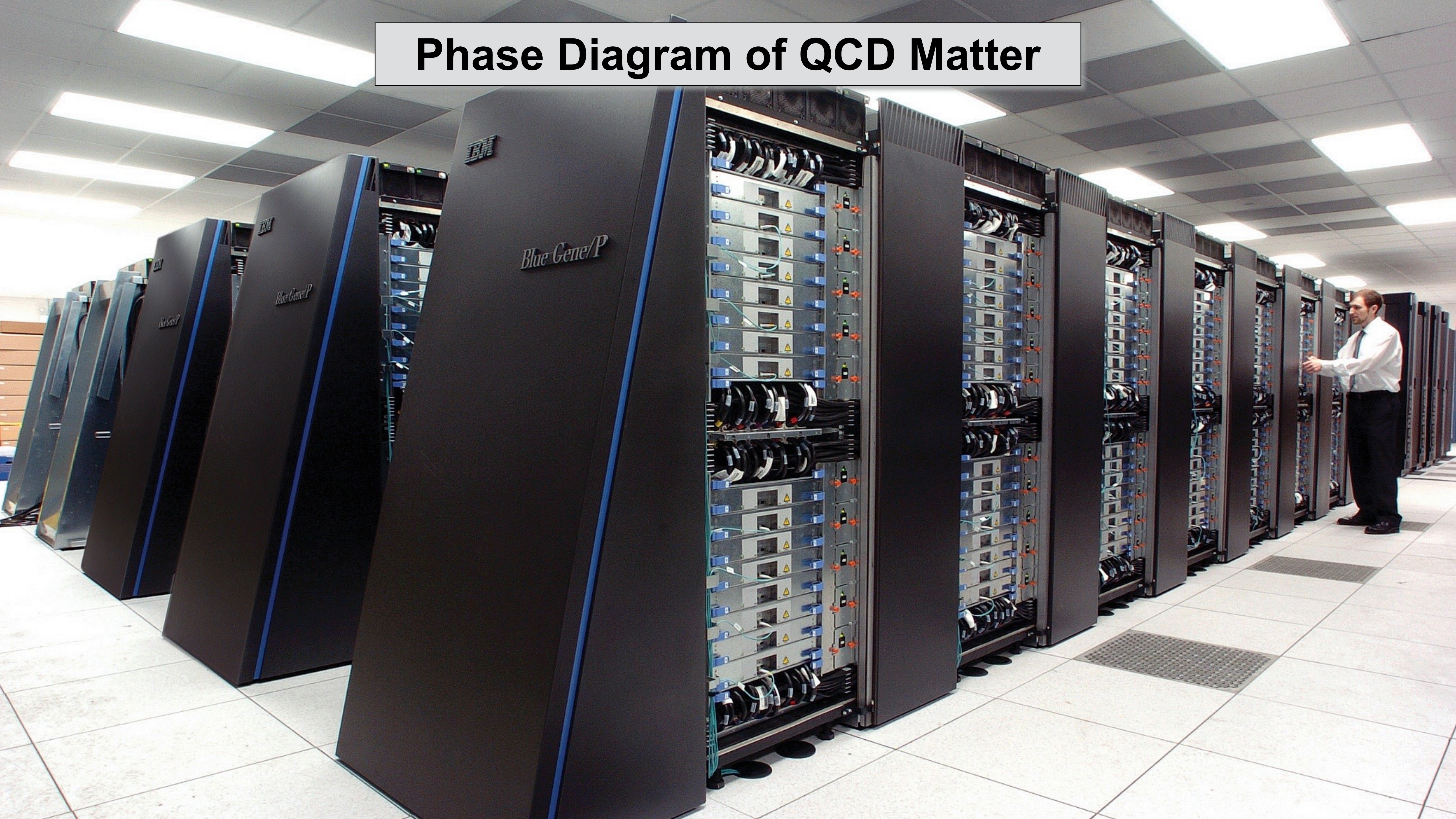


Determination of QGP Parameters from a Global Bayesian Analysis

Steffen A. Bass

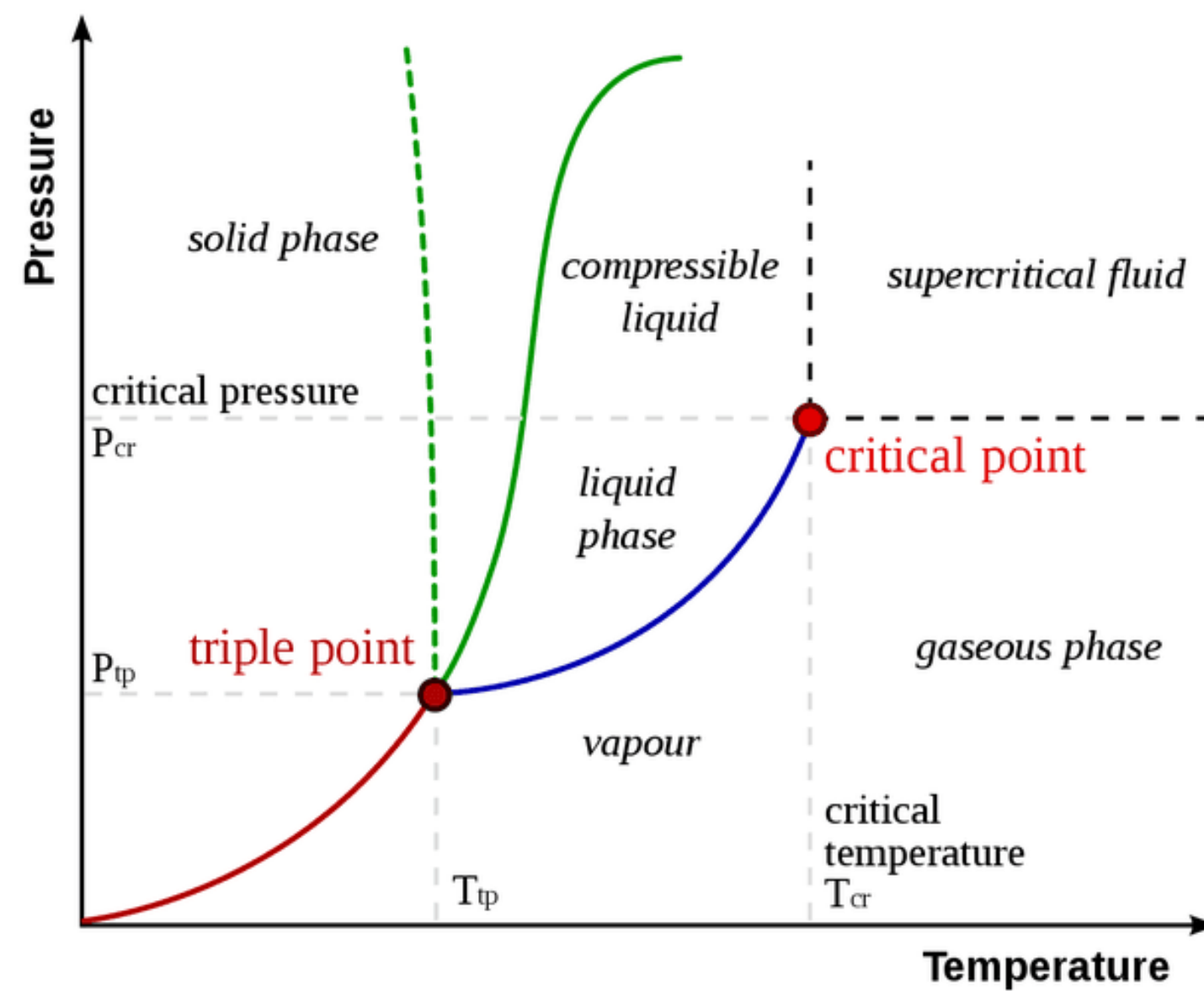
Phase Diagram of QCD Matter



Phase Diagram of QCD Matter

Ordinary Matter:

- phases determined by (electromagnetic) interaction between molecules
- apply heat & pressure to study phase-diagram
- calculate via derivatives of partition function



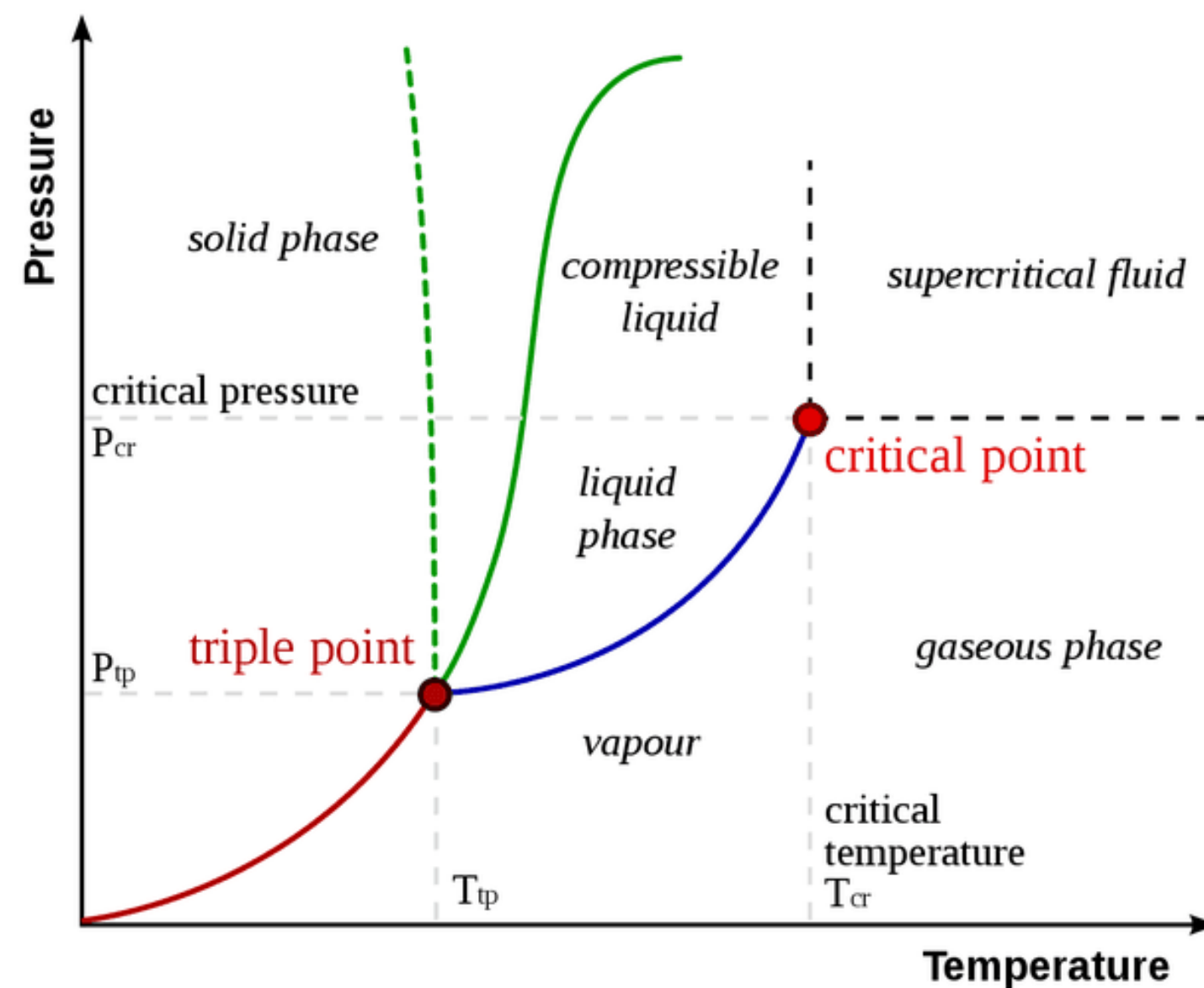
Blue Gene/P



Phase Diagram of QCD Matter

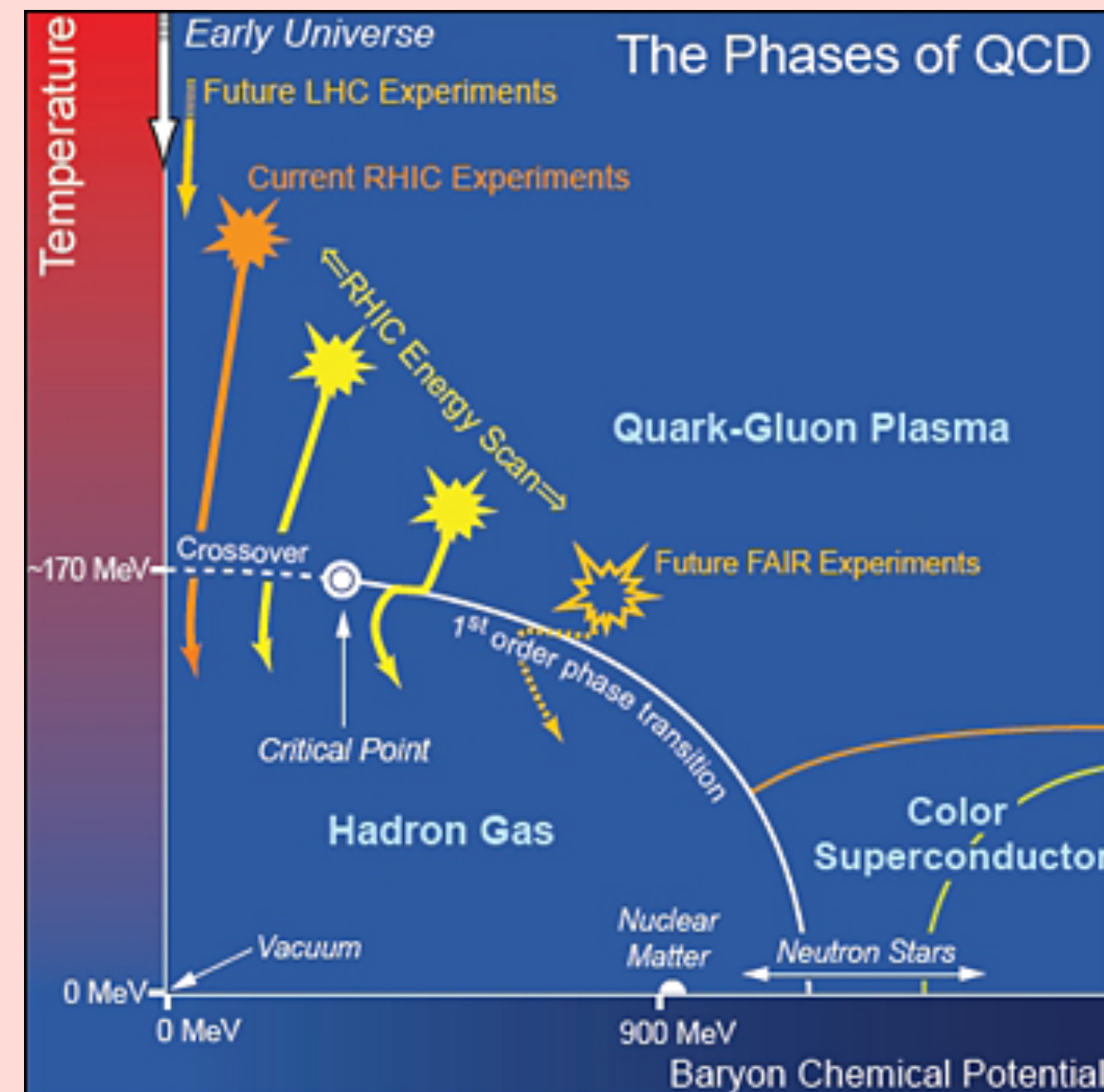
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Phases of QCD matter:

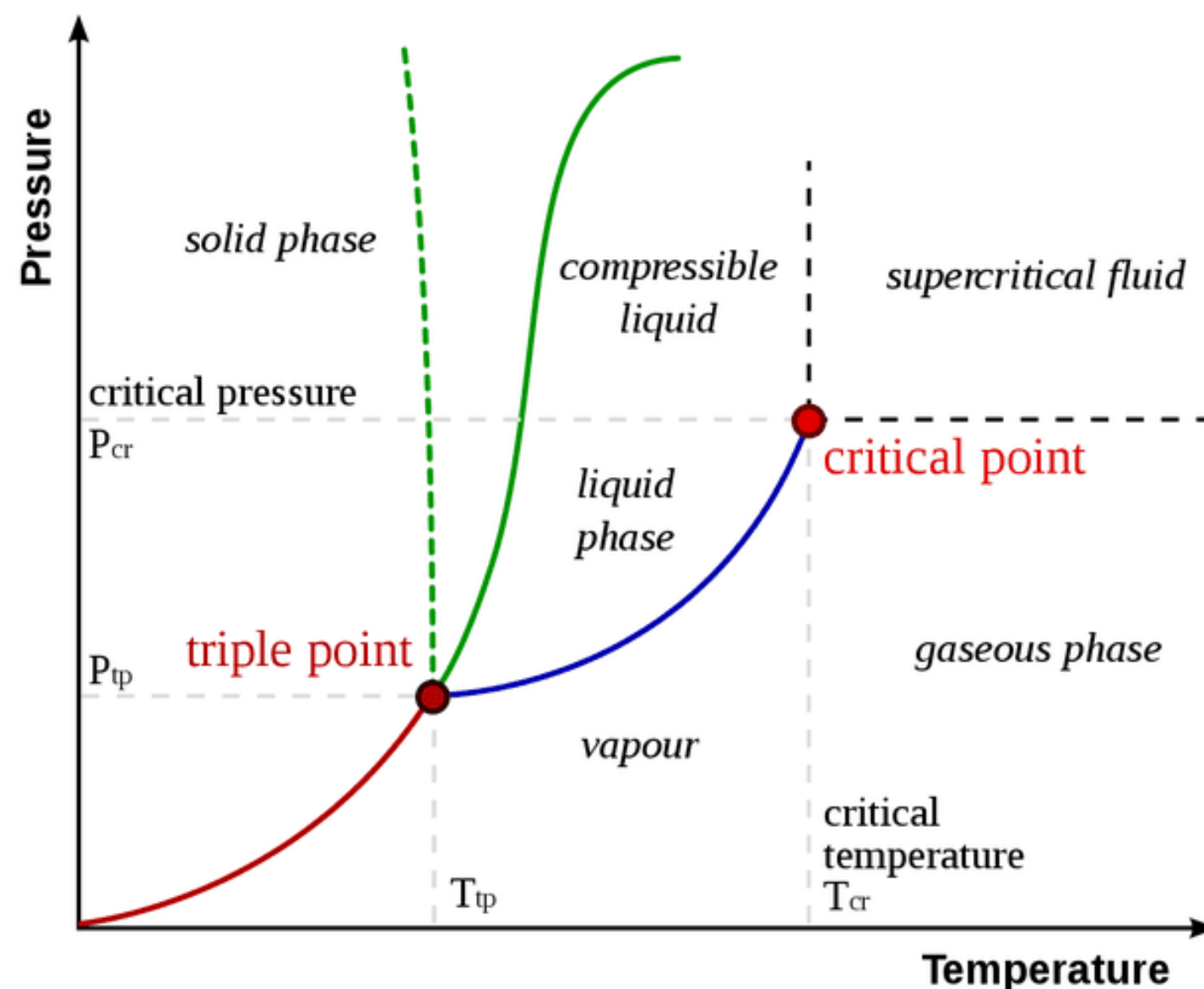
- heat & compress QCD matter:
 - collide heavy atomic nuclei
- numerical simulations:
 - solve partition function (Lattice Field Theory)



Phase Diagram of QCD Matter

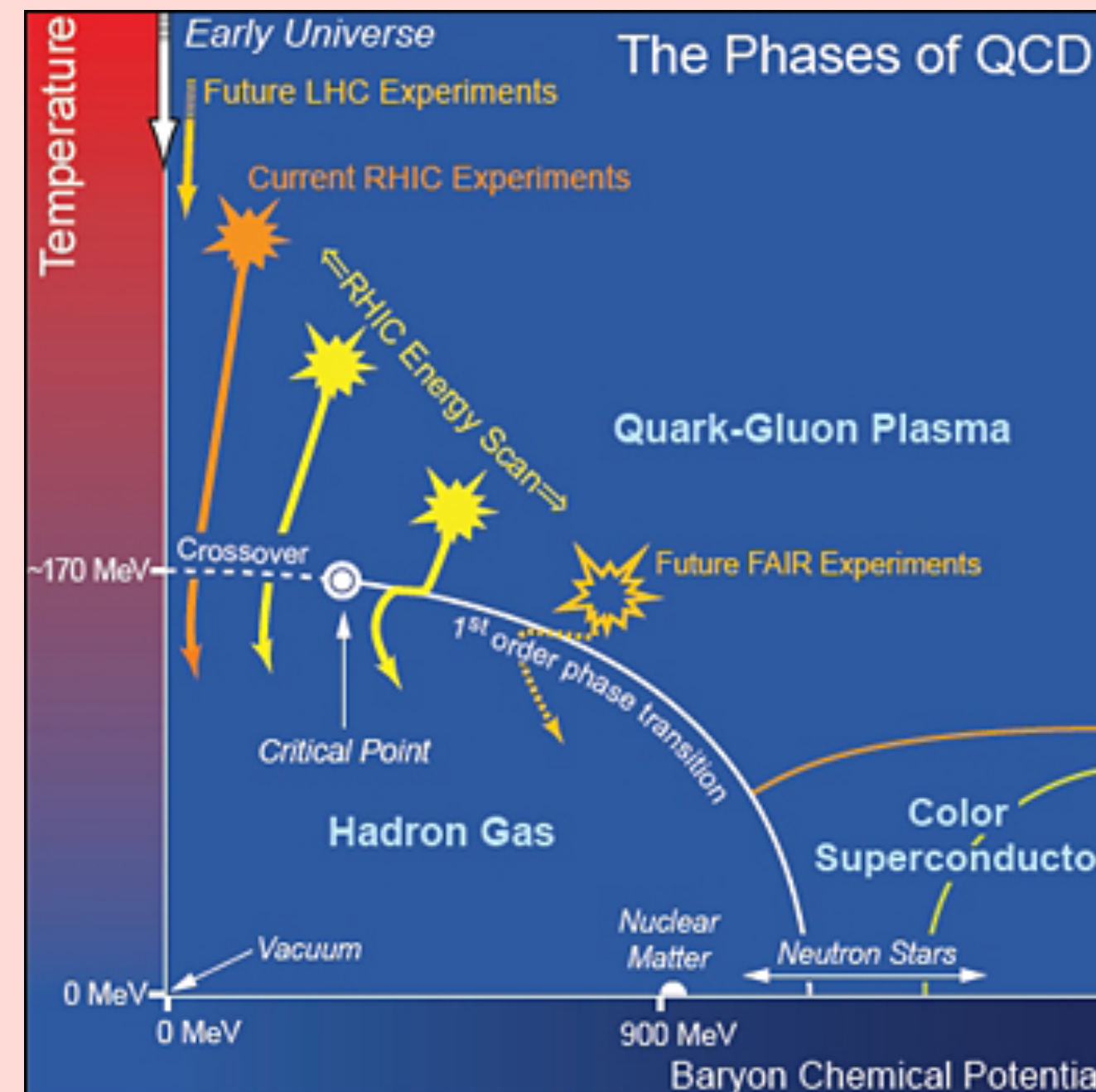
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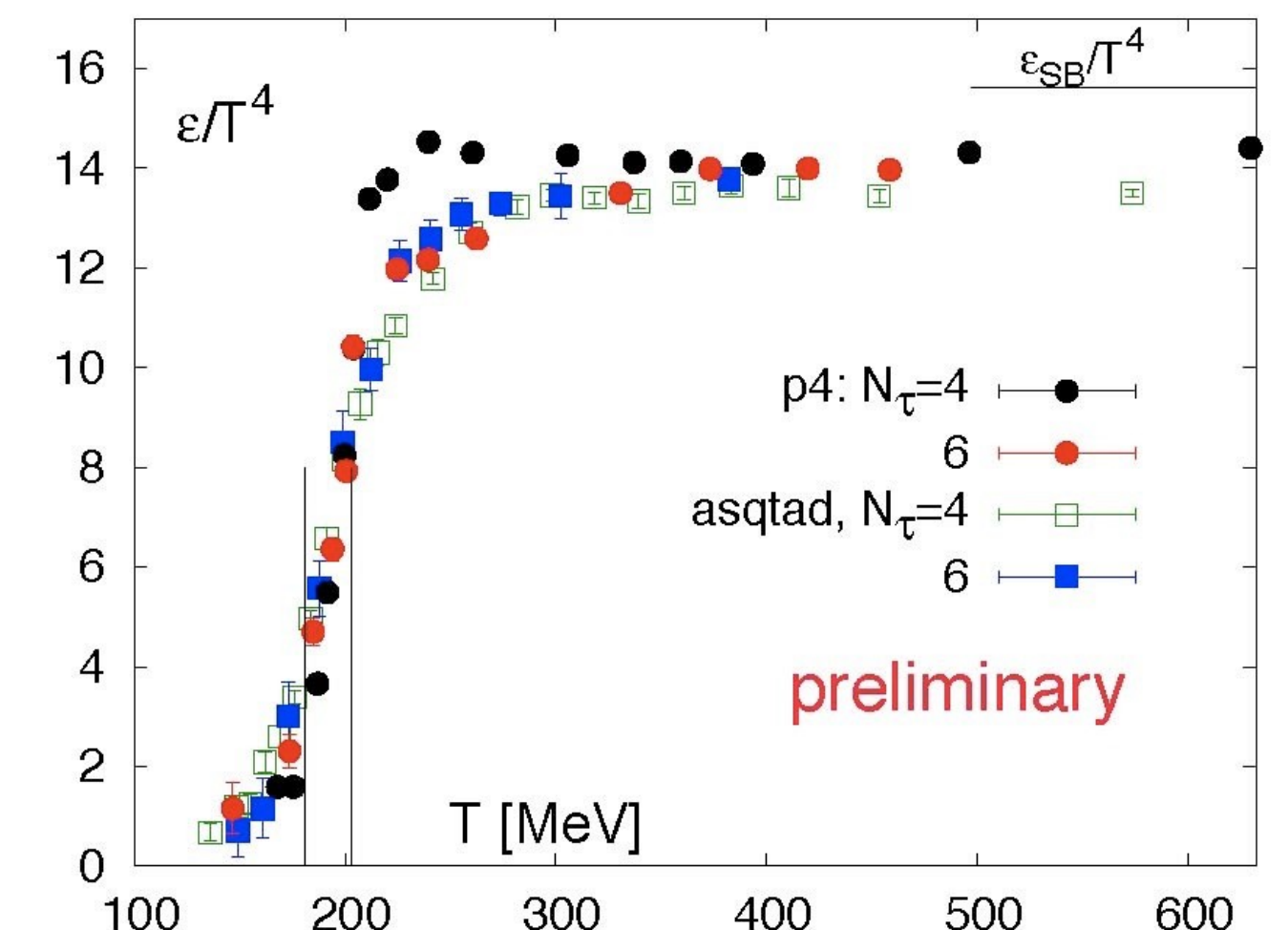


Equation of State for an ideal QGP:

$$\varepsilon = \frac{\pi^2}{30} g_{\text{DOF}} T^4$$

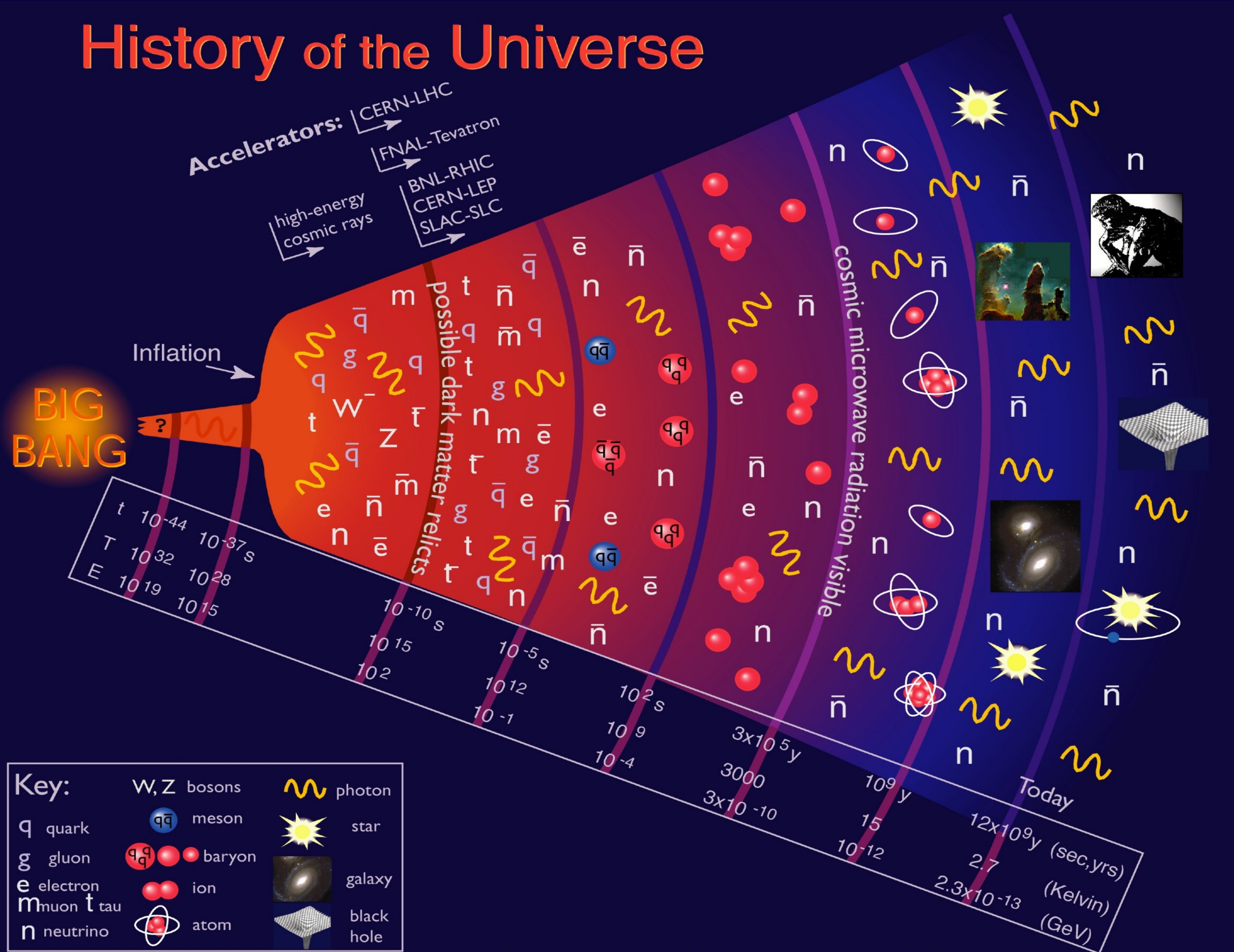
(ultra-relativistic gas of massless bosons)

- LGT predicts a phase-transition to a state of deconfined nearly massless quarks and gluons
- QCD becomes simple at high temperature and/or density



The Early Universe: Quark-Gluon-Plasma

History of the Universe



- a few microseconds after the Big Bang the entire Universe was in a QGP state
- compressing & heating nuclear matter allows to investigate the history of the Universe
- the only means of recreating temperatures and densities of the early Universe is by colliding beams of ultra-relativistic heavy-ions

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**:

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

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

A. Nakamura & S. Sakai: Phys. Rev. Lett. **94** (2005) 072305
Harvey B. Meyer: Phys. Rev. **D79** (2009) 011502
Harvey B. Meyer: [arXiv:0809.5202](#) [hep-lat]

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

Standing on the Shoulders of Giants

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. McLerran⁴

¹Section for Theoretical Physics, Department of Physics, University of Bergen, Allegaten 55, 5007 Bergen, Norway

²MTA-KFKI, Research Institute of Particle and Nuclear Physics, 1525 Budapest 114, P. O. Box 49, Hungary

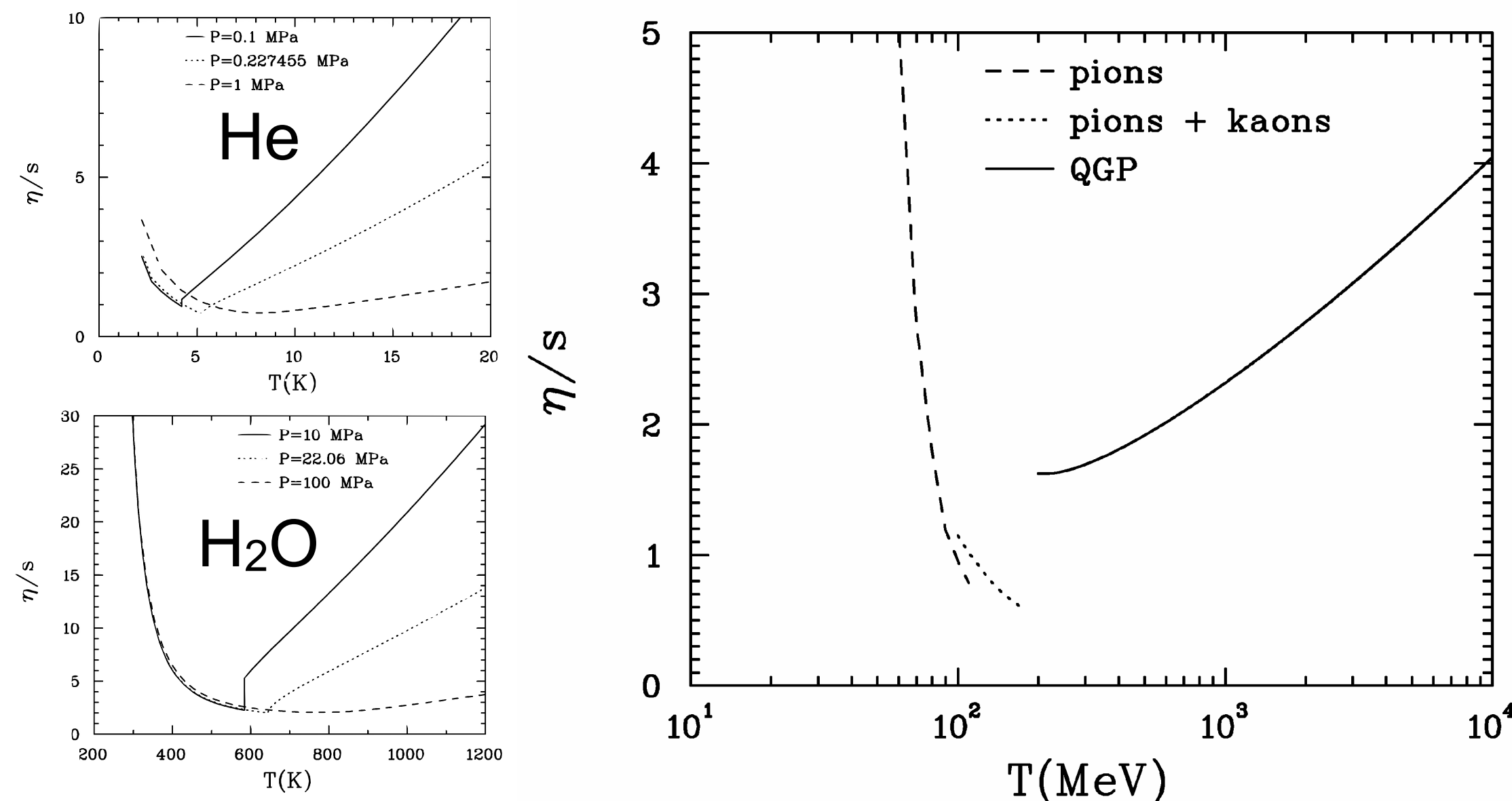
³School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA

⁴Nuclear Theory Group and Riken Brookhaven Center, Brookhaven National Laboratory, Bldg. 510A, Upton, New York 11973, USA
(Received 12 April 2006; published 12 October 2006)

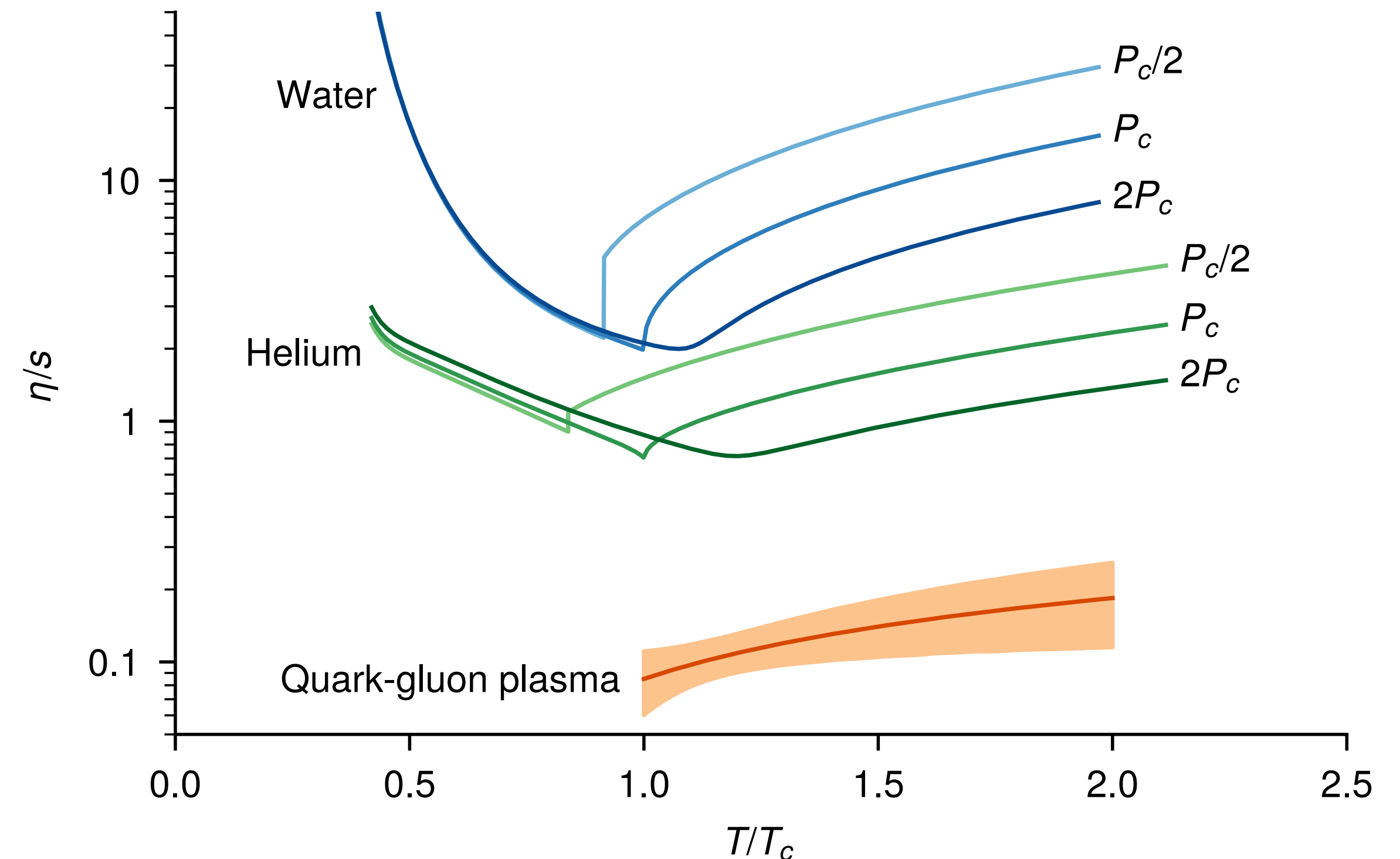
Substantial collective flow is observed in collisions between large nuclei at BNL RHIC (Relativistic Heavy Ion Collider) as evidenced by single-particle transverse momentum distributions and by azimuthal correlations among the produced particles. The data are well reproduced by perfect fluid dynamics. 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](https://doi.org/10.1103/PhysRevLett.97.152303)

PACS numbers: 12.38.Mh, 24.10.Nz, 25.75.Nq, 51.20.+d

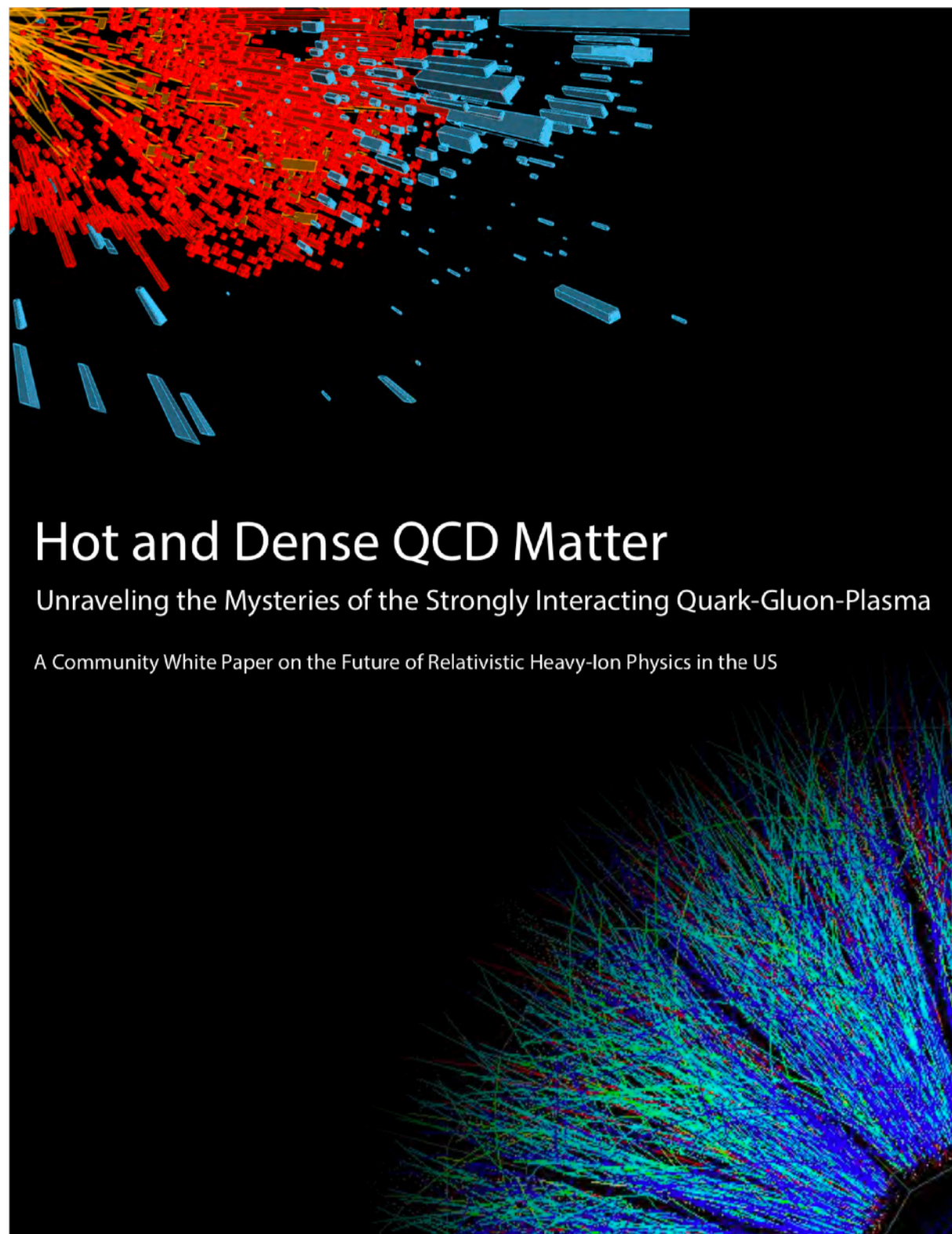


Jonah E. Bernhard, J. Scott Moreland & Steffen A. Bass,
to appear in **Nature Physics** on August 12th 2019



- 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

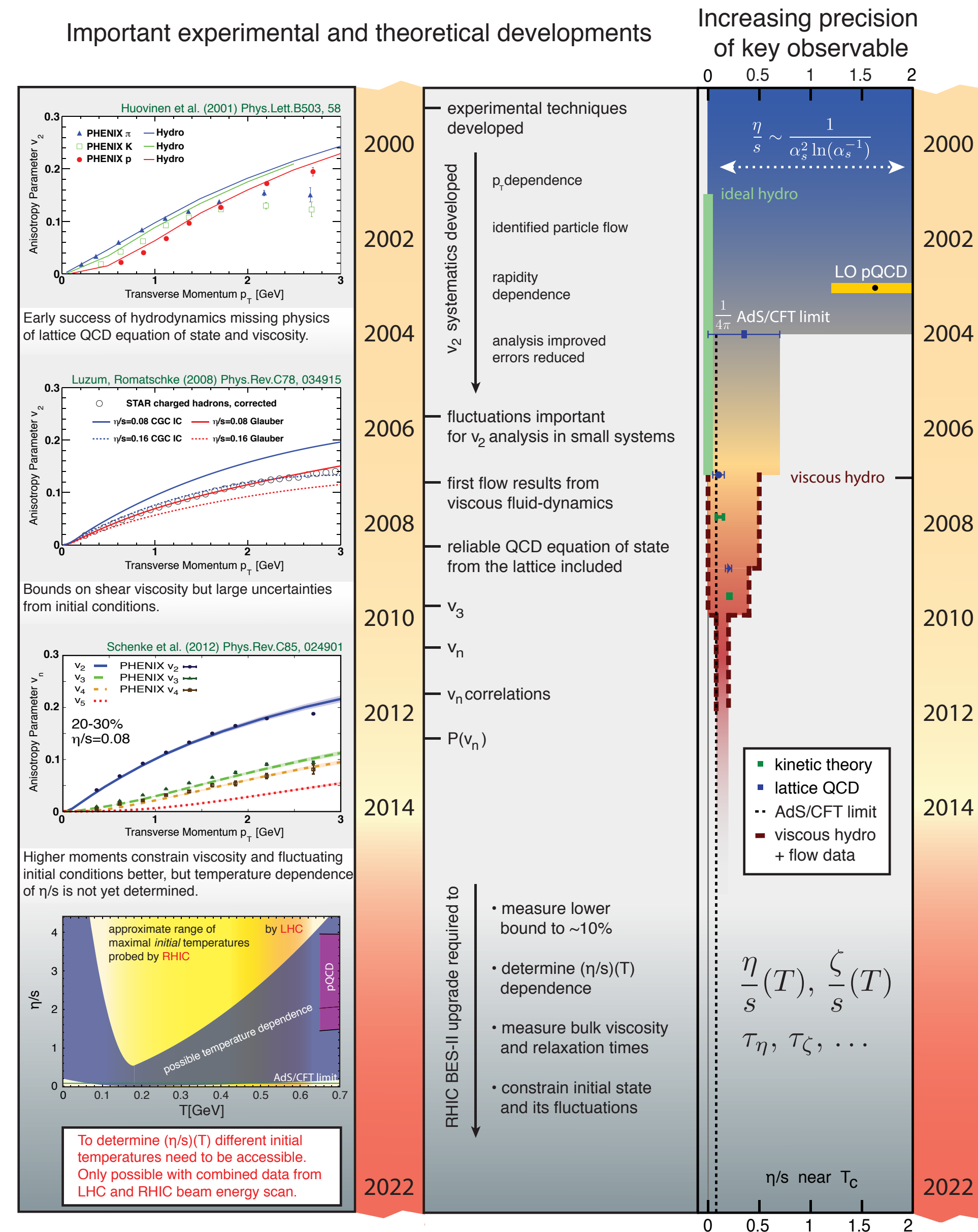


2012 response of the US relativistic heavy-ion community to the request for comments by the NSAC subcommittee, that was tasked to recommend *optimizations* to the US Nuclear Science Program over the following five years.

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. $\hat{q}$ and $\hat{e}$)

We are well on our way deliver on these goals!



Telescopes for the Early Universe: Heavy-Ion Collider Facilities

Heating & Compressing QCD Matter

The only way to heat & compress QCD matter under controlled laboratory conditions is by colliding two heavy atomic nuclei!

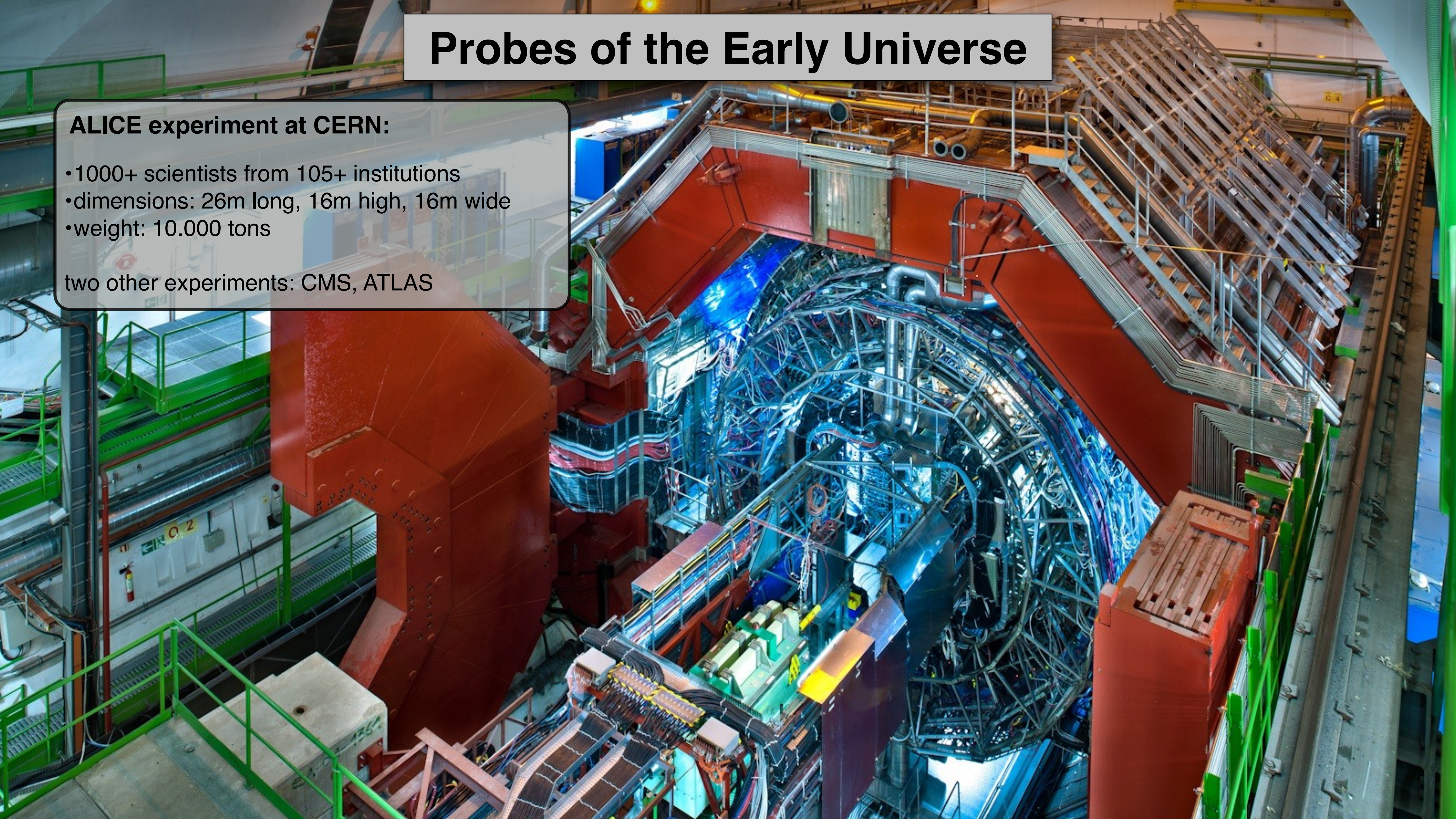


Probes of the Early Universe

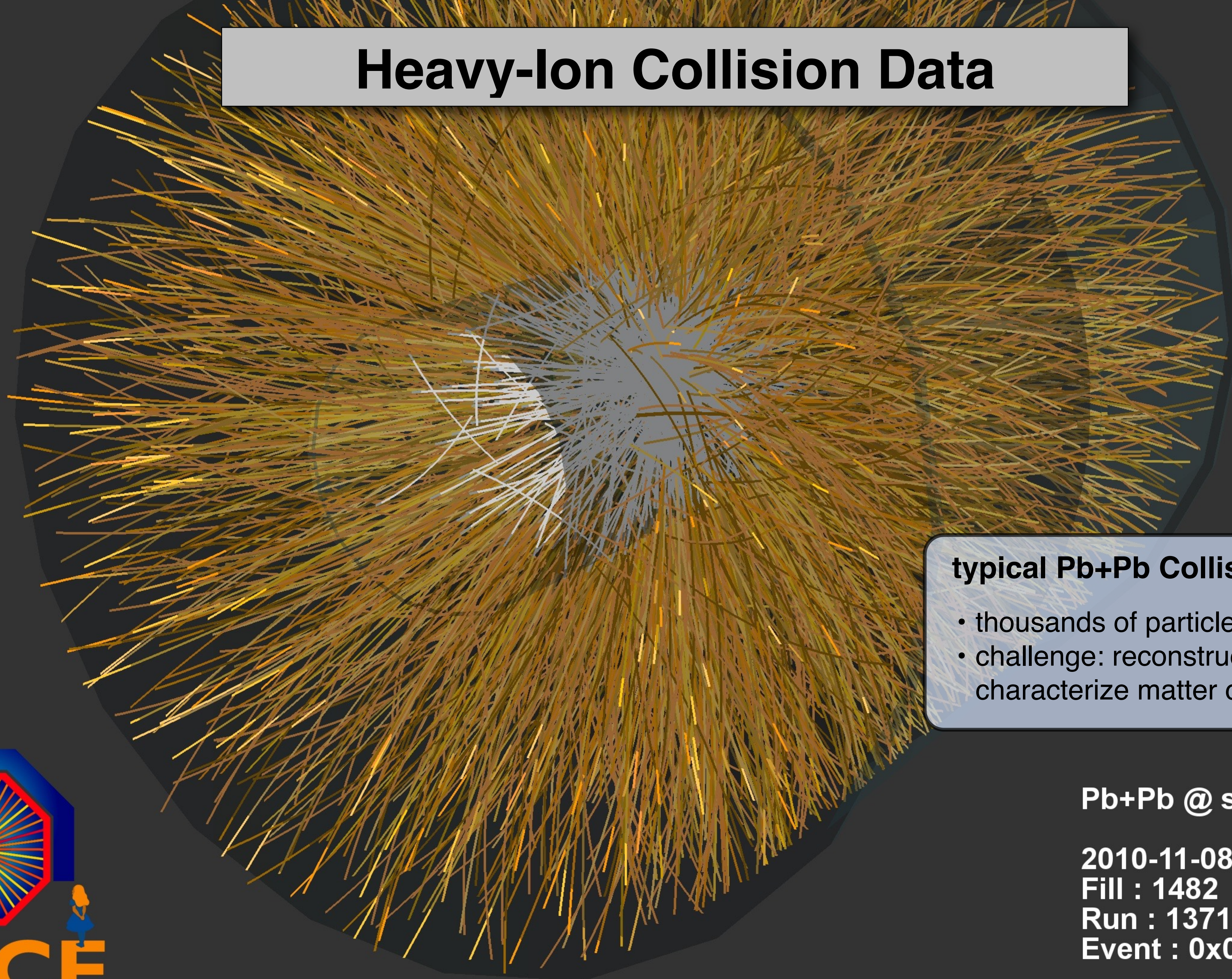
ALICE experiment at CERN:

- 1000+ scientists from 105+ institutions
- dimensions: 26m long, 16m high, 16m wide
- weight: 10.000 tons

two other experiments: CMS, ATLAS



Heavy-Ion Collision Data



typical Pb+Pb Collision at the LHC:

- thousands of particle tracks
- challenge: reconstruction of final state to characterize matter created in collision

Pb+Pb @ $\sqrt{s} = 2.76$ ATeV

2010-11-08 11:29:52

Fill : 1482

Run : 137124

Event : 0x0000000042B1B693



Transport Theory: Connecting Data to Knowledge

Transport Theory

microscopic transport models based on the Boltzmann Equation:

- transport of a system of microscopic particles
- all interactions are based on **binary scattering**

$$\left[\frac{\partial}{\partial t} + \frac{\vec{p}}{E} \times \frac{\partial}{\partial \vec{r}} \right] f_1(\vec{p}, \vec{r}, t) = \sum_{\text{processes}} C(\vec{p}, \vec{r}, t)$$

diffusive transport models based on the Langevin Equation:

- transport of a system of microscopic particles in a thermal medium
- interactions contain a **drag term** related to the properties of the medium and a **noise term** representing random collisions

$$\vec{p}(t + \Delta t) = \vec{p}(t) - \frac{\kappa}{2T} \vec{v} \cdot \Delta t + \vec{\xi}(t) \Delta t$$

(viscous) relativistic fluid dynamics:

- transport of macroscopic degrees of freedom
- based on conservation laws:

$$\begin{aligned} \partial_\mu T^{\mu\nu} &= 0 \\ T_{ik} &= \varepsilon u_i u_k + P (\delta_{ik} + u_i u_k) \\ &\quad - \eta \left(\nabla_i u_k + \nabla_k u_i - \frac{2}{3} \delta_{ik} \nabla \cdot u \right) \\ &\quad + \zeta \delta_{ik} \nabla \cdot u \end{aligned}$$

(plus an additional 9 eqns. for dissipative flows)

hybrid transport models:

- combine microscopic & macroscopic degrees of freedom
- current state of the art for RHIC modeling

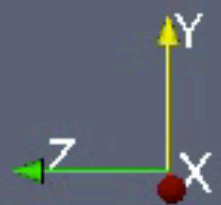
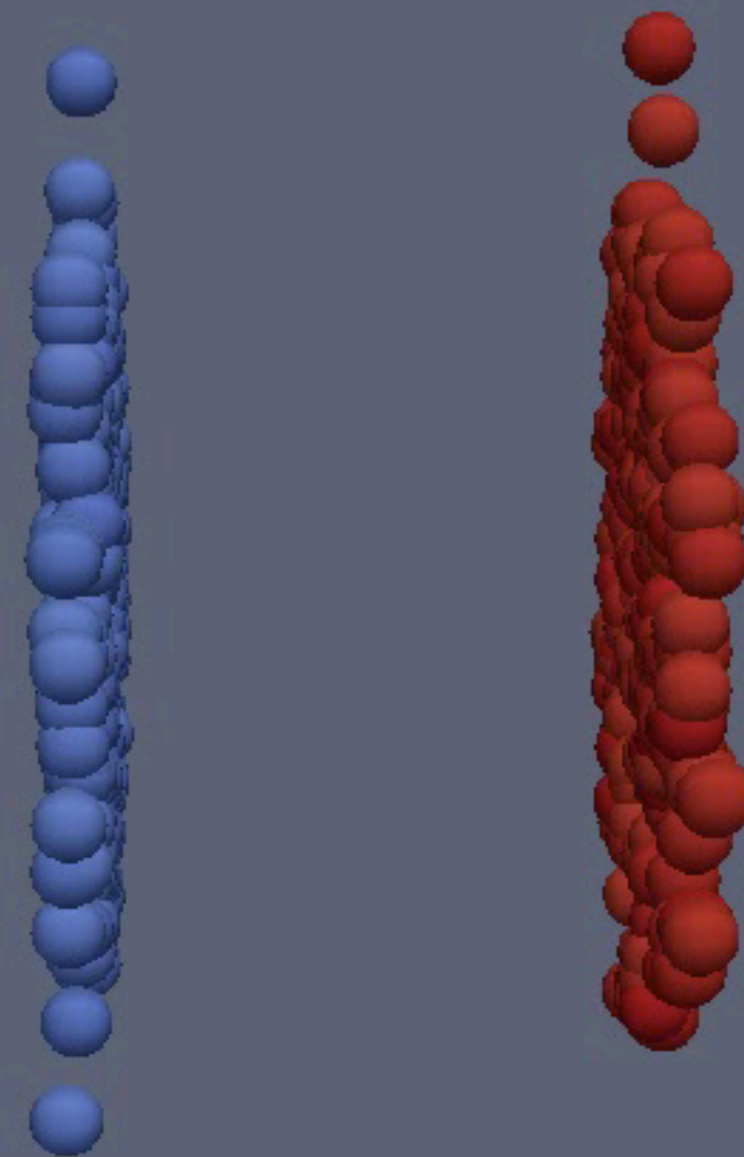
Each transport model relies on roughly a dozen physics parameters to describe the time-evolution of the collision and its final state. These physics parameters act as a representation of the information we wish to extract from RHIC & LHC.

Computational Modeling

Time: 0.10

3+1D Hydro + Boltzmann Hybrid

rapidity



MADAI.us

Computational Modeling

Time: 0.10

3+1D Hydro + Boltzmann Hybrid

rapidity

5.9

5

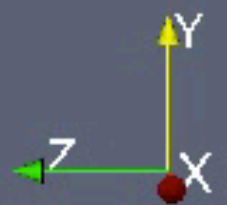
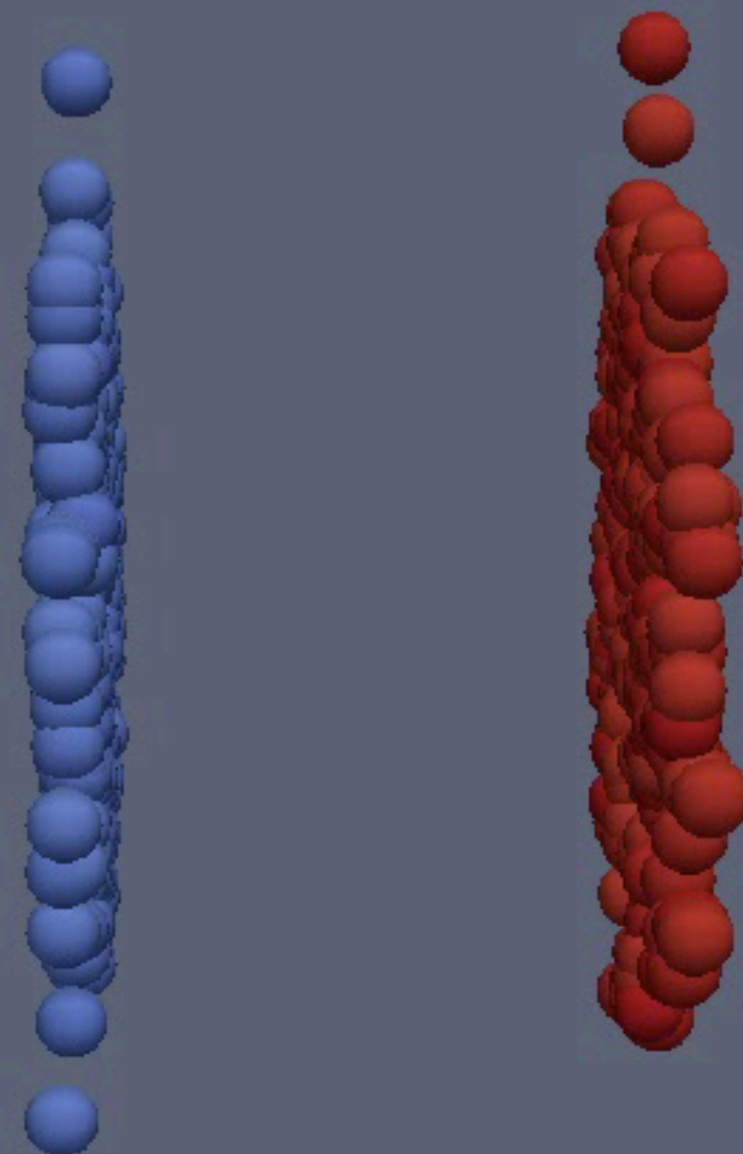
2.5

0

-2.5

-5

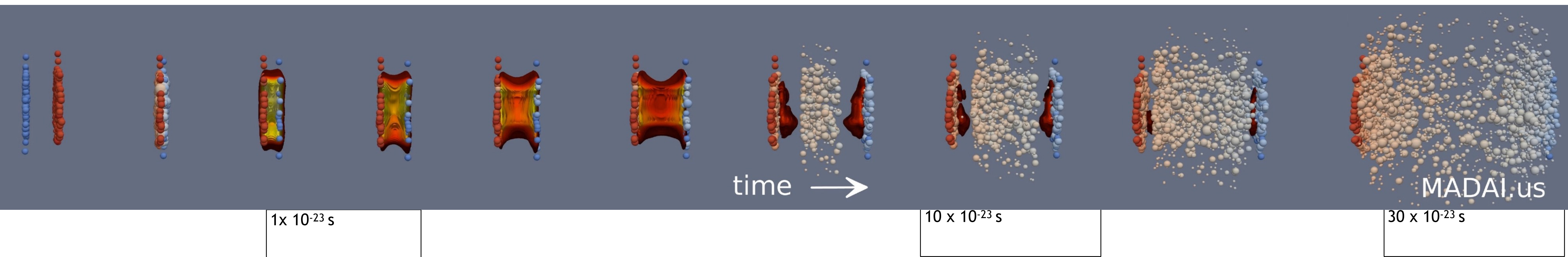
-7



MADAI.us

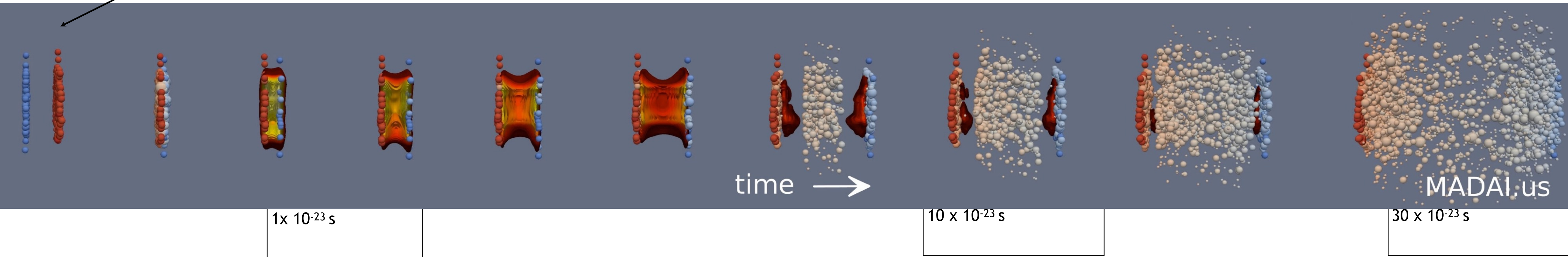
Probing the QGP in Relativistic Heavy-Ion Collisions

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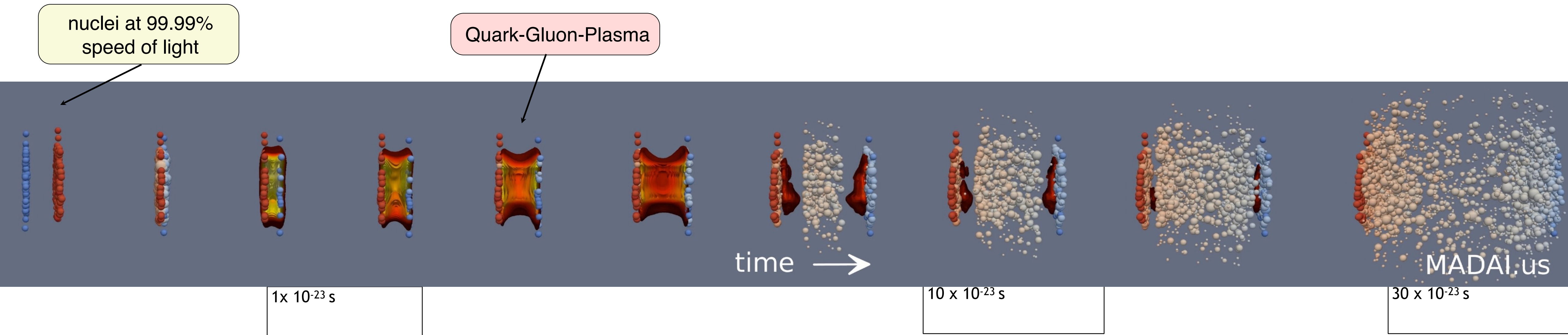


Probing the QGP in Relativistic Heavy-Ion Collisions

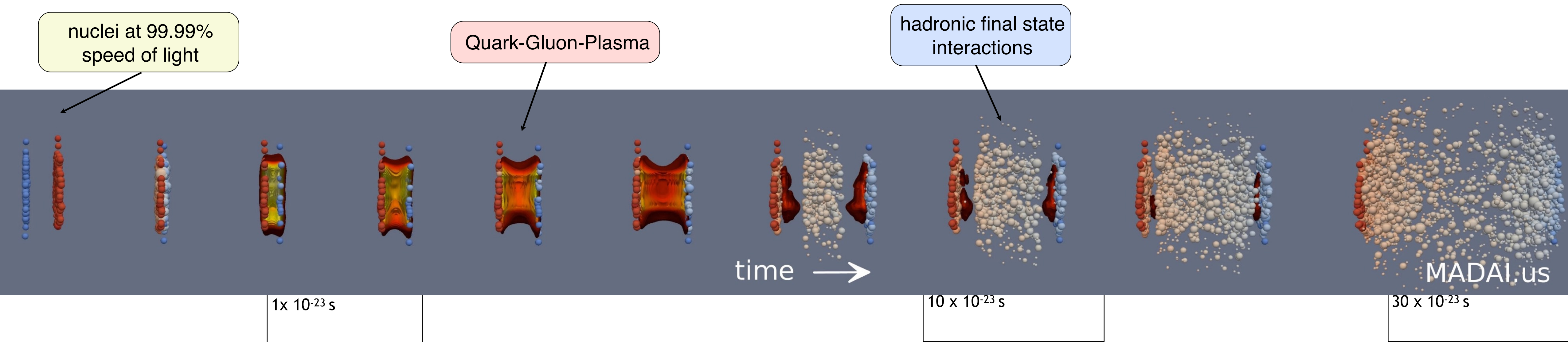
nuclei at 99.99%
speed of light



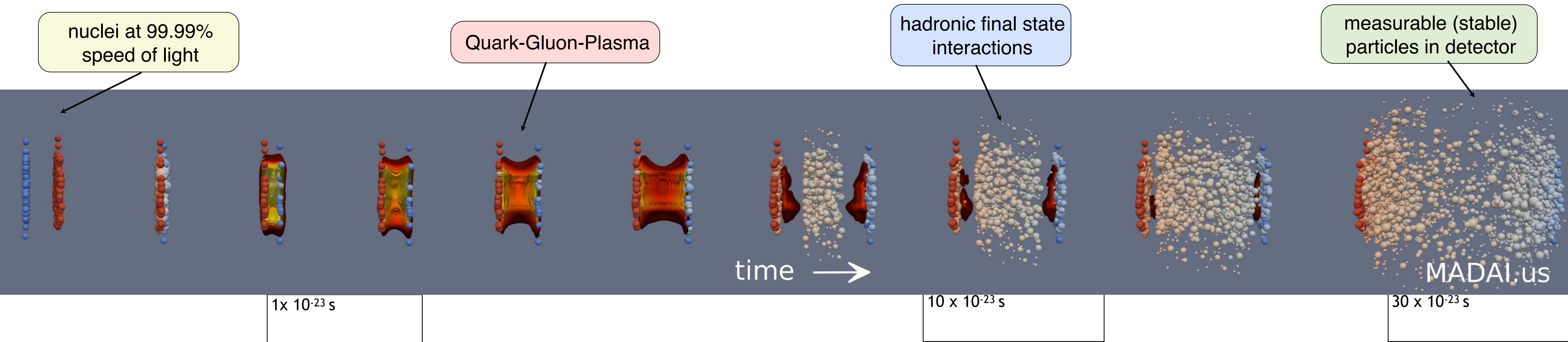
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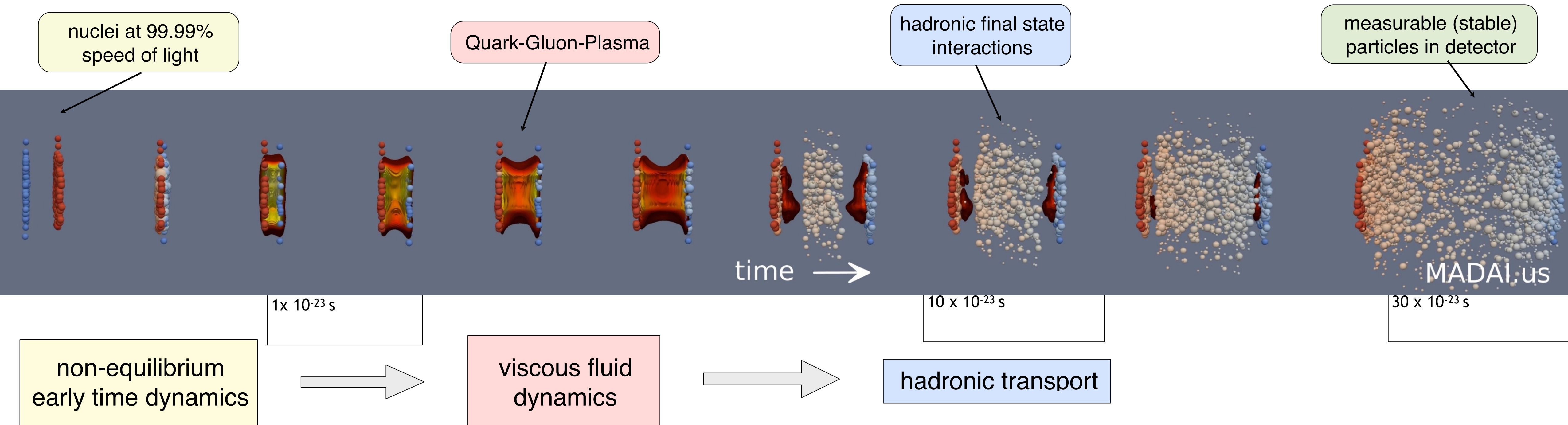
Probing the QGP in Relativistic Heavy-Ion Collisions



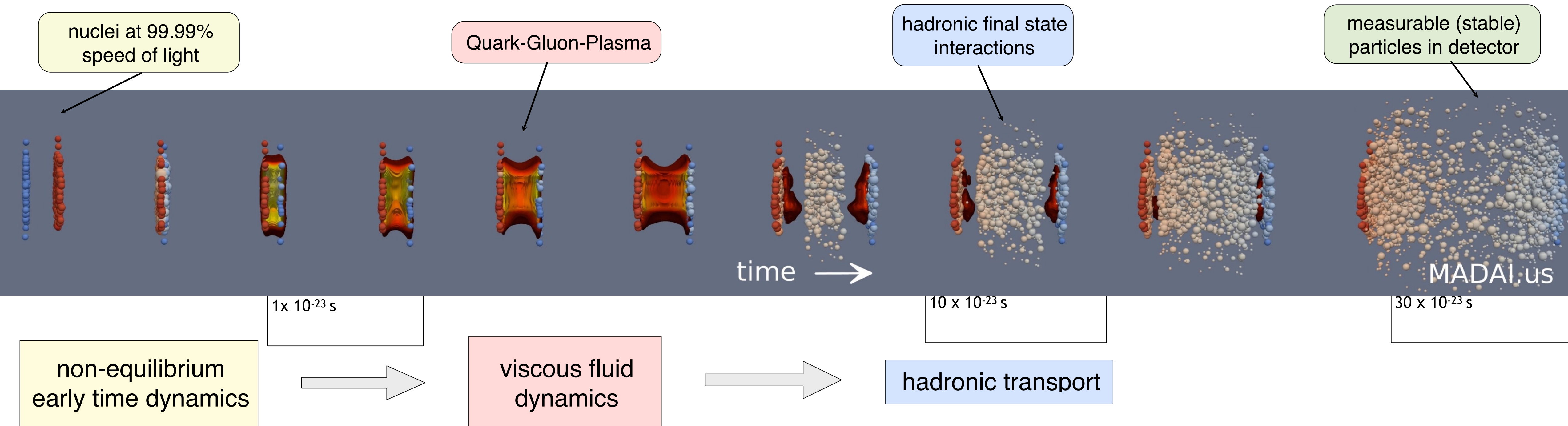
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Probing the QGP in Relativistic Heavy-Ion Collisions



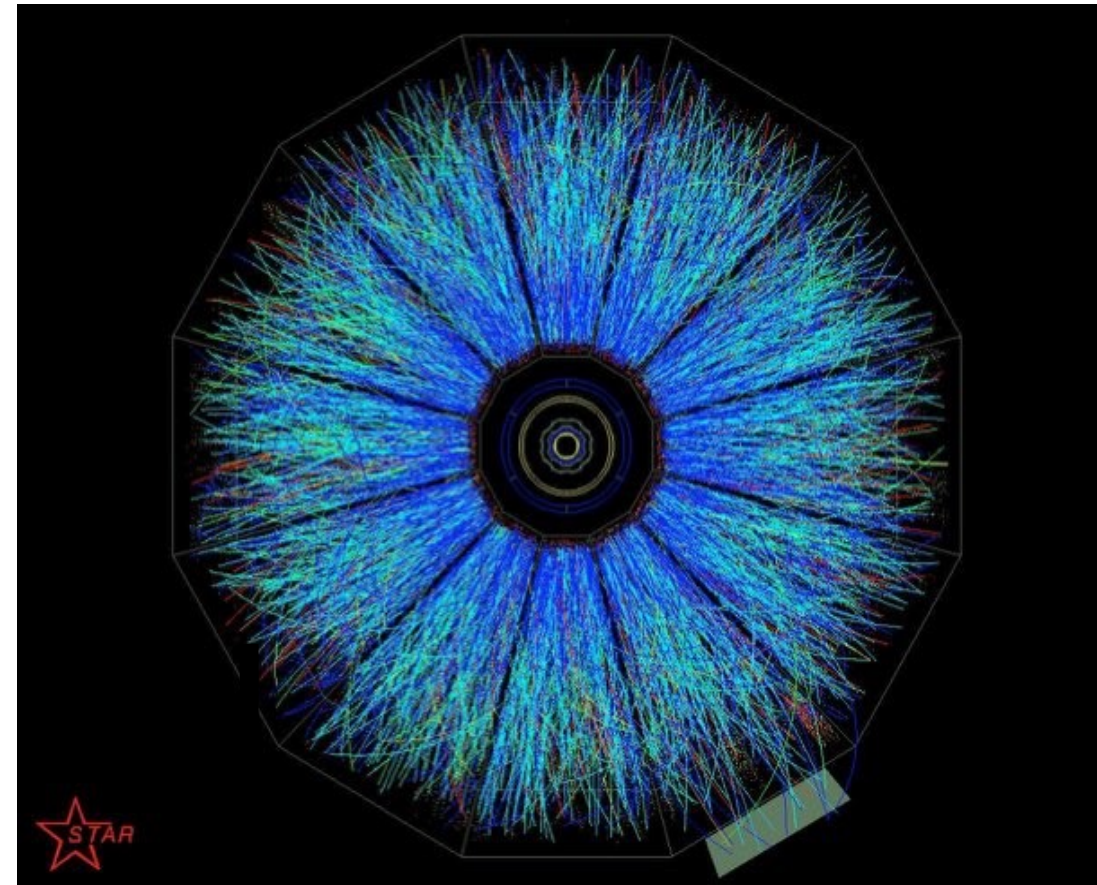
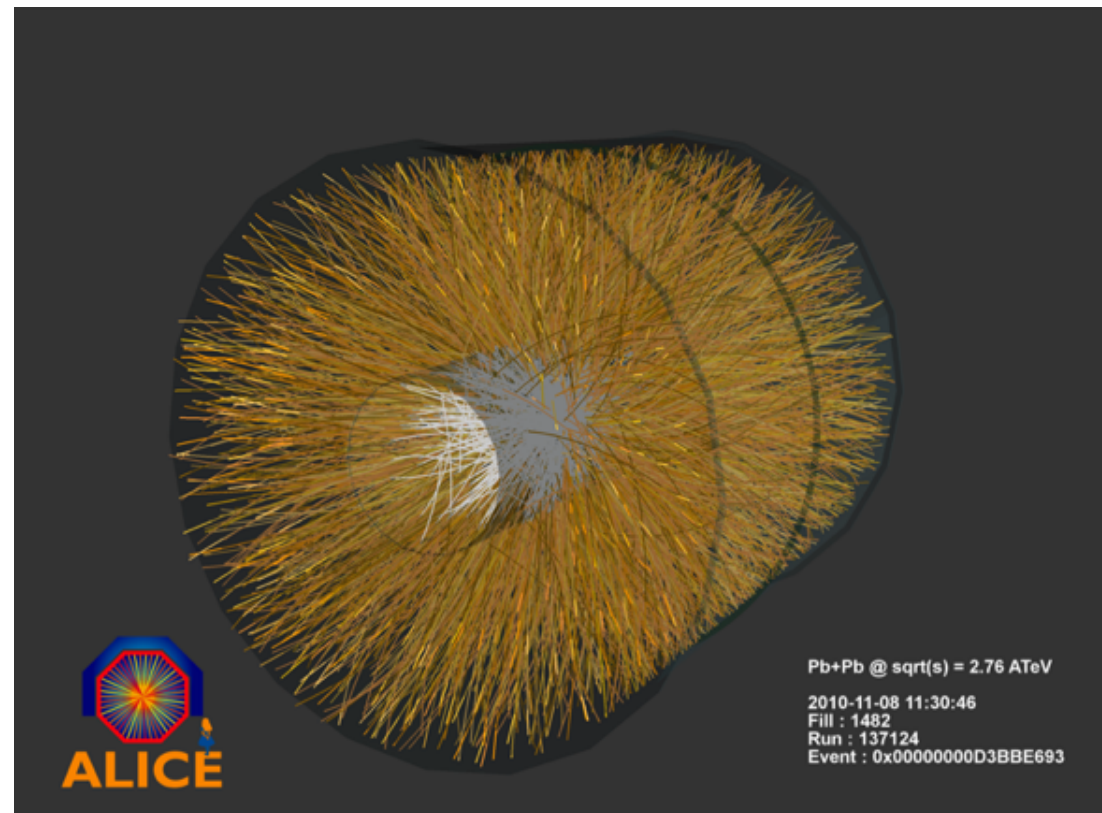
Principal Challenges of Probing the QGP with Heavy-Ion Collisions:

- 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 needed to connect the experiments to QGP properties!**

Knowledge Extraction from Relativistic Heavy-Ion Collisions

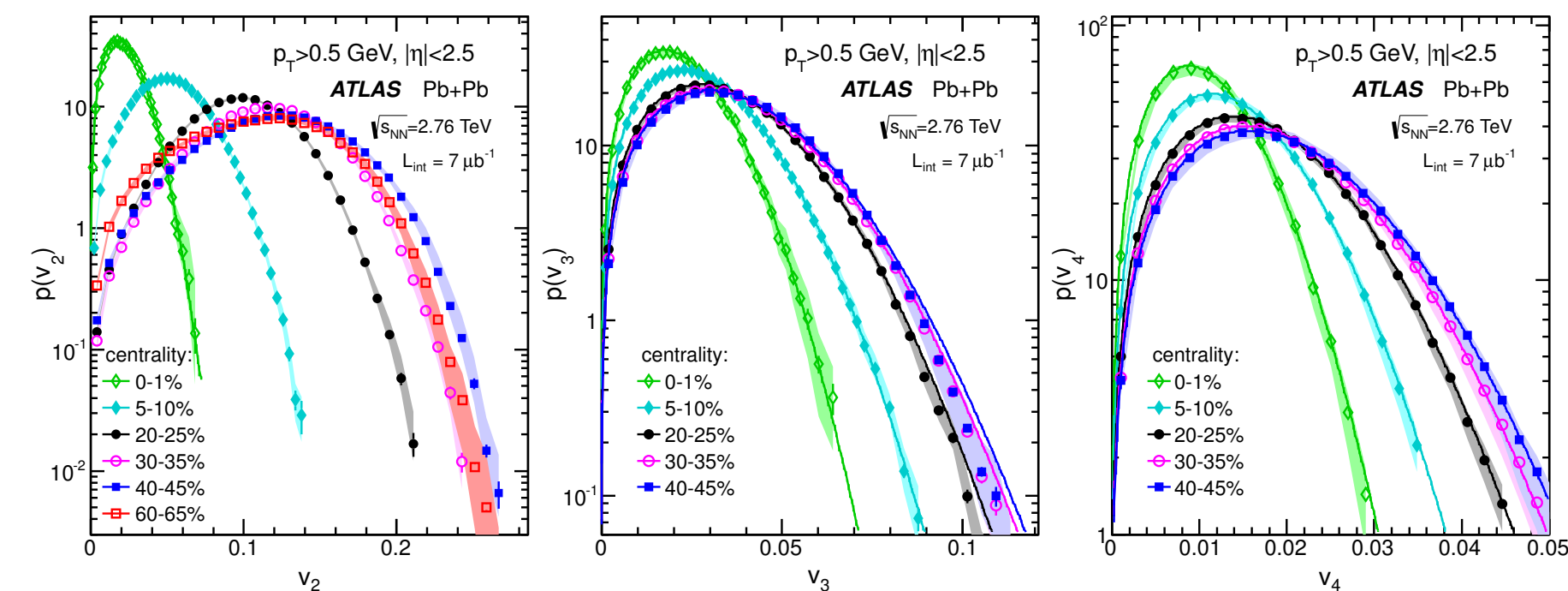
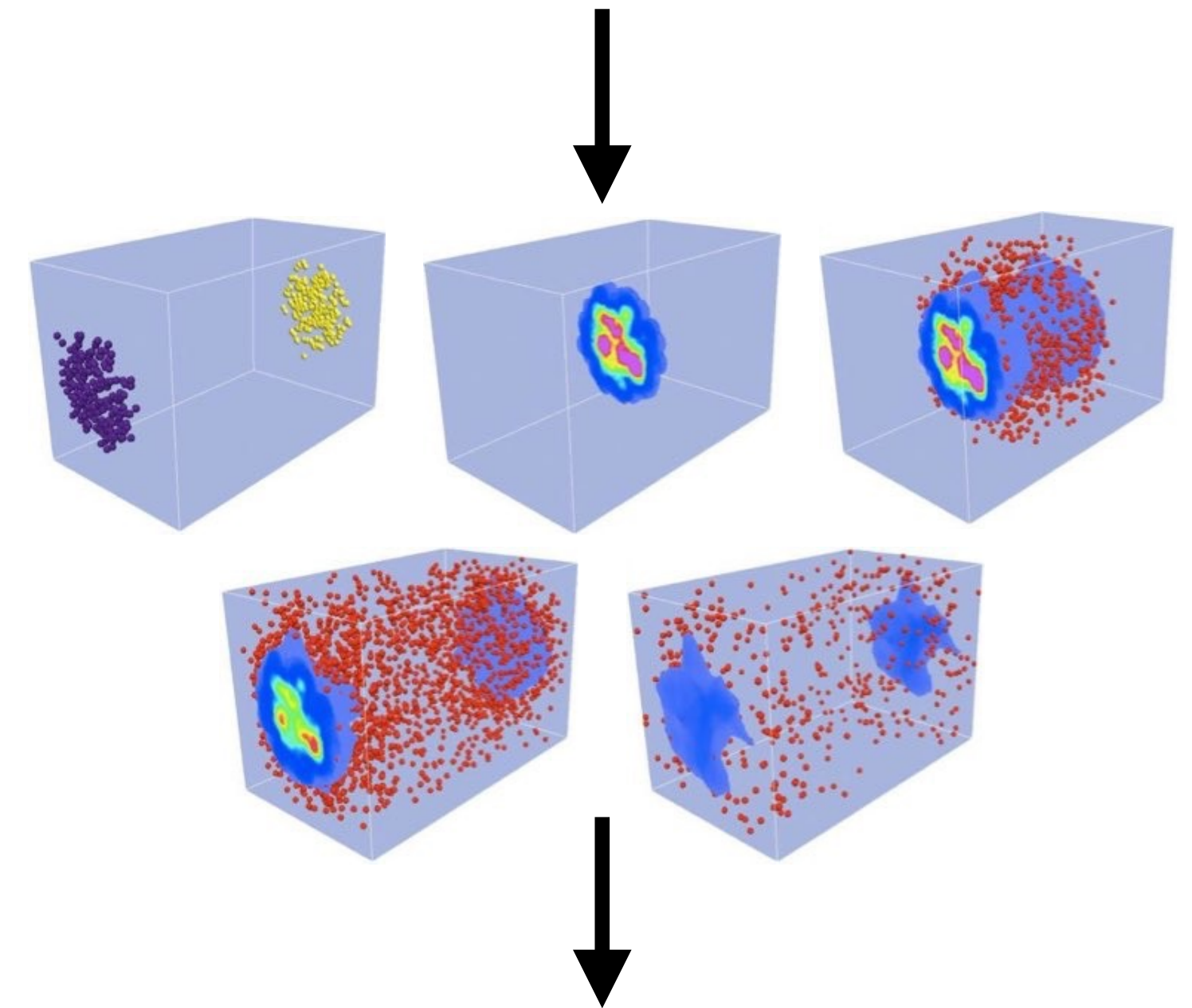
Probing QCD in Heavy-Ion Collisions

Data:

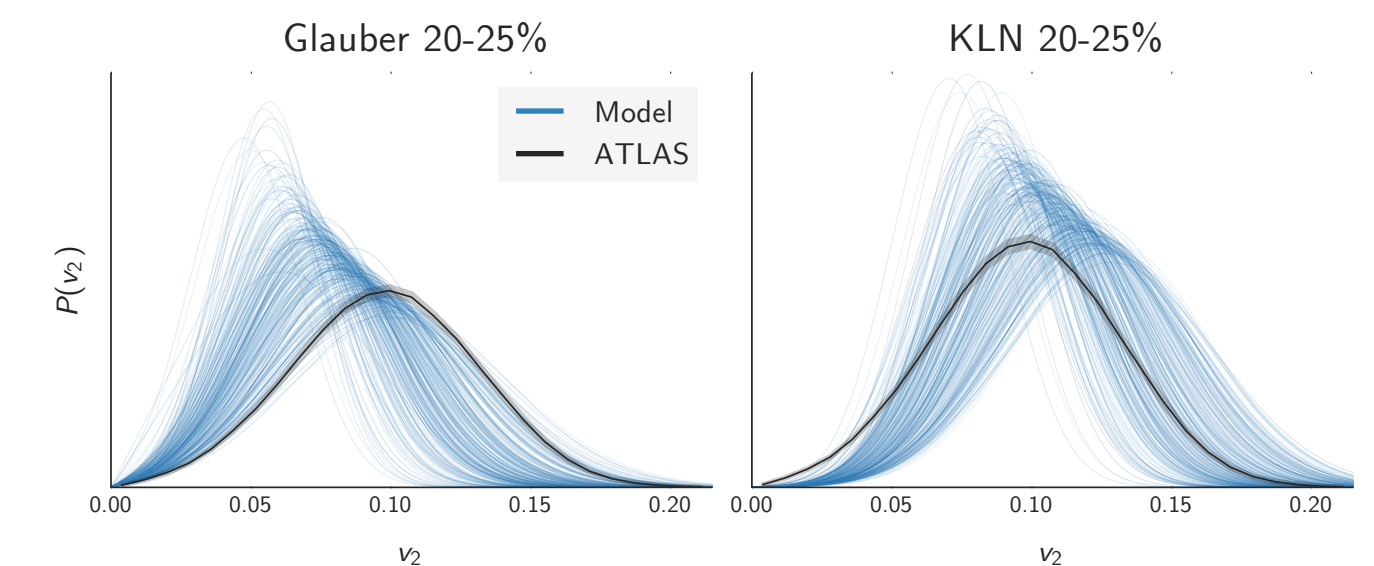


Model:

initial conditions, τ_0 , η/s , ζ/s ,



extracted QGP properties: η/s , ...



Determining the QGP Properties via a Model to Data Comparison

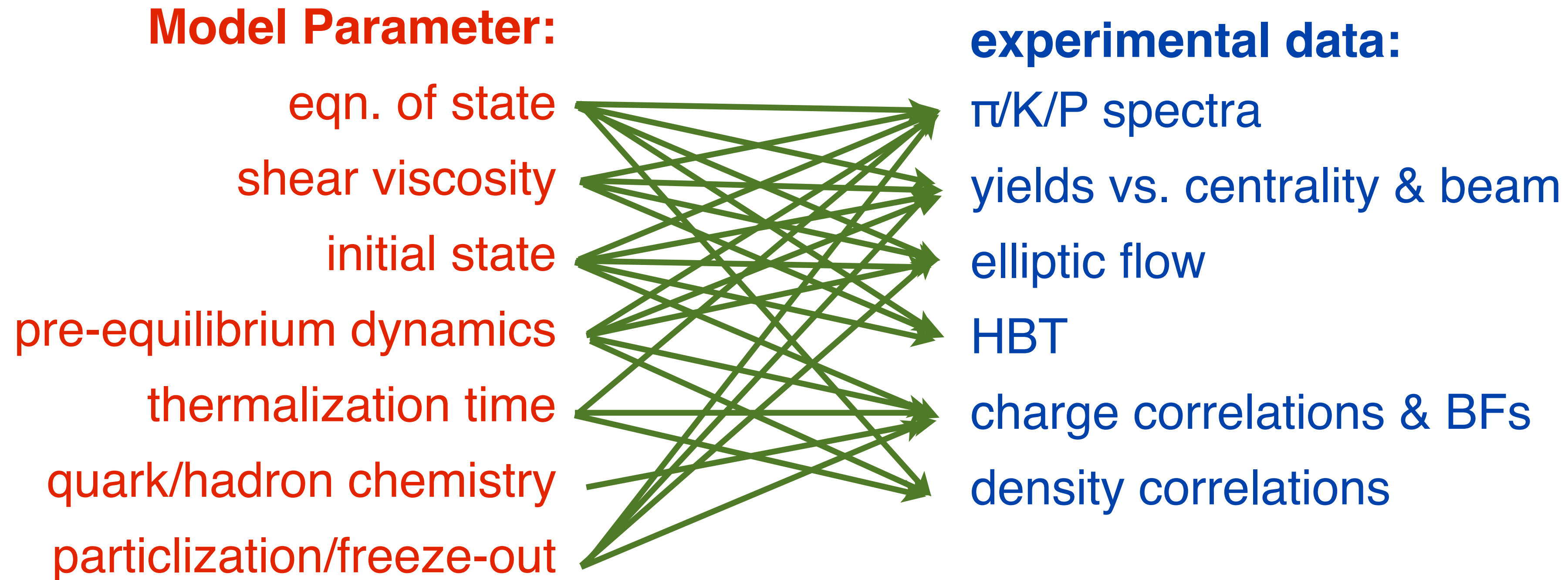
Model Parameter:

eqn. of state
shear viscosity
initial state
pre-equilibrium dynamics
thermalization time
quark/hadron chemistry
particlization/freeze-out

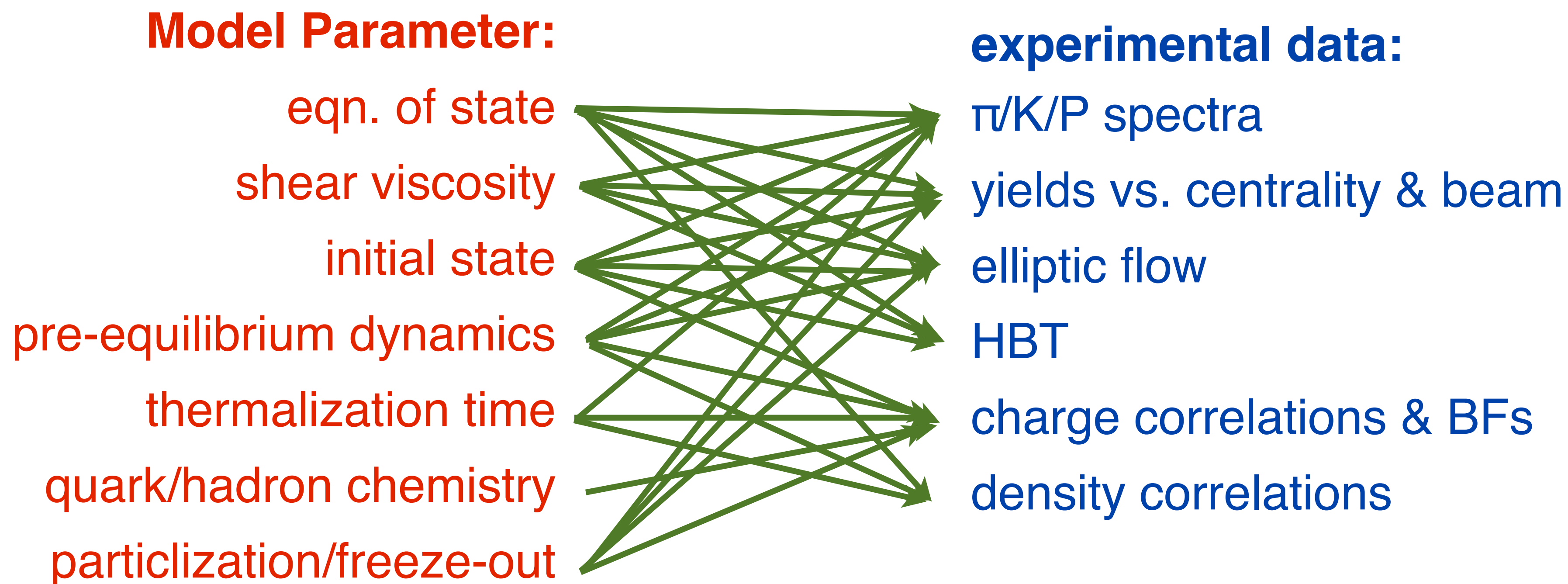
experimental data:

π /K/P spectra
yields vs. centrality & beam
elliptic flow
HBT
charge correlations & BFs
density correlations

Determining the QGP Properties via a Model to Data Comparison



Determining the QGP Properties via a Model to Data Comparison



- 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 RHIC & LHC.

Model Parameters - System Properties

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

Physics Model:

- Trento
- iEBE-VISHNU

Experimental Data

- ALICE flow & spectra

estimate or calculate parameters

calculate observables & compare to data

Bayesian Analysis

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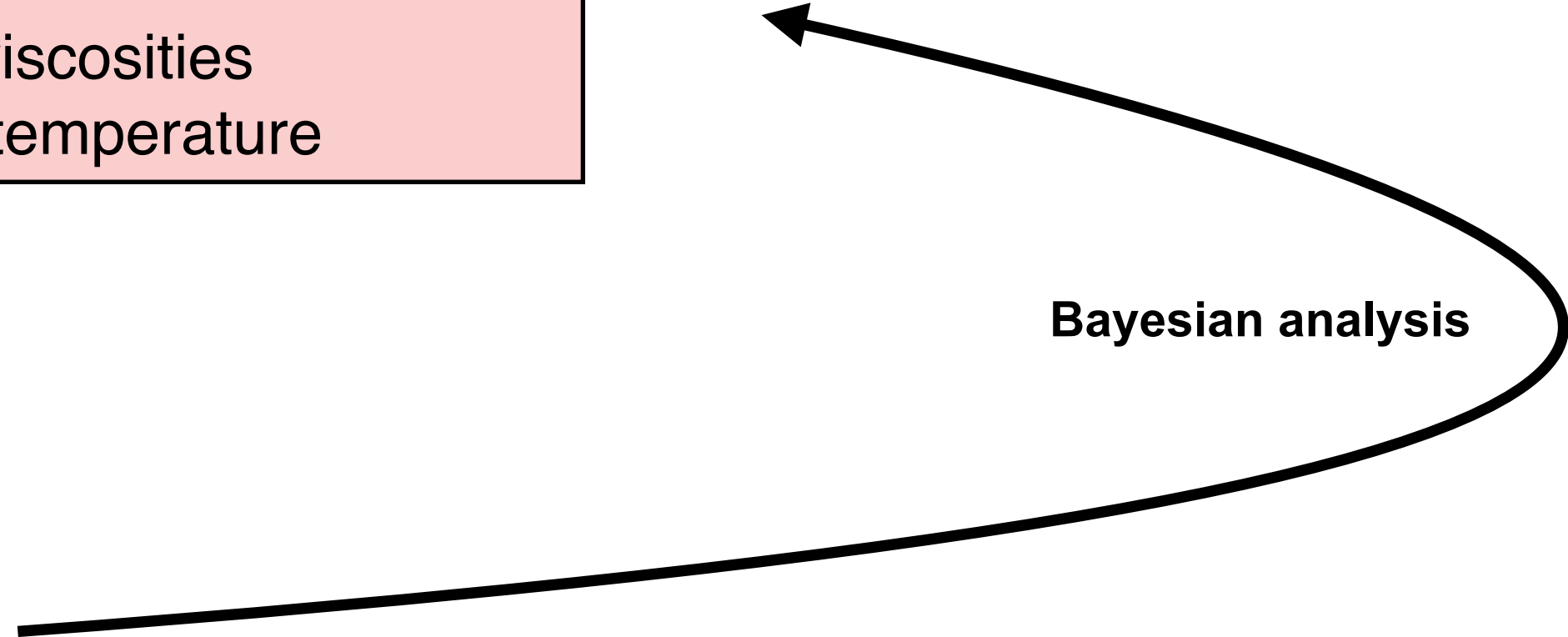
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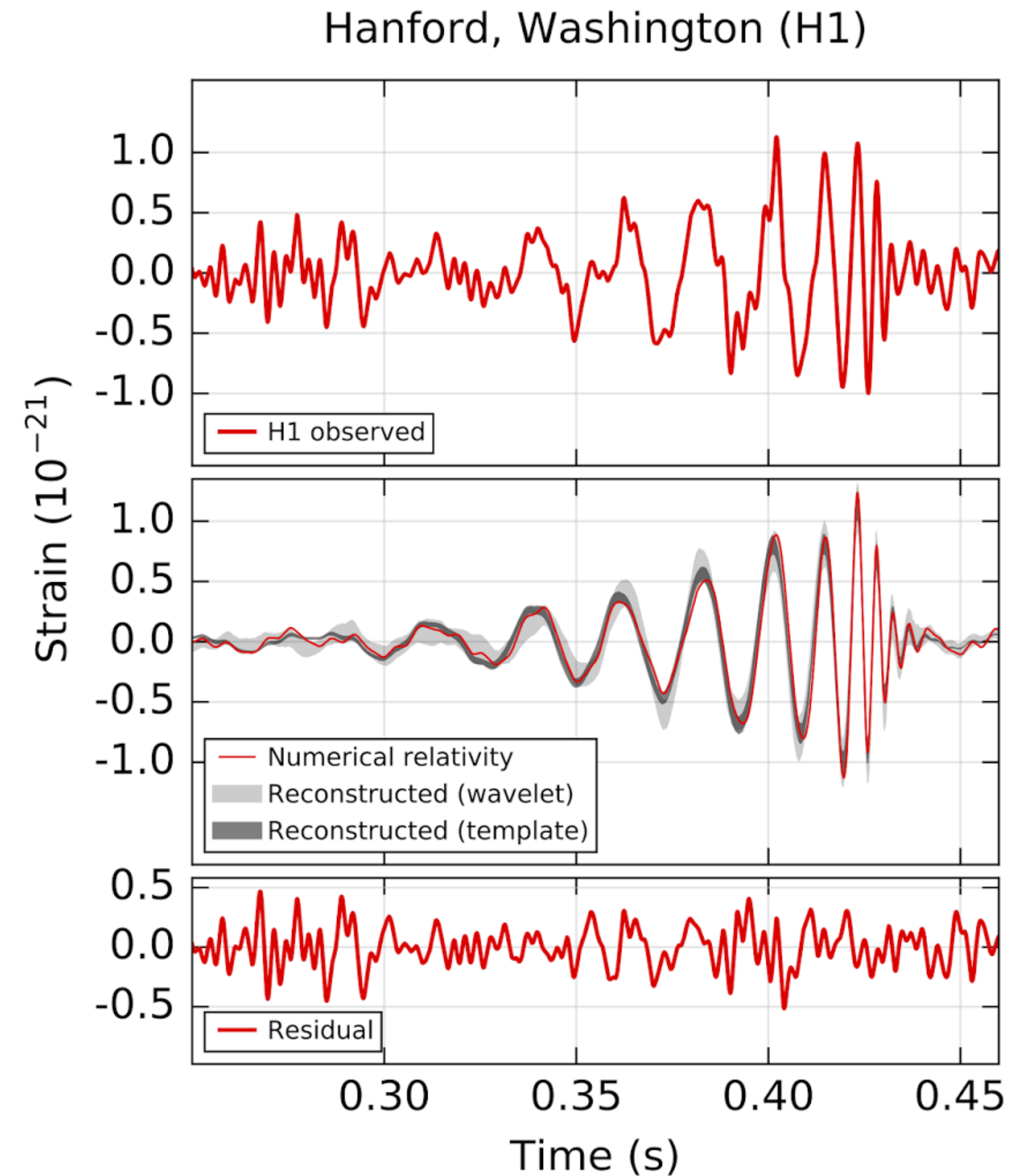
Experimental Data

- ALICE flow & spectra

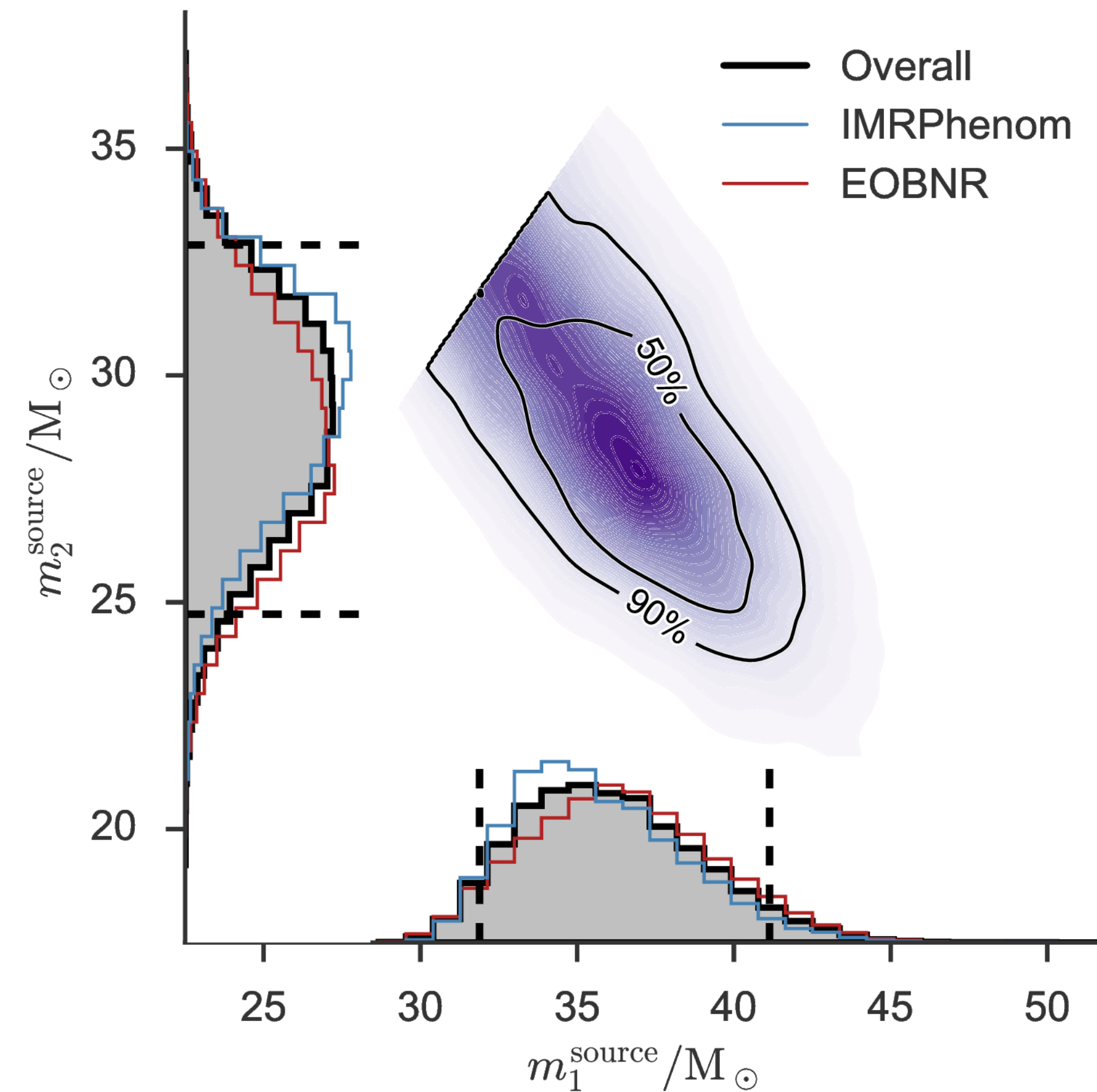
- Bayesian analysis allows us to simultaneously calibrate all model parameters via a model-to-data comparison
- determine parameter values such that the model best describes experimental observables
- extract the probability distributions of all parameters

Example: Gravitational Waves

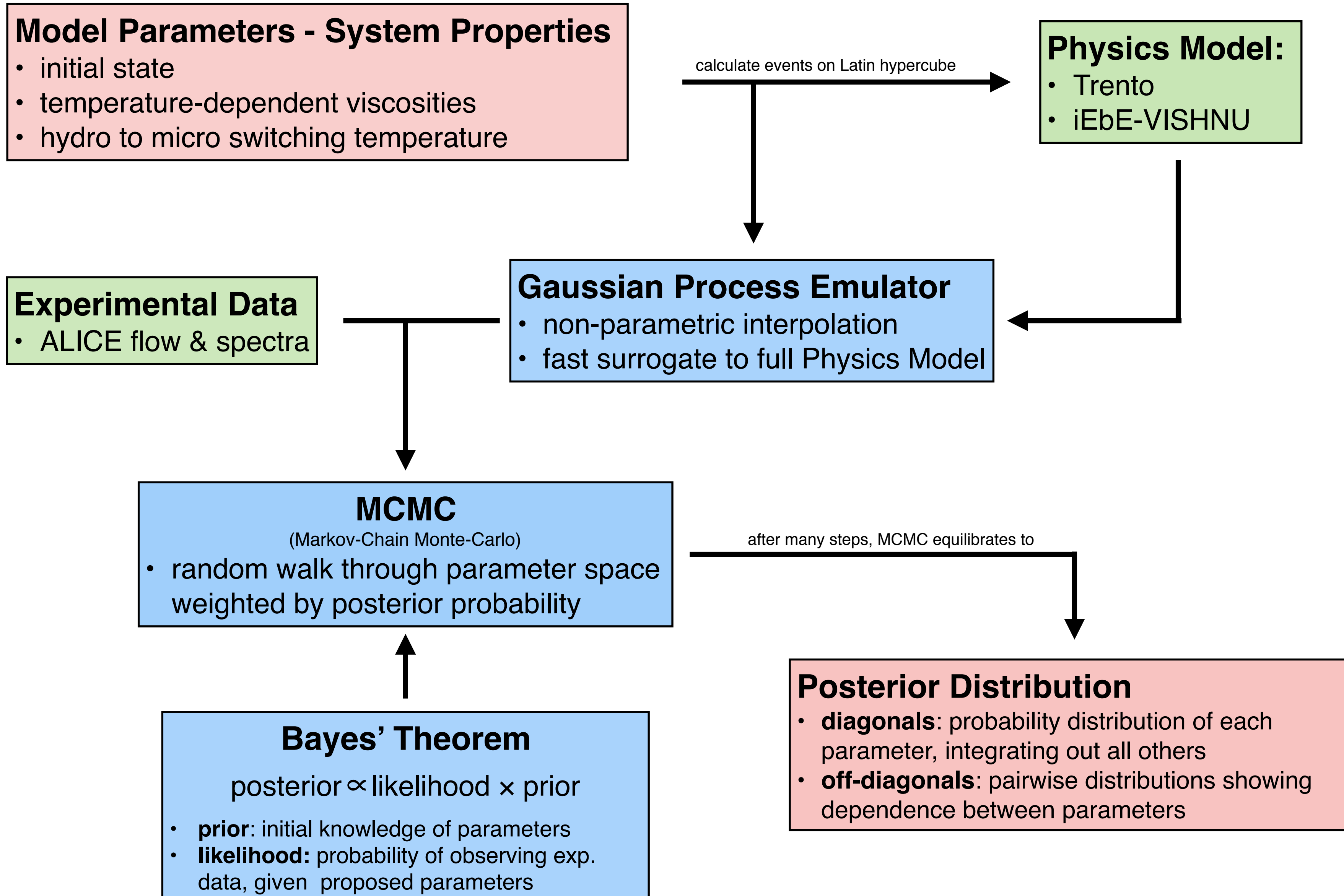
LIGO gravitational wave signal:



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

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

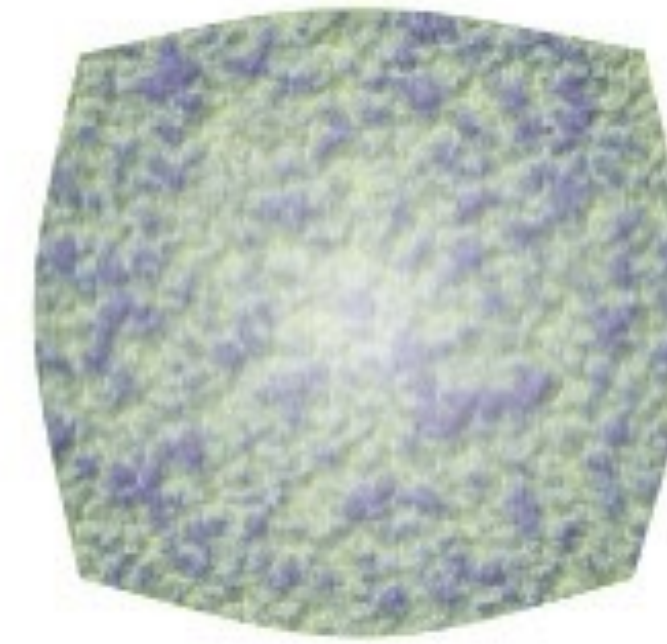
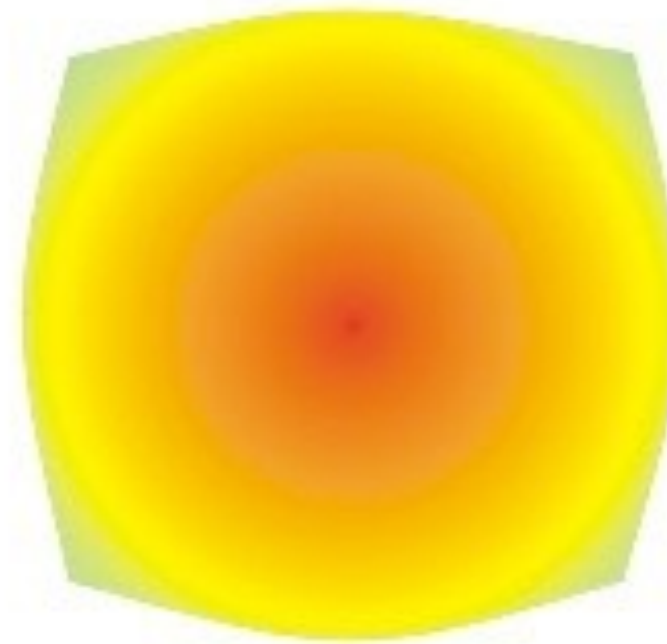
- **prior:** initial knowledge of parameters
- **likelihood:** probability of observing exp. data, given proposed parameters

Physics Model: Trento + iEbE-VISHNU

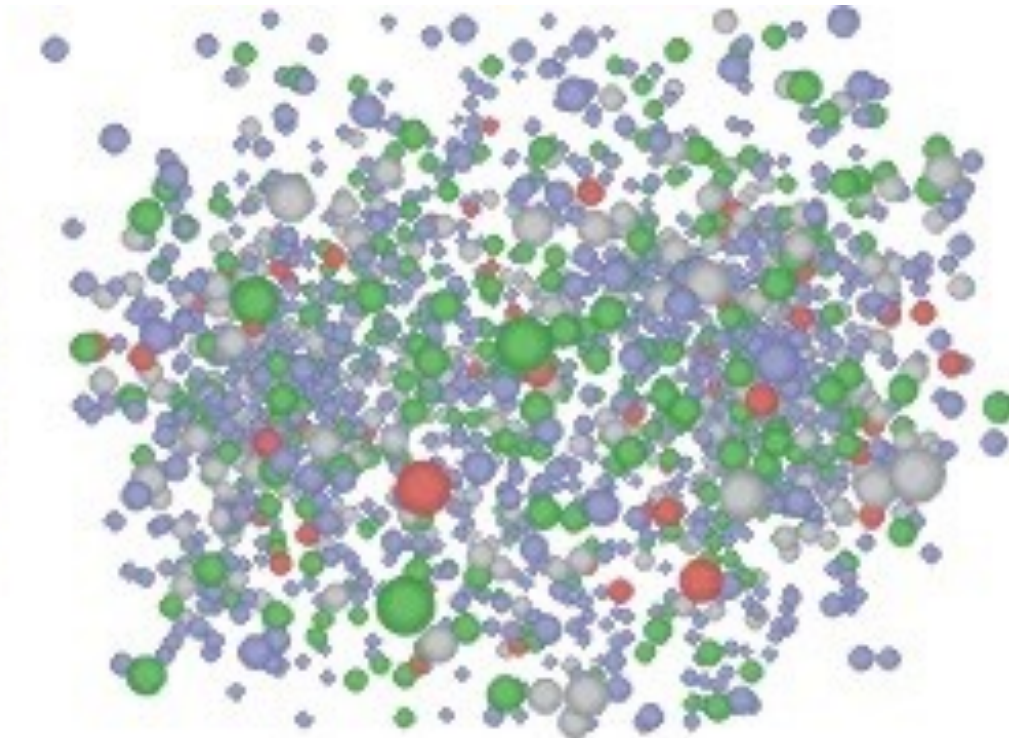
QGP and
hydrodynamic expansion

hadronic phase
and freeze-out

parameterized
initial QGP state

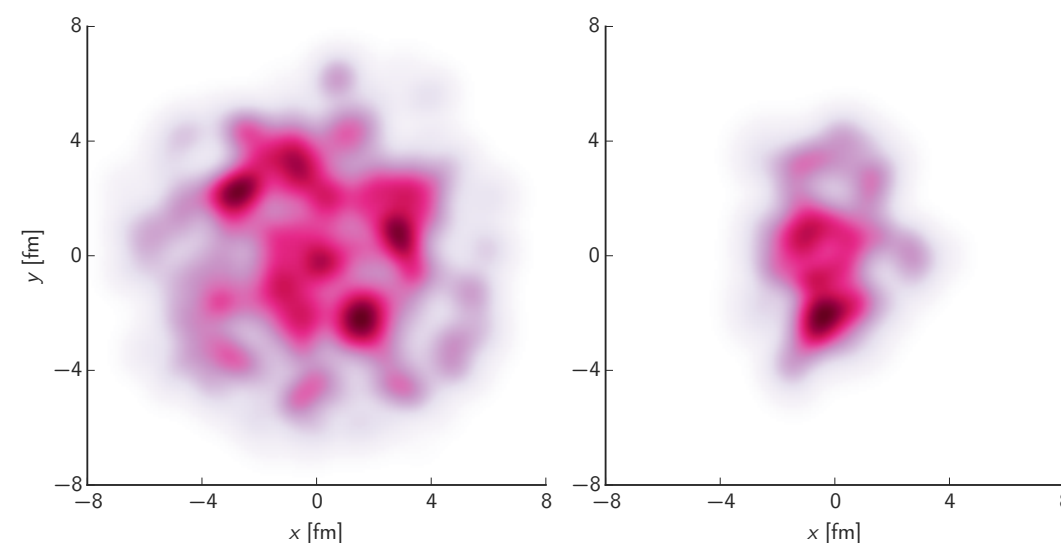


hadronization



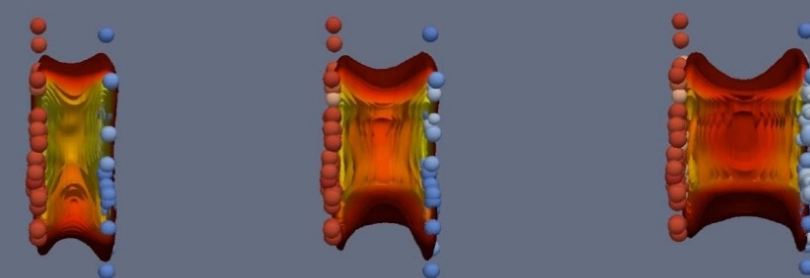
Trento:

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



iEbE-VISHnew:

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



UrQMD:

- non-equilibrium evolution of an interacting hadron gas
- hadron gas shear & bulk viscosities are implicitly contained in calculation

Methodology

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Bayes' Theorem

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Calibration Parameters

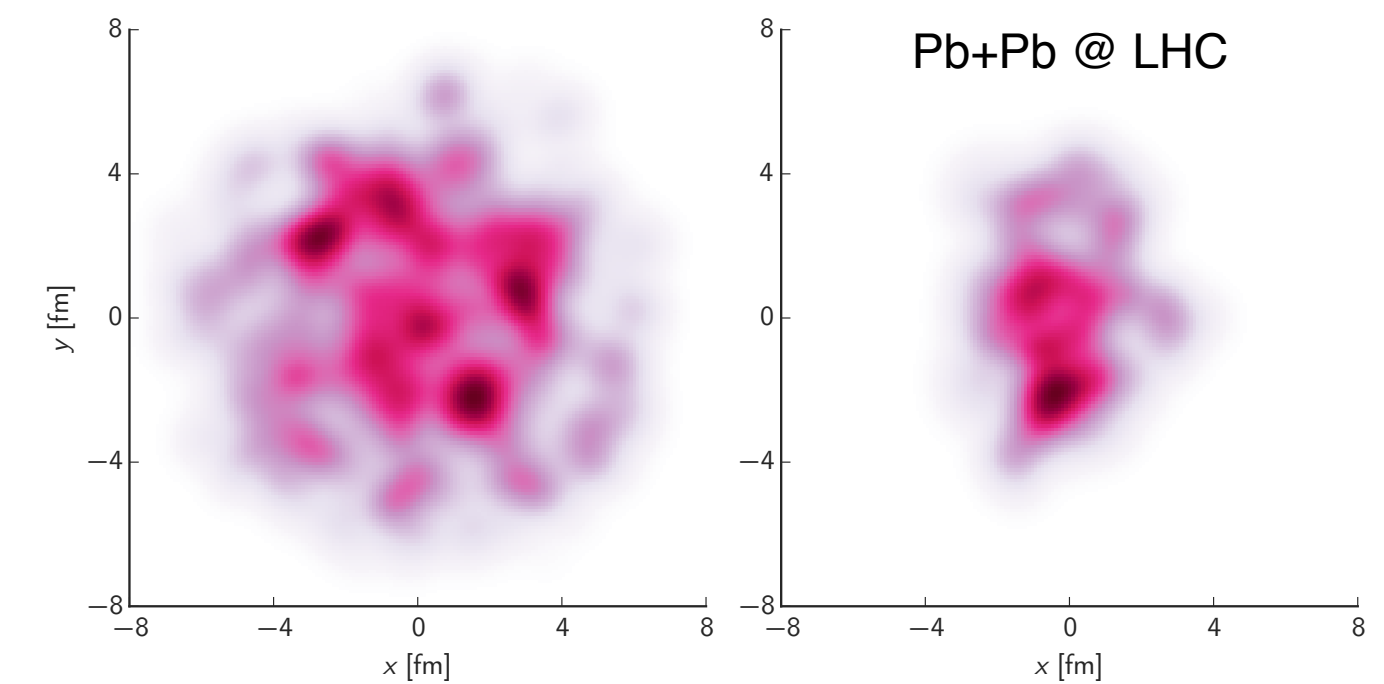
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Trento initial condition:

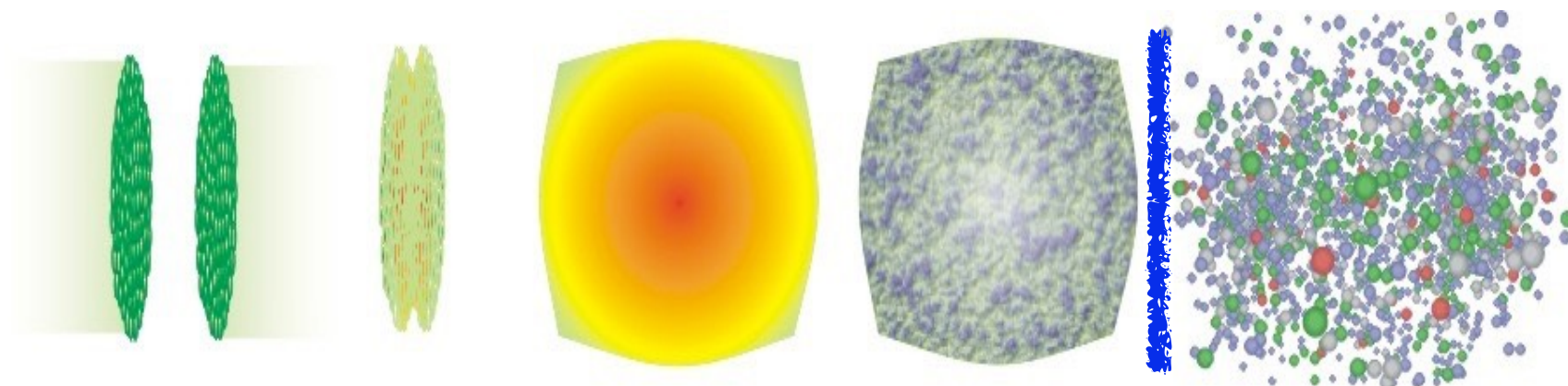
- p : attenuation parameter - entropy deposition
- k : governs fluctuation in nuclear thickness
- w : Gaussian nucleon width



Calibration Parameters

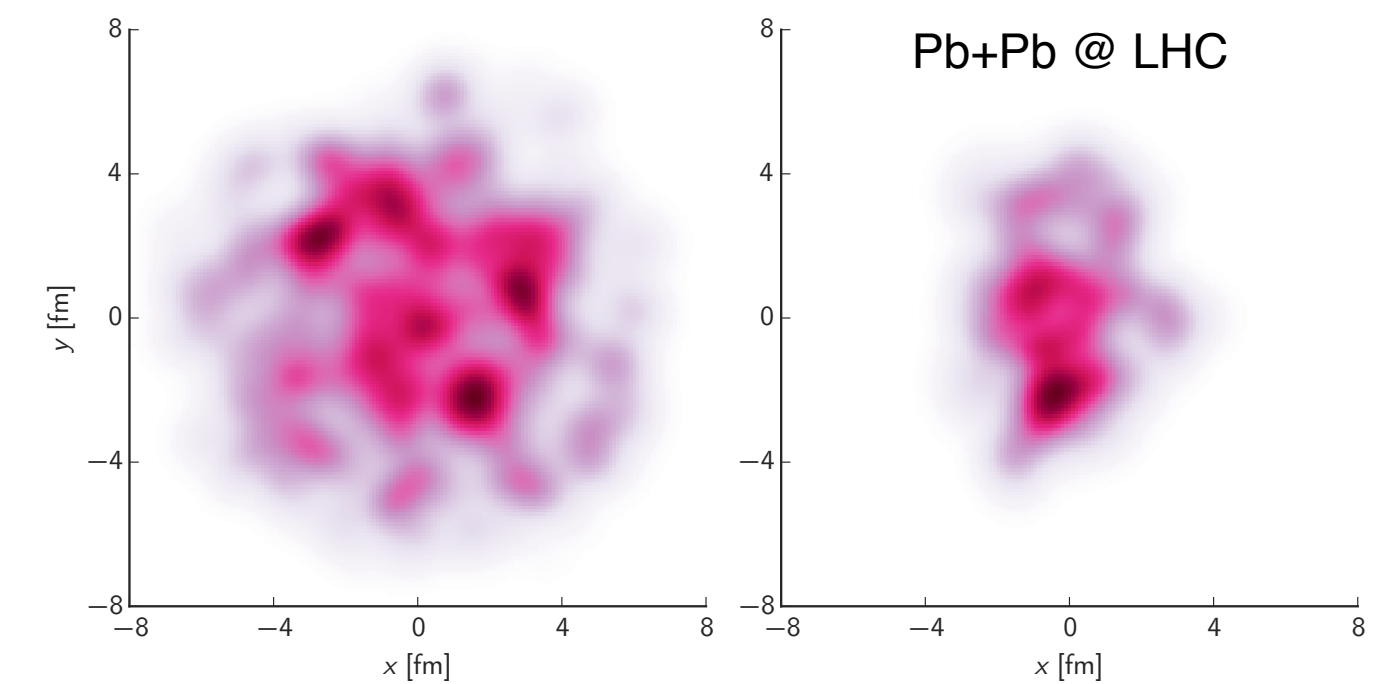
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- hydro to micro switching temperature T_{sw}



Trento initial condition:

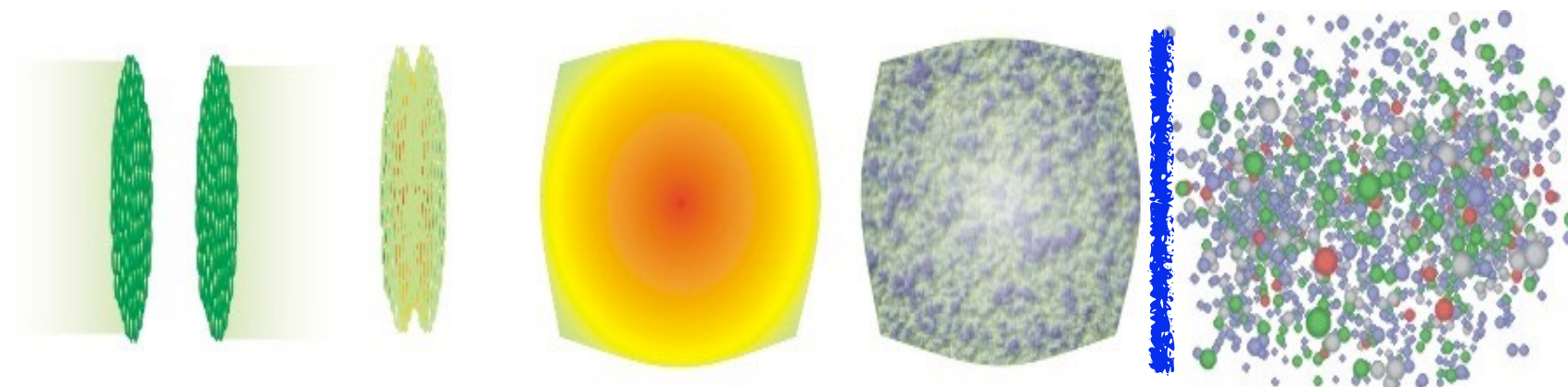
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Calibration Parameters

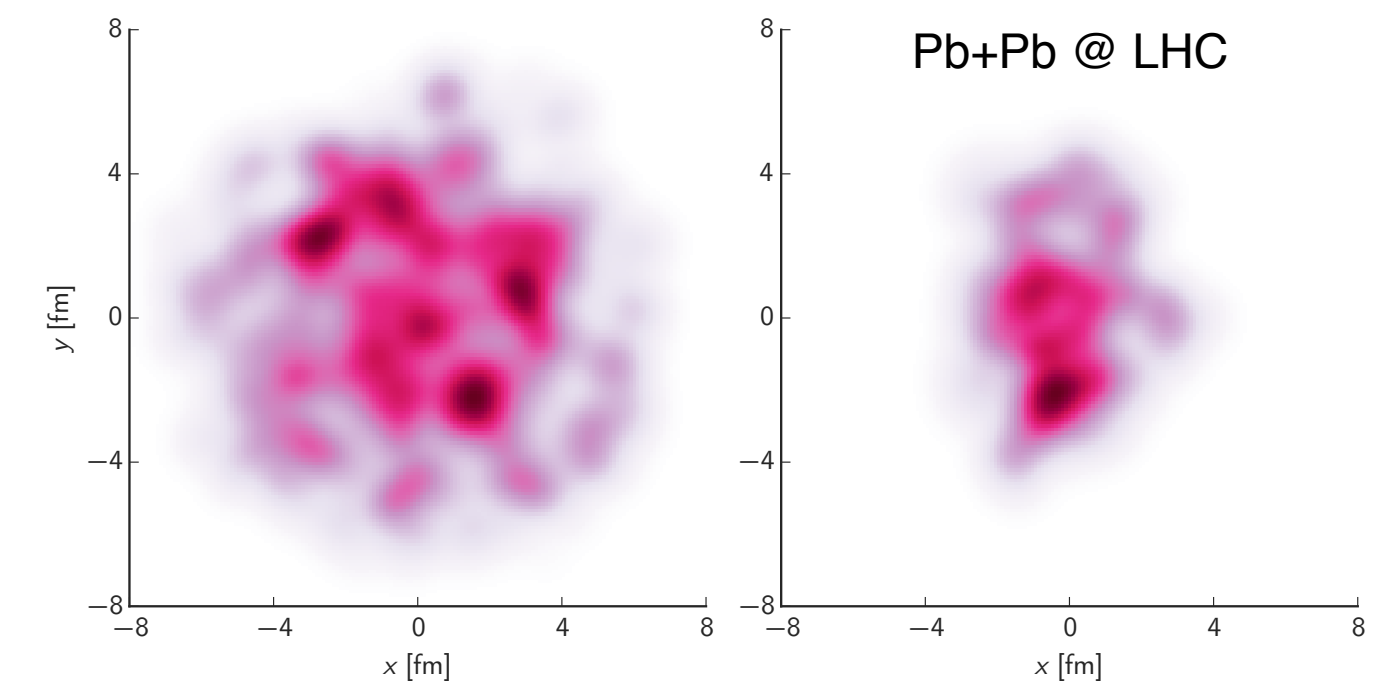
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- k : governs fluctuation in nuclear thickness
- w : Gaussian nucleon width

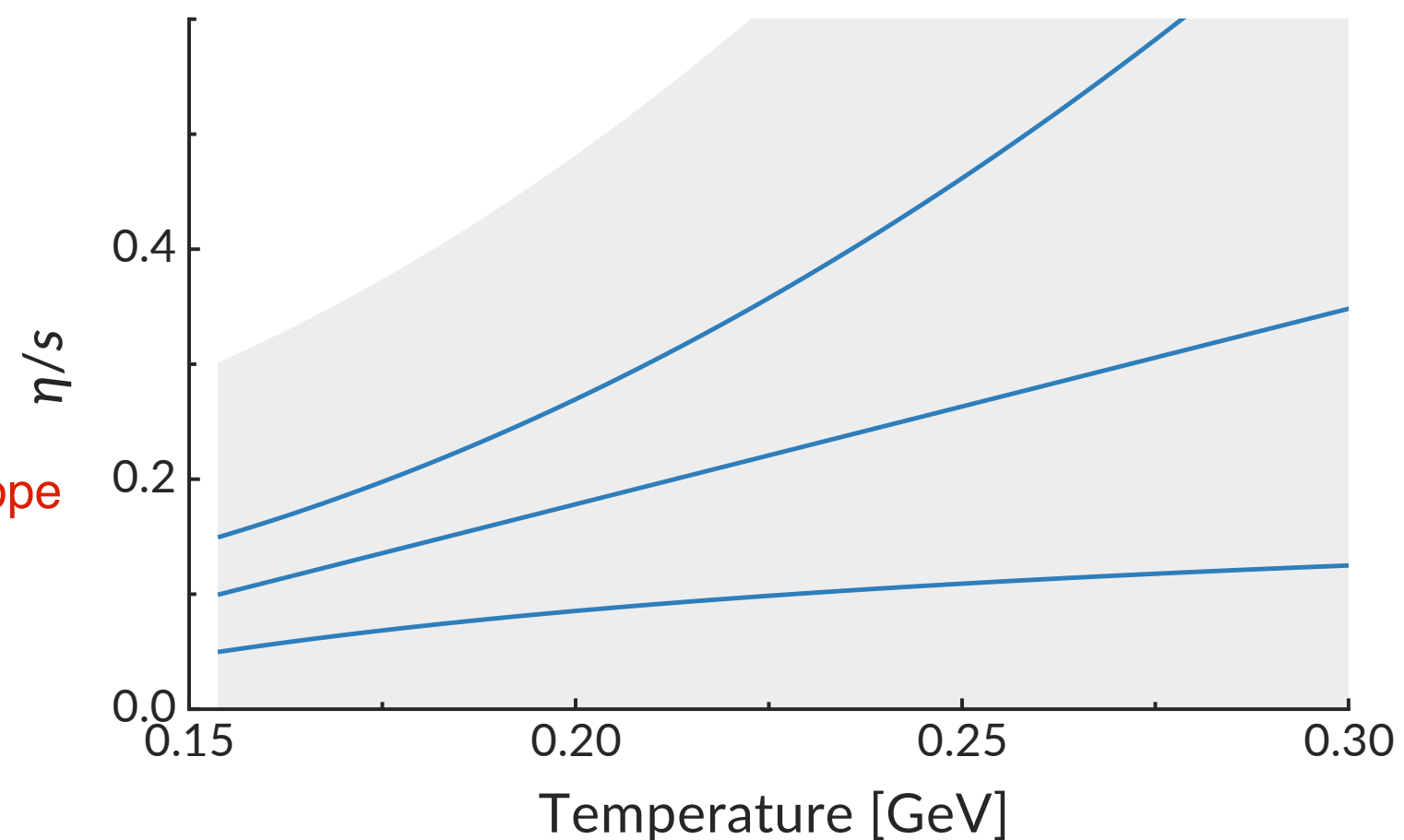


temperature dependent shear viscosity:

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

parameters:

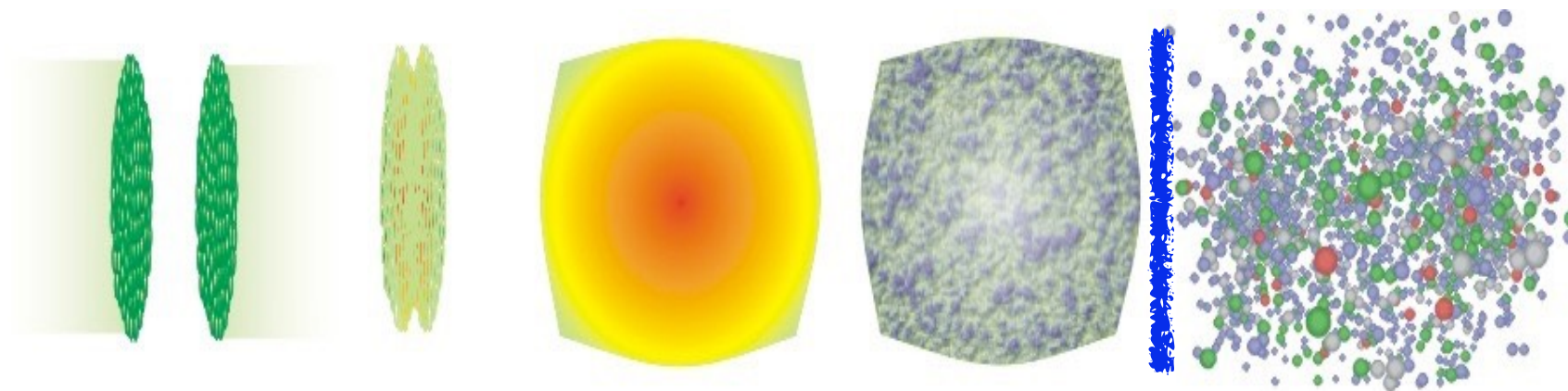
- intercept: $(\eta/s)_{\min}$ at T_C
- slope: $(\eta/s)_{\text{slope}}$
- curvature: β



Calibration Parameters

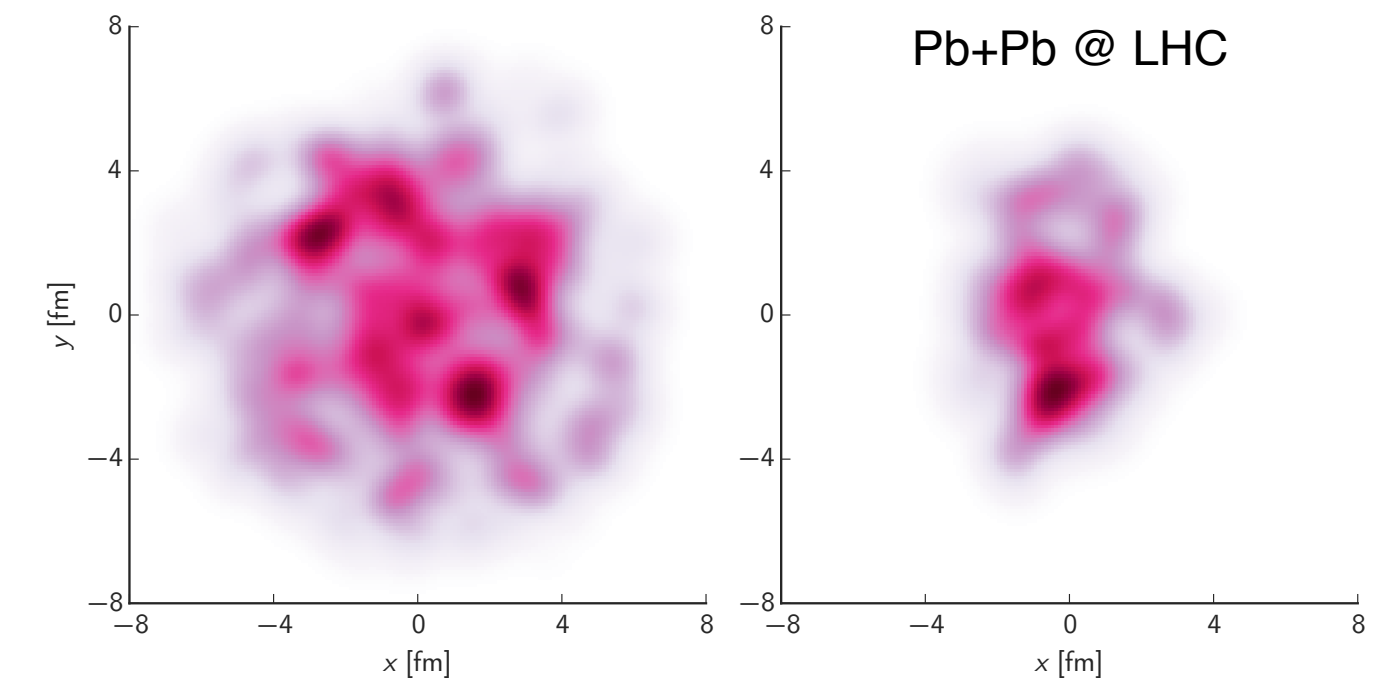
- the calibration parameters are the model parameters that codify the physical properties of the system that we wish to characterize with the analysis

- hydro to micro switching temperature T_{sw}



Trento initial condition:

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

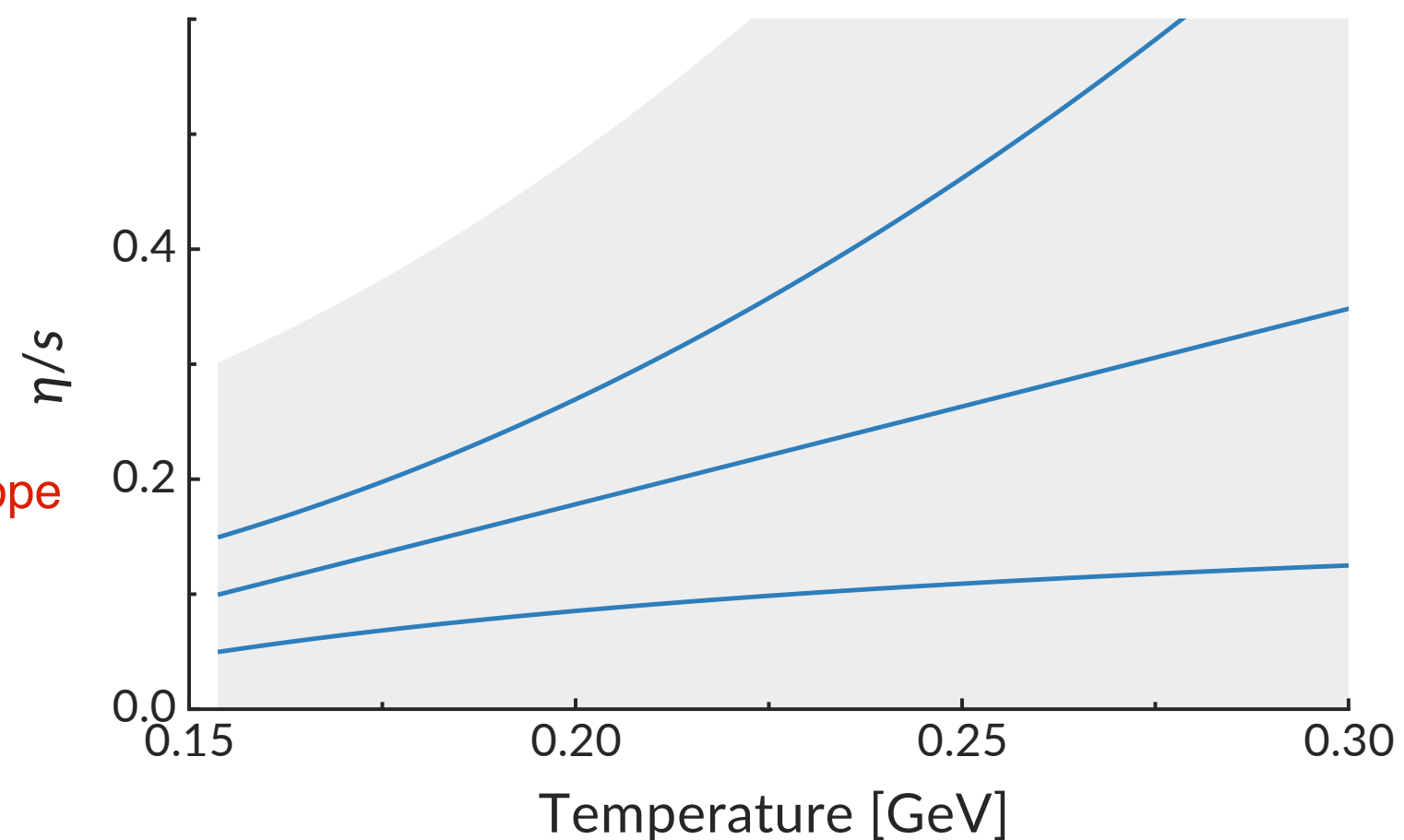


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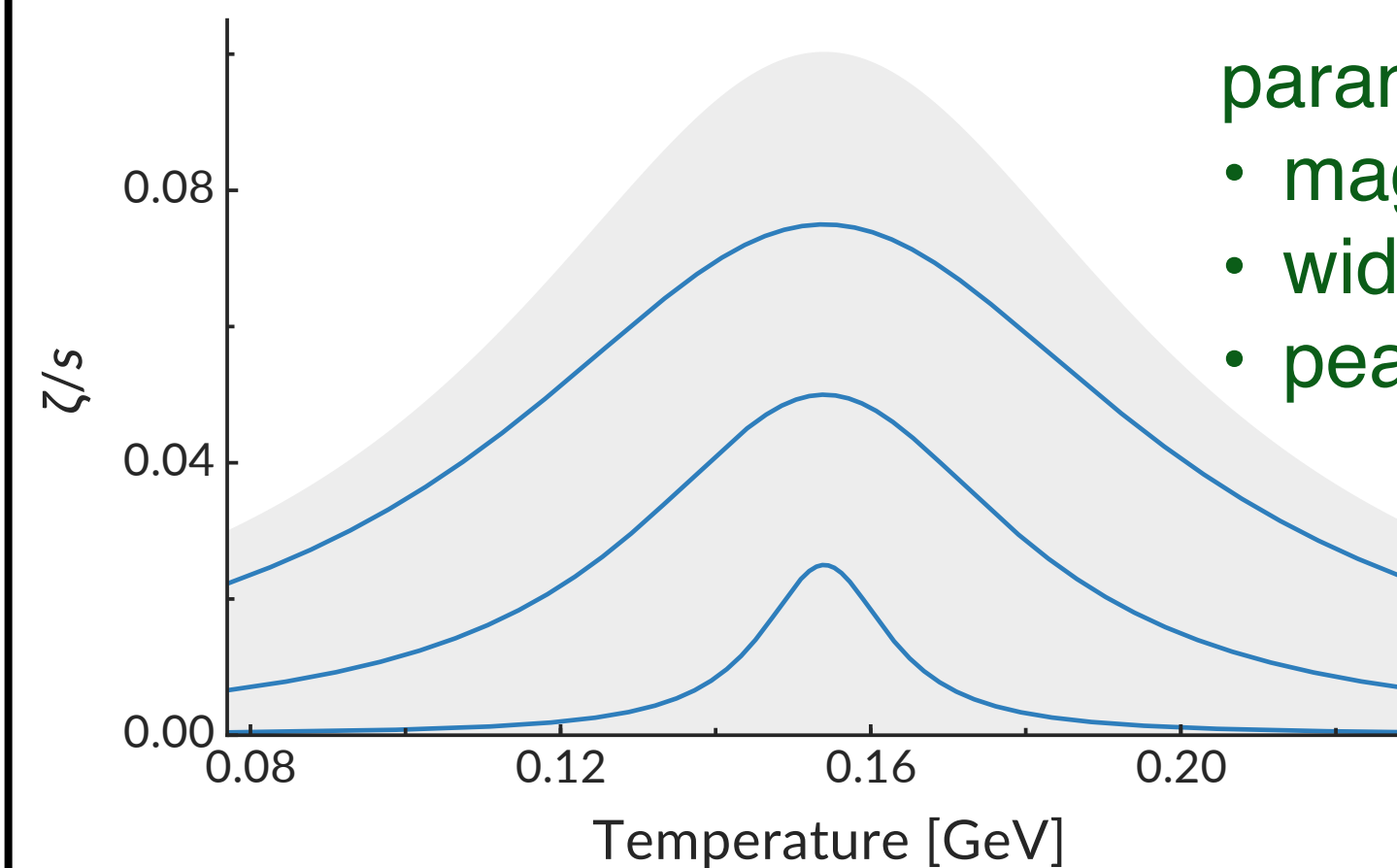


temperature dependent bulk viscosity:

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

parameters:

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



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

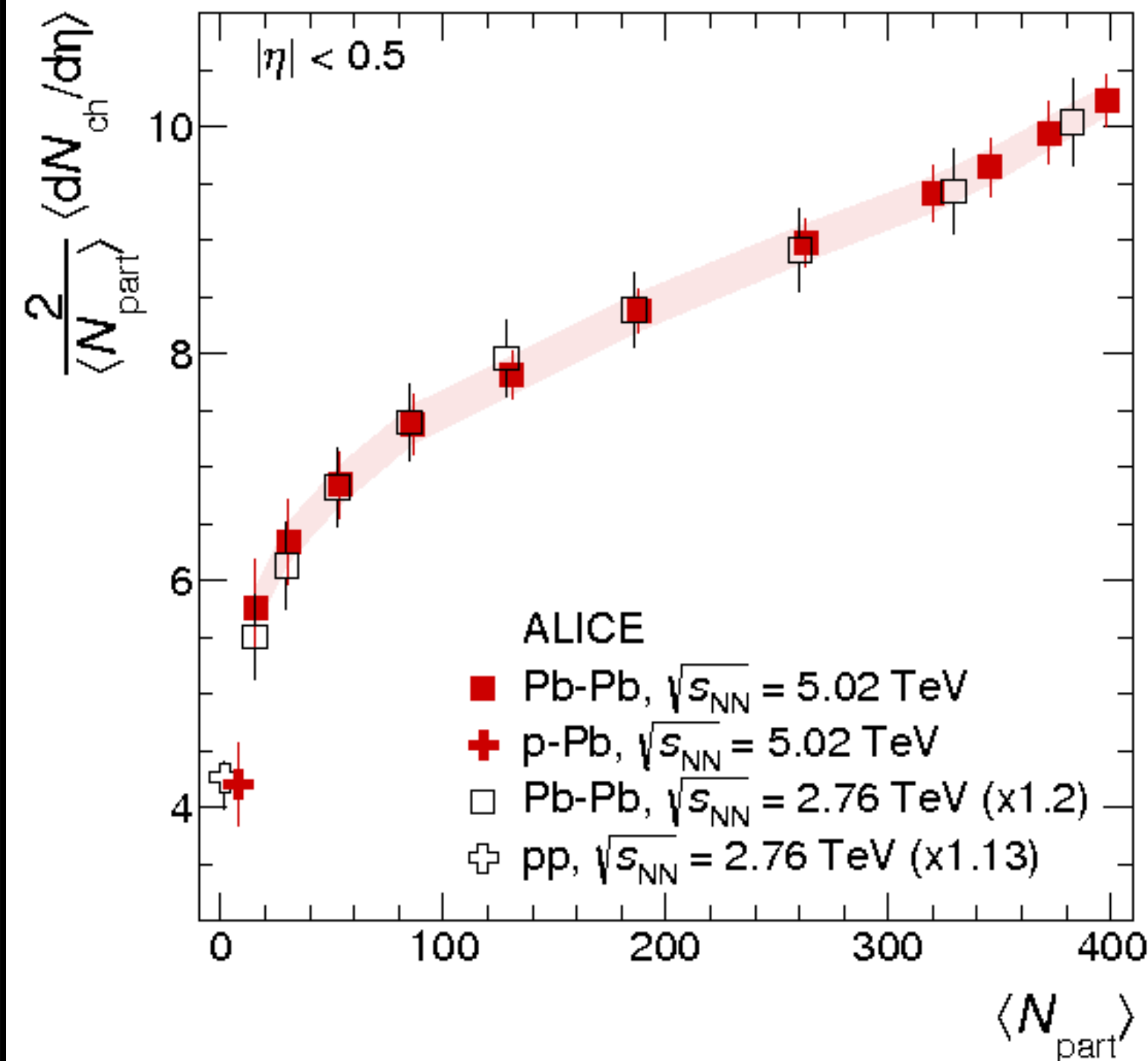
$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

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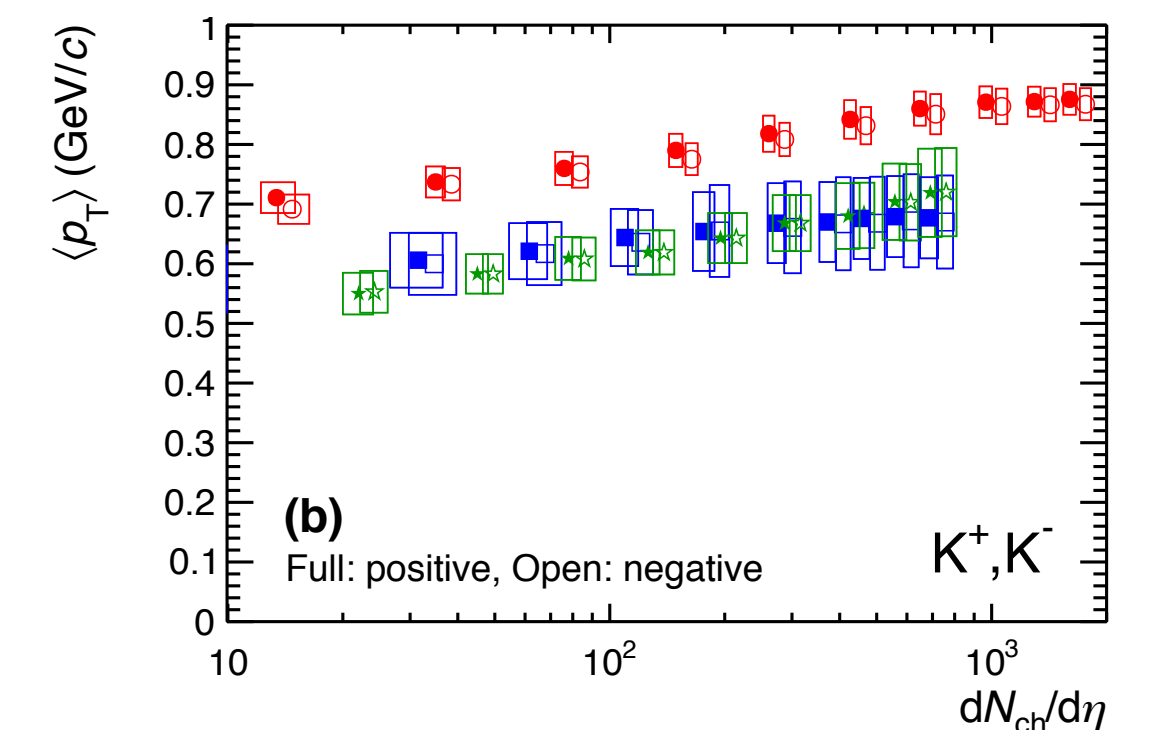
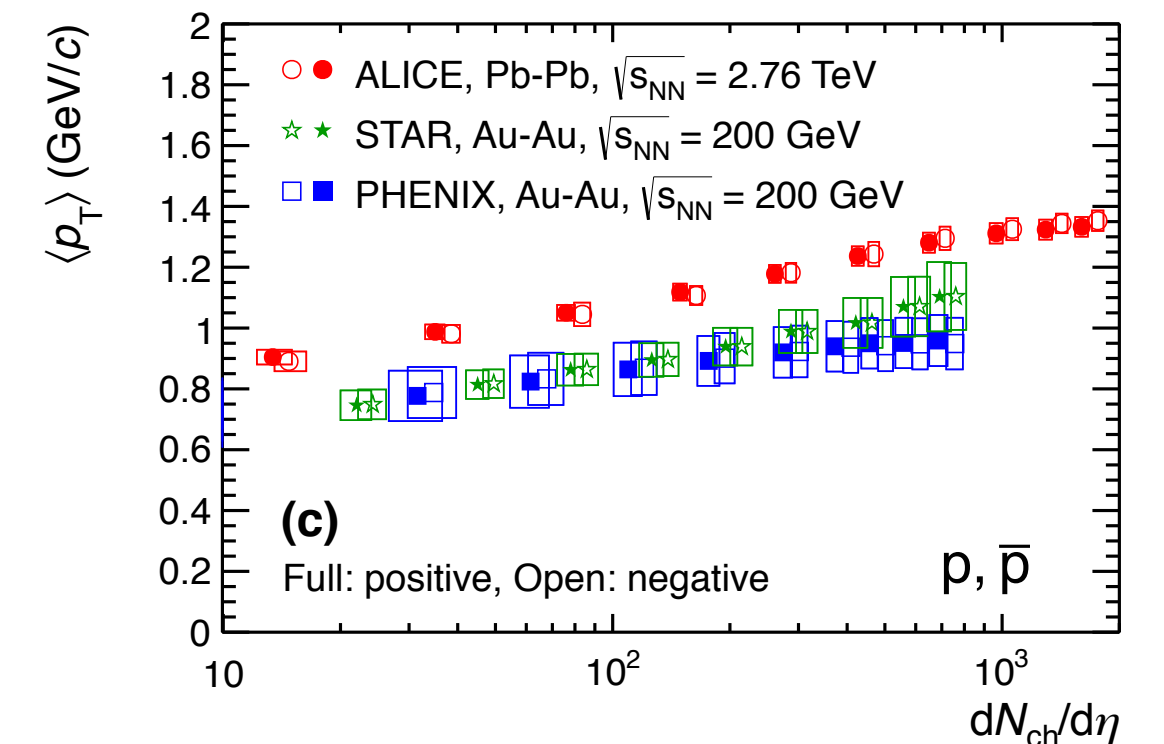
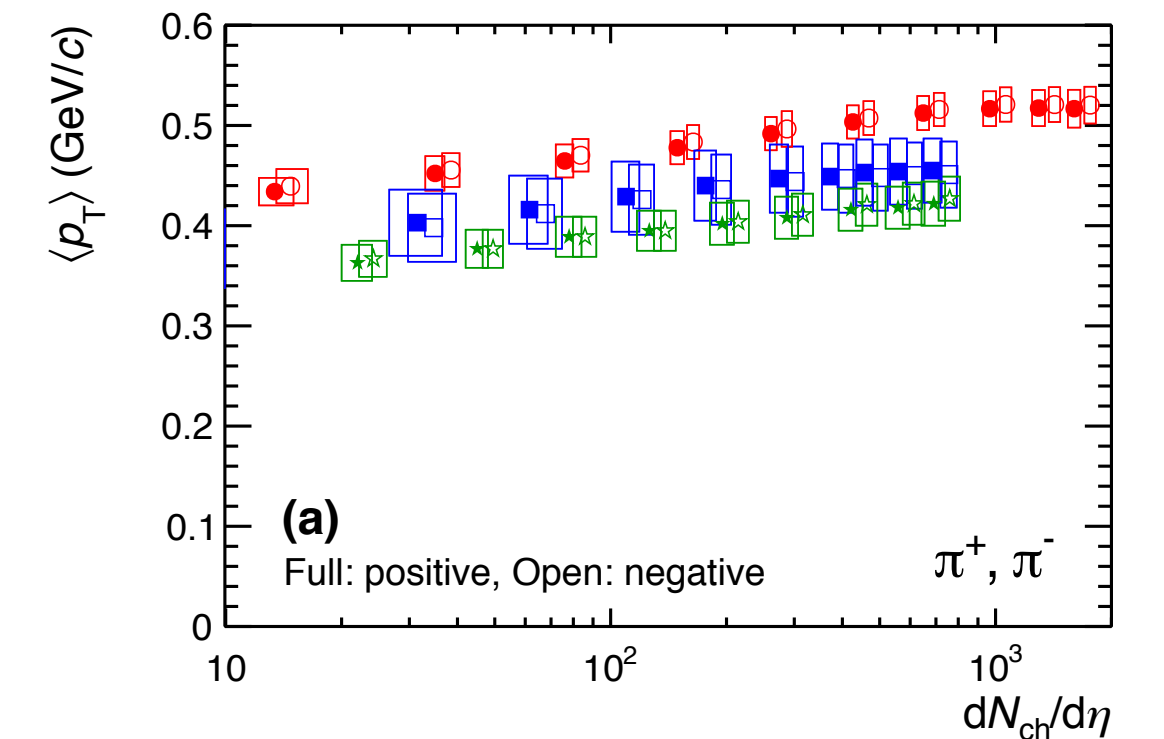
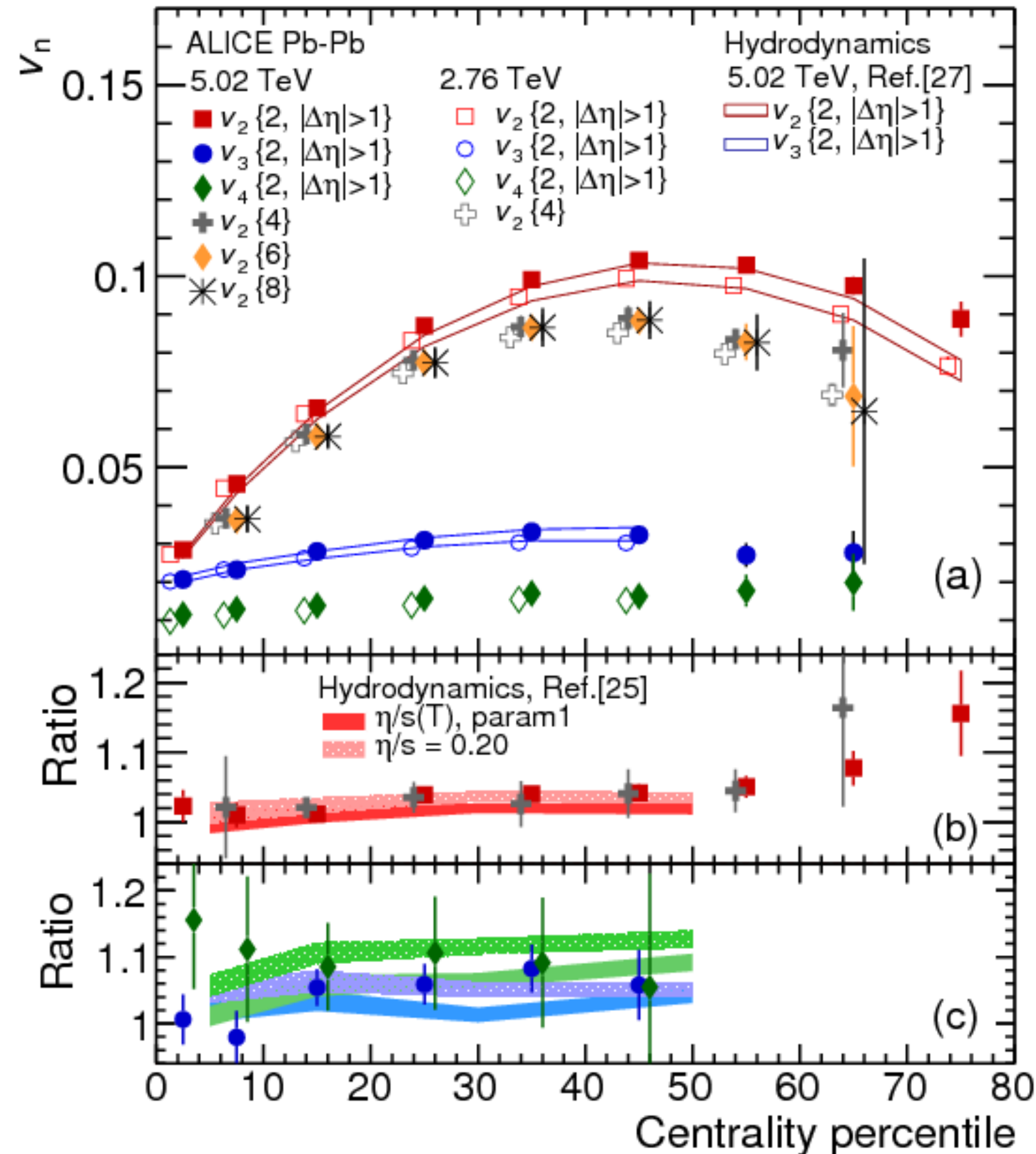
Training Data

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

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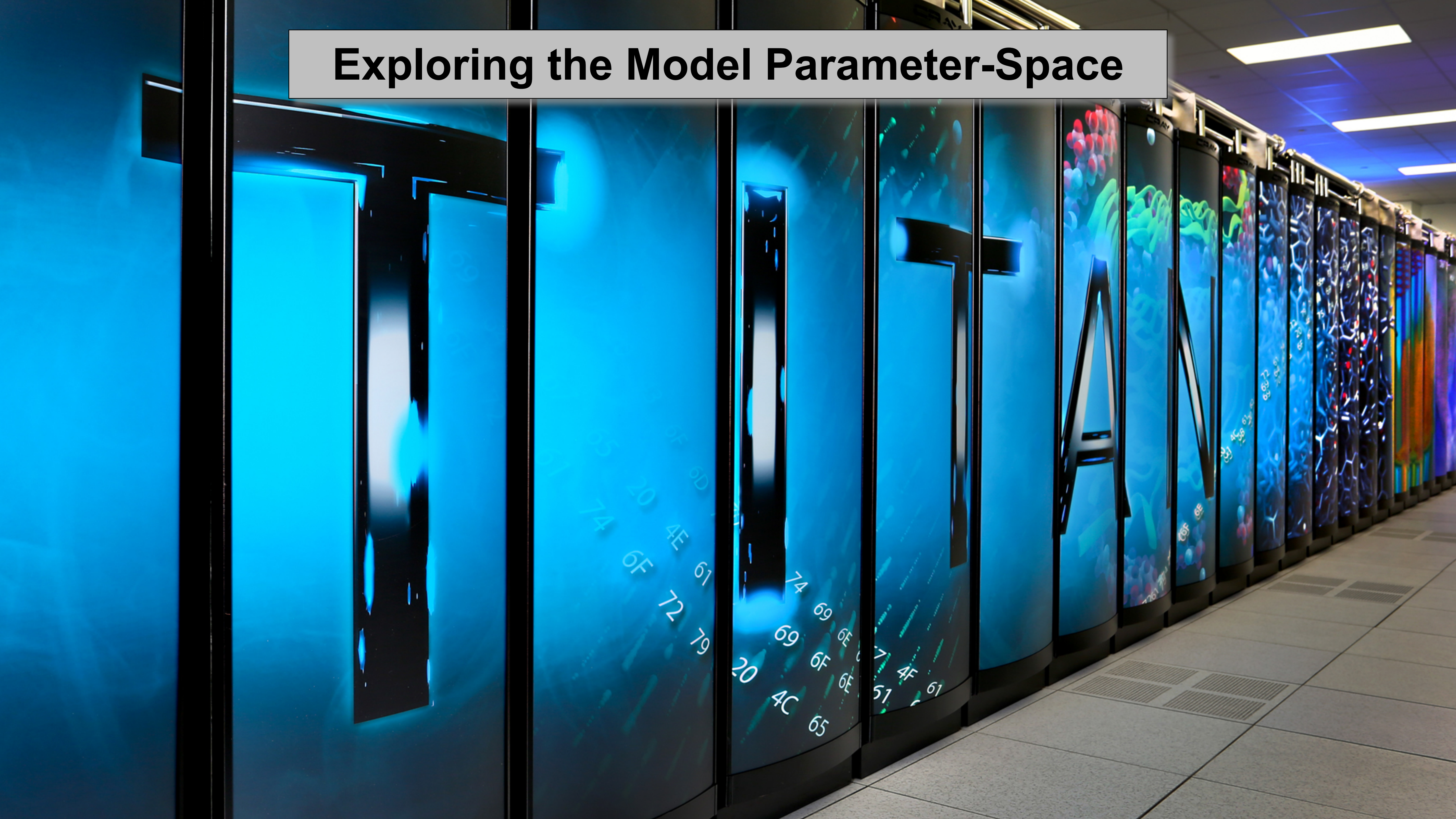
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Exploring the Model Parameter-Space



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)**
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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**

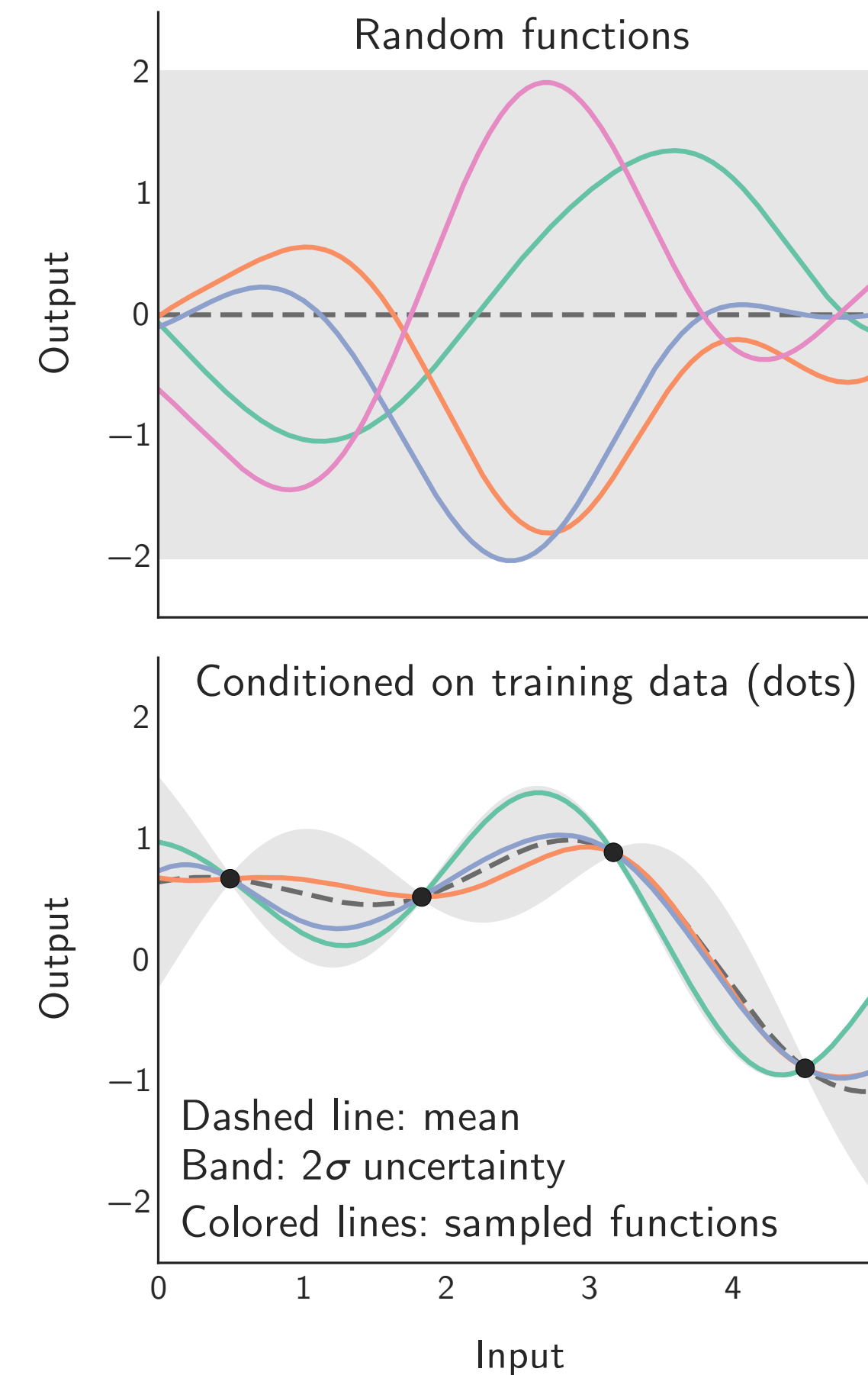
Exploring the Model Parameter-Space

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



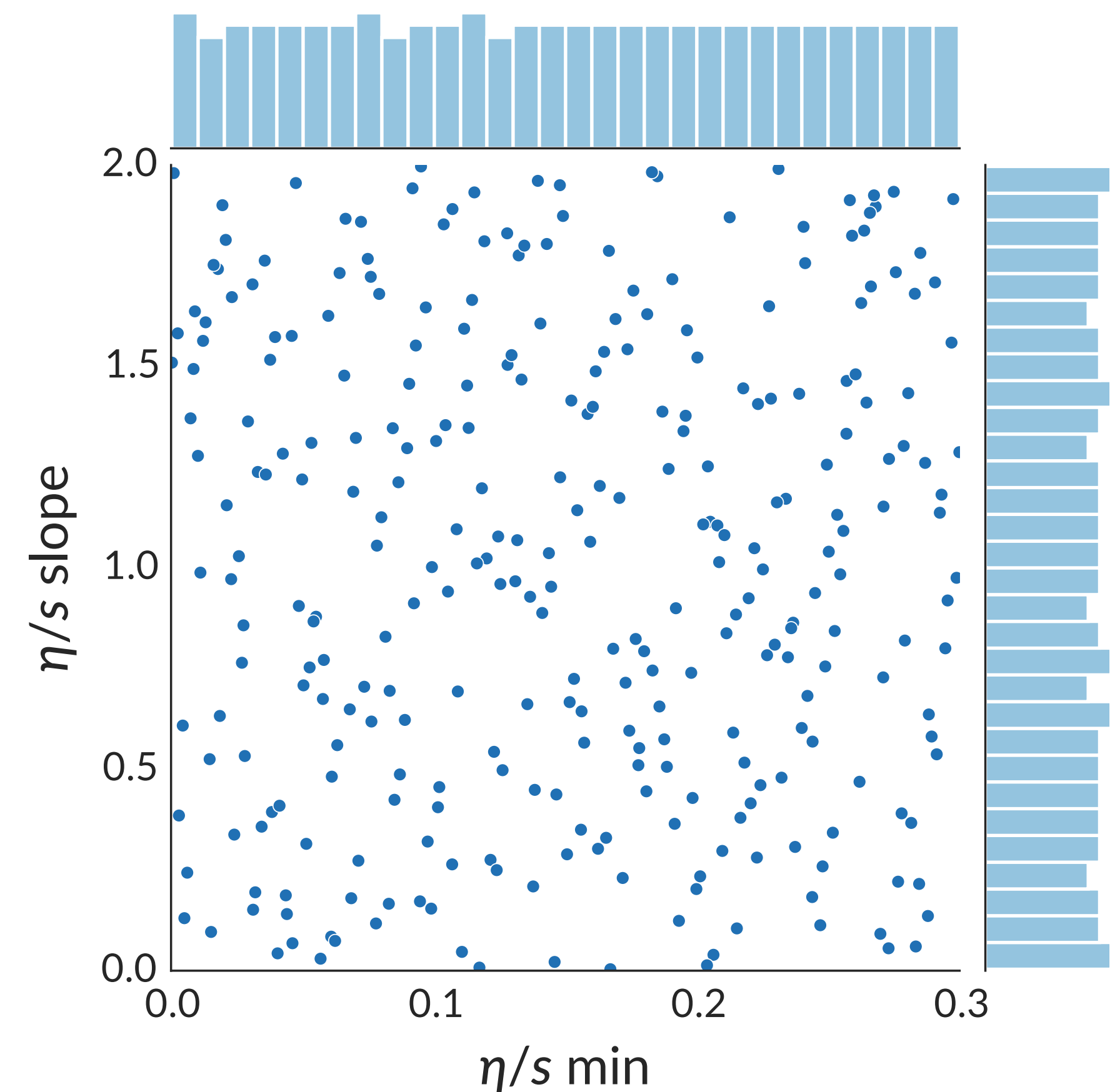
Computer Experiment Design

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



Computer Experiment Design

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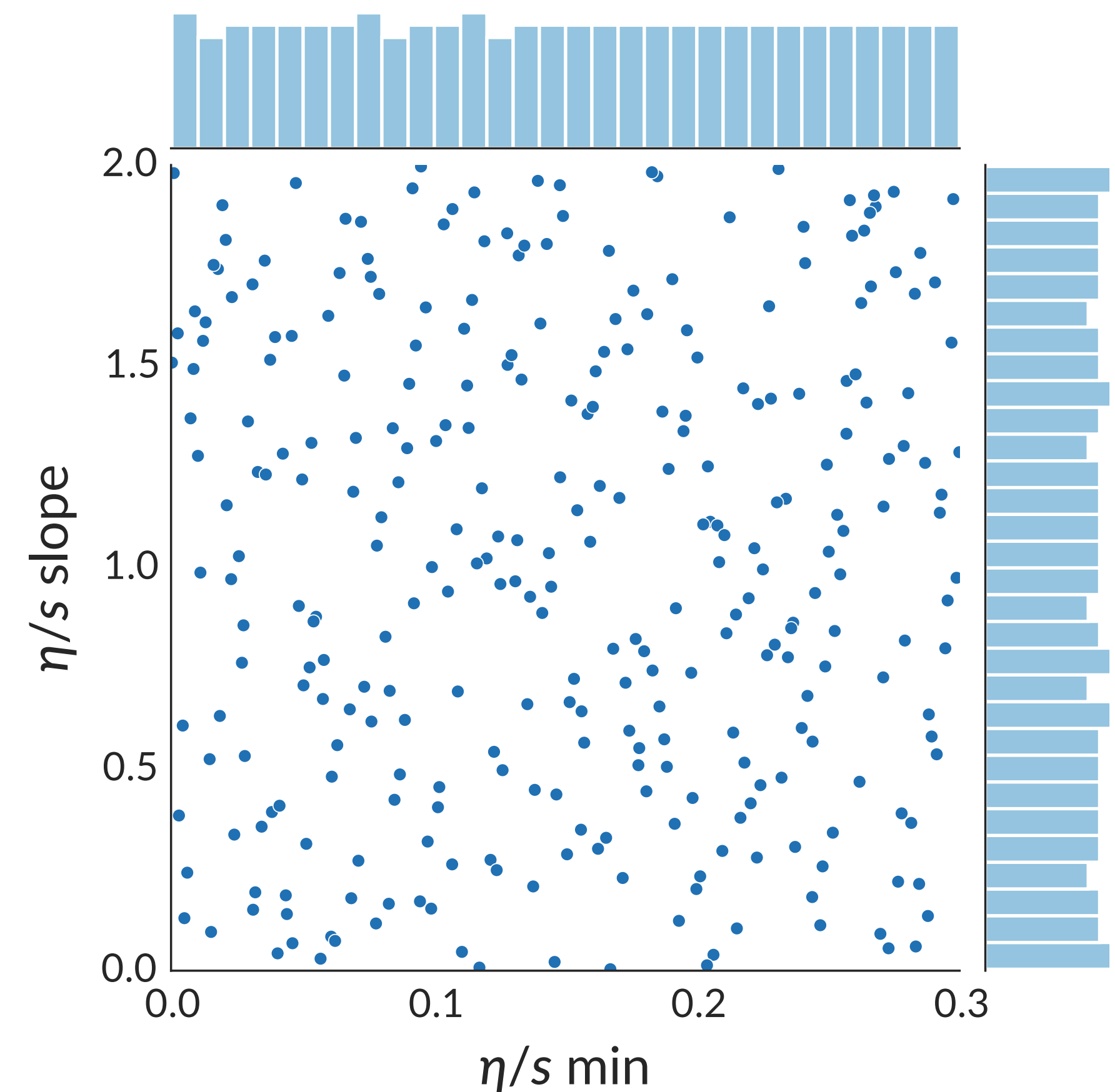
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- all parameters varied simultaneously
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this design:

- $n=15$ 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



Computer Experiment Execution

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

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

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

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

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

- $P(X, Y, \mathbf{y}_{\text{exp}} | \mathbf{x}_\star)$ = likelihood
 $\Rightarrow$ probability of observing $(X, Y, \mathbf{y}_{\text{exp}})$ given proposed $\mathbf{x}_\star$

- $P(\mathbf{x}_\star)$ = prior
 $\Rightarrow$ initial knowledge of $\mathbf{x}_\star$

Markov-Chain Monte-Carlo:

- 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
- posterior $\sim$ likelihood within design range, zero outside

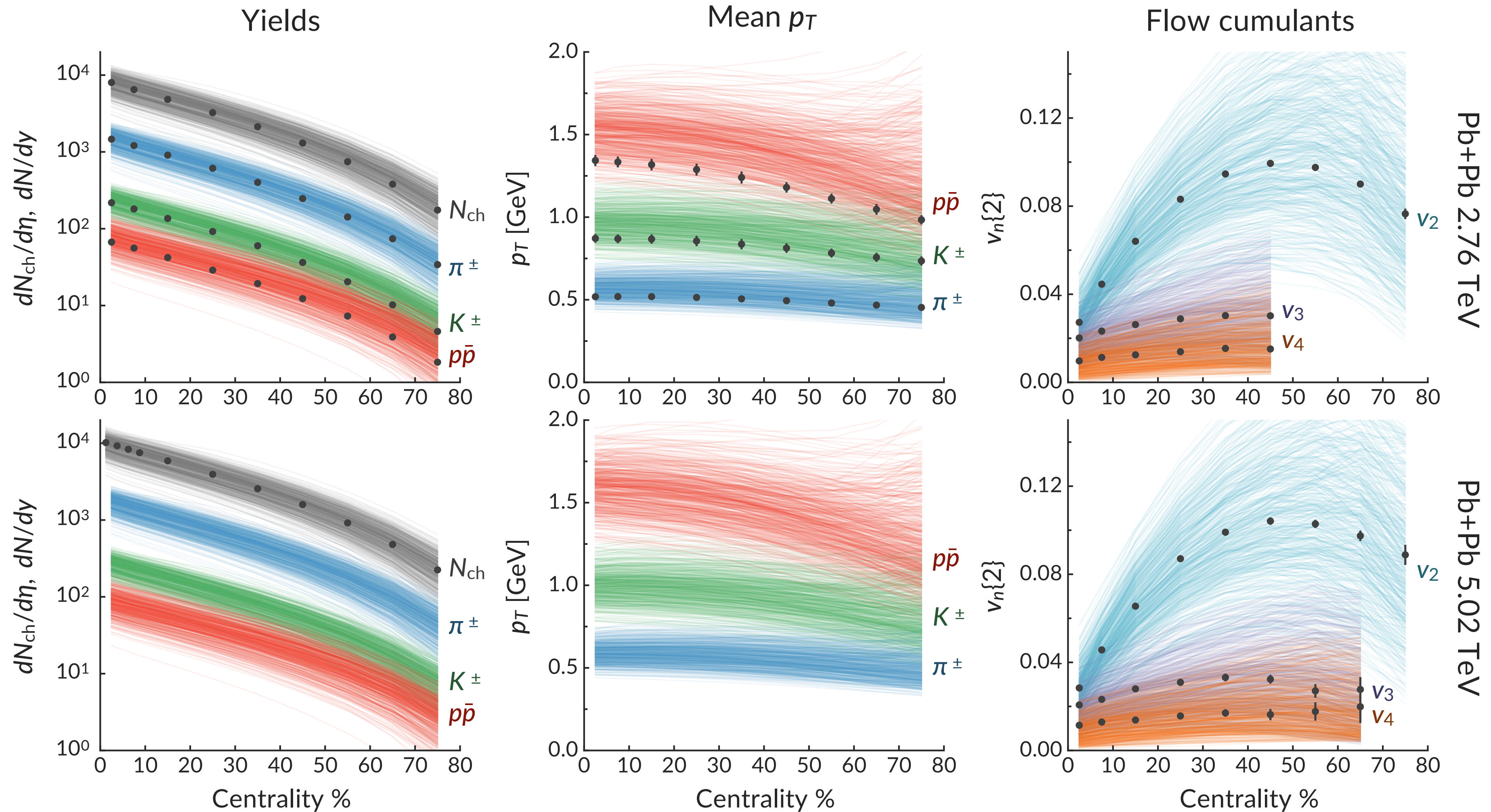
Likelihood and Uncertainty Quantification:

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

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

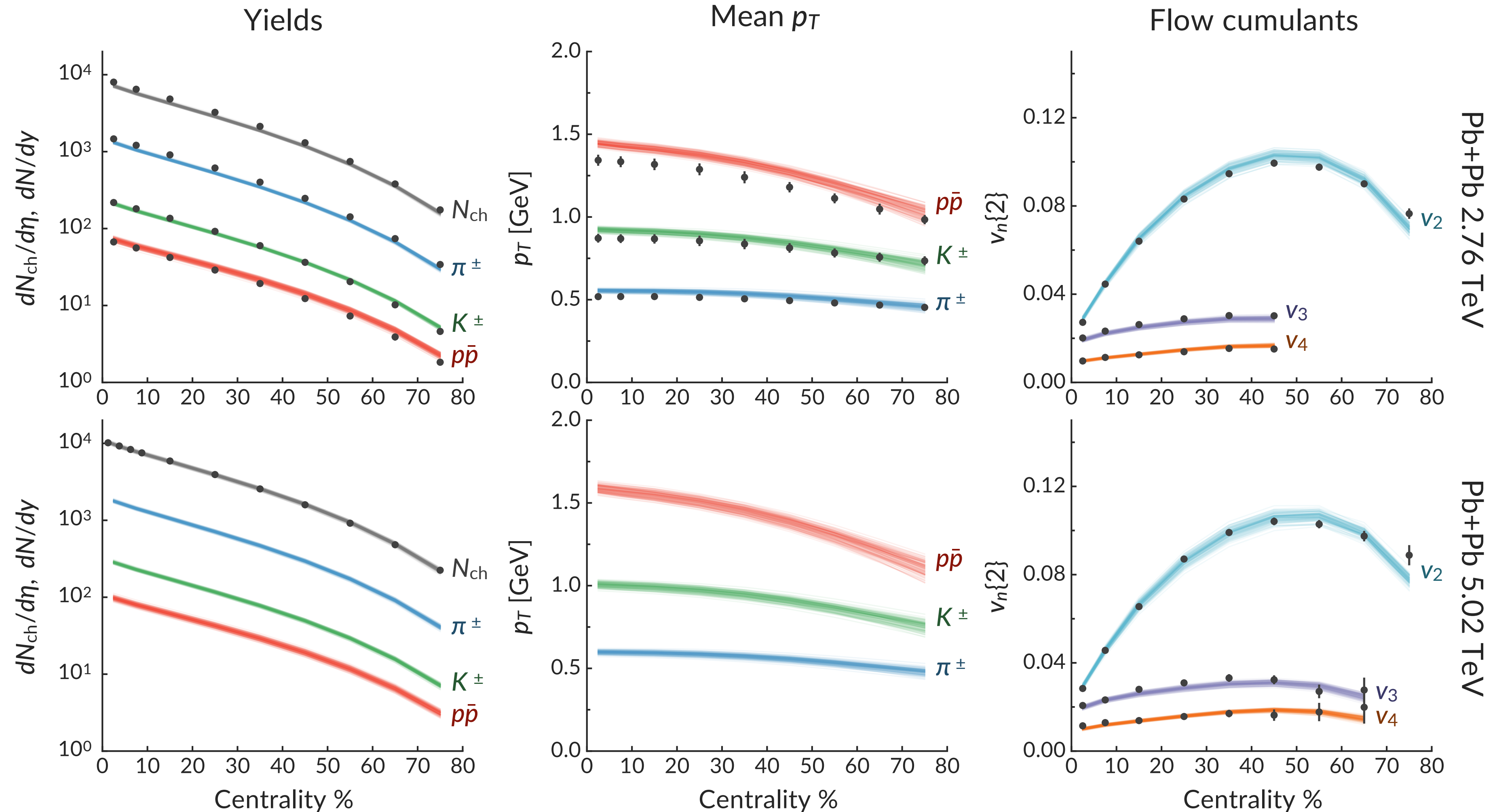
Prior vs. Posterior

Prior: model calculations evenly distributed over full design space



Prior vs. Posterior

Posterior: emulator predictions for highest likelihood parameter values



Analysis Results

Methodology

Model Parameters - System Properties

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

calculate events on Latin hypercube

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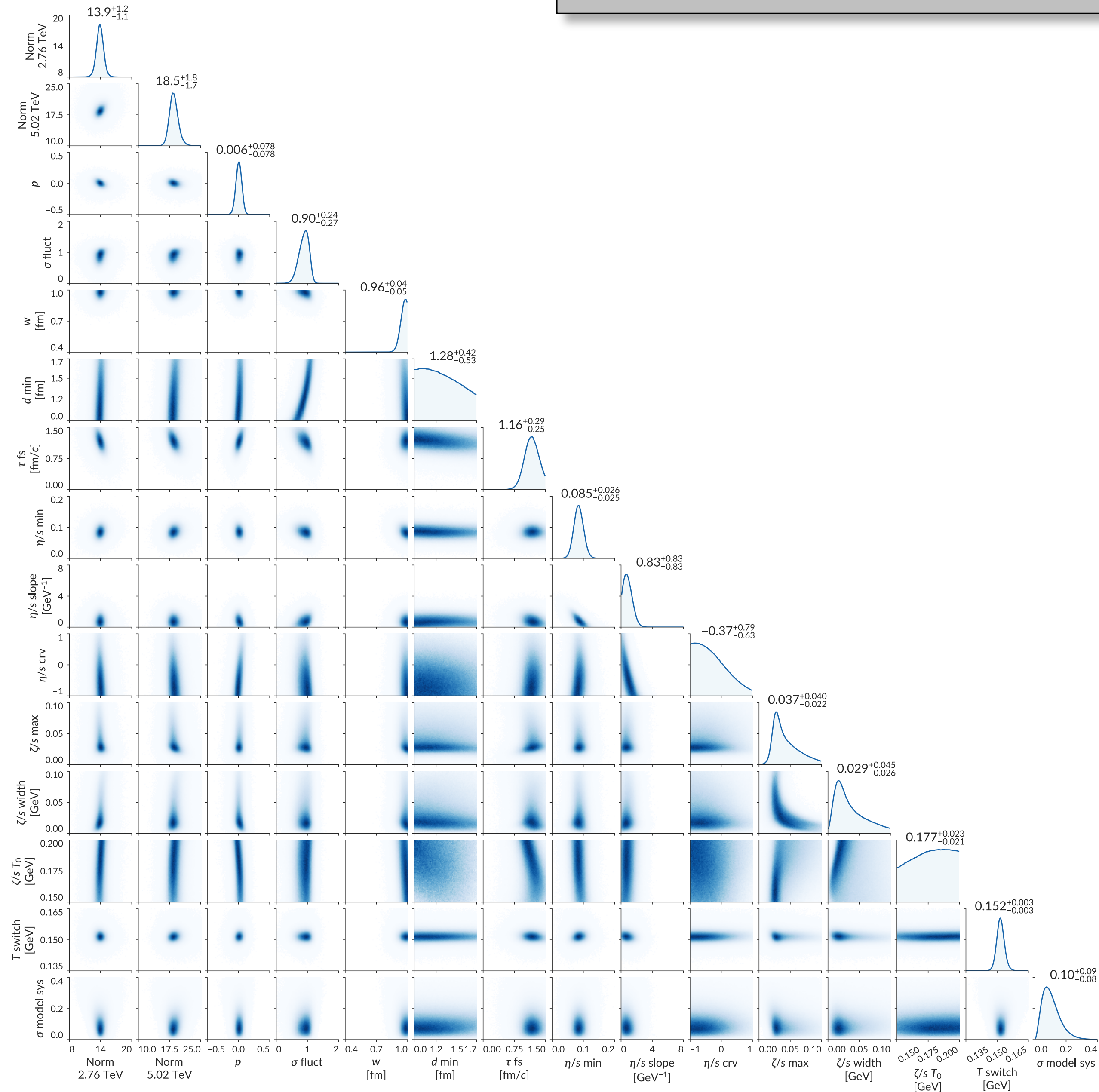
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$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

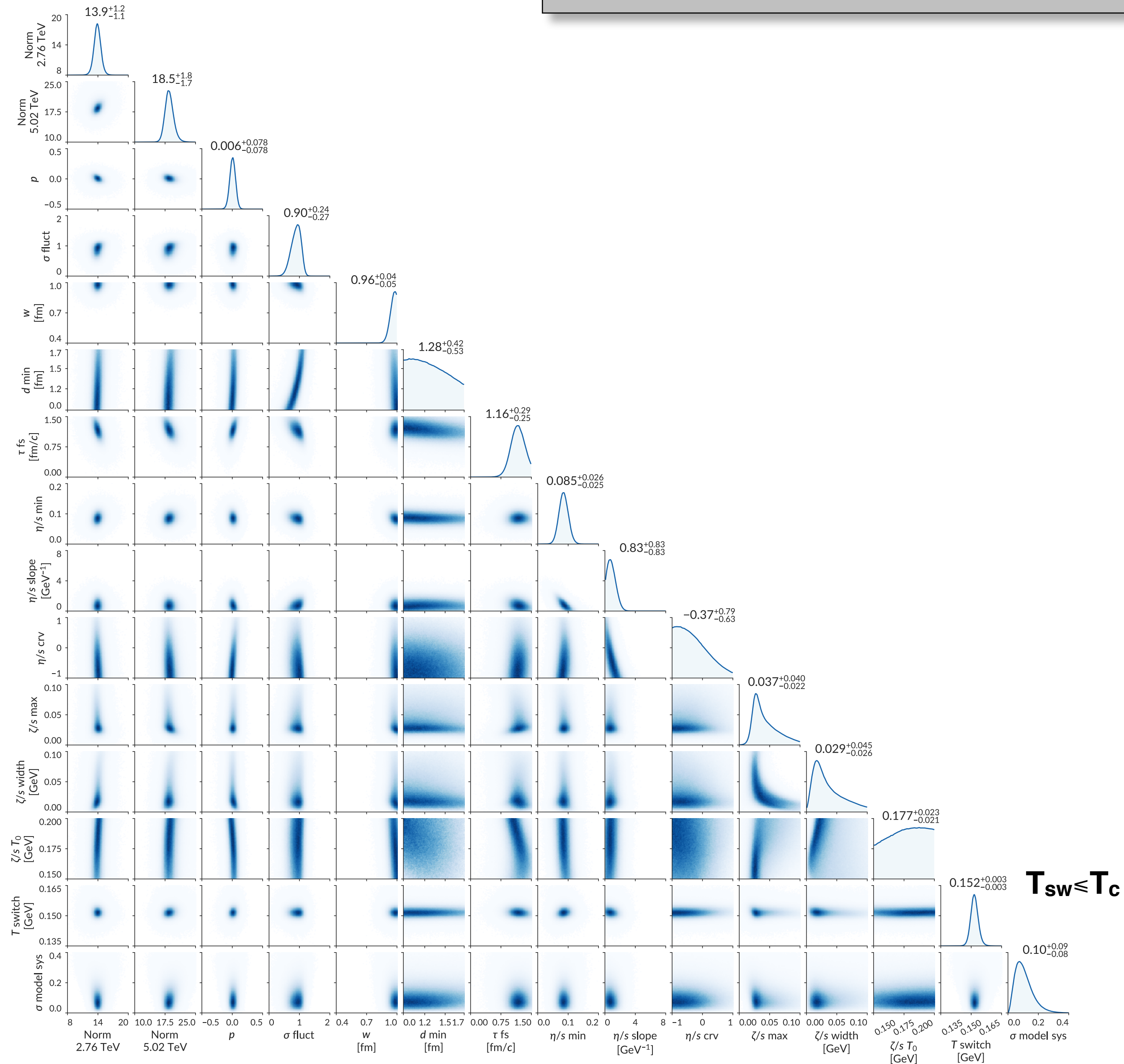
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Calibrated Posterior Distribution



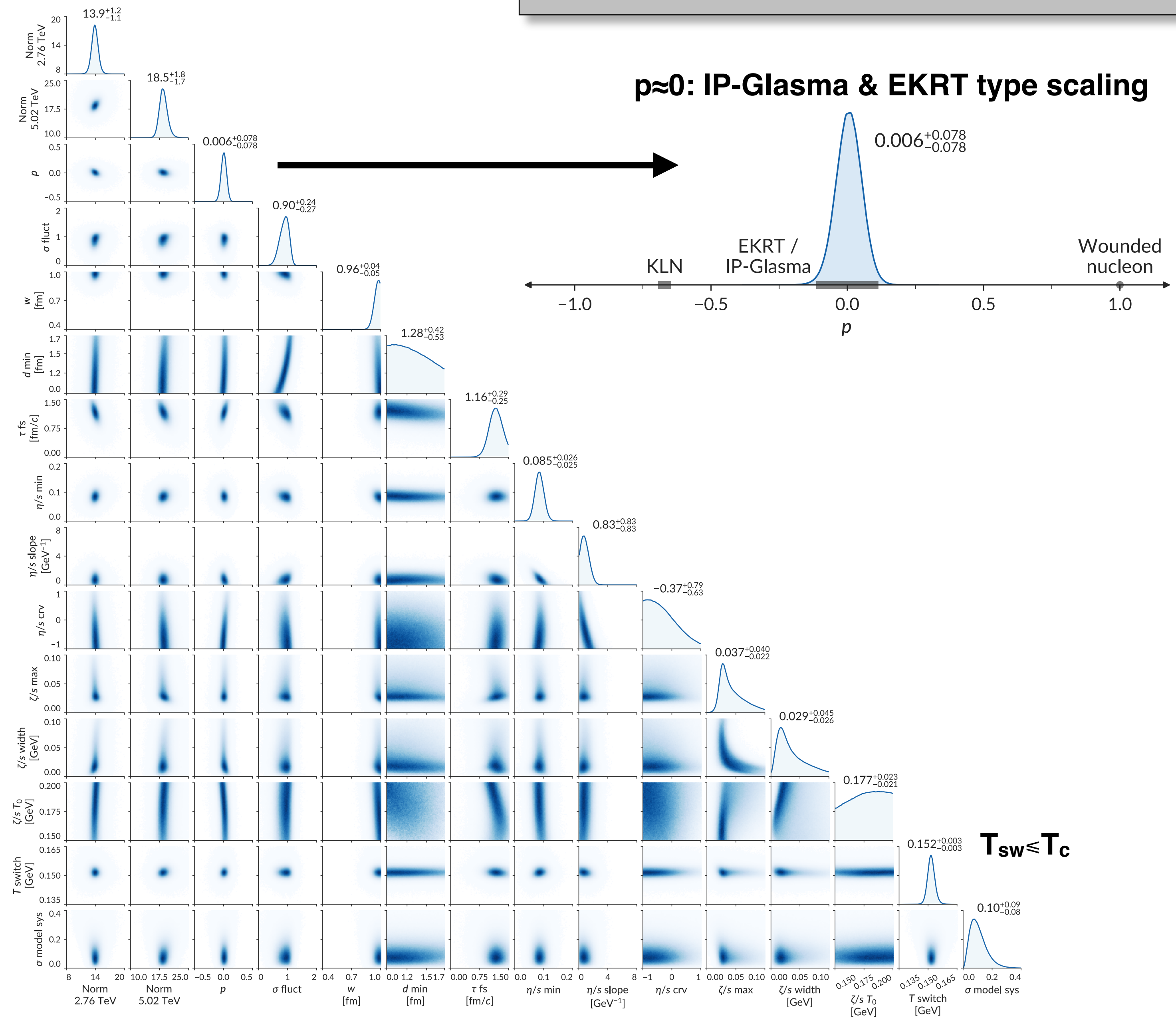
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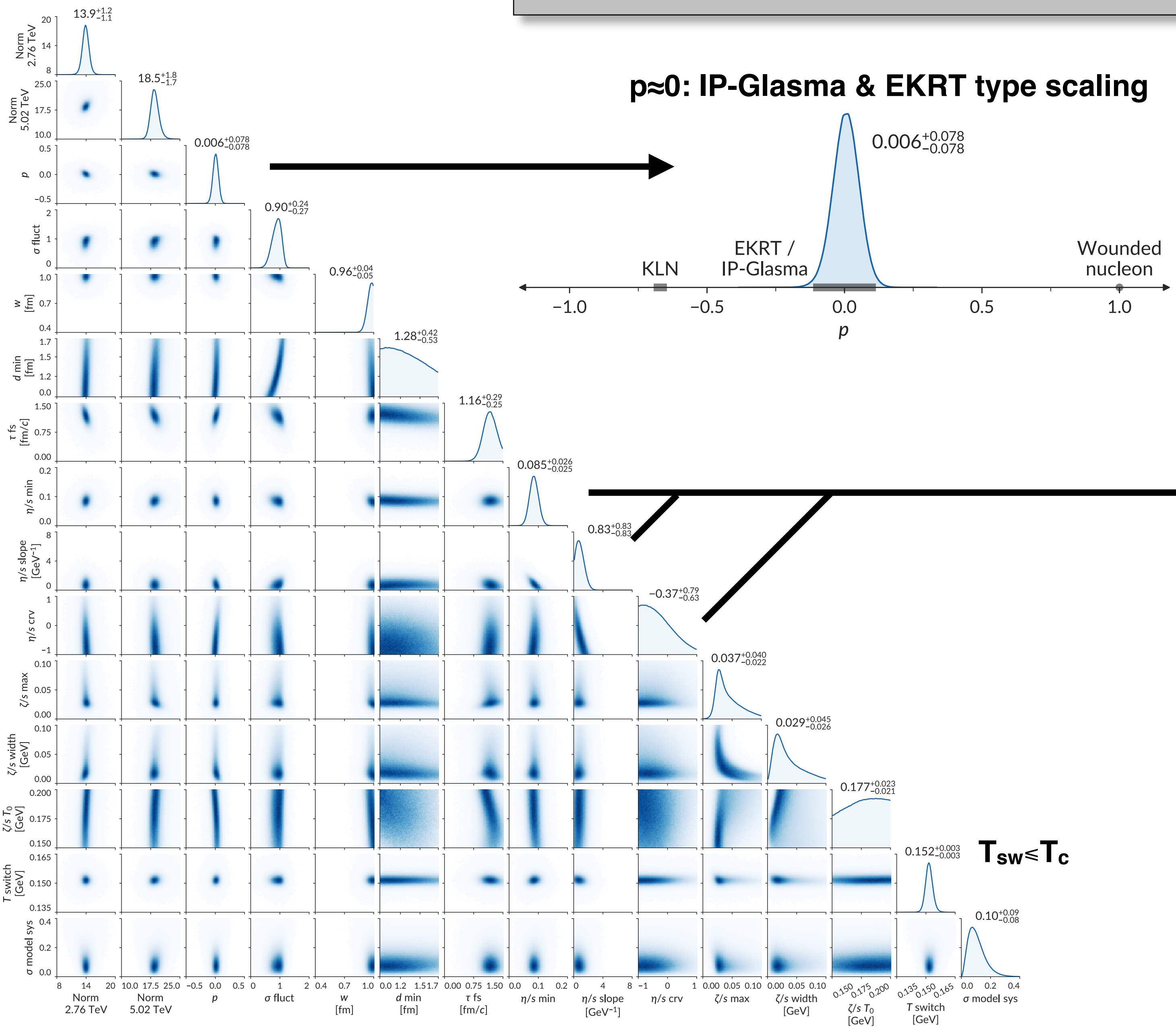
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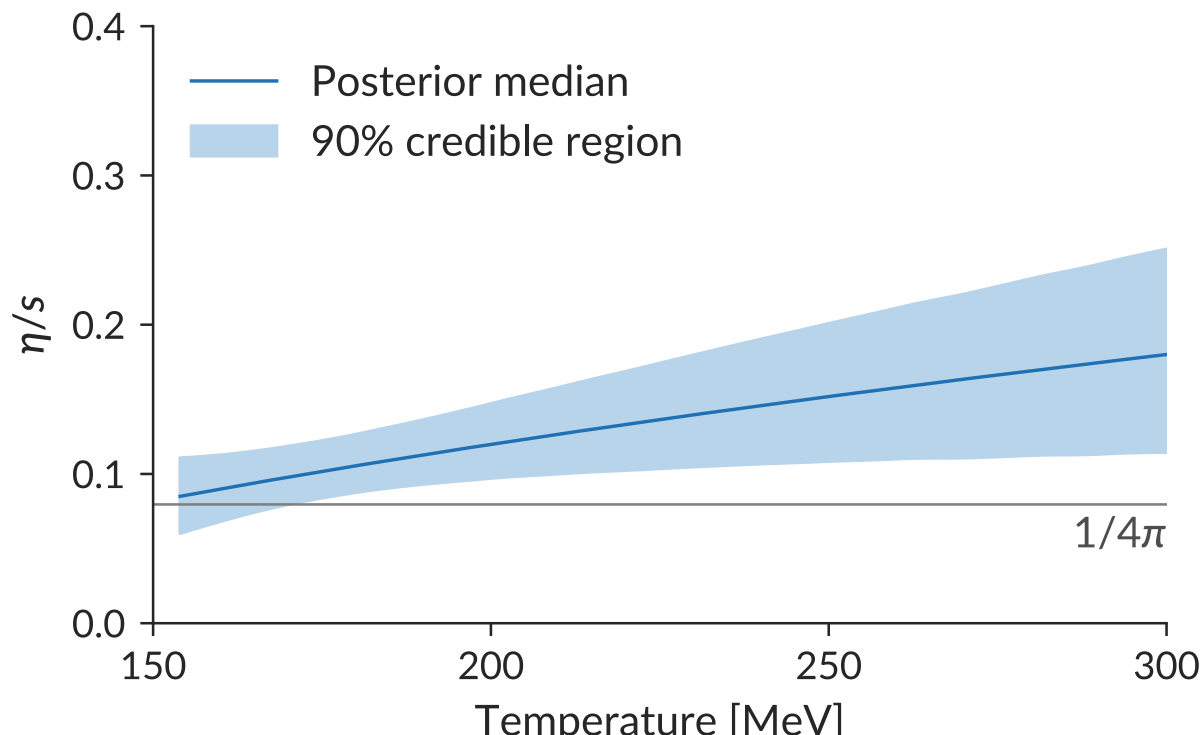
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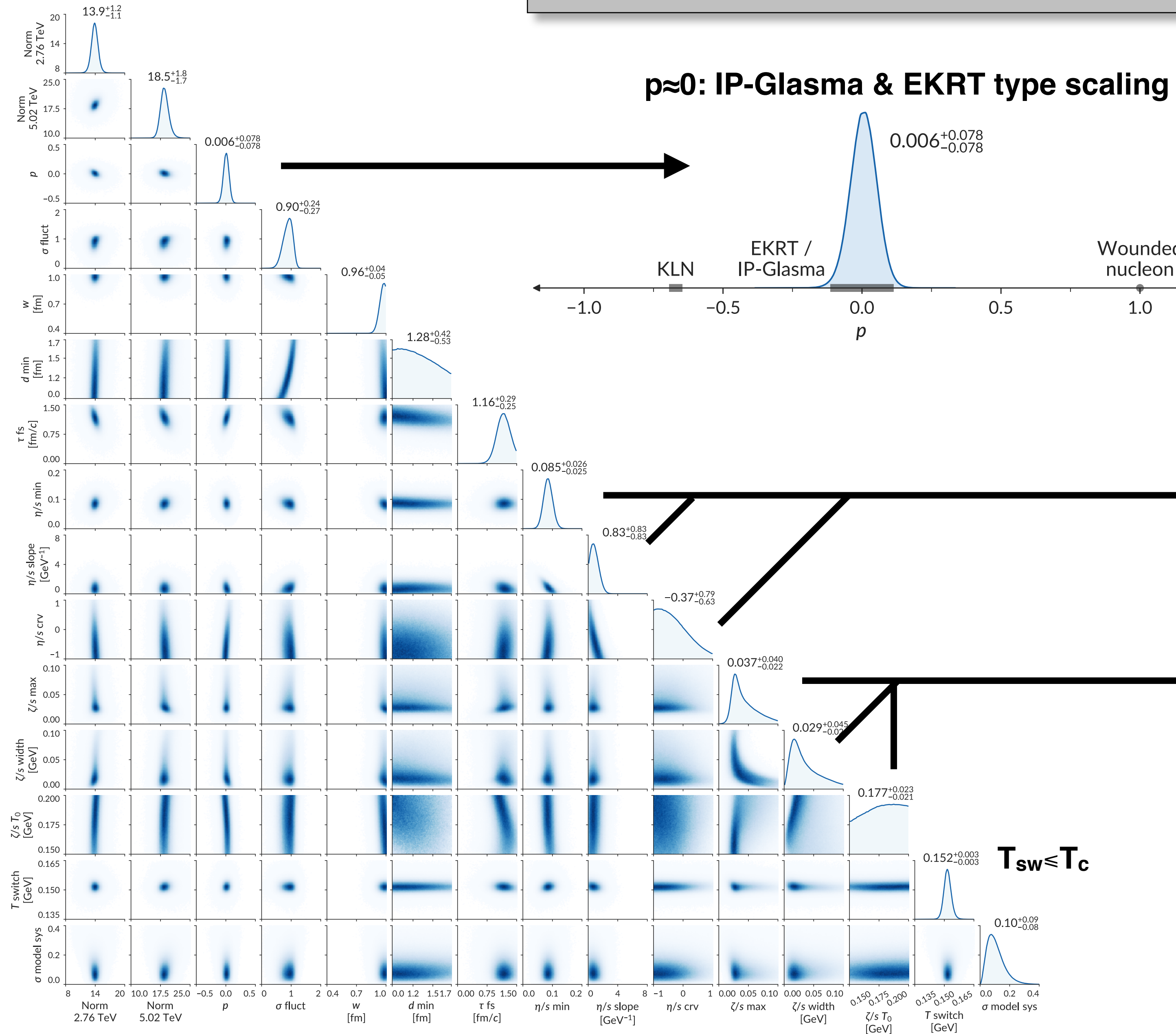


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temperature-dependent viscosities:

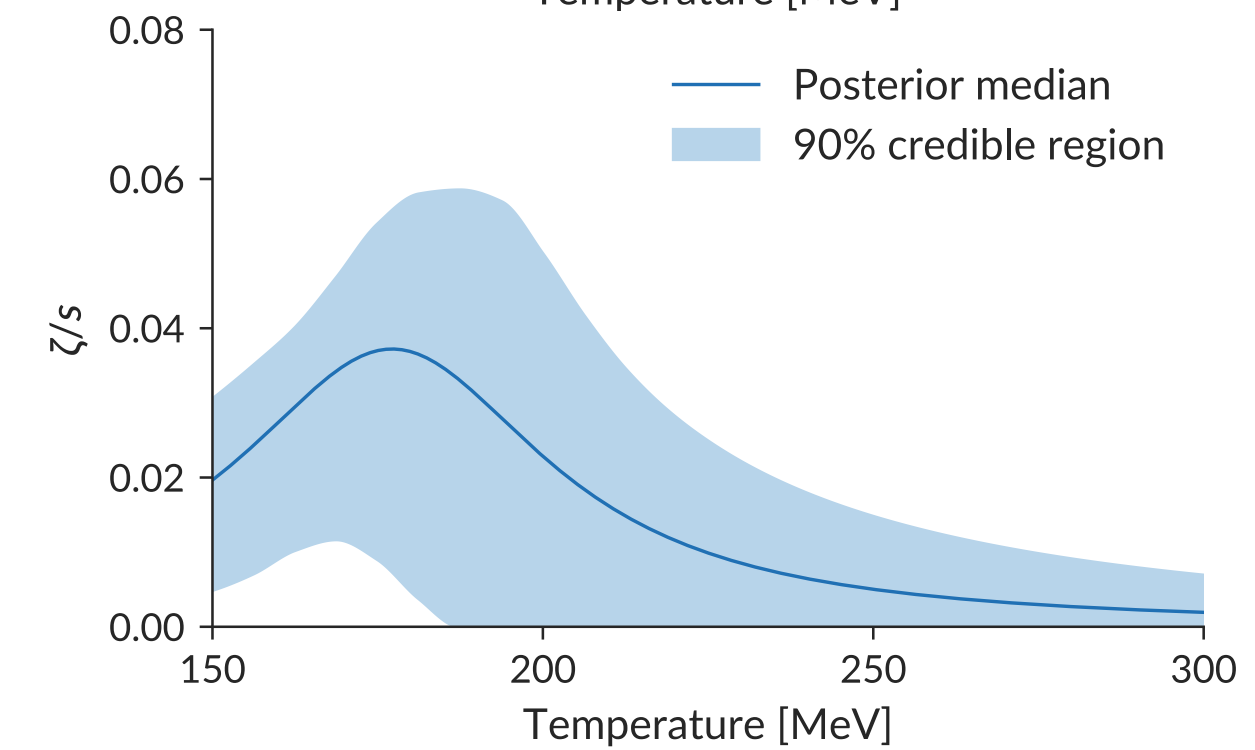
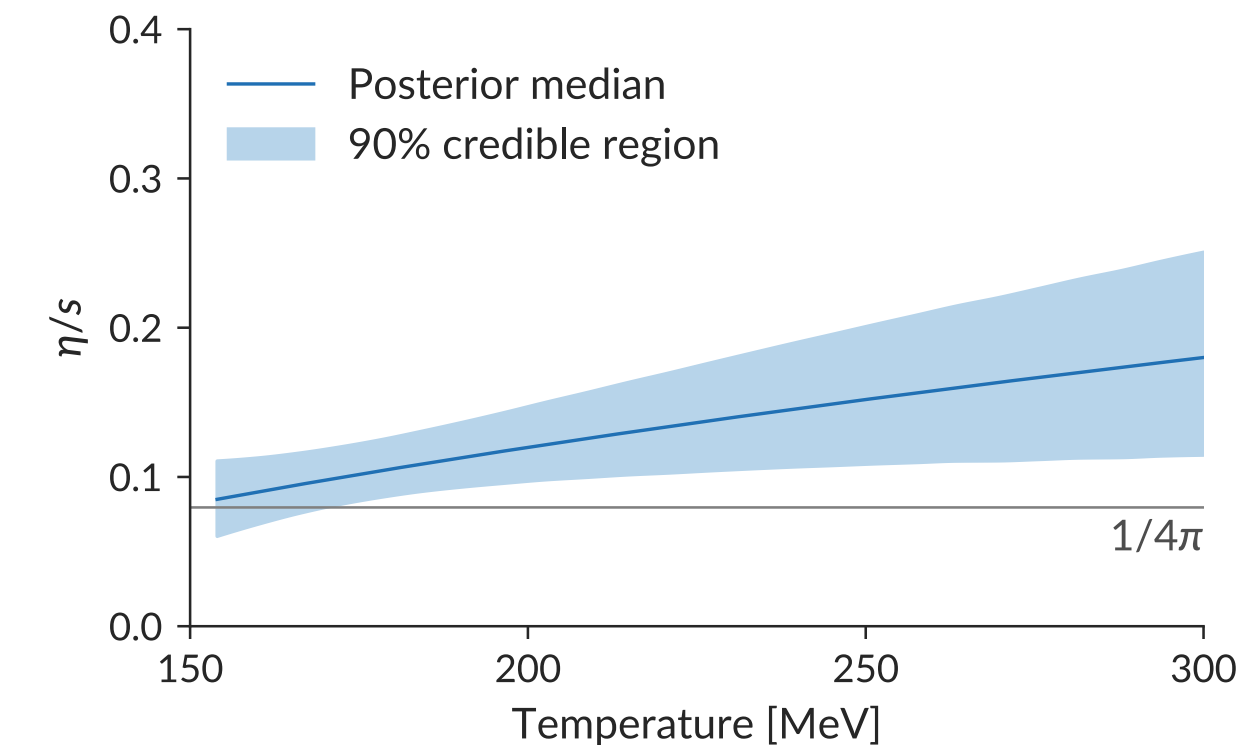


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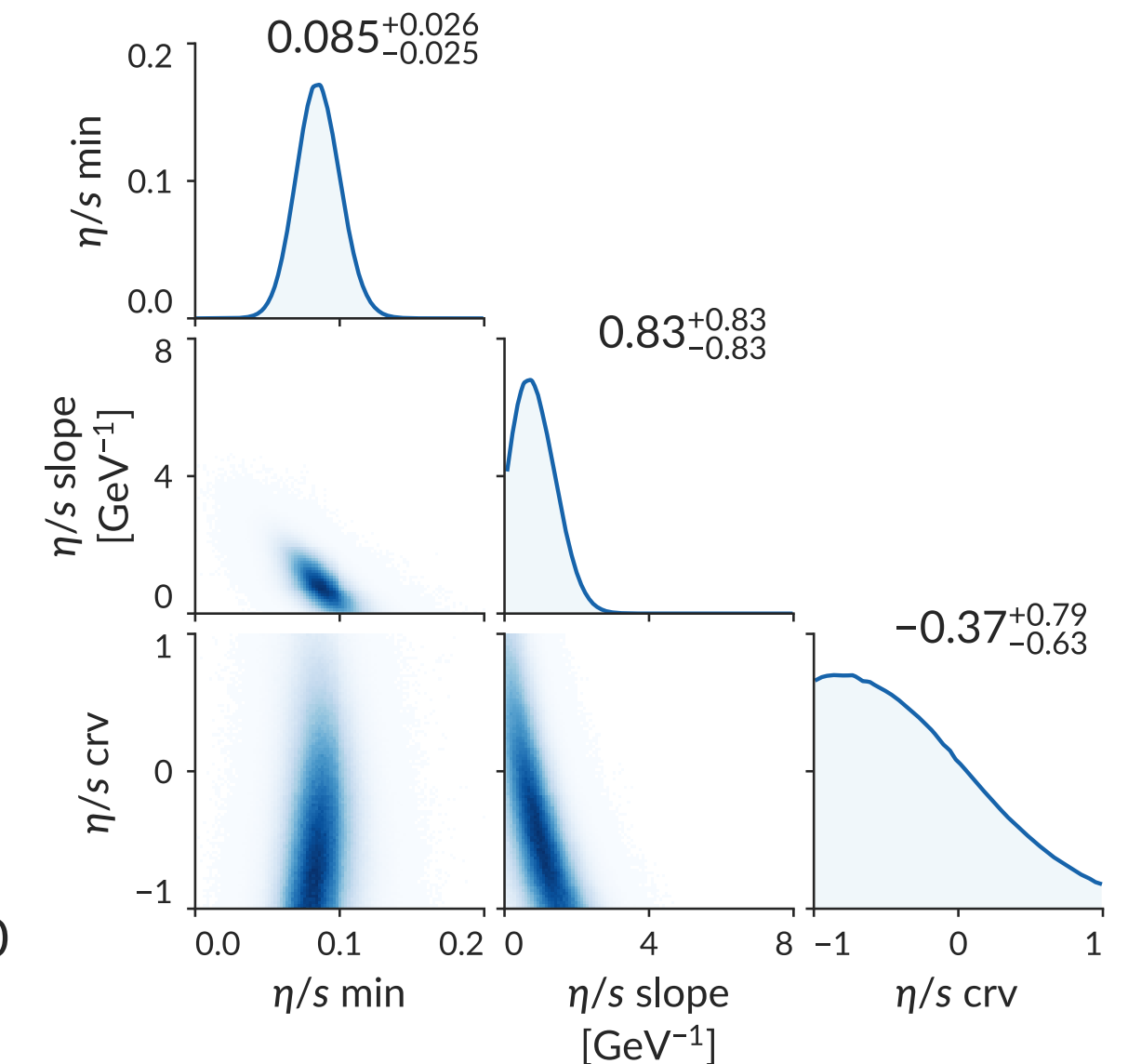
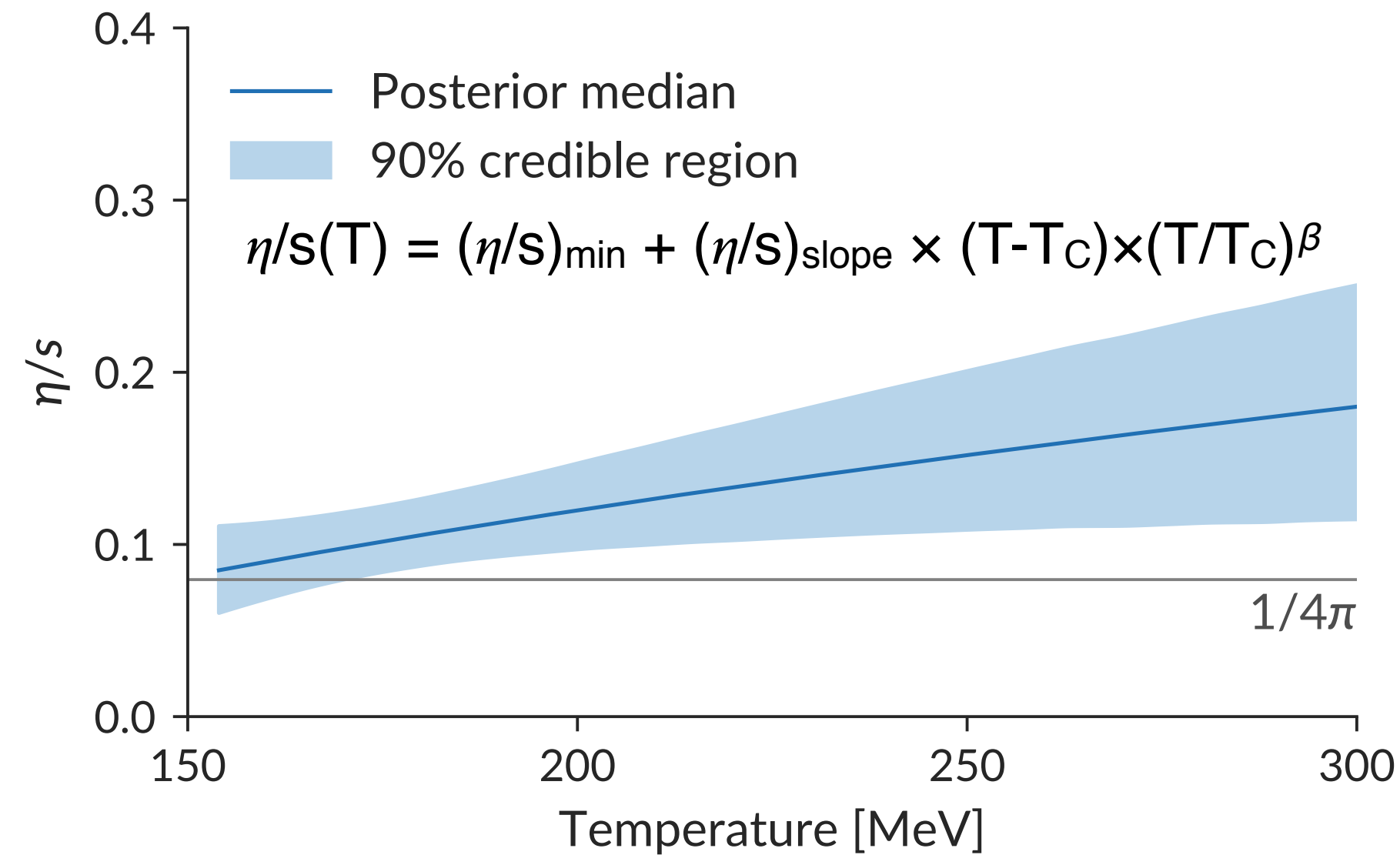
temperature-dependent viscosities:



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 $(\eta/s)_{\text{slope}}$ slope and intercept $(\eta/s)_{\text{min}}$
 - insufficient data to obtain sharply peaked likelihood distributions for $(\eta/s)_{\text{slope}}$ and curvature β independently
- current analysis most sensitive to $T < 0.23$ GeV
 - RHIC data may disambiguate further

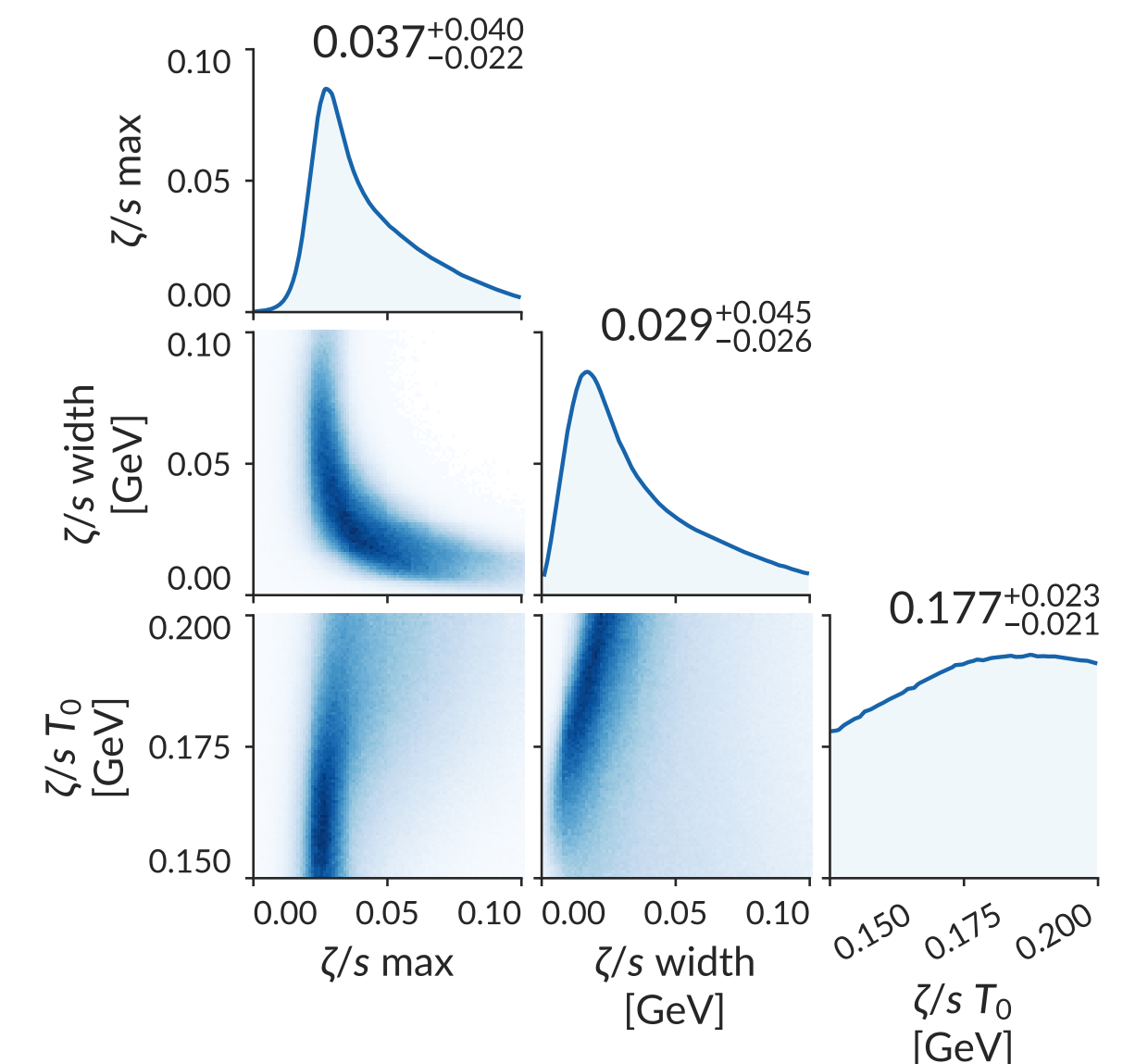
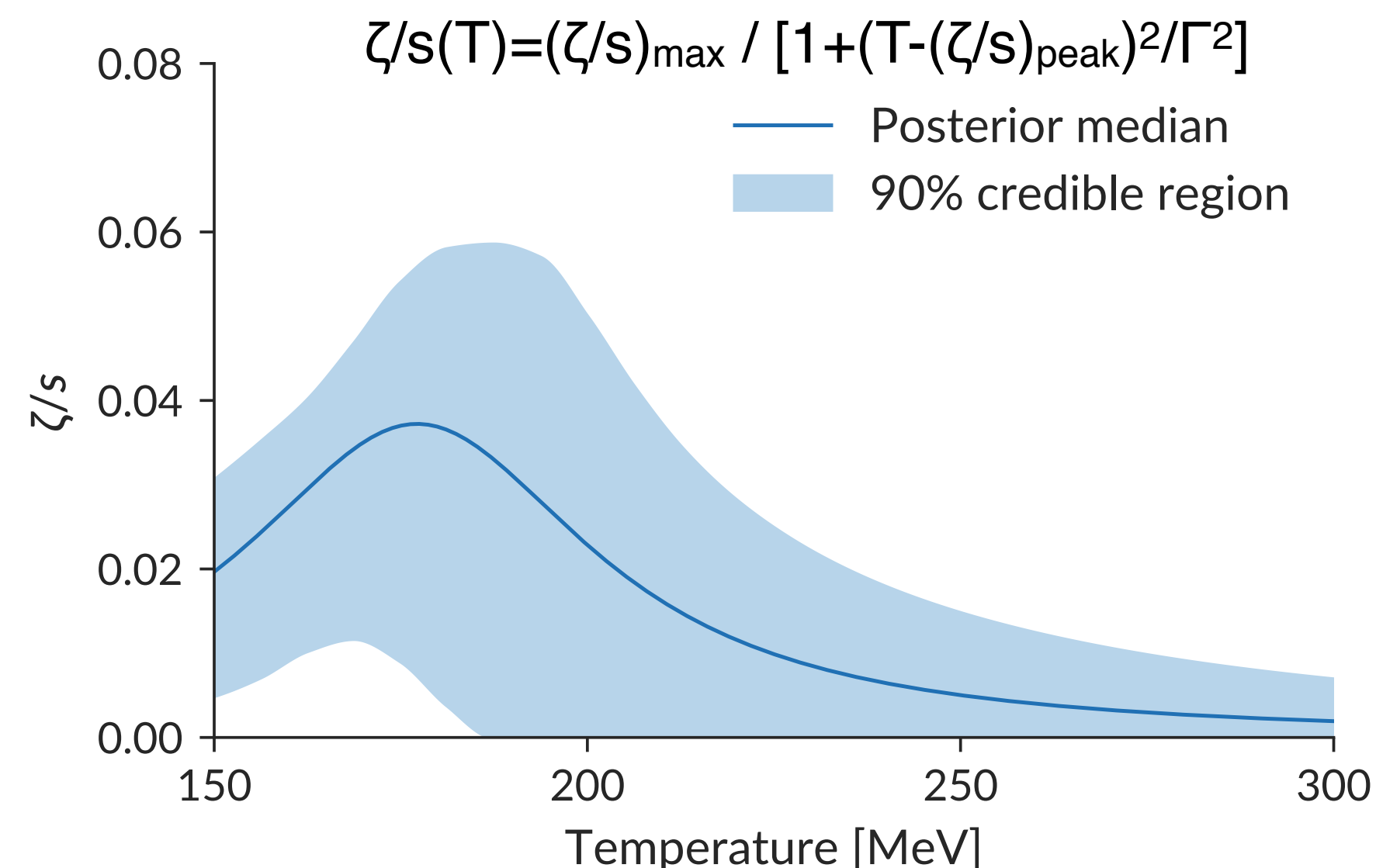


temperature dependent bulk viscosity:

- 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



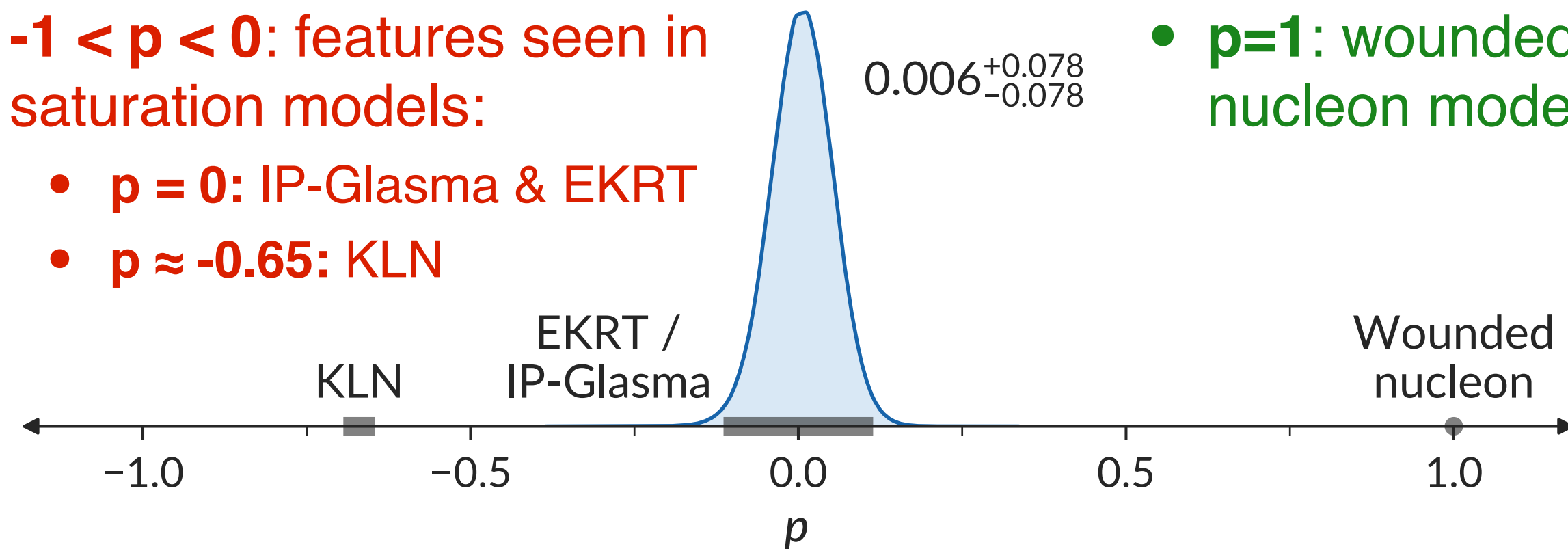
Constraining the Initial State

p quantifies the attenuation of entropy production in the off-diagonal regions of $dS/dy \propto T_R(p; T_A, T_B)$:

- $-1 < p < 0$: features seen in saturation models:

- $p = 0$: IP-Glasma & EKRT
- $p \approx -0.65$: KLN

- $p=1$: wounded nucleon model



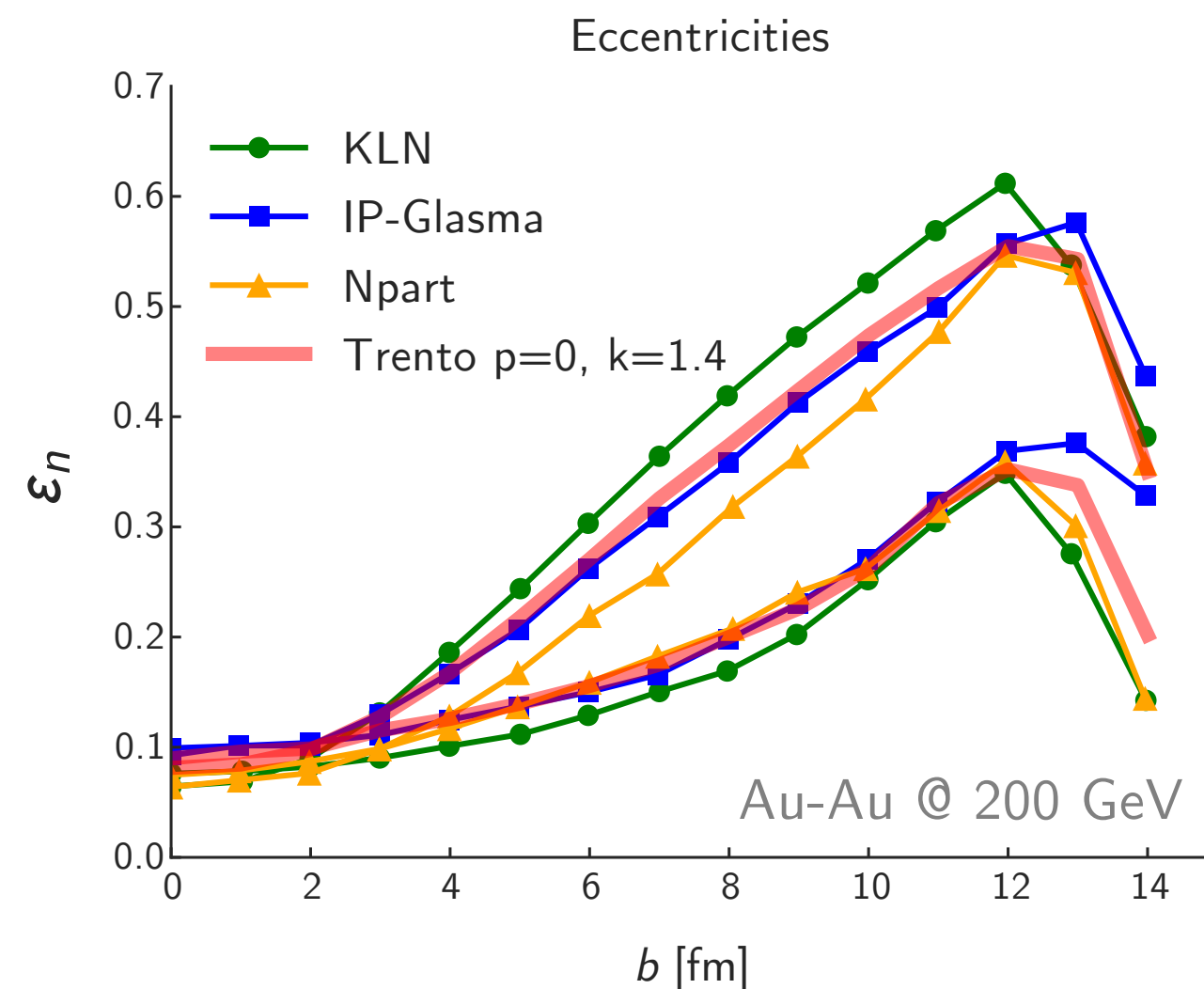
► **analysis strongly favors eccentricity scaling and entropy deposition seen in the EKRT & IP-Glasma models**

► **wounded nucleon and KLN models disfavored**

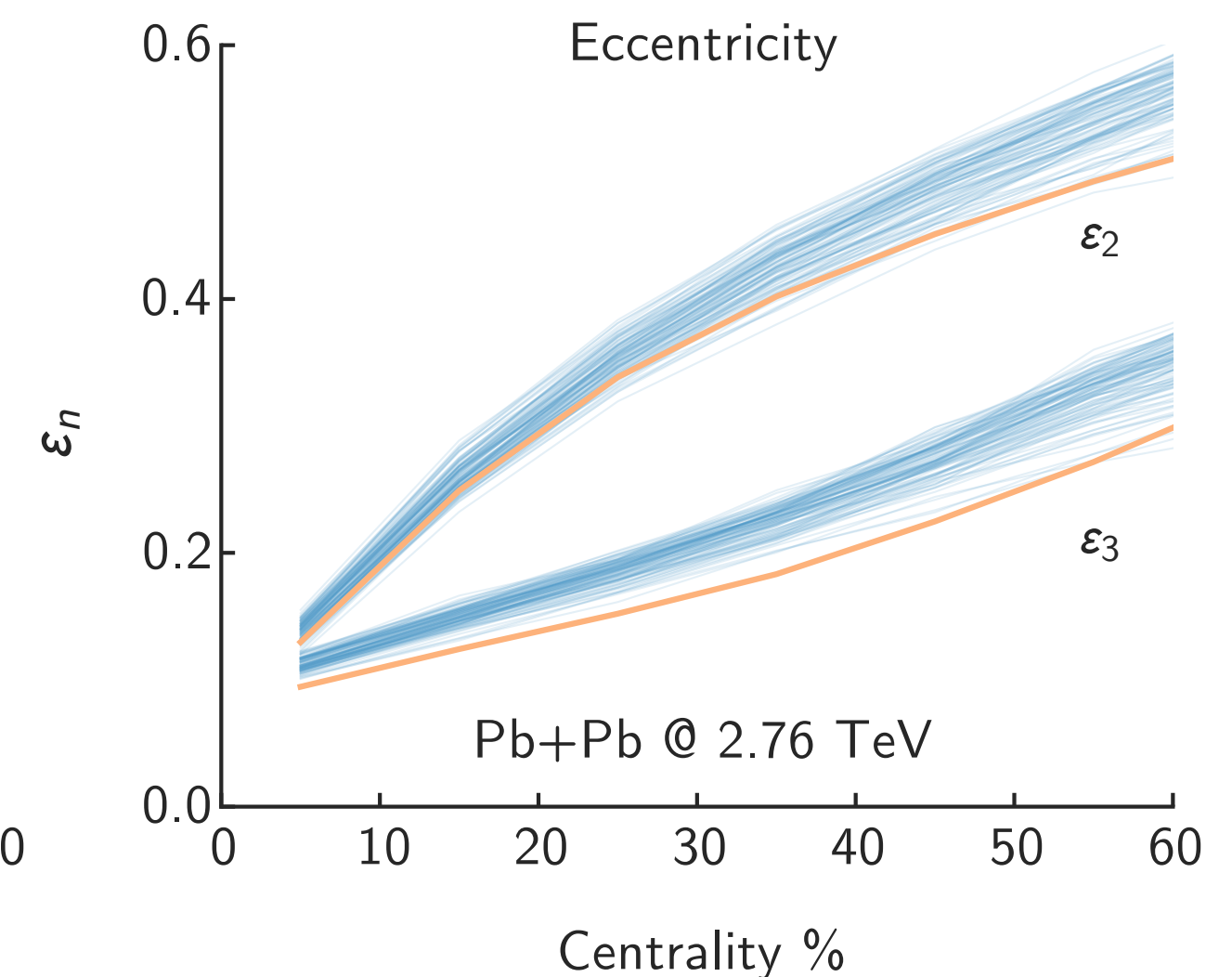
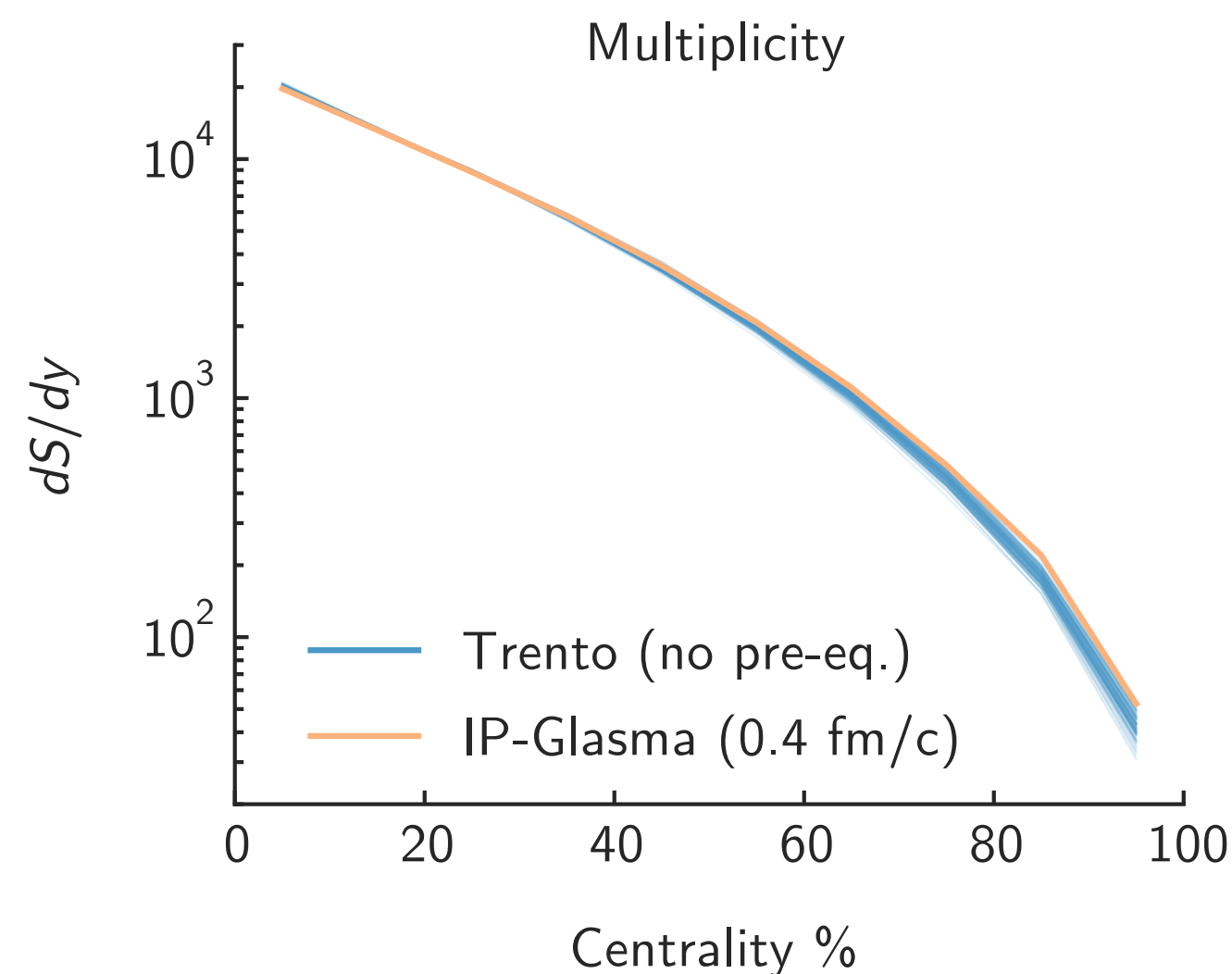
► **no conclusion yet on 2 component WN+BC model**

- **still need to corroborate scale of fluctuations being probed**

Trento vs. IP-Glasma:



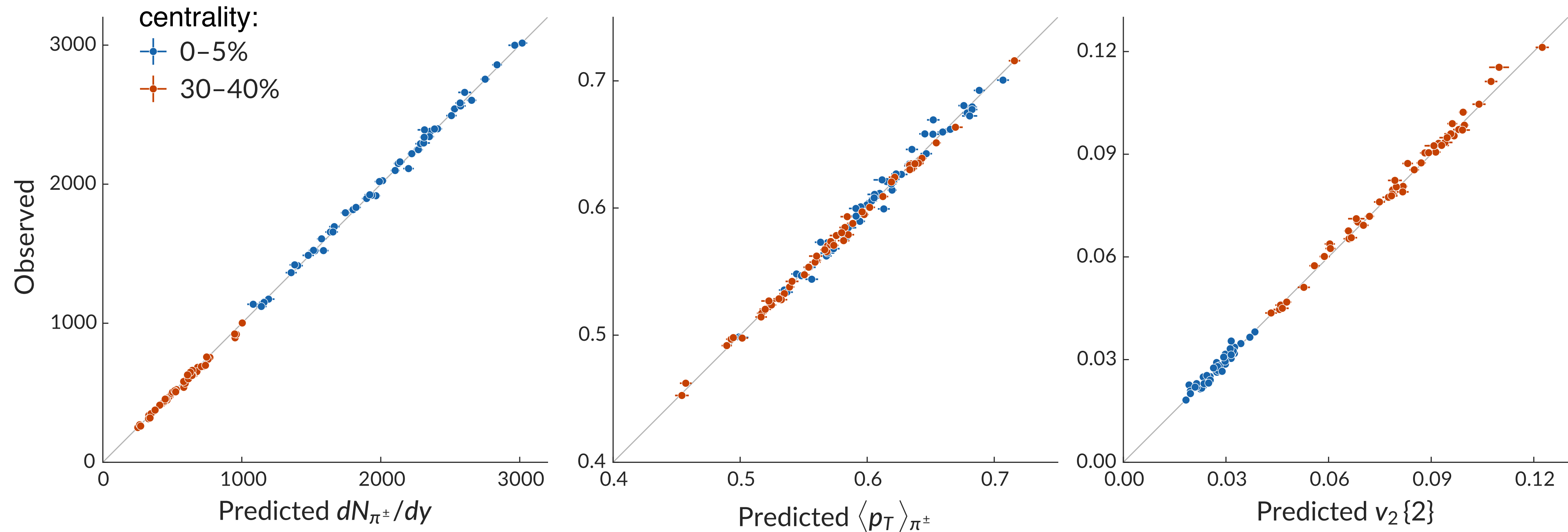
note: no pre-equilibrium flow in the current Trento analysis, may account for larger ε_n



**Precision Science
or
“Smoke & Mirrors”?**

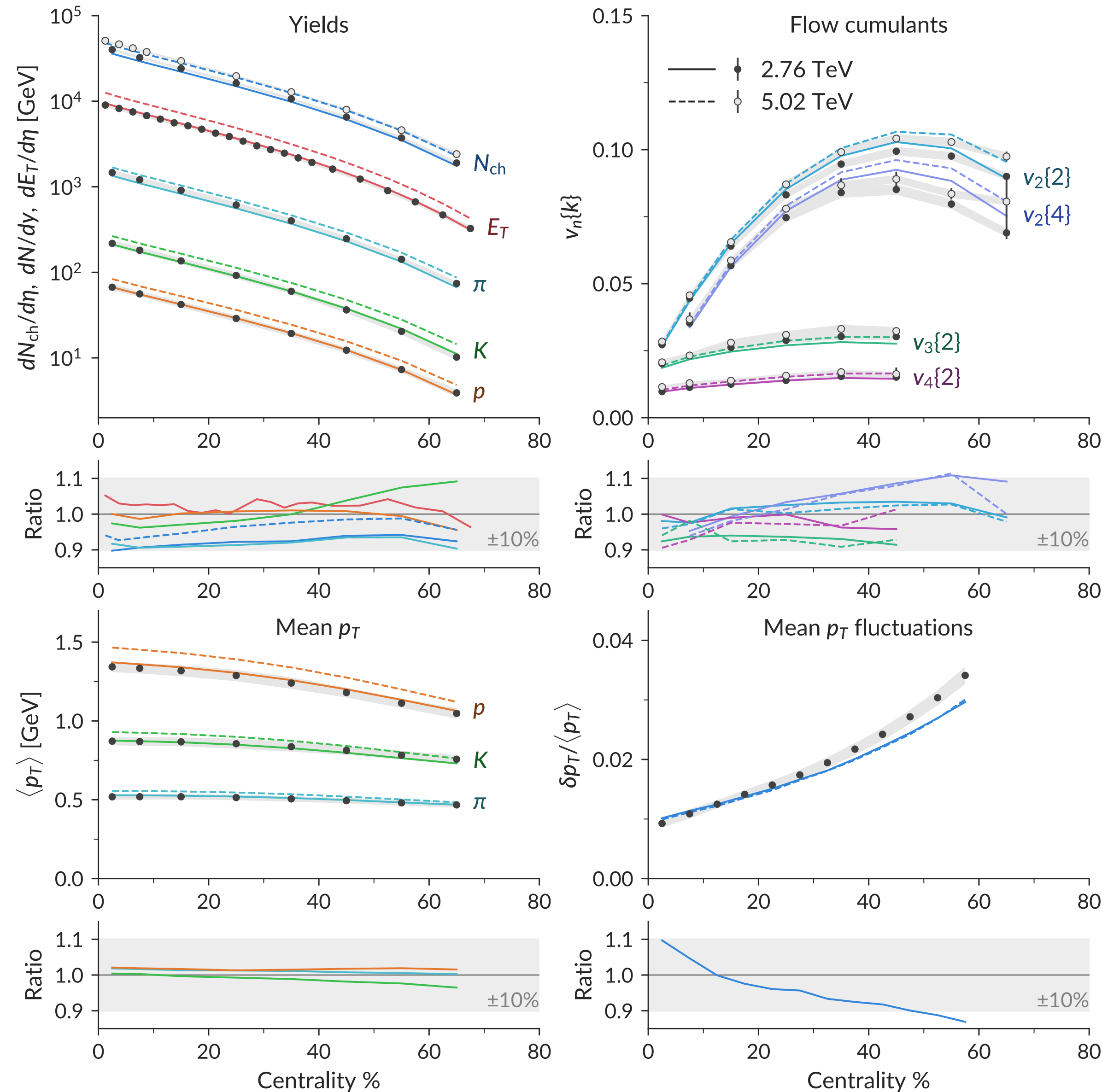
Validation

- 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



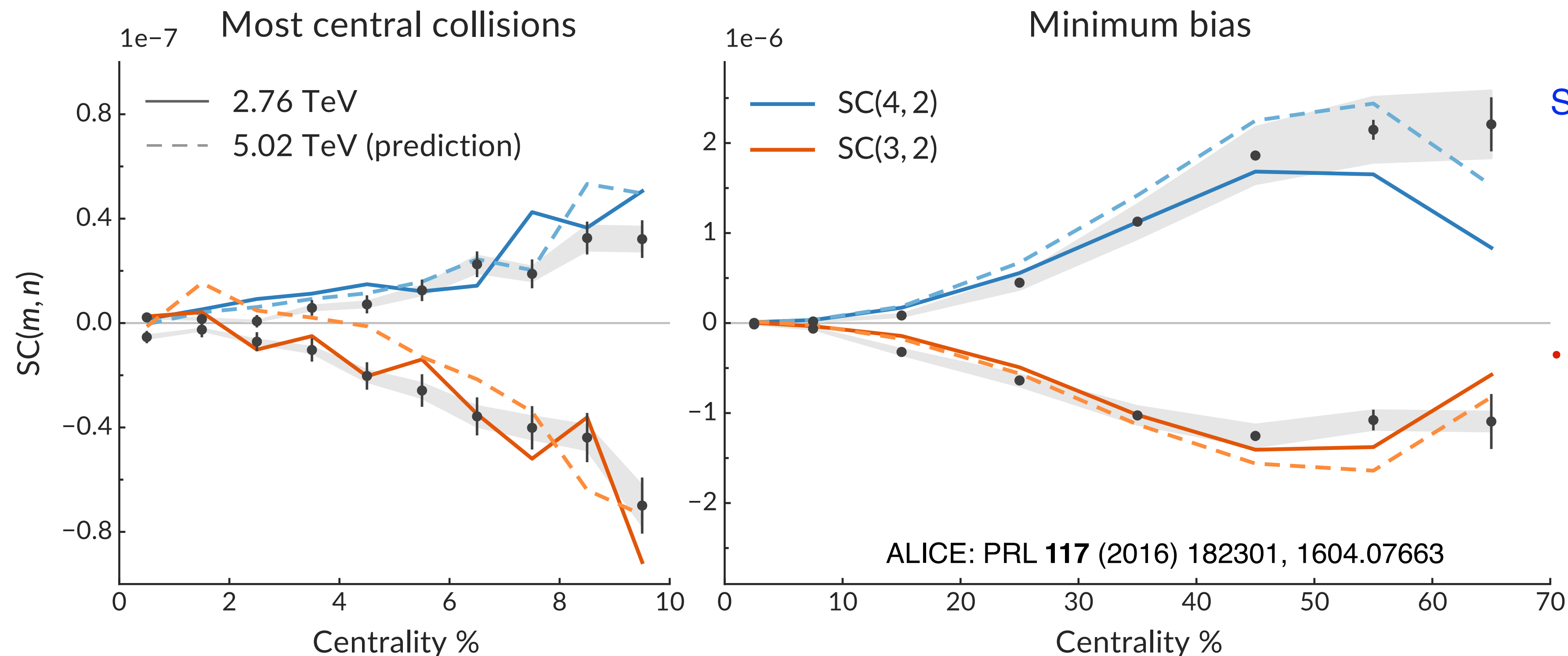
- explicit physics model calculations (no emulator) with parameter values set to the maximum of the posterior probability distributions yield excellent agreement with data!
- description of data to within $\pm 10\%$ accuracy

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

$$SC(m,n) = \langle v_m^2 v_n^2 \rangle - \langle v_m^2 \rangle \langle v_n^2 \rangle$$



$SC(m,n)$ are sensitive to:

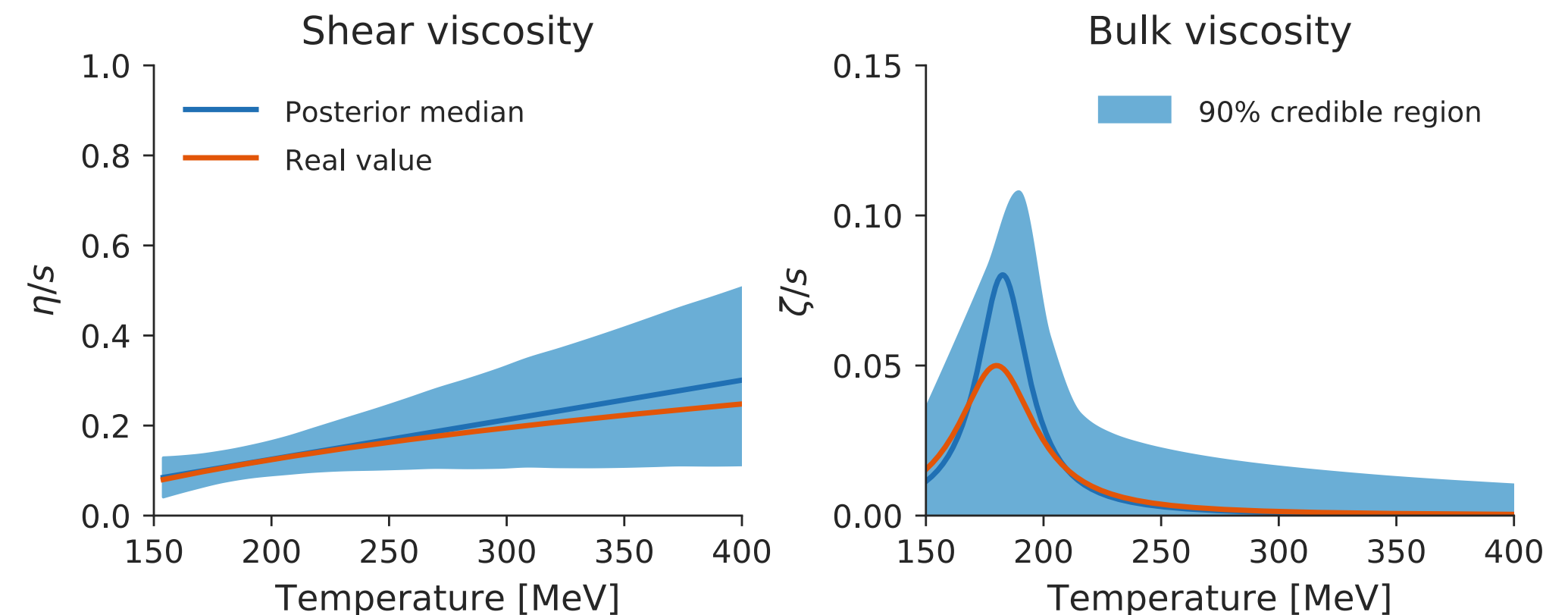
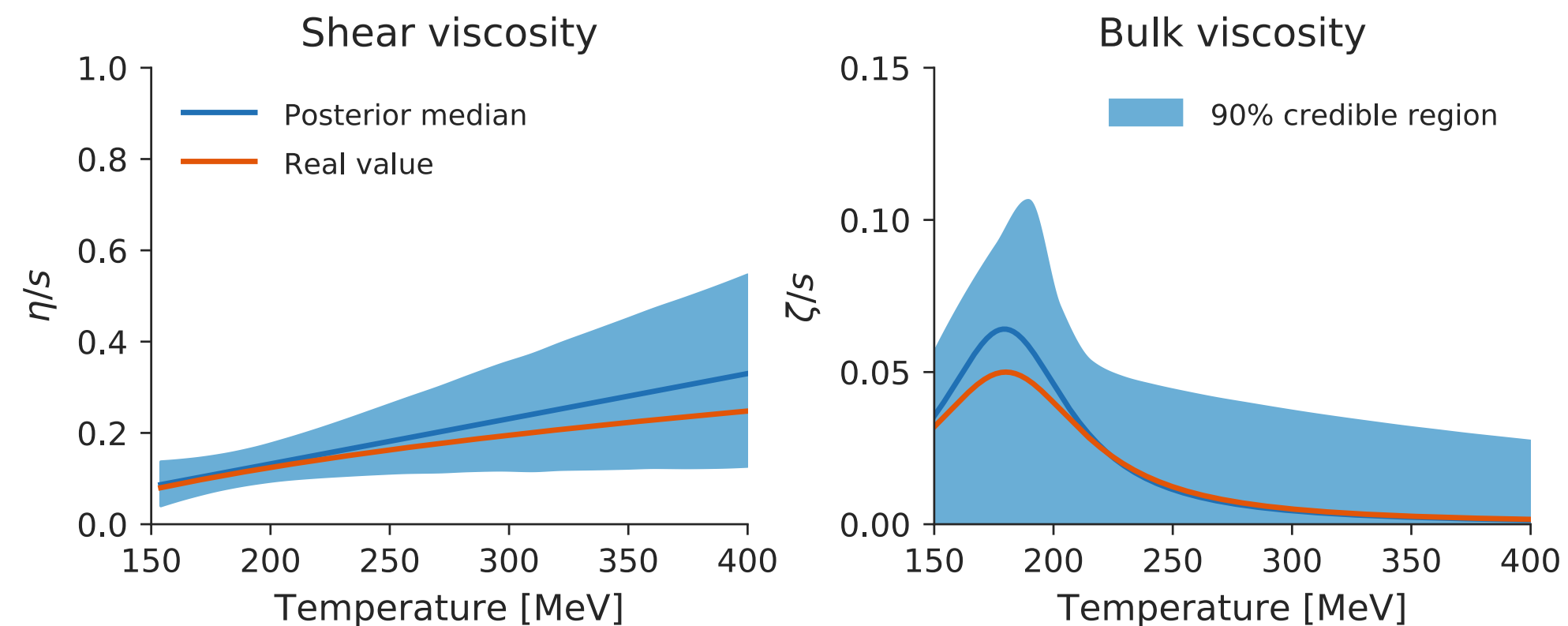
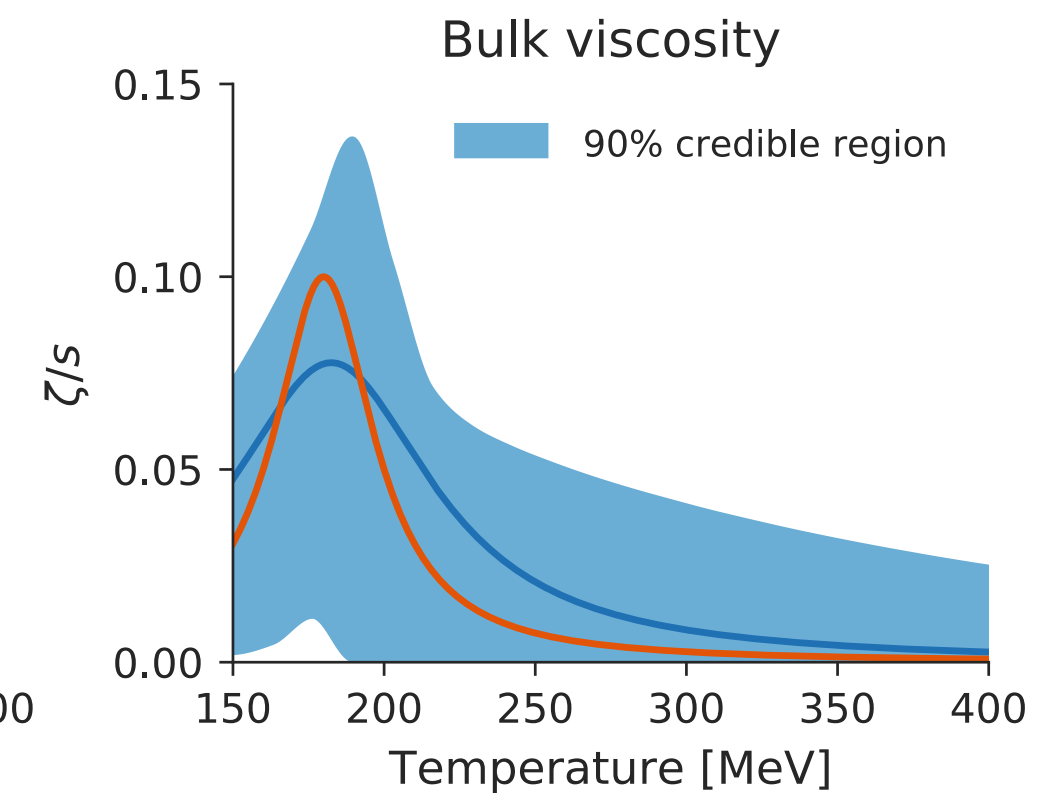
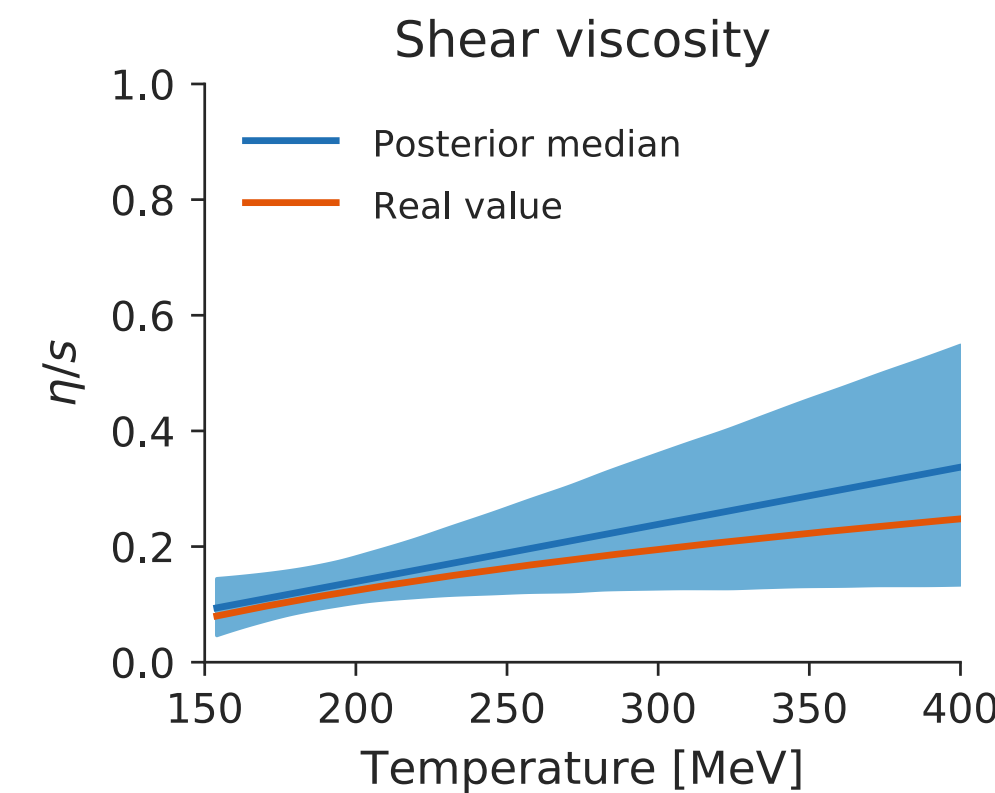
- initial conditions
- evolution model
- QGP transport coefficients

• 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!

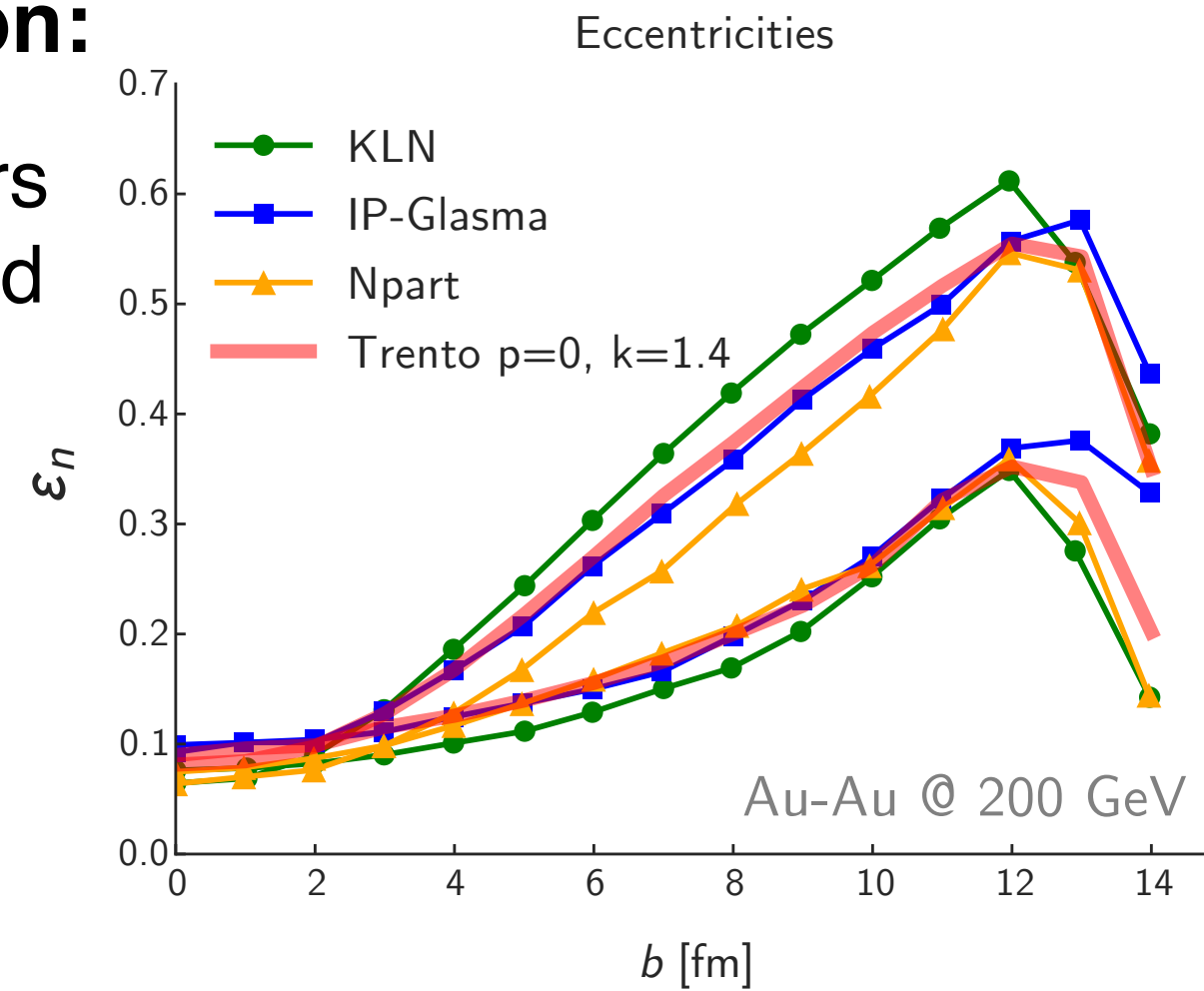
- both, smooth functions as well as peaked functions, can be reproduced well within the 90% CR
- note: due to reduction of information when going from model output to observables & model/GP uncertainties one should not expect a one-to-one reconstruction
- bulk analysis is mostly sensitive to area under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



Summary I: Key Physics Results

Trento initial condition:

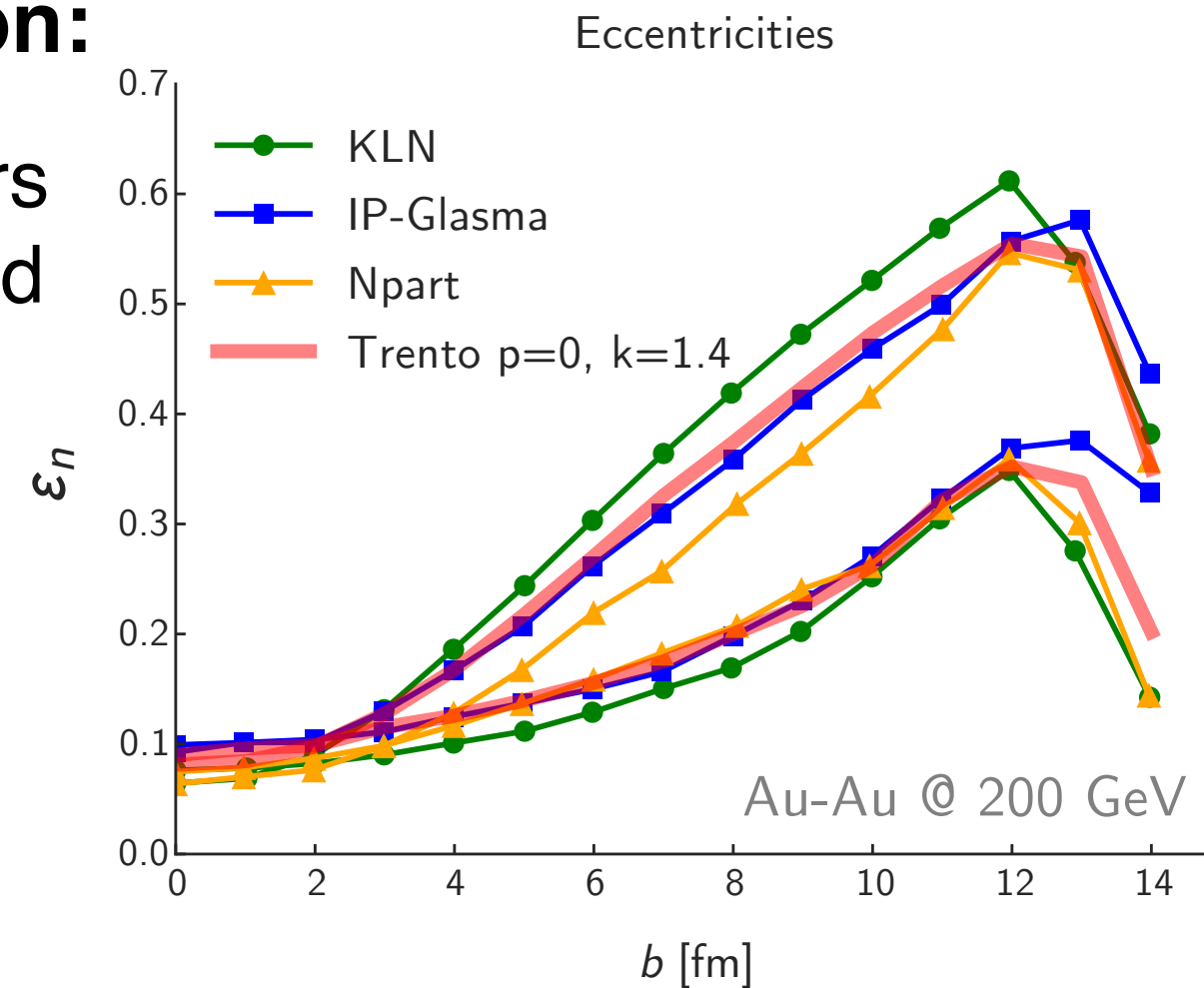
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- Glauber and KLN models strongly disfavored



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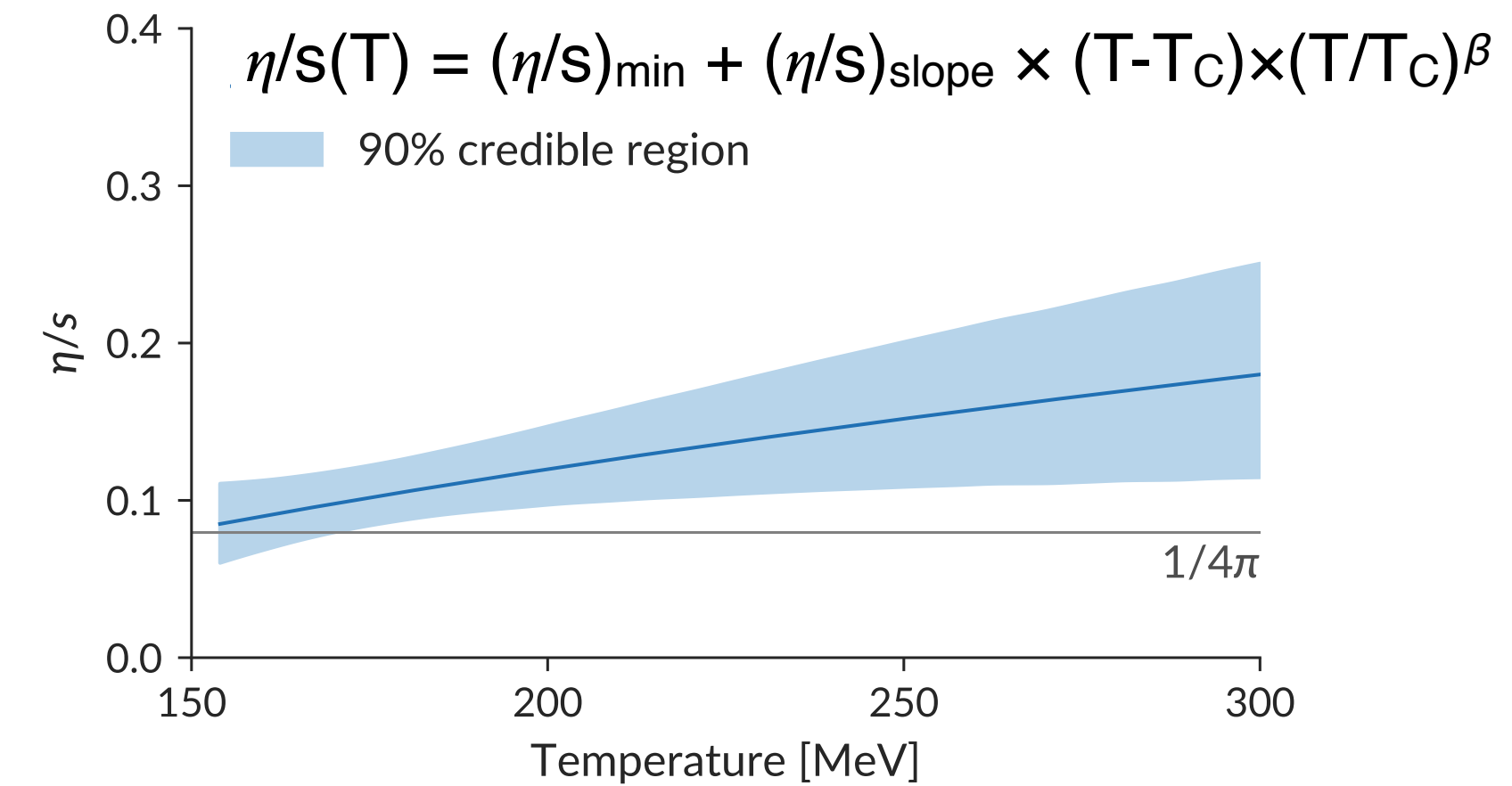
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temperature dependent shear viscosity:

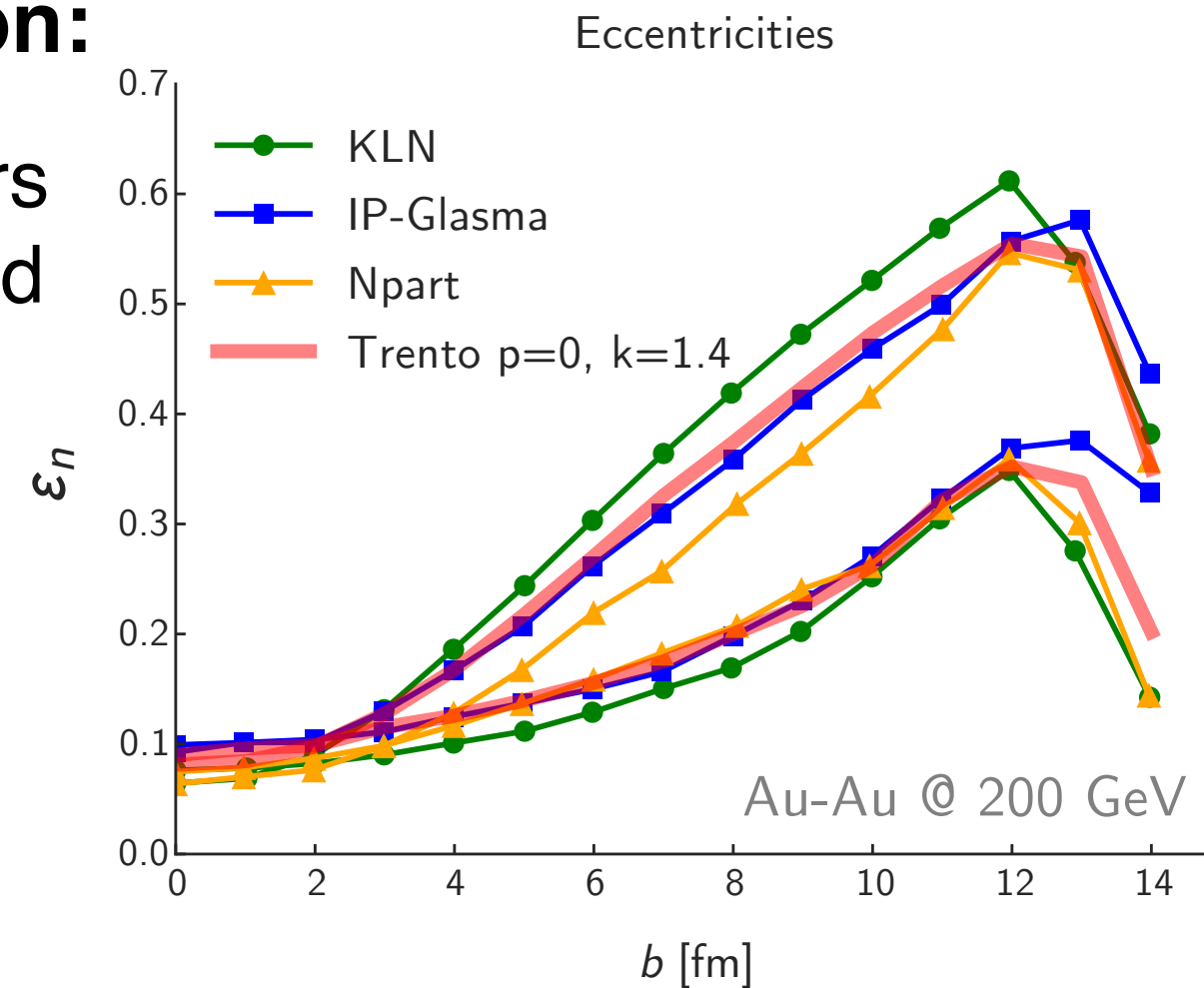
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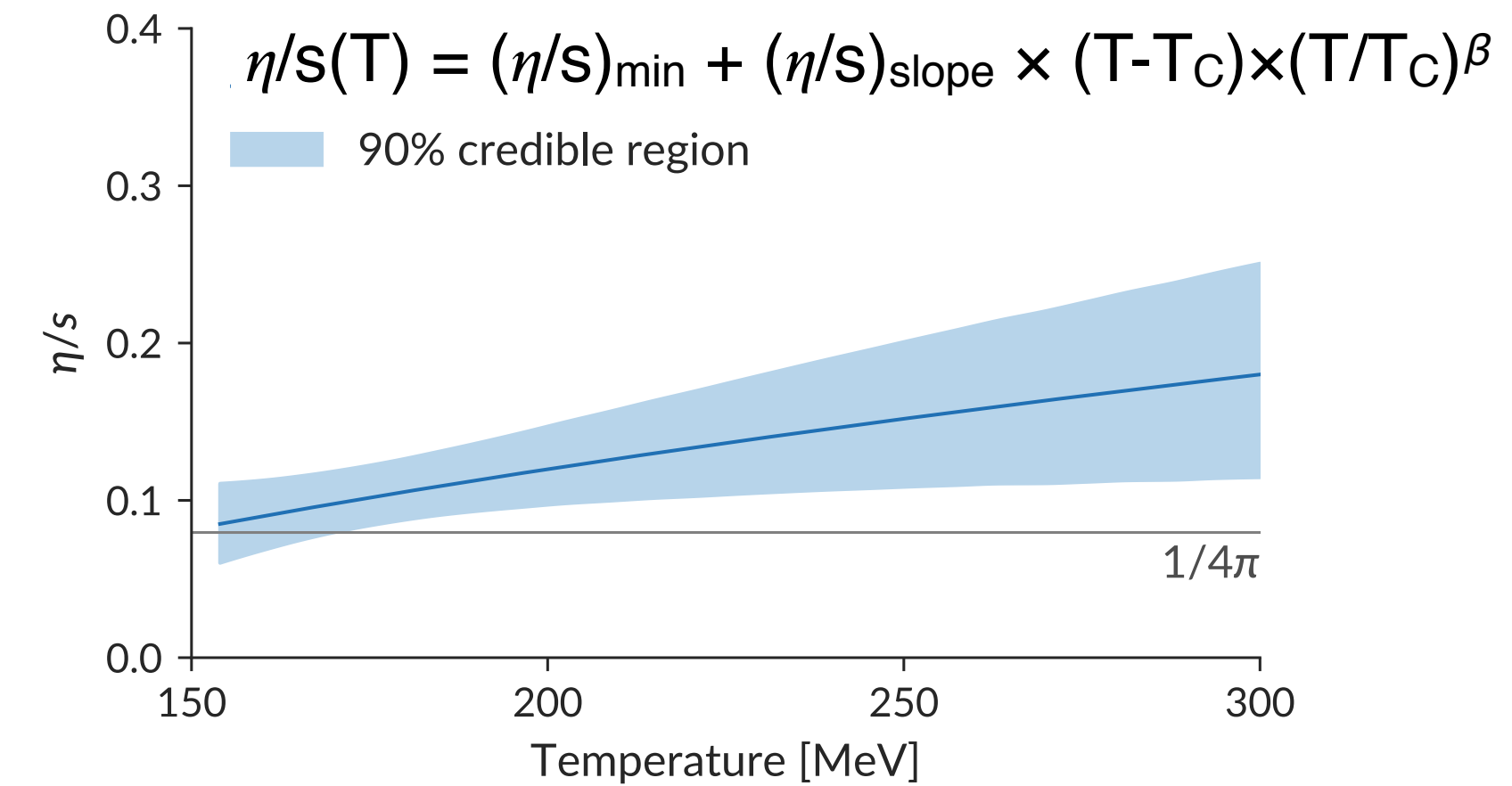
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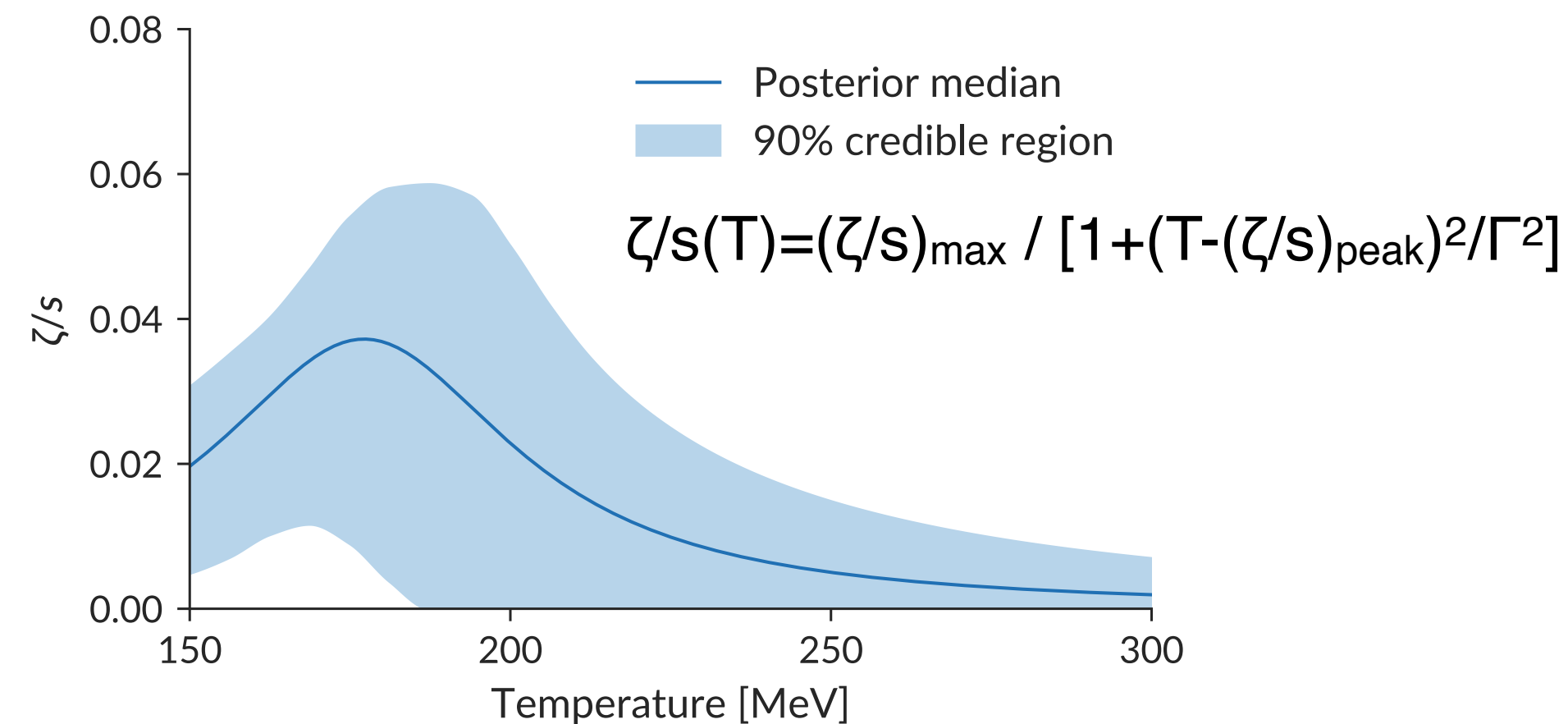
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temperature dependent bulk viscosity:

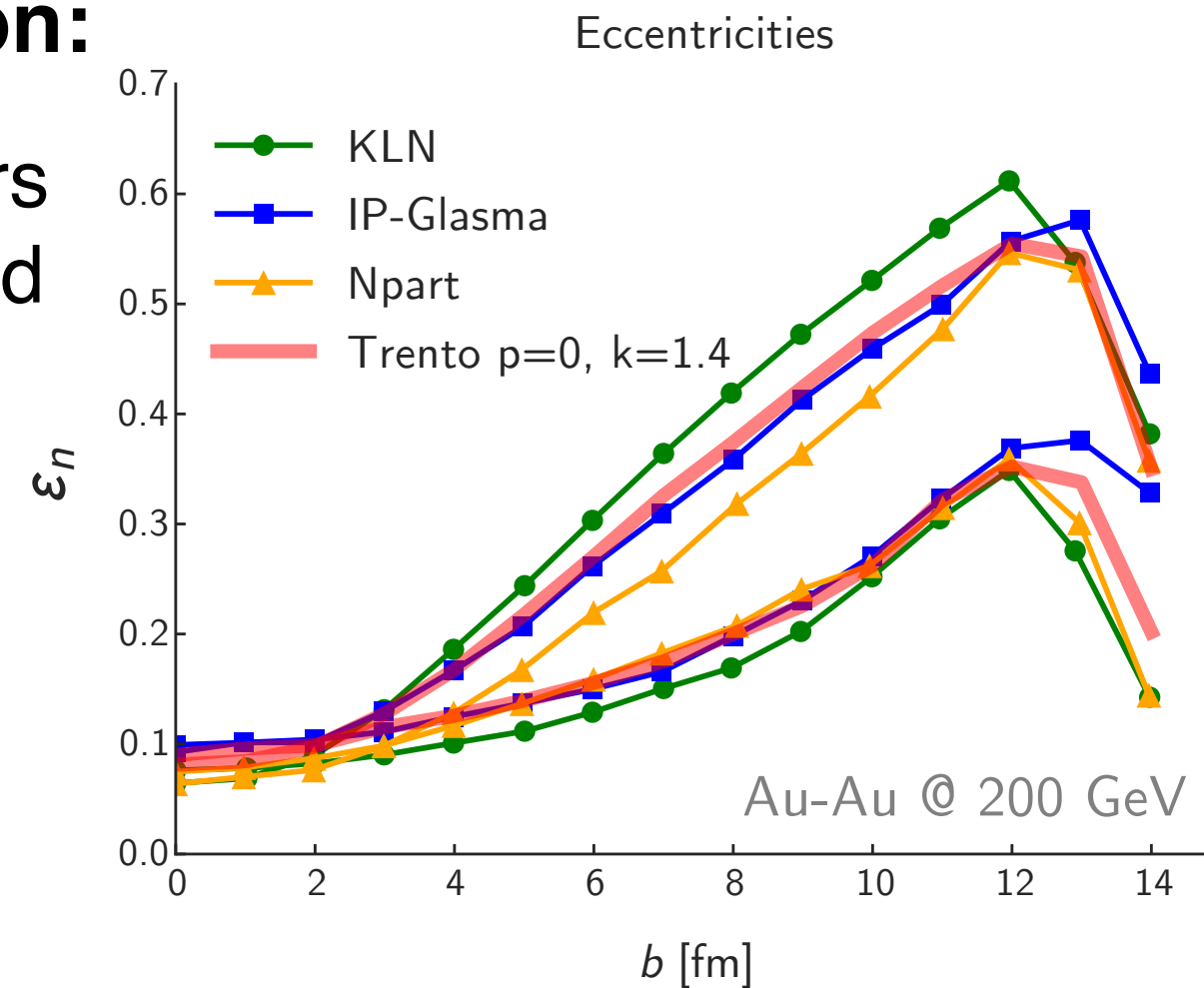
- non-zero value near T_C favored
- ambiguities exist for peak high vs. width



Summary I: Key Physics Results

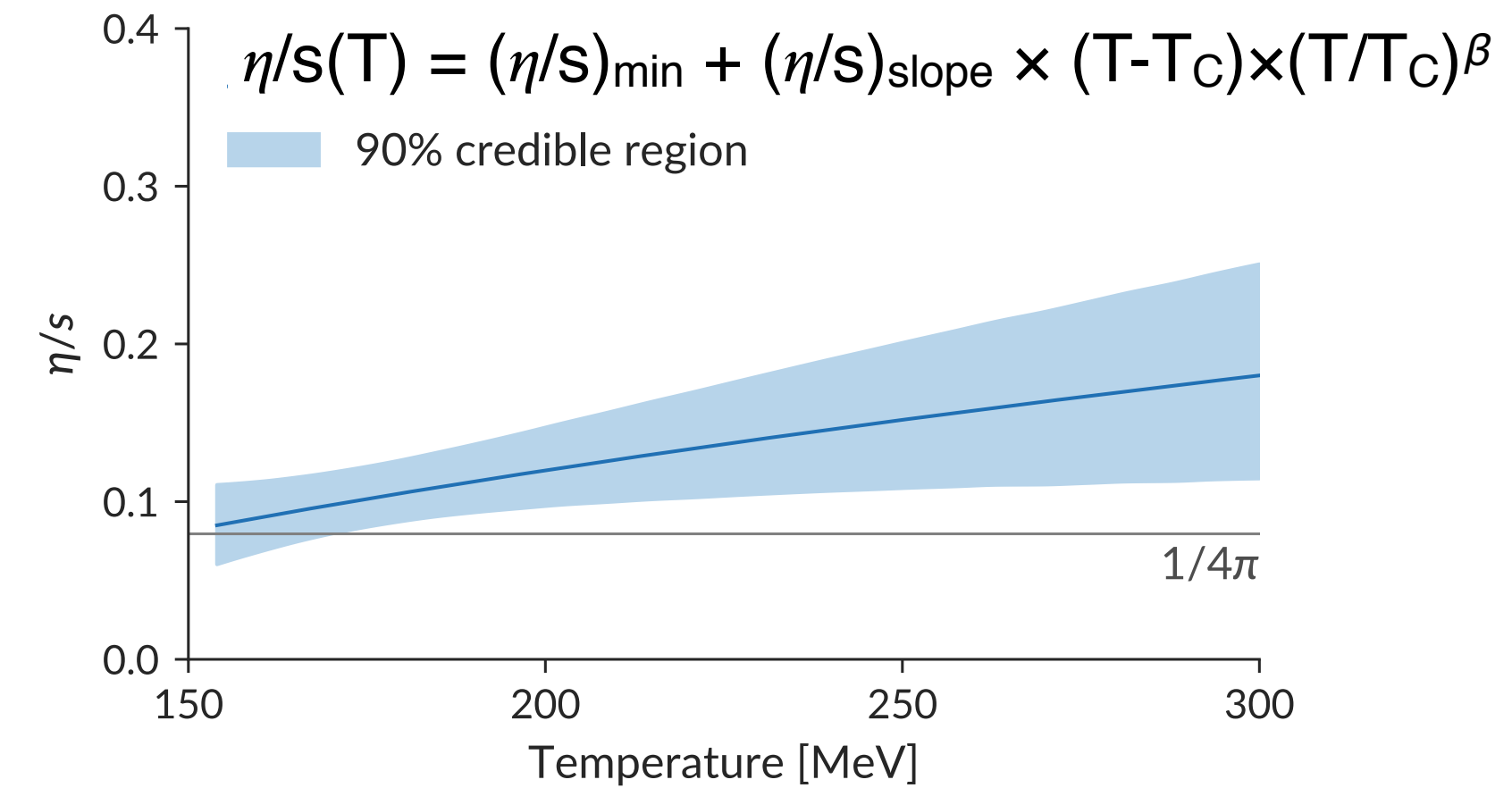
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- analysis strongly favors eccentricity scaling and entropy deposition of EKRT & IP-Glasma model
- Glauber and KLN models strongly disfavored



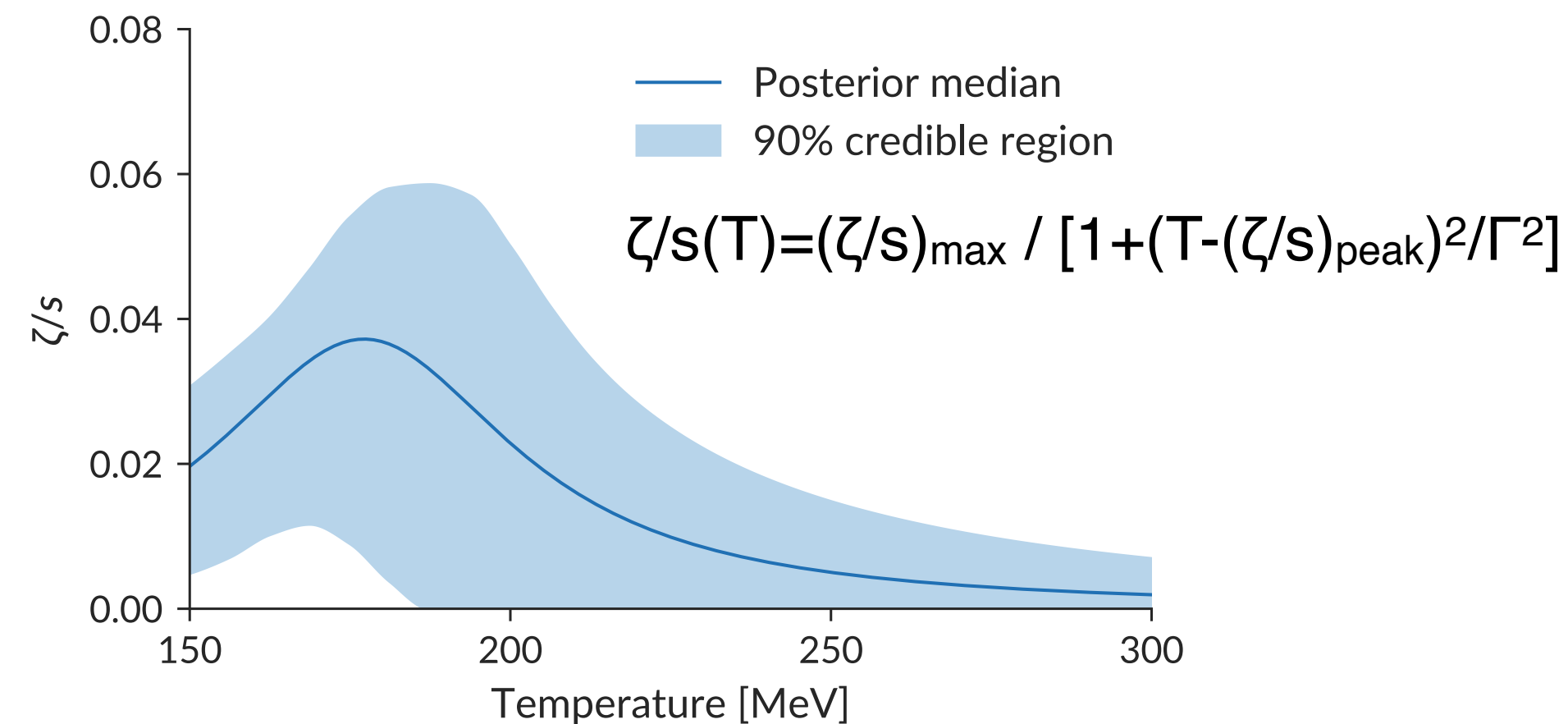
temperature dependent shear viscosity:

- analysis favors small value and shallow rise
- slope vs. curvature needs disambiguation



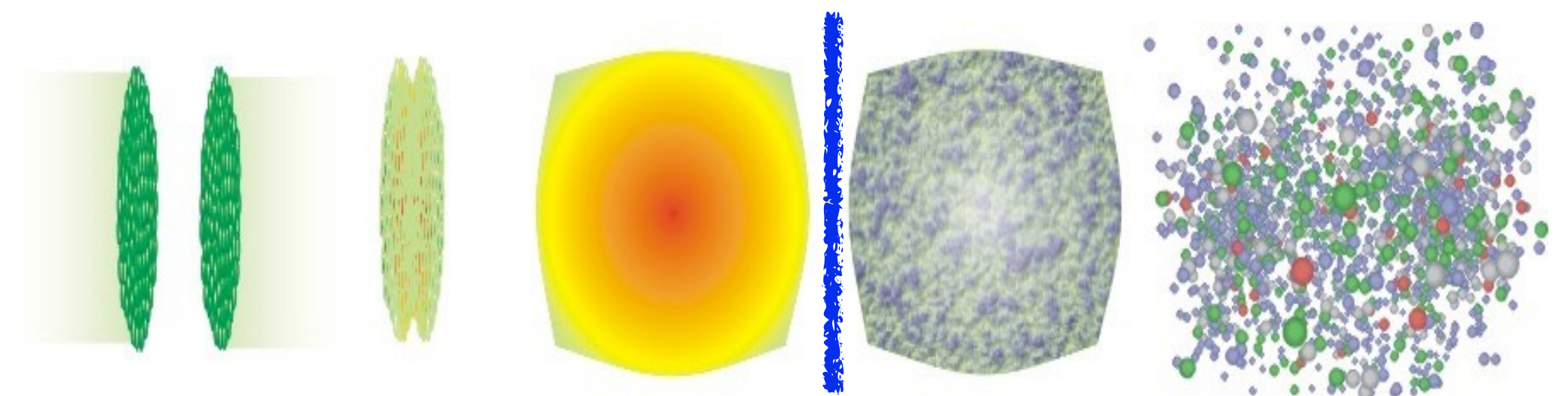
temperature dependent bulk viscosity:

- non-zero value near T_C favored
- ambiguities exist for peak height vs. width



hydro to micro switching temperature T_{sw}

- strong likelihood for a value of T_{sw} just around T_C
- indicative of the non-equilibrium nature and dynamical breakup of the hadronic system



Summary II: 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

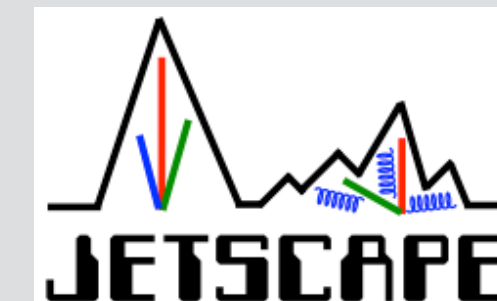
$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

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

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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Scientific Computing Center

Past & Present Collaborators & Sponsors

Duke QCD Group:

- Jonah Bernhard (now Lowe's Corporate)
- J. Scott Moreland
- Weiyao Ke
- Yingru Xu
- Jean-Francois Paquet

Duke Dept. of Statistical Sciences:

- Robert E. Wolpert
- Jake Coleman

Ohio State Nuclear Theory:

- Ulrich W. Heinz
- Jia Liu (now SAP)
- Chun Shen (now BNL)

U. of Wyoming Dept. of Statistics:

- Snehalata Huzurbazar
- Peter W. Marcy (now LANL)

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US Dept. of Energy



National Science
Foundation



Open Science Grid



NERSC



SAMSI



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:

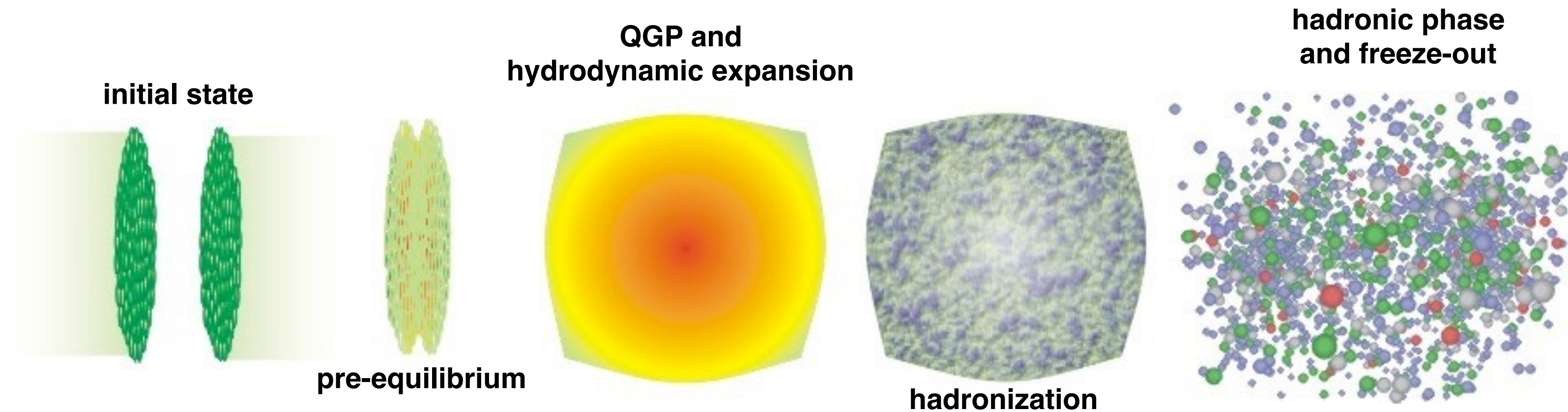
- Visualization and Bayesian Analysis packages
- <https://madai-public.cs.unc.edu>

Duke Bayesian Analysis Package:

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

The End

Time Evolution of a Heavy-Ion Collision



• Initial State:

- fluctuates event-by-event
- classical color-field dynamics

• QGP and hydrodynamic expansion:

- proceeds via 3D viscous RFD
- EoS from Lattice QCD

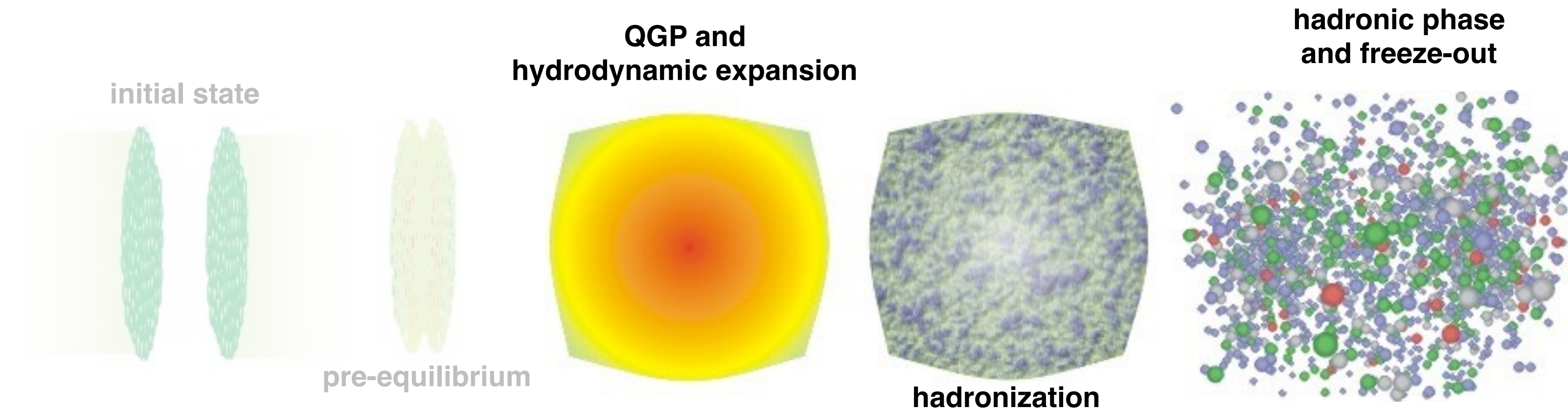
• Pre-equilibrium:

- rapid change-over from glue-field dominated initial state to thermalized QGP
- time scale: 0.15 to 2 fm/c in duration
- build-up of transverse velocity fields?

• hadronic phase & freeze-out

- interacting hadron gas
- separation of chemical and kinetic freeze-out

Constraining the IS of Heavy-Ion Collisions



- treatment of QGP evolution and hadronic freeze-out is well established and largely understood
- major success: first extraction of QGP properties such as η/s
- major challenges:
 - quantify uncertainties in extracted QGP properties
 - temperature dependence of transport coefficients

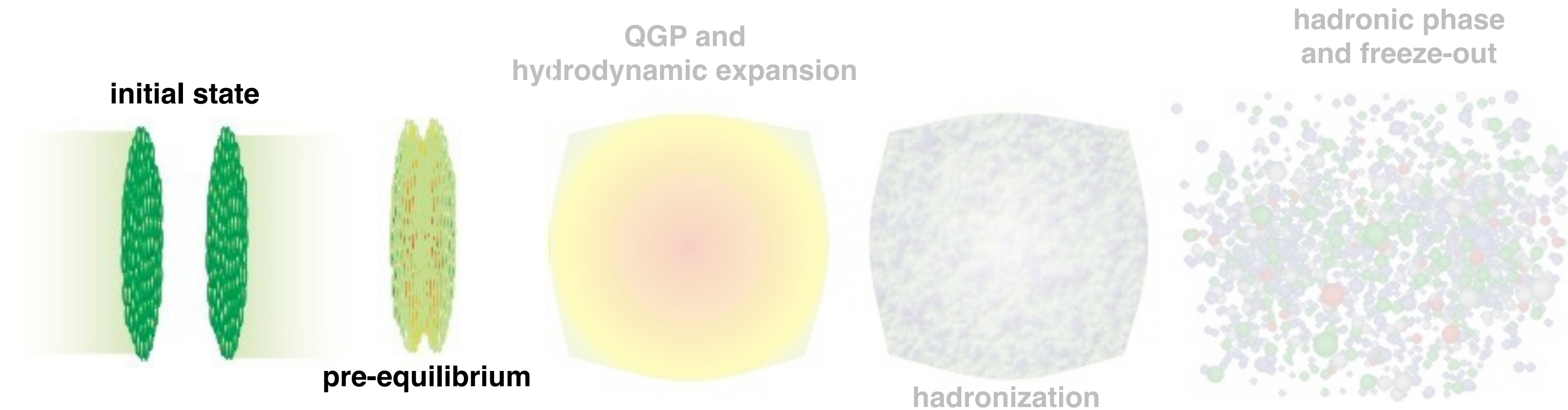
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Constraining the IS of Heavy-Ion Collisions



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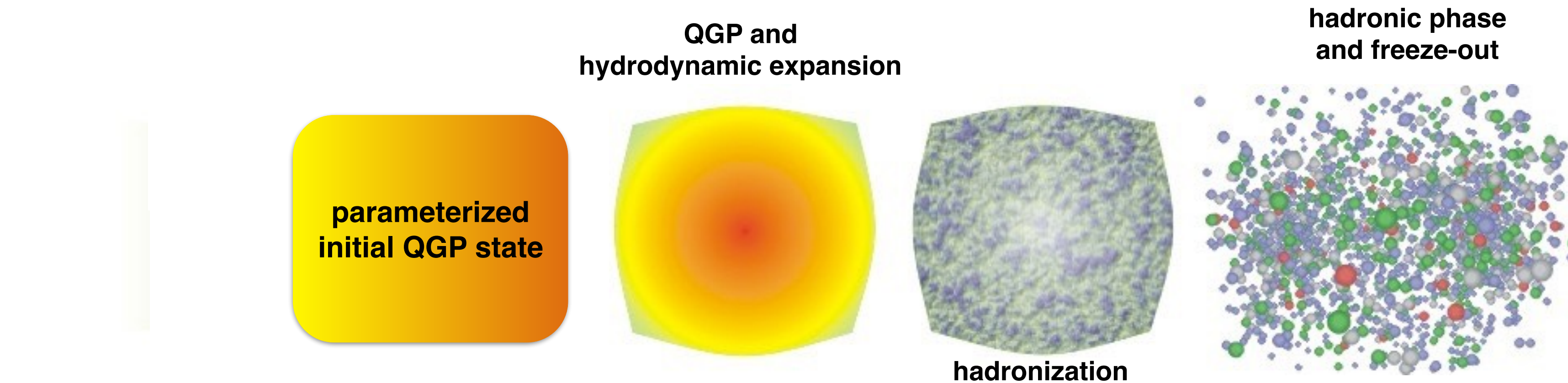
- rapid change-over from glue-field dominated initial state to thermalized QGP
- time scale: 0.15 to 2 fm/c in duration
- build-up of transverse velocity fields?

- physics of initial state and pre-equilibrium dynamics are still conceptually challenging with many open questions

- what processes drive the system towards equilibration?
- on what timescale?
- ...

- **a major source of uncertainty for the extraction of QGP properties**

Constraining the IS of Heavy-Ion Collisions



parameterized initial QGP state:

- based on simple phenomenological ideas for entropy deposition
- constrained by global model to data fit
- provides guidance to ab-initio IS models on features needed to describe the data

• QGP and hydrodynamic expansion:

- proceeds via 3D viscous RFD
- EoS from Lattice QCD

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Initial Condition Model: Trento

- effective, parametric, description of entropy production prior to thermalization
- based on **reduced thickness*** T_R as ansatz for dS/dy :

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

- determine participant nucleons in A, B by sampling for each nucleon pair:

$$P_{\text{coll}} = 1 - \exp \left[-\sigma_{gg} \int dx dy \int dz \rho_A \int dz \rho_B \right]$$

Nuclear Thickness*:

$$T_A = \sum_i \gamma_i \int dz \rho_{\text{nucleon}}(x - x_i, y - y_i, z - z_i)$$

- sum is over participant nucleons with positions sampled from an uncorrelated Woods-Saxon distribution or correlated nuclear configurations when available
- introduce fluctuations via γ_i , sampled from a gamma distribution with unit mean:
- nucleon density ρ_{nucleon} modeled as Gaussian in transverse plane

$$P_k(\gamma) = \frac{k^k}{\Gamma(k)} \gamma^{k-1} e^{-k\gamma}$$

$$\int dz \rho_{\text{proton}} = \frac{1}{2\pi w^2} \exp \left(-\frac{x^2 + y^2}{2w^2} \right)$$

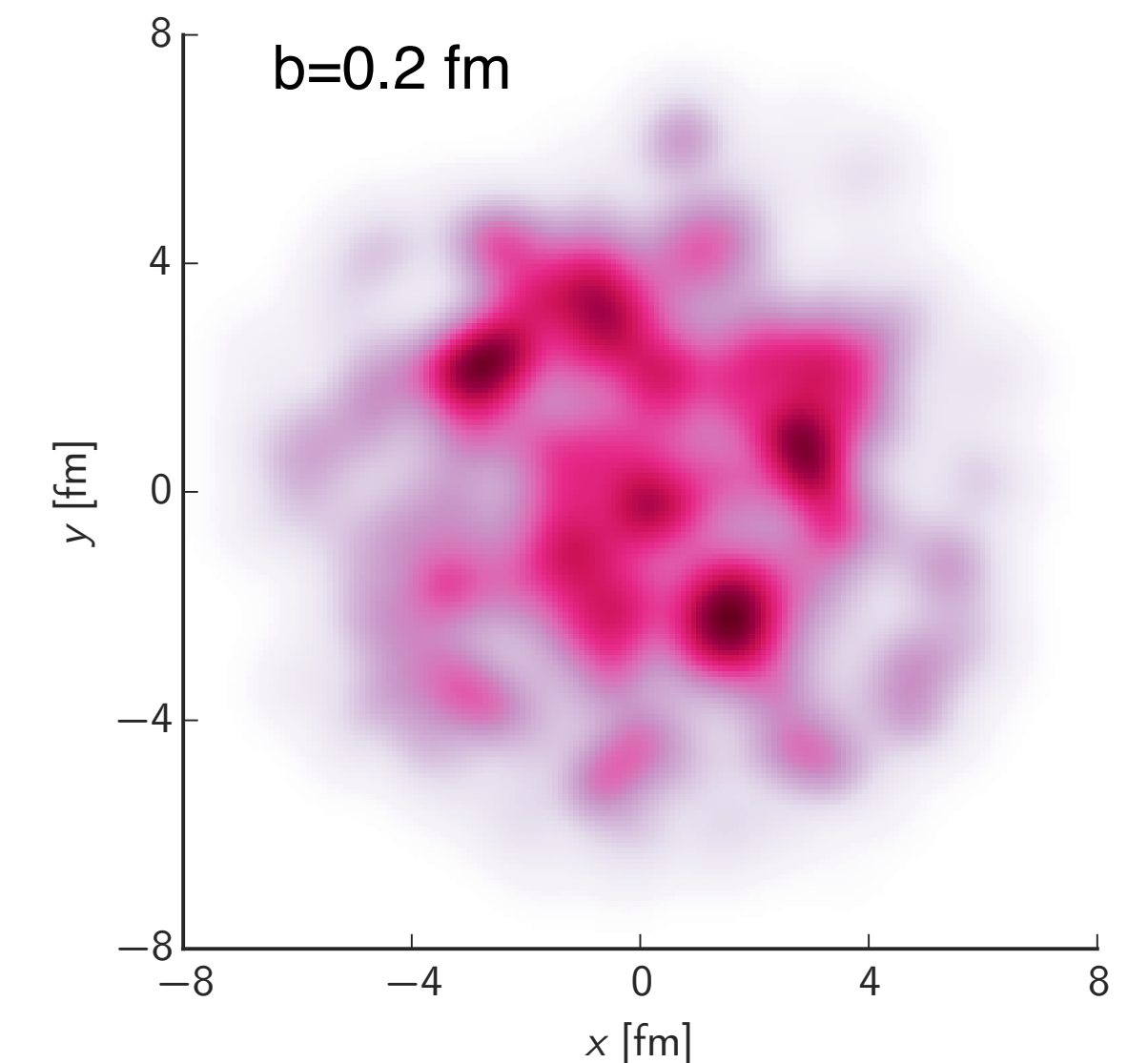
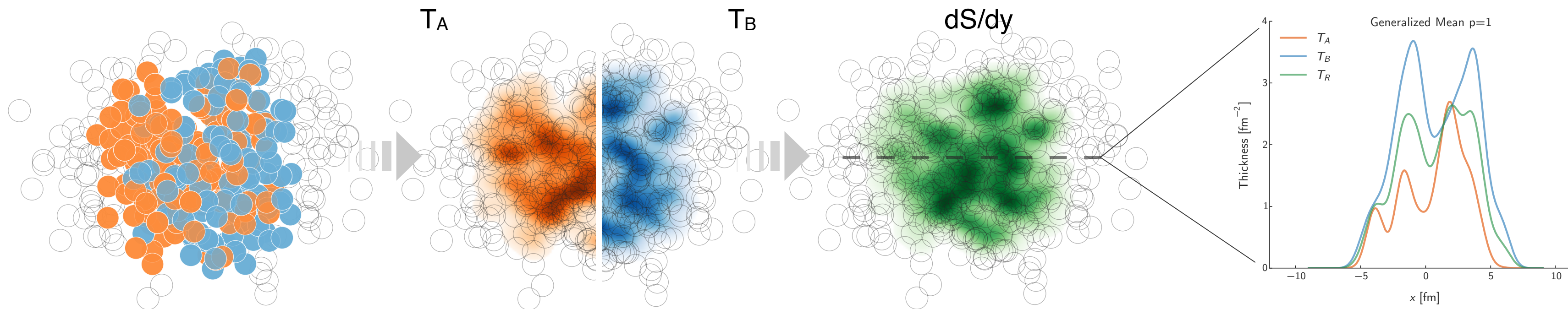
model parameters:

- attenuation parameter: p
- fluctuation parameter: k
- width of nucleon: w
- overall normalization: C_{norm}

model output:

- event by event spatial entropy density distribution at mid-rapidity at thermalization time τ_0

(1) determine participants: (2) construct thickness functions: (3) calculate entropy deposition:



Multivariate Output

Scaling of analysis with # of observables:

- independent emulators for each output?
 - neglects correlations among outputs
 - what if # of outputs scales to 100?
 - ▶ training of individual GPE's may become unfeasible and unnecessary in case of strong correlations

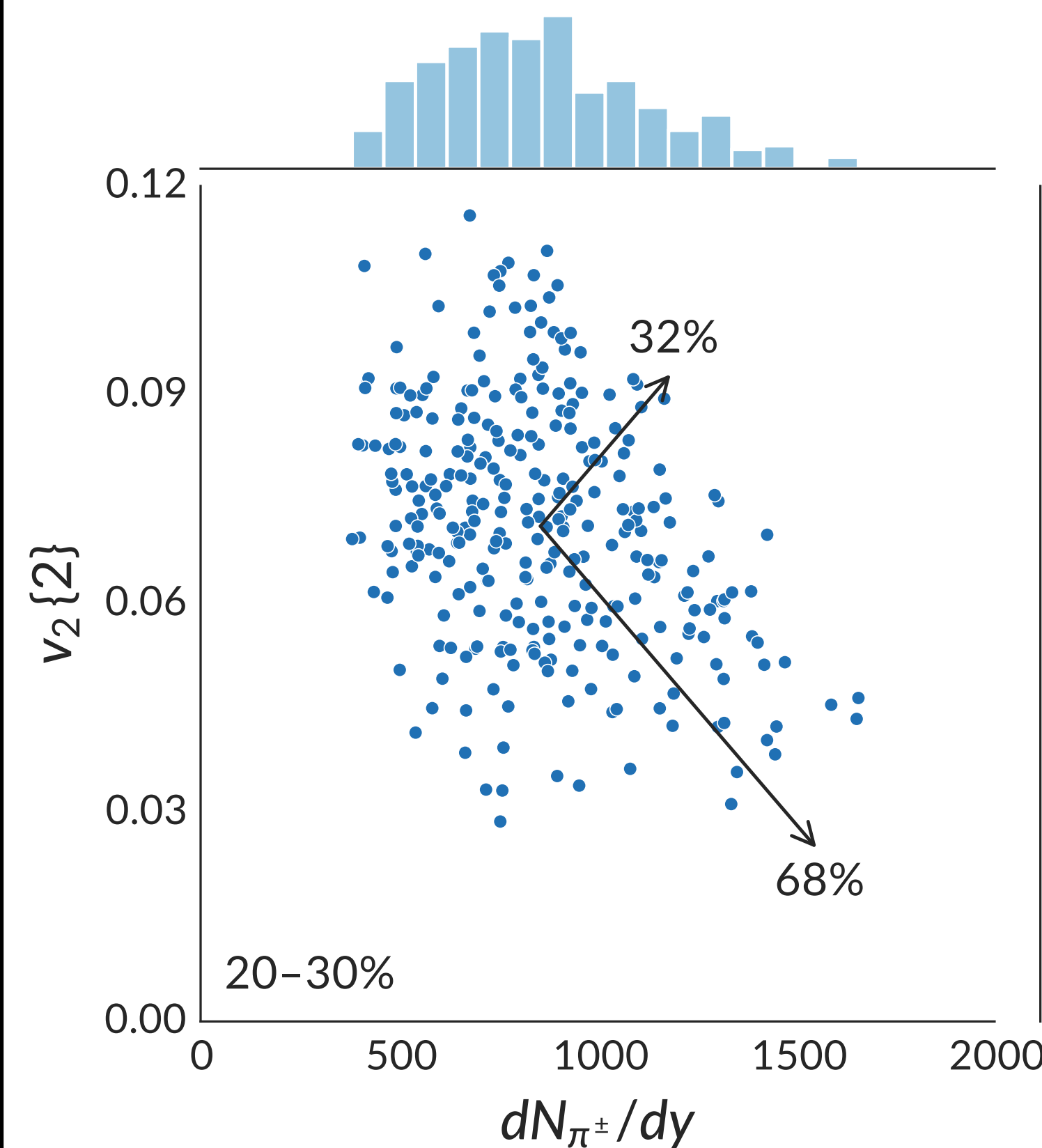
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Principal Components:

- linear combinations of model output
 - orthogonal and uncorrelated
- ⇒ emulate each PC



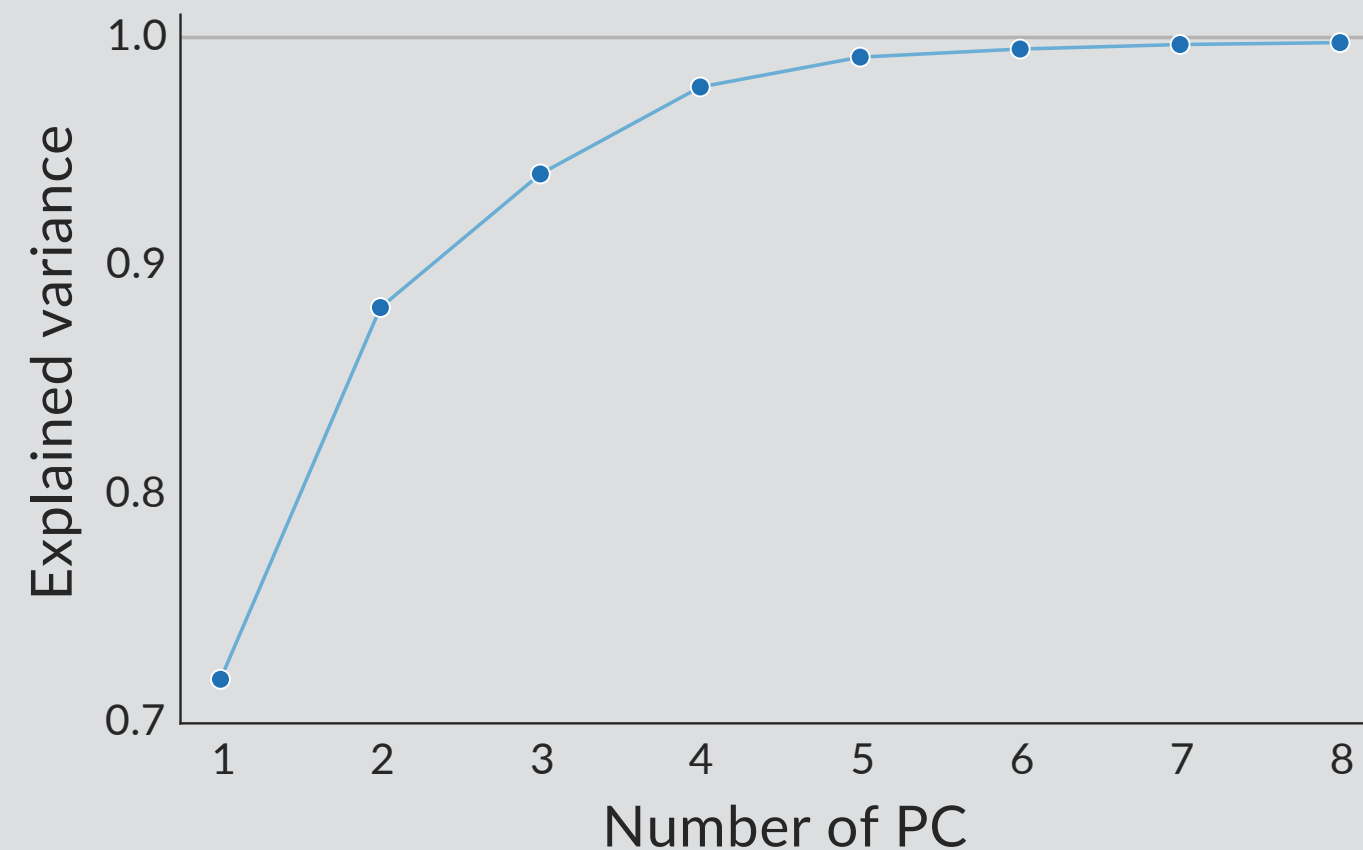
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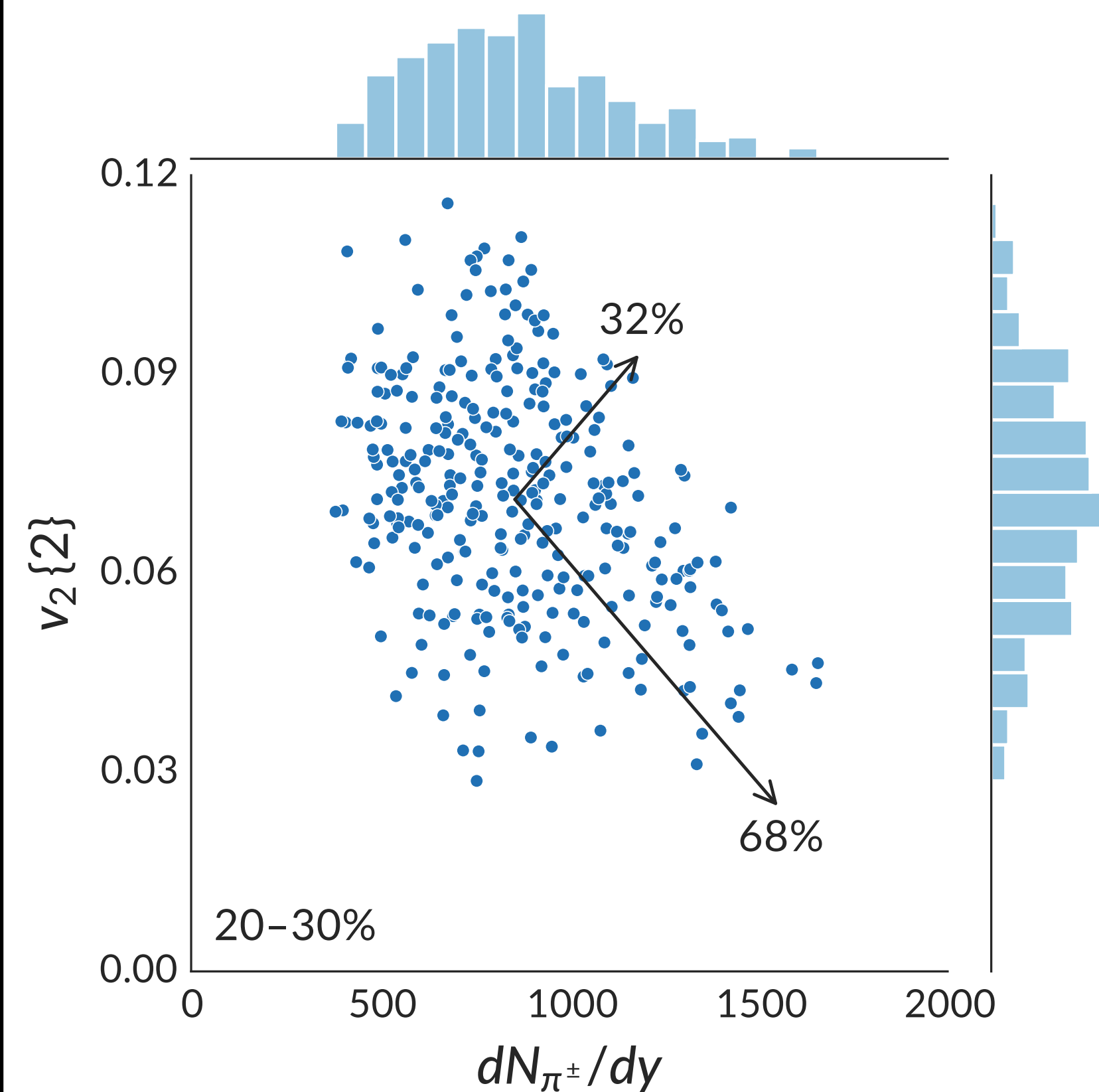
this analysis:

- model outputs are yields, $\langle p_T \rangle$, v_2 , v_3 and v_4
- 68 original output dimensions
- 8 principal components used



Principal Components:

- linear combinations of model output
 - orthogonal and uncorrelated
- ⇒ emulate each PC



Next steps:

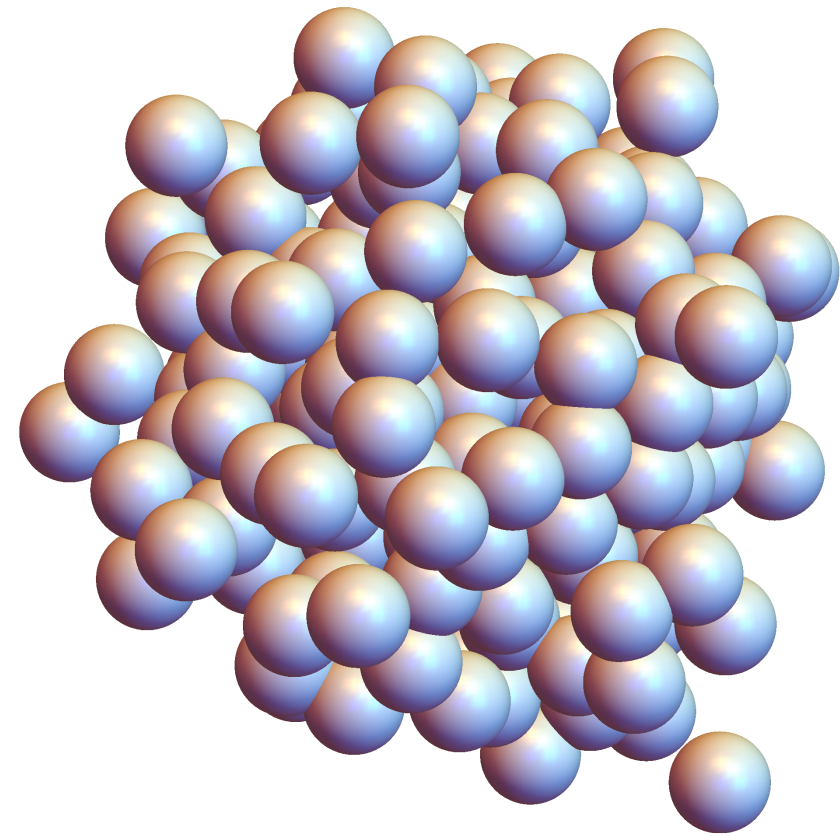
- **sub-nucleon degrees of freedom**
- **forward/backward rapidity**

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:

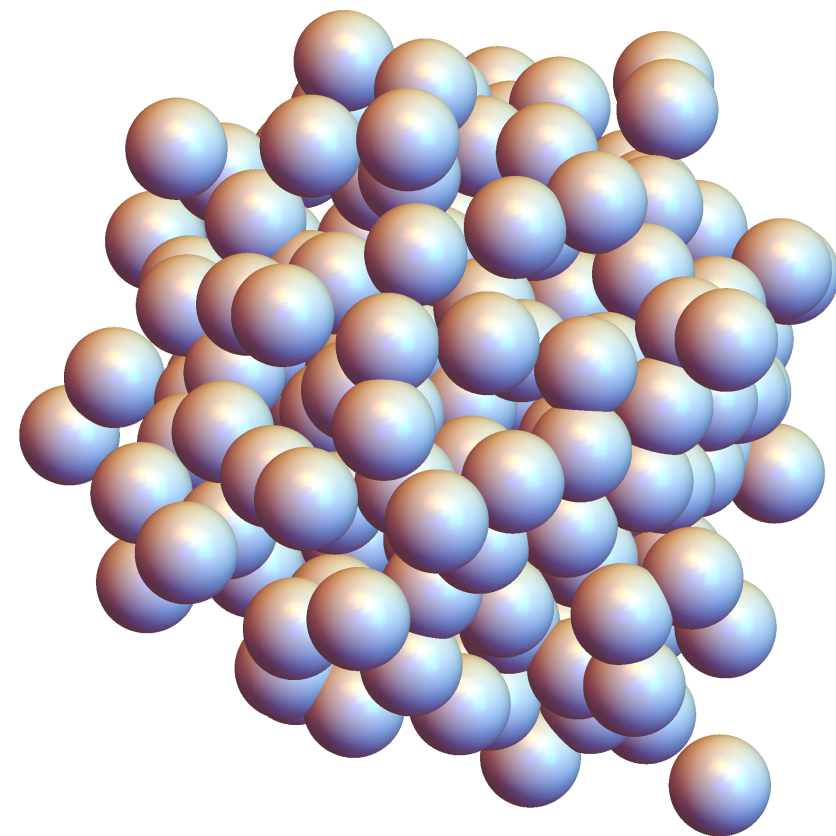
- spherical protons do not allow for proper eccentricities in p+A or small/asymmetric collision systems

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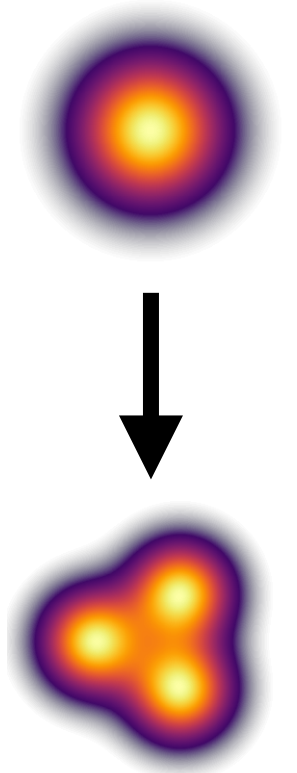


Caveat:

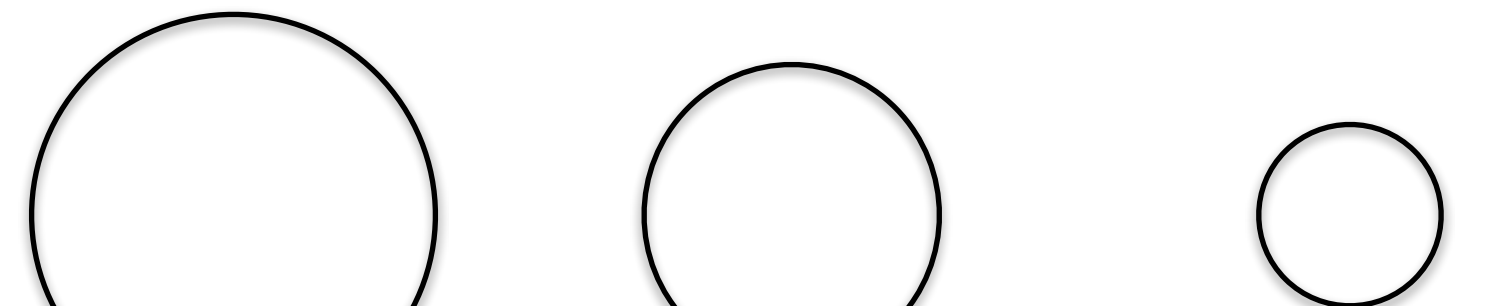
- spherical protons do not allow for proper eccentricities in p+A or small/asymmetric collision systems

Trento with nucleon substructure:

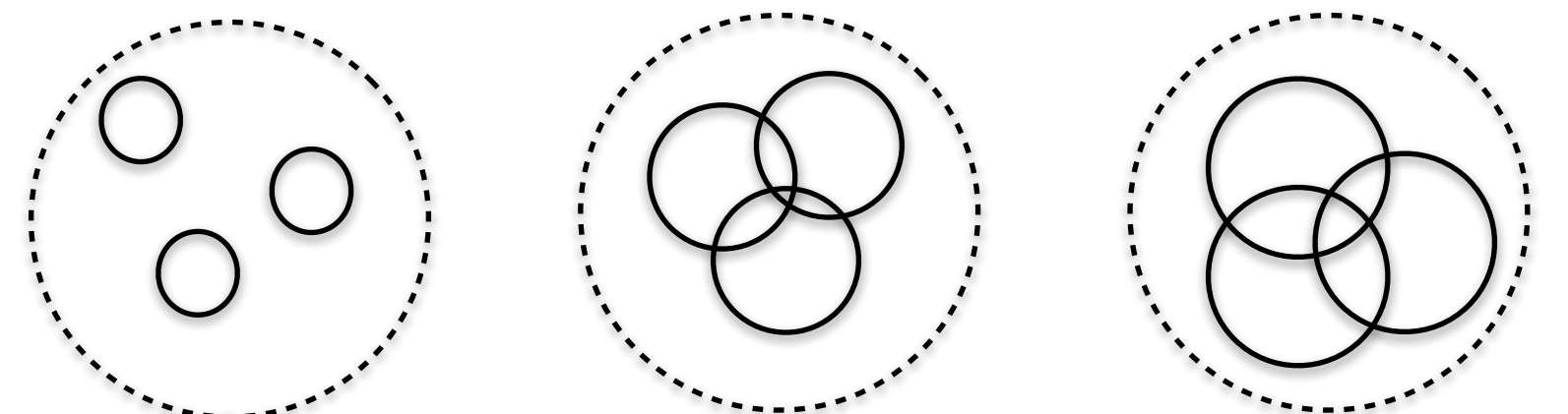
- trade Gaussian nucleons for lumpy nucleons
- additional parameters:
 - sampling radius of constituent positions
 - constituent Gaussian width
 - number of constituents in each nucleon



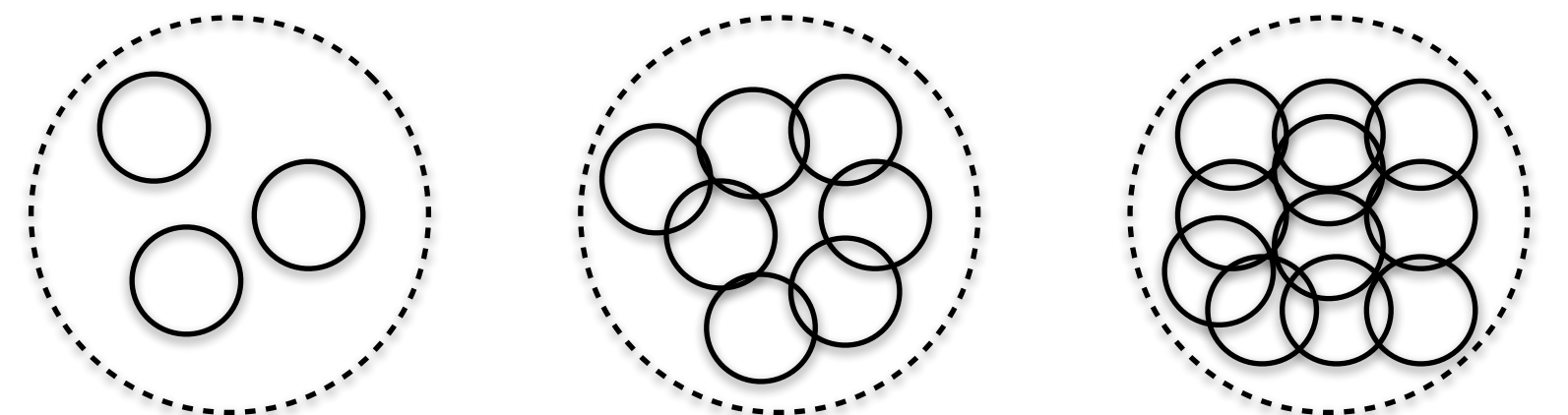
sampling radius:



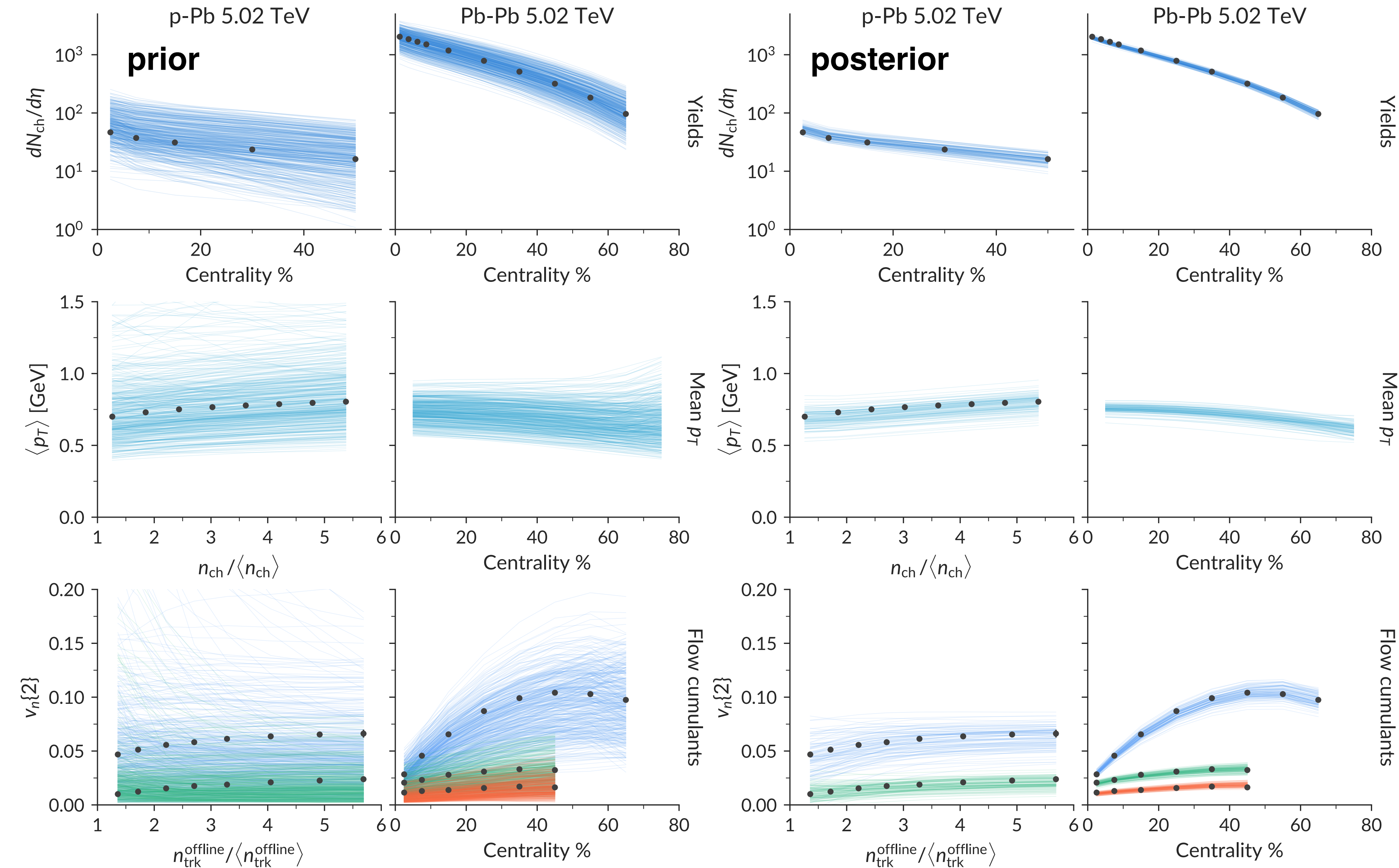
constituent width:



of constituents:

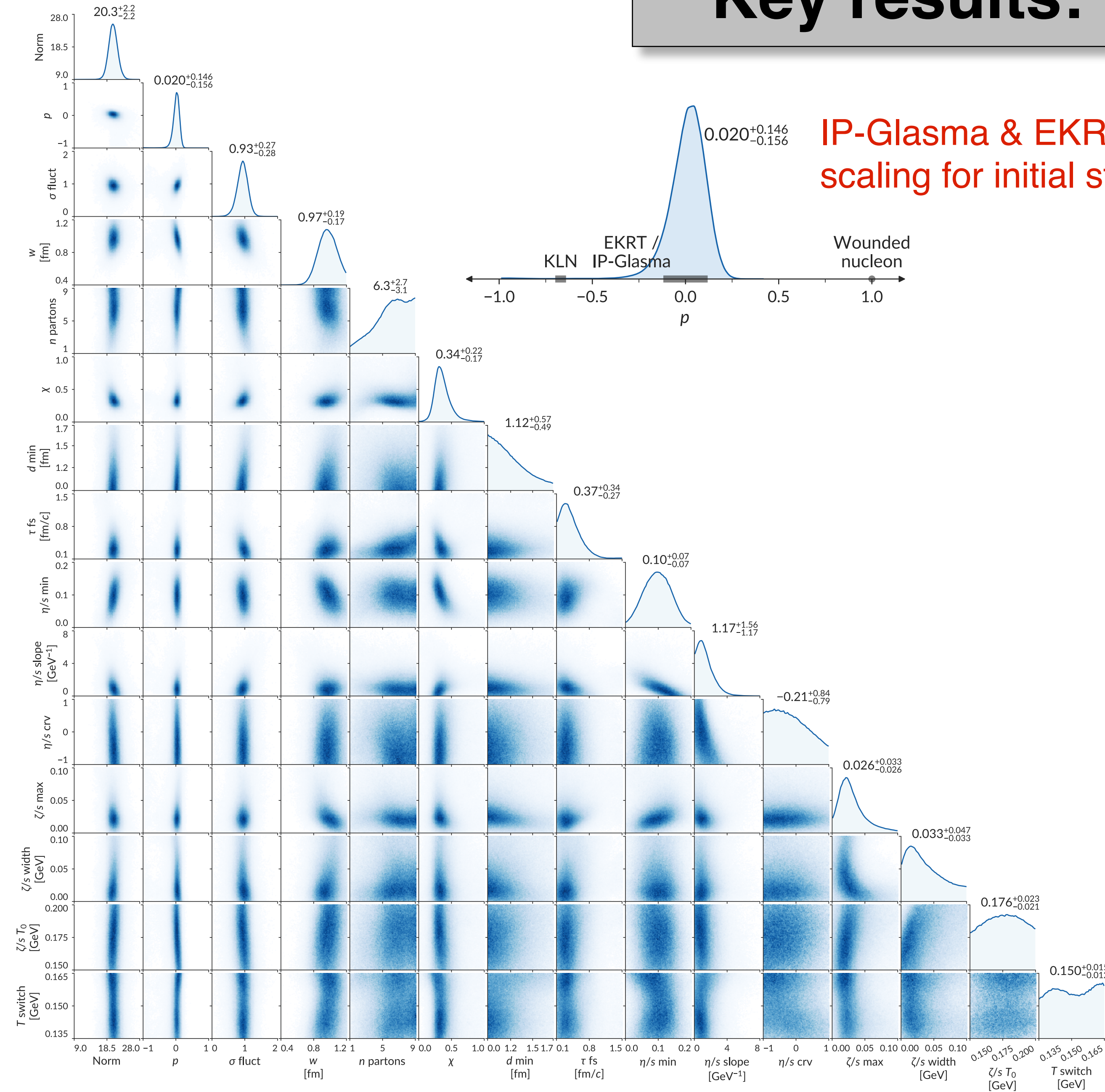


Simultaneous Calibration on AA and pA

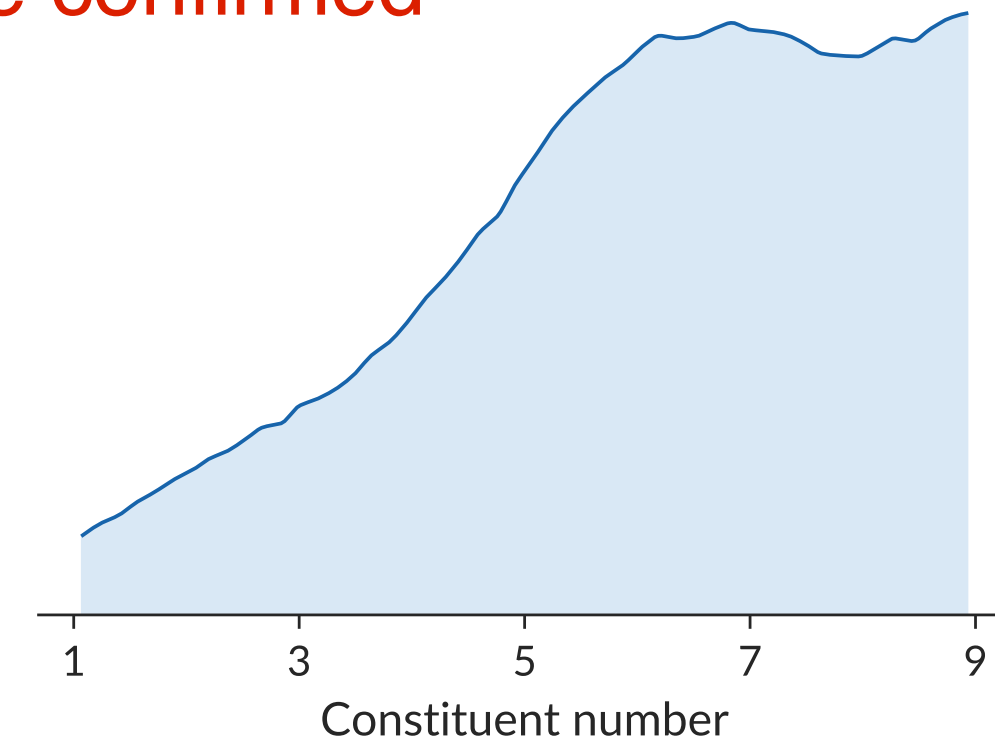
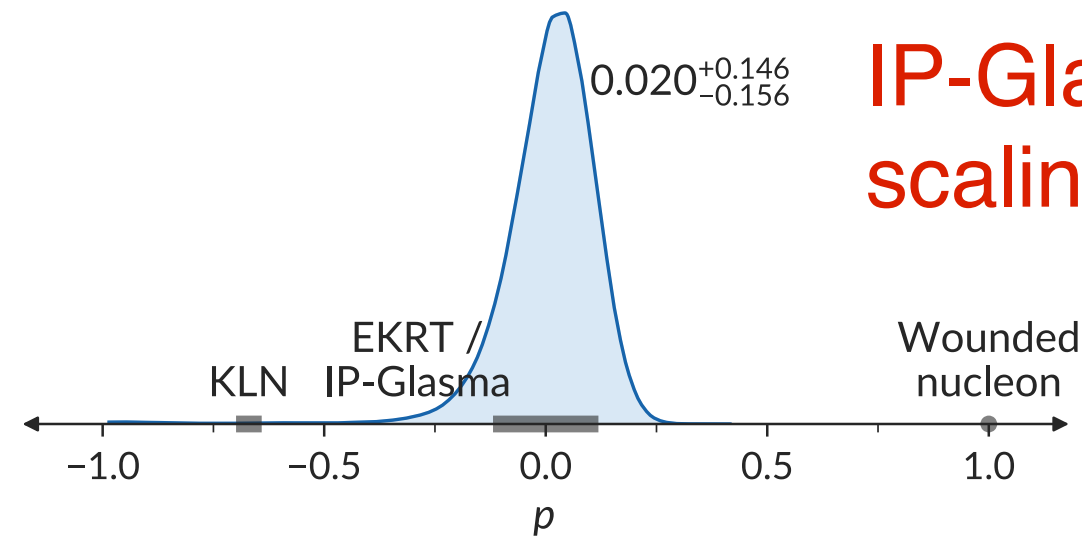


- ALICE & CMS data for AA & pA at 5.02 TeV
- calibration on 15 parameters, for initial state, shear and bulk viscosities
- restriction on 1 energy to keep computational effort reasonable
- generally larger uncertainties in posterior, due to less data than in the AA calibrations for 2 energies...

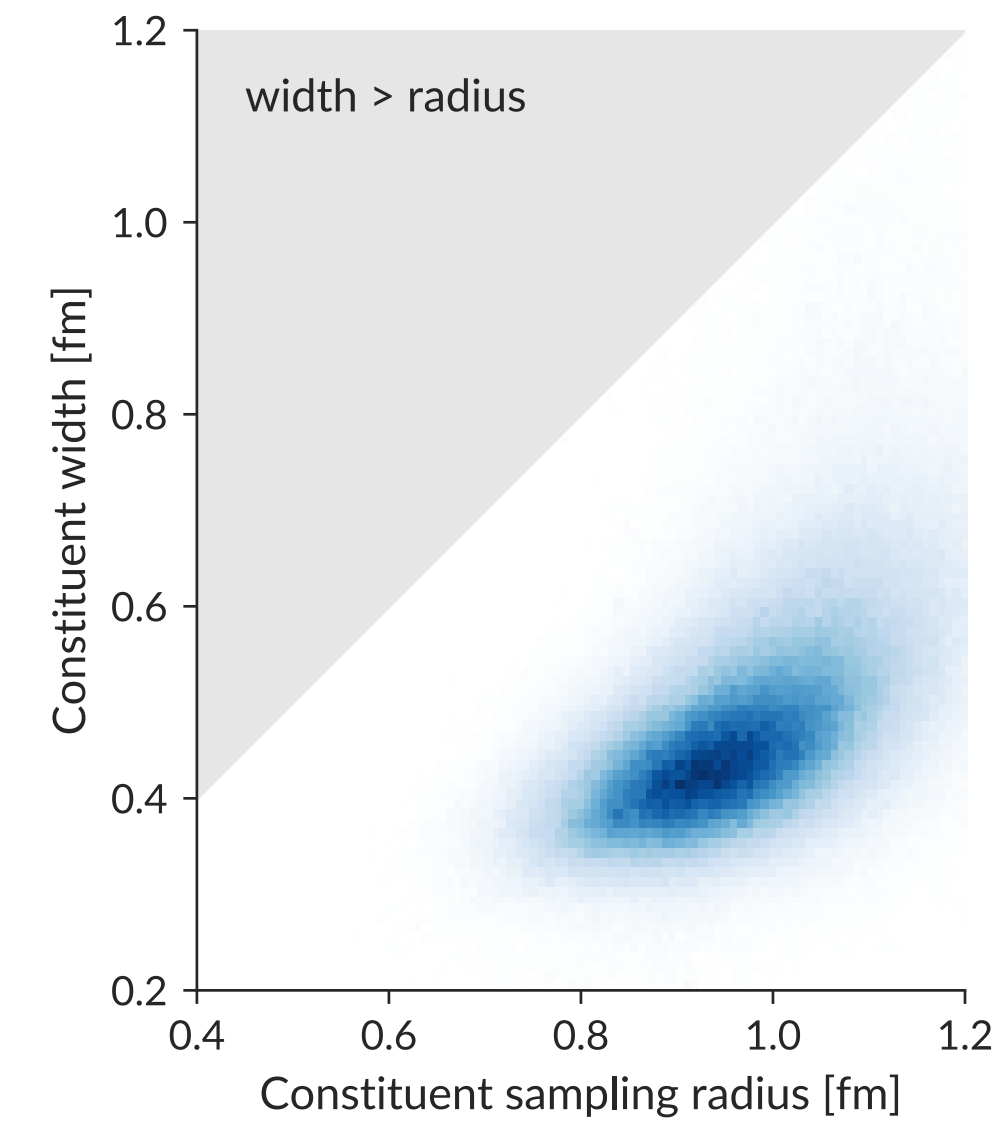
Key results: initial state



IP-Glasma & EKRT eccentricity scaling for initial state confirmed



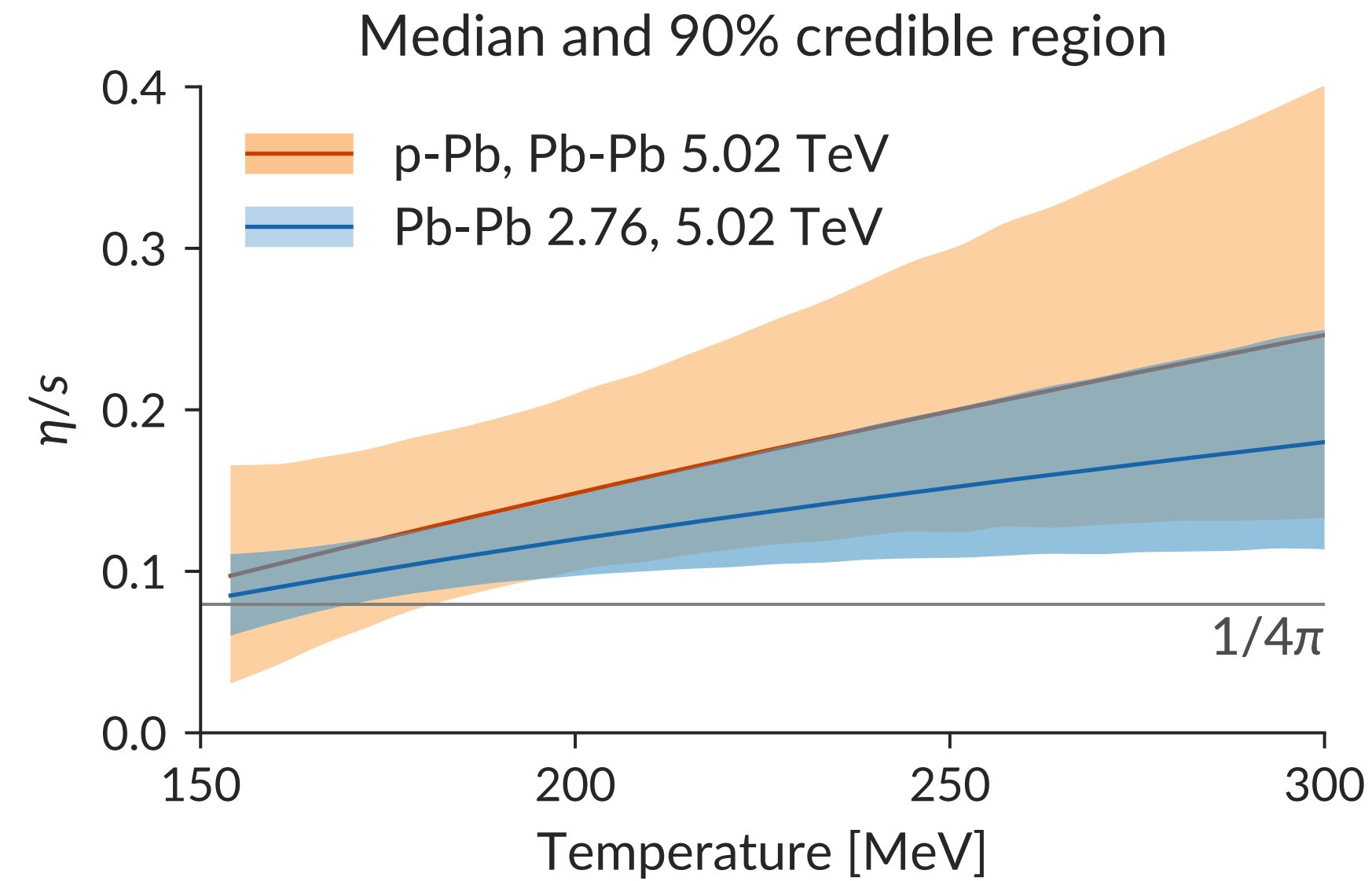
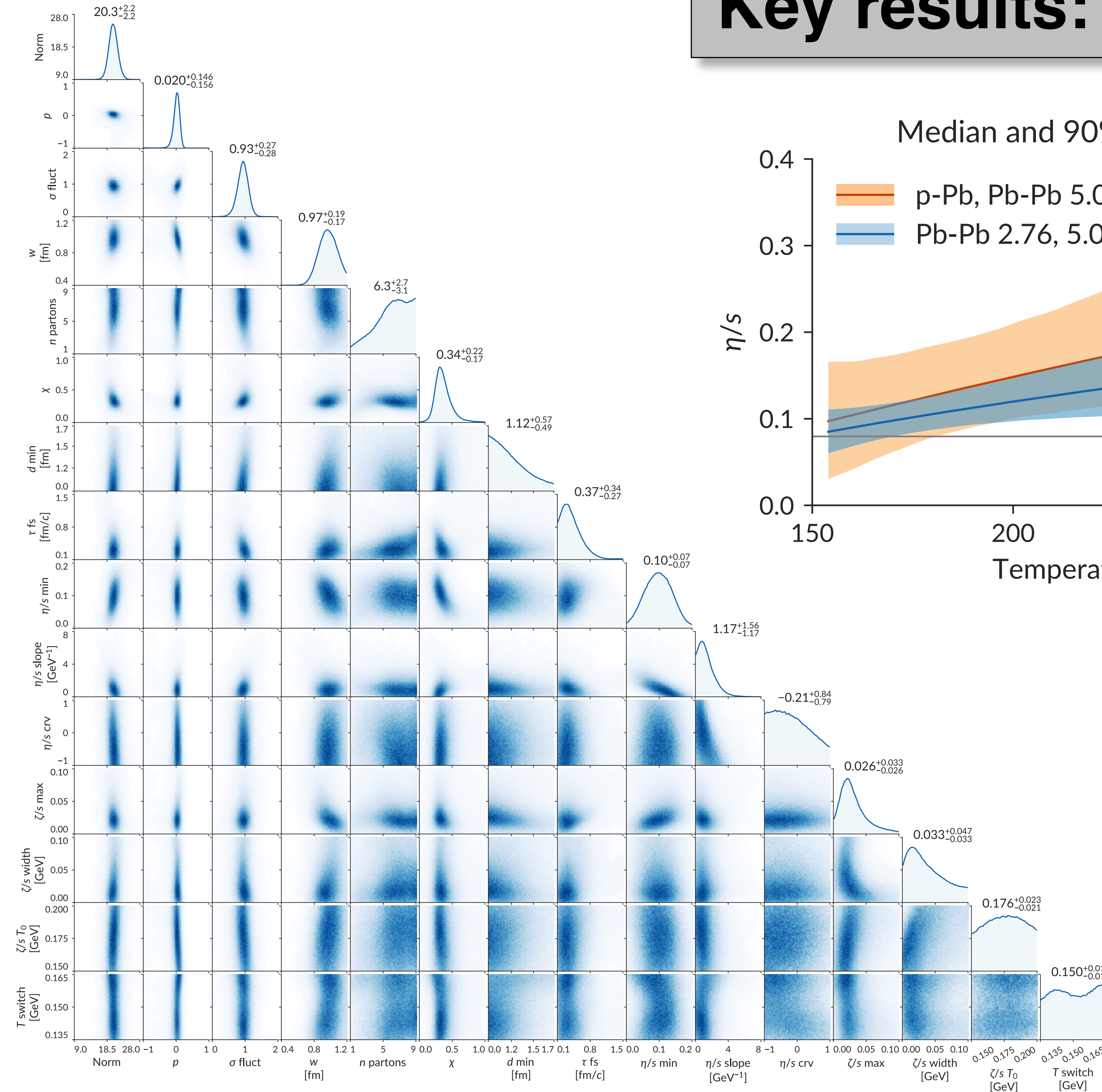
no strong preference for a particular constituent # as long as $n > 3$



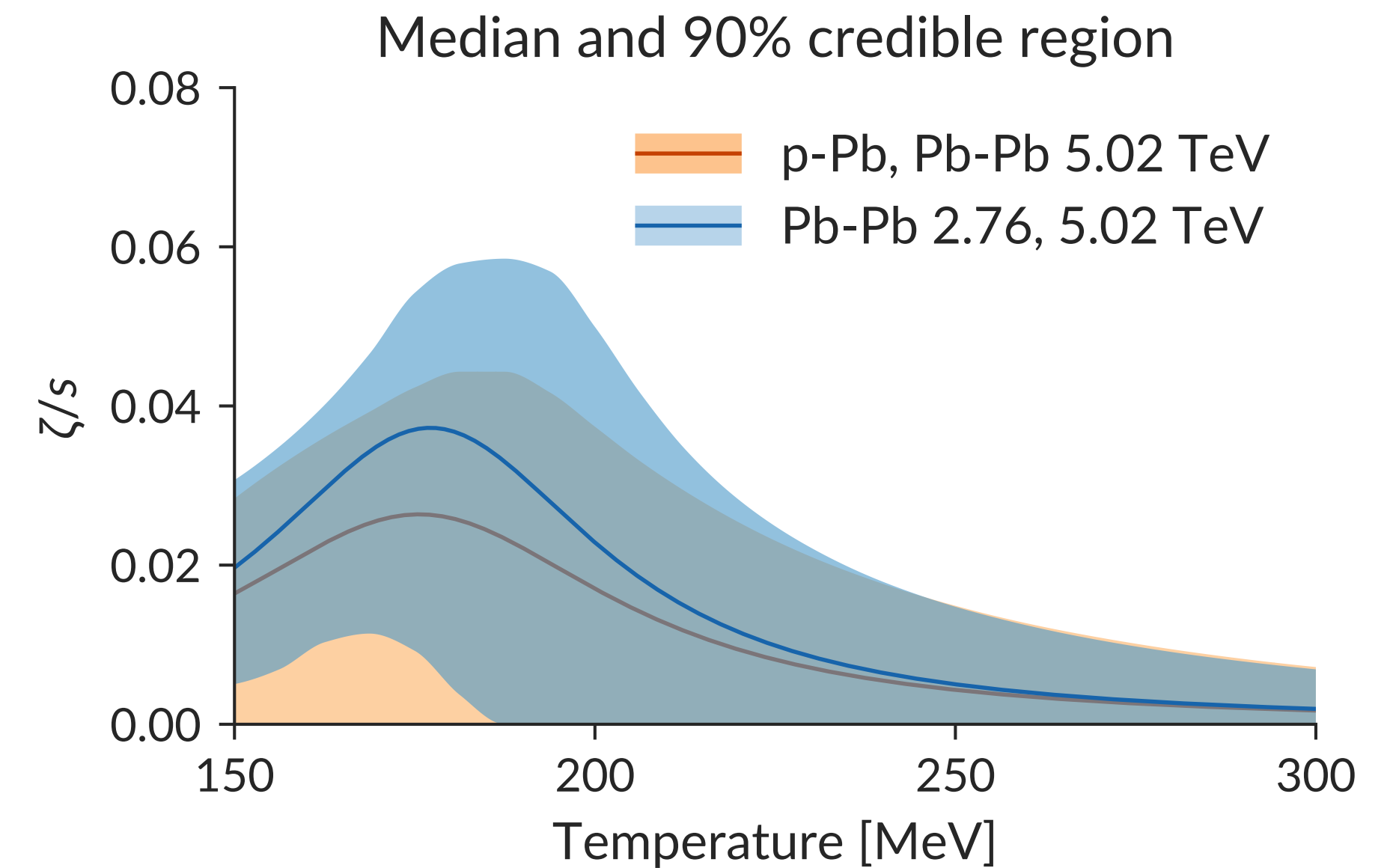
constituent width & sampling radius are well constrained to

- $r = 0.99 \pm 0.16$
- $w = 0.47 \pm 0.18$

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

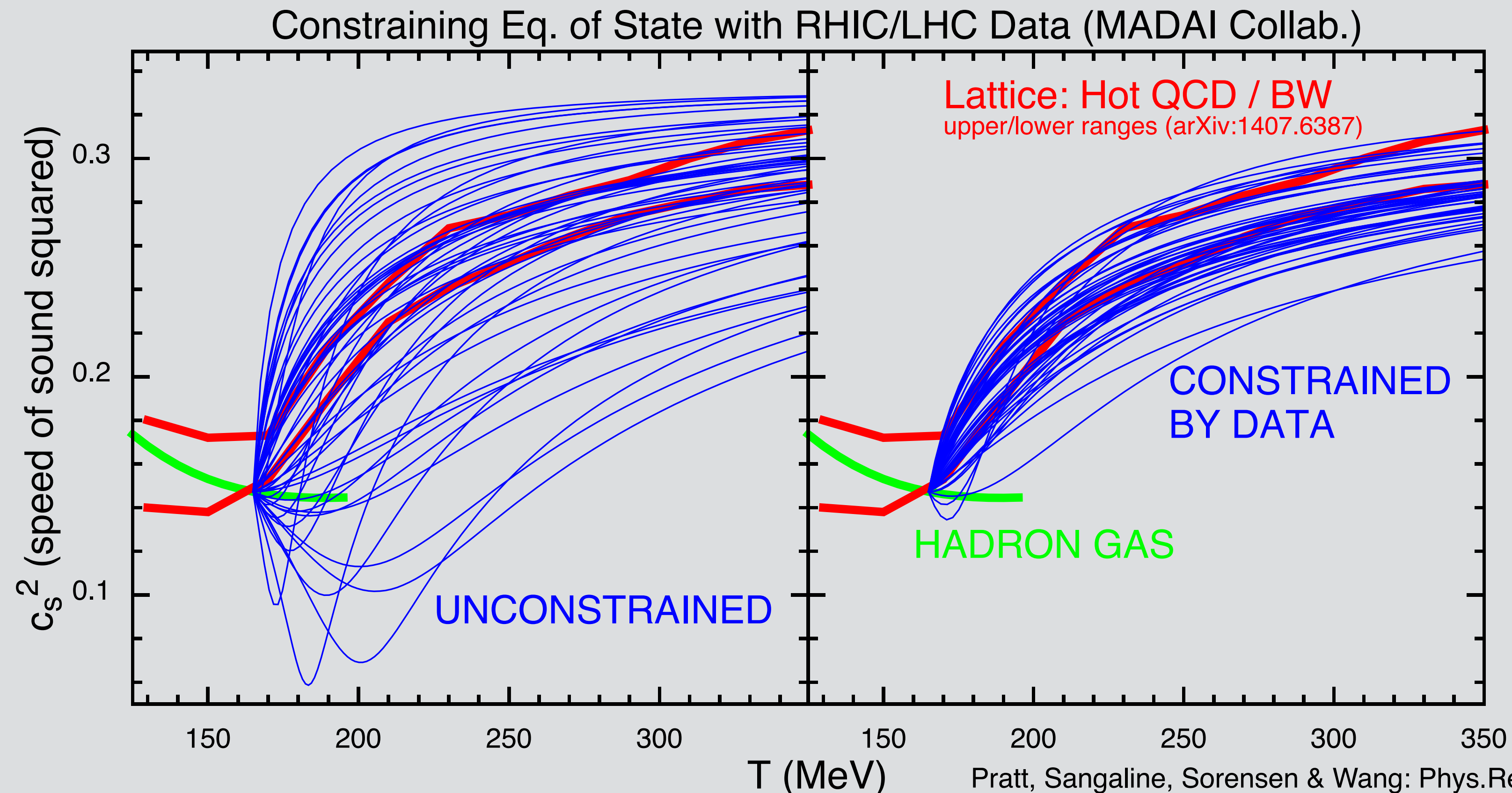


Other Examples: Equation of State

Example: determine the EoS of QGP matter from experimental measurements

what equation of state would the physics model choose to best describe the experimental data?

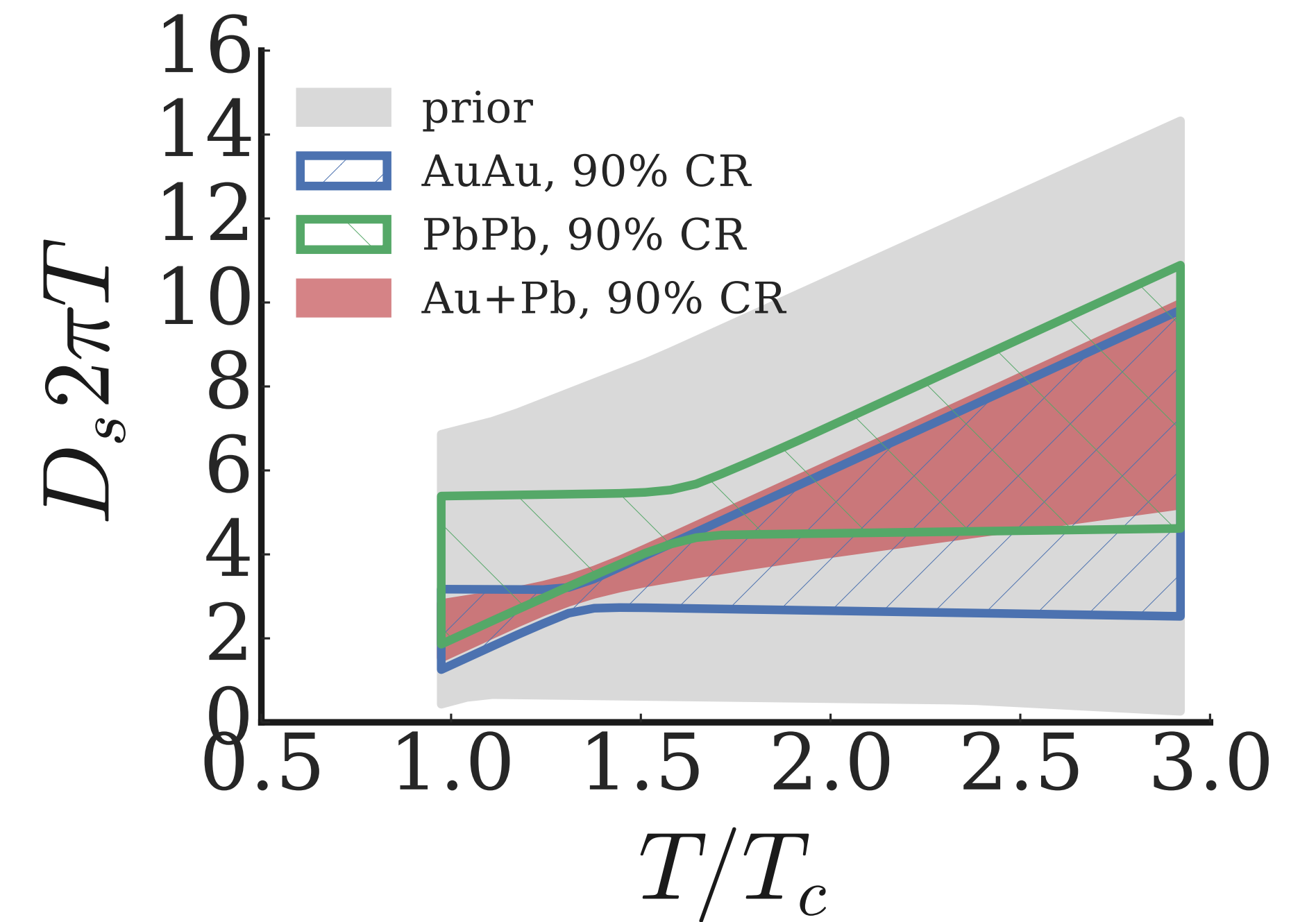
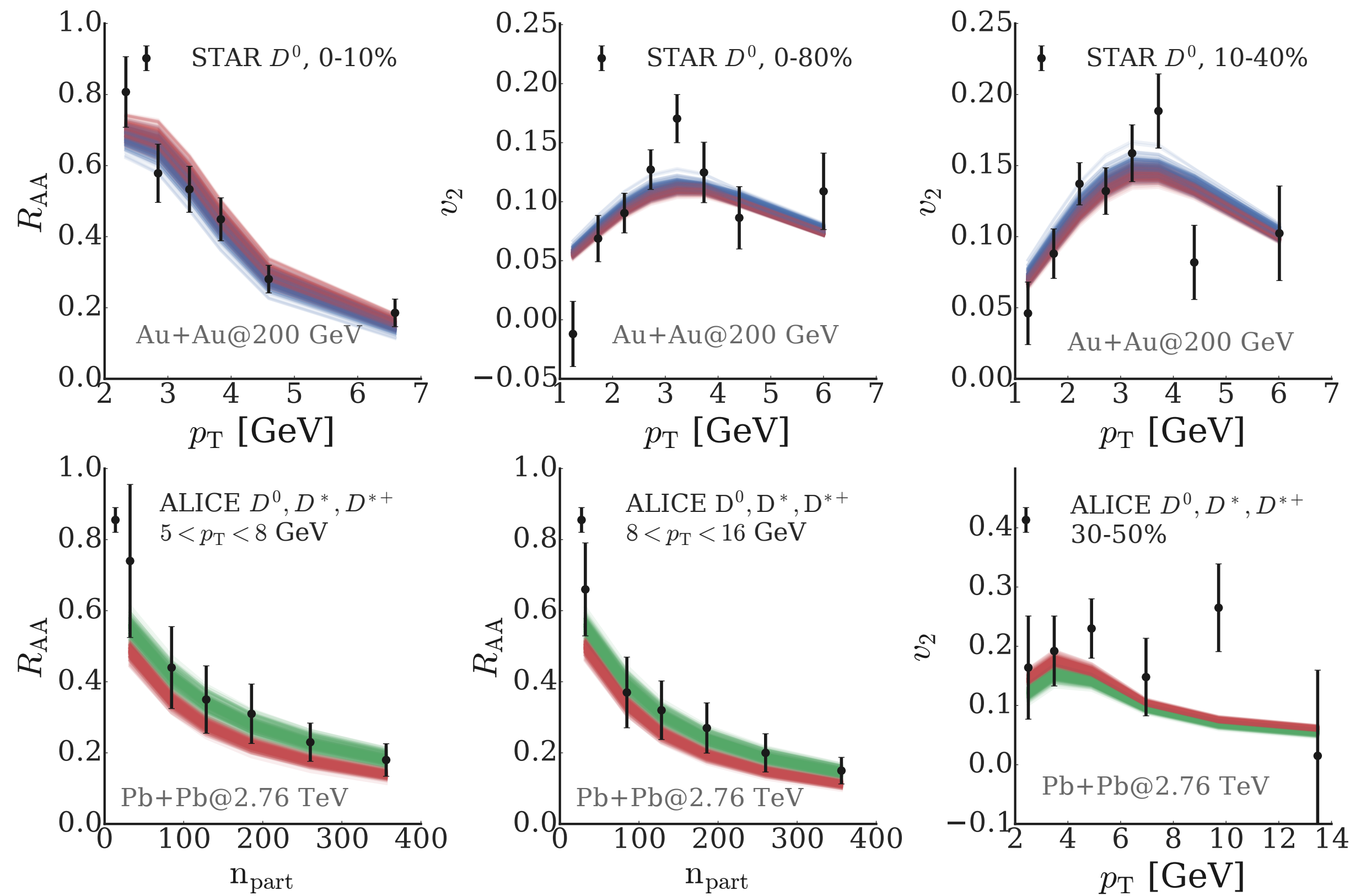
- create set of QCD Equations of State (aka the *prior*)
- run physics model with each EoS
- use comparison with RHIC/LHC data to determine which Equations of State are consistent with data (i.e. the *posterior*)
- ▶ **posterior is very similar to Lattice EoS!!**



Other Examples: Heavy Quarks

Extraction of the Heavy Quark Diffusion Coefficient

- calibration on heavy quark v_2 and R_{AA}



- combining RHIC and LHC data yields significant improvement for the extraction of $D_s(T)$