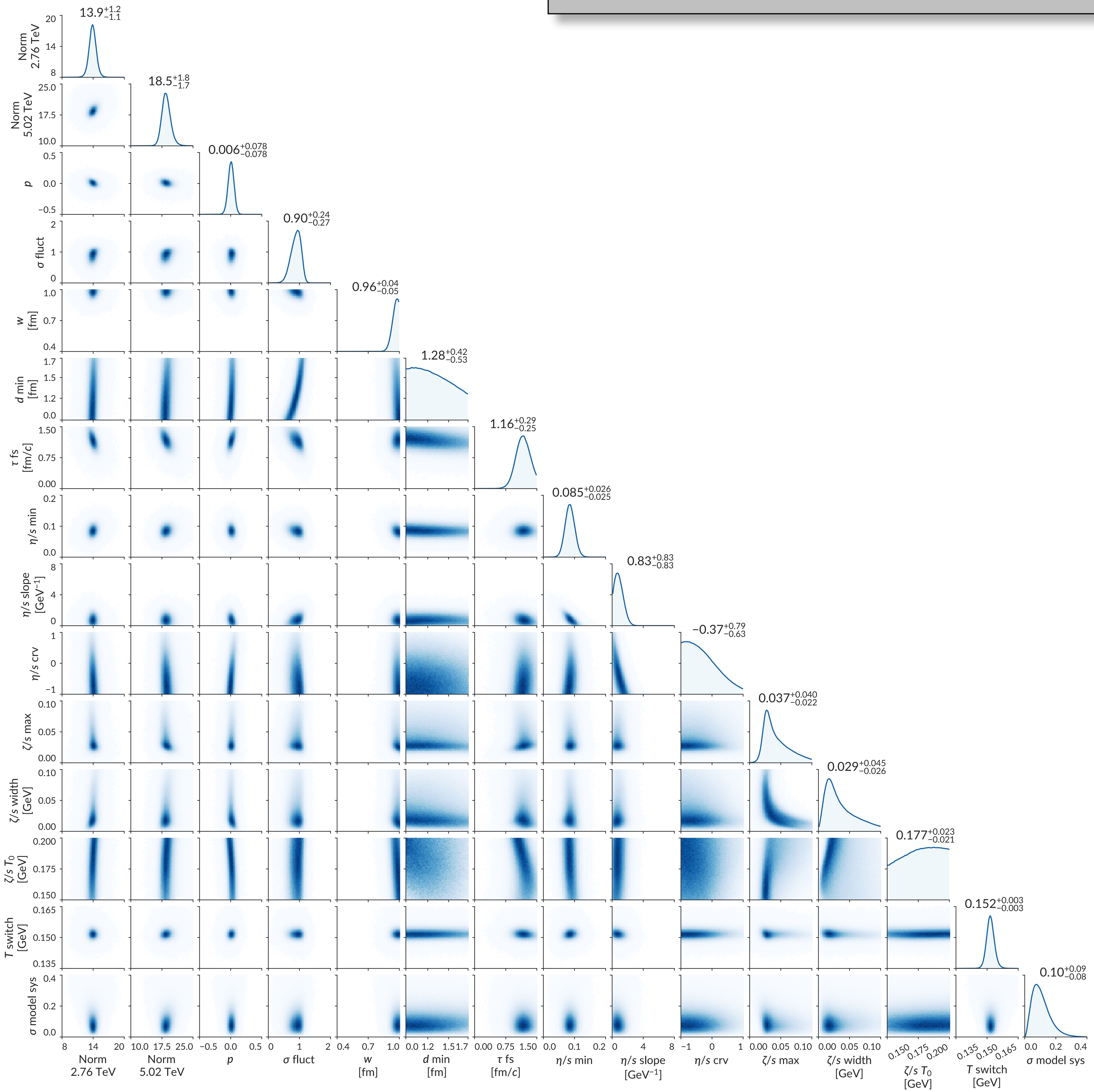
Analysis Results

Methodology: Jonah E. Bernhard, J. Scott Moreland, Steffen A. Bass, Jia Liu, Ulrich Heinz: Phys. Rev. **C94** (2016) 024907, arXiv:1605.03954
Results: Jonah E. Bernhard, PhD thesis arXiv:1804.06469; John Scott Moreland, PhD thesis arXiv:1904.08290
Jonah E. Bernhard, J. Scott Moreland & Steffen A. Bass: *Nature Physics* **15** (2019) 11, 1113-1117

Methodology



Calibrated Posterior Distribution



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

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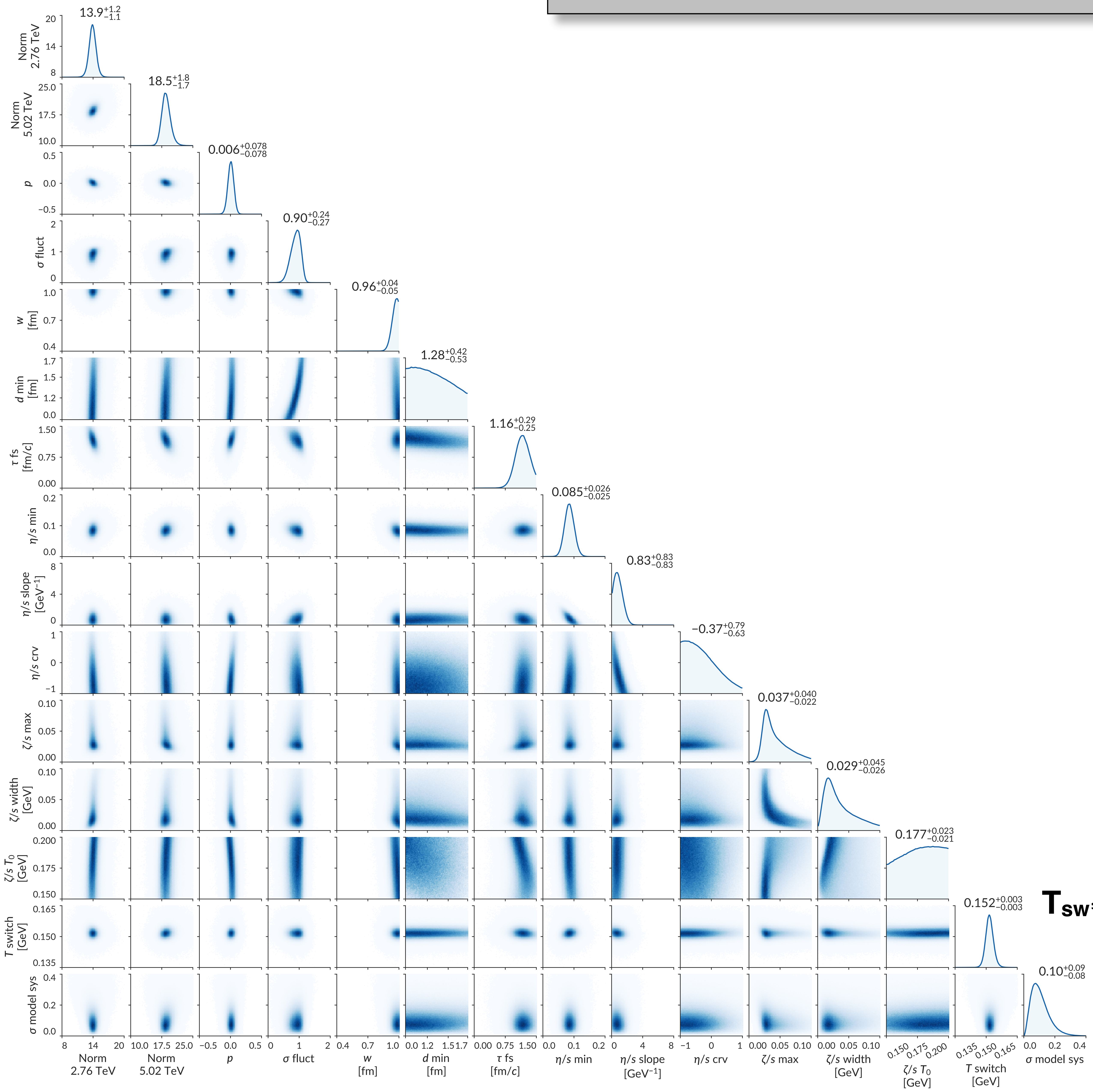

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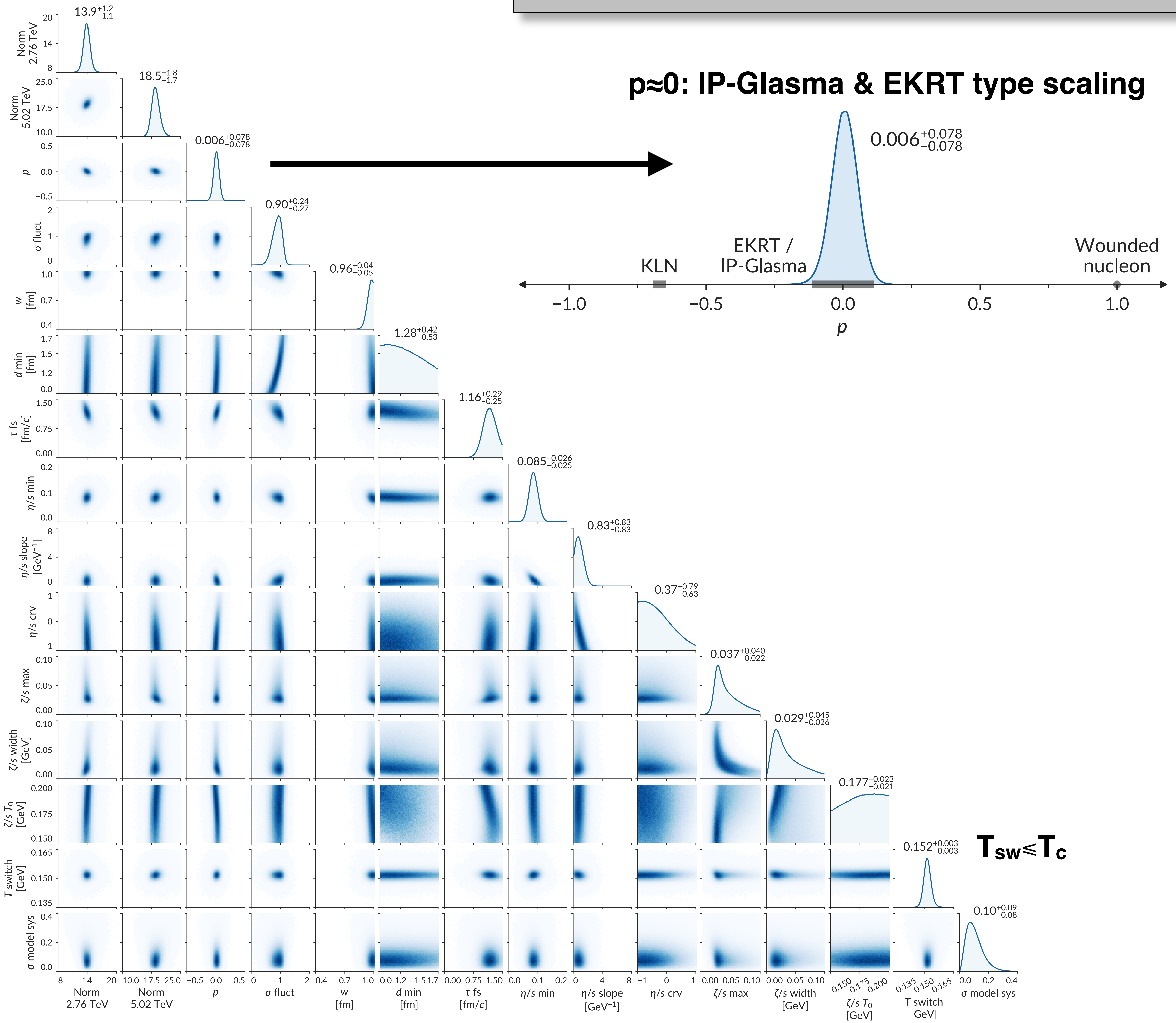

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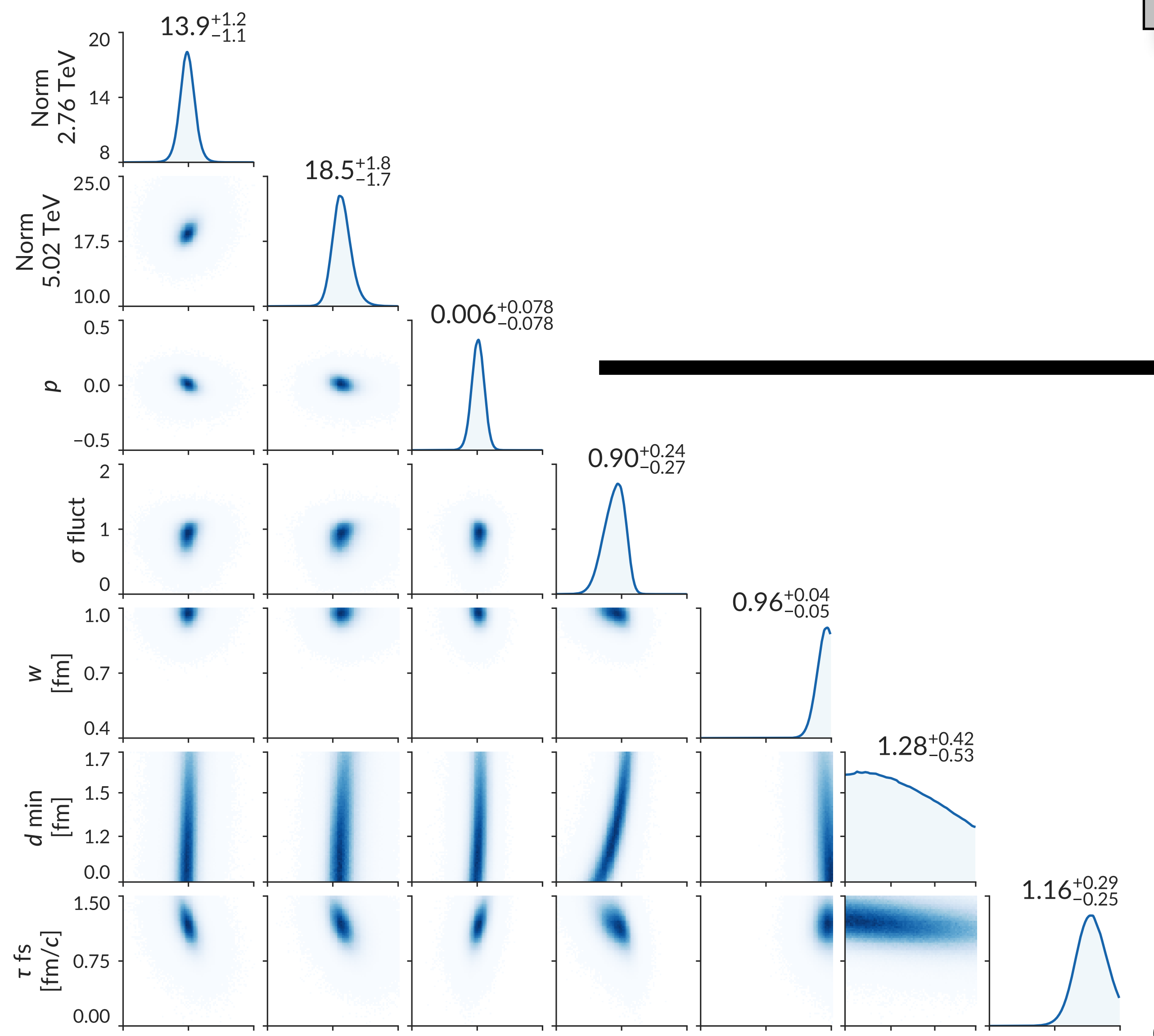
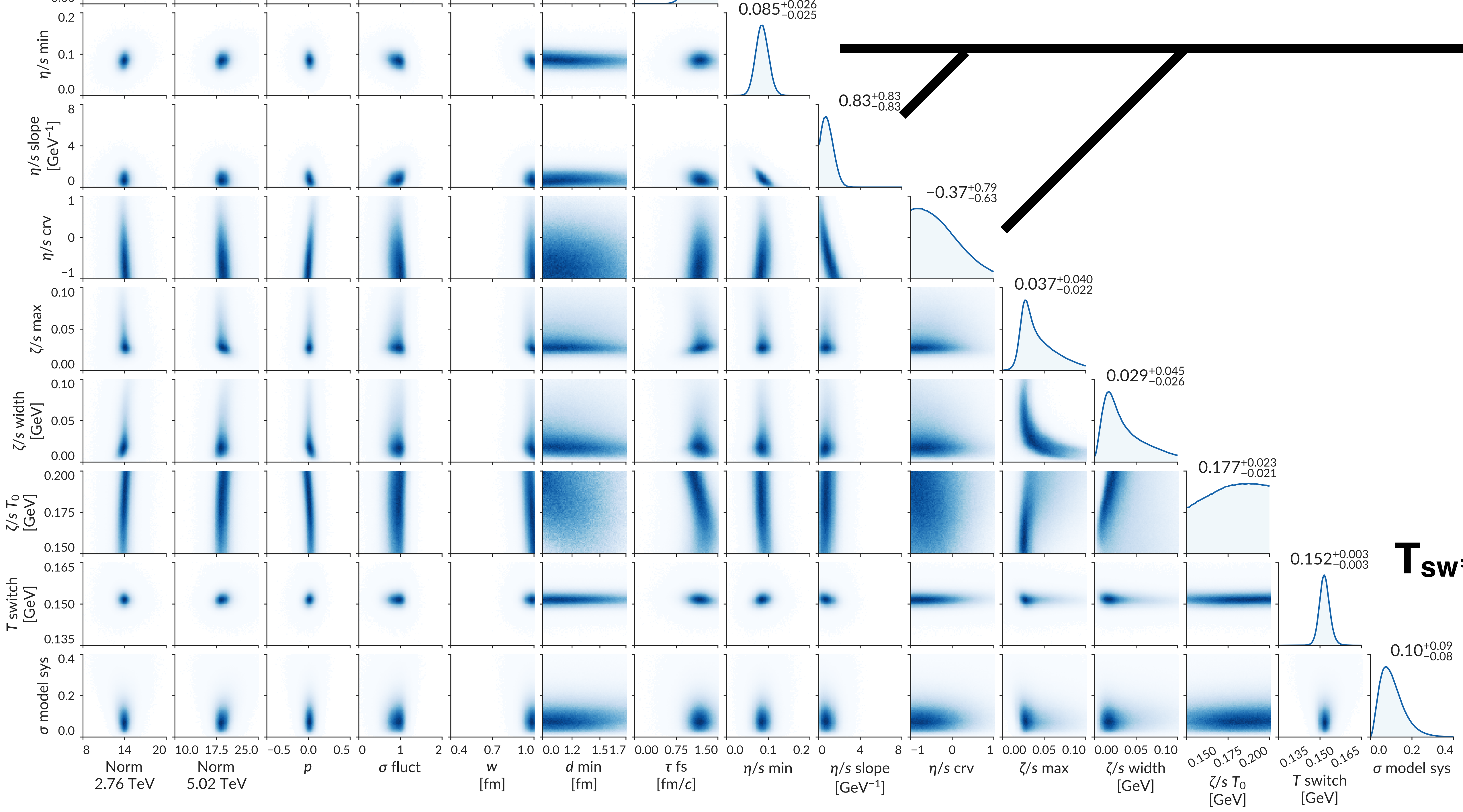

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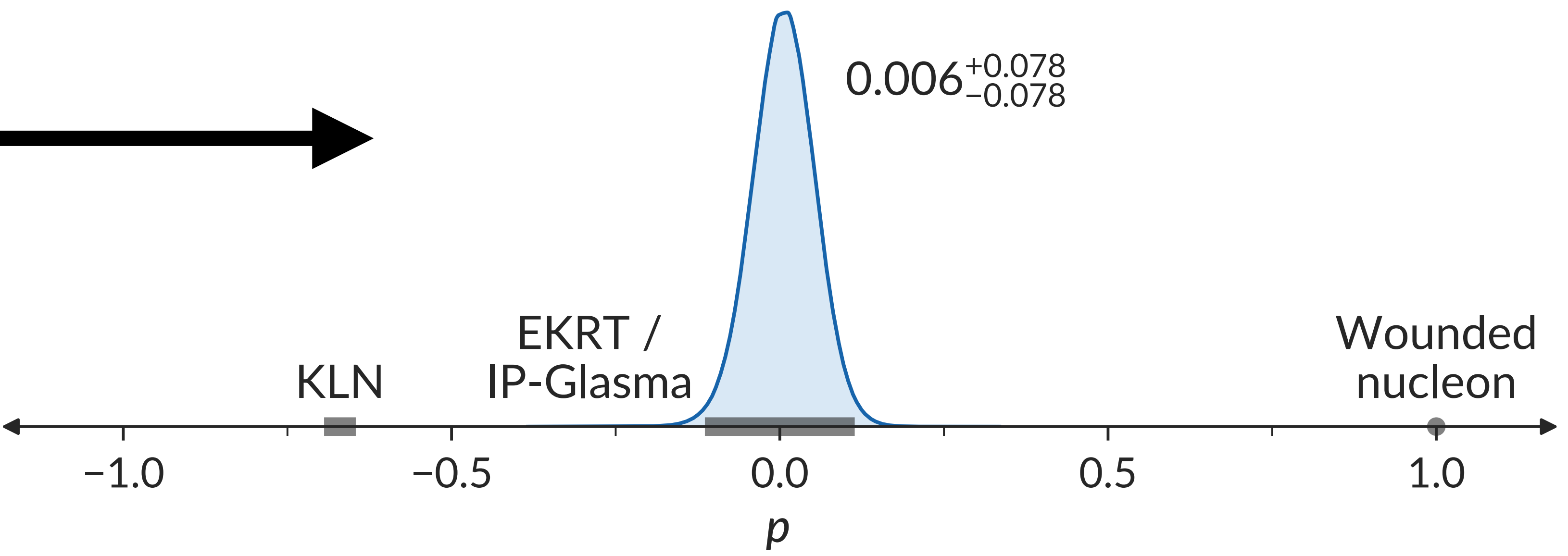

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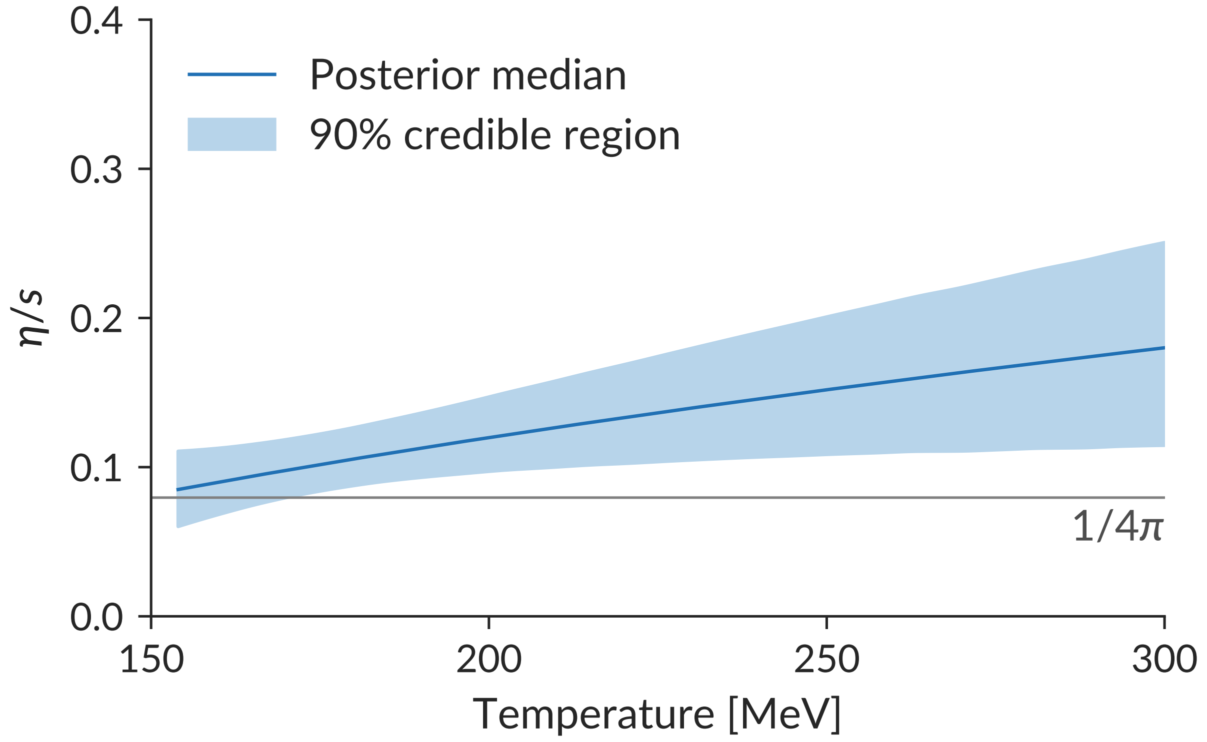
temperature-dependent viscosities:



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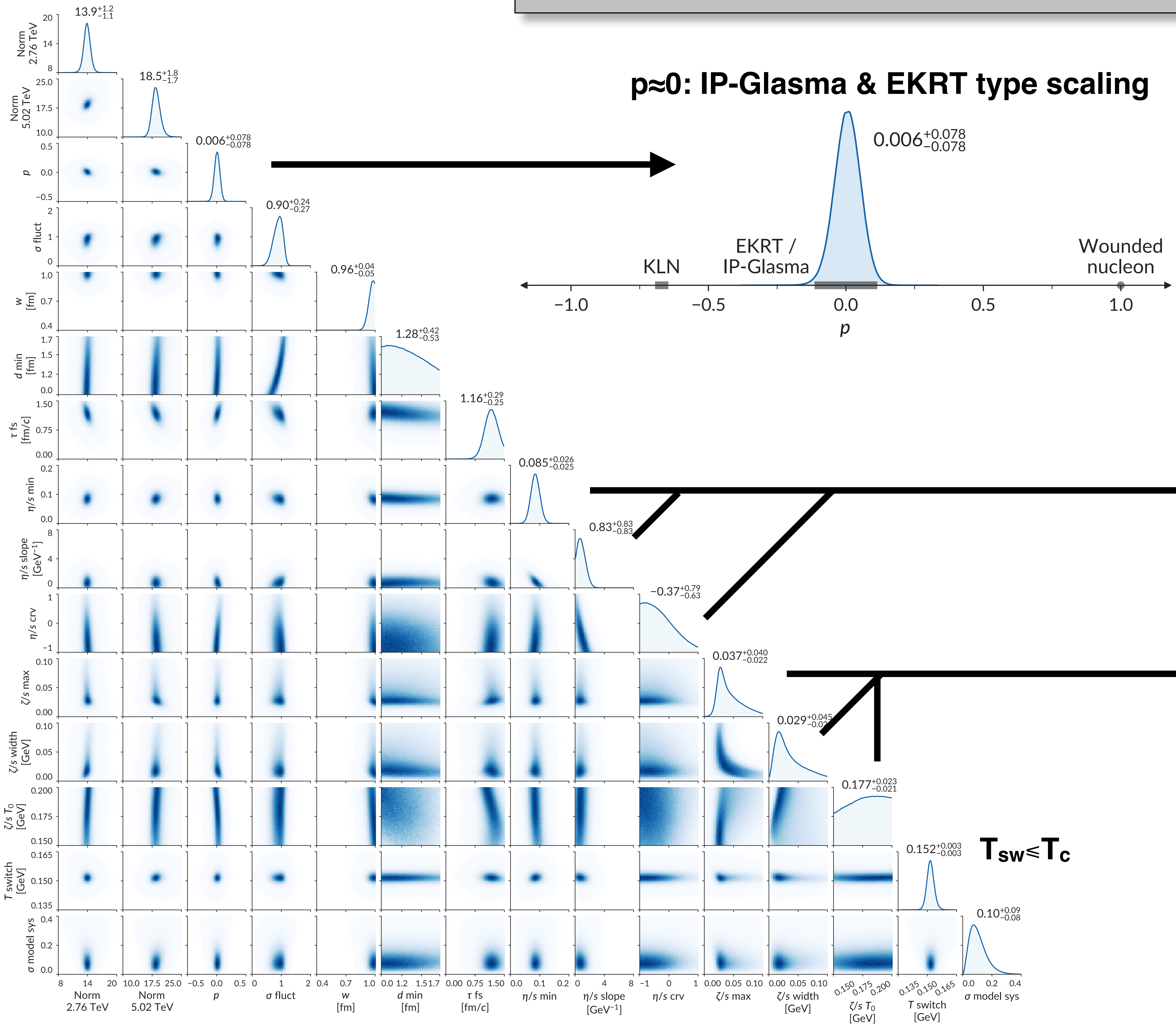

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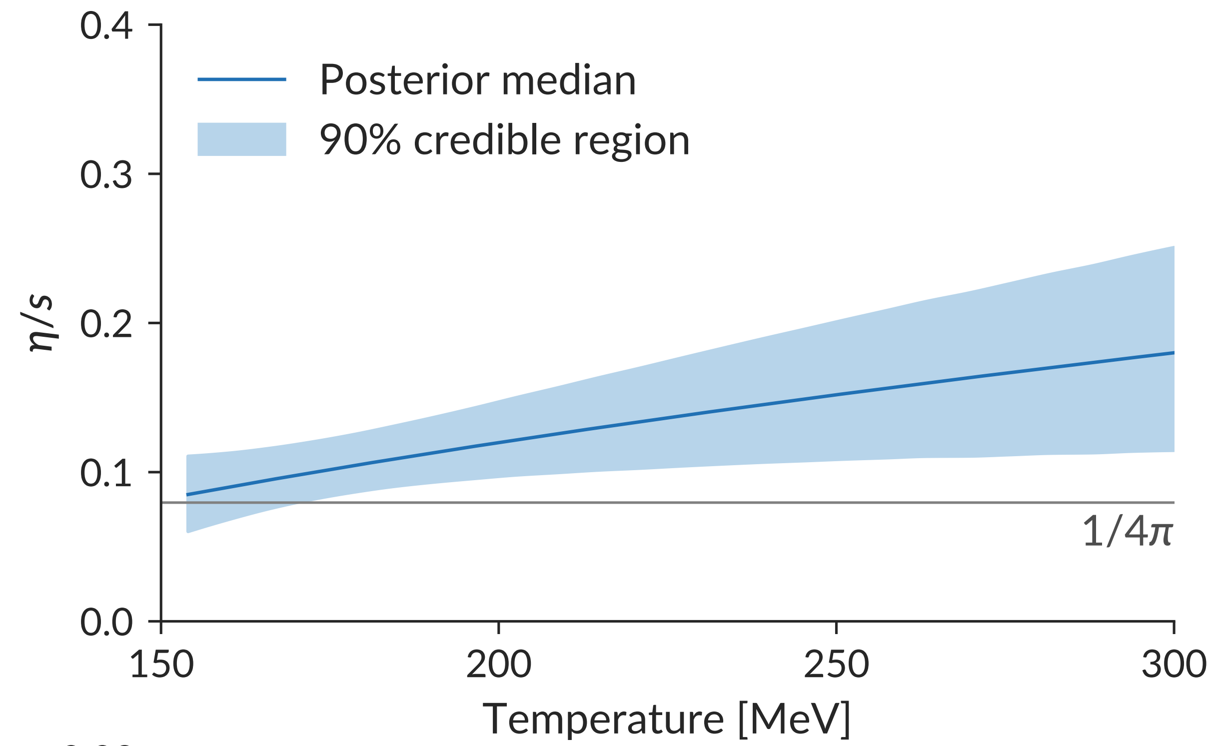
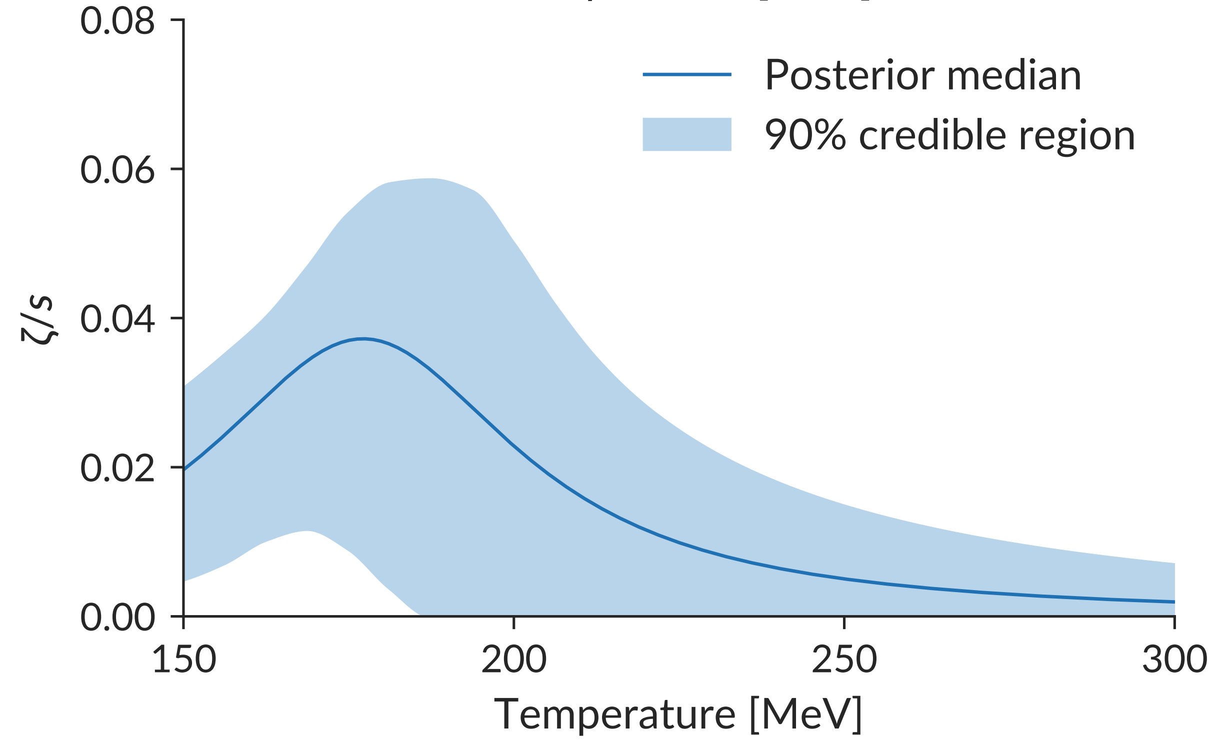


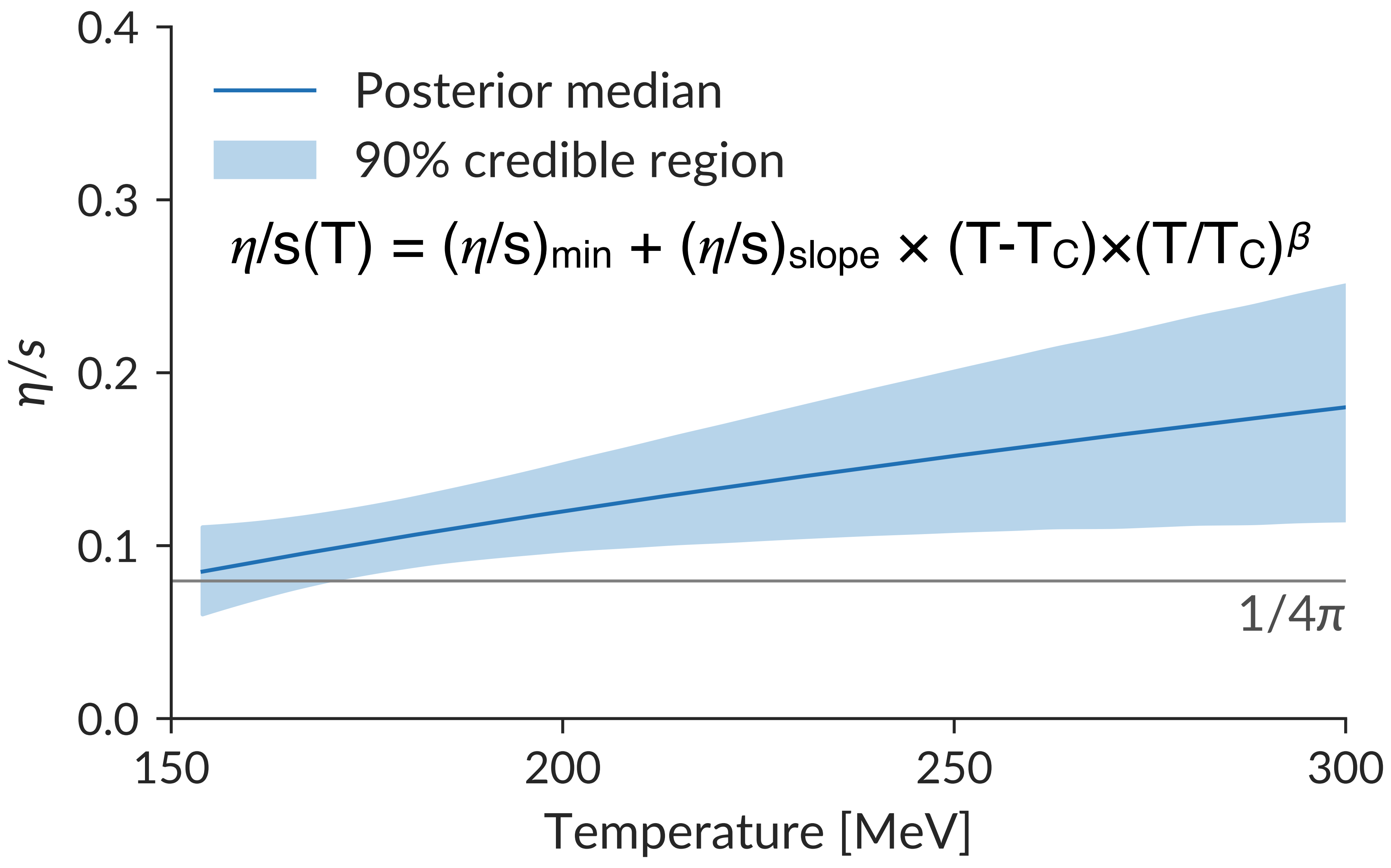


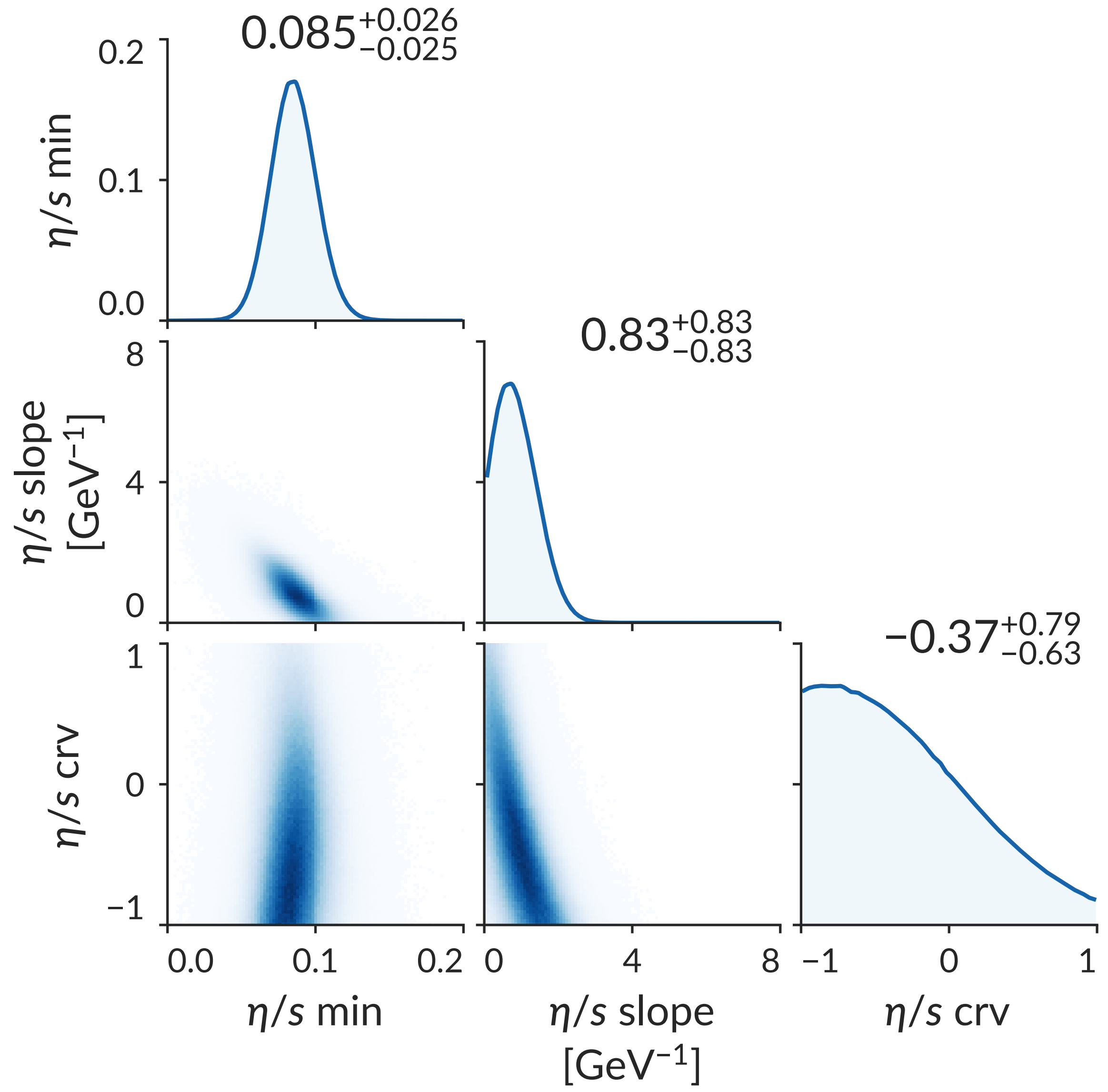
Temperature Dependence of Shear & Bulk Viscosities

temperature dependent shear viscosity:

- analysis favors small value and shallow rise
- results do not fully constrain temperature dependence:
  - inverse correlation between $(\eta/s)_{slope}$ slope and intercept $(\eta/s)_{min}$
  - insufficient data to obtain sharply peaked likelihood distributions for $(\eta/s)_{slope}$ and curvature β independently
- current analysis most sensitive to T< 0.23 GeV

▸ **RHIC data may disambiguate further**



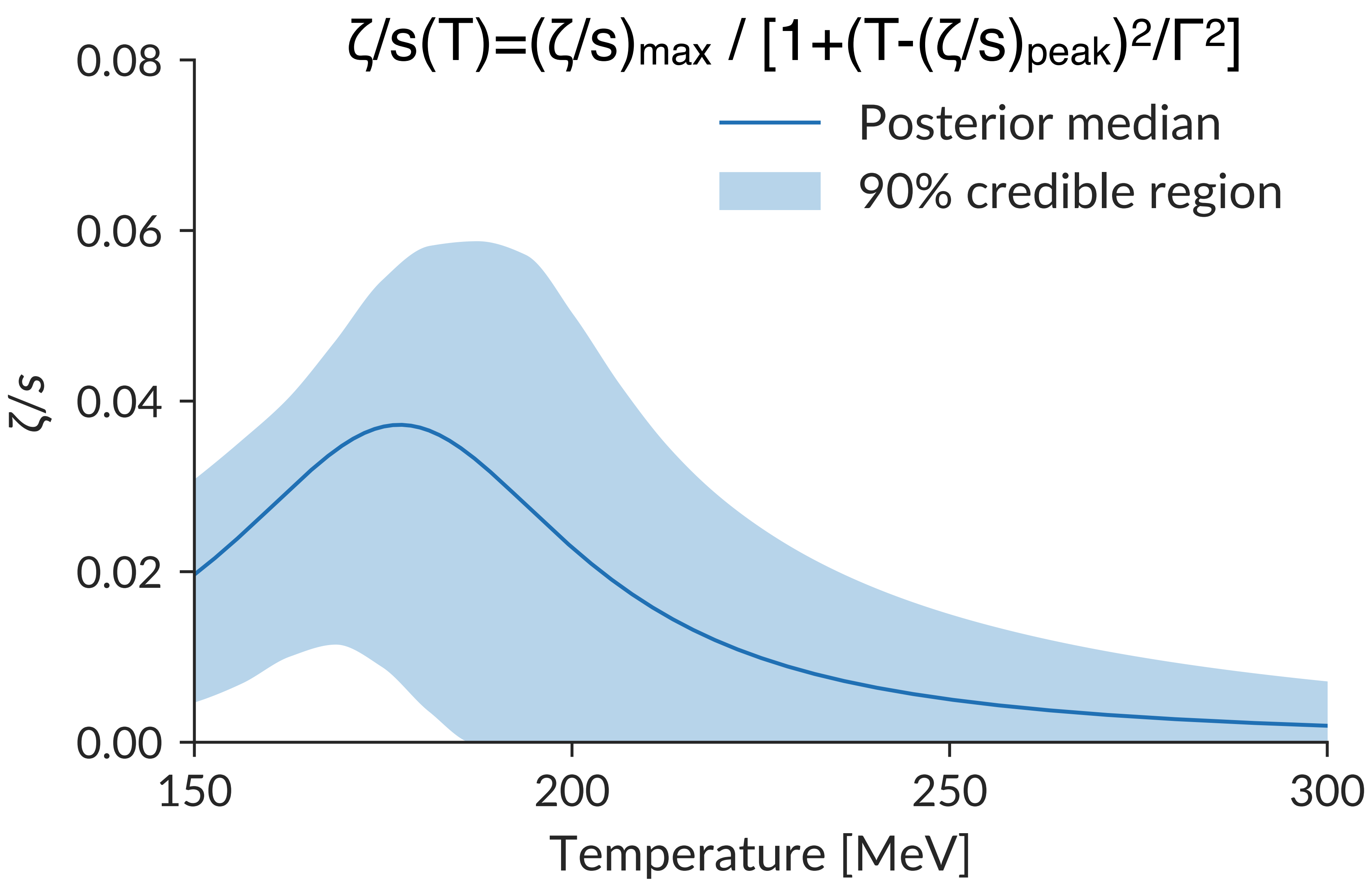


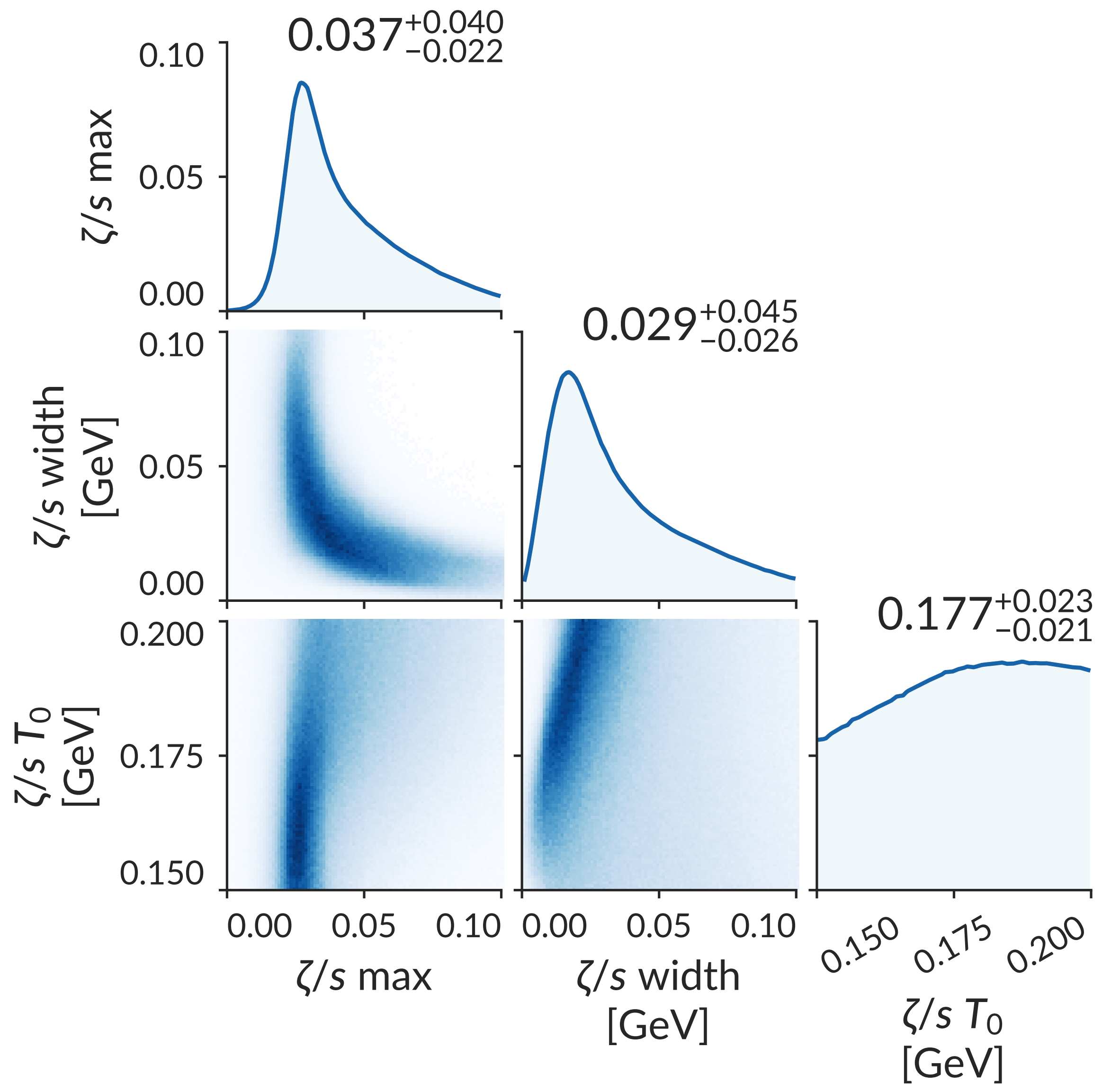
temperature dependent bulk viscosity:

- setup of analysis allows for vanishing value of bulk viscosity
- significant non-zero value near T_C favored, confirming the presence / need for bulk viscosity

caveat of current analysis:

- bulk-viscous corrections are implemented using relaxation-time approximation & regulated to prevent negative particle densities

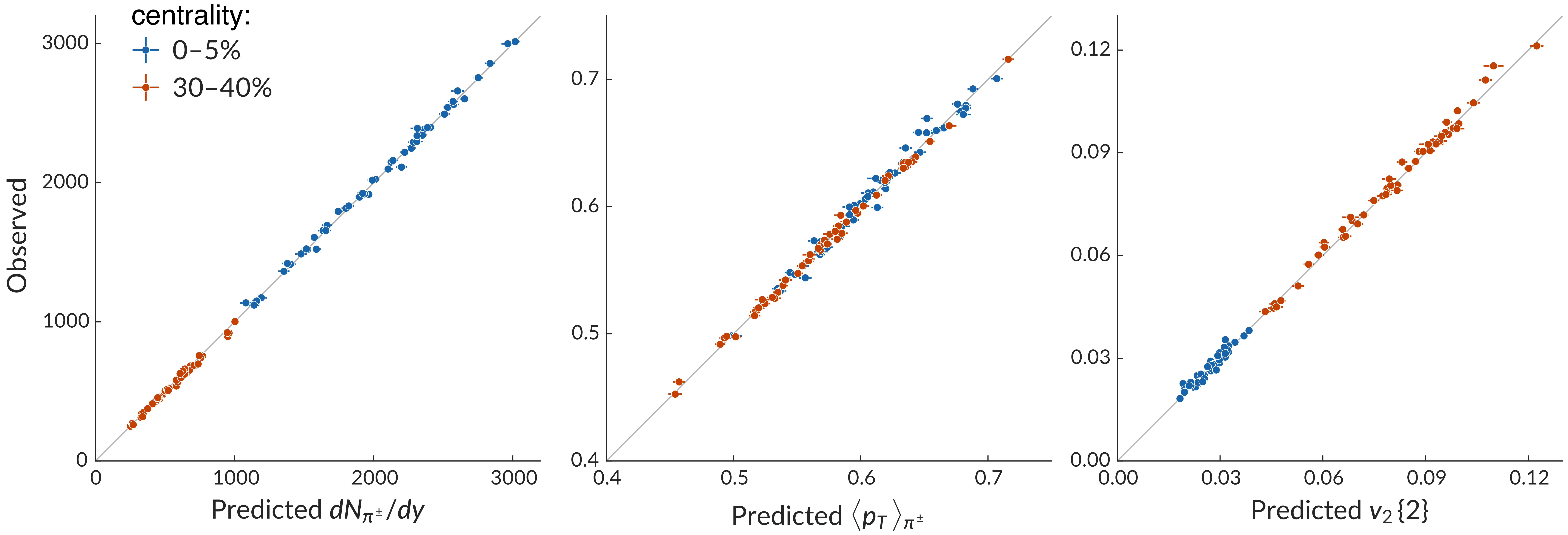




Precision Science
or
“Smoke & Mirrors”?

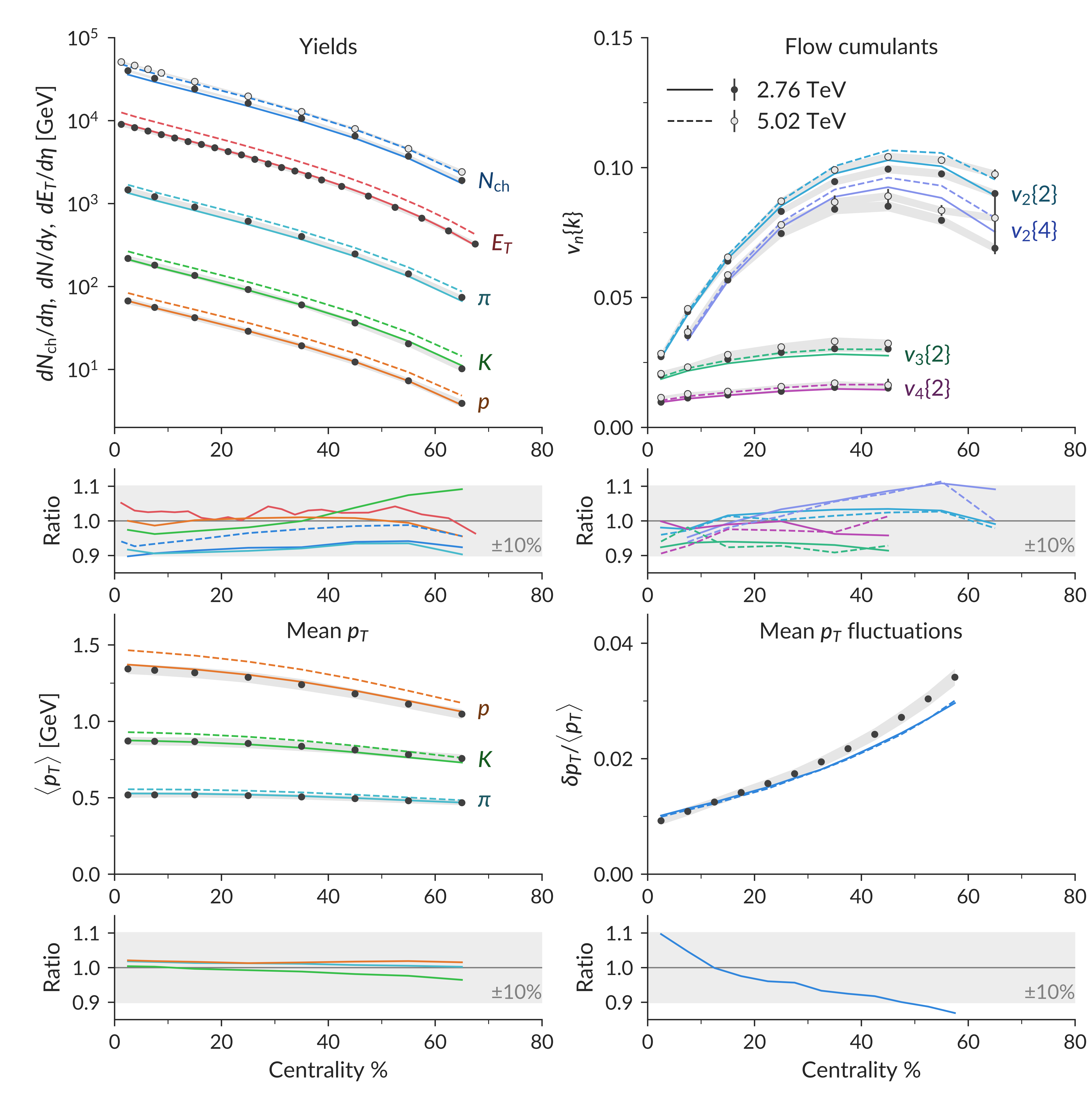
Validation

- generate a separate Latin hypercube validation design with 50 points
- evaluate the full physics model at each validation point
- compare physics model output to that of the previously conditioned GP emulators:



- note that since GPEs are stochastic functions, only ~68% of predictions need to fall within 1 standard deviation

Verification: Explicit Model Calculation



- explicit physics model calculations (no emulator) with parameter values set to the maximum of the posterior probability distributions yield excellent agreement with data!

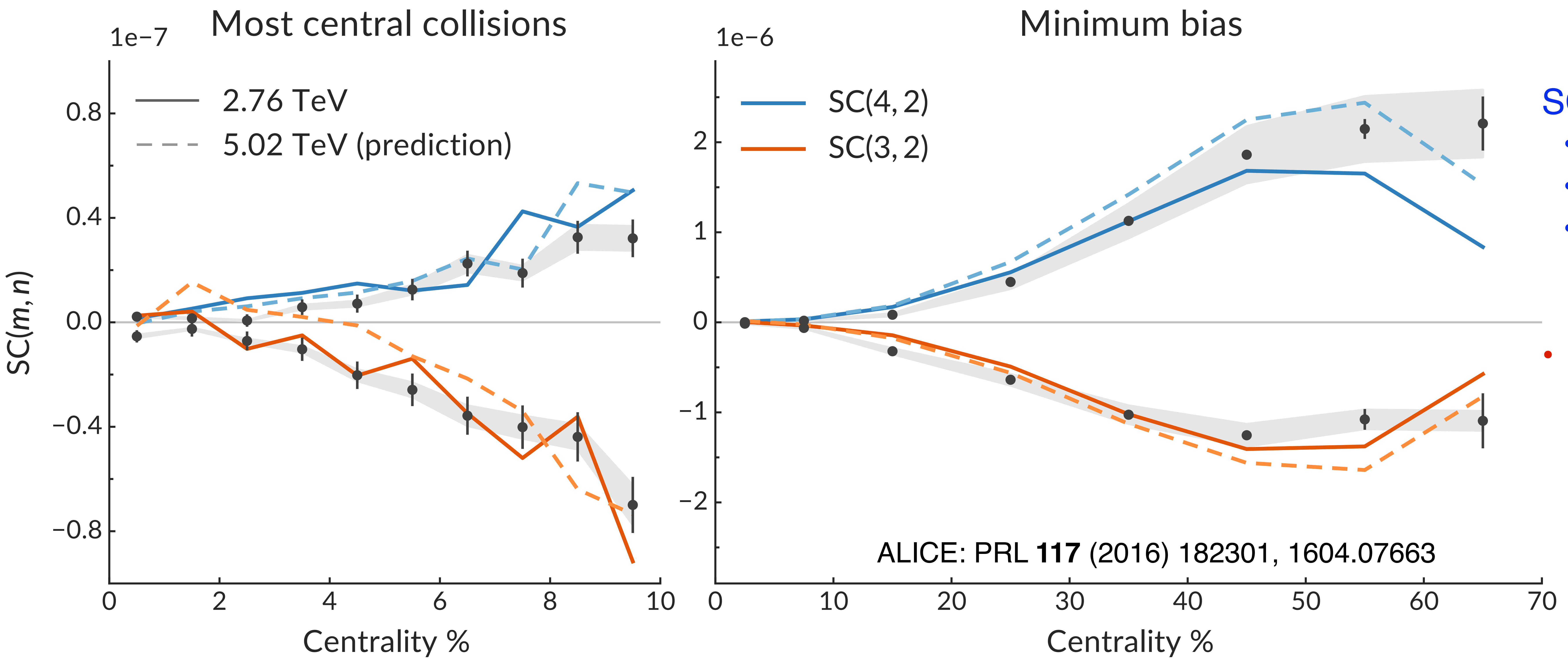
- description of data to within ±10% accuracy

Prediction: Non-Calibrated Observables

The robustness and quality of the Physics Model can be tested by making predictions on observables not used during calibration using highest likelihood parameter values.

Example: correlations between event-by-event fluctuations of flow harmonics

$SC(m,n) = \langle v^2_m v^2_n \rangle - \langle v^2_m \rangle \langle v^2_n \rangle$



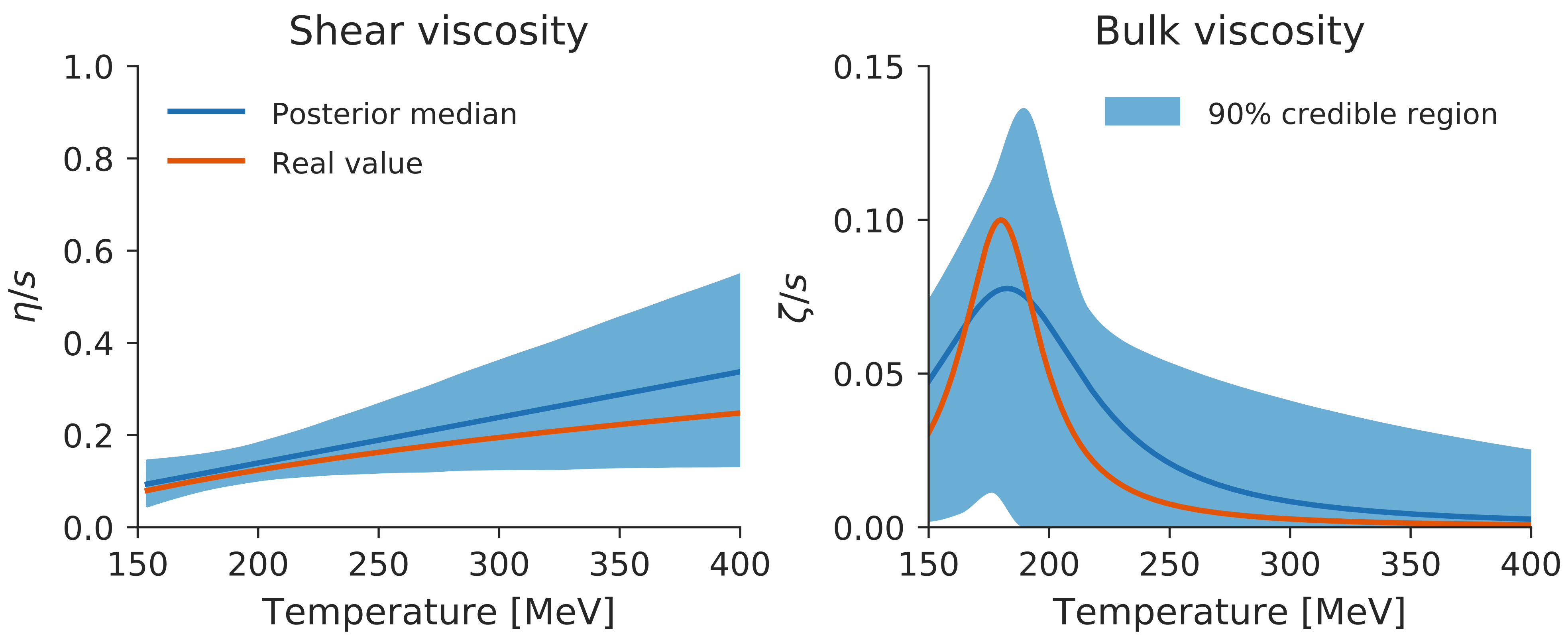
SC(m,n) are sensitive to:
- initial conditions
- evolution model
- QGP transport coefficients

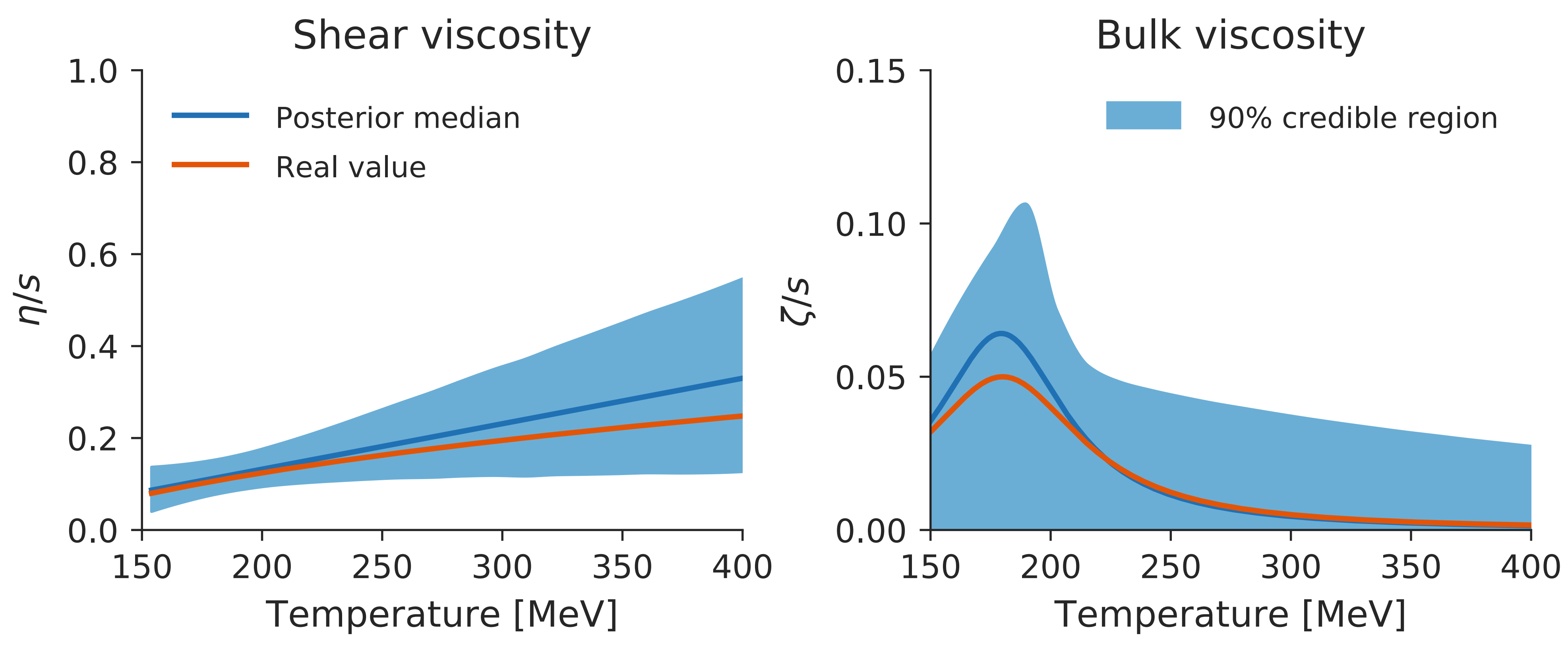
- excellent agreement of model prediction to data!

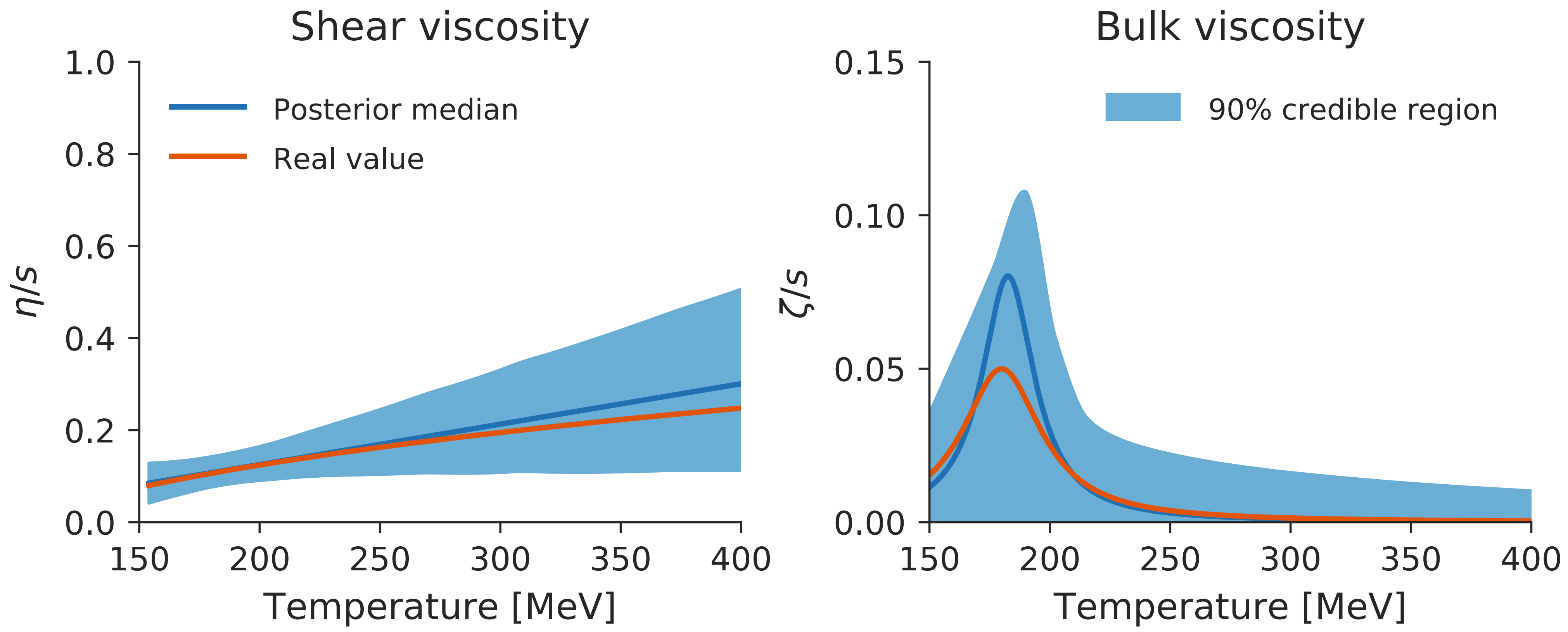
Closure Test

Need to verify that analysis can recover “true” values for the parameters: run physics model with chosen set of parameters, generate “fake data” from model output and then conduct analysis on that fake data to test if the input parameters can be recovered!

- both, smooth functions as well as peaked functions, can be reproduced well within the 90% CR
- note: due to reduction of information when going from model output to observables & model/GP uncertainties one should not expect a one-to-one reconstruction
- bulk analysis is mostly sensitive to area under bulk peak, not peak position, height & width independently







Next steps:

- **sub-nucleon degrees of freedom**
- **forward/backward rapidity**

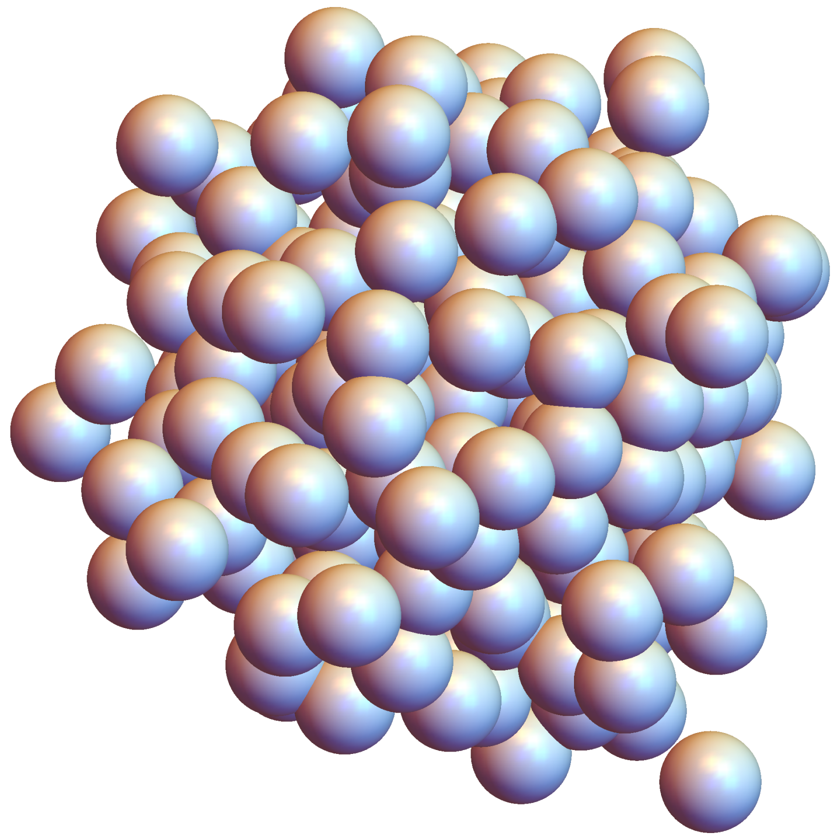
W. Ke, J.S. Moreland, J.E. Bernhard & S.A. Bass: Phys. Rev. **C96** (2017) 044912, arXiv:1610.08490
J.S. Moreland, J.E. Bernhard & S.A. Bass: Phys. Rev. **C101** (2020) 024911, arXiv 1808.02106

Nucleon Substructure

Original Trento model:

- sample nucleon positions from spherical or deformed Woods-Saxon distributions
- solid angles resampled to preserve minimum distance d_{min}
- Gaussian nucleons of width w
- works very well for large nuclei

^{208}Pb nucleus



Caveat:

- spherical protons do not allow for proper eccentricities in p+A or small/asymmetric collision systems

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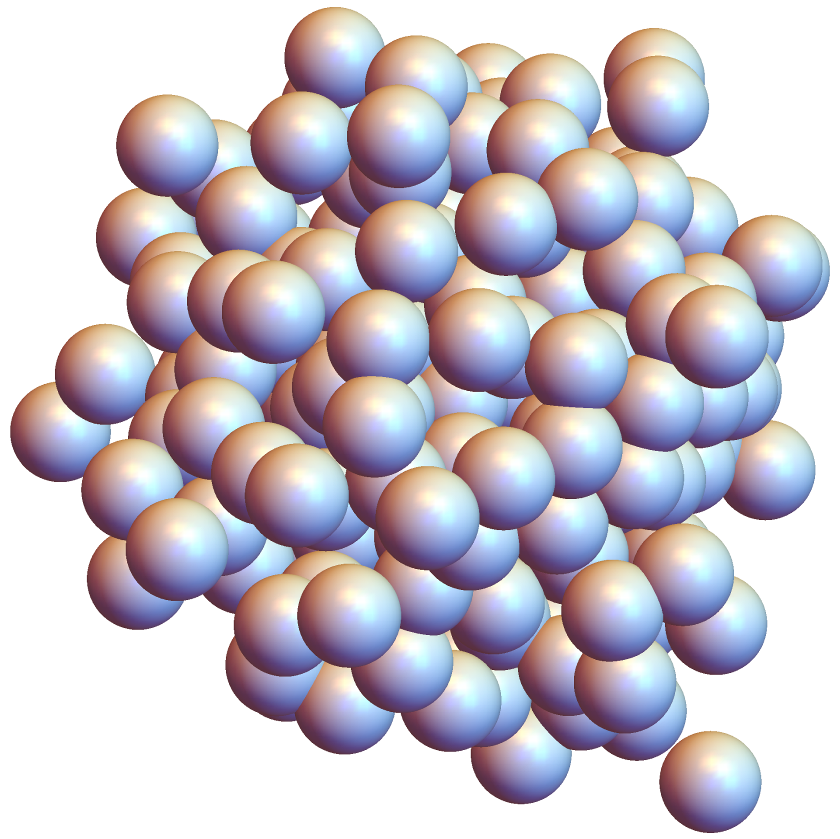

Caveat:

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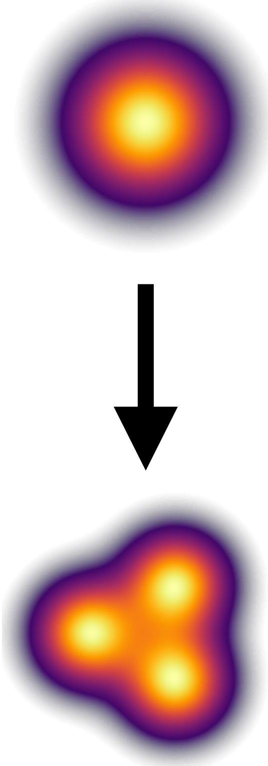
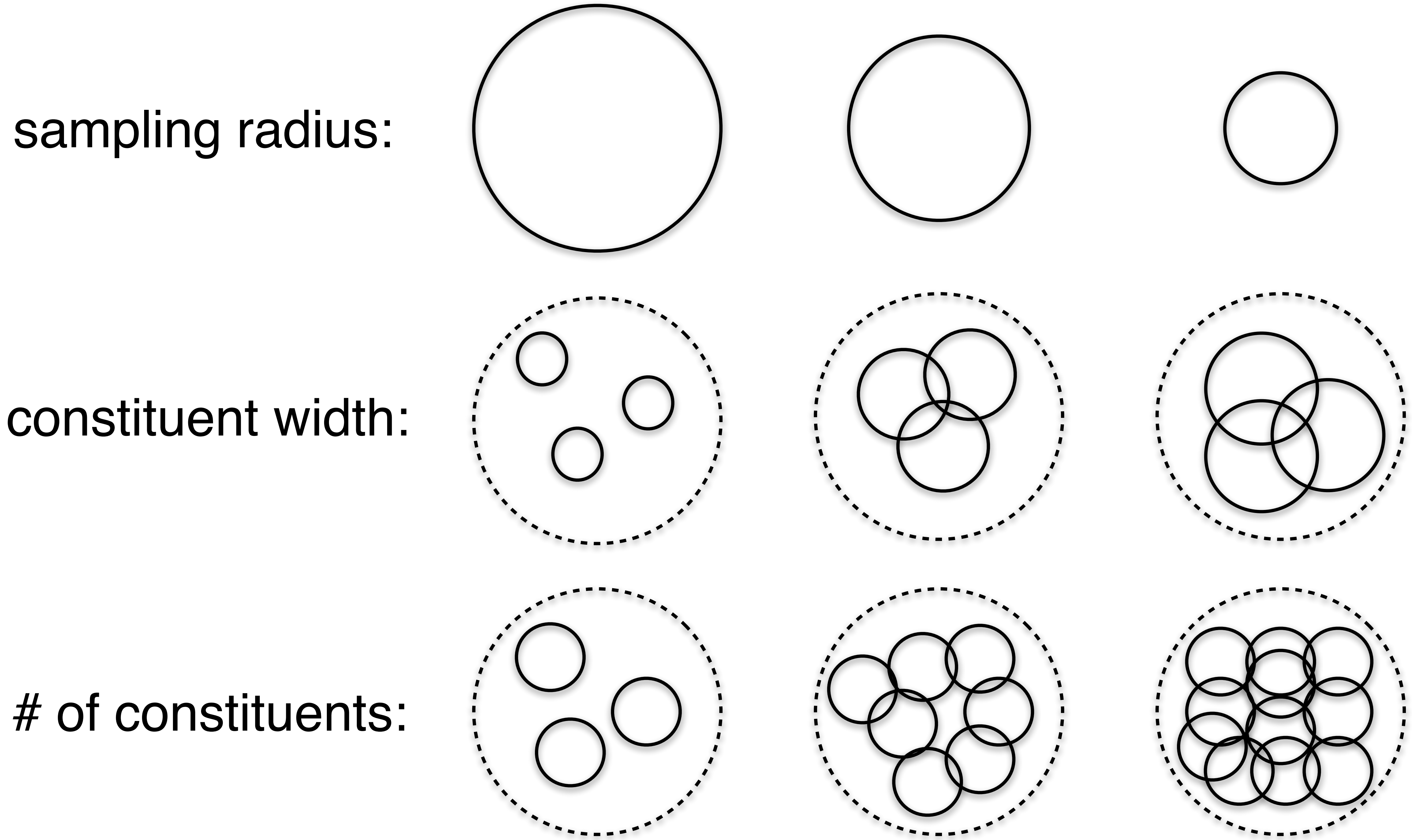
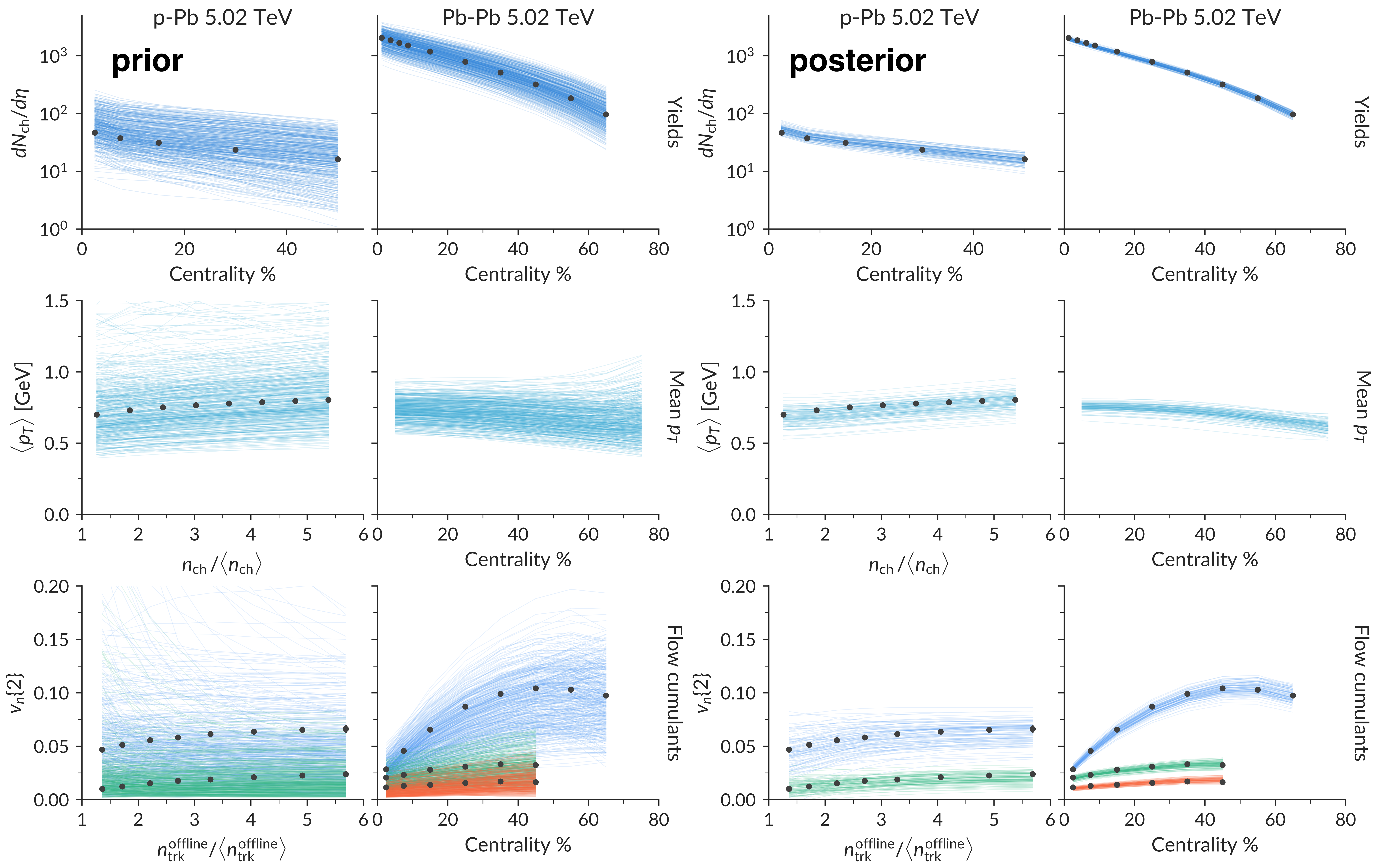
Trento with nucleon substructure:

- trade Gaussian nucleons for lumpy nucleons
- additional parameters:
  - sampling radius of constituent positions
  - constituent Gaussian width
  - number of constituents in each nucleon



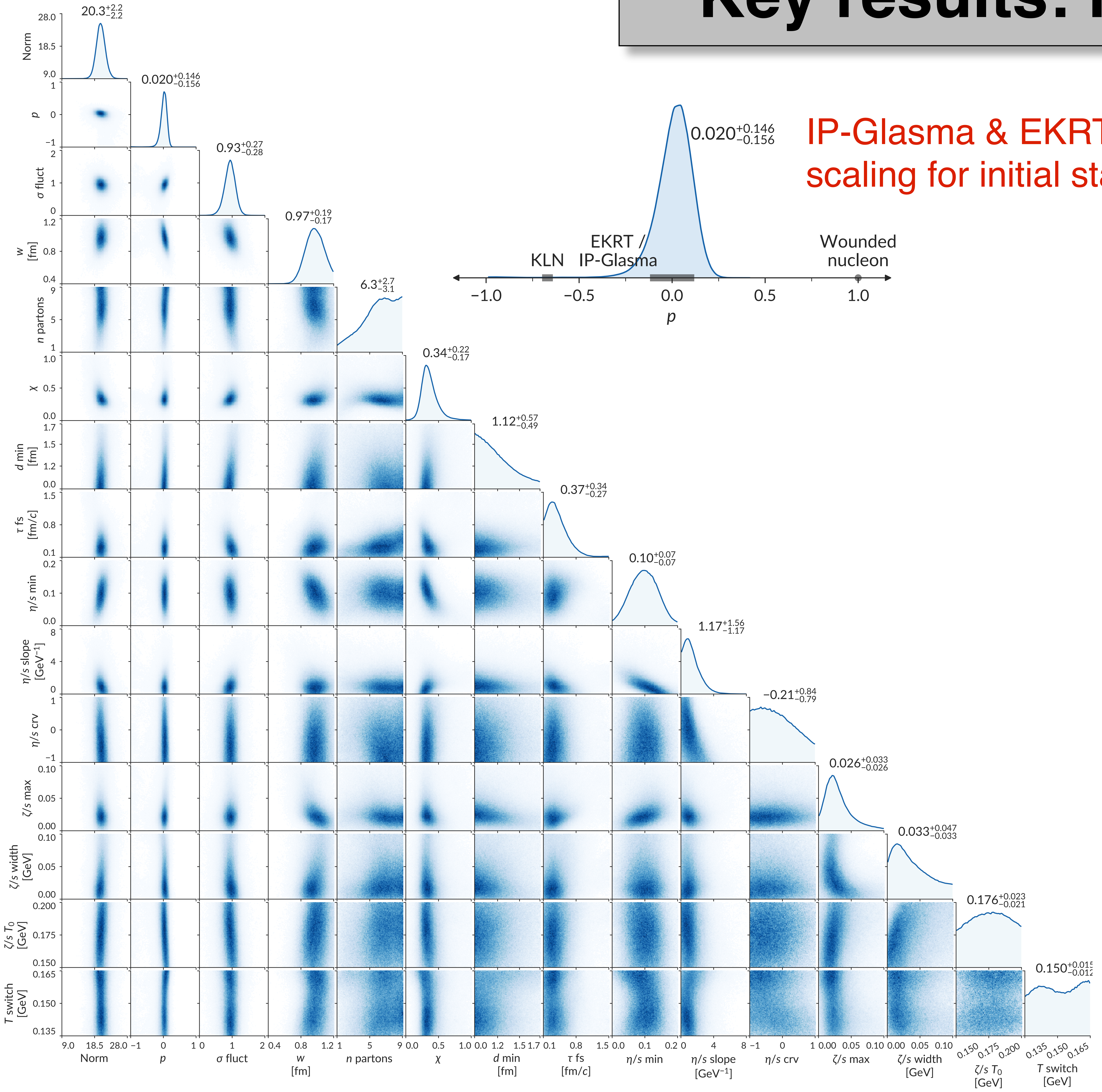


Simultaneous Calibration on AA and pA

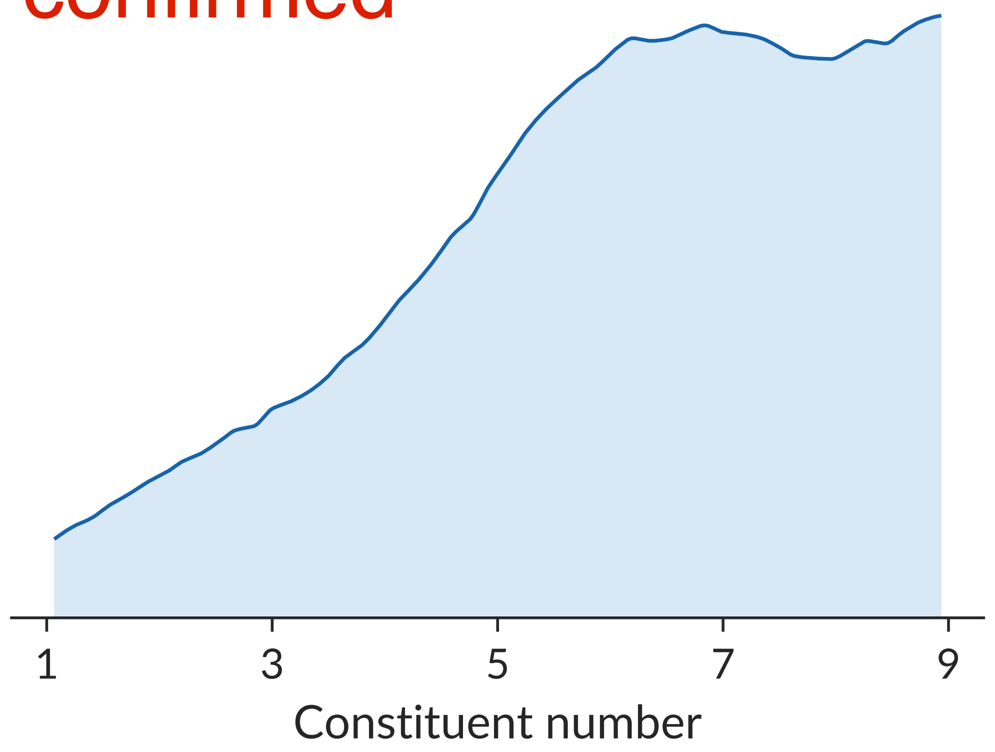


- ALICE & CMS data for AA & pA at 5.02 TeV
- calibration on 15 parameters, for initial state, shear and bulk viscosities
- restriction on 1 energy to keep computational effort reasonable
- generally larger uncertainties in posterior, due to less data than in the AA calibrations for 2 energies…

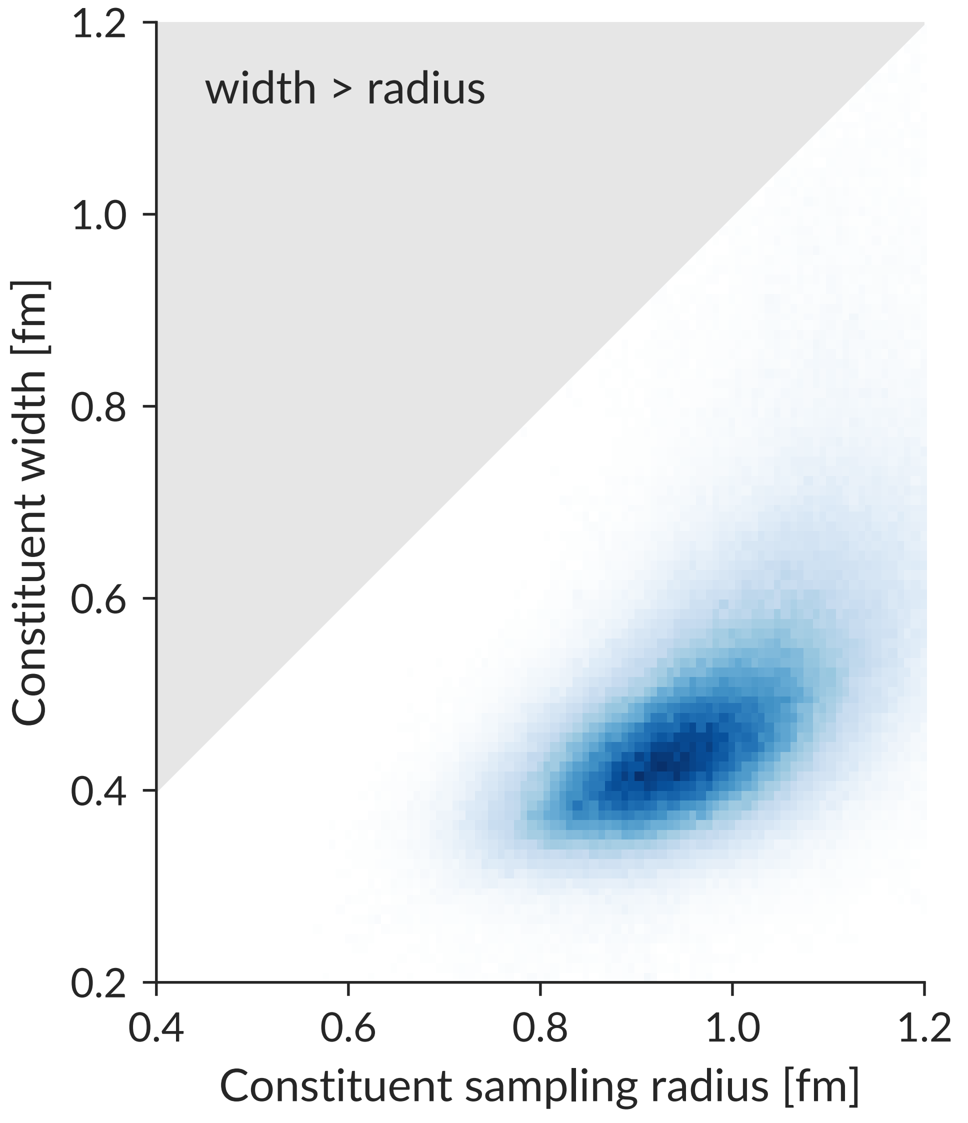
Key results: initial state



IP-Glasma & EKRT eccentricity scaling for initial state confirmed



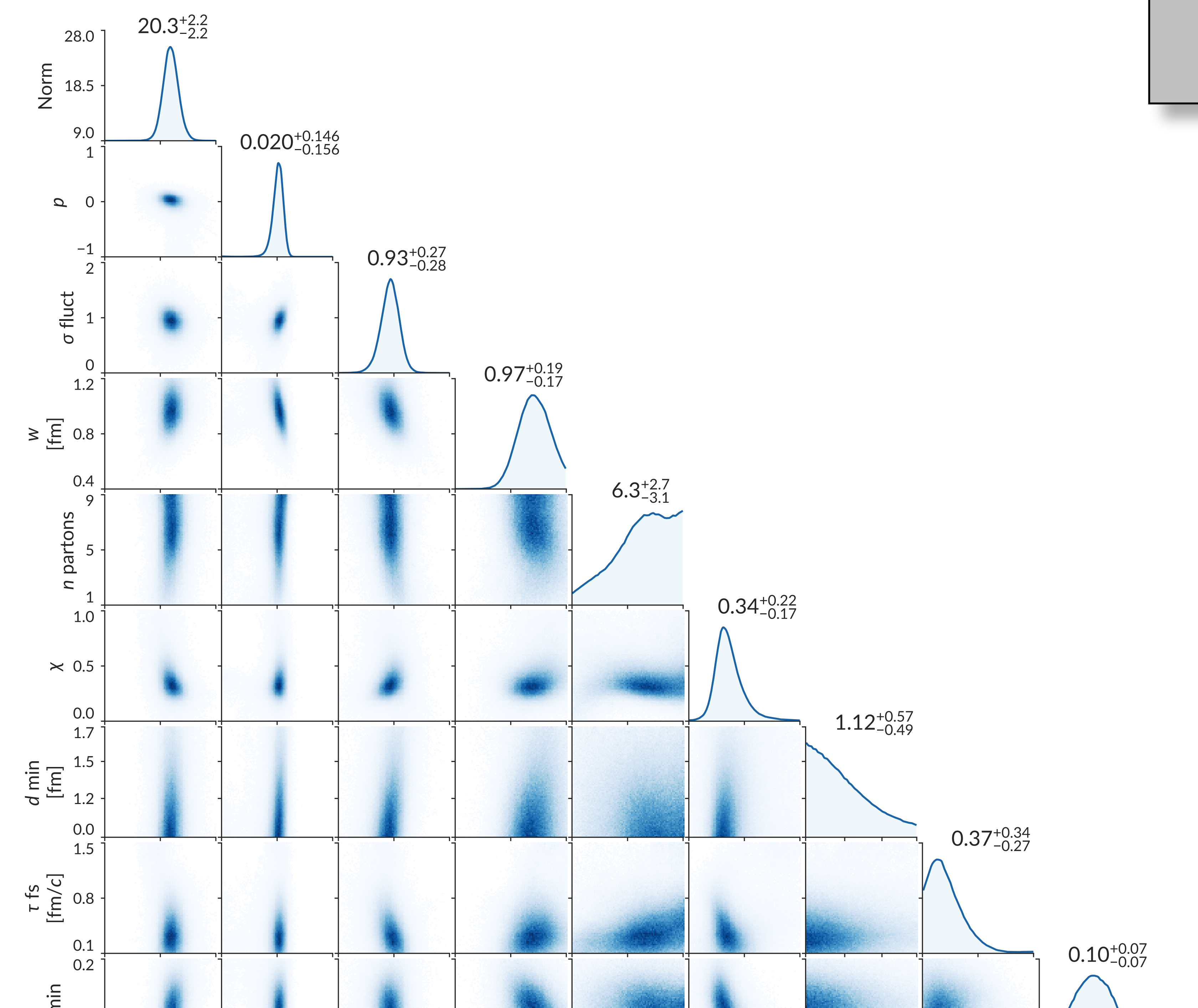
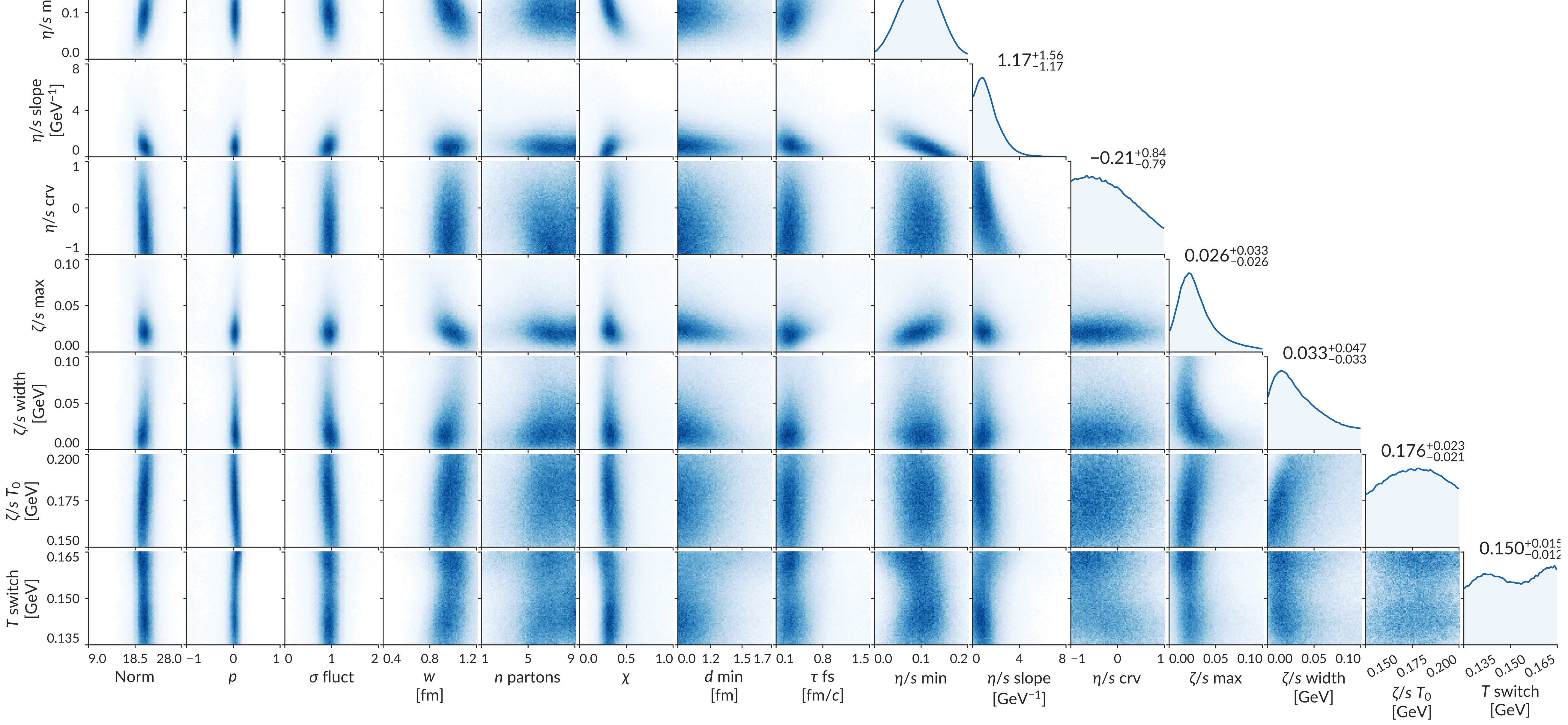
no strong preference for a particular constituent # as long as n>3

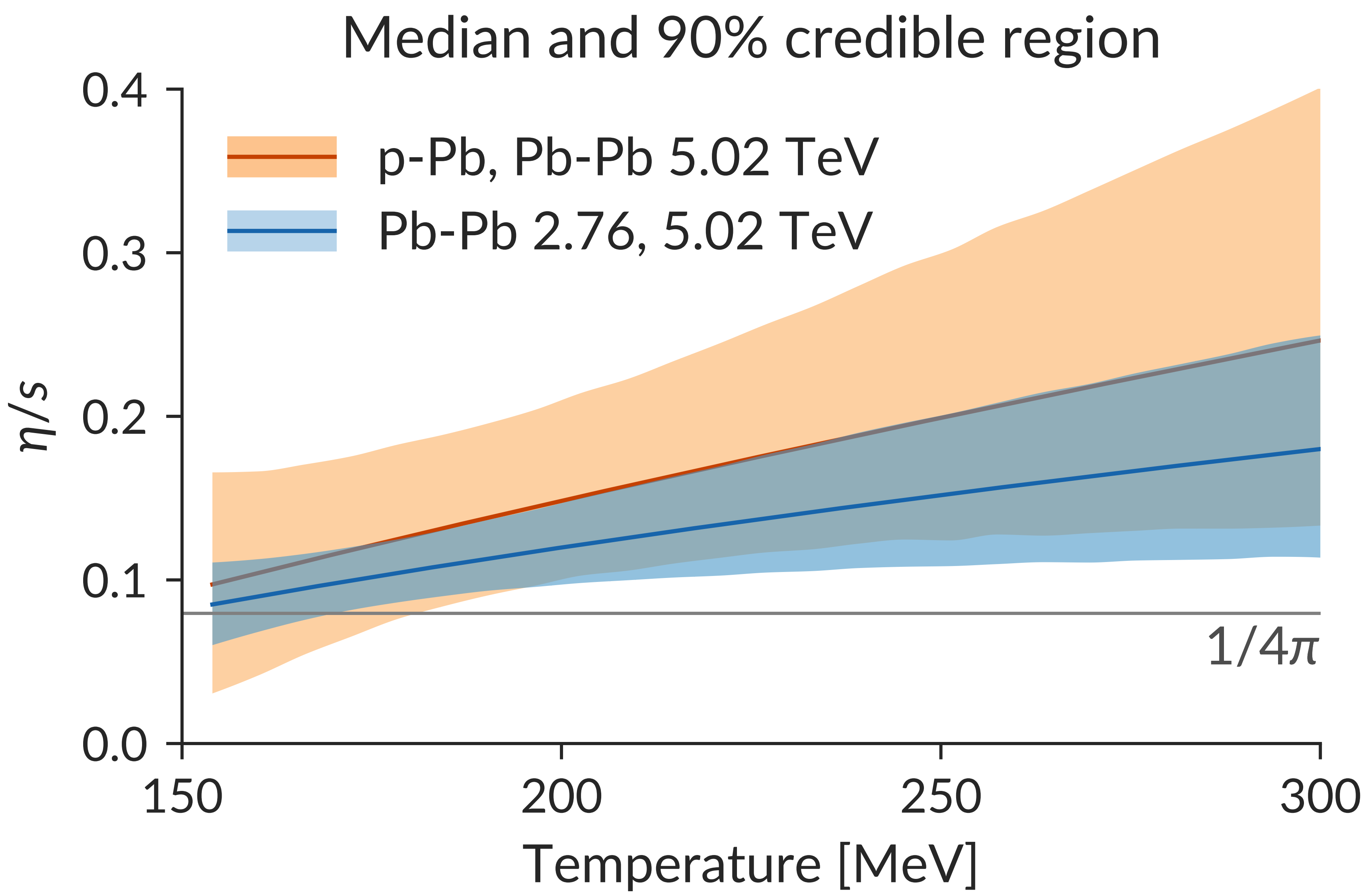


constituent width & sampling radius are well constrained to

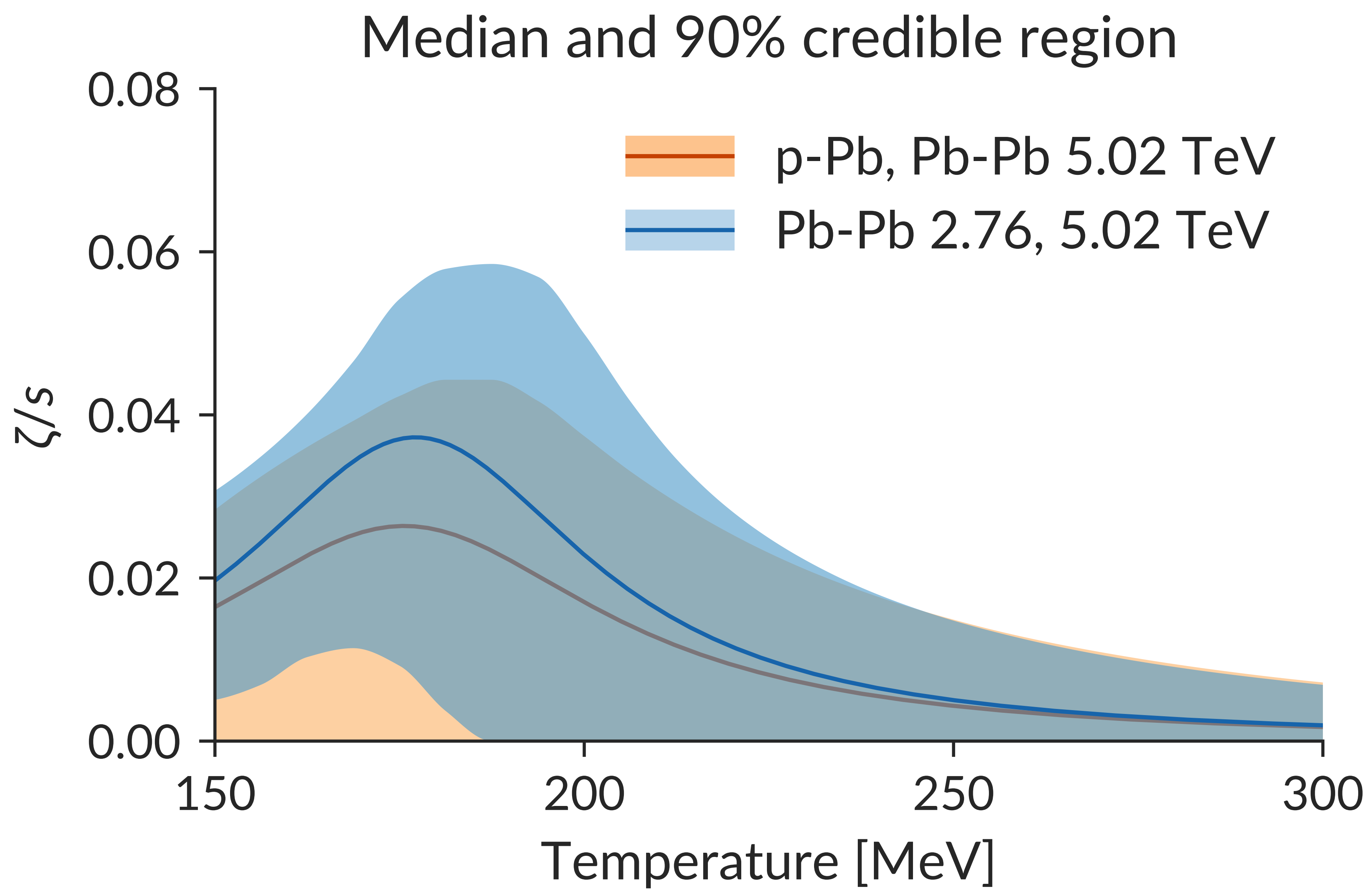
- r = 0.99 ± 0.16
- w = 0.47 ± 0.18

Key results: viscosities



- shear and bulk viscosities are fully compatible with previous calibration on Pb+Pb @ 2.76 TeV & 5.02 TeV
- uncertainty bands are larger in AA + pA analysis due to focus on single beam energy
- for bulk properties, multiple beam energies are more important than inclusion of small systems



Summary:

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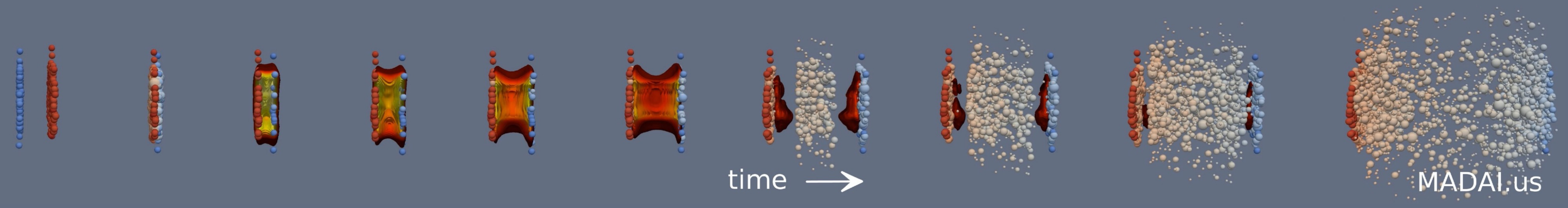
- created a comprehensive set of computational models to describe the dynamical evolution of ultra-relativistic heavy-ion collisions



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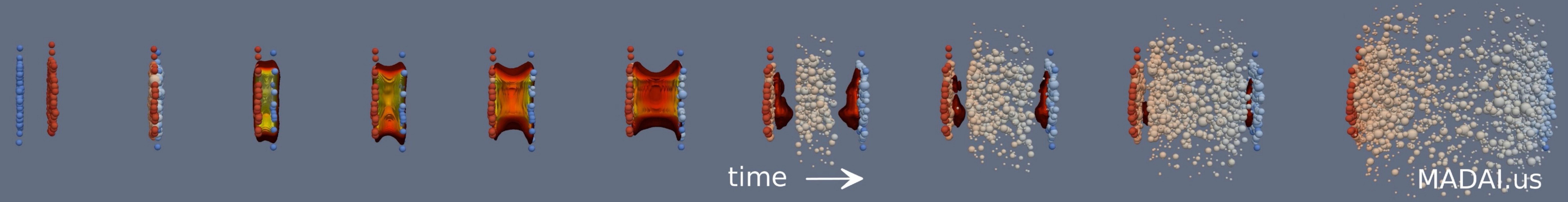
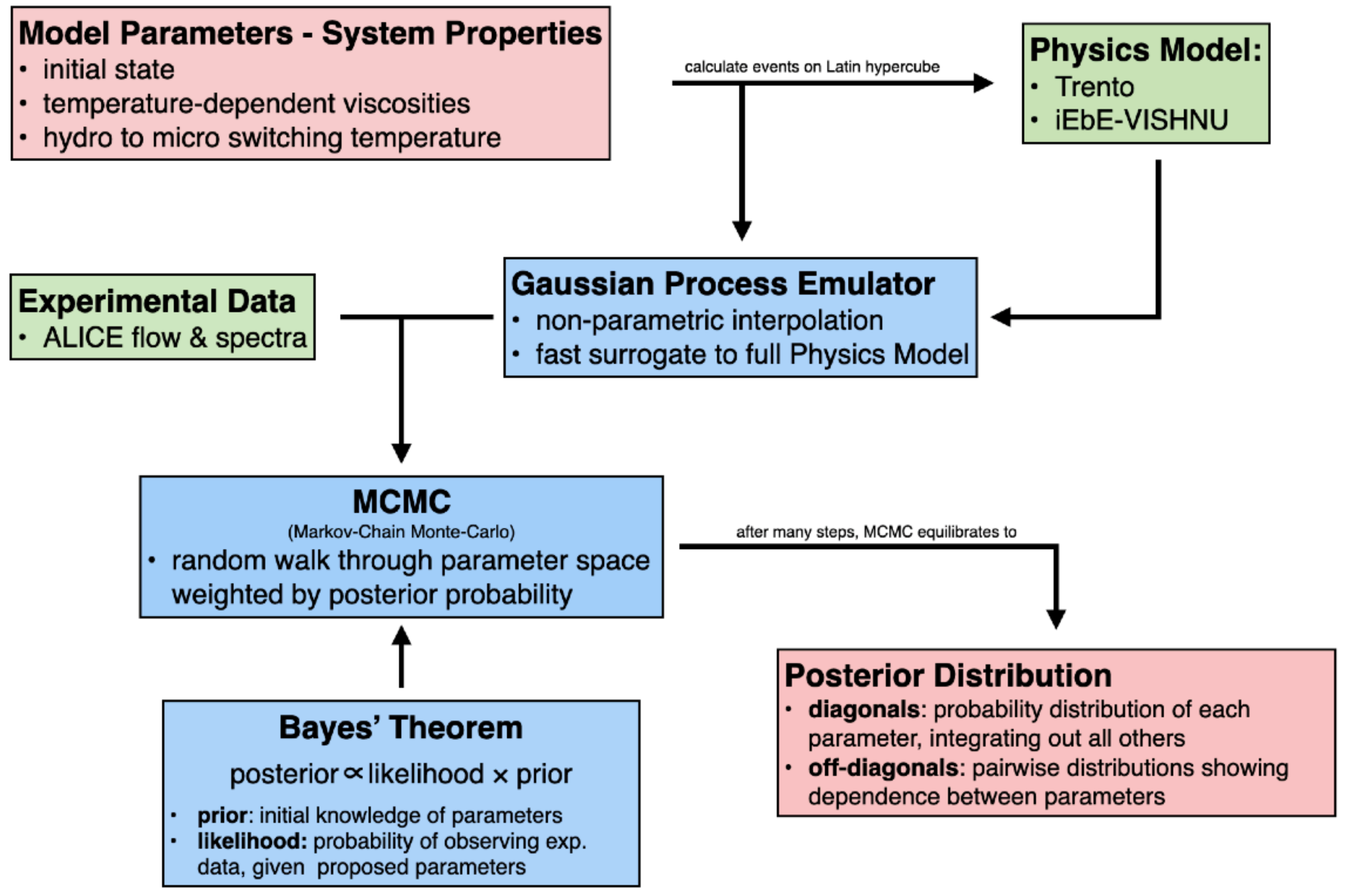


• developed a framework, utilizing Bayesian Statistics and high performance computing, to execute model-to-data calibrations with uncertainty quantification:



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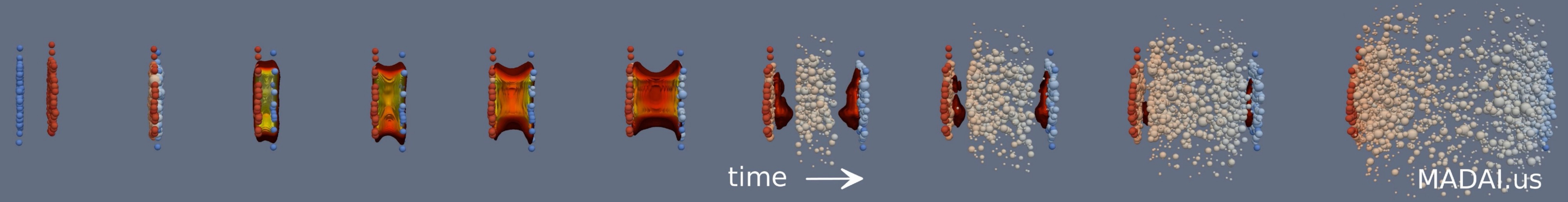
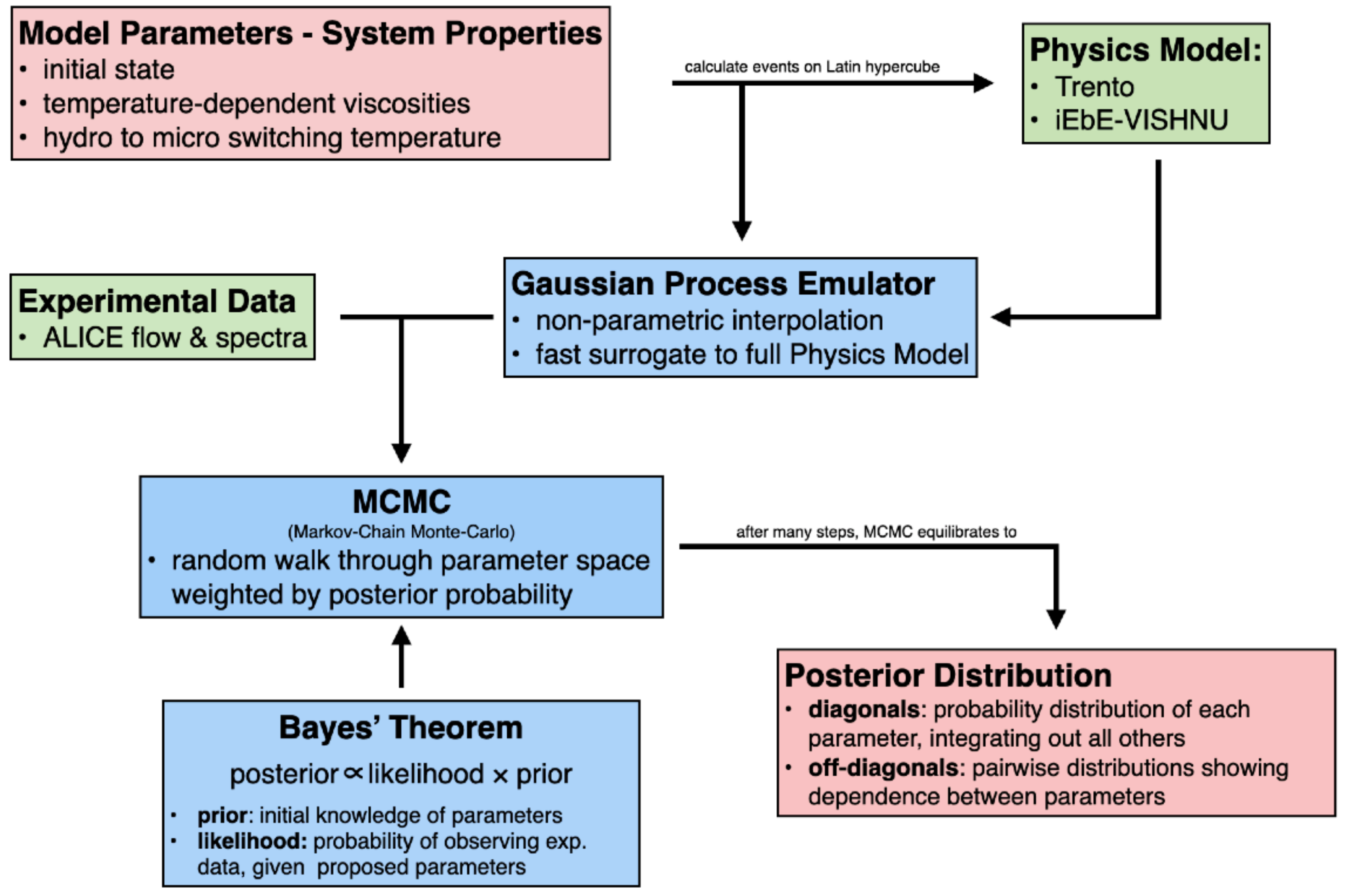
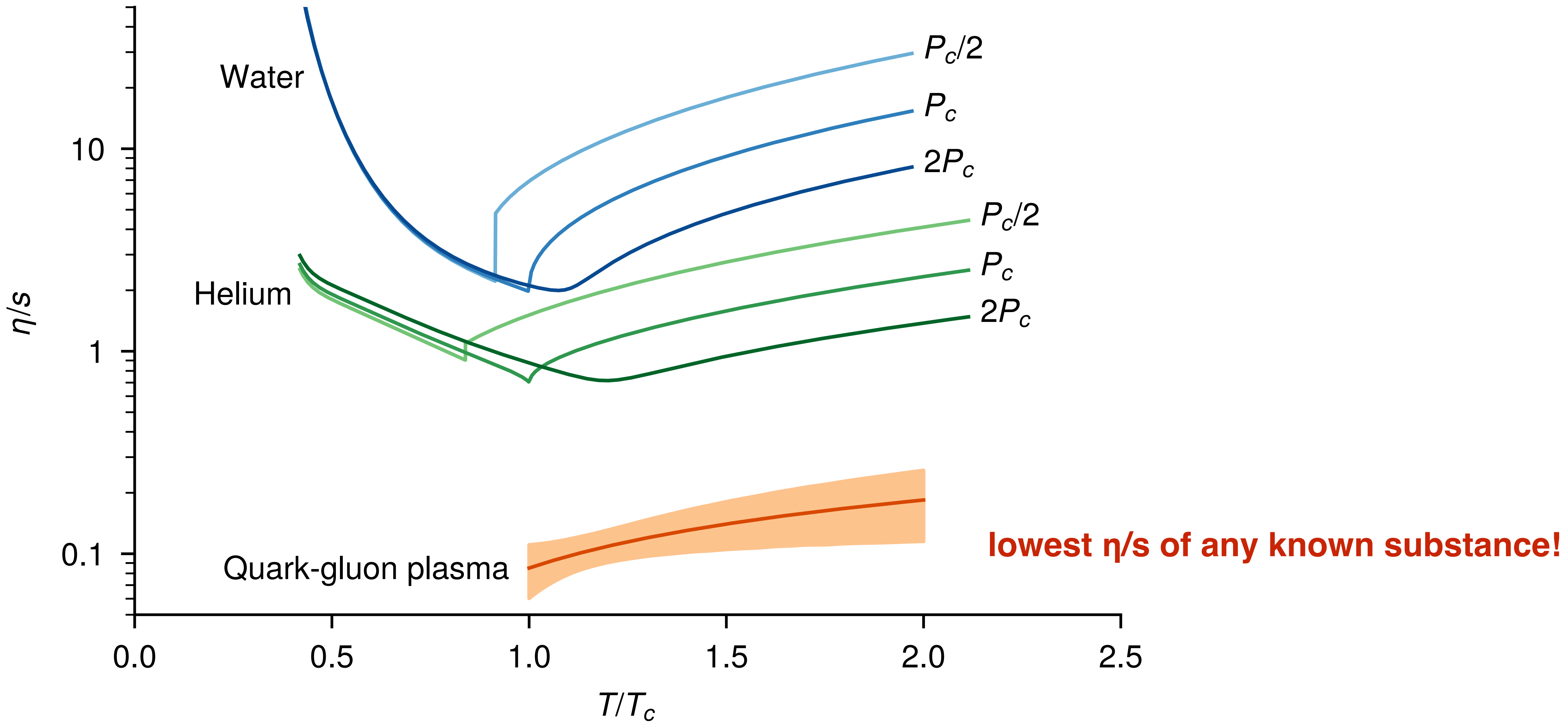


- developed a framework, utilizing Bayesian Statistics and high performance computing, to execute model-to-data calibrations with uncertainty quantification:



- applied models and framework for the first quantitative determination of the temperature-dependence of the QGP specific shear-viscosity



Outlook & Future Directions

current analysis focus was on the properties of bulk QCD matter and utilized only LHC data on soft hadrons. The analysis needs to be extended to:

- **include data from lower beam energies**
  - necessary for determination of the temperature and μ_B dependence of transport coefficients
- **include asymmetric collision systems (p+A, d+A, 3He+A, A+B)**
  - generate improved understanding of the initial state
- **include hard probes (jets and heavy quark observables)**
  - consistent determination of jet and heavy flavor transport coefficients
- **include other physics models**
  - analysis is model agnostic, allows for quantitative comparison among different models and verification/falsification of models/conceptual approaches

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NERSC National Energy Research Scientific Computing Center

Past & Present Collaborators & Sponsors

Duke QCD Group:
- Jonah Bernhard (now Lowe's Corporate)
- J. Scott Moreland (now at IQVIA)
- Weiyao Ke (now at LBNL)
- Yingru Xu (now at Capital One)
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Pioneering work by the MADAI Collaboration, led by Scott E. Pratt, MSU (2009-2014)

Resources

Trento:

- J. Scott Moreland, Jonah E. Bernhard & Steffen A. Bass: Phys. Rev. C 92, 011901(R)
- https://github.com/Duke-QCD/trento

iEbE-VISHNU:

- Chun Shen, Zhi Qiu, Huichao Song, Jonah Bernhard, Steffen A. Bass & Ulrich Heinz: Computer Physics Communications in print, arXiv:1409.8164
- http://u.osu.edu/vishnu/

UrQMD:

- Steffen A. Bass et al. Prog. Part. Nucl. Phys. 41 (1998) 225-370 , arXiv:nucl-th/9803035
- Marcus Bleicher et al. J.Phys. G25 (1999) 1859-1896 , arXiv:hep-ph/9909407
- http://urqmd.org

MADAI Collaboration:

- Visualization and Bayesian Analysis packages
- https://madai-public.cs.unc.edu

Duke Bayesian Analysis Package:

- https://github.com/jbernhard/mtd

The End