Bayesian methods and uncertainty quantification in heavy-ion physics

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The Ohio State University, Columbus

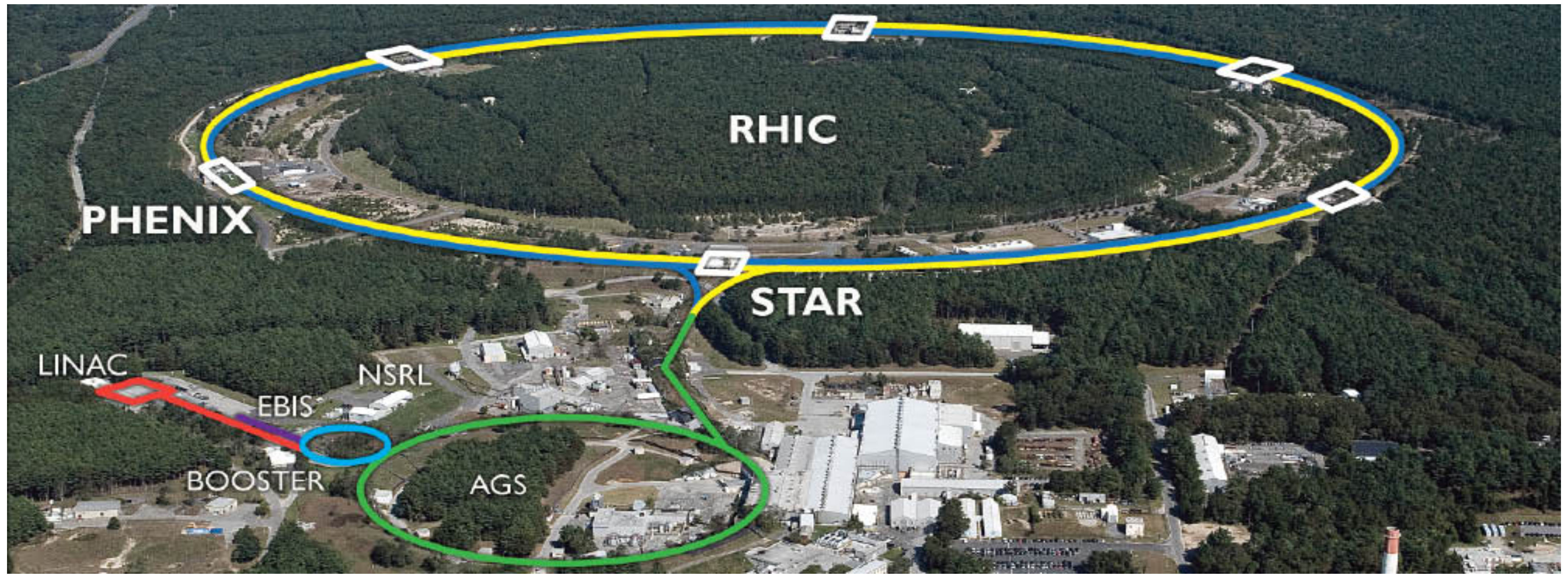
June 27, 2024

Overview

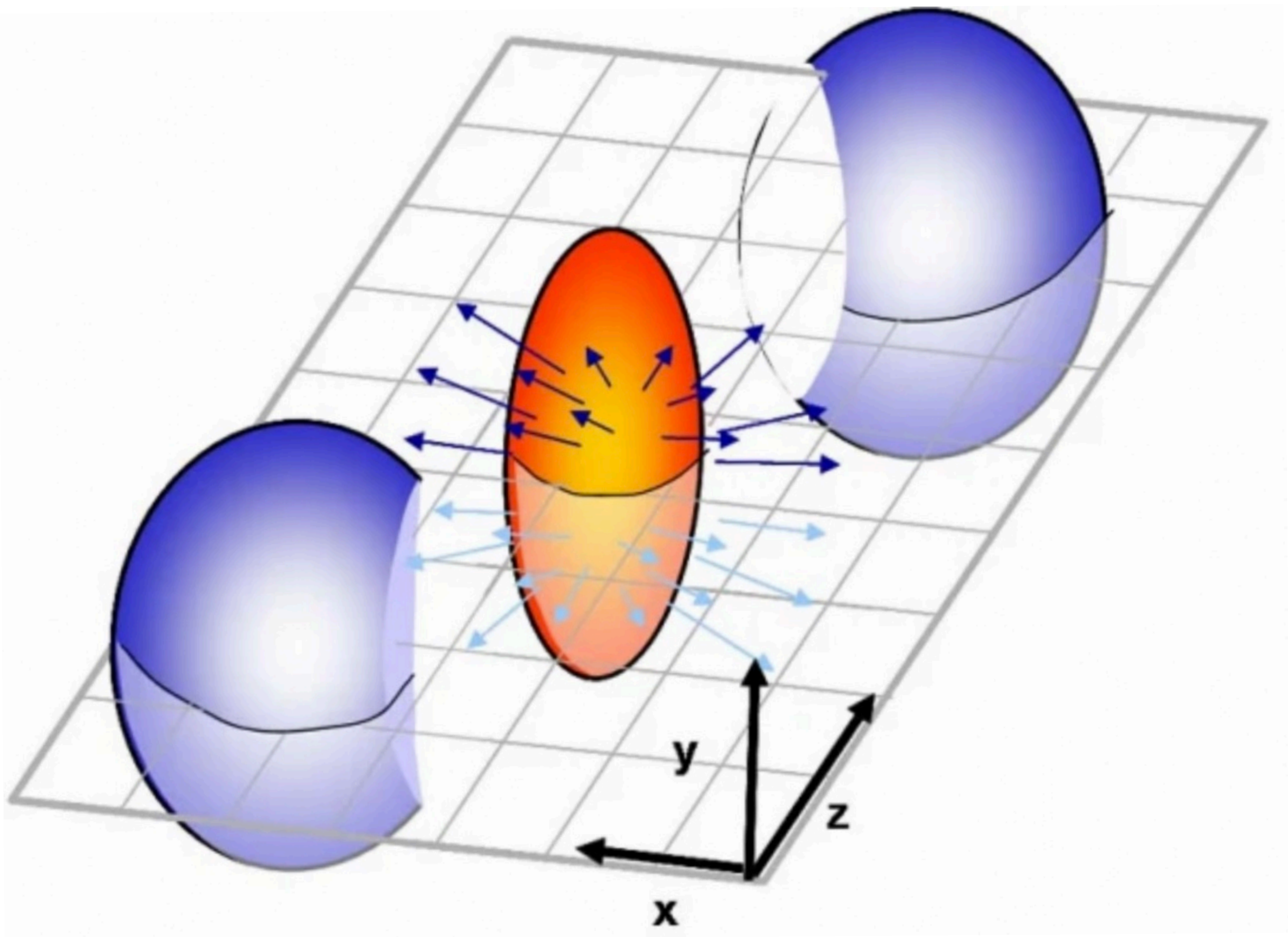
- Heavy-ion collisions and multi-stage physics models
- Model emulators
- Results of Bayesian parameter estimation from different studies
- Quantifying theoretical uncertainties: Model discrepancy
- Challenges

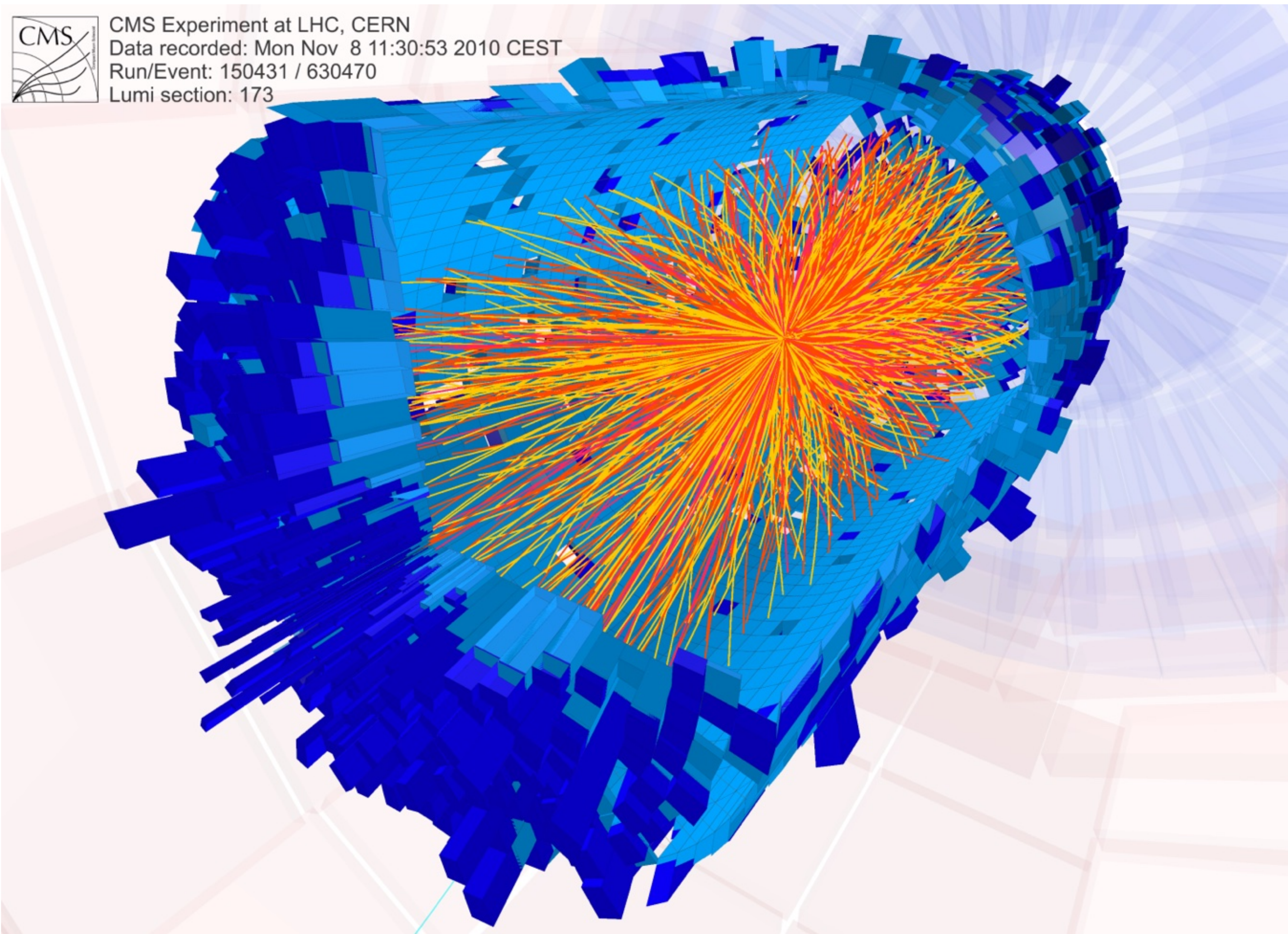
Heavy-ion collision

The Large Hadron Collider (LHC) in Europe (27 Km circumference)



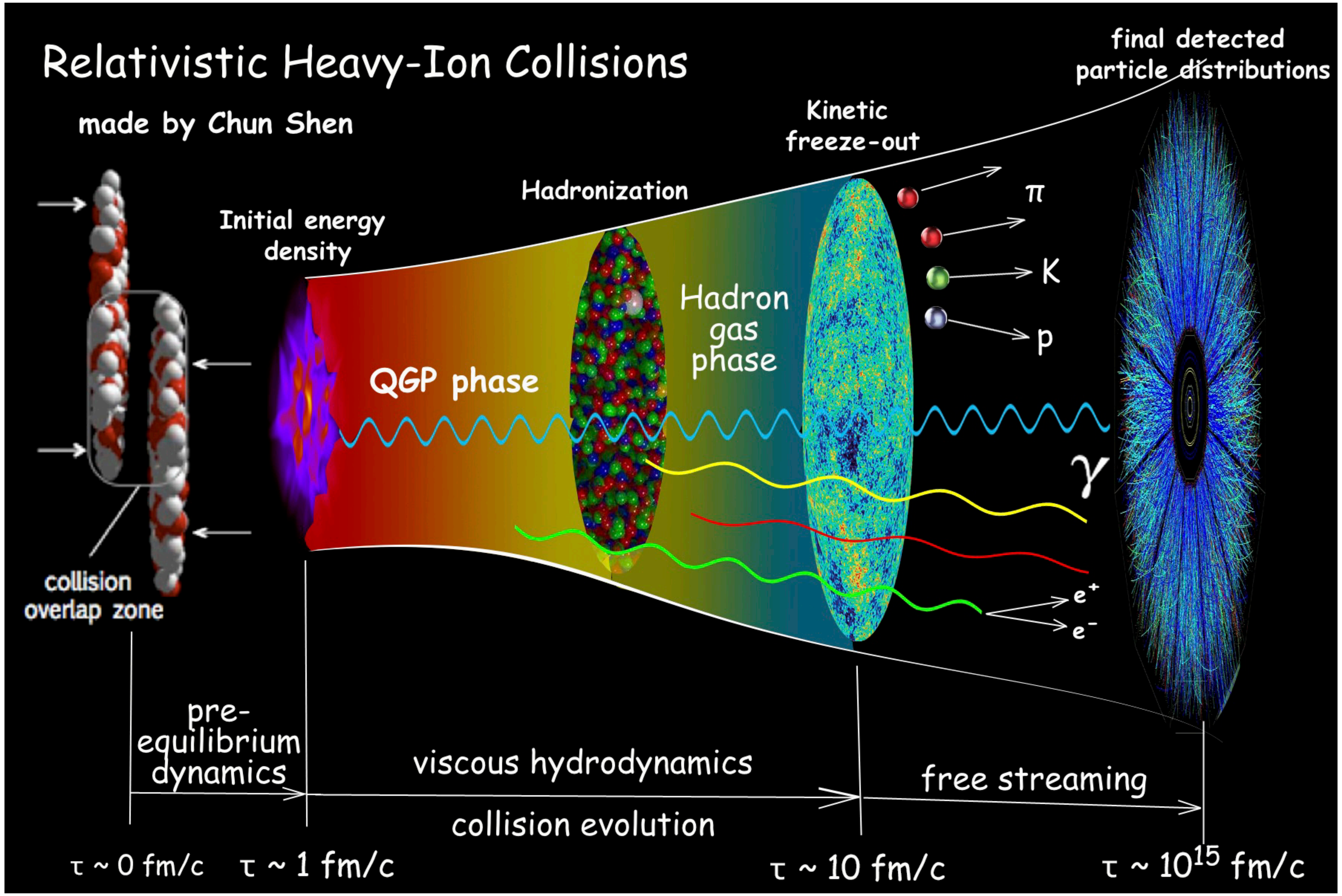
The Relativistic Heavy Ion Collider in US (3.8 Km circumference)



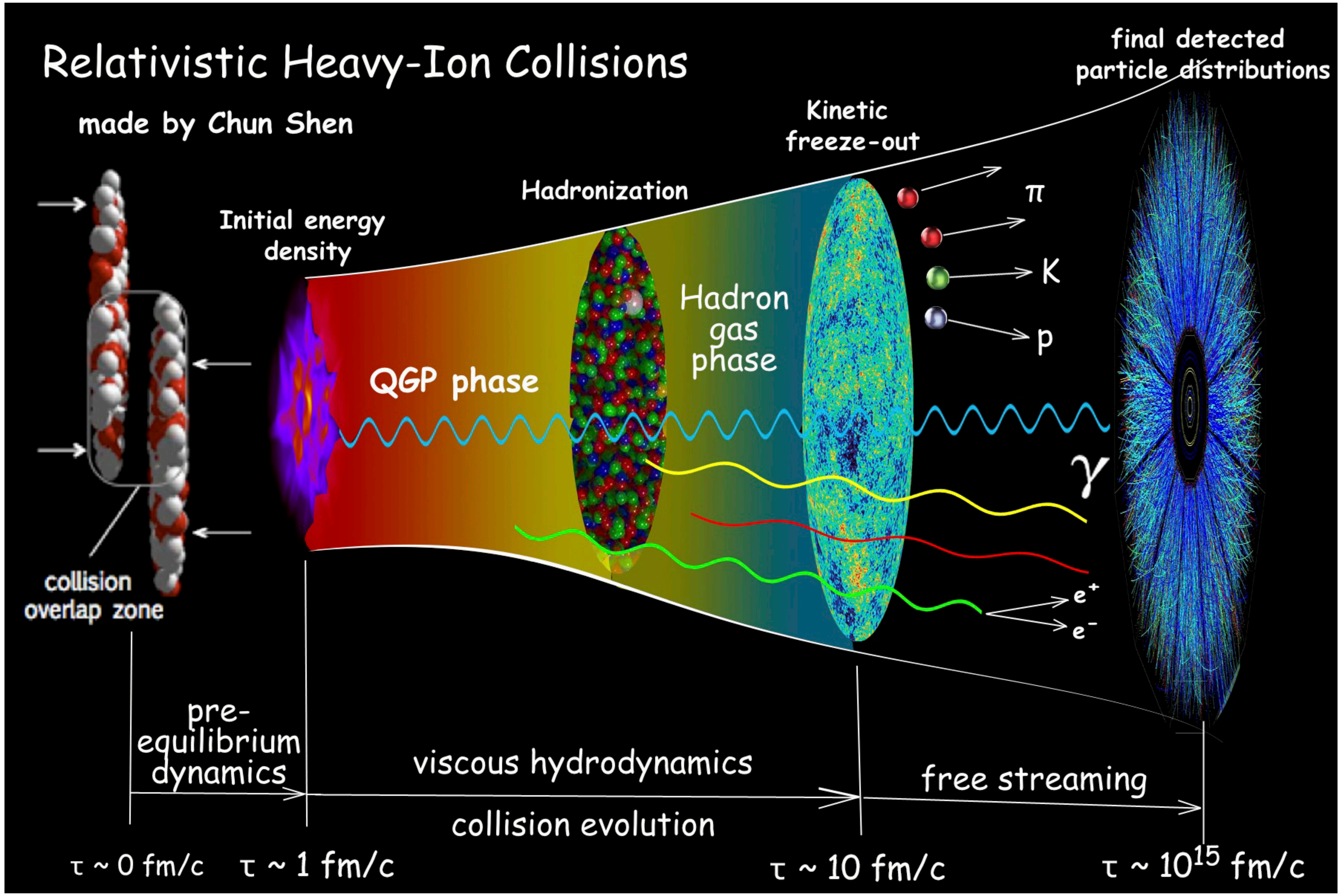


CMS collision events: first lead ion collisions - CERN Document Server

Many stages of heavy-ion collisions



Physics goals



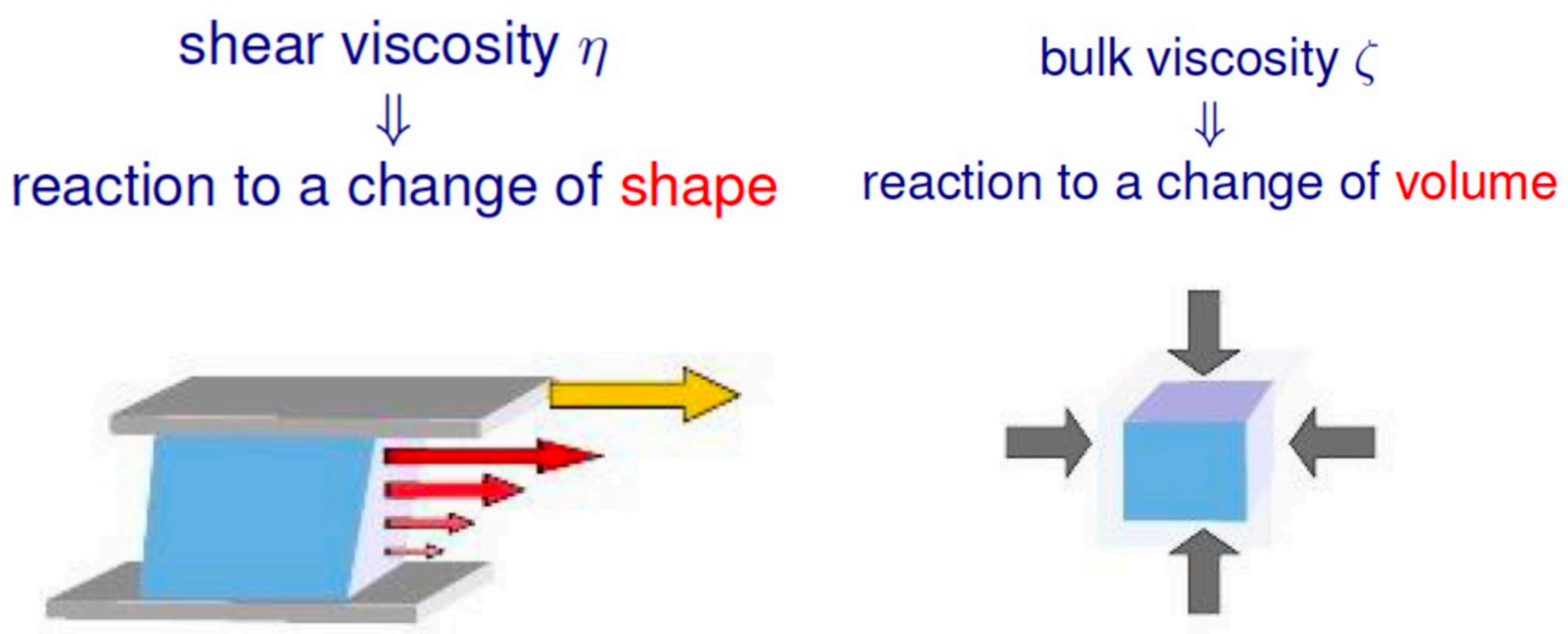
Quark Gluon Plasma (QGP) phase:

Hints of "fluid" formation.

Two decades of research

- Equation of state? $P(T, \mu)$, $\epsilon(T, \mu)$
  Taken from lattice results for hydro simulation

- Transport properties of formed QGP:
  Coefficient of shear viscosity: η
  Coefficient of bulk viscosity: ζ
  First principle calculation have large uncertainties
  Needs to be inferred from experiments



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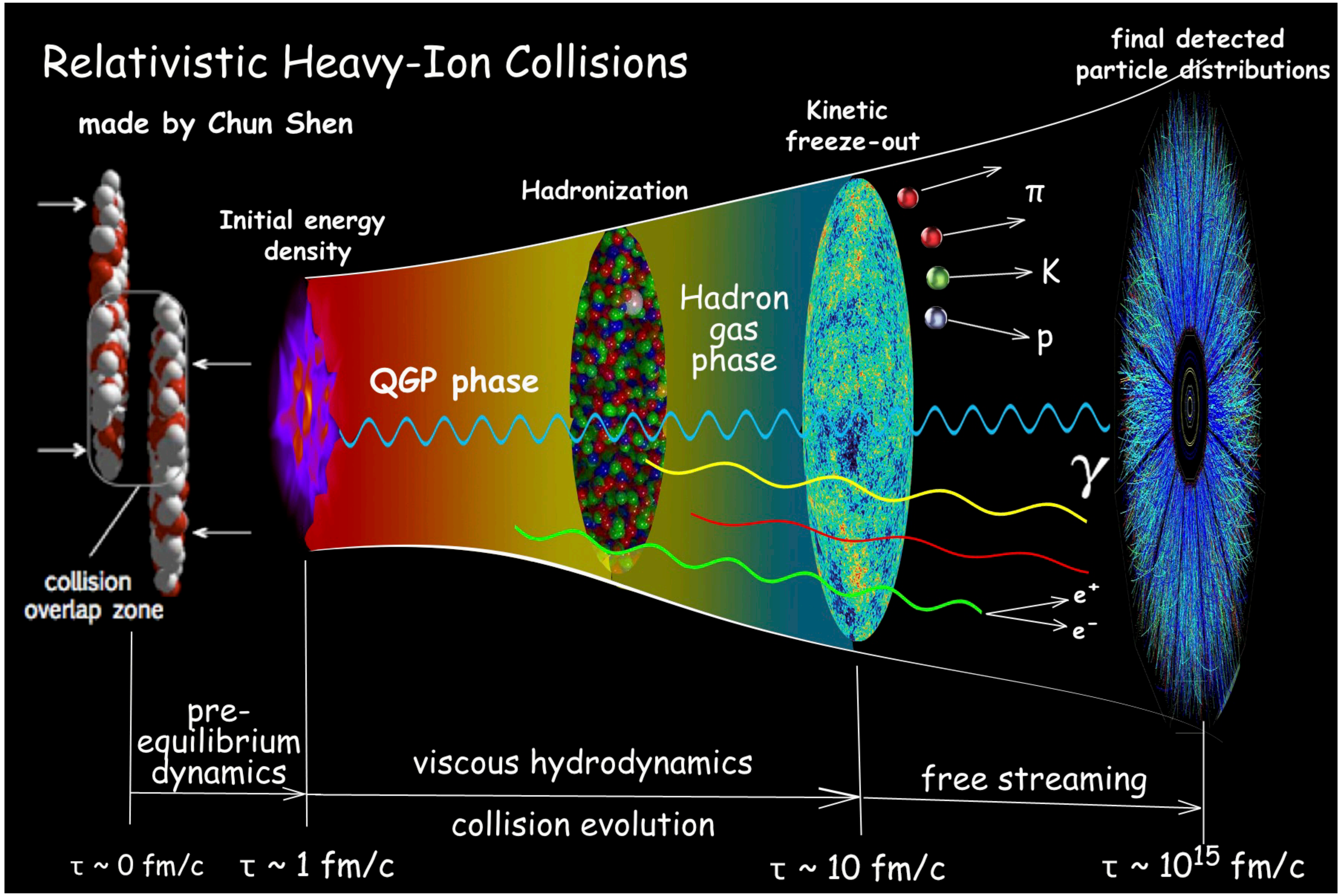

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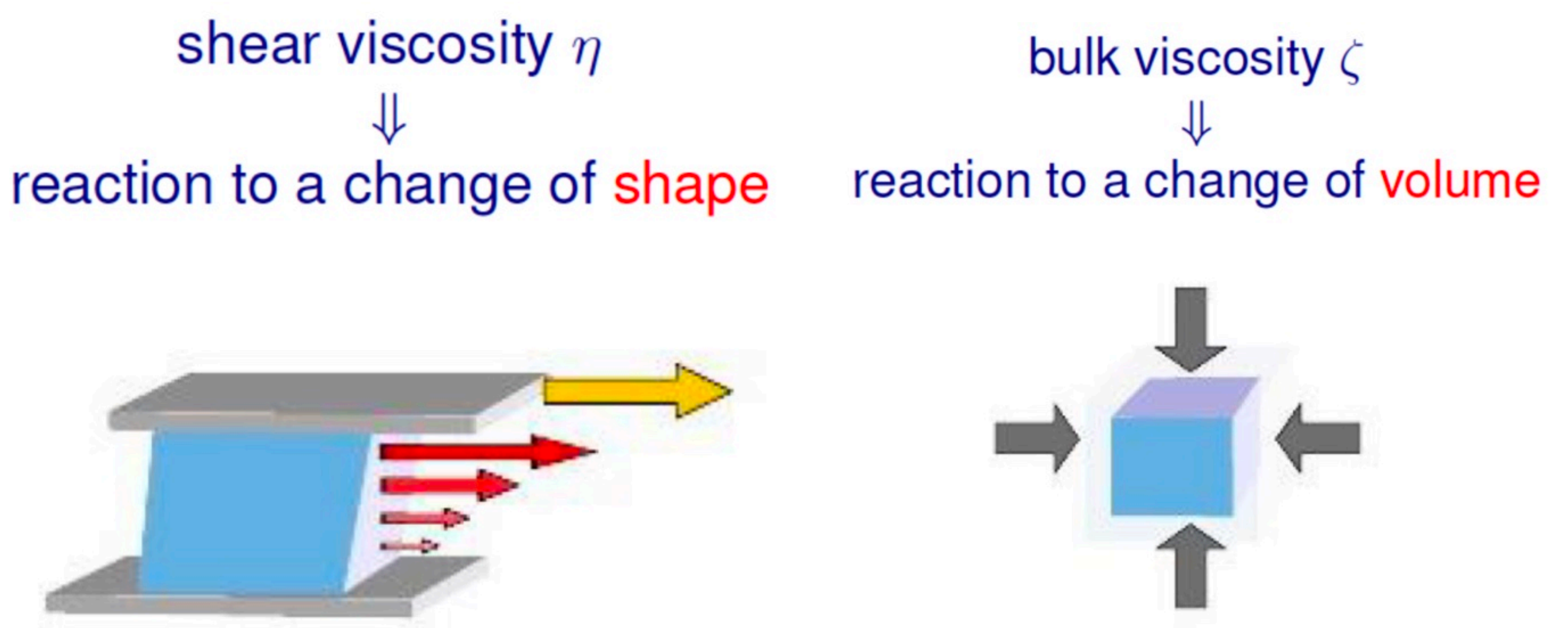


Challenges: models are multi-stage, uncertain, and expensive

Measurements (in transverse plane at midrapidity)

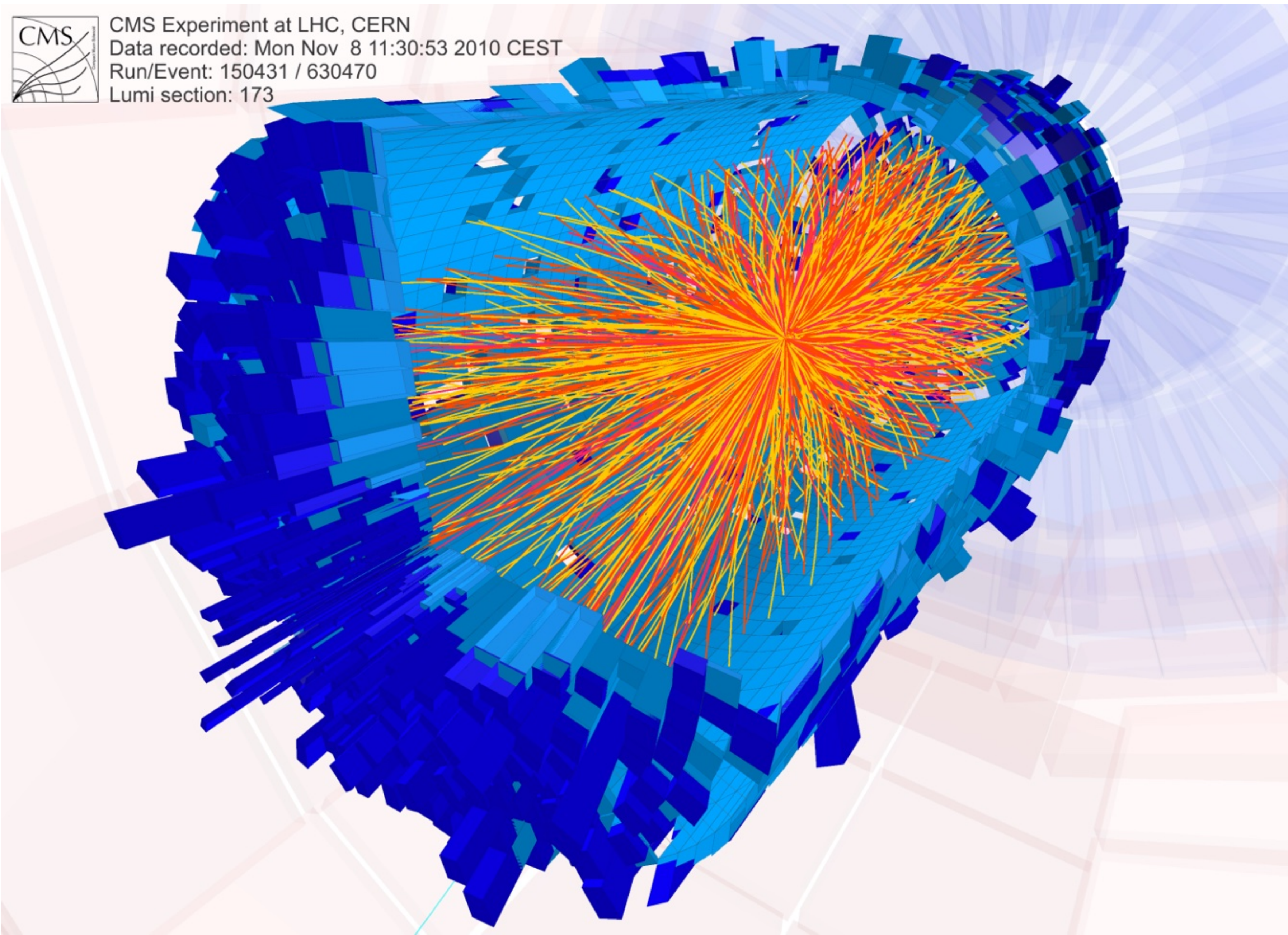
Particle yields for kaons, pions and protons:
$\frac{dN_\pi}{dy}, \frac{dN_K}{dy}, \frac{dN_p}{dy}$

Charged particle yield:
$dN_{ch}/d\eta$

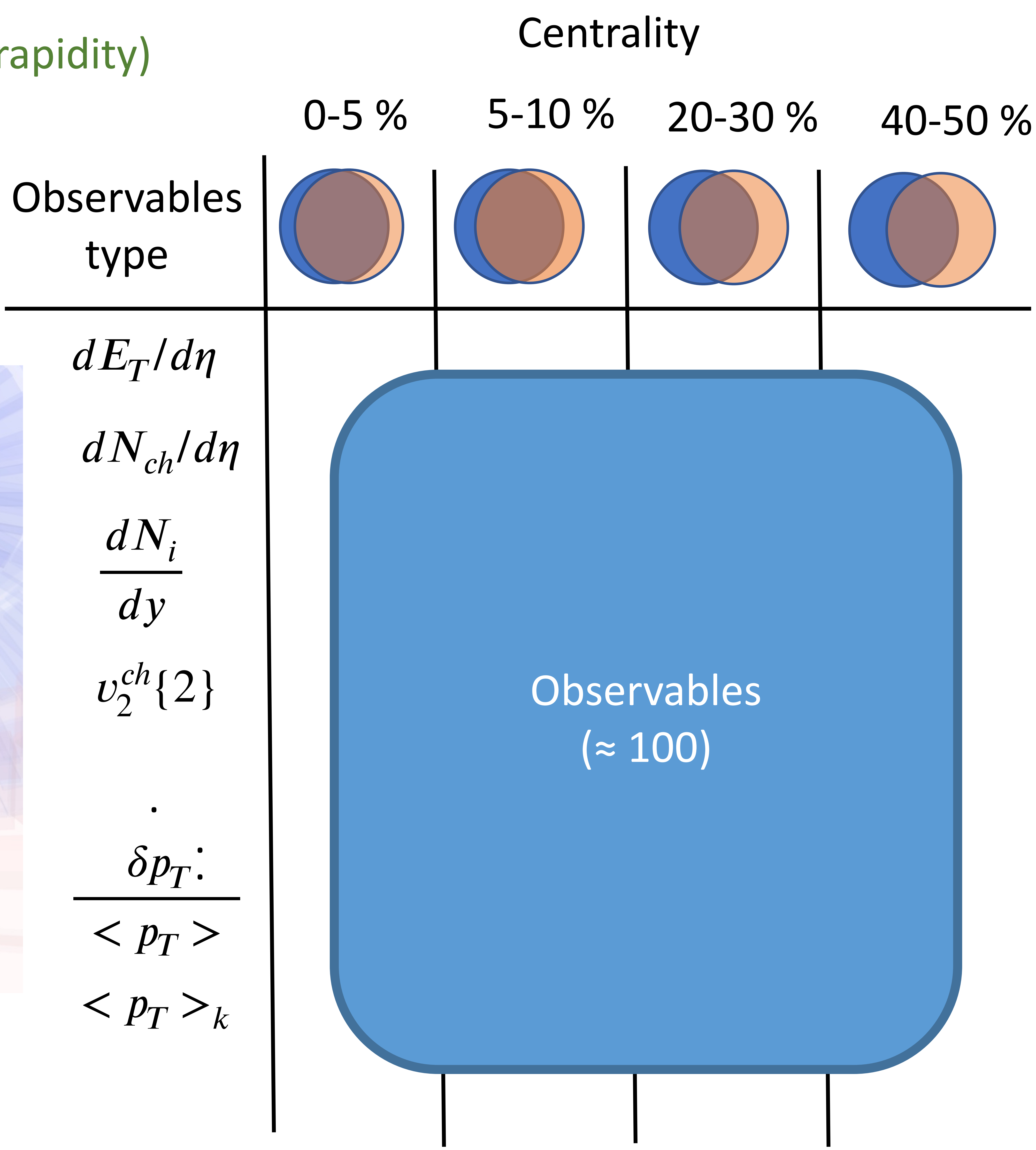
Mean transverse energy:
$dE_T/d\eta$

Elliptic, triangular and quadrangular flows:
$v_2^{ch}\{2\}, v_3^{ch}\{2\}, v_4^{ch}\{2\}$

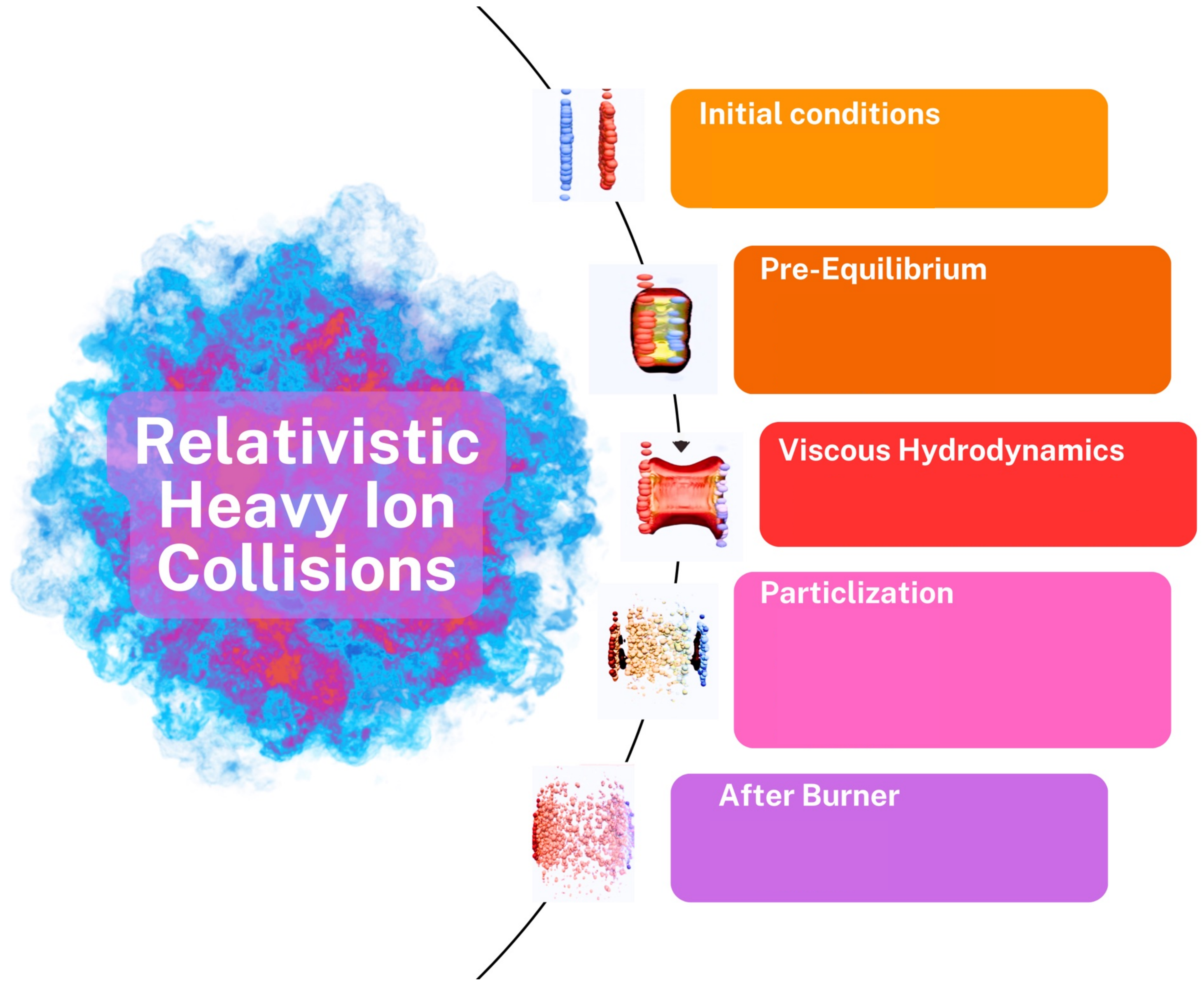
Mean transverse momentum fluctuations:
$\frac{\delta p_T}{< p_T >}$



Mean transverse momenta of kaons, pions, protons:
$\langle p_T \rangle \pi, \langle p_T \rangle K, \langle p_T \rangle p$



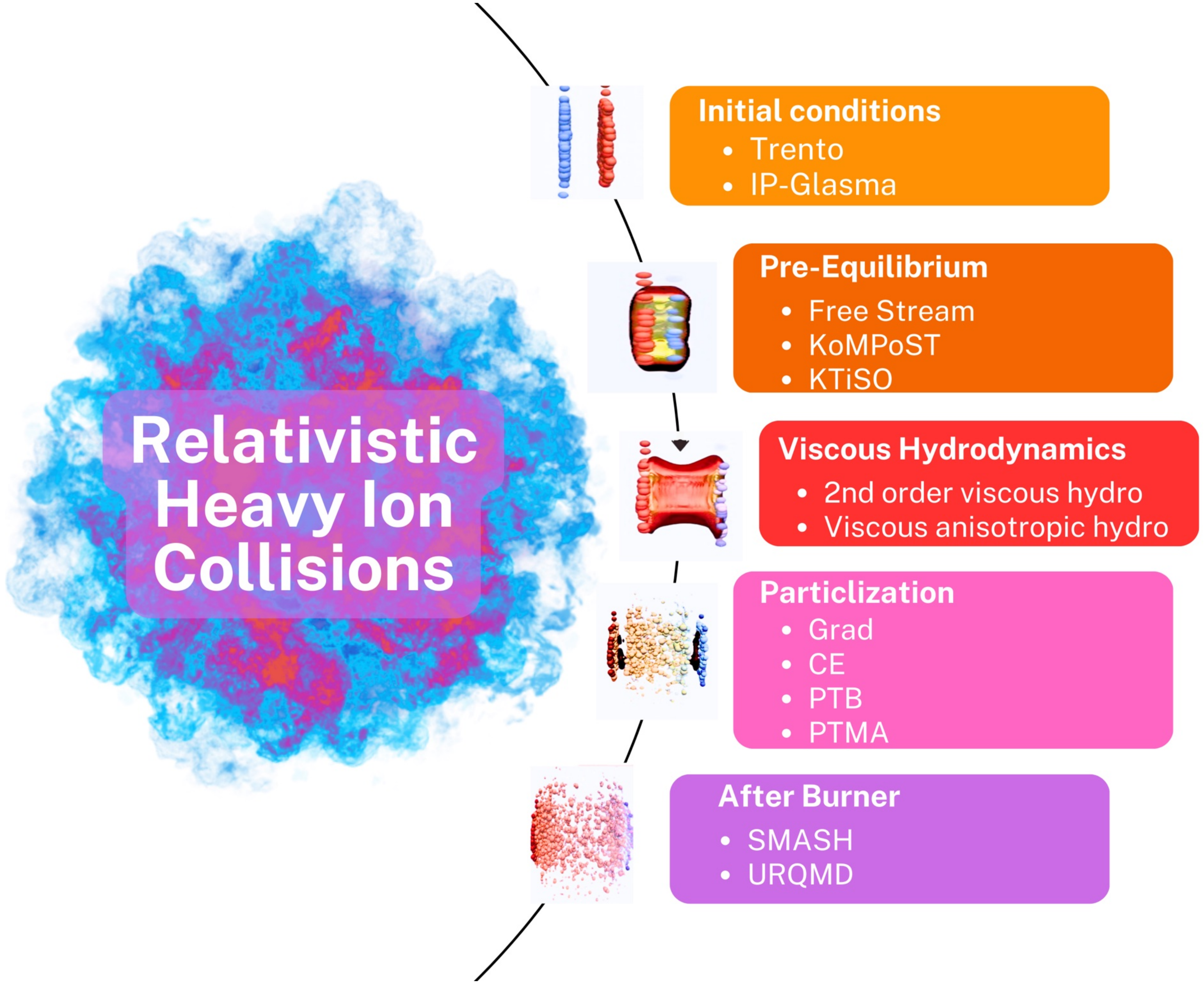
Simulation models



multi-stage models

Slide adapted from D. Liyanage

Simulation models



multi-stage models

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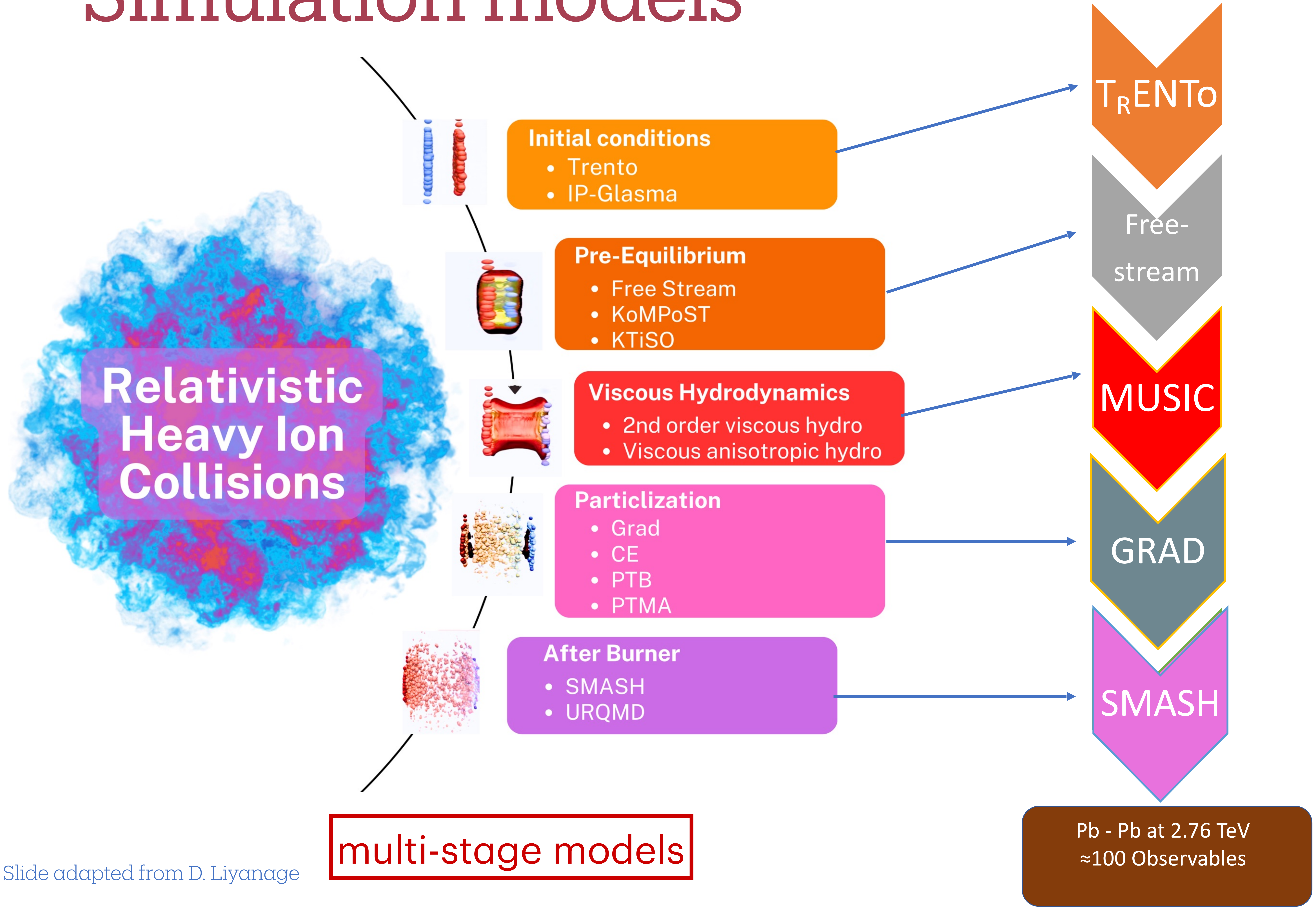
Simulation models

JETSCAPE SIMS calibration

D. Everett *et al.* 2010.03928, 2011.01430



multi-stage models

Slide adapted from D. Liyanage

Simulation models

Initial conditions
- Trento
- IP-Glasma

Pre-Equilibrium
- Free Stream
- KoMPoST
- KTiSO

Viscous Hydrodynamics
- 2nd order viscous hydro
- Viscous anisotropic hydro

Particlization
- Grad
- CE
- PTB
- PTMA

After Burner
- SMASH
- URQMD

multi-stage models

JETSCAPE SIMS calibration
D. Everett *et al.* 2010.03928, 2011.01430

TRENTo → Free-stream → MUSIC → GRAD → SMASH

Viscous Anisotropic Hydrodynamics Model
M. McNelis *et al.* 2101.02827
D. Liyanage *et al.* 2302.14184

VAH → PTMA

Pb - Pb at 2.76 TeV
≈100 Observables

Many more models..

iEBE-MUSIC
https://github.com/chunshen1987/iEBE-MUSIC

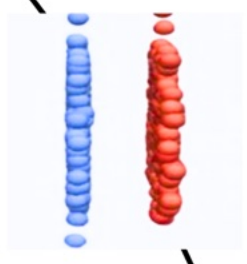
Trajectum
G. Nijs *et al.* 2010.15134

AMPT
Z. Lin *et al.* nucl-th/0411110

. . .

Slide adapted from D. Liyanage

Model parameters



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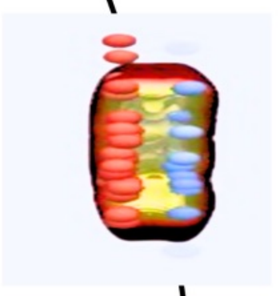

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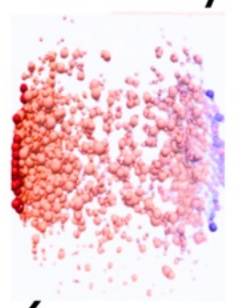

After Burner
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multi-stage models

JETSCAPE SIMS calibration

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T$_R$ENTo
- N : normalization
- p : generalized mean power
- w : nucleon width
- σ_k : multiplicity fluct. variance
- d_{min} : min. dist. betw. nucleons

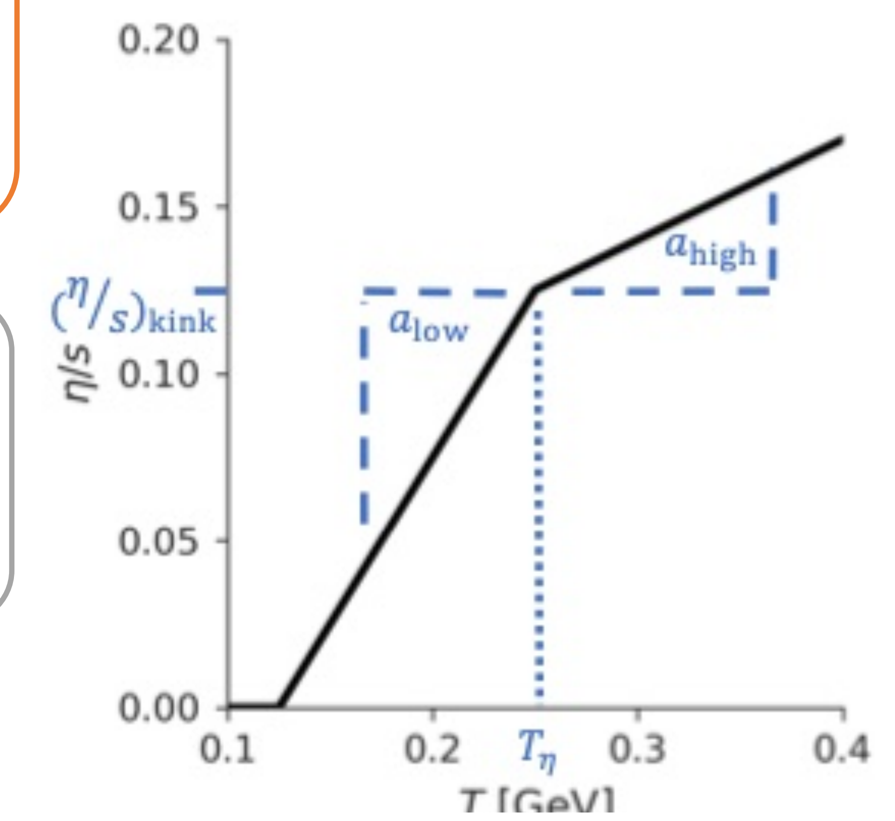
Free-stream
- τ_r : free-stream time scale
- α_s : energy density scaling of τ_r

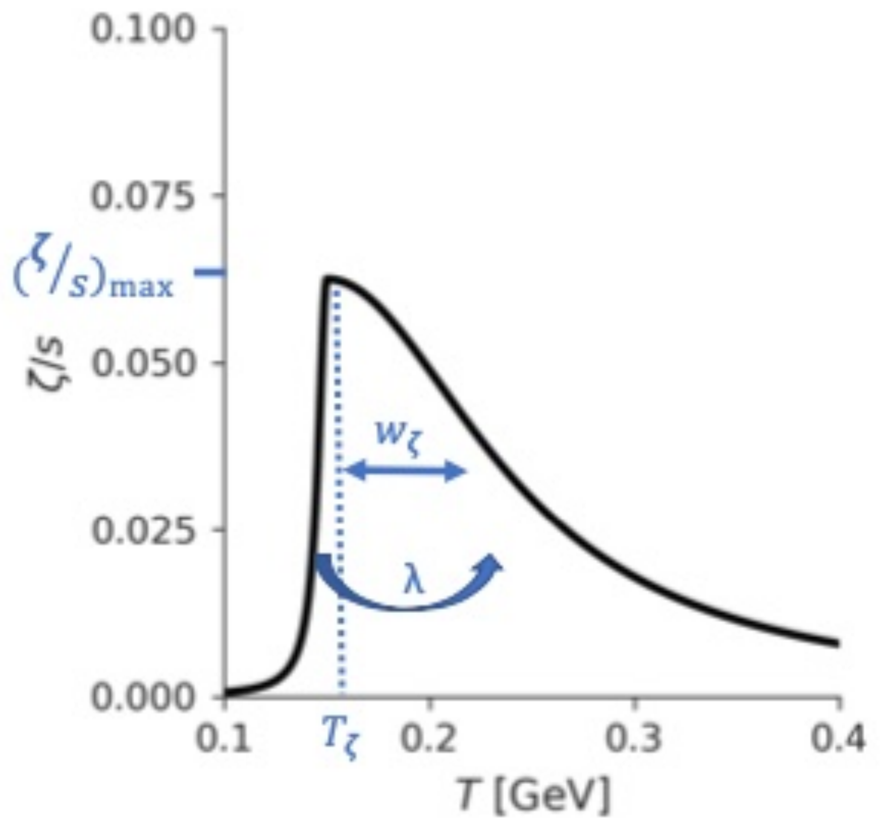
MUSIC
- T_{sw} : switching temperature
- $(\eta/s)(T)$: shear viscosity
- $(\zeta/s)(T)$: bulk viscosity

GRAD

SMASH

Pb - Pb at 2.76 TeV
≈100 Observables
≈15 model parameters





Slide adapted from D. Liyanage

Simulation models: typical numbers

- The model parameter θ is a vector of length ℓ (≈15).

- The multi-stage model is stochastic: For a given θ, model simulations $\mathbf{y}_{\mathrm{sim}}(\theta)$ results in distributions of d (≈100) observables of interest. **uncertain**

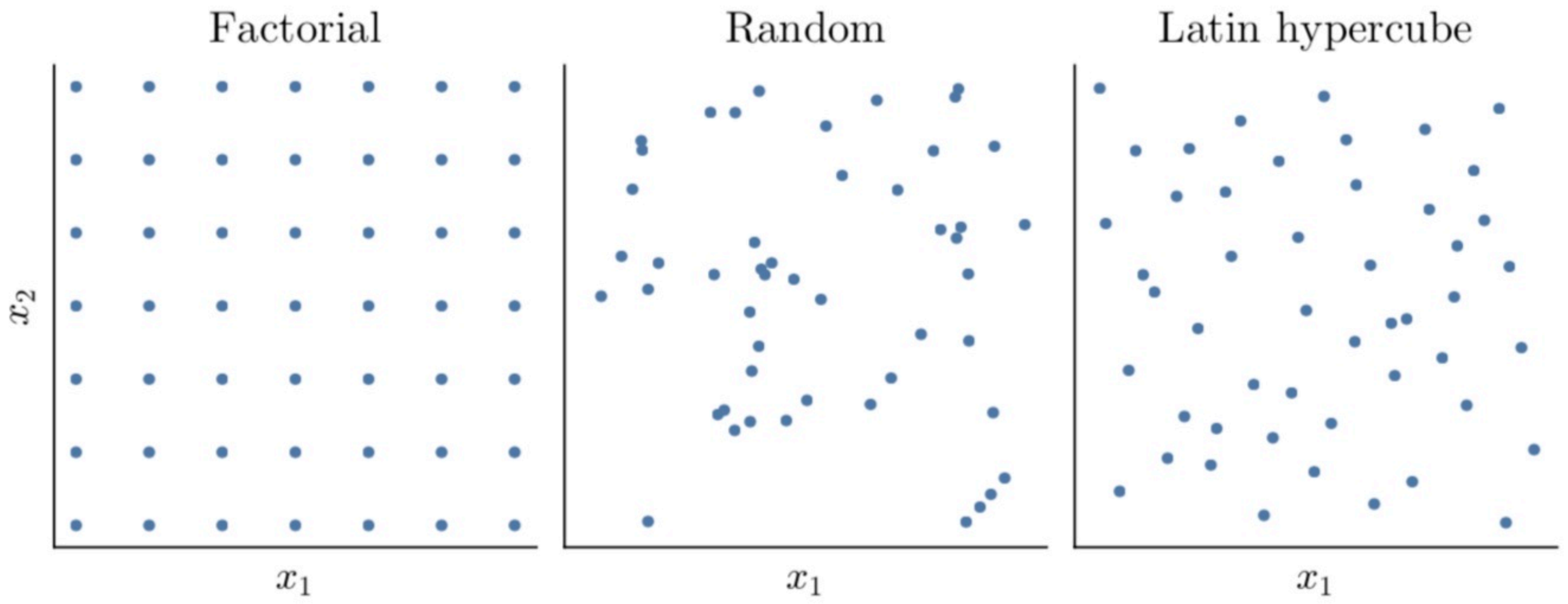
- Model is computationally expensive: ≈1000 CPU hours needed for a given parameter setting θ (≈3000 events for each θ). Many model observables still have large statistical uncertainty even after ≈1000 CPU hours. **expensive**

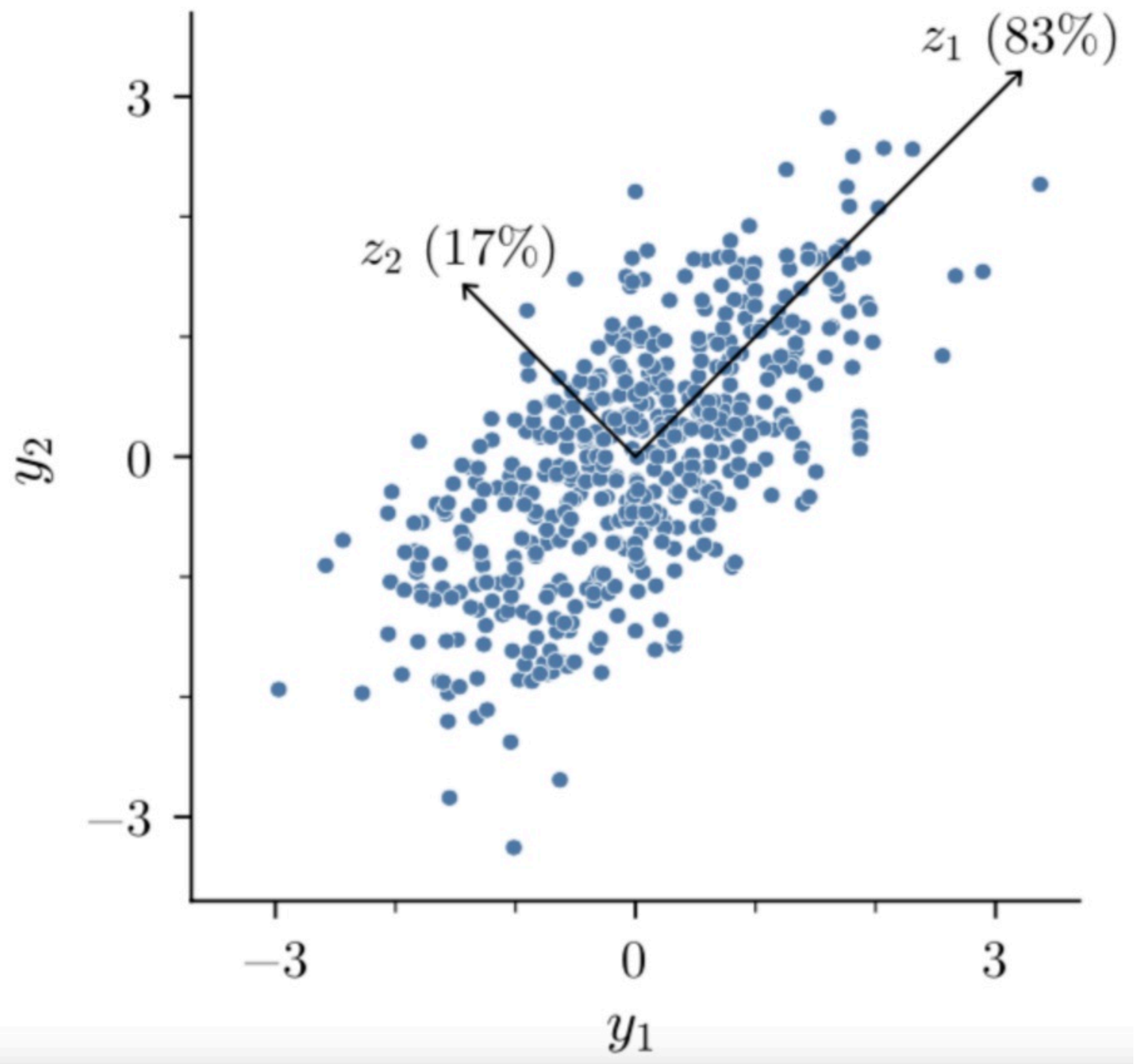
- Posterior inference requires model simulations at $> 10^6$ samples of parameter space. Inference is out of reach without emulation.

- Need for fast and accurate model surrogates to perform any Bayesian study.

Gaussian Process based model emulators

- We want emulators to "interpolate" in the ℓ (≈15) dimensional parameter space.
  - Consider the mean values of the d (≈100) distributions for each $\theta_\mathbf{i}$: $\bar{\mathbf{y}}_{\text{sim}}(\theta_\mathbf{i})$.
  - For n (≈1000) training set $\{\theta_\mathbf{1}, \ldots, \theta_\mathbf{n}\}$ (LHS), define a $n \times d$ matrix: $\Xi \equiv \{\bar{\mathbf{y}}_{\text{sim}}(\theta_\mathbf{1}), \ldots, \bar{\mathbf{y}}_{\text{sim}}(\theta_\mathbf{n})\}$
  - Standardize dataset by removing mean and scaling to unit variance for all d-distributions: $\Xi \to \tilde{\Xi}$
  - Principal Component Analysis → Reduce dimensionality of dataset
  - Transform by doing PCA and keep $p < d$ principal components. In most applications, $p \ll d$ is sufficient to describe almost all the variance in the original dataset.
- Train p independent Gaussian process corresponding to the p reduced observables (means). Each Gaussian process is ℓ (≈15) dimensional.





Emulator: Challenges

- GP training does not take into account the inherent stochastic uncertainty.
- Principal Component Stochastic Kriging (PCSK) takes into account the variance to some extent.

BAND SURMISE package
M. Plumlee, Ö. Sürer, S. Wild, M. Chan
https://surmise.readthedocs.io

D. Liyanage, Ö. Sürer *et al.* 2302.14184
Hendrik Roch, Syed Afrid Jahan, Chun Shen: 2405.12019

- We need a way to reduce dimensionality of dataset *consisting of distributions.*
- Efficient emulator training through Transfer Learning. D. Liyanage, *et.al.* (JETSCAPE Collaboration) 2201.07302
- Current status: model emulators are fast, but not precise (Next slide ⟶)

Comparison of different emulators

Hendrik Roch, Syed Afrid Jahan, Chun Shen: 2405.12019

- For Au-Au collision for 3 different $\sqrt{S_{NN}}$
- Overall 544 experimental observables

Error in prediction (mean):

$$\mathcal{E} \equiv \sqrt{\left\langle \left(\frac{\text{prediction} - \text{truth}}{\text{truth}} \right)^2 \right\rangle}$$

PCGP, PCSK

BAND `SURMISE` package

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https://surmise.readthedocs.io

970 training sets. 30 validation sets

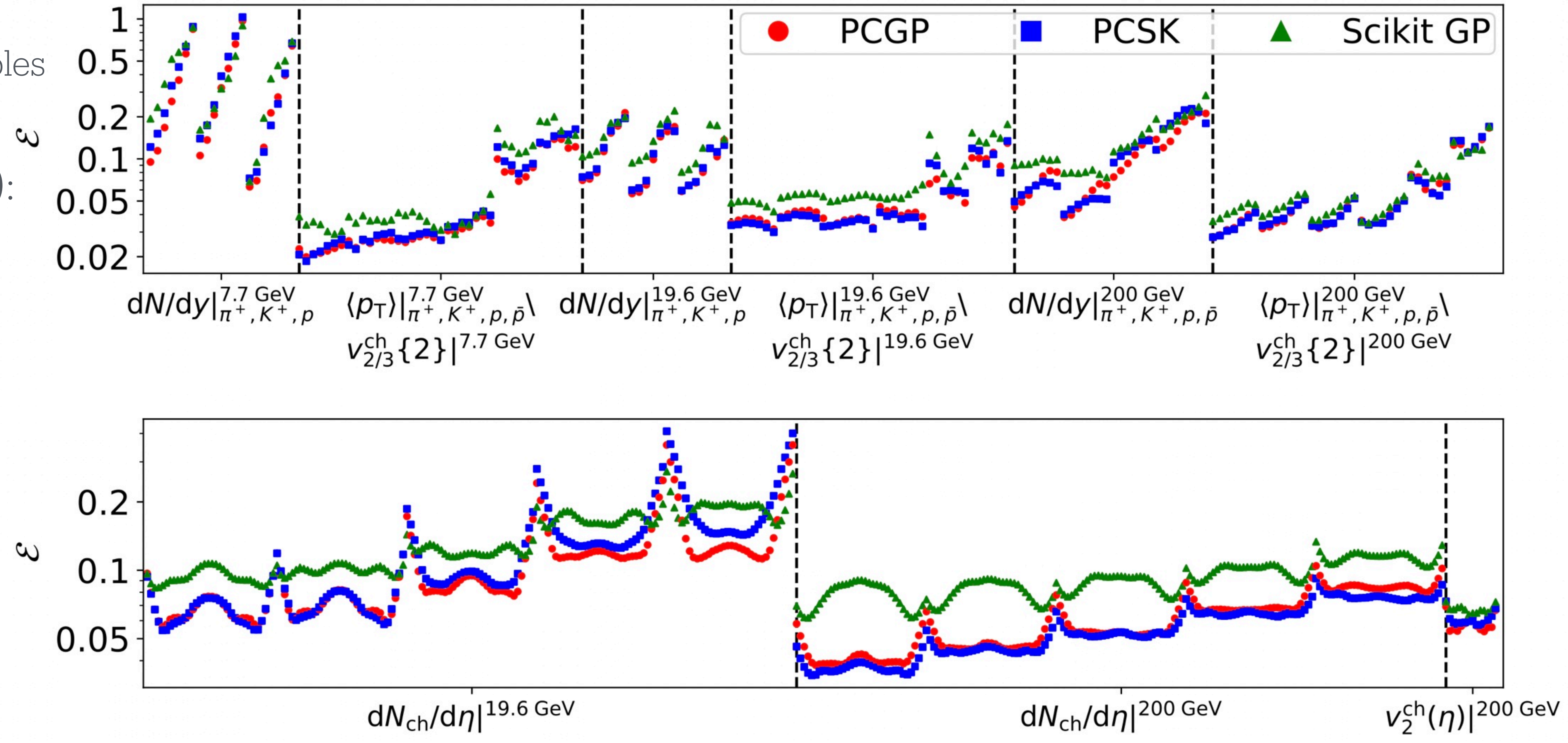

FIG. 2. (Color Online) The averaged RMS errors $\mathcal{E}$ for the three different types of GP emulators. Different training sets are separated by black lines. All emulators are trained with the same 970 LHD points.

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Normalized residuals:

$$\mathcal{H} \equiv \ln\left(\sqrt{\left\langle\left(\frac{\text{prediction} - \text{truth}}{\text{prediction uncertainty}}\right)^2\right\rangle}\right).$$

For an accurate prediction, we expect the values of $\mathcal{E} \to 0$ and $\mathcal{H} \to 0$. In the case where $\mathcal{H} > 0$, the emulator gives uncertainties that are too small compared to the actual error away from the true values; when $\mathcal{H} < 0$, the returned uncertainty estimates are too conservative.

Better metric for comparison can be KL divergence

970 training sets. 30 validation sets

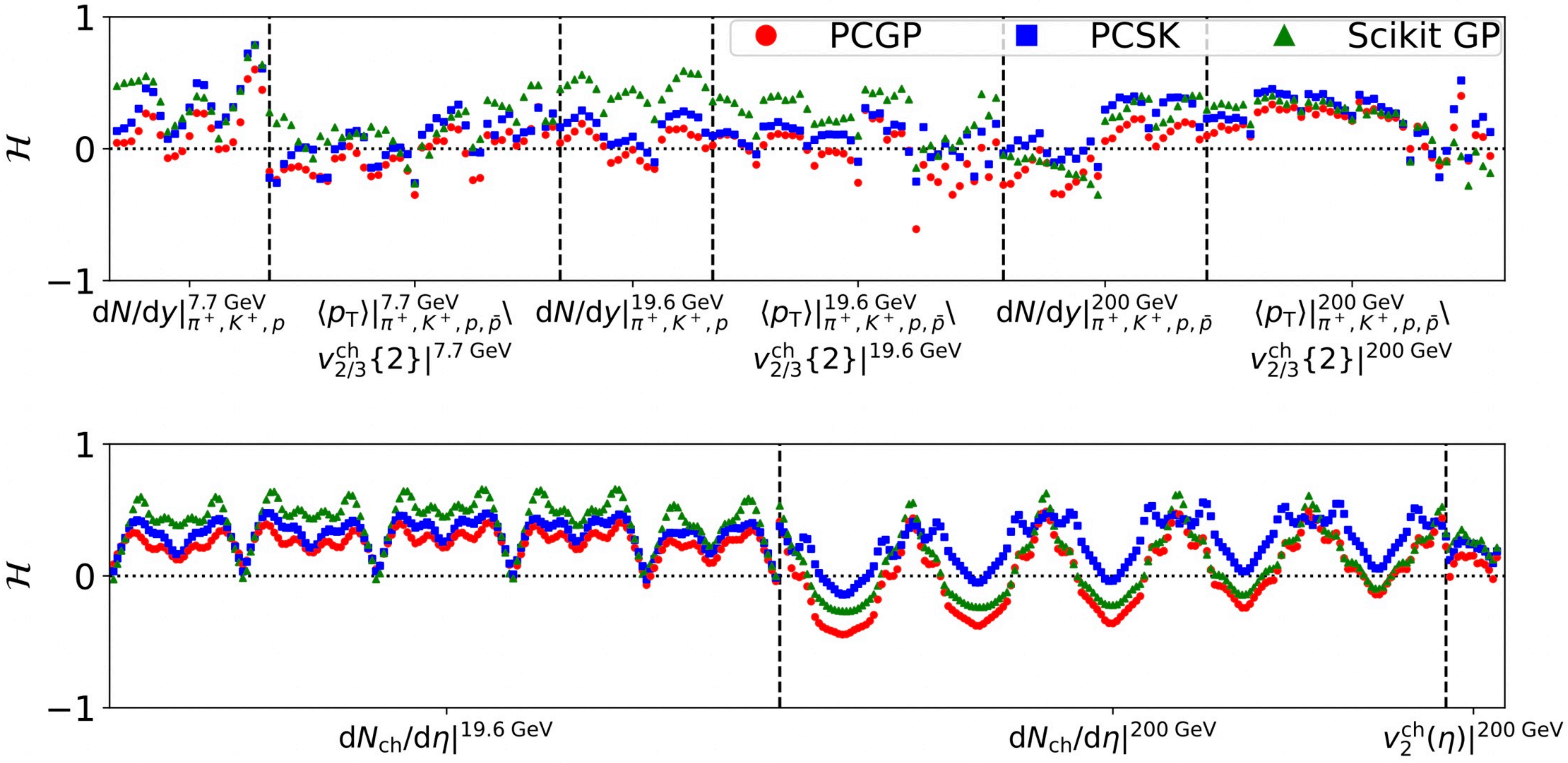
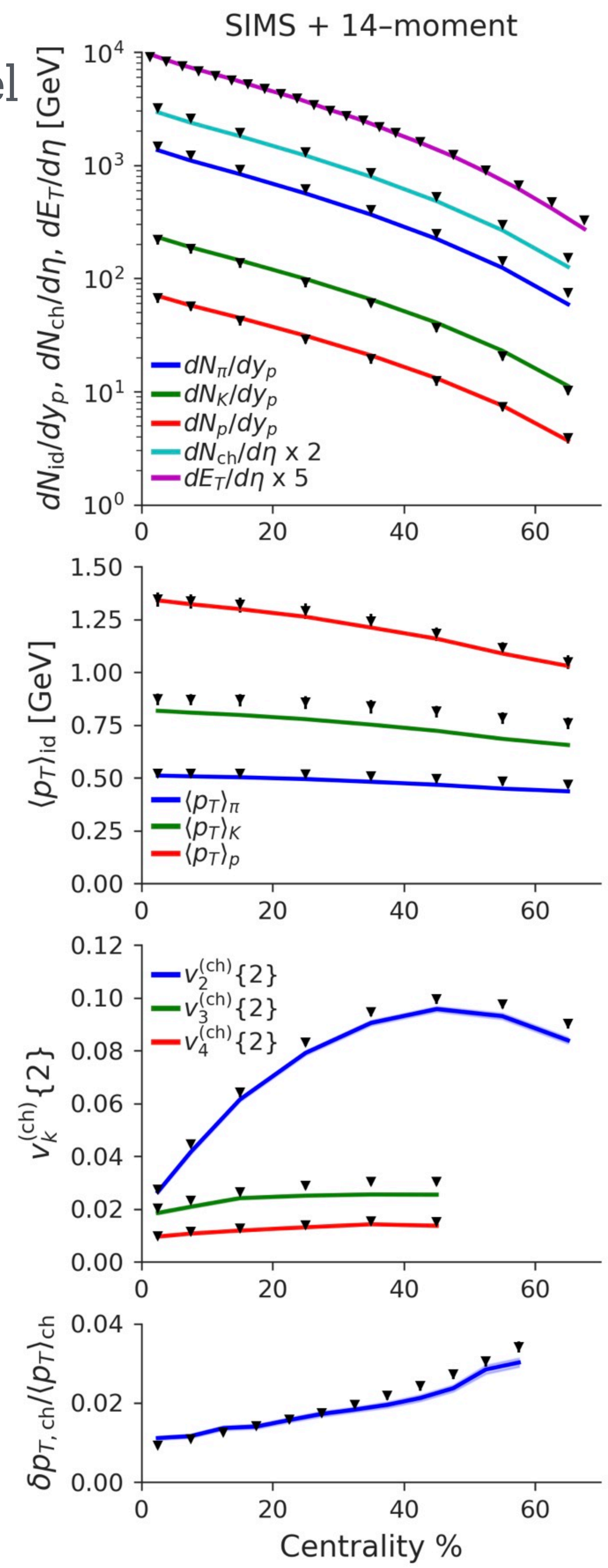


FIG. 3. (Color Online) The metric for emulator uncertainty estimation $\mathcal{H}$ for the three different types of GP emulators. Black lines separate different training sets. All emulators are trained with the same 970 LHD points.

Model prediction

Best fit (MAP) output from the calibrated Models:

Scikit GP
RBF kernel



D. Everett et al. (JETSCAPE Collaboration), Phys. Rev. C 103, 054904 (2021)

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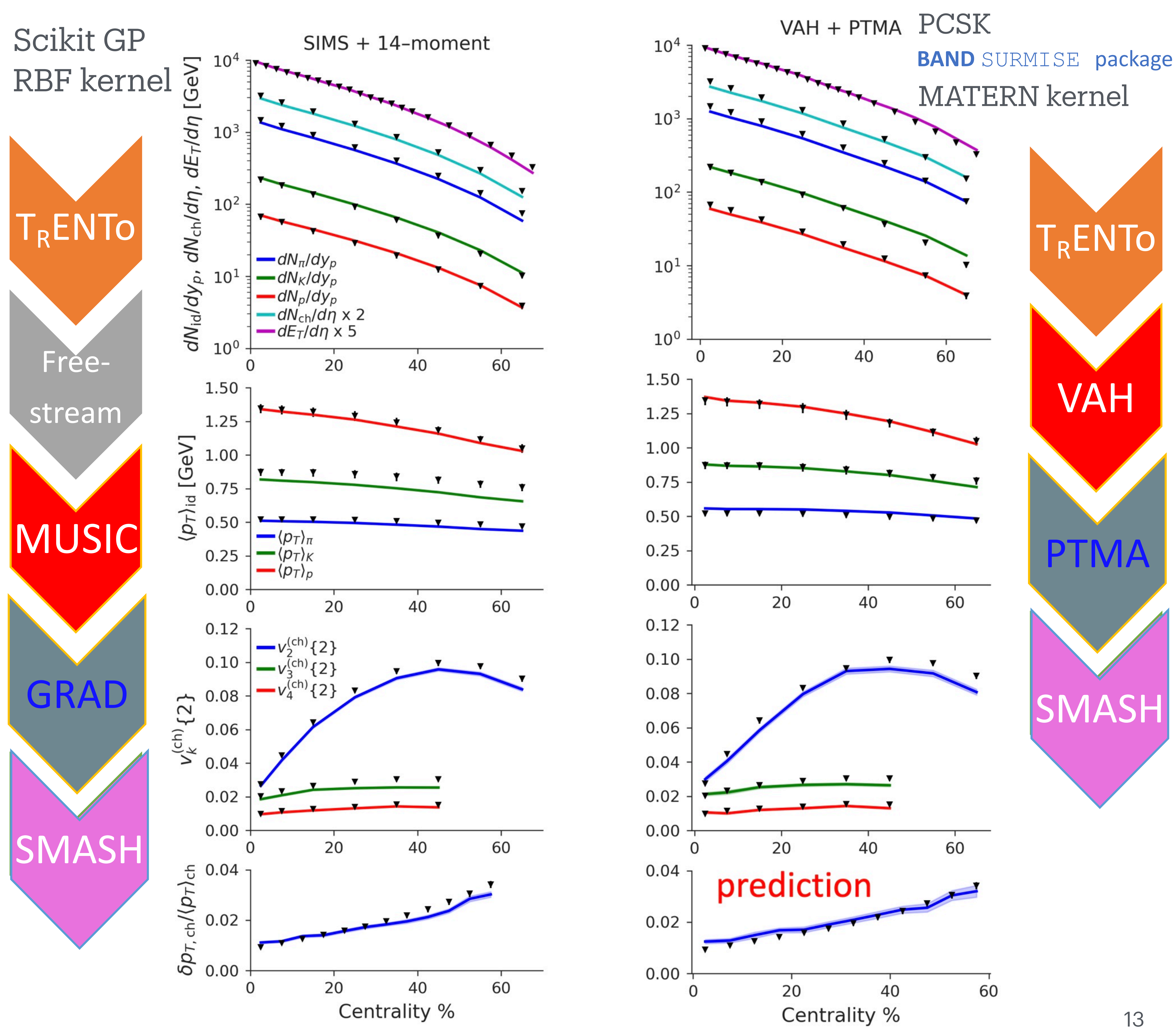

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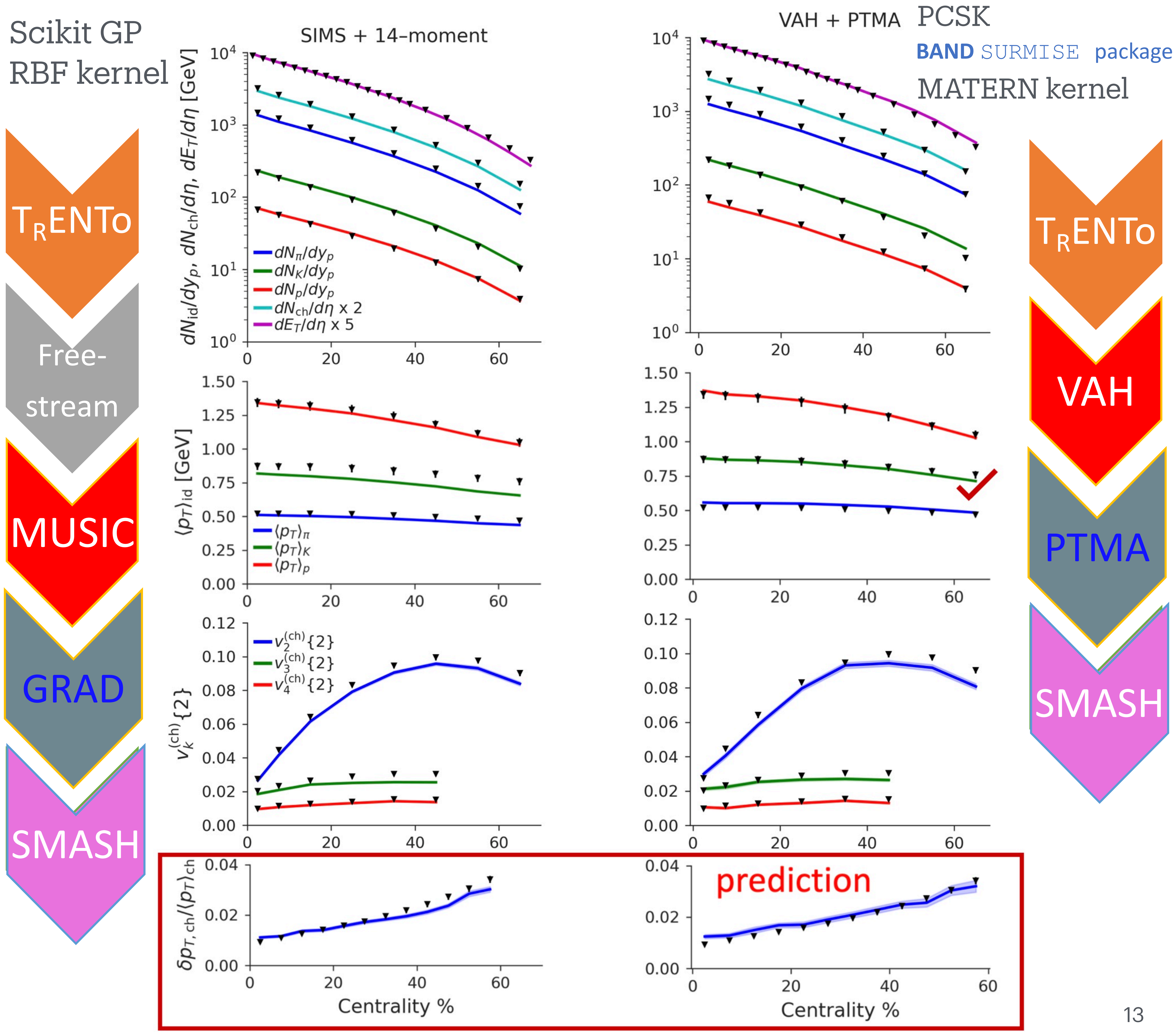

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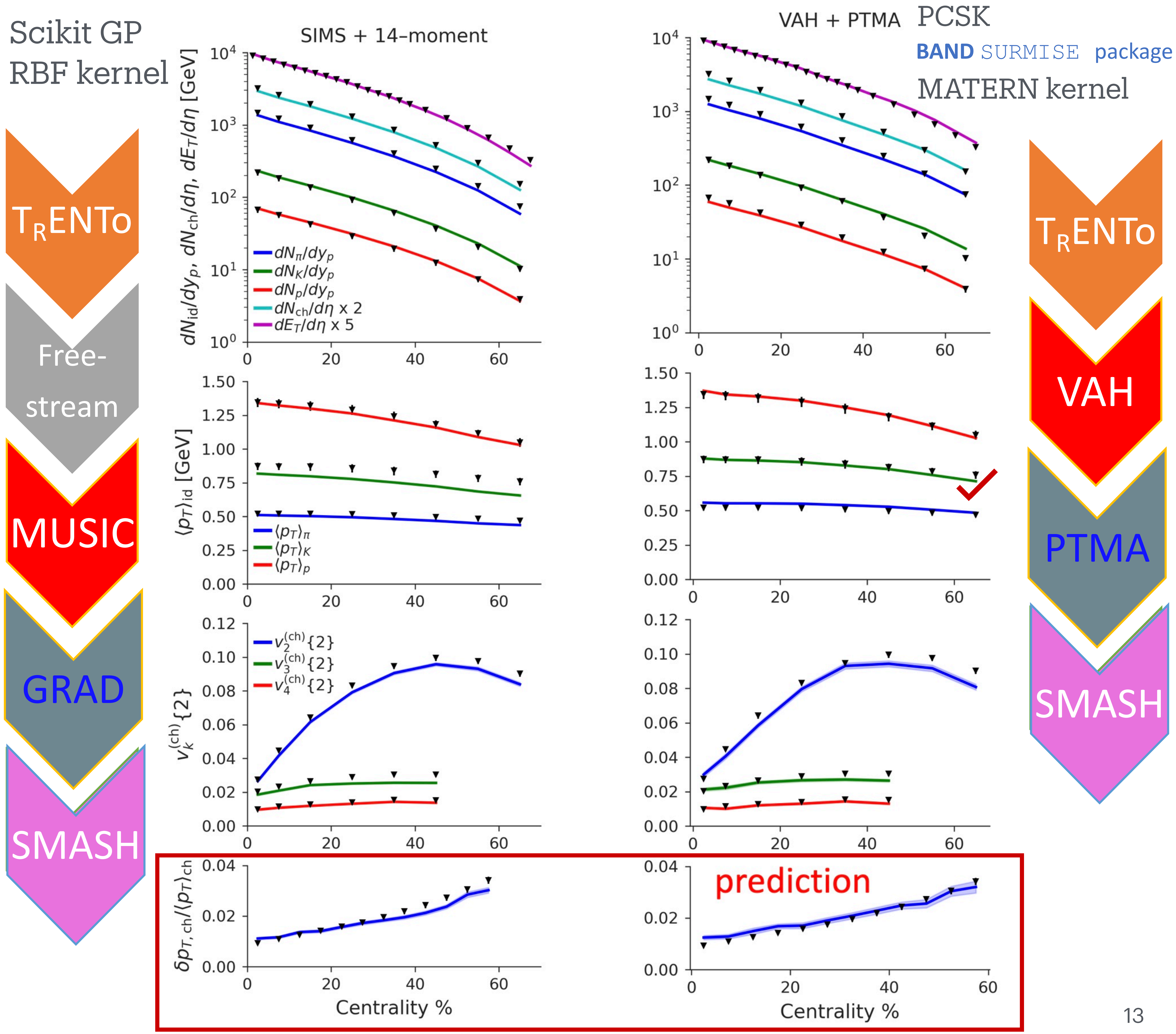
- MAP predictions for VAH+PTMA are in better agreement with SIMS+14-moment model.
- Our aim — Correct inference of physical parameters.



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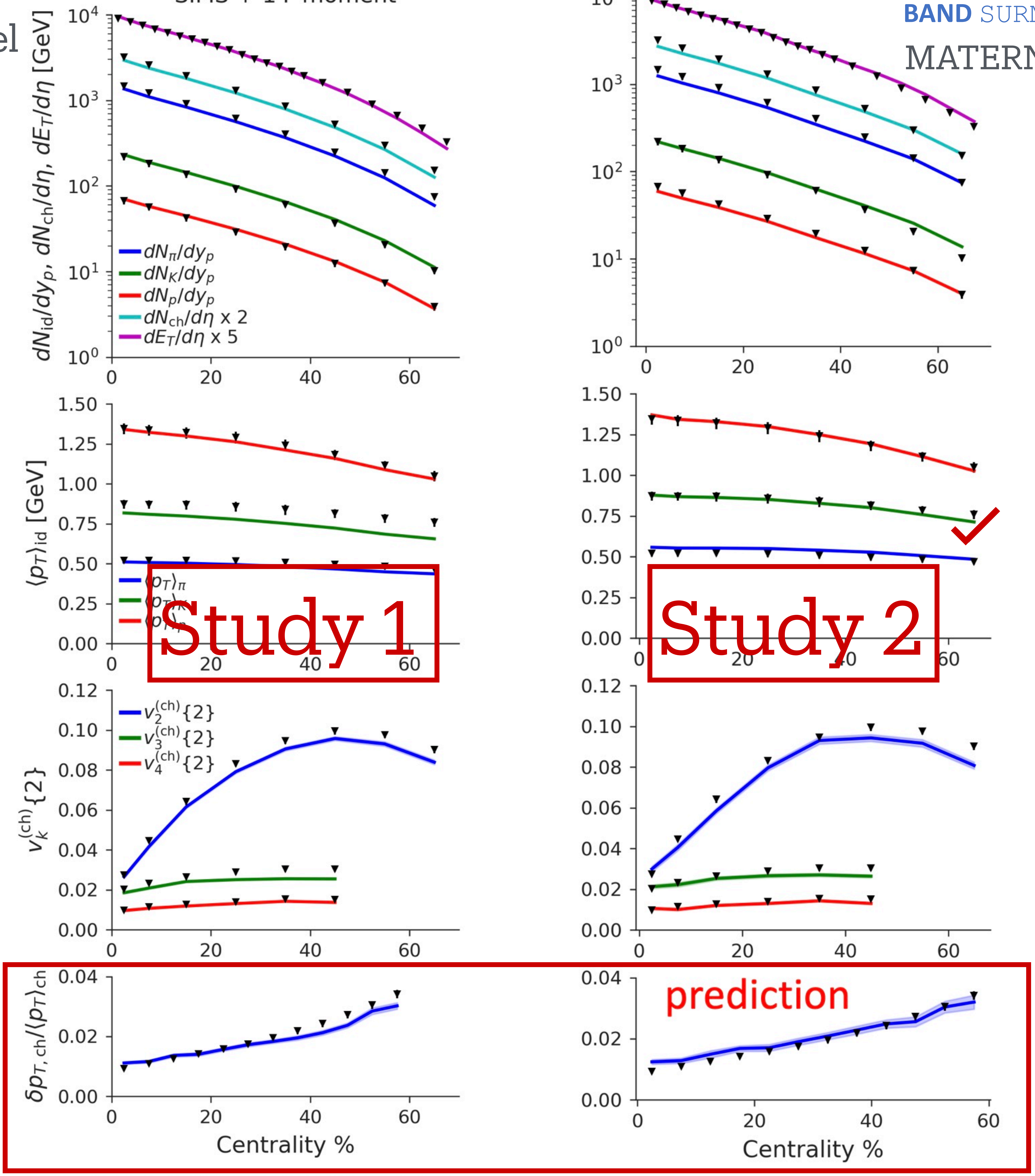

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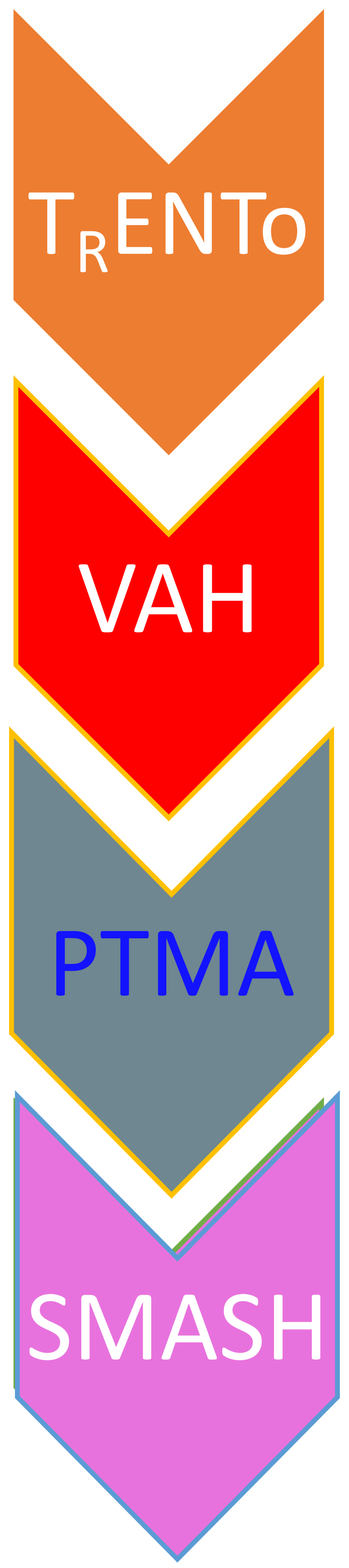

D. Everett et al. (JETSCAPE Collaboration), Phys. Rev. C 103, 054904 (2021)

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JETSCAPE SIMS model parameters

D. Everett et al. (JETSCAPE Collaboration),
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Pb - Pb at 2.76 TeV
≈100 Observables
≈15 model parameters

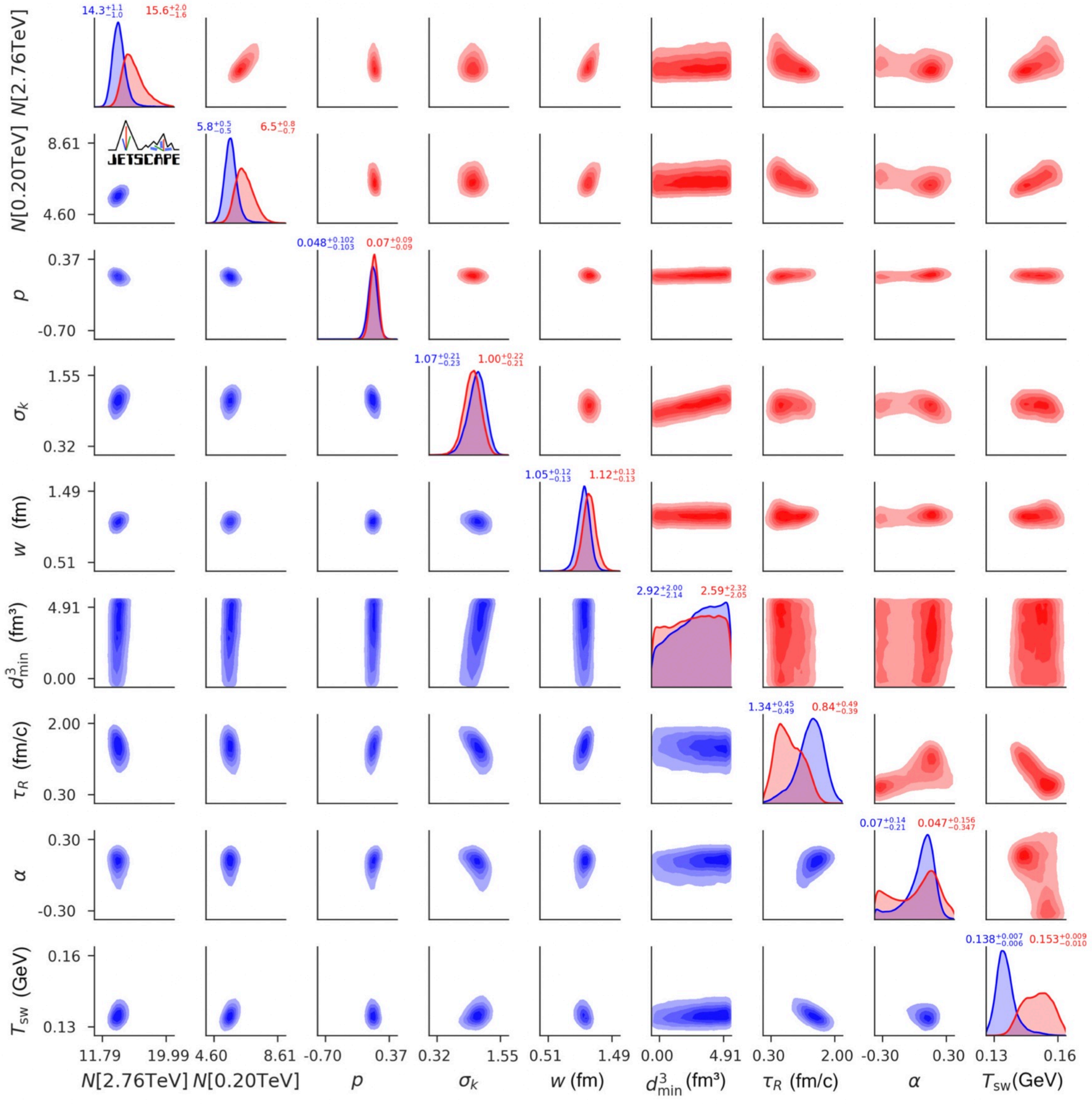

FIG. 10. The posterior for Grad (blue) and Chapman-Enskog (red) viscous corrections for select parameters related to the initial state, prehydrodynamic evolution, and switching temperature. The histograms on the diagonal are the marginal distributions for each parameter,

- Two different viscous corrections: 14-moment Grad, CE

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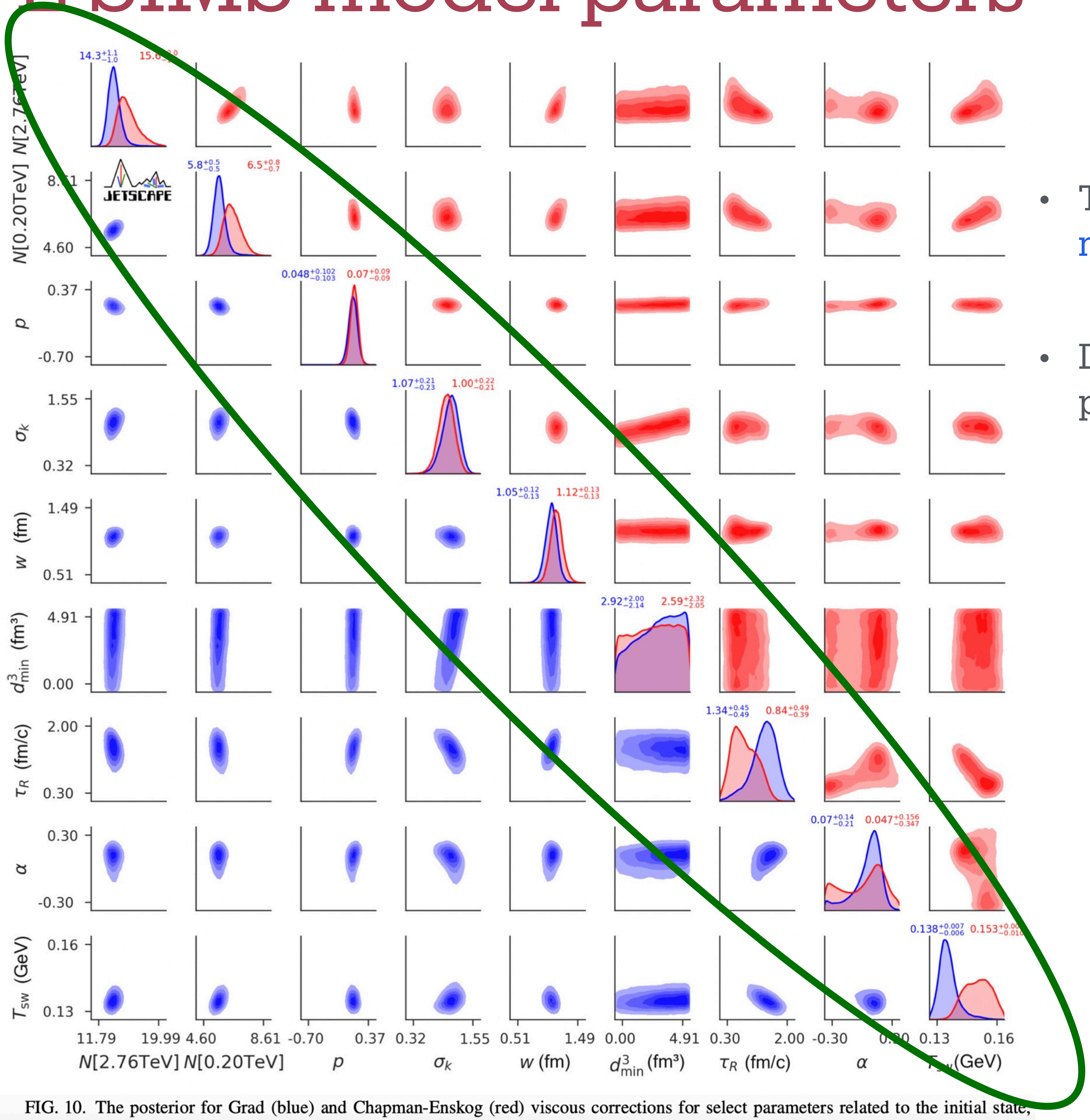

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- Different posterior distributions of the parameters for the two different schemes.

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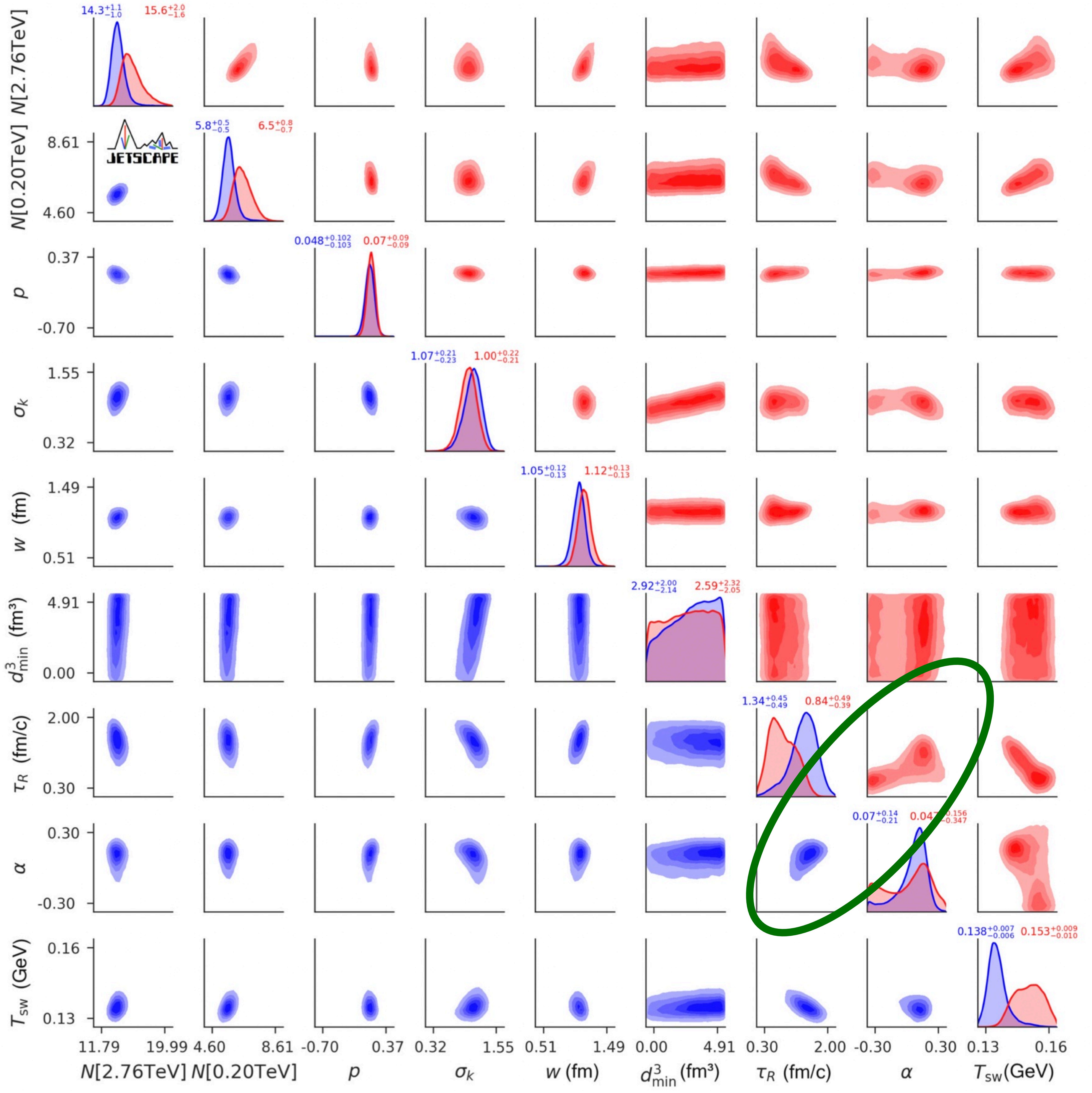

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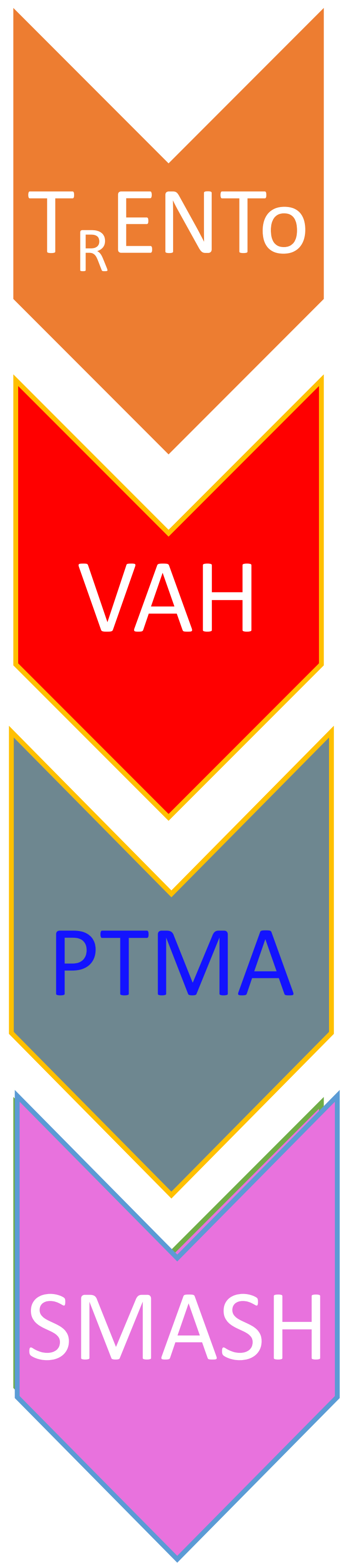
- Two different viscous corrections: 14-moment Grad, CE
- Different posterior distributions of the parameters for the two different schemes.
- Correlation between parameters also differ.
  Note: rotate red contours by 90 degrees for comparison with blue.

VAH+PTMA model parameters

D. Liyanage *et al.*, 2302.14184



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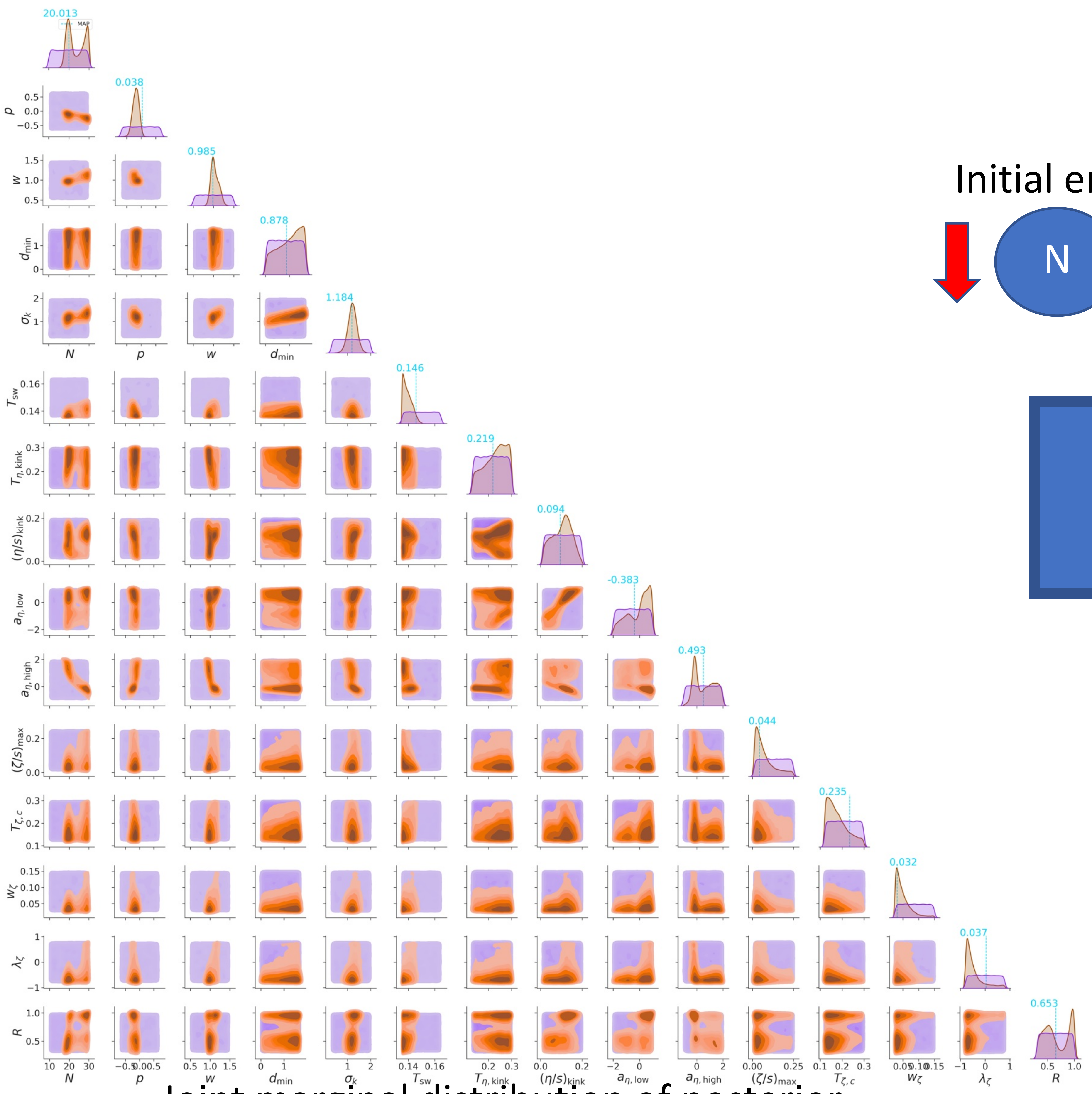
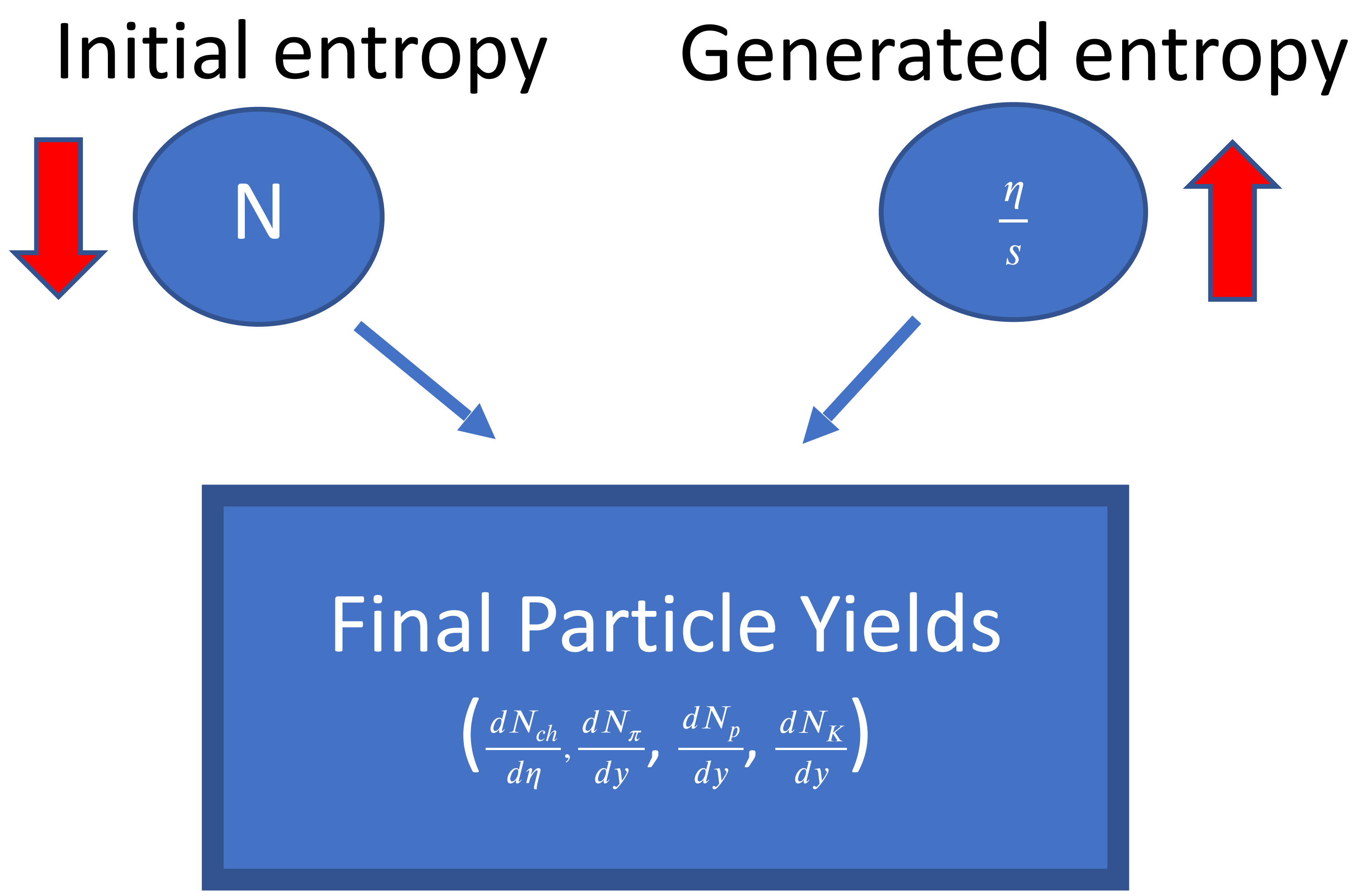


Joint marginal distribution of posterior

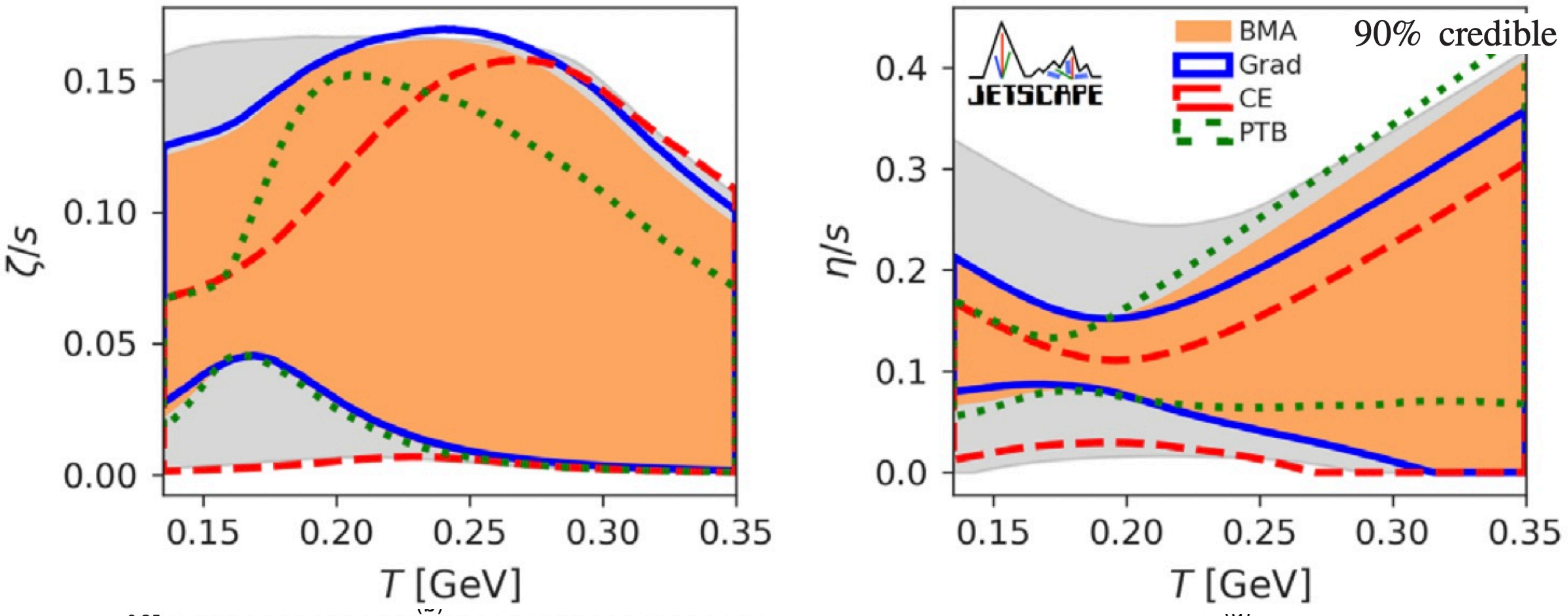


- Posterior distributions of the common parameters differ substantially from the JETSCAPE SIMS model

Tension between different studies

Coefficient of bulk viscosity: ζ

Coefficient of shear viscosity: η



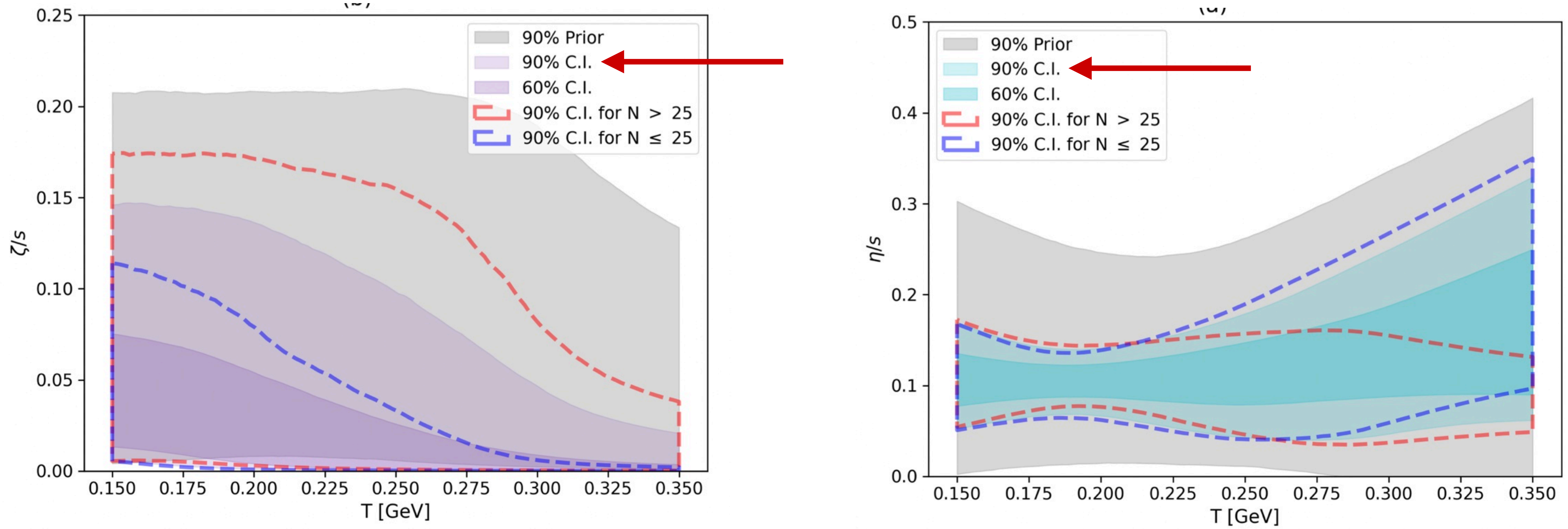
JETSCAPE SIMS calibration

D. Everett *et al.* 2010.03928, 2011.01430

Three different models: Grad, CE, PTB

η/s seems to be in agreement

ζ/s varies for different studies



Viscous Anisotropic Hydrodynamics Model

M. McNelis *et al.* 2101.02827
D. Liyanage, O. Surer, *et al.* 2302.14184

Accounting for theoretical uncertainties: Model discrepancy

- All models are approximations of reality and should only be used within their valid domains to fit experimental data. Extending a model beyond its intended scope leads to incorrect parameter values, making them mere fitting variables. Therefore, it is crucial to account for the theory's uncertainty.

- Consideration of theoretical uncertainties for the complex multi-stage heavy-ion models are beyond current theoretical capabilities. We need a statistical framework to model this uncertainty.

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- Possible framework: GP based model discrepancy by O'Hagan *et. al.*

M. Kennedy, A. O'Hagan, Bayesian calibration of computer models, https://doi.org/10.1111/1467-9868.00294

D. Higdon, M. Kennedy, *et. al.*, https://doi.org/10.1137/S1064827503426693

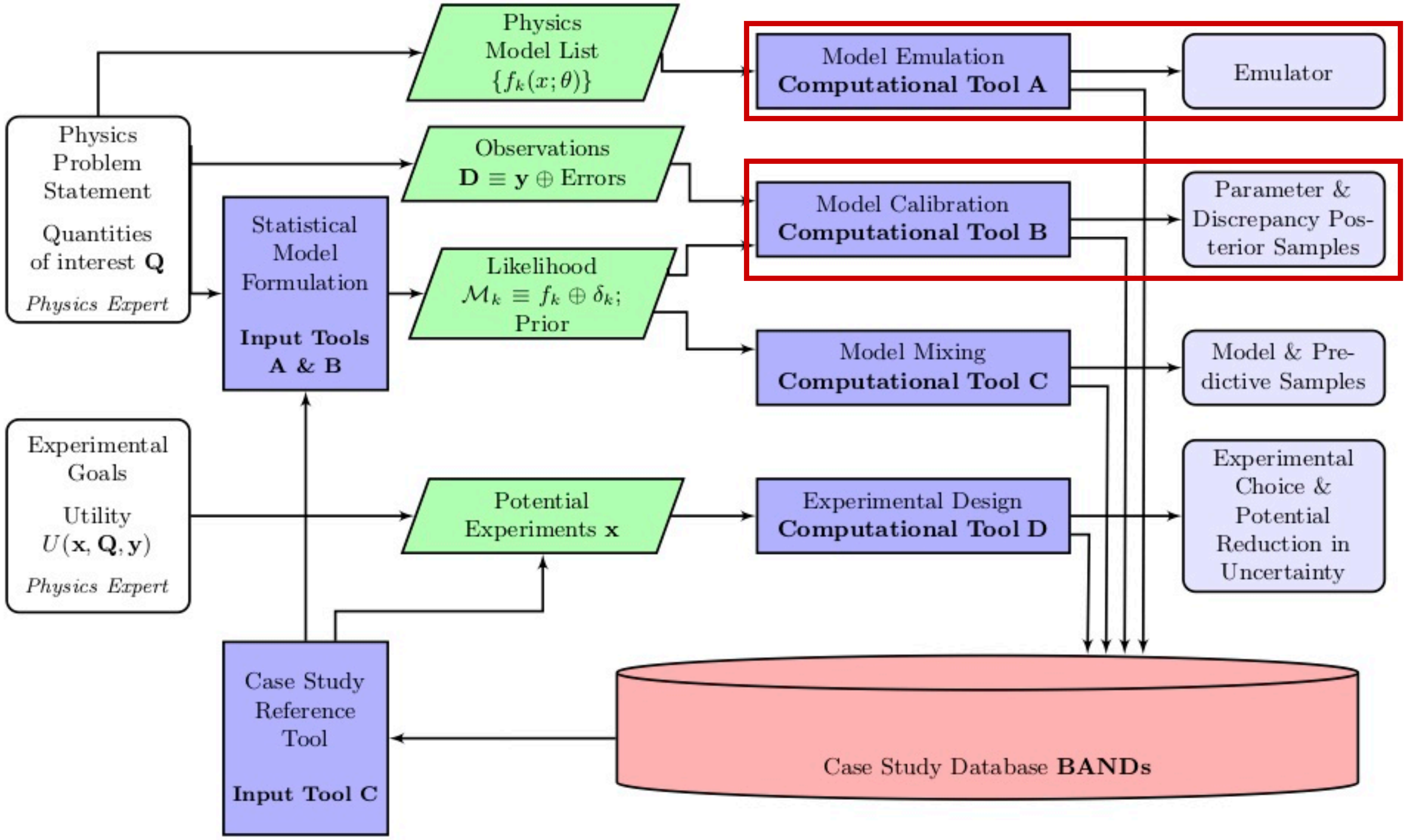
$$\underbrace{y(x_i)}_{\text{Physical observation}} = \underbrace{\eta(x_i, \theta)}_{\text{Model}} + \underbrace{\delta(x_i)}_{\text{Accounts for discrepancy between model and truth}} + \underbrace{\epsilon(x_i)}_{\text{Observation error}}$$

Model $\delta(x_i)$ as a gaussian process. Choice of covariance kernel motivated from the physics.

Work in progress...

Challenges

- Expensive heavy-ion model simulations demands fast and accurate model emulators.
- Quantifying theoretical uncertainties is a *necessity* for correct parameter estimation.

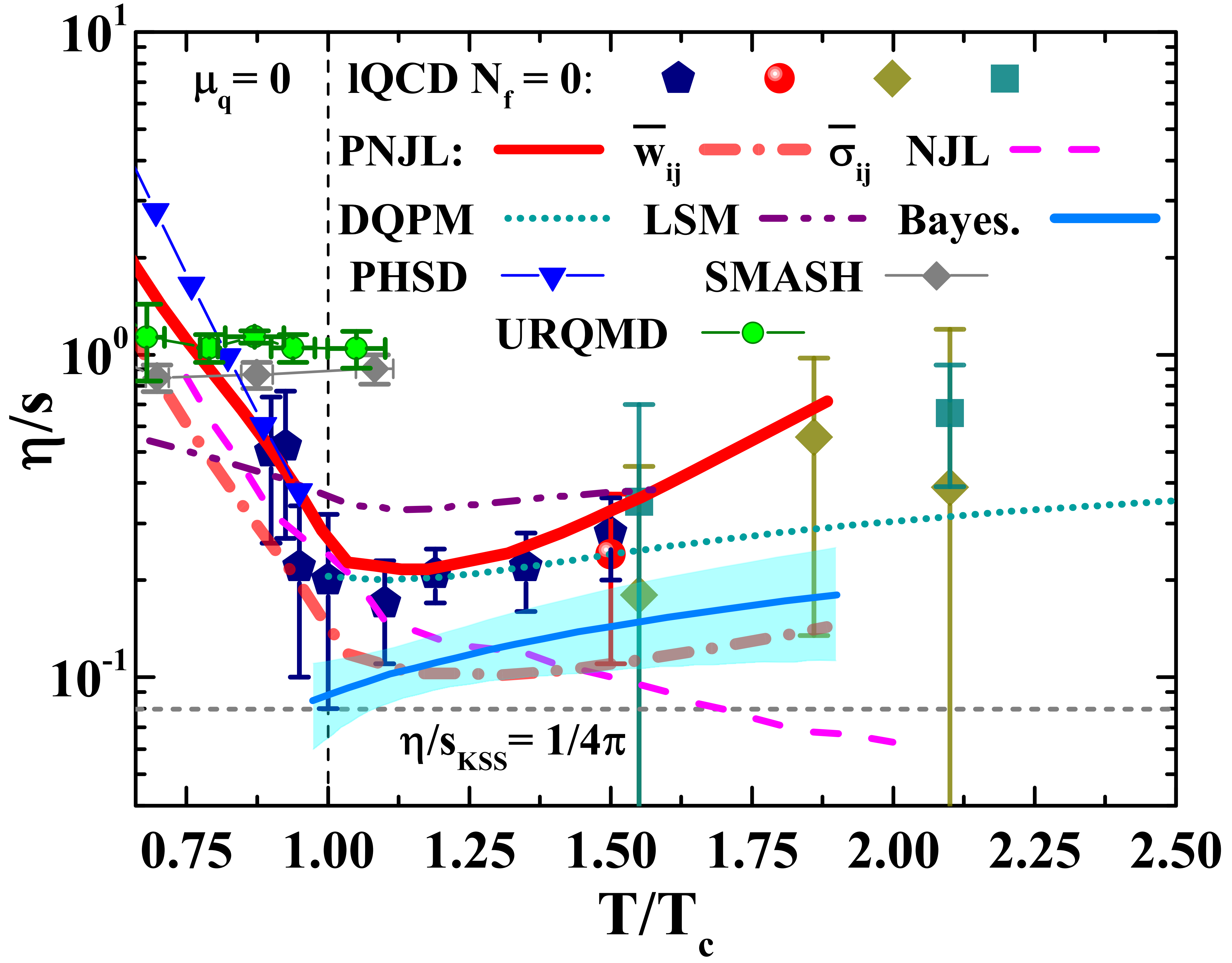


Bayesian Analysis of Nuclear Dynamics

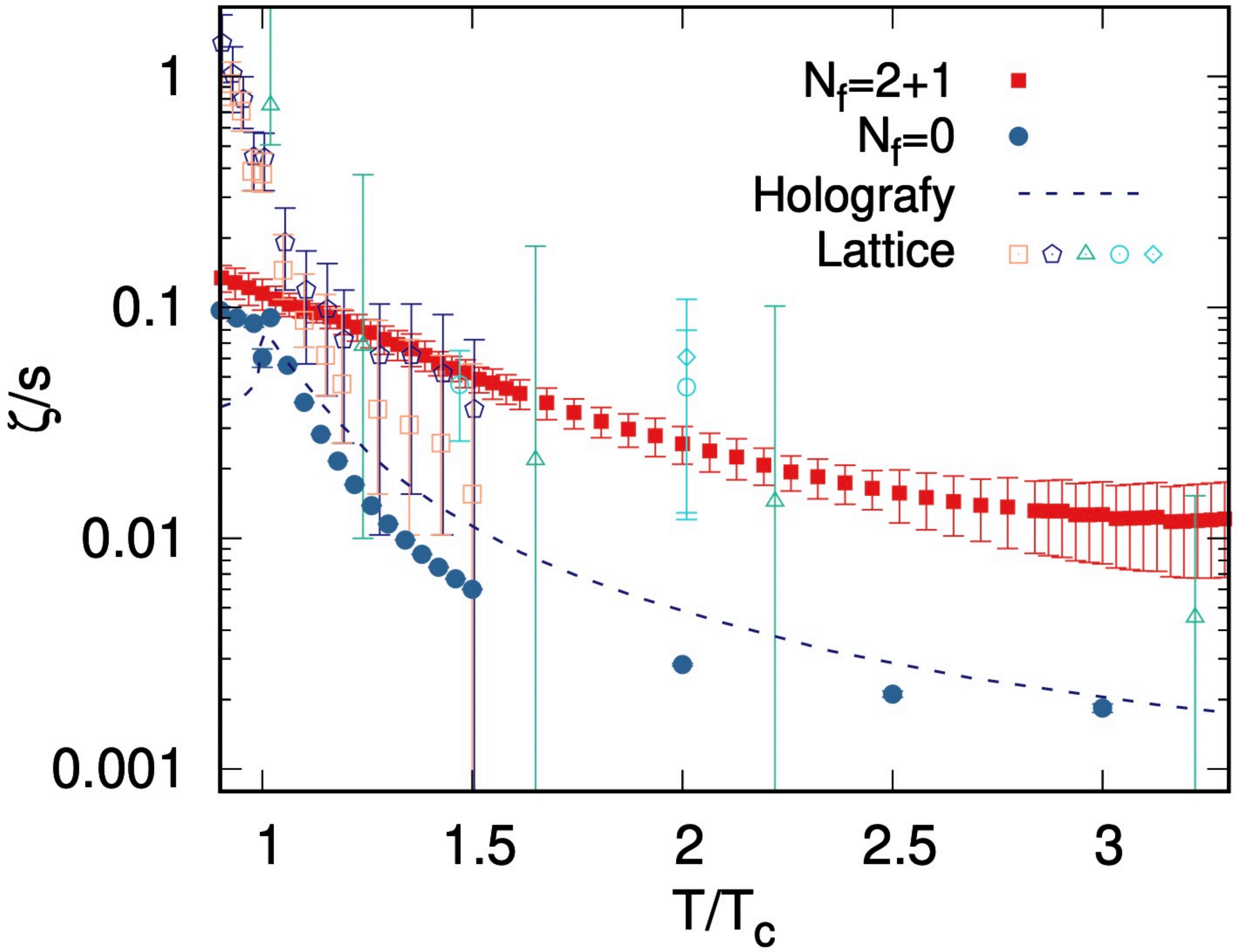
Thank You!

Backup

Transport coefficients from different calculations



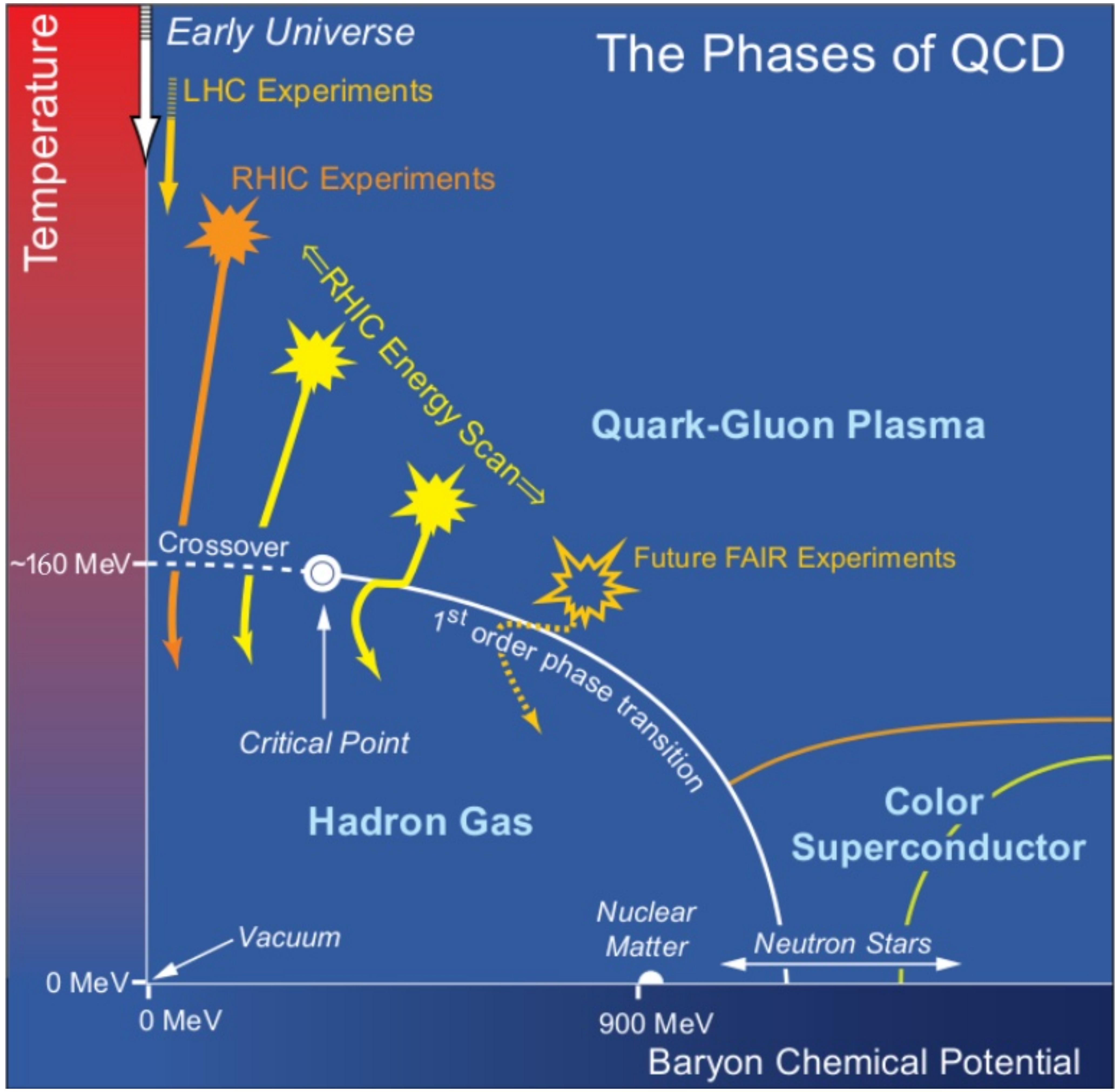
O. Soloveva, D. Fuseau, J. Aichelin, E. Bratkovskaya, 2011.03505



Valeriya Mykhaylova Thesis

Large Uncertainties

QCD phase diagram

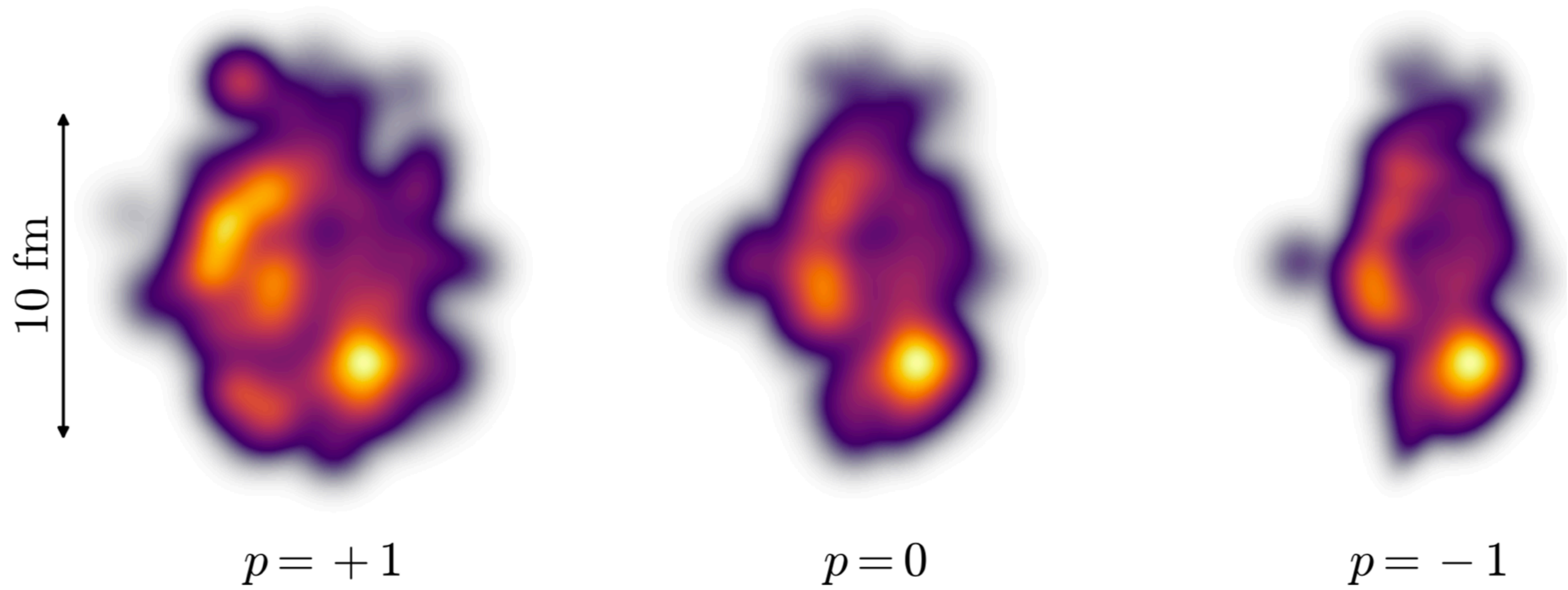


Foka, Panagiota *et al* - arXiv:1702.07233

Initial Energy Deposition (TRENTO)

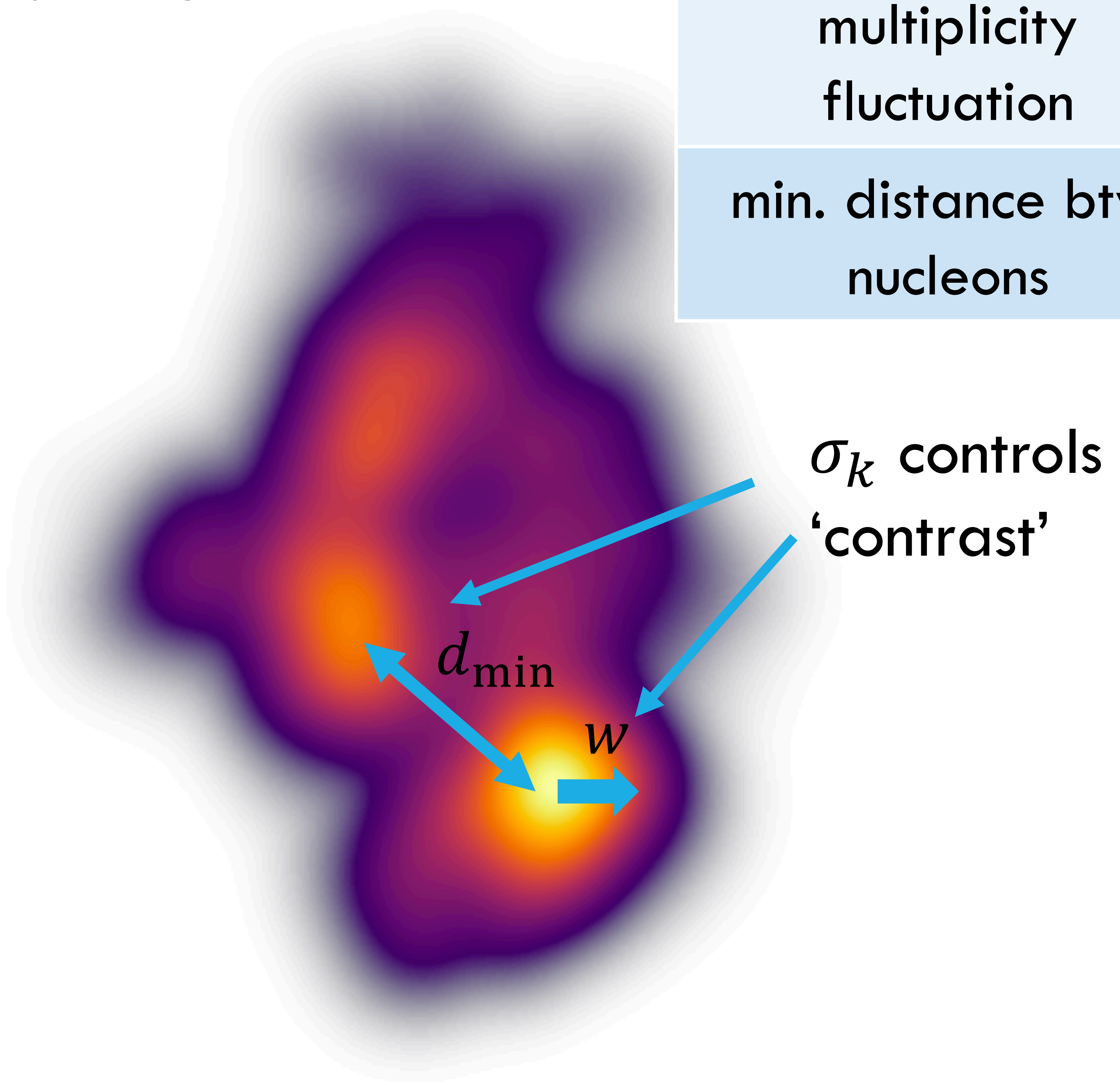
Parameter	Symbol
reduced thickness	p
nucleon width	w
energy normalization	N
multiplicity fluctuation	σ_k
min. distance btw. nucleons	$d_{\min}$

Parametrization for energy deposition at proper time $\tau = 0^+$



Pb-Pb @ 2.76 TeV $w = 0.4$fm

arXiv:1904.08290v1



Slide adapted from D. Everett

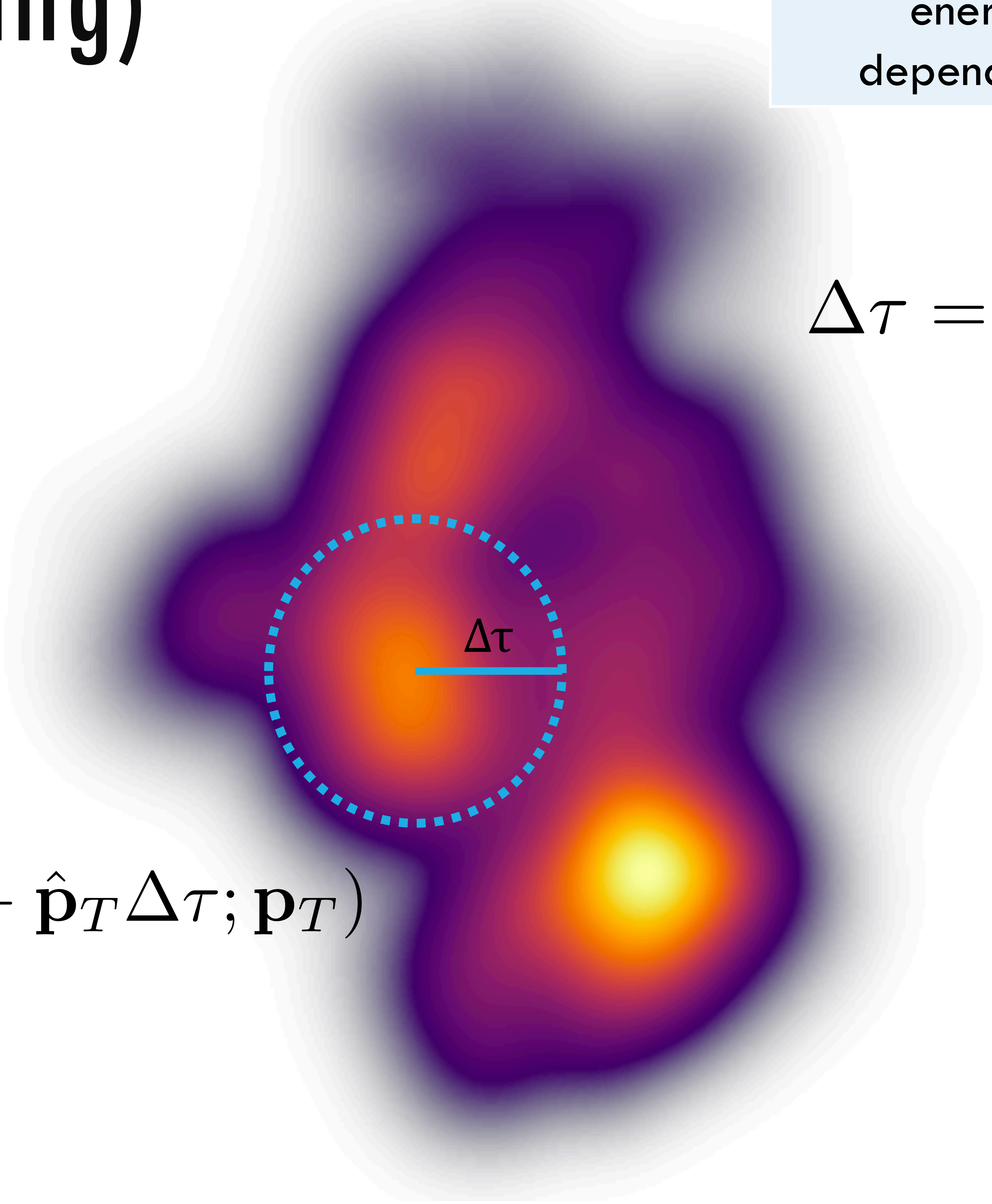
Parameter	Symbol
ref. proper time	τ_R
energy dependence	α

Pre-hydro (freestreaming)

Freestream massless particles:

$$f(t, \mathbf{x}; \mathbf{p}) = f(t_0, \mathbf{x} - \mathbf{v}\Delta t; \mathbf{p})$$

$$\Delta\tau = \tau_R \left(\frac{\langle \epsilon \rangle}{\epsilon_R} \right)^{\alpha}$$



Take initial momentum-distribution isotropic in transverse plane

$$T^{\mu\nu}(\tau_h) = \frac{\tau_0}{\tau_h} \int \frac{d\phi}{2\pi} \hat{p}^{\mu} \hat{p}^{\nu} T^{\tau\tau}(\tau_0, \mathbf{x}_T - \hat{\mathbf{p}}_T \Delta\tau; \mathbf{p}_T)$$

Slide adapted from D. Everett

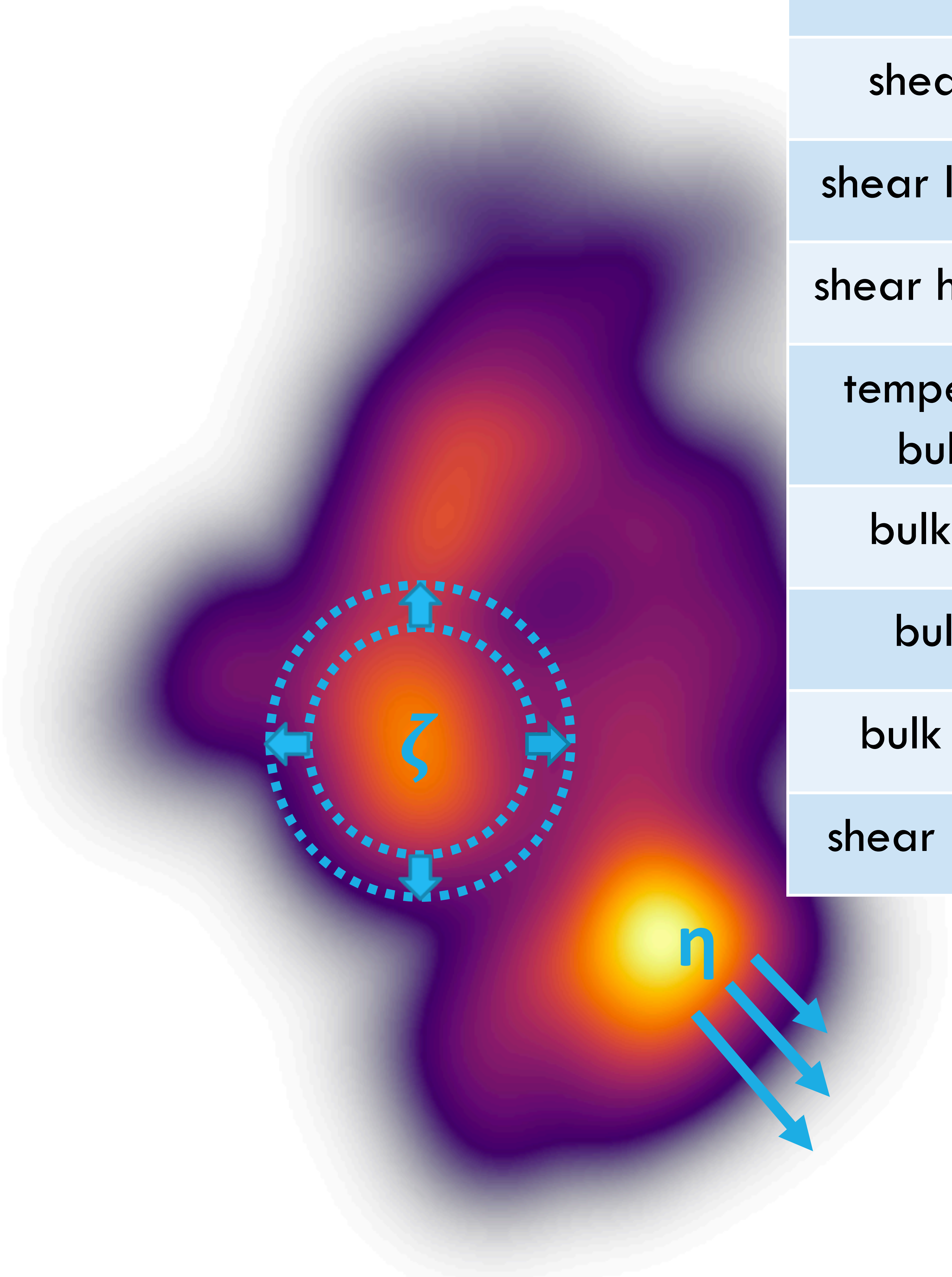
Viscous Hydro

The viscosity of QGP:

$$\tau_\Pi \dot{\Pi} + \Pi = -\zeta\theta + \ldots$$

$$\tau_\pi \dot{\pi}^{\langle\mu\nu\rangle} + \pi^{\mu\nu} = 2\eta\sigma^{\mu\nu} + \ldots$$

Quantify transport properties :
shear and bulk viscosities

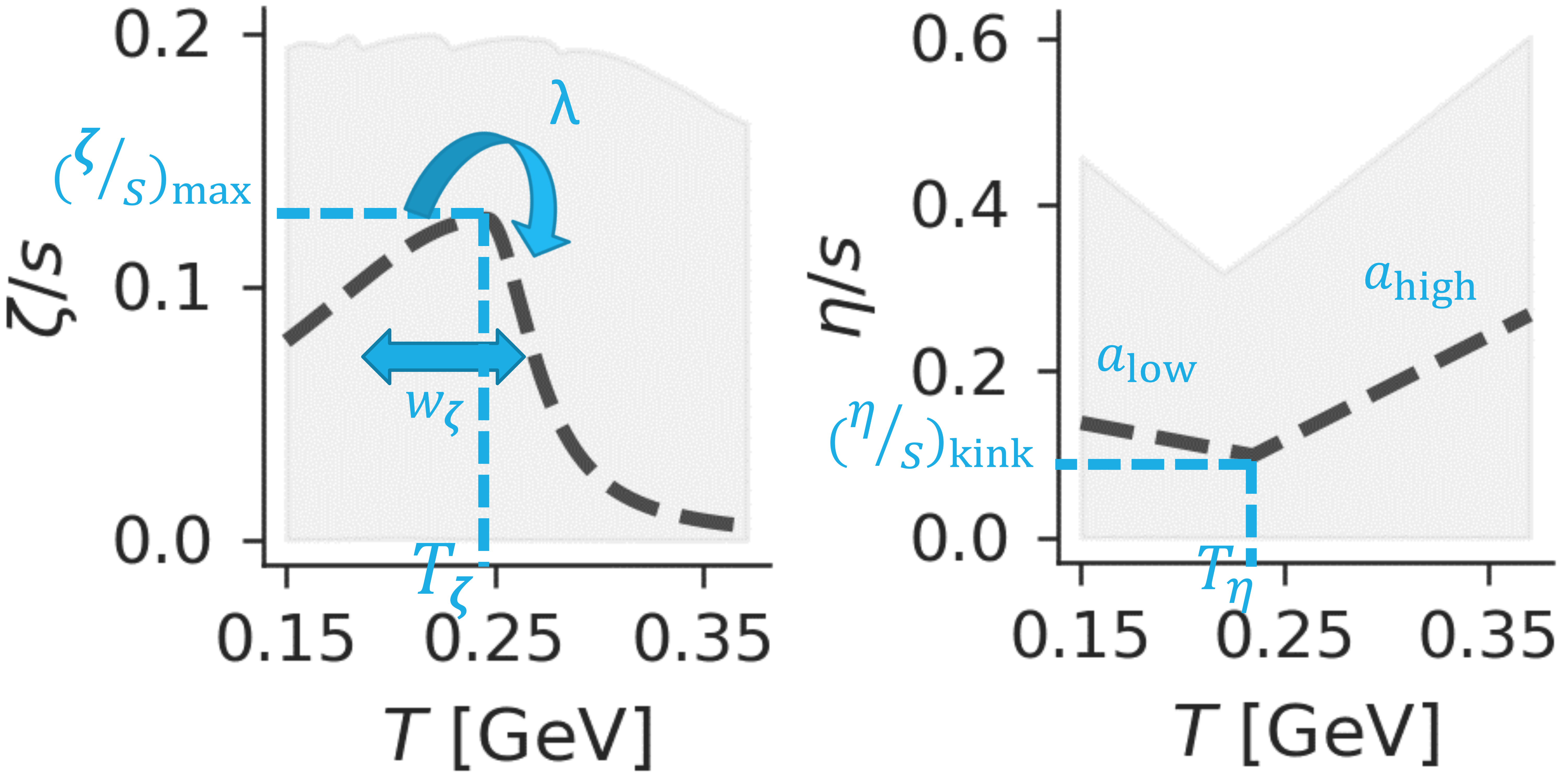


Parameter	Symbol
temperature of kink	T_η
shear at kink	$(\eta/s)_{\rm kink}$
shear low-T slope	$a_{\rm low}$
shear high-T slope	$a_{\rm high}$
temperature of bulk peak	T_ζ
bulk at peak	$(\zeta/s)_{\max}$
bulk width	w_ζ
bulk skewness	λ
shear relax. time	b_π

Slide adapted from D. Everett

Viscous Hydro

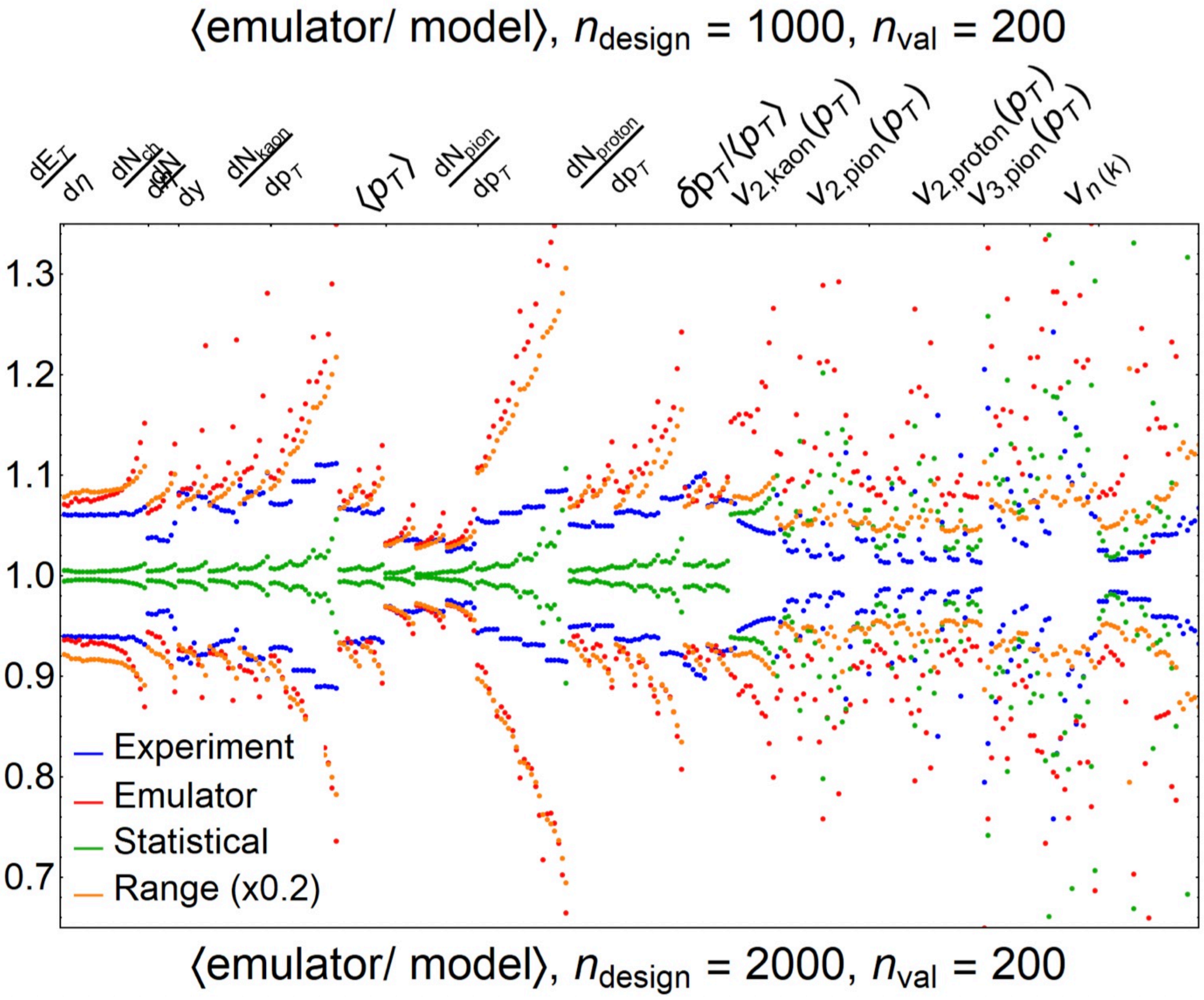
Viscosity parameterizations:



Parameter	Symbol
temperature of kink	T_η
shear at kink	$(\eta/s)_{\mathrm{kink}}$
shear low-T slope	a_{low}
shear high-T slope	a_{high}
temperature of bulk peak	T_ζ
bulk at peak	$(\zeta/s)_{\max}$
bulk width	w_ζ
bulk skewness	λ
shear relax. time	b_π

Slide adapted from D. Everett

Emulator: challenges



the experimental error of the data point (blue), the average statistical error of our model (green) and the range of model predictions given our prior range, defined as the standard deviation over the mean (orange). Ideally the

Trajectum
G. Nijs *et al.* 2010.15134