

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

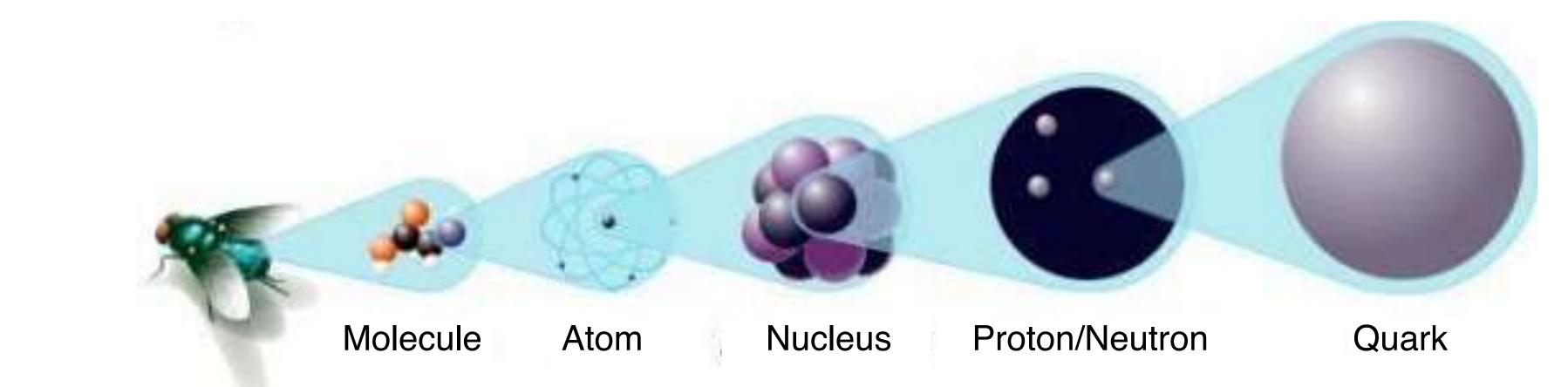
Steffen A. Bass

http://www.facebook.com/DukeQCD

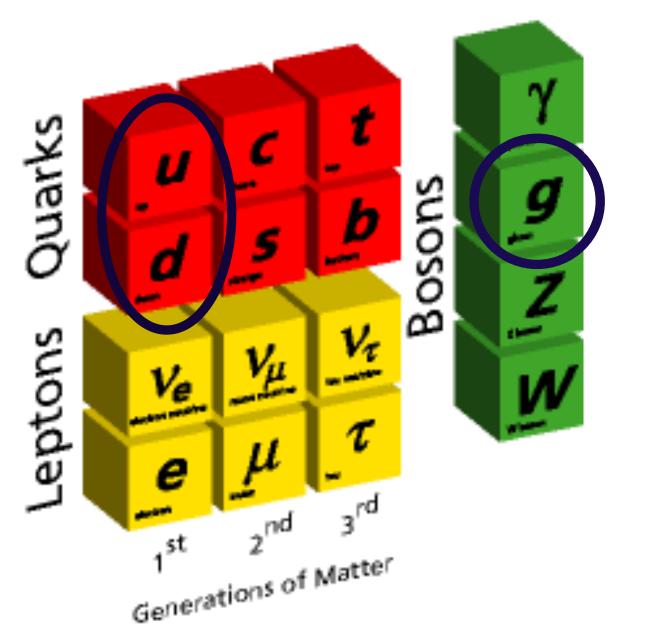
**@Steffen\_Bass** 



### **Quarks & Gluons: Elementary Building-Blocks of Matter**



### **Elementary Particles:**

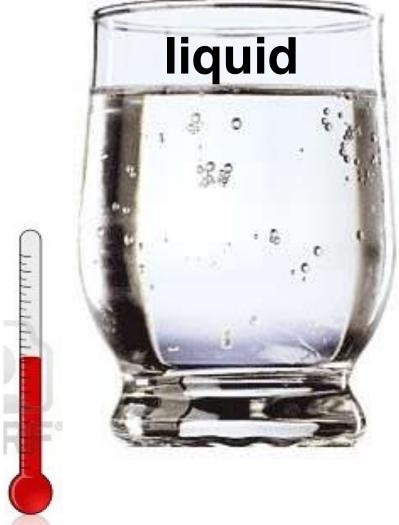


• 12 elementary building blocks of nature (plus anti-particles) • only need three for creation of ordinary matter (u, d, e) strong force mediates the interaction between quarks via exchange of gluons: Quantum-Chromo-Dynamics (QCD)



### **Phases of Matter**

### by adding/removing heat, phase of matter can be changed between solid, liquid and gaseous







### **Pressure plays an important role for the value of** the transition temperature between the phases



### **boiling temperature:**

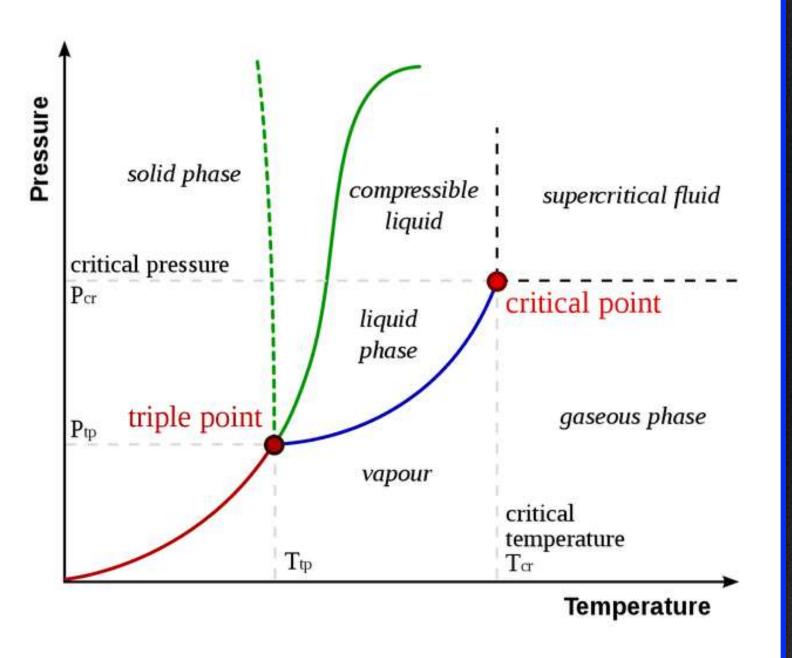
- sea level: 100 °C
- Mt. Everest: 71 °C



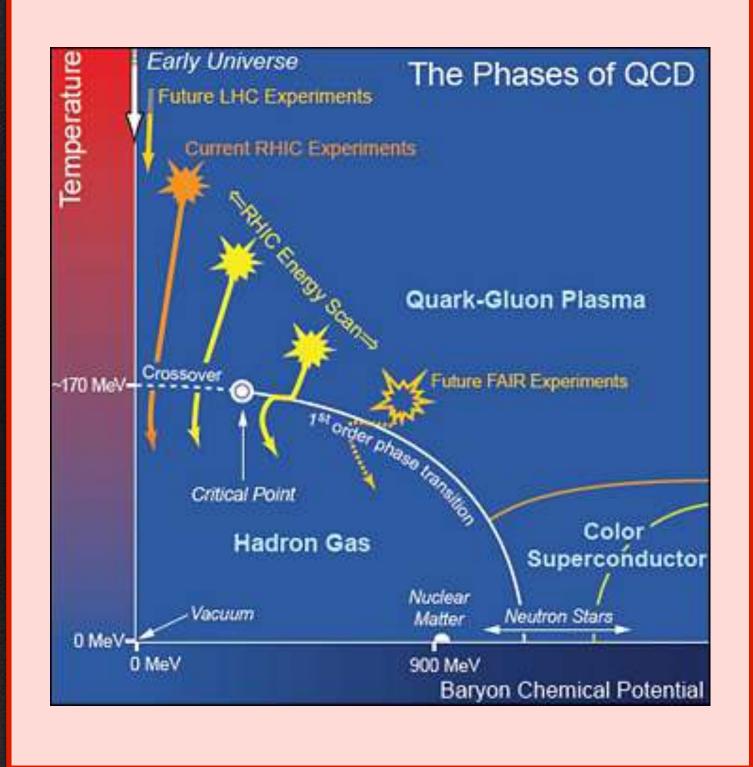
### Phase Diagram of QCD Matter

#### **Ordinary Matter:**

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



numerical simulations: Field Theory)

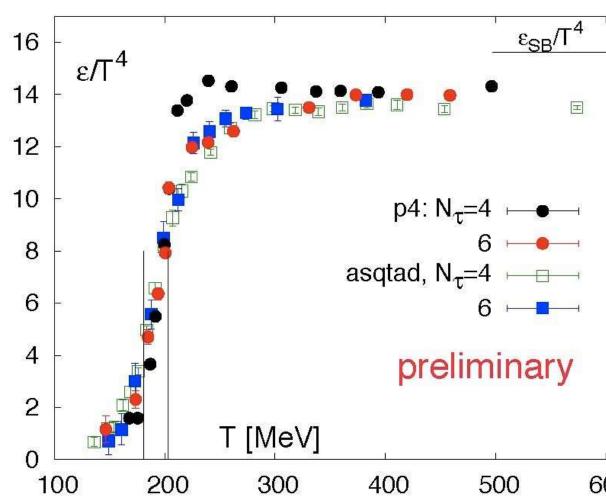


### **Phases of QCD matter:**

- •heat & compress QCD matter: collide heavy atomic nuclei
  - solve partition function (Lattice)

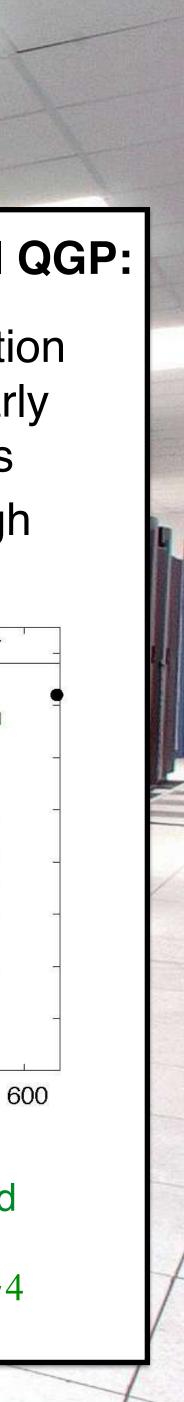
#### Equation of State for an ideal QGP:

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

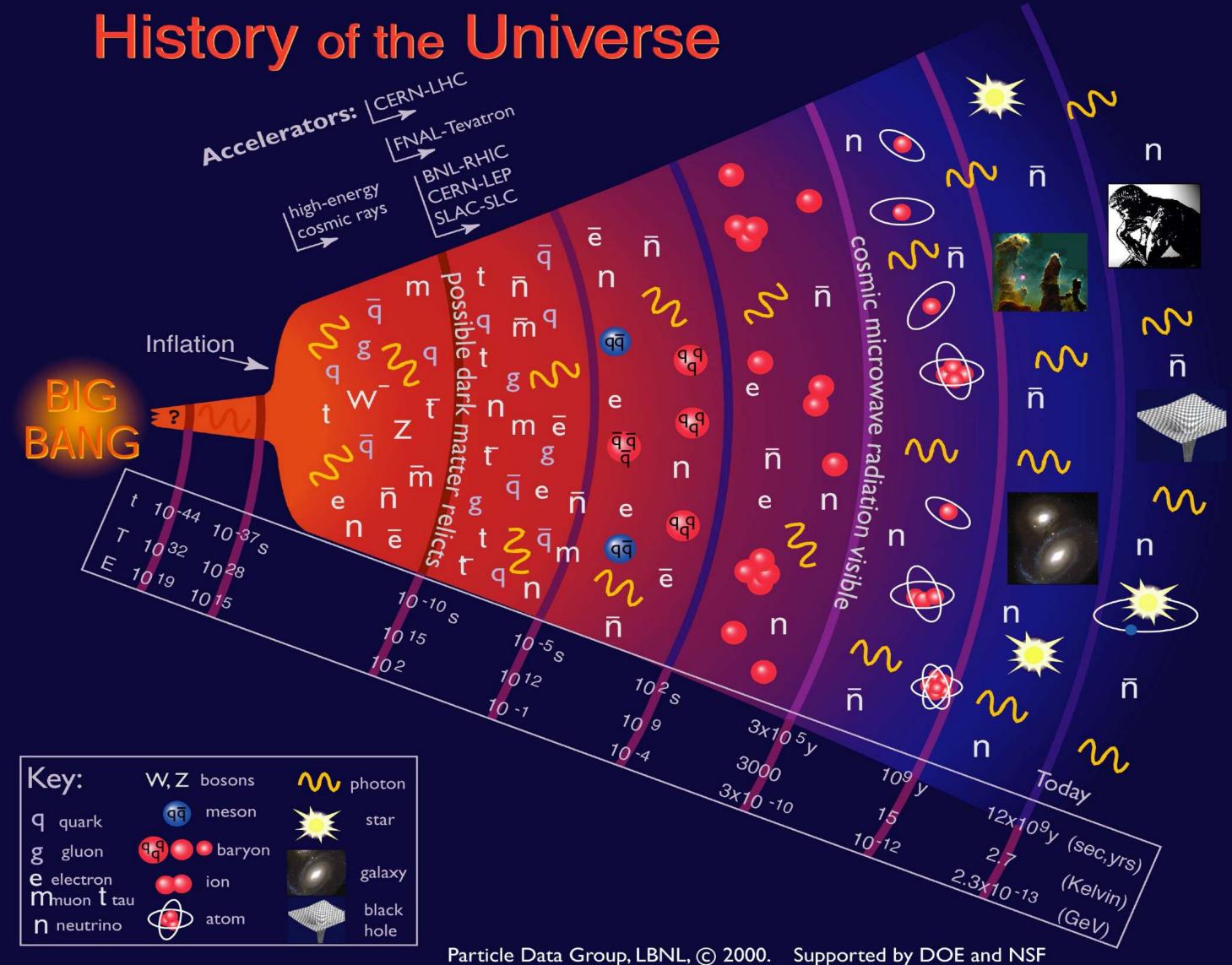


e.g. for a gas of ultra-relativistic massless bosons, steep rise would indicate a change in DOFs:

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



### The Early Universe: Quark-Gluon-Plasma



- •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 ultrarelativistic 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:

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

#### $\eta$ /s from Lattice QCD:



zero momentum limit in an infinite spatial volume, which is numerically not

The confines of the Euklidian Formulation: •extracting  $\eta$ /s formally requires taking the possible...

heavy-ion effort!

#### •preliminary estimates:

Т	1.58 T <sub>C</sub>	2.32 T <sub>C</sub>
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]

#### The determination of the QCD transport coefficients is one of the key goals of the global relativistic



### 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,<sup>1,2</sup> Joseph I. Kapusta,<sup>3</sup> and Larry D. McLerran<sup>4</sup>

<sup>1</sup>Section for Theoretical Physics, Department of Physics, University of Bergen, Allegaten 55, 5007 Bergen, Norway

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

<sup>3</sup>School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA

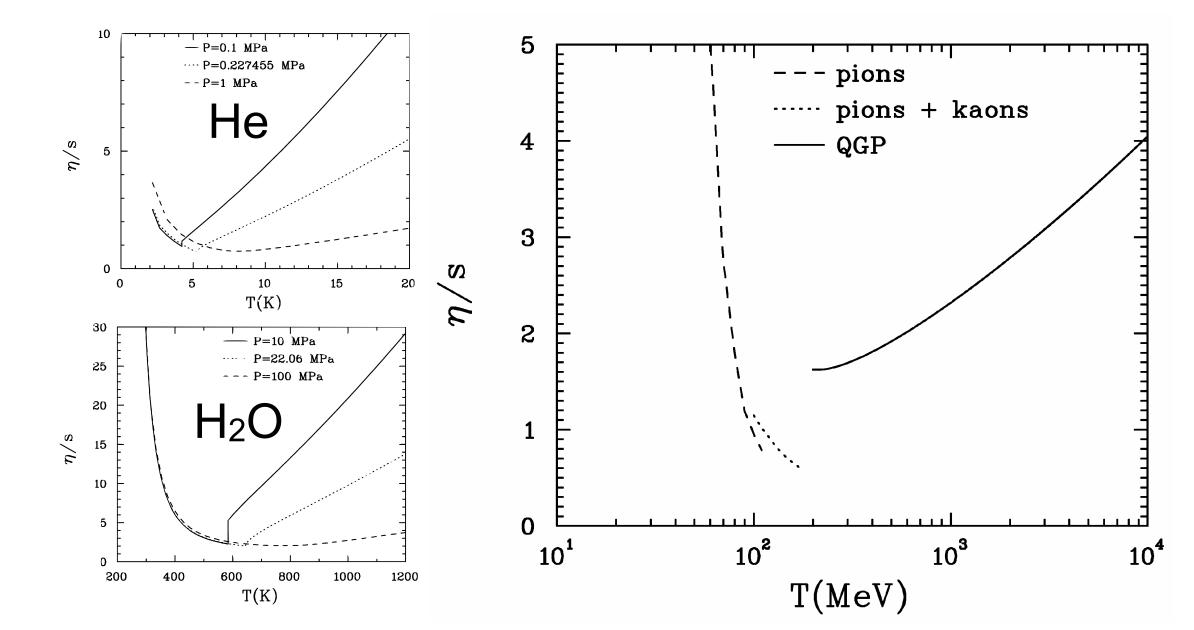
<sup>4</sup>Nuclear Theory Group and Riken Brookhaven Center, Brookhaven National Laboratory, Bldg. 510A, Upton, New York 11973, USA

(Received 12 April 2006; published 12 October 2006)

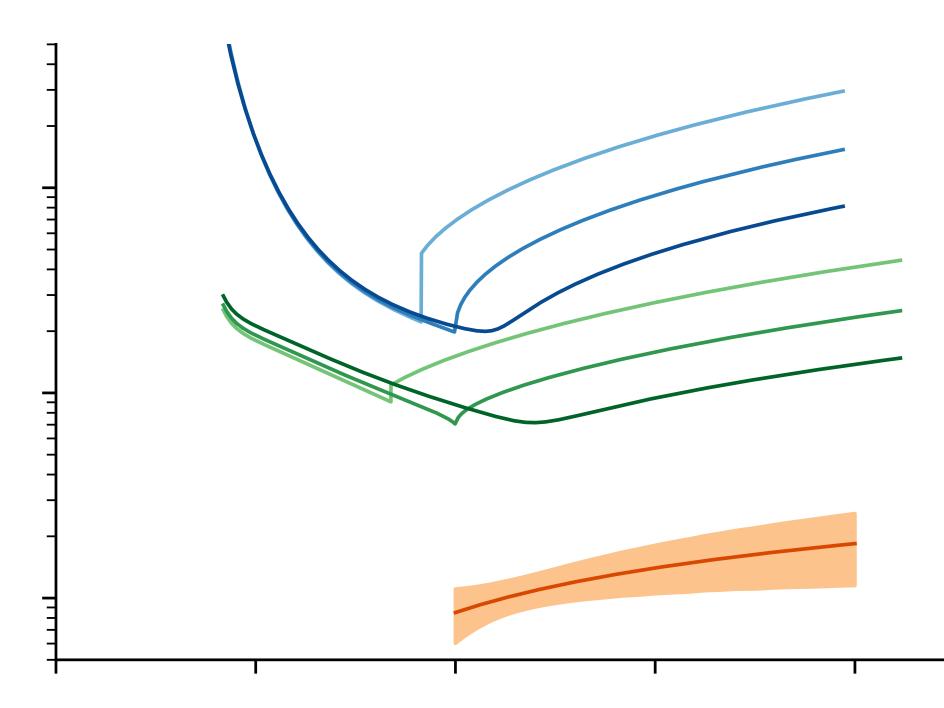
Substantial collective flow is observed in collisions between large nuclei at BNL RHIC (Relativistic Heavy Ion Collider) as evidenced by single-particle transverse momentum distributions and by azimuthal correlations among the produced particles. The data are well reproduced by perfect fluid dynamics. A calculation of the dimensionless ratio of shear viscosity  $\eta$  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  $\eta/s$ . We suggest that experimental measurements can pinpoint the location of this transition or rapid crossover in QCD.

DOI: 10.1103/PhysRevLett.97.152303

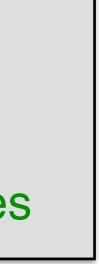
PACS numbers: 12.38.Mh, 24.10.Nz, 25.75.Nq, 51.20.+d



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



### **Telescopes for the Early Universe: Heavy-Ion Collider Facilities**

## Heating & Compressing QCD Matter

CERN Ridensin

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

SUISSE



### **Probes of the Early Universe**

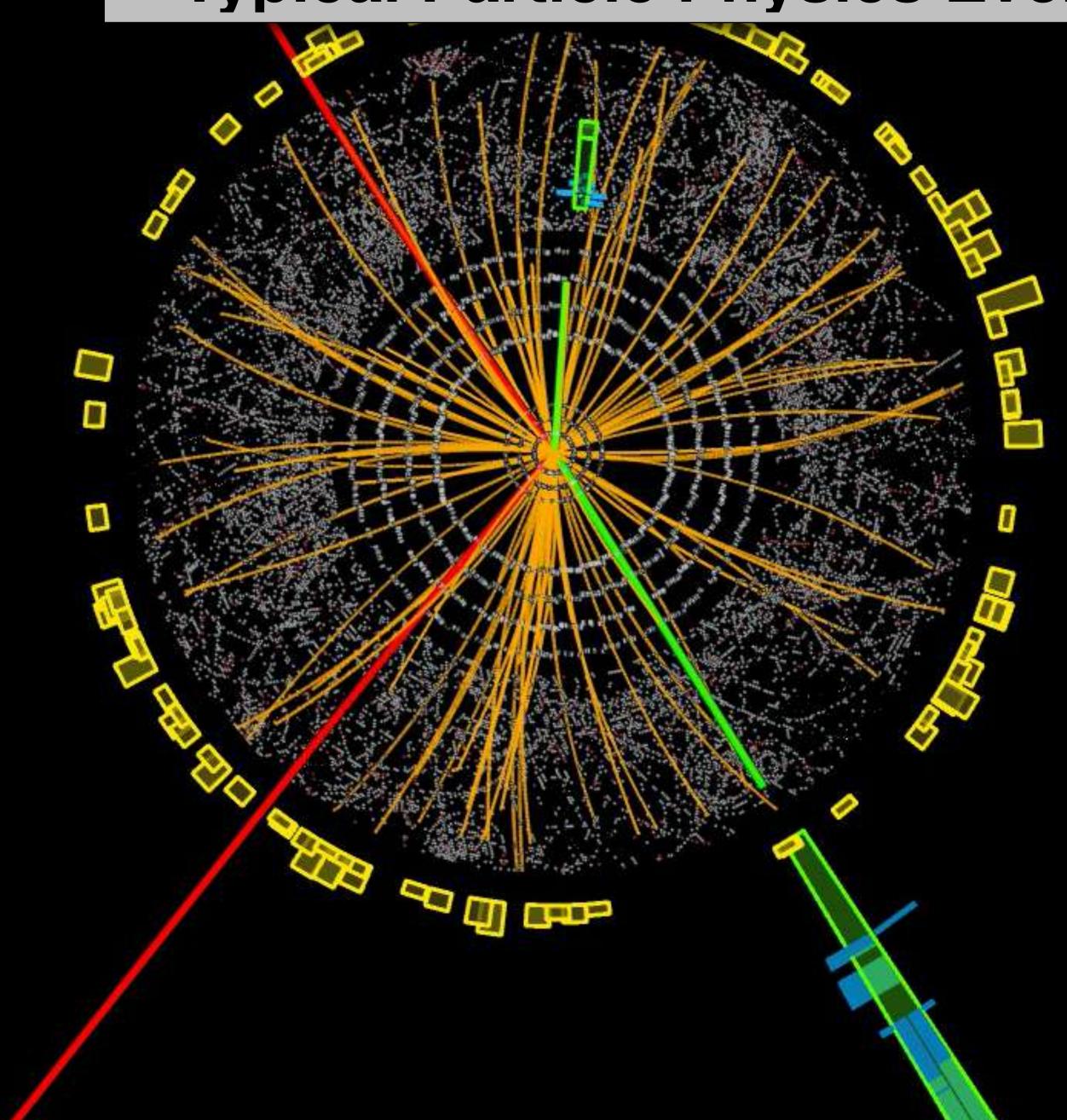
#### **ALICE experiment at CERN:**

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

two other experiments: CMS, ATLAS



### **Typical Particle Physics Event**





### **Typical Heavy-Ion Event**

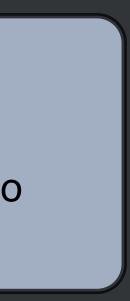


#### **Pb+Pb Collision at the LHC:**

- 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 : 0x000000042B1B693







# **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

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

## 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

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

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.

### (viscous) relativistic fluid dynamics:

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

$$\partial_{\mu}T^{\mu\nu} = 0$$
  

$$T_{ik} = \varepsilon u_{i}u_{k} + P(\delta_{ik} + u_{i}u_{k})$$
  

$$- \eta \left(\nabla_{i}u_{k} + \nabla_{k}u_{i} - \frac{2}{3}\delta_{ik}\nabla \cdot u\right)$$
  

$$+ \varsigma \delta_{ik}\nabla \cdot u$$

(plus an additional 9 eqns. for dissipative flows)

nediur the

#### hybrid transport models:

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



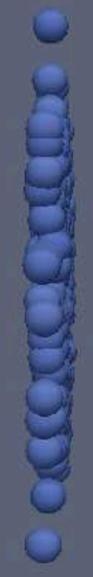




### **Computational Modeling**

## Time: 0.10

rapidity 5.9 52.5 0 -2.5 -5 -7



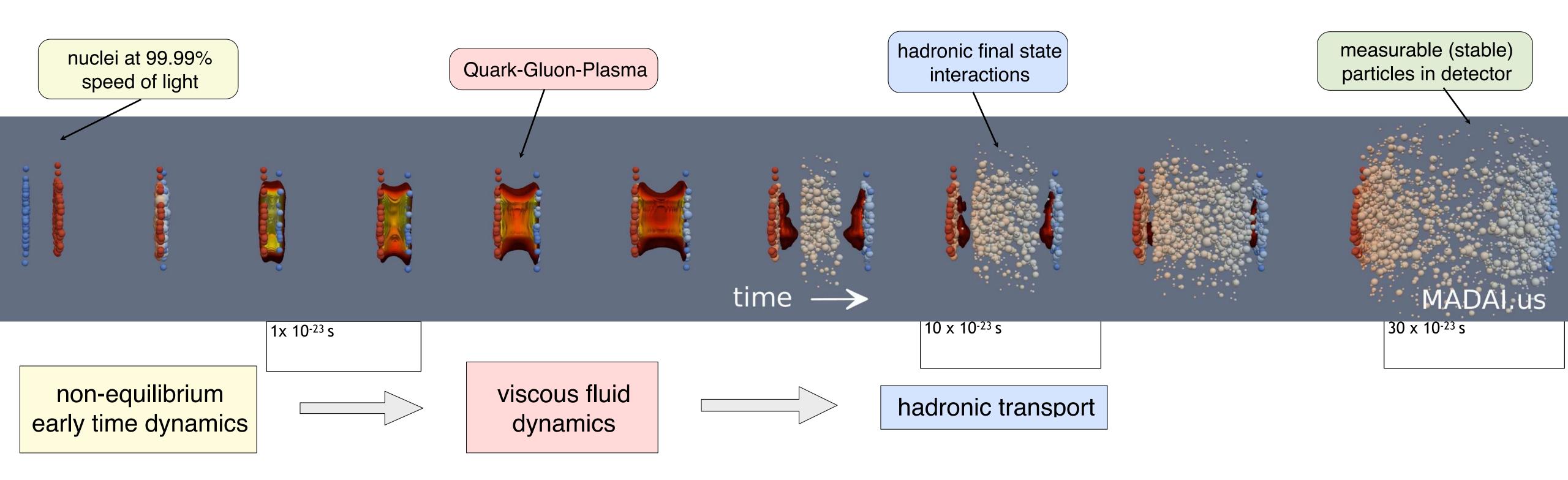


3+1D Hydro + Boltzmann Hybrid





### Probing the QGP in Relativistic Heavy-lon Collisions



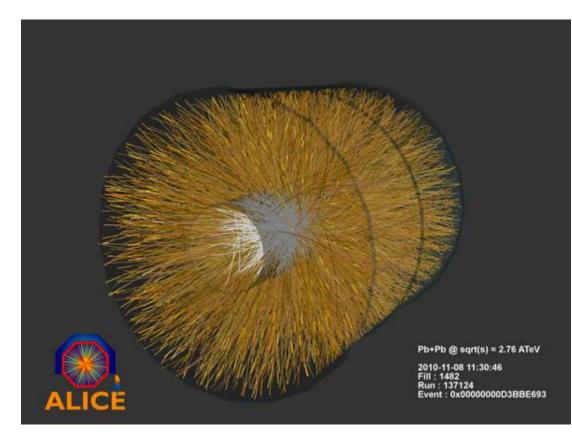
### **Principal Challenges of Probing the QGP with Heavy-Ion Collisions:**

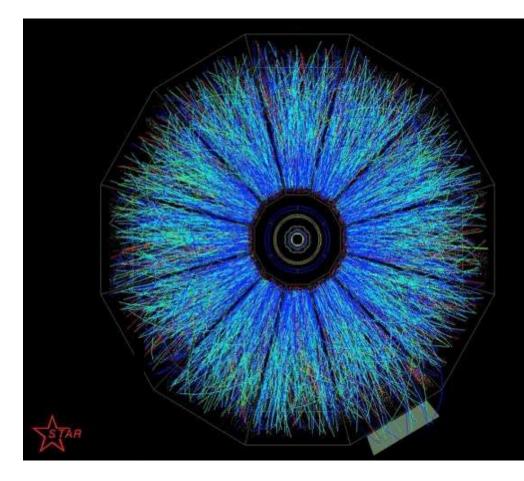
- time-scale of the collision process: 10<sup>-24</sup> seconds! [too short to resolve]
- characteristic length scale: 10<sup>-15</sup> meters! [too small to resolve]
- confinement: quarks & gluons form bound states, experiments don't observe them directly
- computational models are need to connect the experiments to QGP properties!

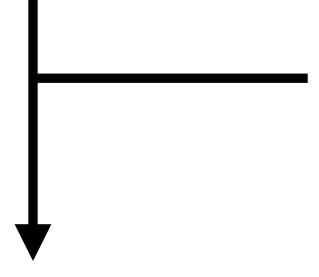
### **Knowledge Extraction from Relativistic Heavy-Ion Collisions**

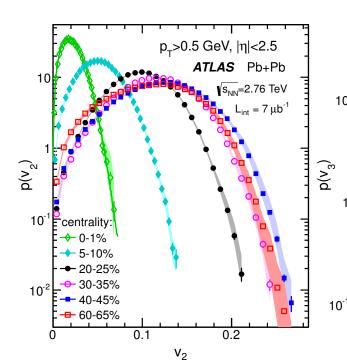
## **Probing QCD in Heavy-Ion Collisions**

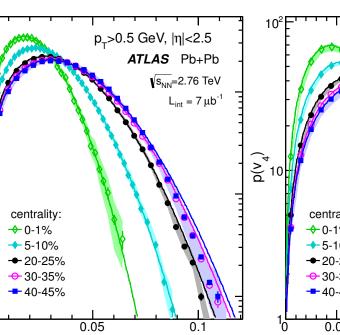
### Data:



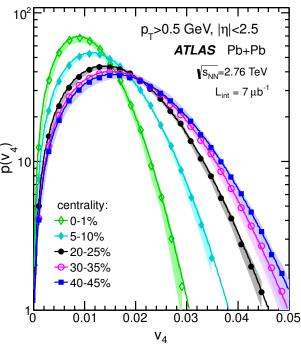


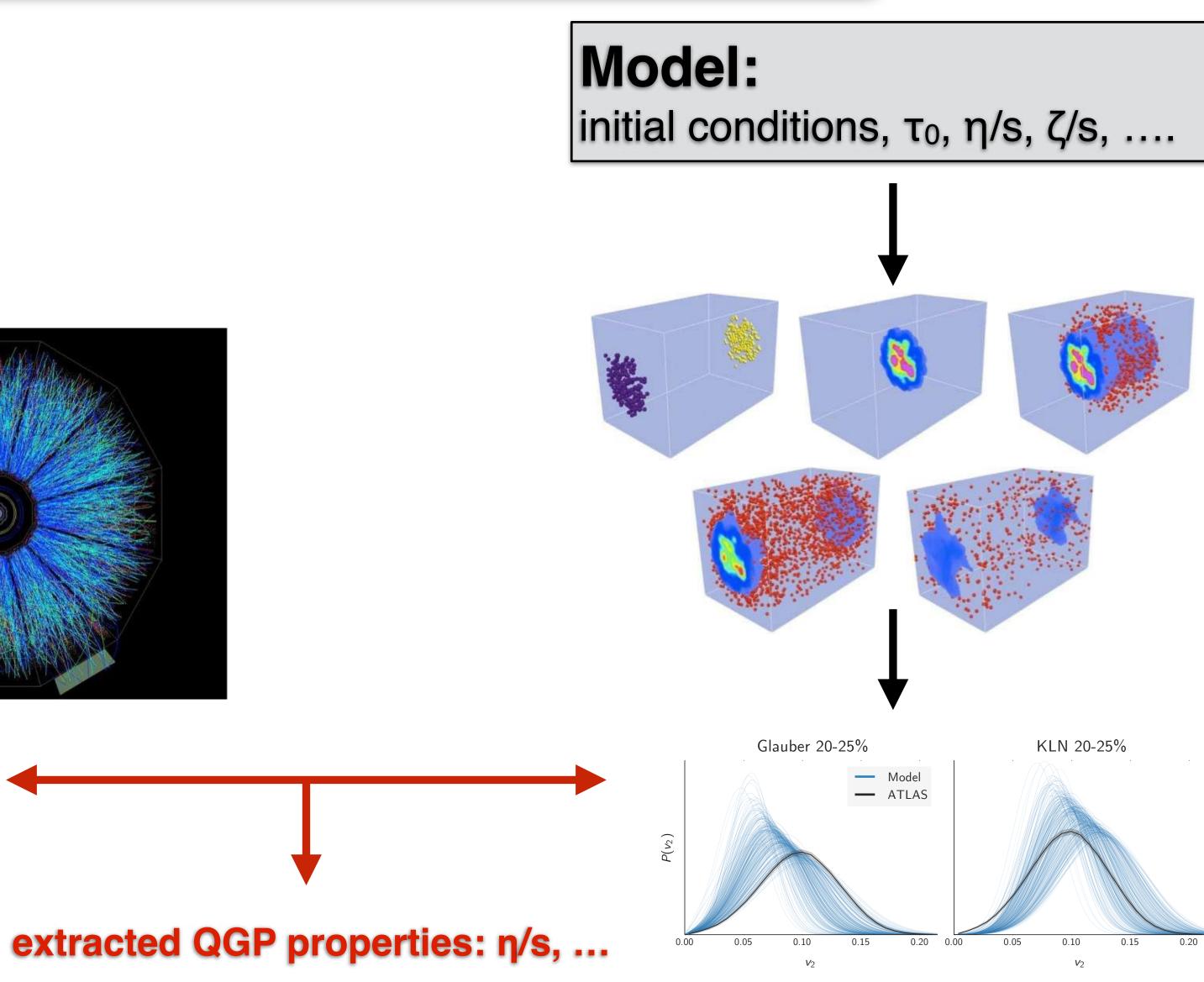






 $V_3$ 







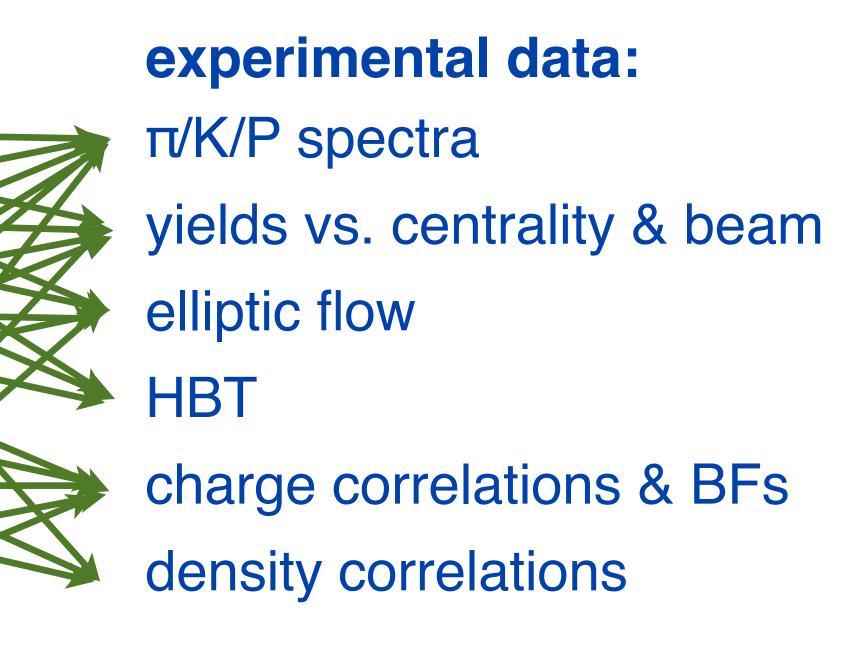
## **Determining the QGP Properties via a Model to Data Comparison**

### **Model Parameter:**

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

particlization/freeze-out

- 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.

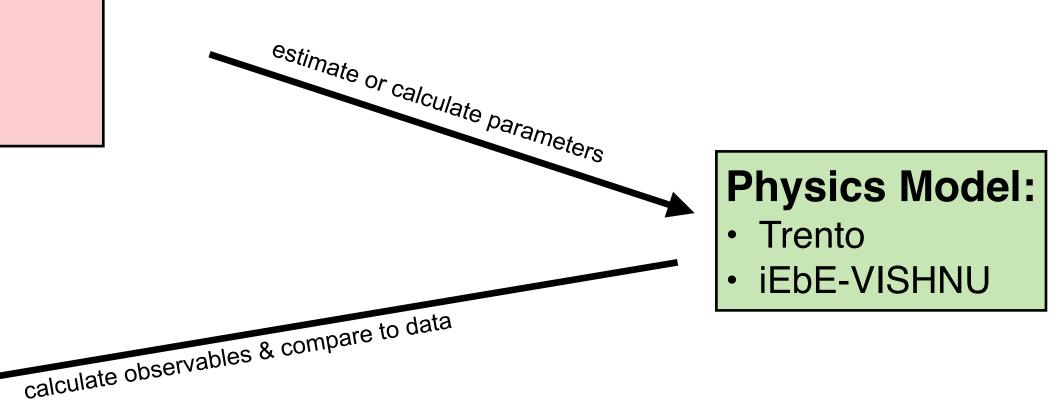
#### **Model Parameters - System Properties**

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

#### **Experimental Data**



ALICE flow & spectra





## **Bayesian Analysis**

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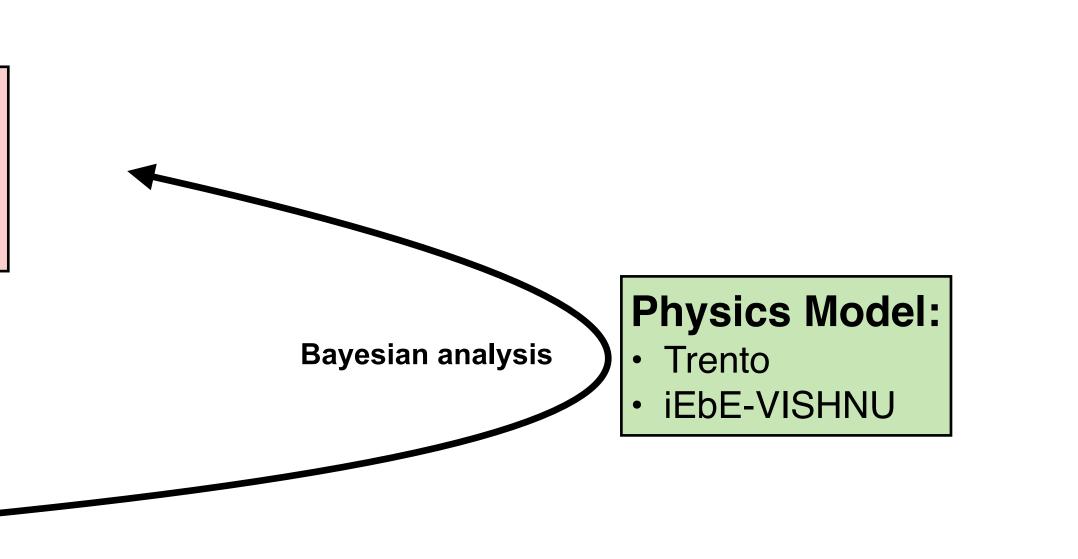
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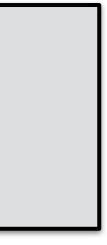
ALICE flow & spectra

- determine parameter values such that the model best describes experimental observables
- extract the probability distributions of all parameters



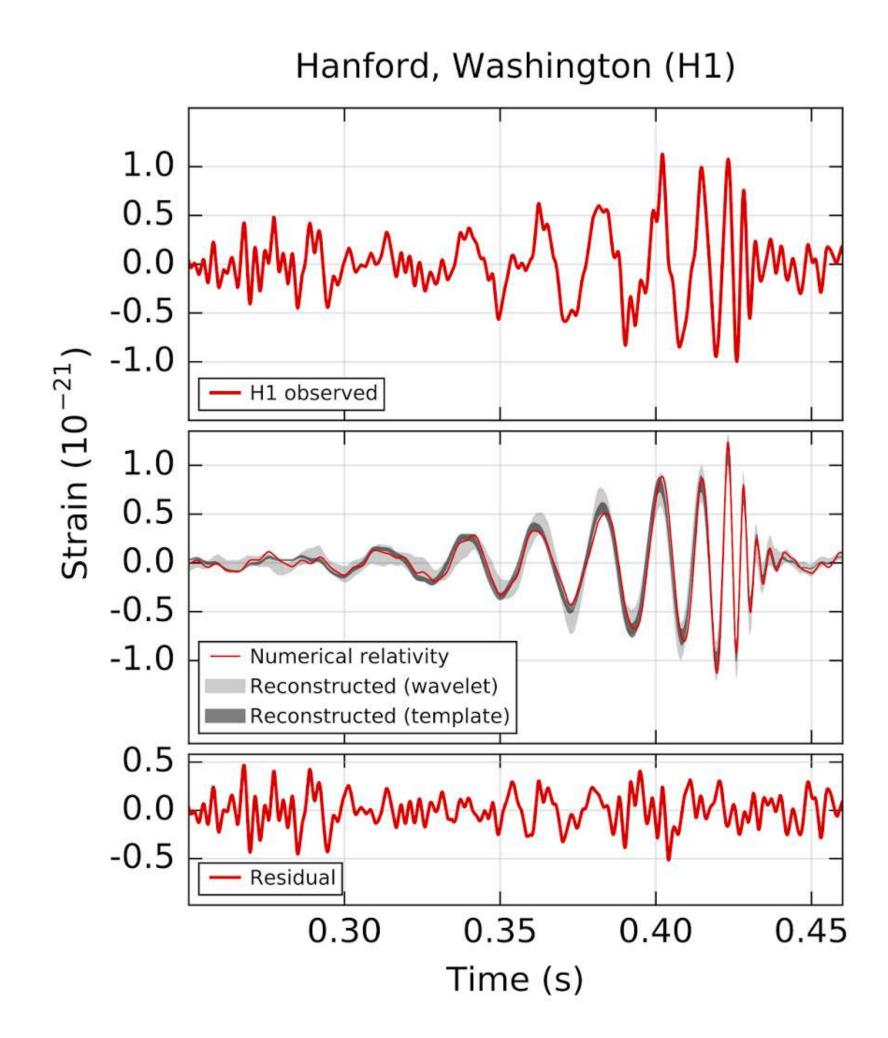
• Bayesian analysis allows us to simultaneously calibrate all model parameters via a model-to-data comparison



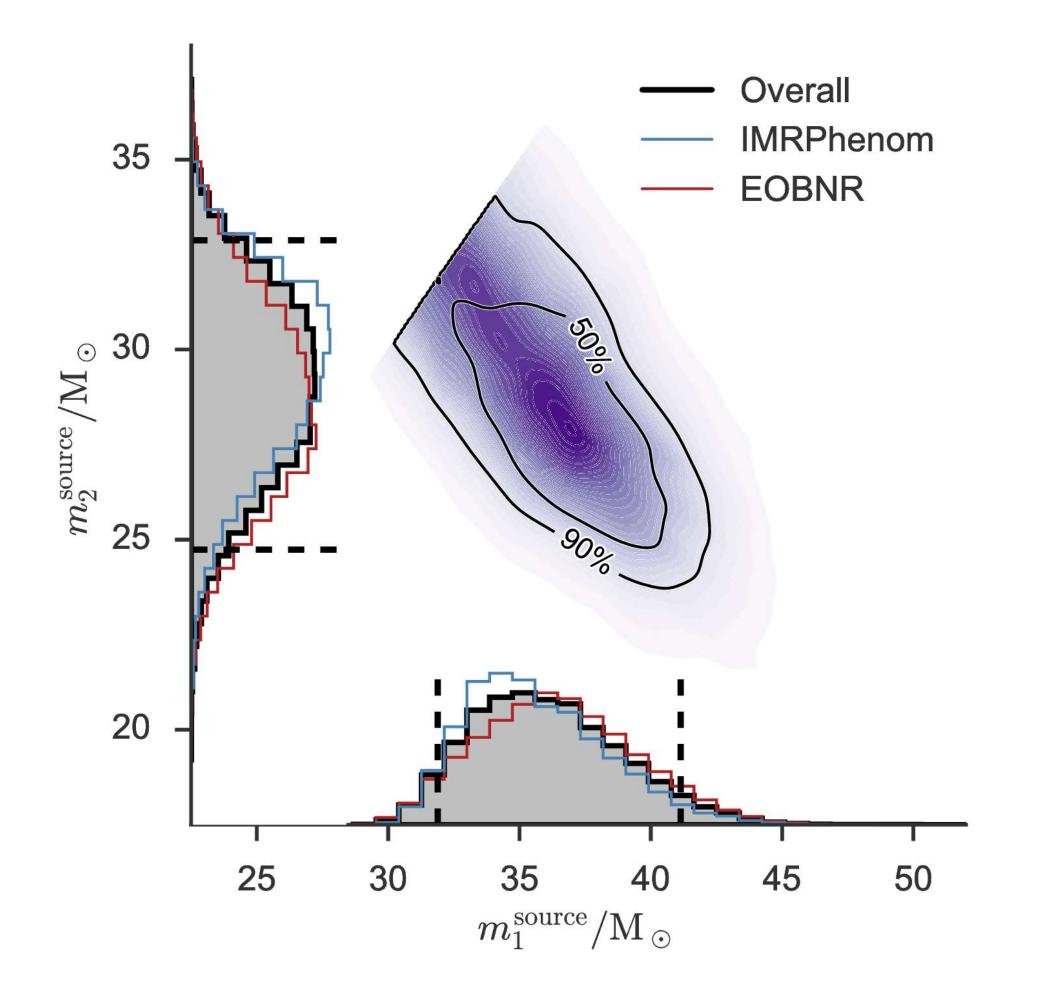


### **Example: Gravitational Waves**

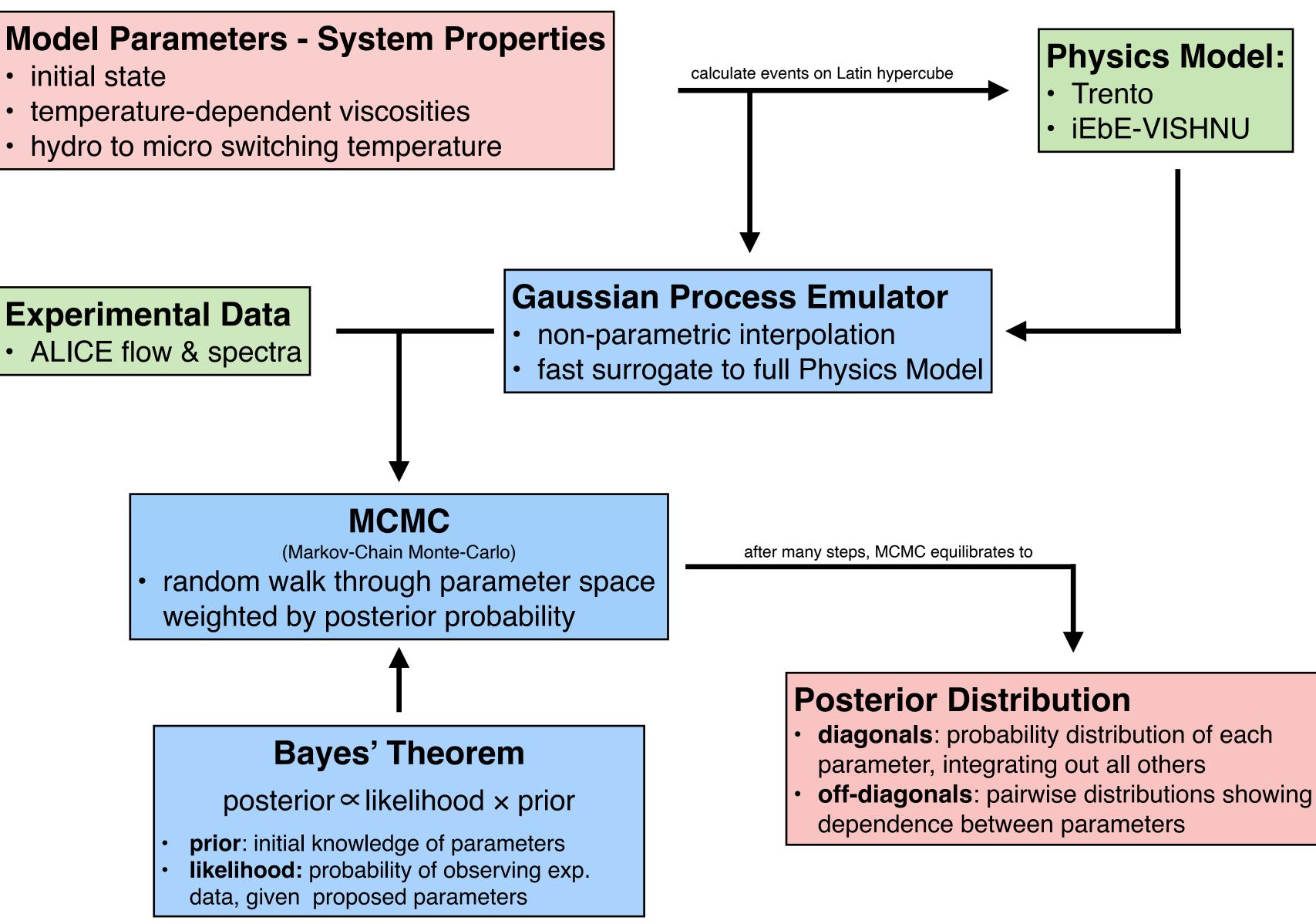
### LIGO gravitational wave signal:



Bayesian analysis of GR model of merging black holes of masses m<sub>1</sub> and m<sub>2</sub> that is capable of reproducing LIGO data:

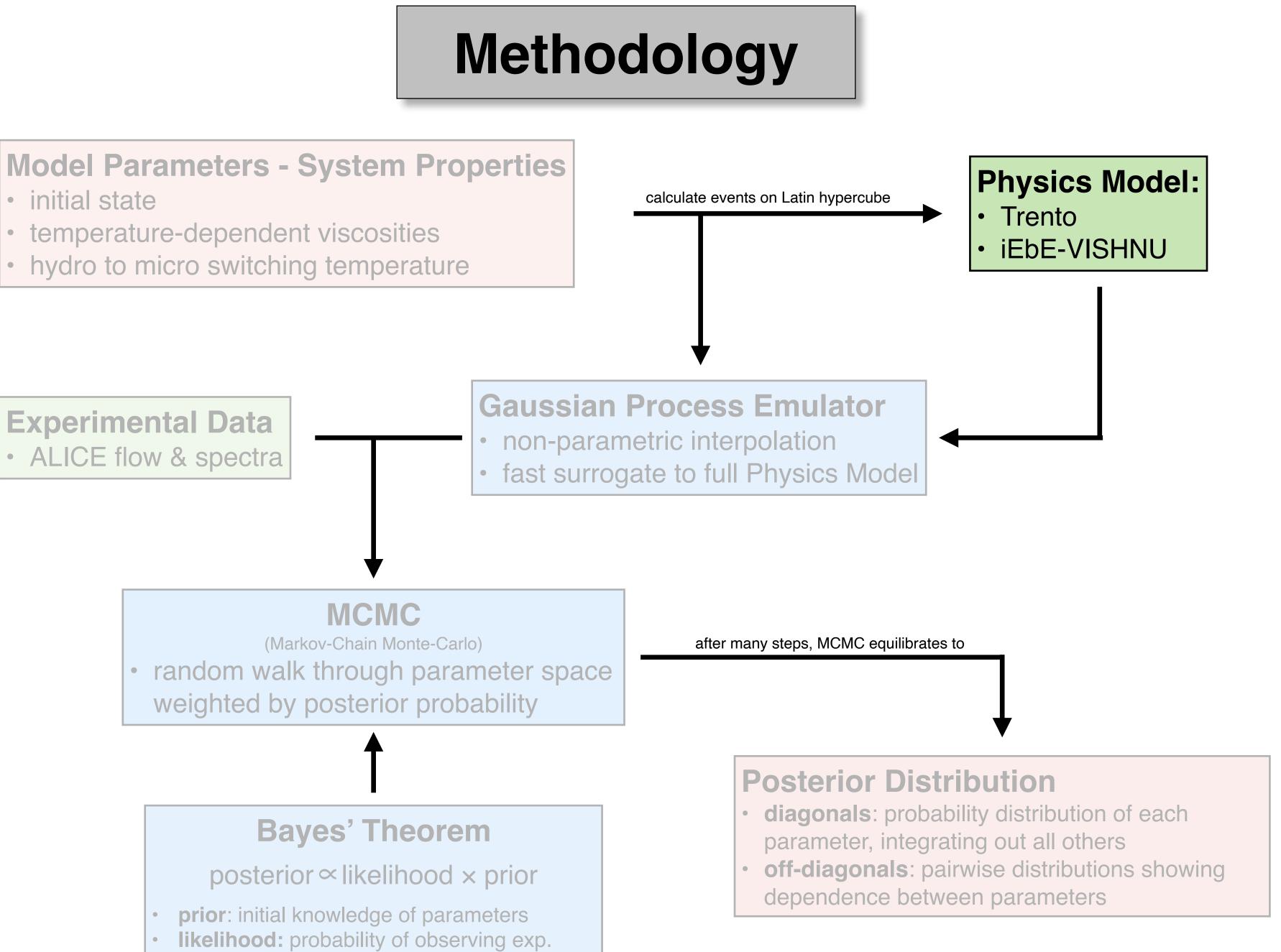


## Setup of a Bayesian Statistical Analysis



### **Components of the Bayesian Analysis**

- hydro to micro switching temperature



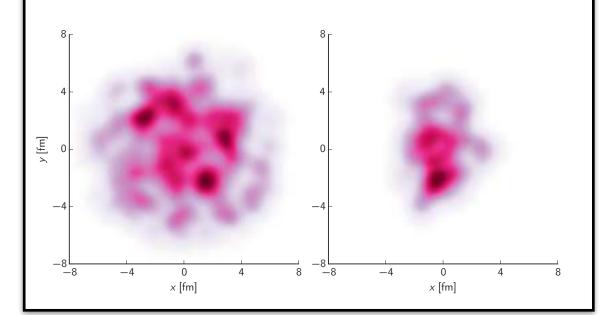


- data, given proposed parameters

### Physics Model: Trento + iEbE-VISHNU

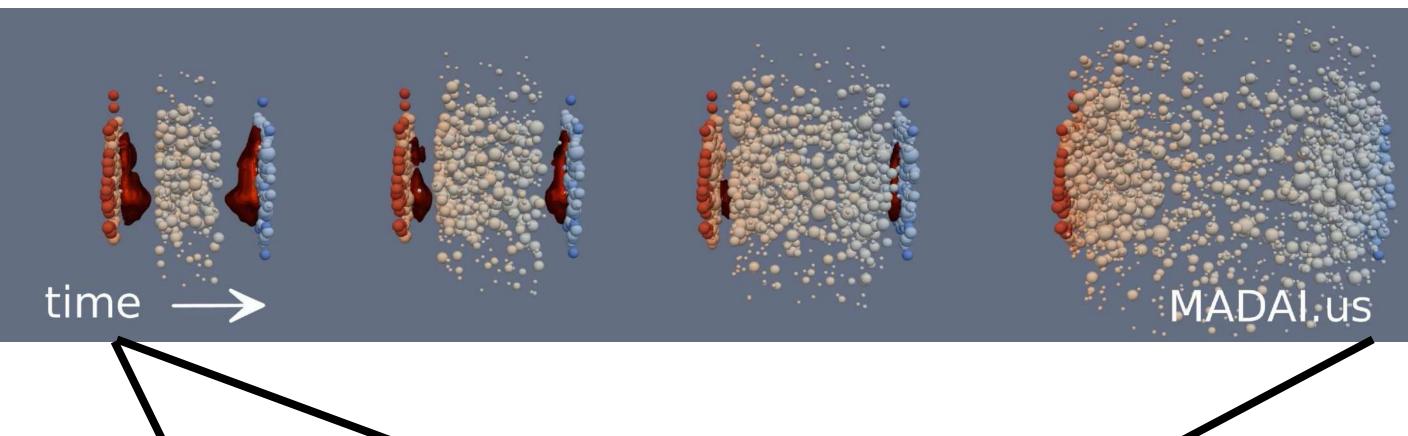
### **Trento:**

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



### iEbE-VISHNU:

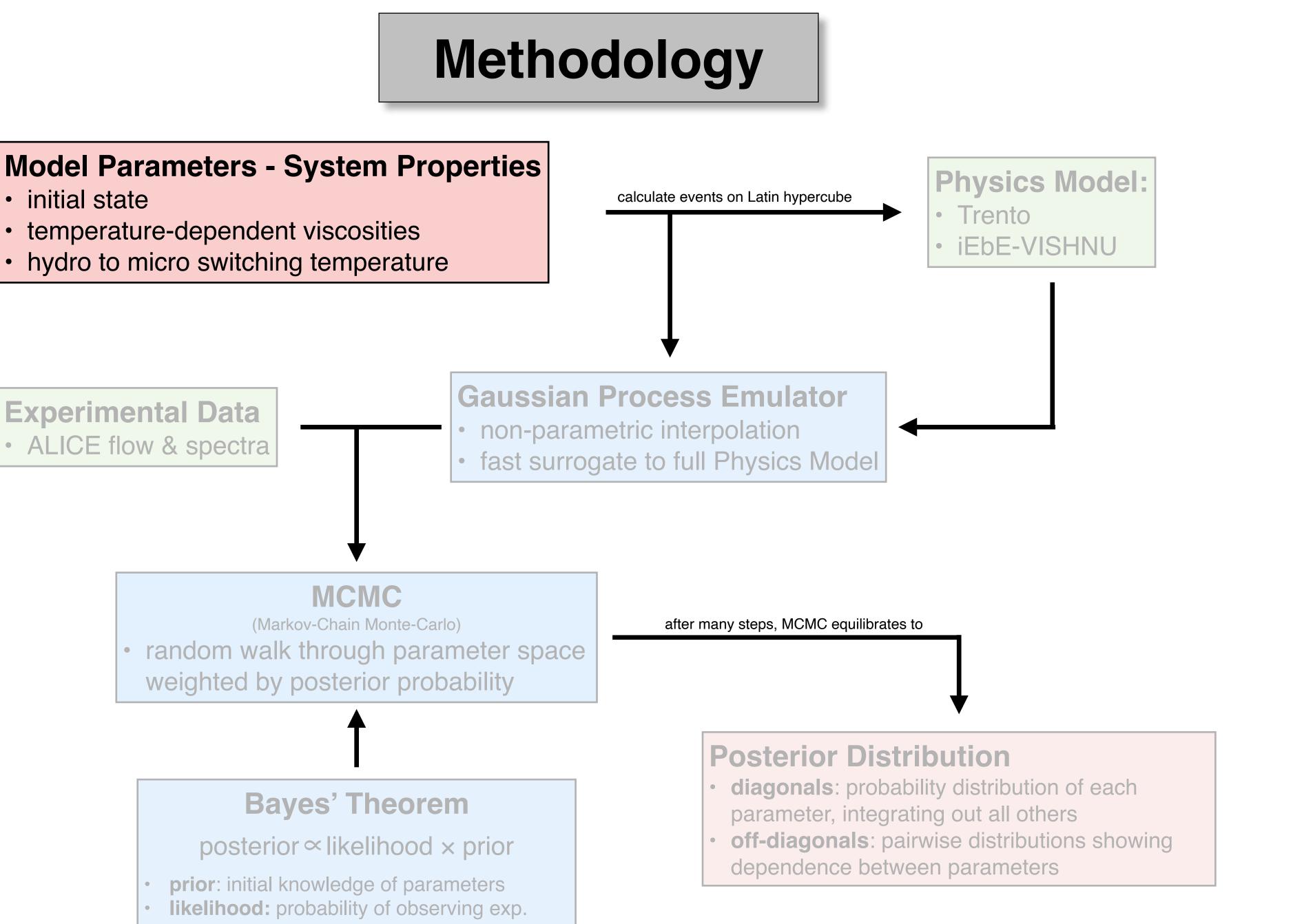
- EbE 2+1D viscous RFD
- describes QGP dynamics & hadronization
- EoS from Lattice QCD
- temperature-dependent shear and bulk viscosity as input



**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

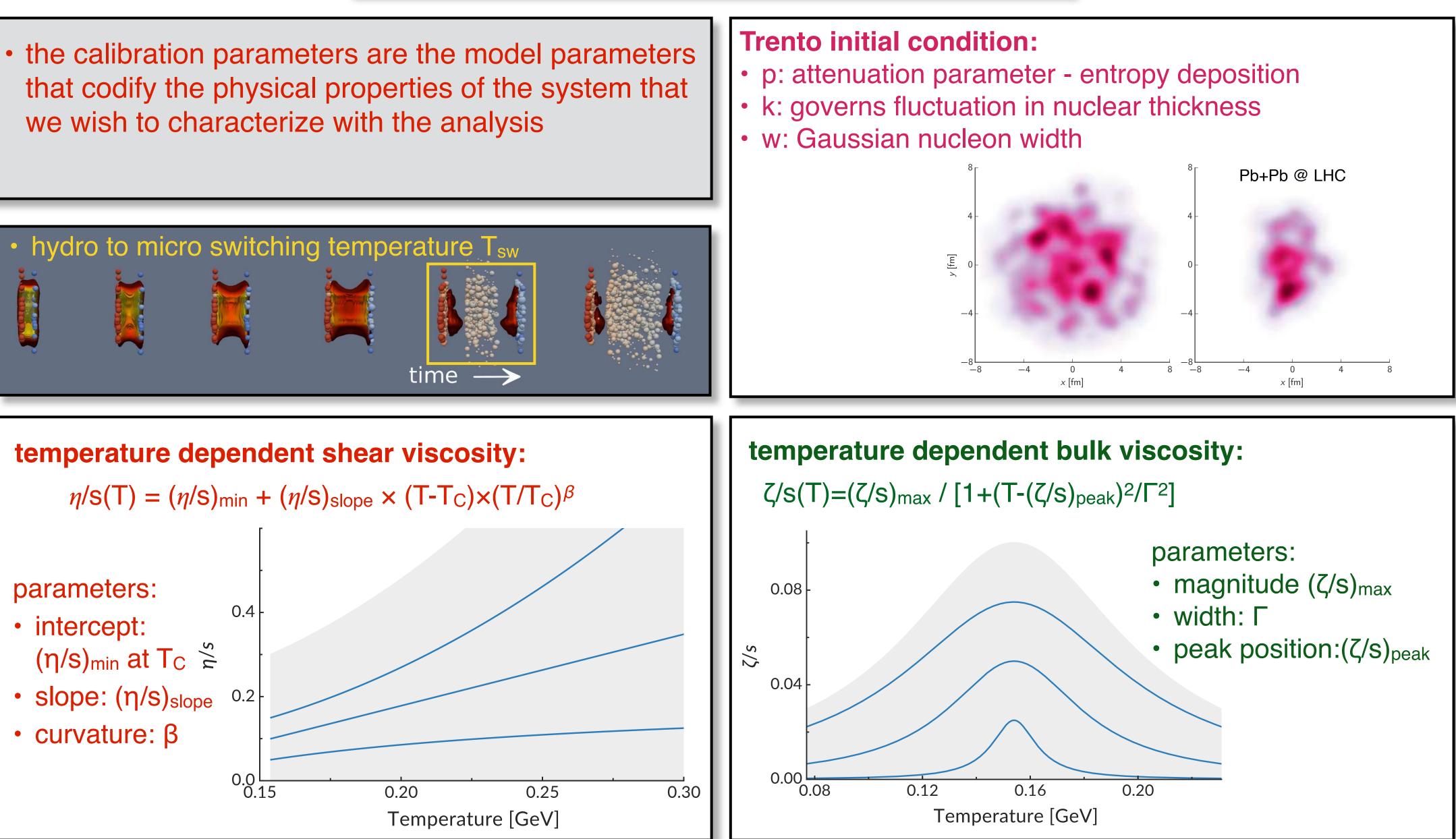
- initial state
- temperature-dependent viscosities
- hydro to micro switching temperature



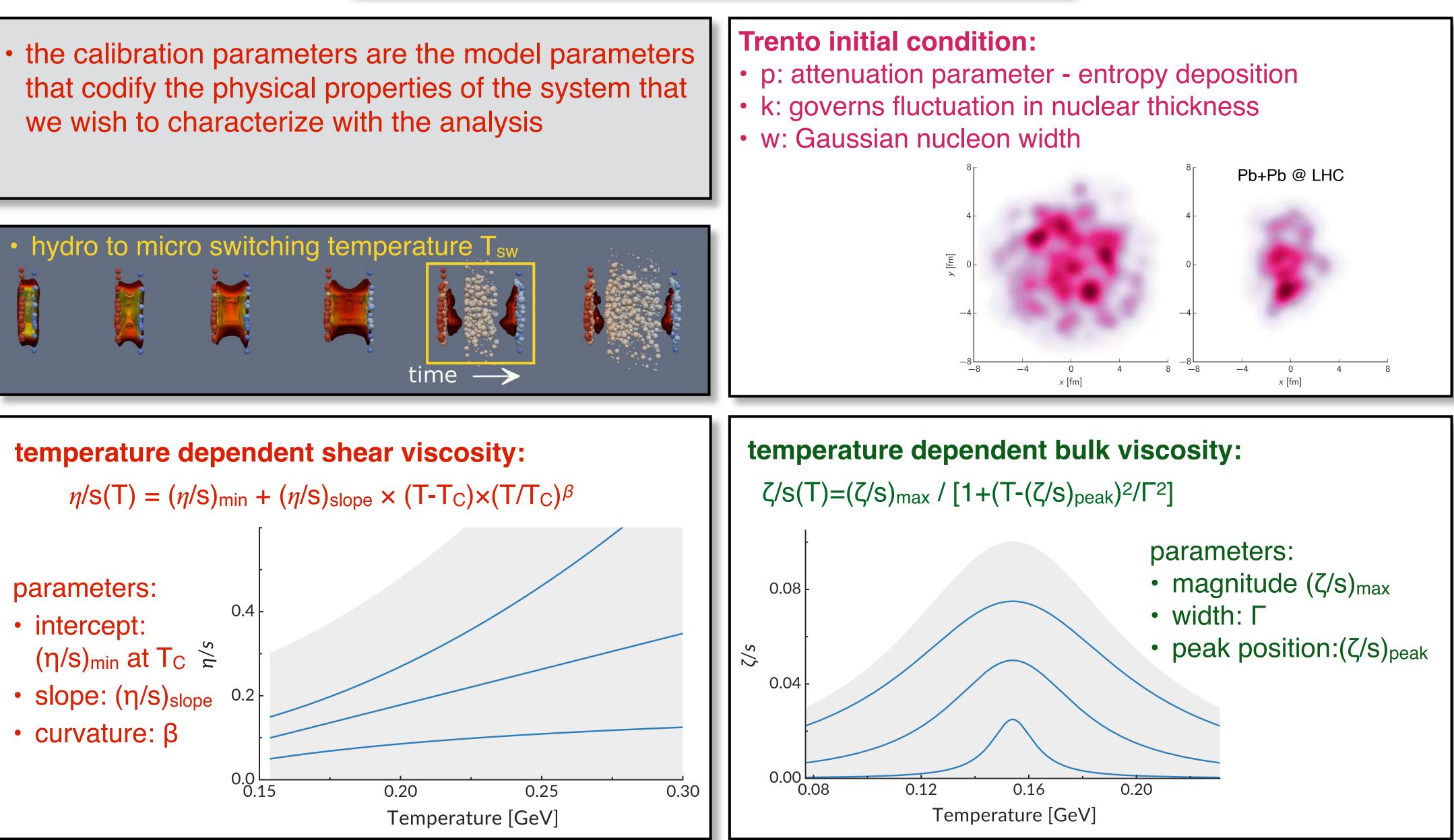
- data, given proposed parameters

### **Calibration Parameters**

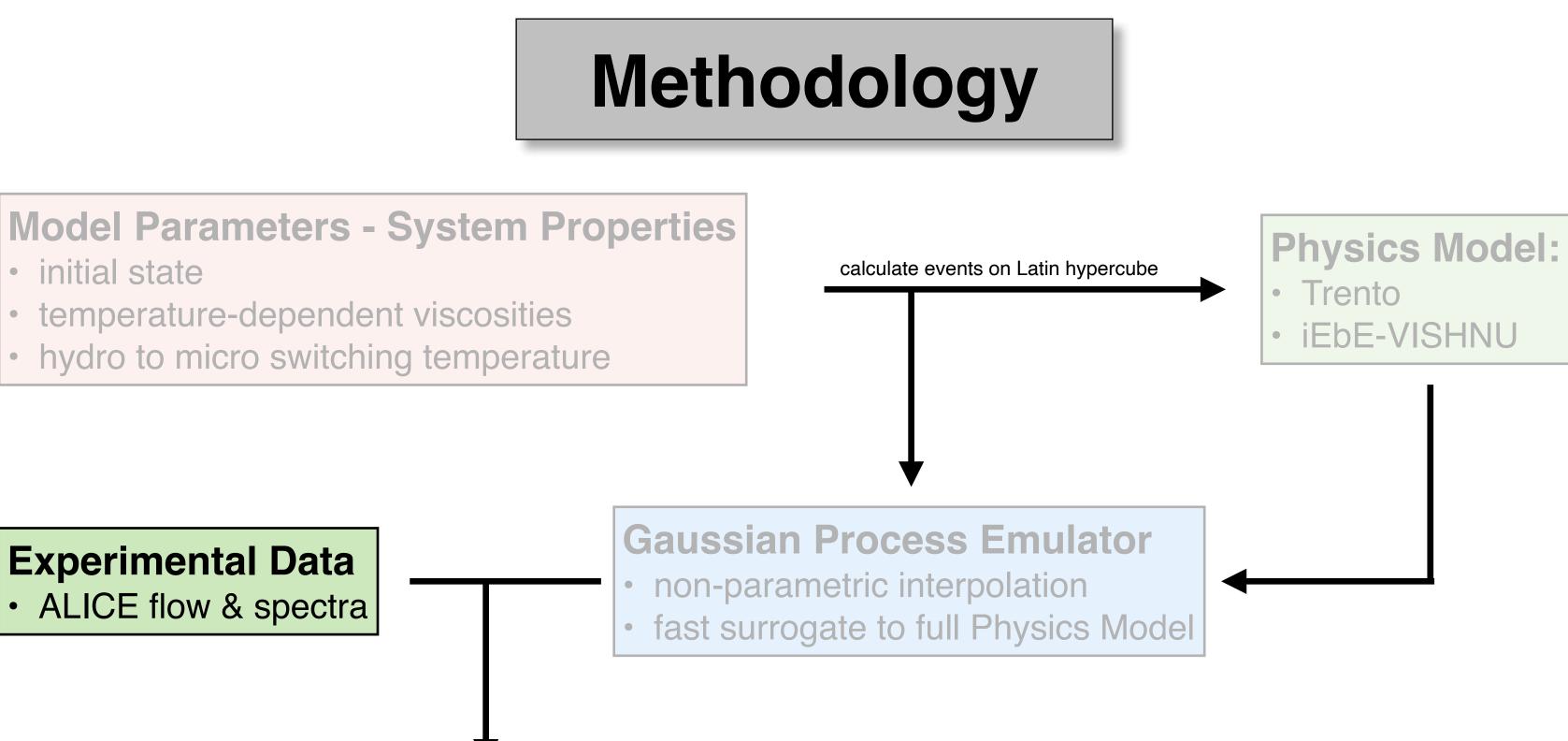
we wish to characterize with the analysis











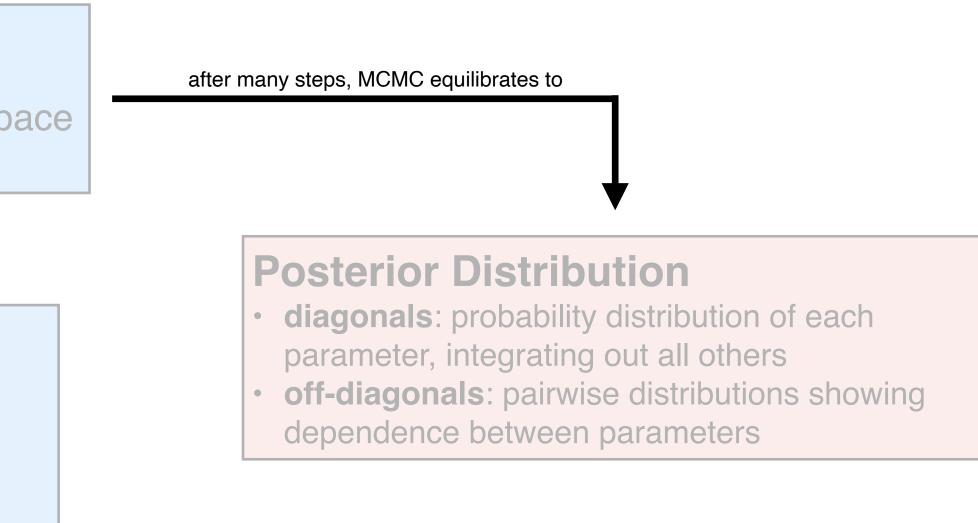
#### MCMC

(Markov-Chain Monte-Carlo) random walk through parameter space weighted by posterior probability

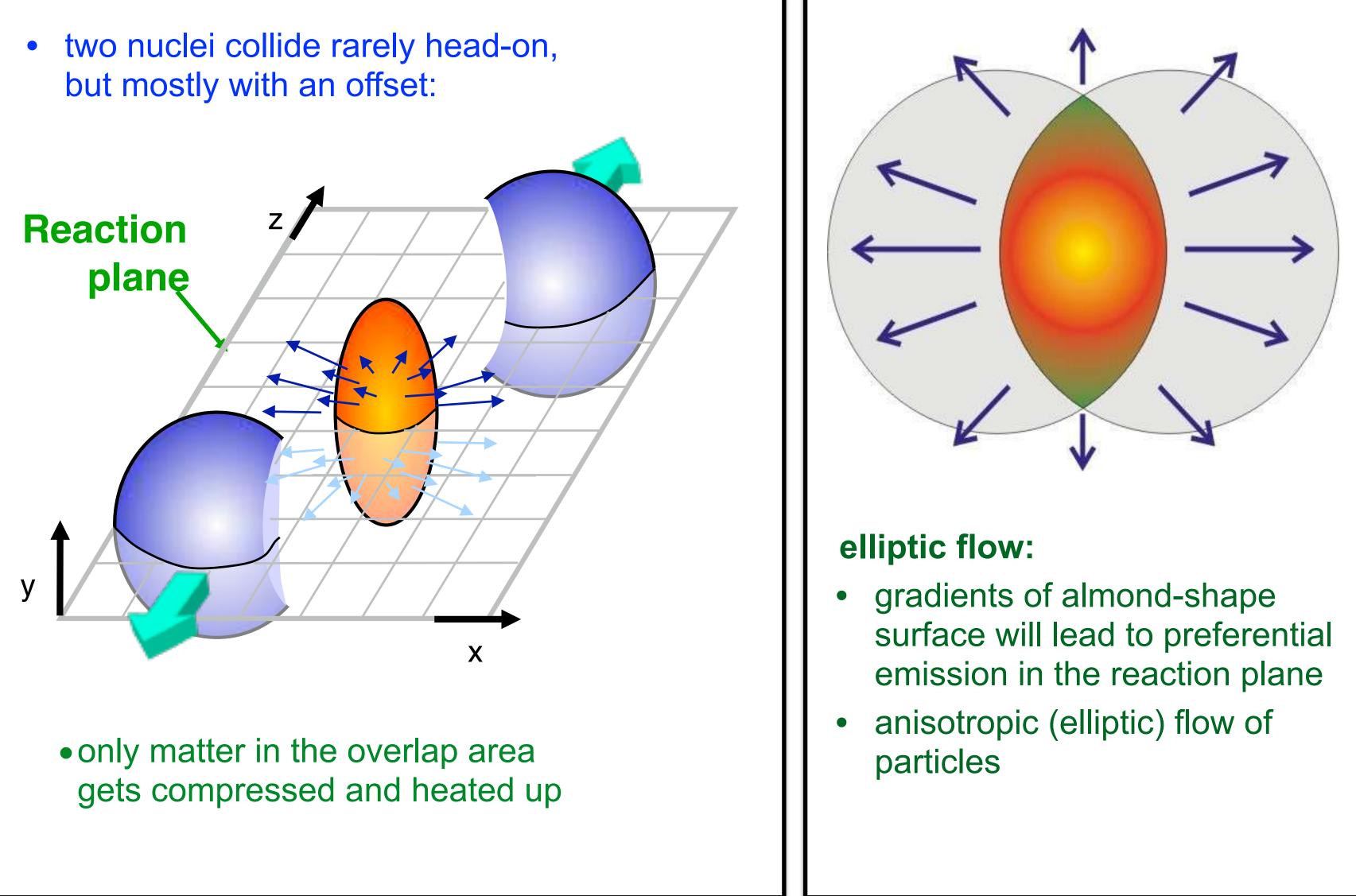
#### **Bayes' Theorem**

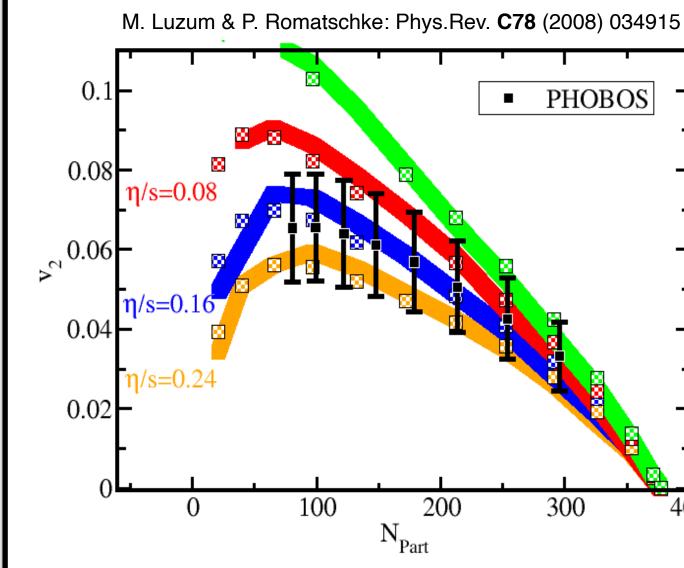
posterior  $\propto$  likelihood  $\times$  prior

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



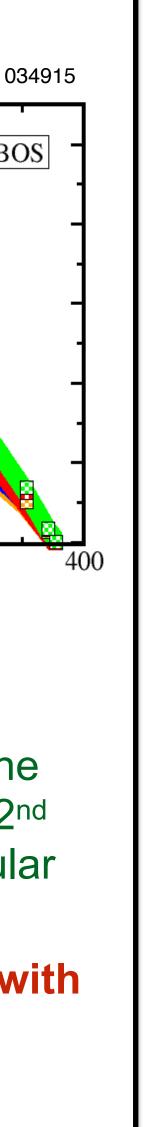
## **Picking the right Data: Elliptic Flow**





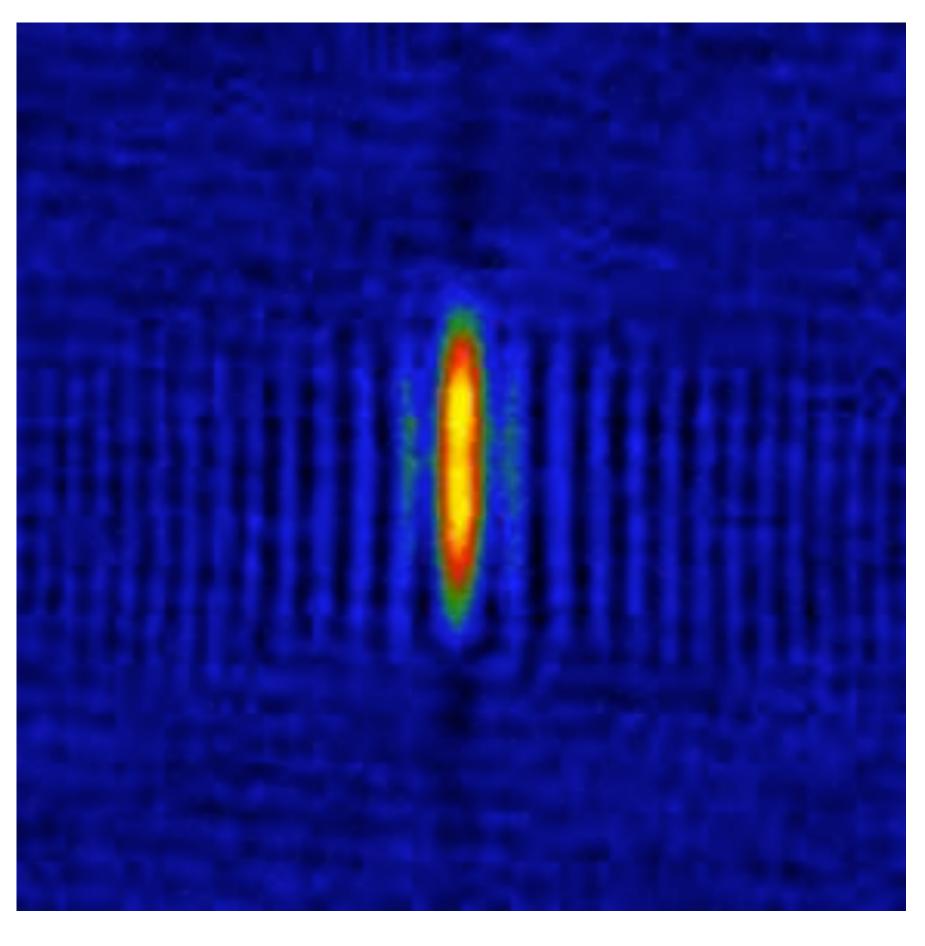
#### elliptic flow $(v_2)$ :

- asymmetry out- vs. in-plane emission is quantified by 2<sup>nd</sup> Fourier coefficient of angular distribution:  $v_2$
- > vRFD: good agreement with data for very small  $\eta/s$



## Elliptic flow: ultra-cold Fermi-Gas

- Li atoms at release from an optical trap:
- initial almond shape, similar to interaction area in heavy-ion collision



- Li-atoms released from an optical trap exhibit elliptic flow analogous to what is observed in ultra-relativistic heavy-ion collisions
- Elliptic flow is a general feature of strongly interacting systems!

100 µs 200 µs 400 μs 600 μs 800 μs 1000 μs 1500 μs 2000 µs

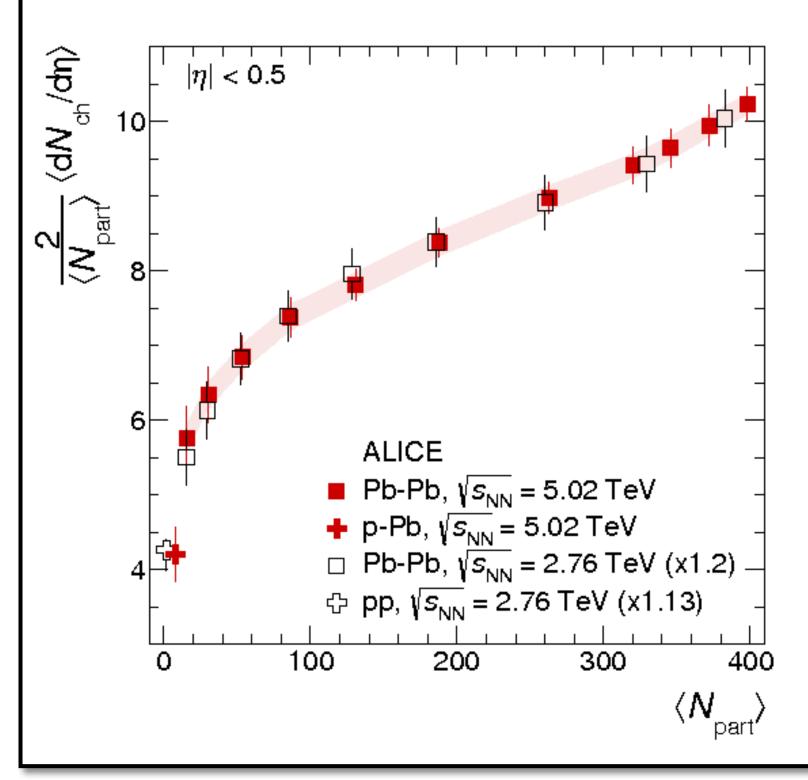
K. M. O'Hara, S. L. Hemmer, M. E. Gehm, S. R. Granade, J. E. Thomas: Science 298 (2002) 2179



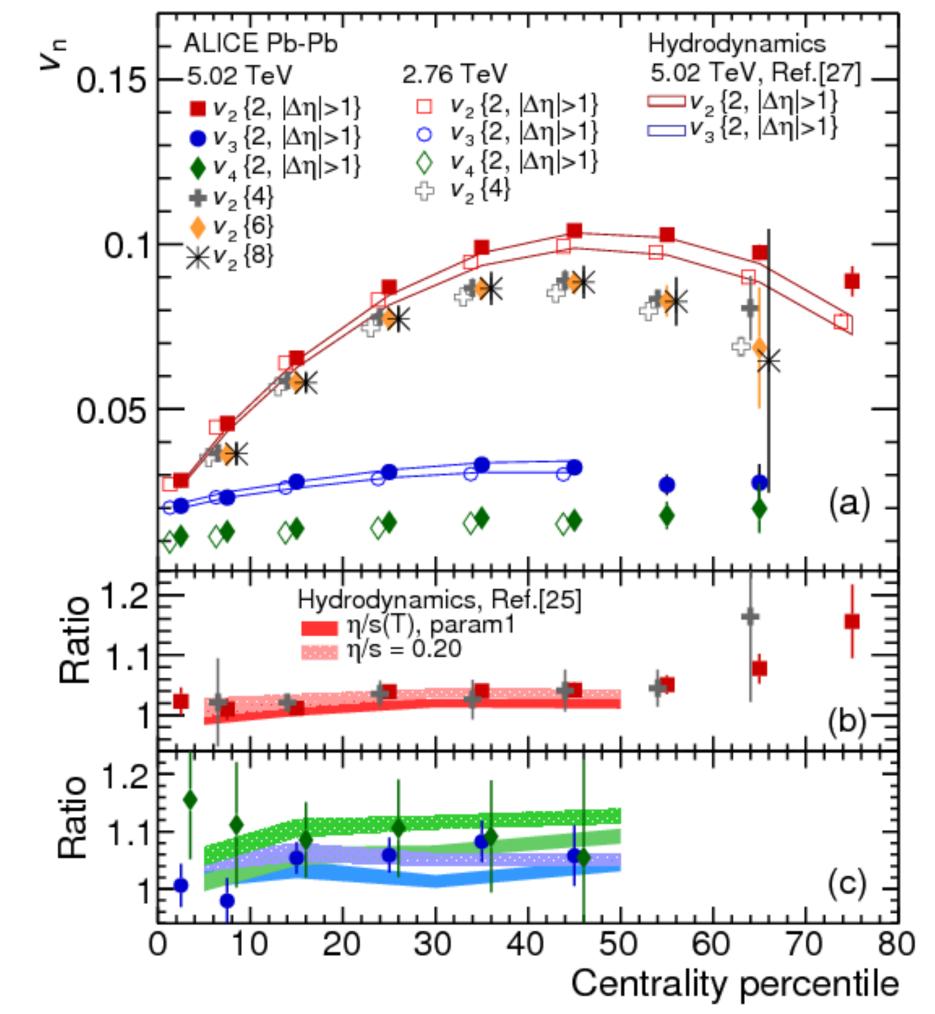
## **Training Data**

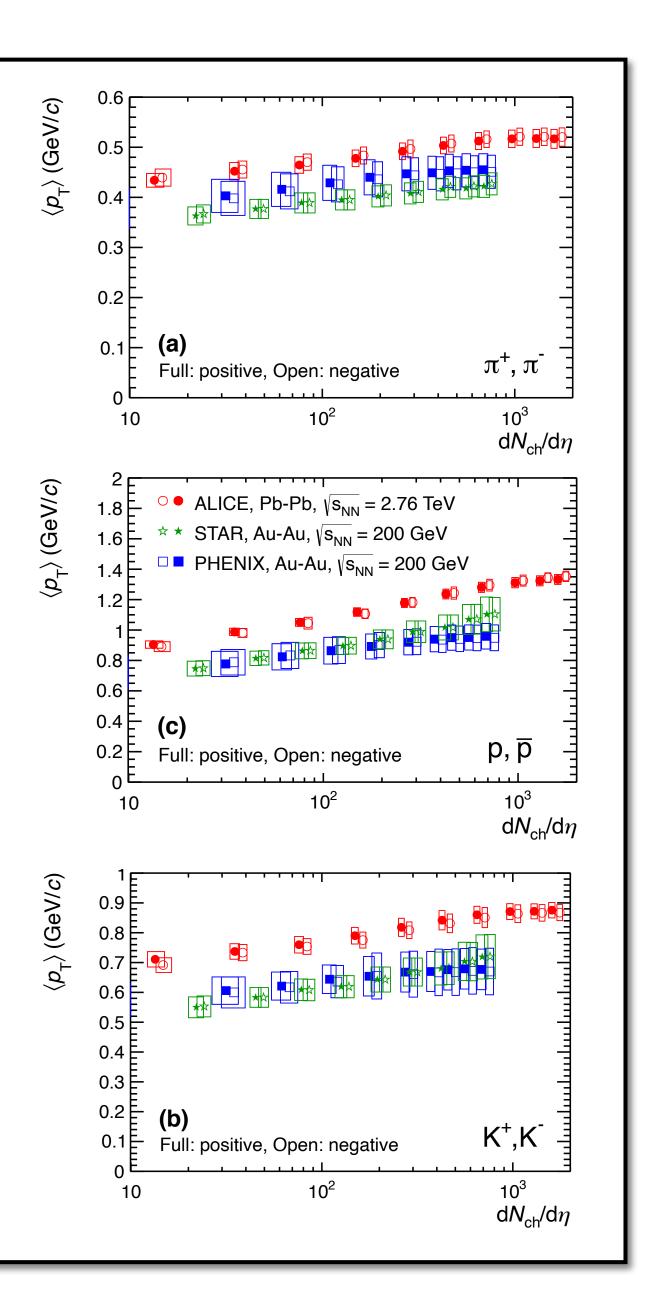
### Data:

- ALICE v<sub>2</sub>, v<sub>3</sub> & v<sub>4</sub> flow cumulants
- identified & charged particle yields
- identified particle mean  $p_T$
- 2 beam energies: 2.76 & 5.02 TeV

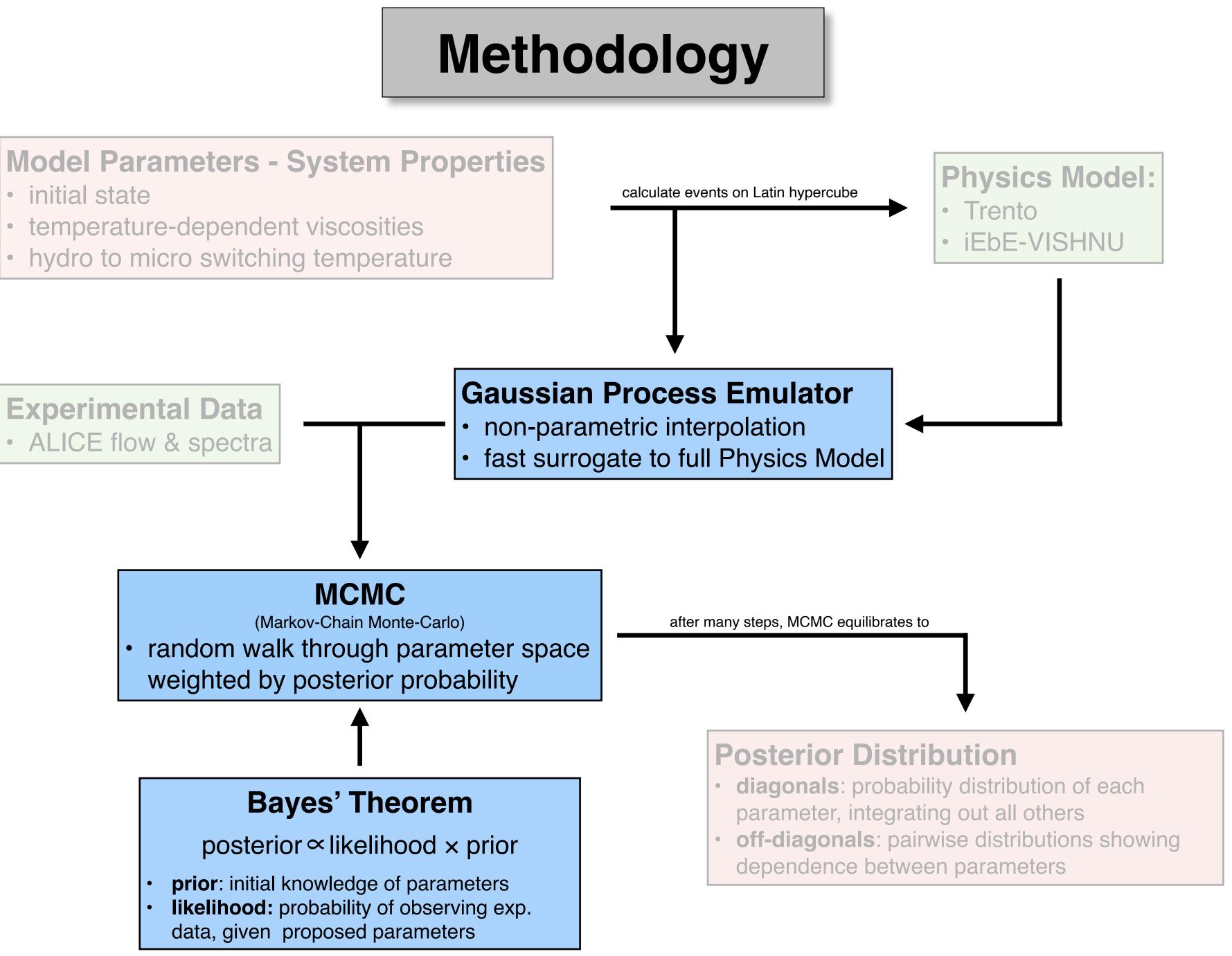


### the entire success of the analysis depends on the quality of the exp. data!





- temperature-dependent viscosities
- hydro to micro switching temperature

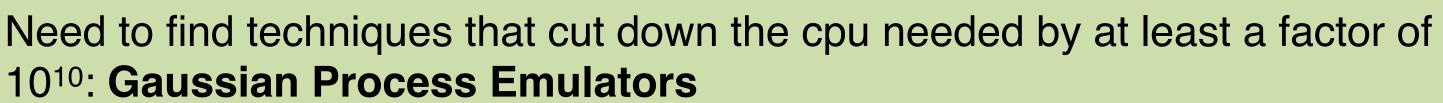


### **Exploring the Model Parameter-Space**

#### brute force analysis:

- 14 model parameters
- 9 centrality bins
- 20 bins per parameter
- need to evaluate model at 9 ×20<sup>14</sup> points
- fluctuating initial conditions:  $\mathcal{O}(10^4)$  events per point  $\rightarrow 10^{18}$  events
- assume 1 cpu hour per event: 10<sup>18</sup> 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...

**1010: Gaussian Process Emulators** 



65

61



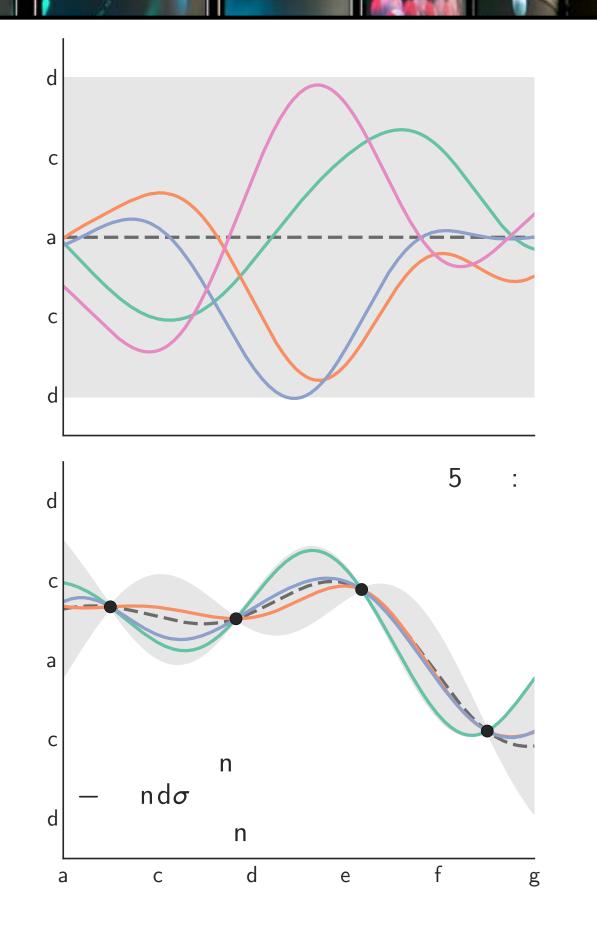
## **Exploring the Model Parameter-Space**

#### **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:

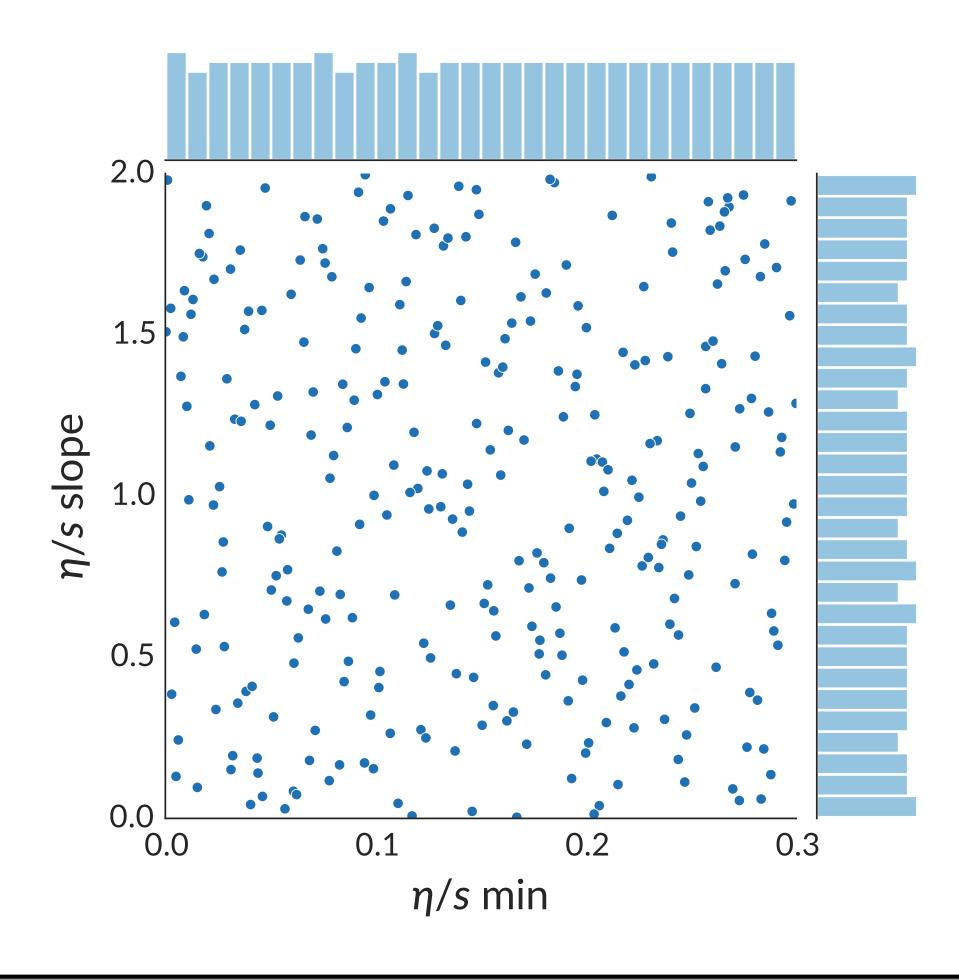
- algorithm for generating semi-randomized, spacefilling points (here: maximin Latin hypercube)
- avoids large gaps and tight clusters
- all parameters varied simultaneously
- needs only *m≥10n* points, with
   n: number of model parameters

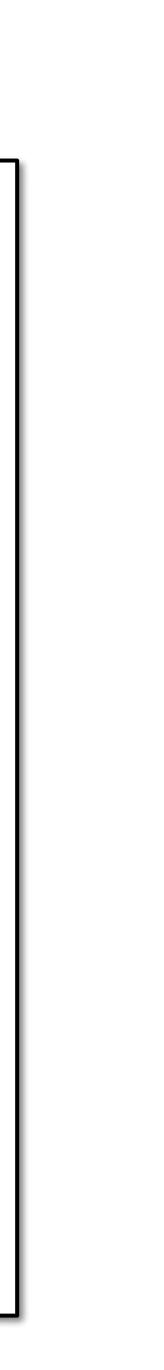
#### this design:

- n=15 model parameters
- 9 centrality bins, 2 energies
- Latin hypercube with m=500 points
- O(10<sup>4</sup>) 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  $\eta$ /s parameters





## **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

## NOW COMPUTING

CFRAN

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

CFRAN

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
			113,074.0
	Cori KNL	1,008	77.000 5
PI: Sudip S. Dosanjh, Lawrence Berkeley National Lab - NERSC			77,866.5
Extraction of QCD transport coefficients from ultra-	Edison	1,000	
relativistic heavy-ion collisions through a Bayesian model to data analysis			443,890.9
PI: Steffen A. Bass, Duke University			
Extraction of QCD transport coefficients from ultra-	Edison	1,000	000 004 0
relativistic heavy-ion collisions through a Bayesian model to data analysis			399,224.3
PI: Steffen A. Bass, Duke University			
Extraction of QCD transport coefficients from ultra-	Edison	750	220 020 2
relativistic heavy-ion collisions through a Bayesian model to data analysis			229,928.2
PI: Steffen A. Bass, Duke University			
NERSC Staff Accounts PI: Sudip S. Dosanjh, Lawrence Berkeley National Lab - NERSC	Cori KNL	512	292 504 2
			282,594.2



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  $\Rightarrow$  find probability distribution for  $\mathbf{x}_{\star}$ 



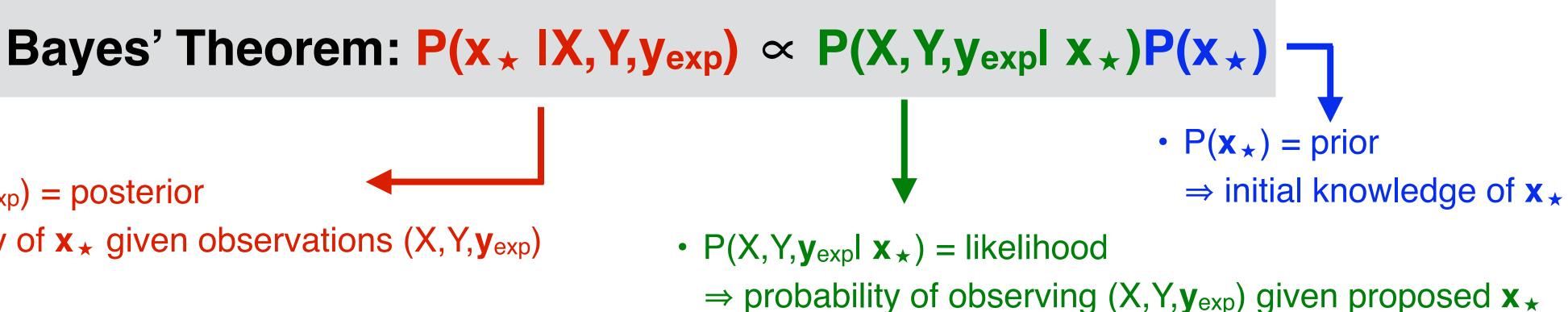
 $\Rightarrow$  probability of  $\mathbf{x}_{\star}$  given observations (X,Y, $\mathbf{y}_{exp}$ )

#### **Markov-Chain Monte-Carlo:**

- random walk through parameter space weighted by posterior
- large number of samples  $\Rightarrow$  chain equilibrates to posterior distribution
- flat prior within design range, zero outside
- posterior ~ likelihood within design range, zero outside

# Calibration

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





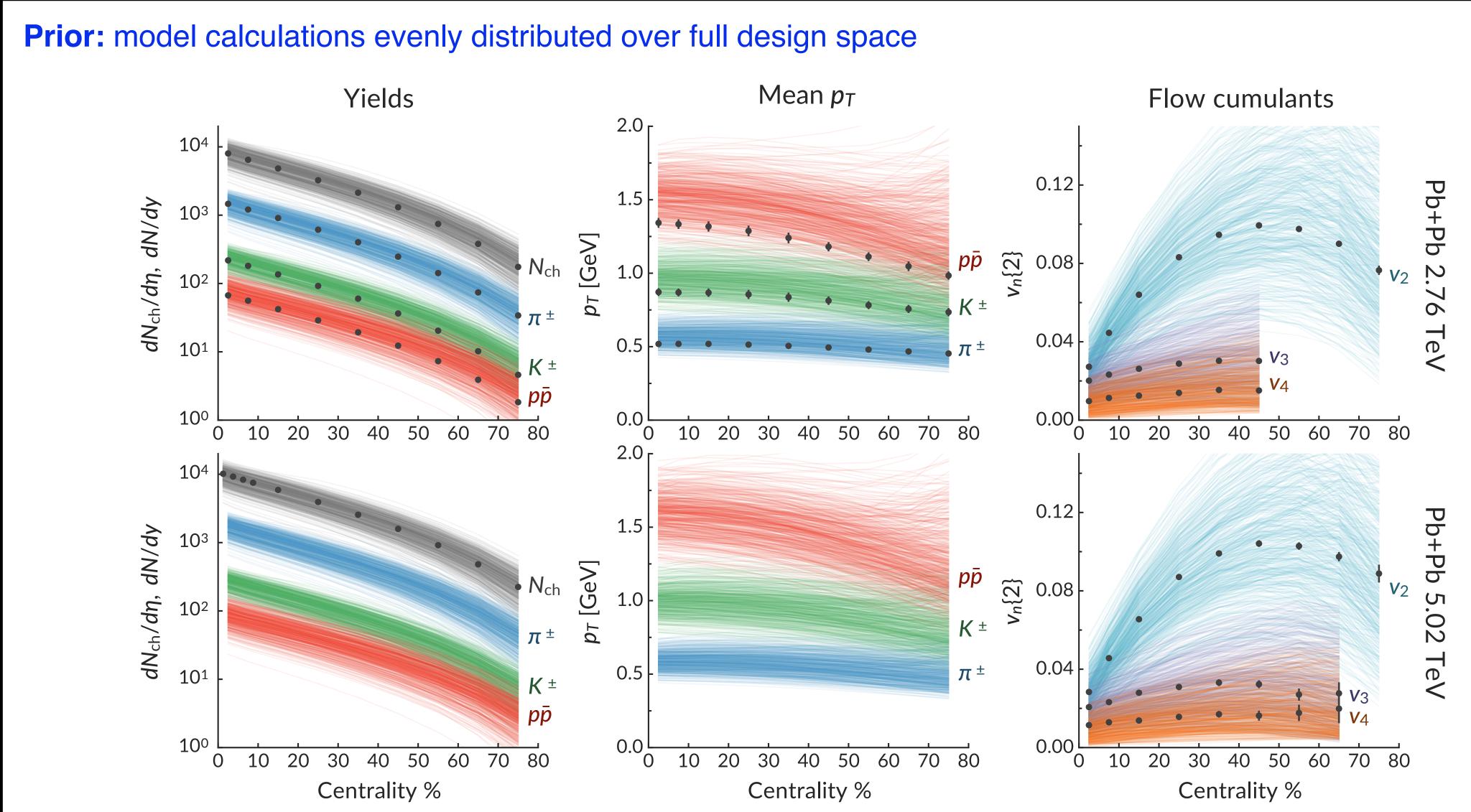
#### Likelihood and Uncertainty Quantification:

- Likelihood  $\propto \exp[-1/2 (\mathbf{y} \mathbf{y}_{exp})^\top \mathbf{\Sigma}^{-1} (\mathbf{y} \mathbf{y}_{exp})]$
- covariance matrix  $\Sigma = \Sigma_{experiment} + \Sigma_{model}$
- Σ<sub>experiment</sub>=stat(diagonal) + sys(non-diagonal)
- Σ<sub>model</sub> conservatively estimated as 5%

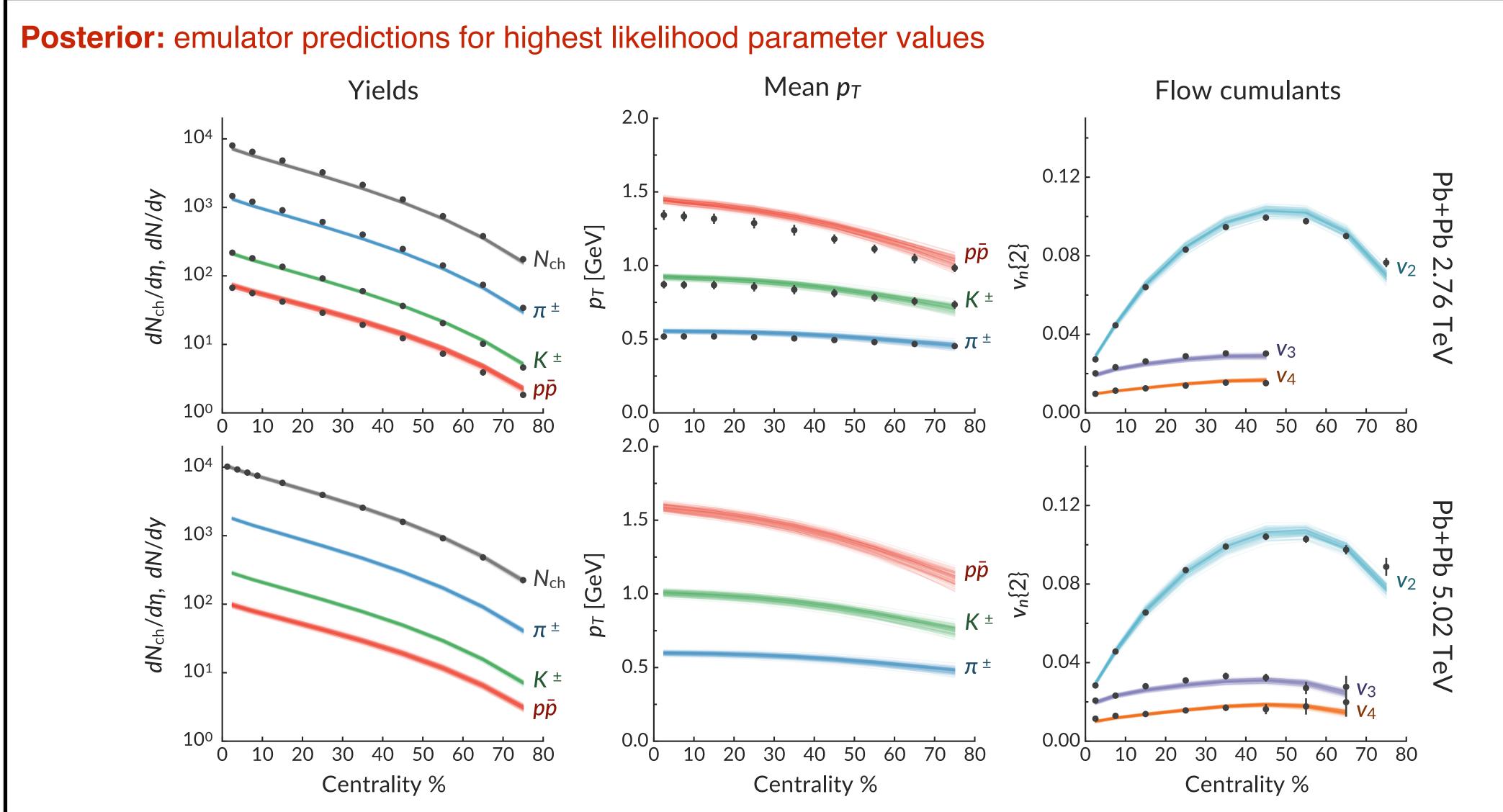




# **Prior vs. Posterior**



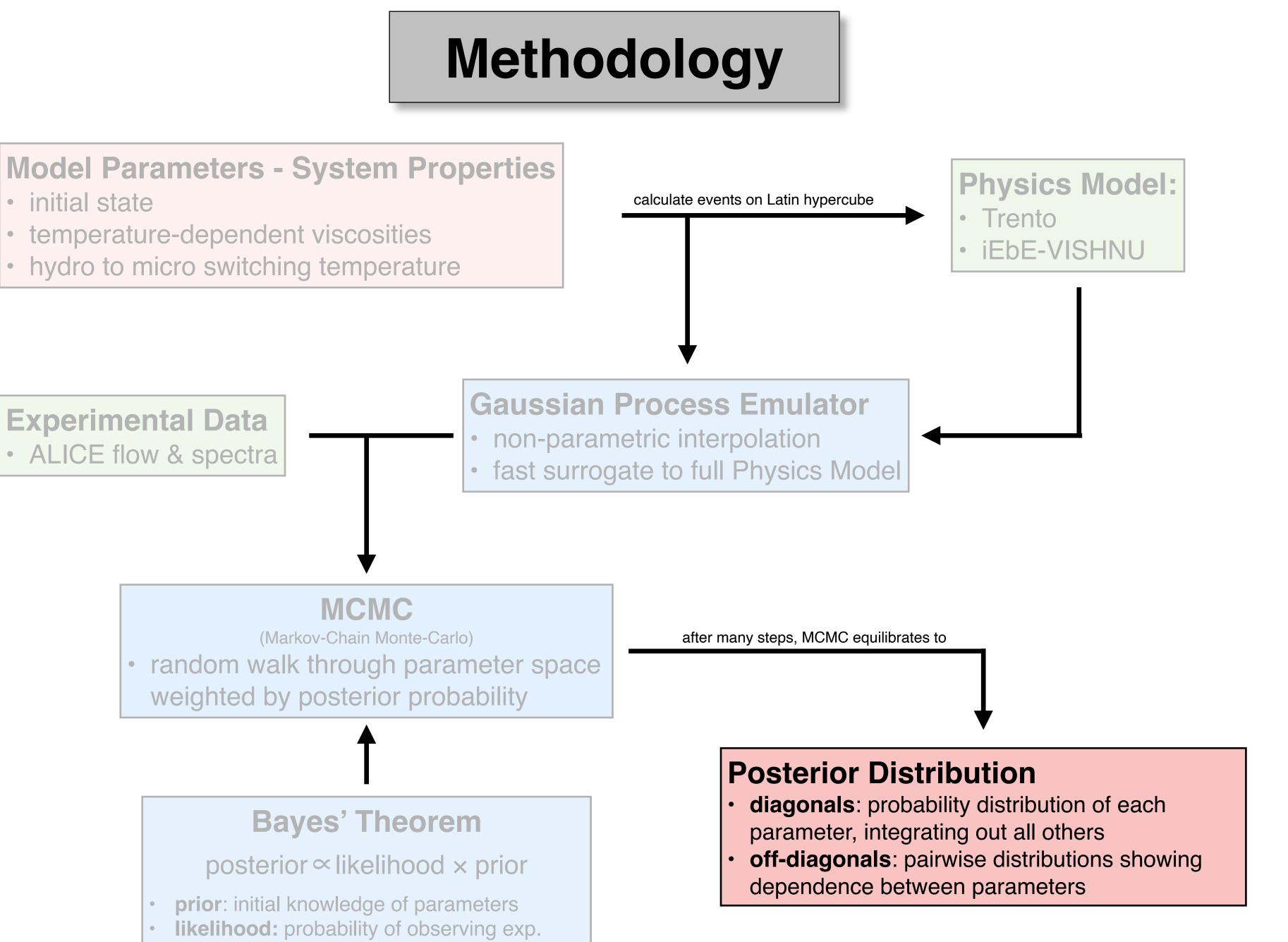
# **Prior vs. Posterior**



# **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

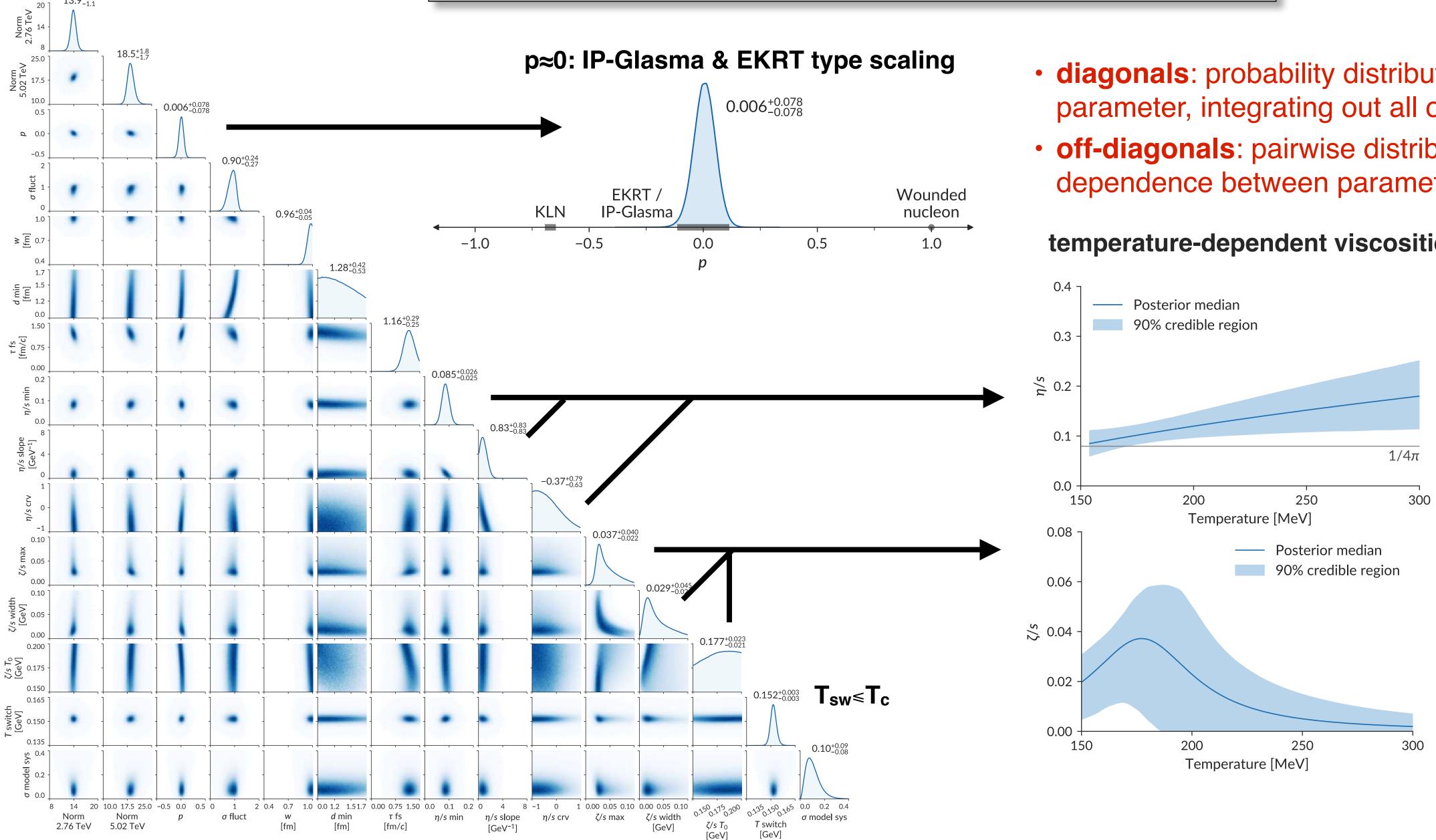
- hydro to micro switching temperature





- data, given proposed parameters

# **Calibrated Posterior Distribution**



 $13.9^{+1.2}_{-1.1}$ 

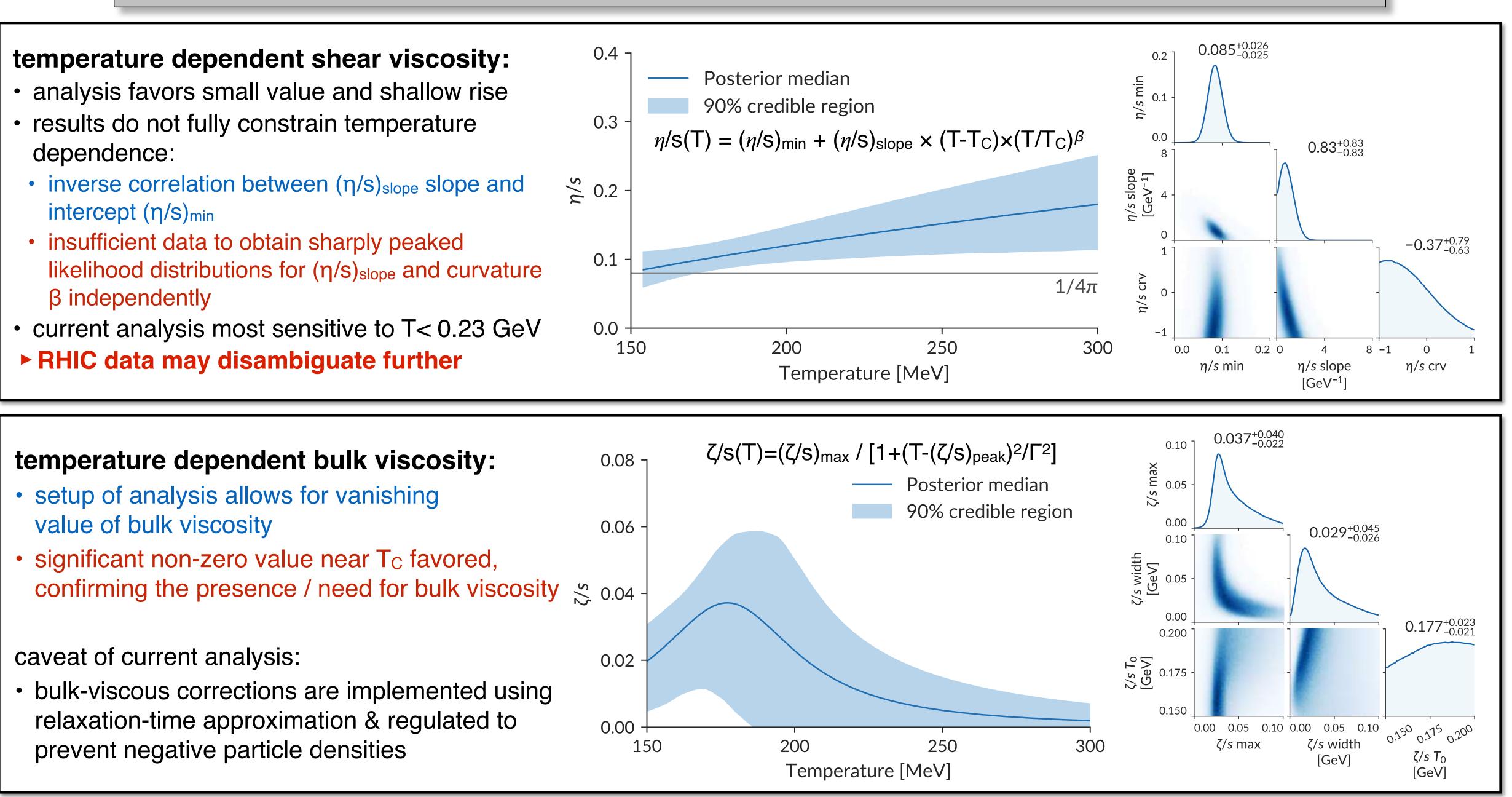
- **diagonals**: probability distribution of each parameter, integrating out all others
- off-diagonals: pairwise distributions showing dependence between parameters

#### temperature-dependent viscosities:



# **Temperature Dependence of Shear & Bulk Viscosities**

S

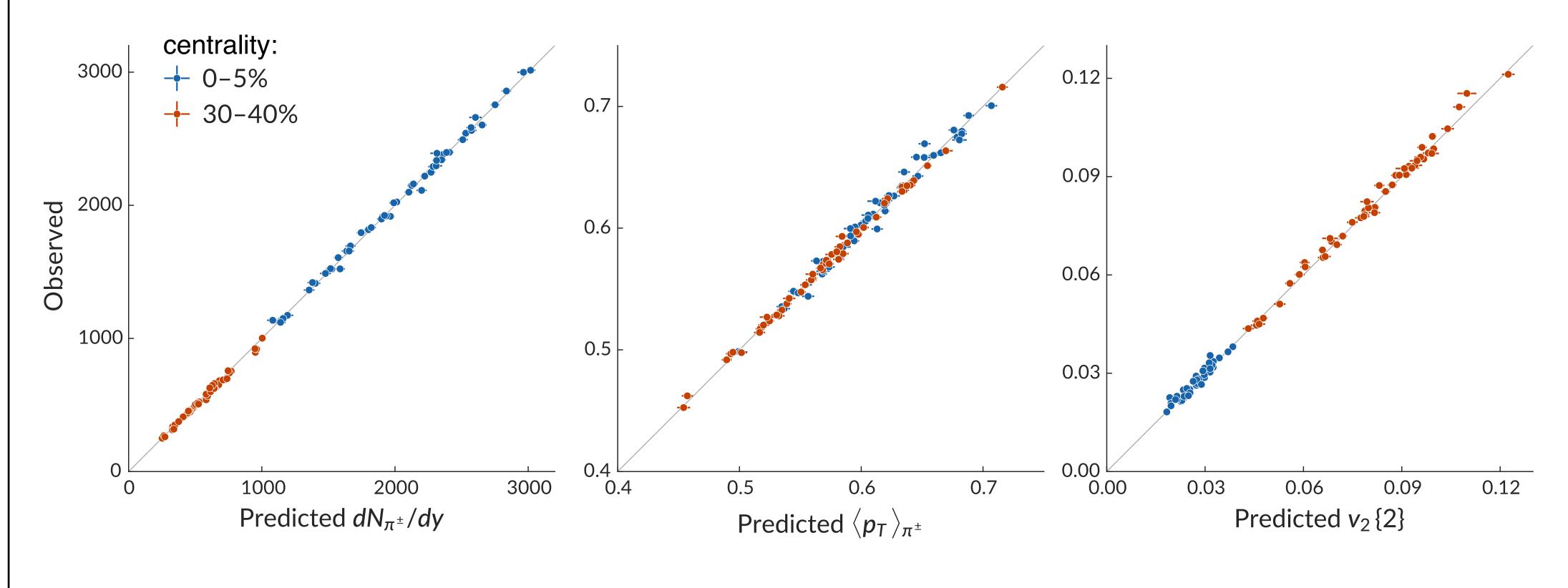


temperature dependent bulk viscosity:	0.08 7
<ul> <li>setup of analysis allows for vanishing value of bulk viscosity</li> </ul>	0.06 -
<ul> <li>significant non-zero value near T<sub>C</sub> favored, confirming the presence / need for bulk viscosity</li> </ul>	\$∕∑ 0.04 -
caveat of current analysis:	0.02
<ul> <li>bulk-viscous corrections are implemented using relaxation-time approximation &amp; regulated to prevent negative particle densities</li> </ul>	0.00

# Or

# **Precision Science** "Smoke & Mirrors"?

- 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:

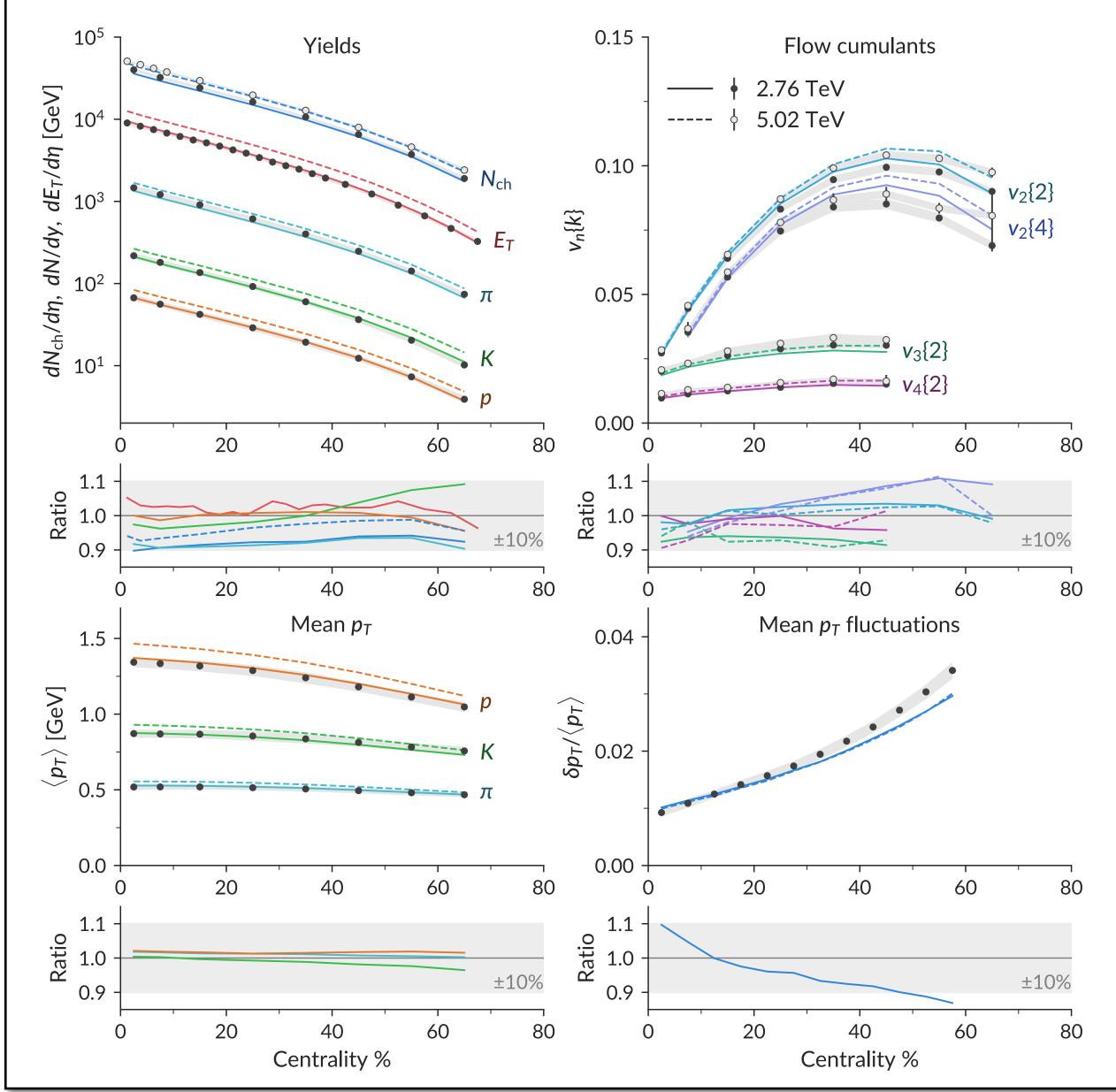


# Validation

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



# Verification: Explicit Model Calculation



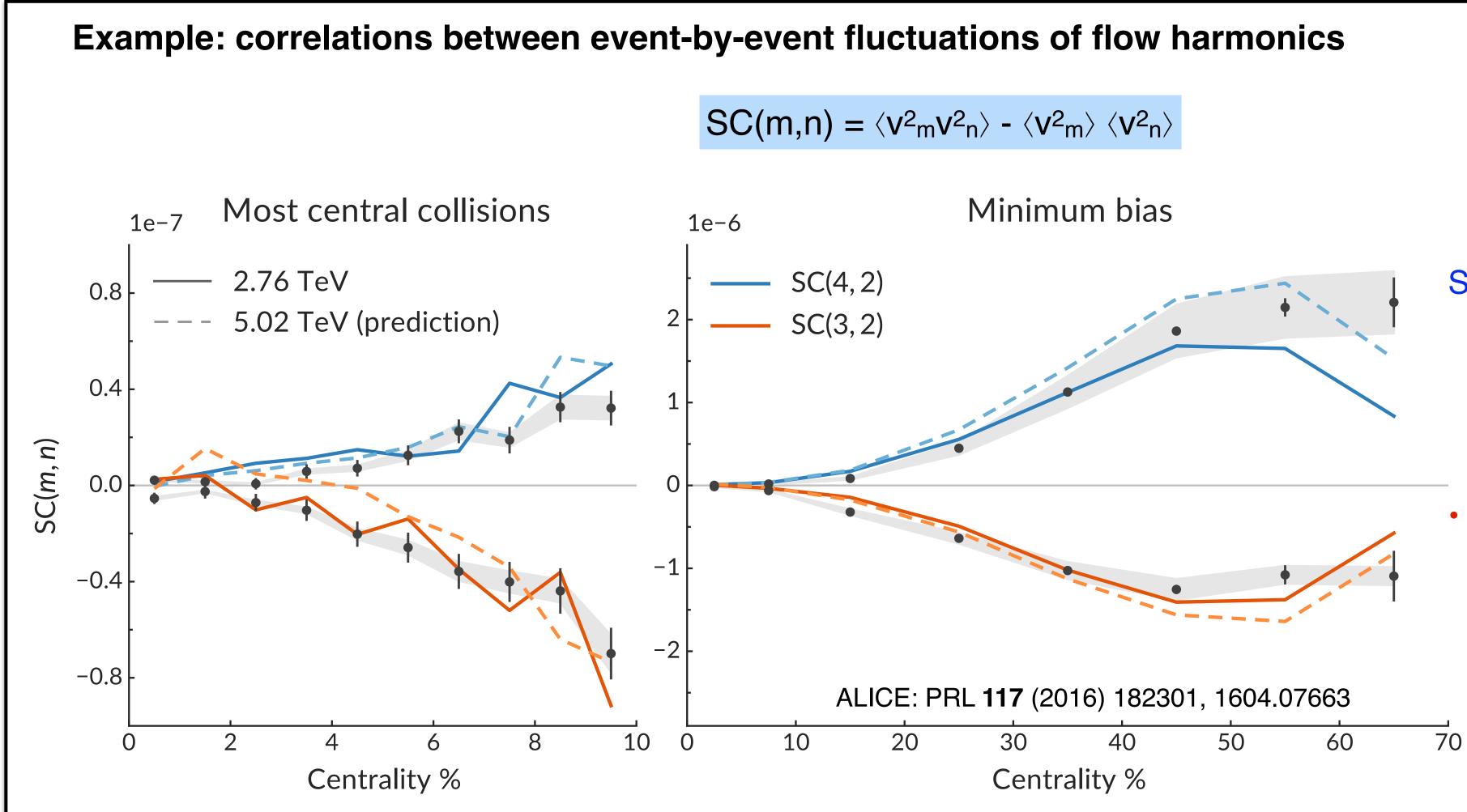
 explicit physics model calculations (no emulator) with parameter values set to the maximum of the posterior probability distributions yield excellent agreement with data!





# **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.



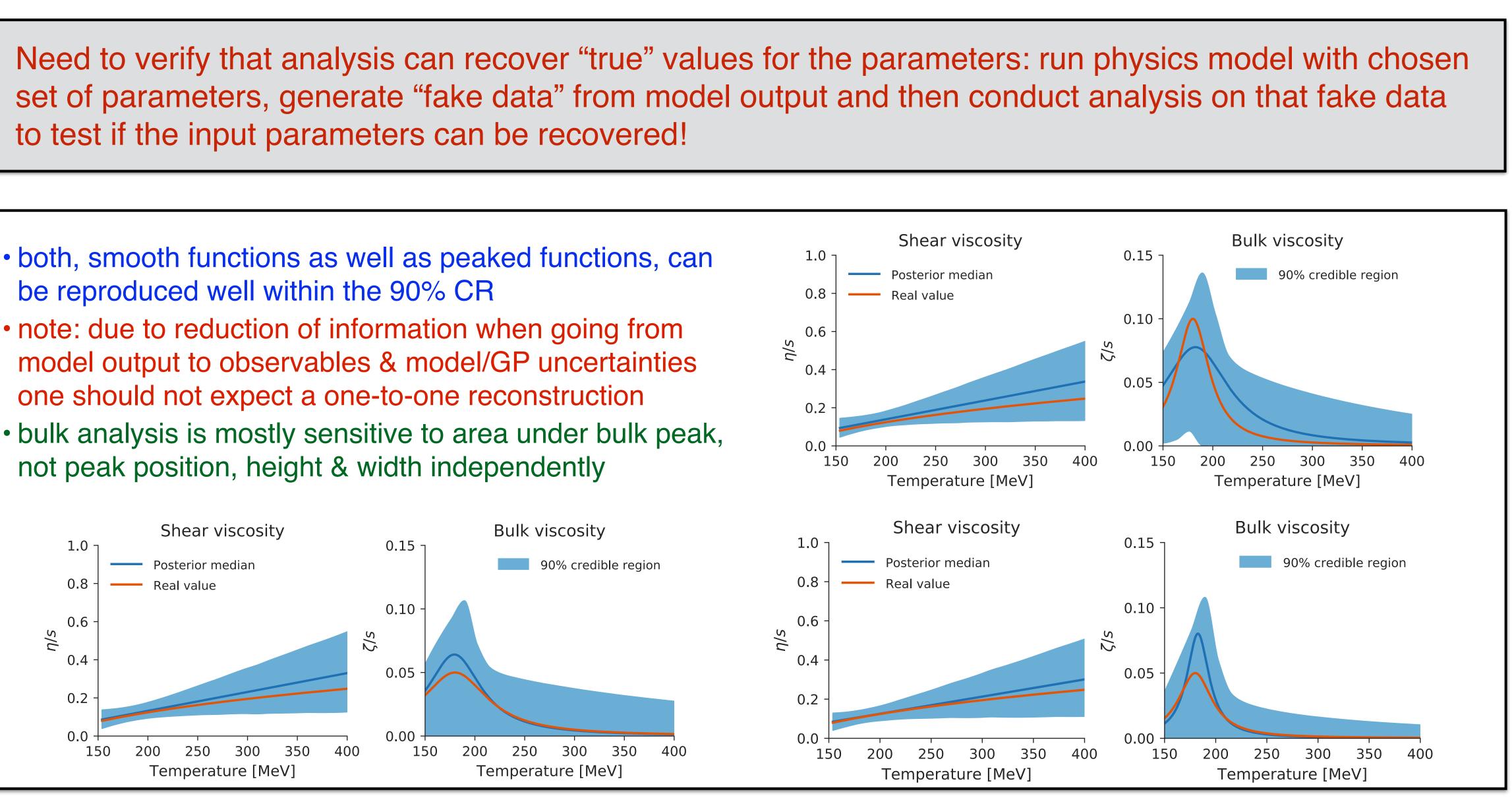
SC(m,n) are sensitive to:

- initial conditions
- evolution model
- QGP transport coefficients
- excellent agreement of model prediction to data!



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!

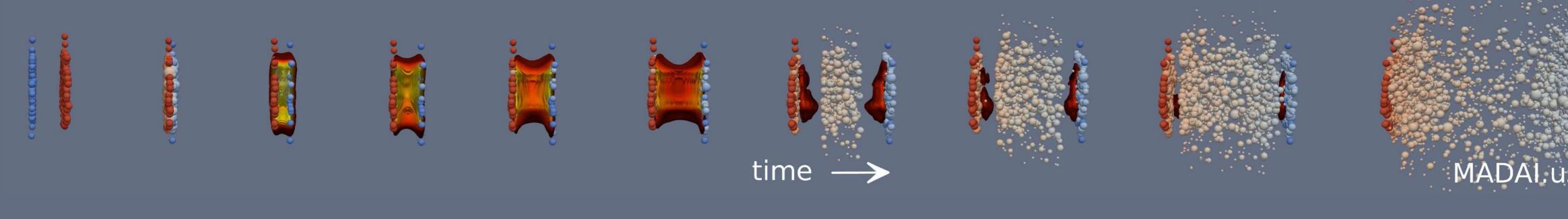
- both, smooth functions as well as peaked functions, can be reproduced well within the 90% CR
- note: due to reduction of information when going from model output to observables & model/GP uncertainties one should not expect a one-to-one reconstruction
- not peak position, height & width independently



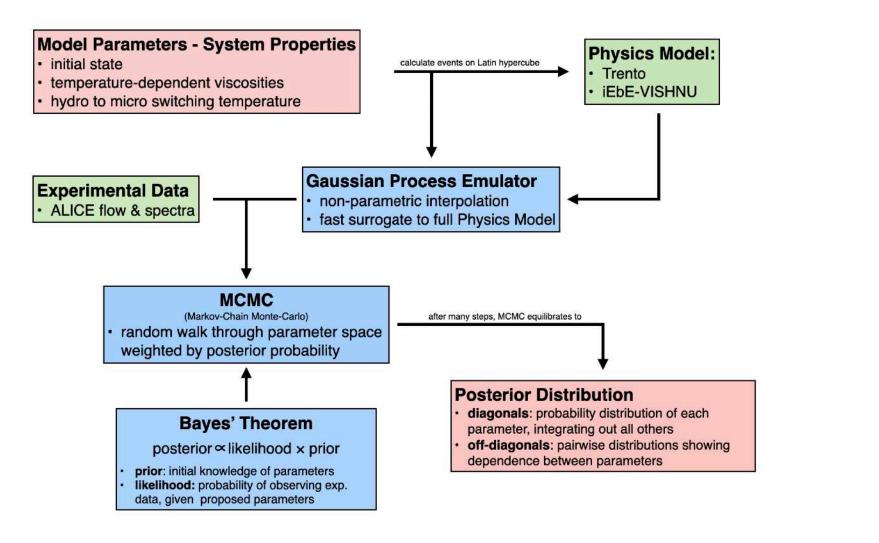
# **Closure Test**

# **Summary:**

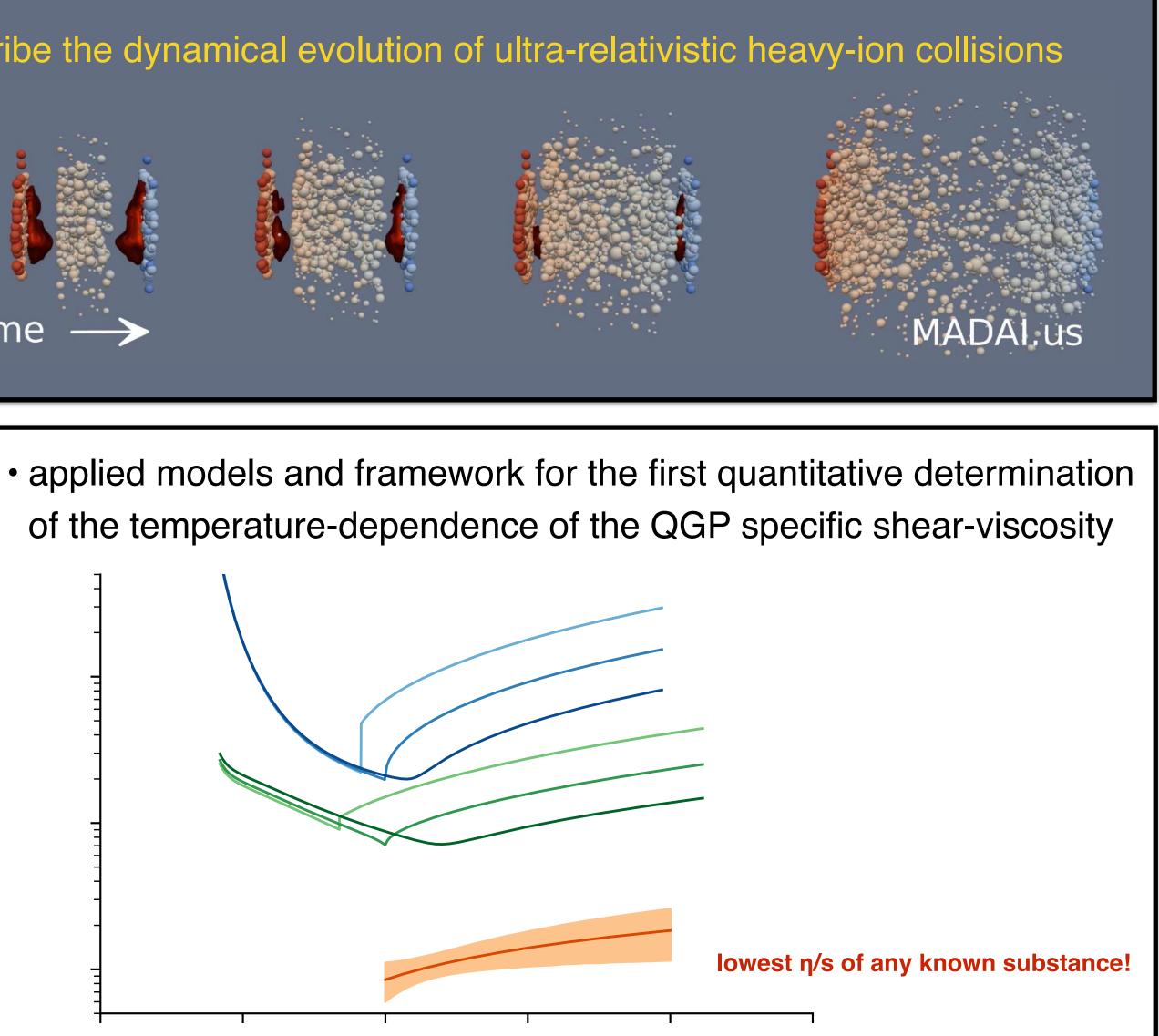
• created a comprehensive set of computational models to describe the dynamical evolution of ultra-relativistic heavy-ion collisions



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



## **Summary:**



# **Outlook & Future Directions**

# 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  $\mu_{\rm B}$  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



current analysis focus was on the properties of bulk QCD matter and utilized only











# 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)
- Jean-Francois Paquet (still at Duke)

#### **Duke Dept. of Statistical Sciences:**

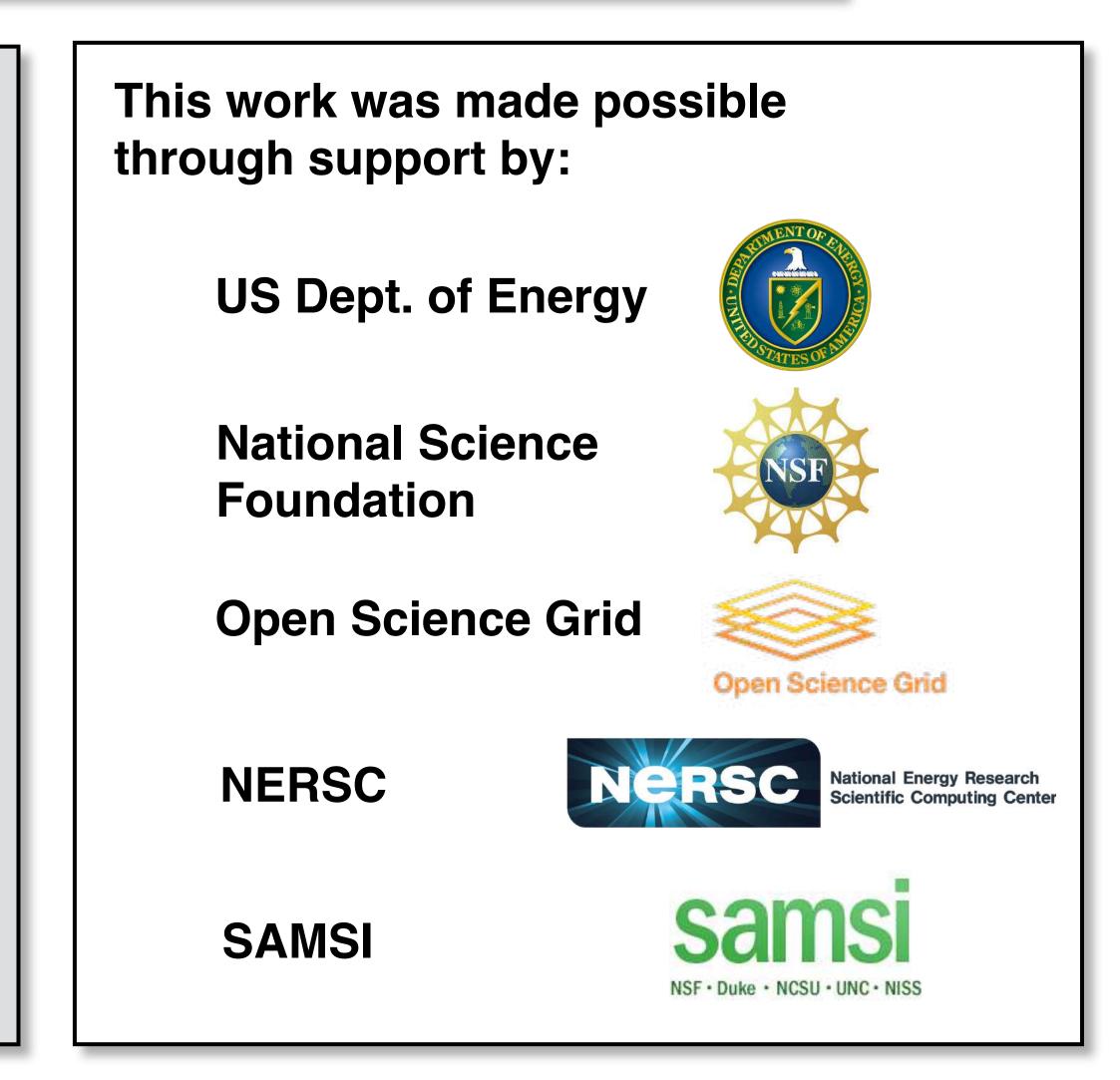
- Robert E. Wolpert
- Jake Coleman (now w/ LA Dodgers)

#### **Ohio State Nuclear Theory:**

- Ulrich W. Heinz
- Jia Liu (now SAP)
- Chun Shen (now faculty at Wayne State)

## **U. of Wyoming Dept. of Statistics:**

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



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: <u>Phys. Rev. C 92, 011901(R)</u>
- <u>https://github.com/Duke-QCD/trento</u>

## iEbE-VISHNU:

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

## **UrQMD**:

- Marcus Bleicher et al. <u>J.Phys. G25 (1999) 1859-1896</u>, <u>arXiv:hep-ph/9909407</u>
- <u>http://urqmd.org</u>

## **MADAI Collaboration:**

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

## **Duke Bayesian Analysis Package:**

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

• Steffen A. Bass et al. Prog. Part. Nucl. Phys. 41 (1998) 225-370, arXiv:nucl-th/9803035



## The End