arXiv:2302.14184

ISNET 9

BAND
Bayesian Analysis of Nuclear Dynamics

Bayesian Parameter Estimation of VAH simulations of Heavy-ion Collisions

Dananjaya (Dan) Liyanage

Özge Surer

Derek Everett

Ulrich Heinz

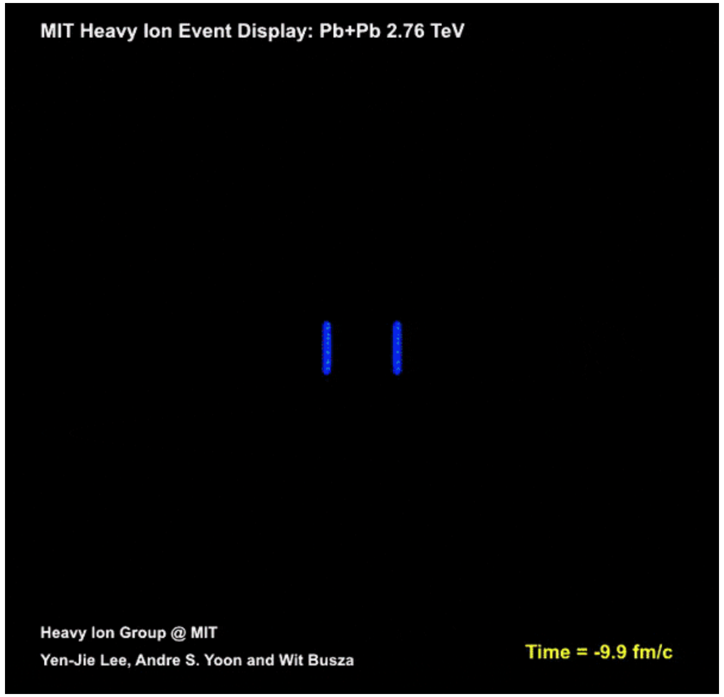
Mike McNelis

Matt Plumlee

Stefan Wild

Agenda

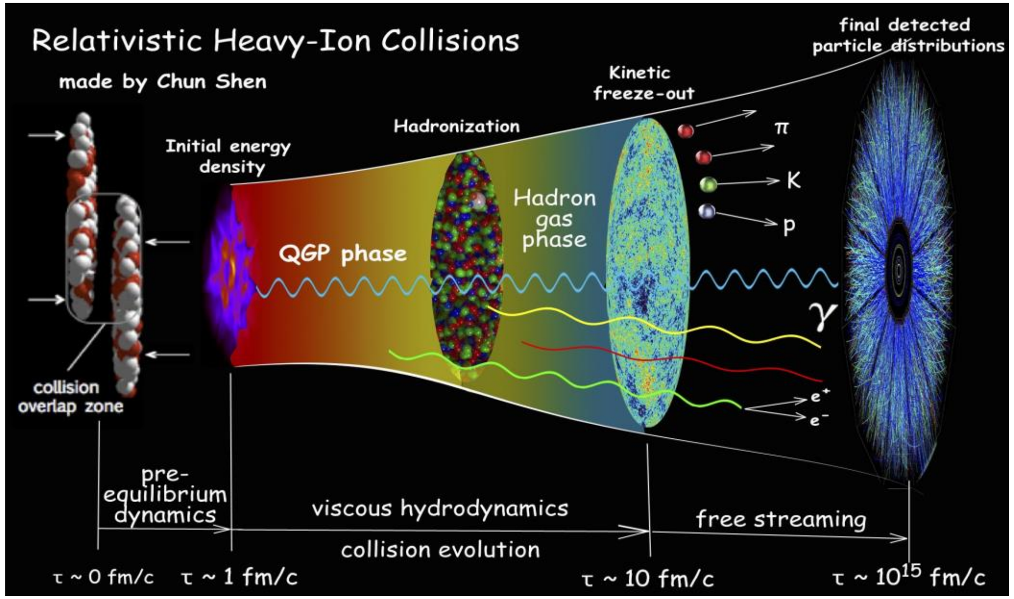
1. Physics Model Overview
2. Bayesian Parameter Estimation
3. Generating Simulation Data
4. Machine Learning Models (Emulators)
5. Results



Relativistic Heavy Ion Collision
http://web.mit.edu/mithig/movies/LHCanmation.mov

Model Overview

- Relativistic heavy-ion collisions are simulated with multiple stages
- Old : JETSCAPE SIMS model
- New : Replace “Free Stream” + “MUSIC” by Viscous Anisotropic Hydrodynamics (“VAH”)
- Calibrate on “Pb Pb collisions at 2.76 TeV”.
  - Viscosity
  - N : the initial energy deposition
  - …



98 Observables

- Charged particle yield
- Mean momentum of kaons, pions, protons
- …

T_RENTo → Free Stream → MUSIC → iS3D → SMASH

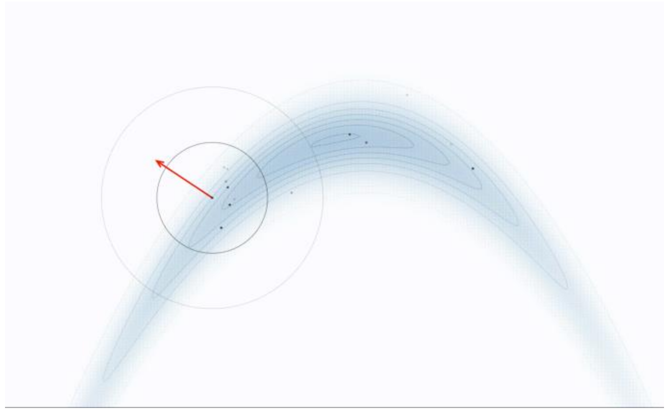
Initial cond. | Particlization | Transport

VAH

M. McNelis, D. Bazow, and U. Heinz, Computer Physics Communications 267, 108077 (2021)
D. Everett et al. (JETSCAPE Collaboration), Phys. Rev. C 103, 054904 (2021)

Bayesian Parameter Estimation

MCMC



Likelihood   Prior

$$P(\theta|Y_{exp}, M_1) = \frac{P(Y_{exp}|\theta, M_1)\, P(\theta|M_1)}{P(Y_{exp}|M_1)}$$

Posterior   Marginal Likelihood

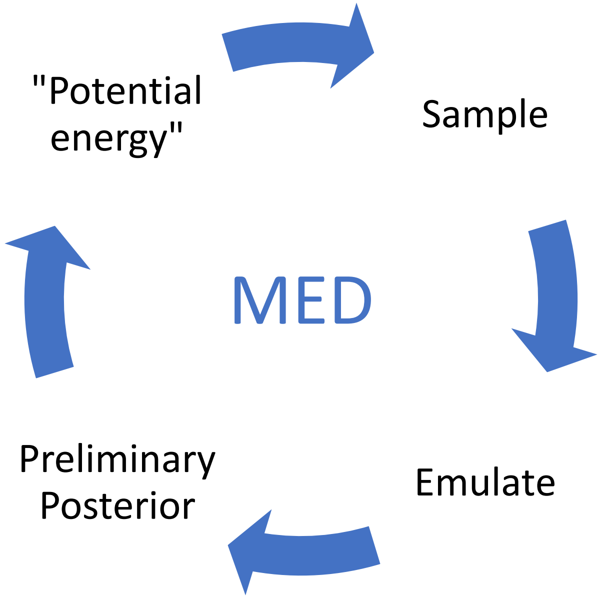
$$P(Y_{exp}|\theta, M_1) \propto \frac{\exp\left\{-\left[Y_{exp} - Y_{sim}(\theta)\right]^T \Sigma^{-1}\left[Y_{exp} - Y_{sim}(\theta)\right]\right\}}{\sqrt{|\Sigma|}}$$

- MCMC sampling require millions of simulation evaluations.
- Simulation is very computationally expensive ($O(1000)$ core hours).
- Need to build fast surrogates for the simulation!
- Gaussian Process (GP) emulators are the most popular choice.

Training Data for Emulators

- "Uniformly" sampling the parameter space : Latin Hypercube Design (LHD)
- Sampling high posterior regions with more weight : Minimum Energy Design (MED)

Batch	Number of design points	Events per Design
A - LHD	300	200
B - LHD (test set)	90	800
C - MED	90	800
D - MED	90	800
E - MED	70	1600
F - MED	30	1600



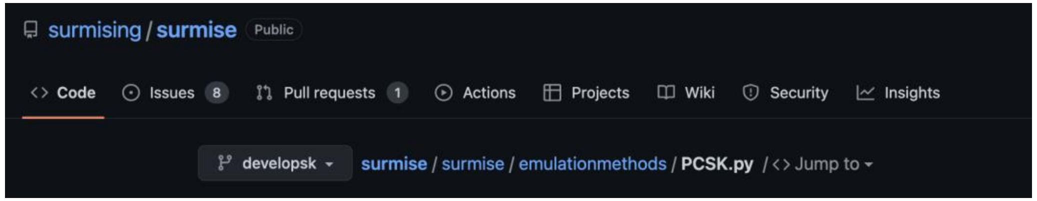
V. R. Joseph, T. Dasgupta, R. Tuo, and C. F. J. Wu, Technometrics 57, 64 (2015).
V. R. Joseph, D. Wang, L. Gu, S. Lyu, and R. Tuo, Technometrics 61, 297 (2019).

Emulators

Emulator Accuracy from R^2 score (Explained variance)

Choose Principal Components Stochastic Kriging (PCSK)

BAND
Bayesian Analysis of Nuclear Dynamics

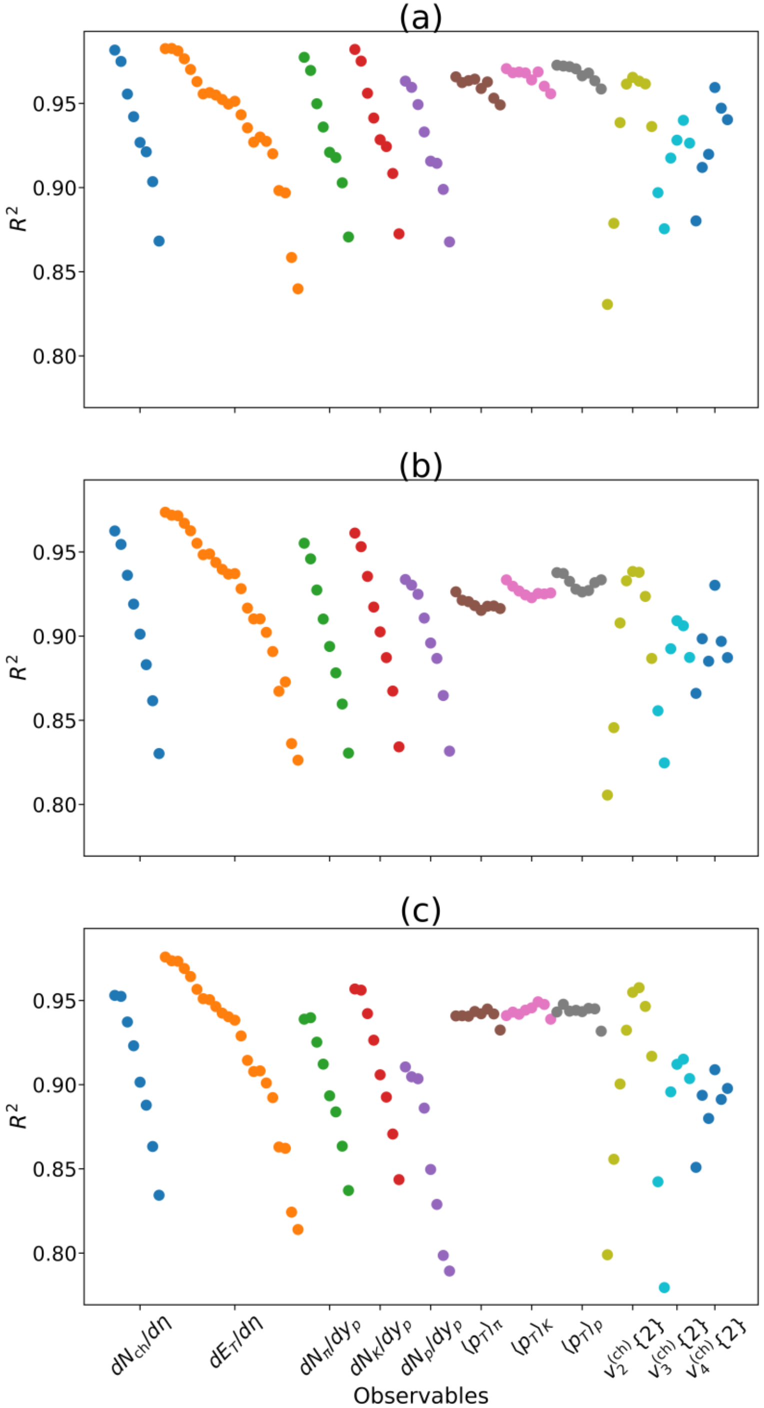


B. Ankenman, B. Nelson, J. Staum (2010), Stochastic kriging for simulation metamodeling

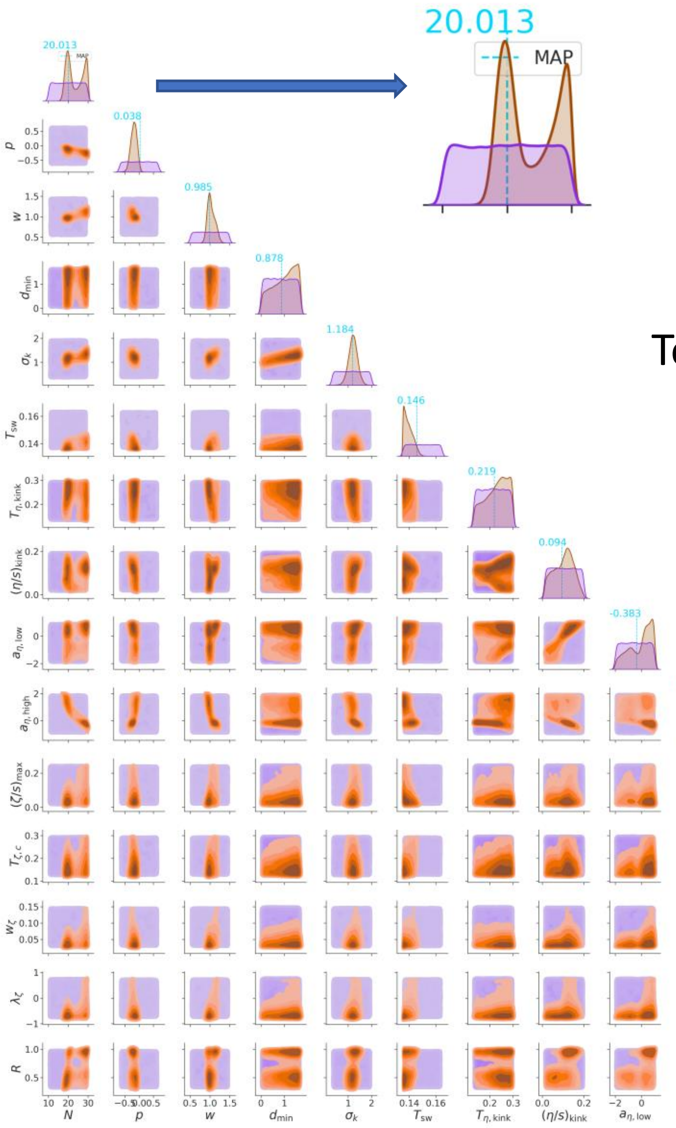
PCSK

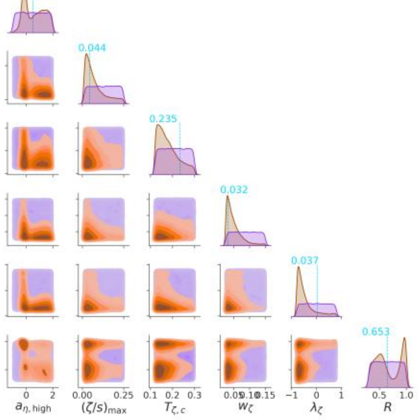
PCGPR

PCGPR Grouped



Results from Parameter Estimation



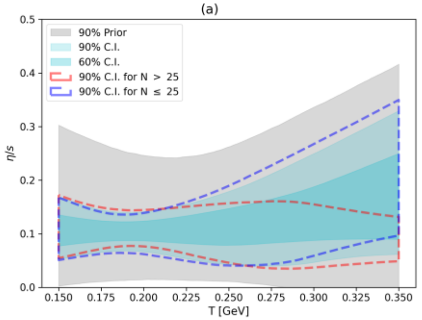


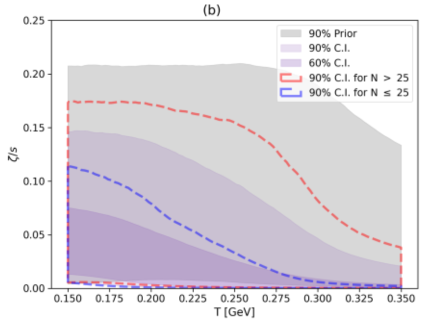
Bi-Modality
- Very interesting but why?

Joint Marginal Distributions
- Too many correlations

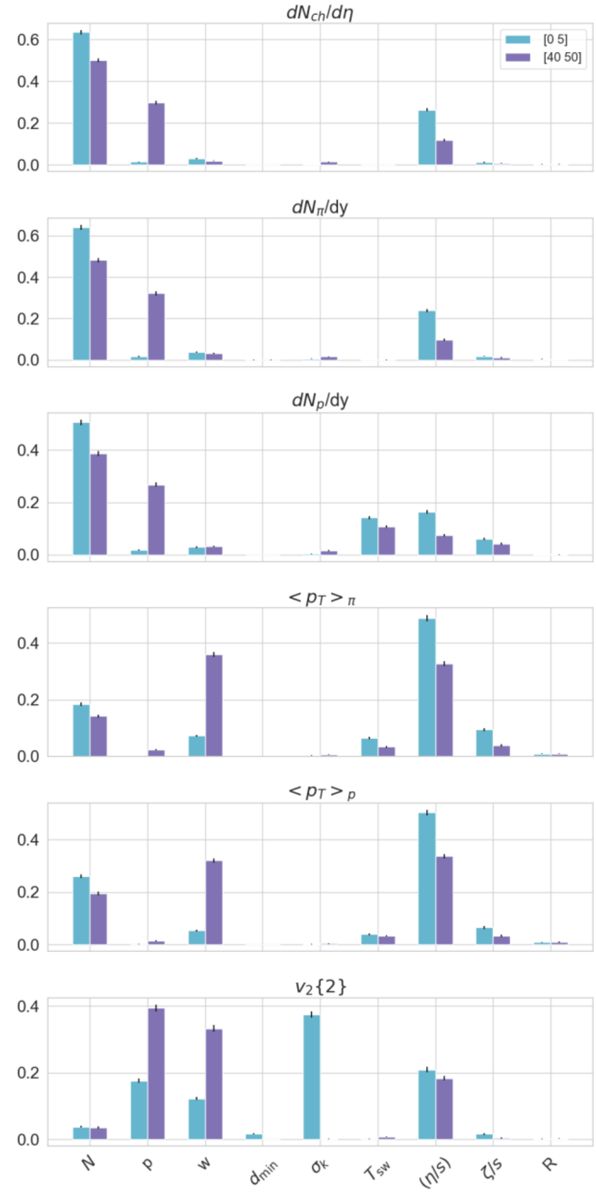
Sensitivity Analysis
- Viscosity!

Temperature Dependent Viscosities





Sensitivity Analysis



Conclusion

- Challenges and (Statistical tools) Answers
  - Limited resources : Adaptive Sampling
  - Heteroscedastic simulation data: PCSK
  - Understand posterior : S'obol sensitivity analysis
- Better constraints for specific bulk viscosity and shear viscosity at high temperatures using VAH.
- Codes/data are public!

  github.com/danOSU/Bayesian_parameter_inferece_for_VAH

https://share.streamlit.io/danosu/visualization_vah/main/streamlit_widget.py

arXiv:2302.14184

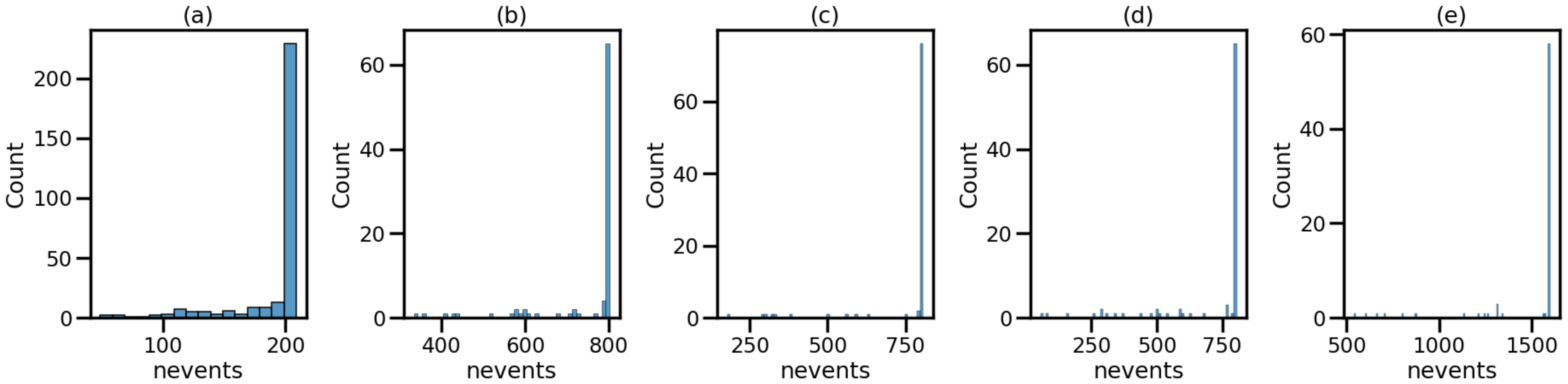
Backup slides

Sequential Design Strategy

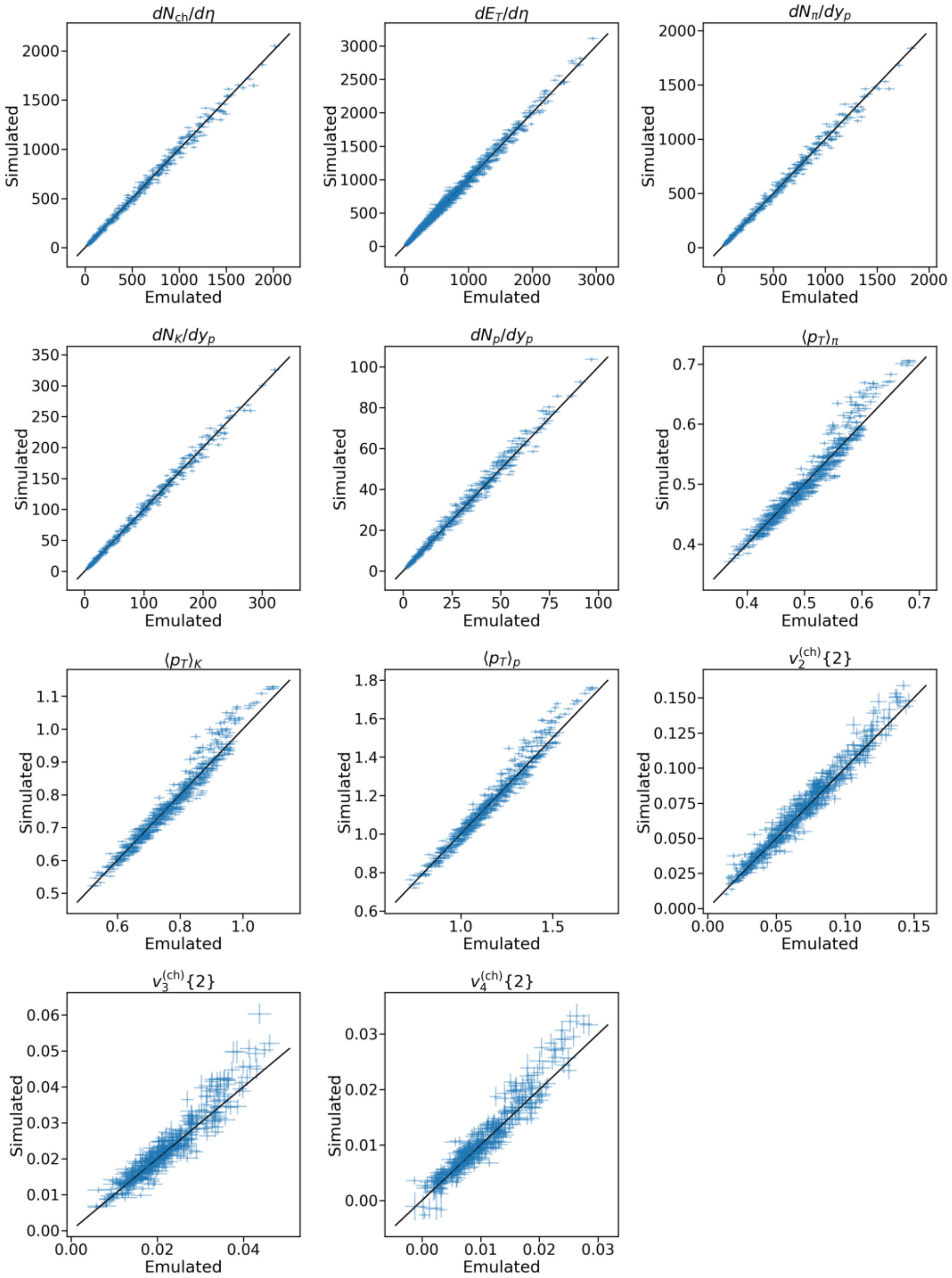
- In the 15-dimensional space, we are mostly interested in the high likelihood region.

$$\mathbf{x}_{j+1} = \arg\max_{\mathbf{x}\in\mathcal{L}} \min_{i=1:j} \mathcal{P}^{1/2q}(\mathbf{y}_{\exp}|\mathbf{x})\mathcal{P}^{1/2q}(\mathbf{y}_{\exp}|\mathbf{x}_i)d(\mathbf{x},\mathbf{x}_i)$$

Low accuracy	Testing	Batch 1	Batch 2	High Accuracy
300 LHD	90 LHD	90 MED	90 MED	90 MED



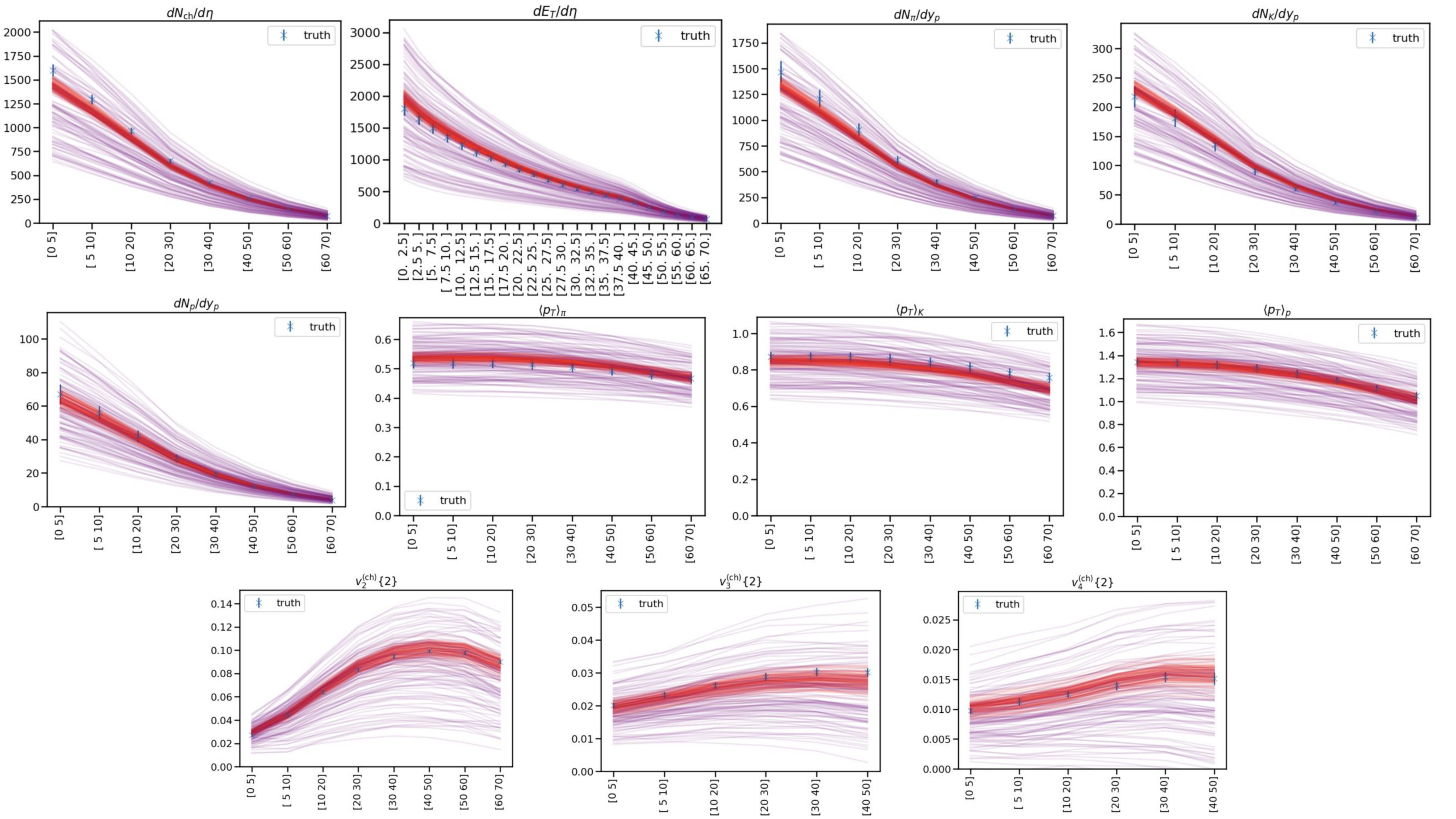
V. Roshan Joseph, Dianpeng Wang, Li Gu, Shiji Lyu & Rui Tuo (2019) Deterministic Sampling of Expensive Posteriors Using Minimum Energy Designs



R^2 Score

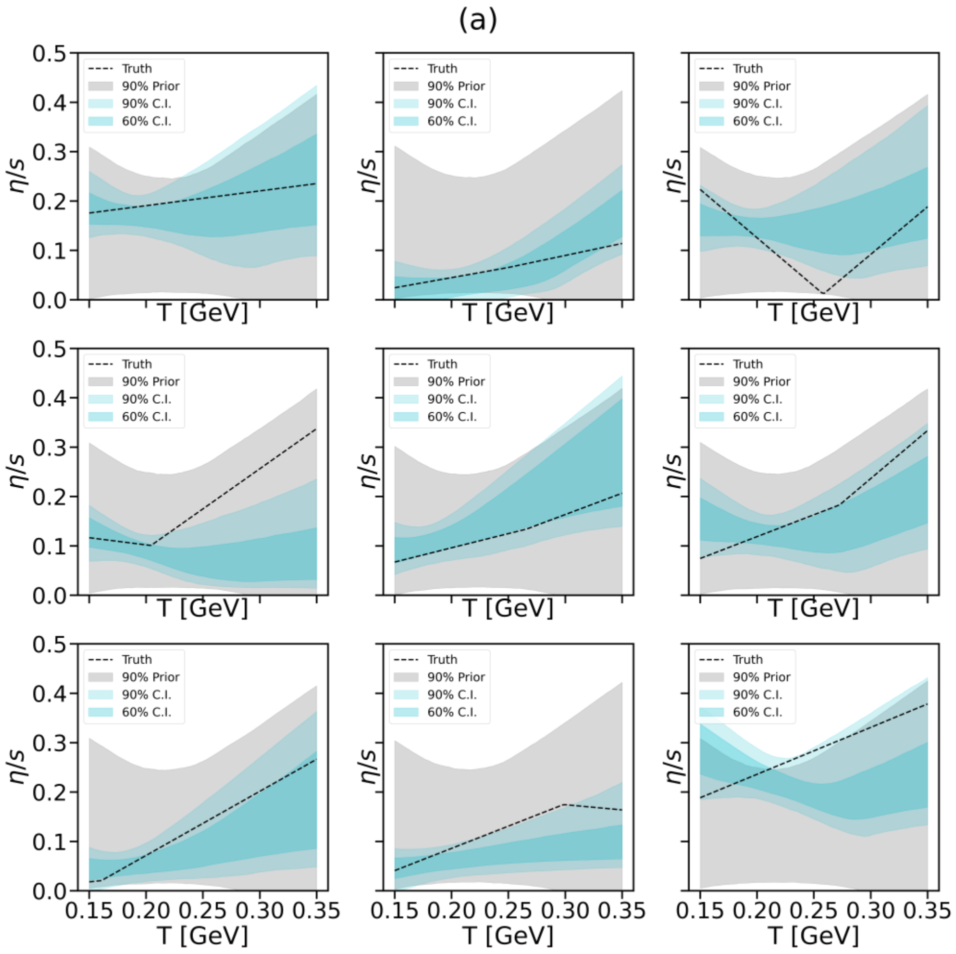
$$\mathrm{R}_j^2 = 1 - \frac{\sum_{i=1}^{m} (y_{i,j}^{test} - y_{i,j}^{emulation})^2}{\sum_{i=1}^{m} (y_{i,j}^{test} - \mu_j)^2}$$

$$\mu_j = \frac{\sum_{i=1}^{m} y_{i,j}^{test}}{m}$$

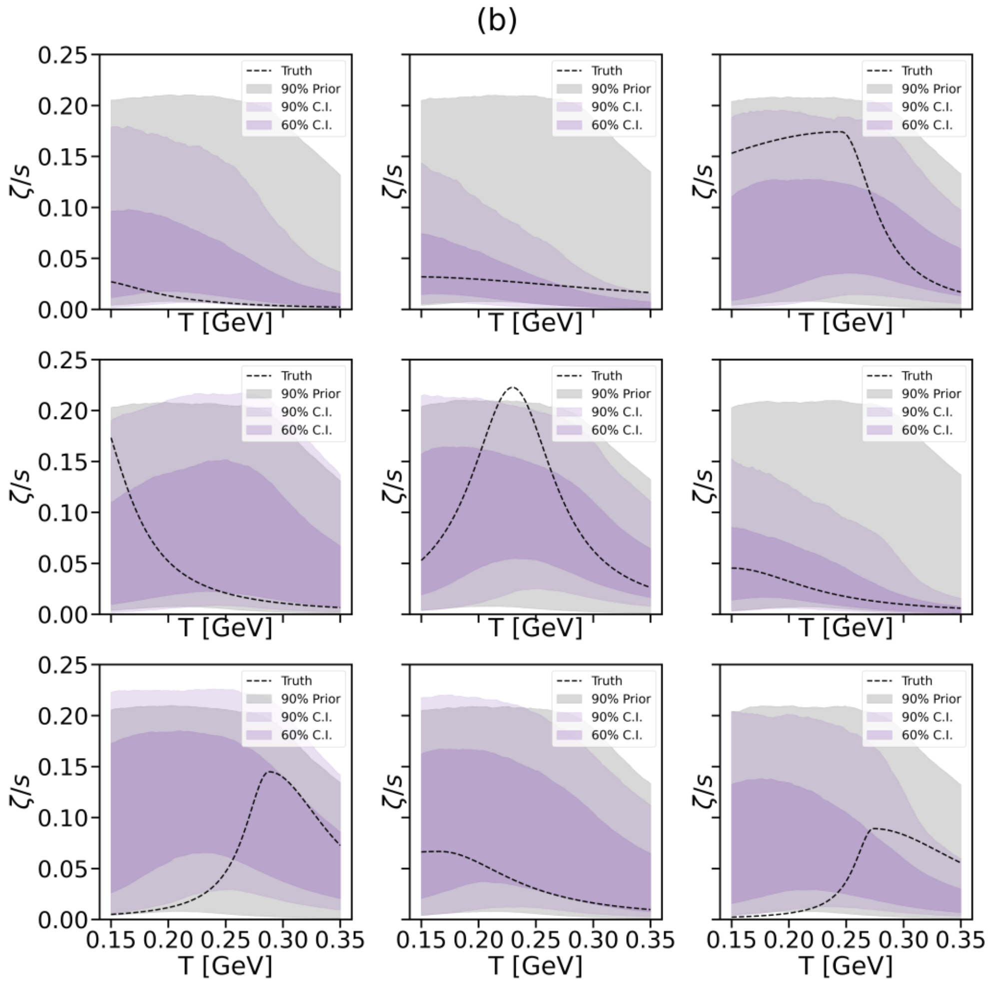


$dN_{ch}/d\eta$
$dE_T/d\eta$
dN_π/dy_p
dN_K/dy_p
dN_p/dy_p
$\langle p_T \rangle_\pi$
$\langle p_T \rangle_K$
$\langle p_T \rangle_p$
$v_2^{(ch)}\{2\}$
$v_3^{(ch)}\{2\}$
$v_4^{(ch)}\{2\}$
truth
[0 5]
[5 10]
[10 20]
[20 30]
[30 40]
[40 50]
[50 60]
[60 70]
[0. 2.5]
[2.5 5.]
[5. 7.5]
[7.5 10.]
[10. 12.5]
[12.5 15.]
[15. 17.5]
[17.5 20.]
[20. 22.5]
[22.5 25.]
[25. 27.5]
[27.5 30.]
[30. 32.5]
[32.5 35.]
[35. 37.5]
[37.5 40.]
[40. 45.]
[45. 50.]
[50. 55.]
[55. 60.]
[60. 65.]
[65. 70.]

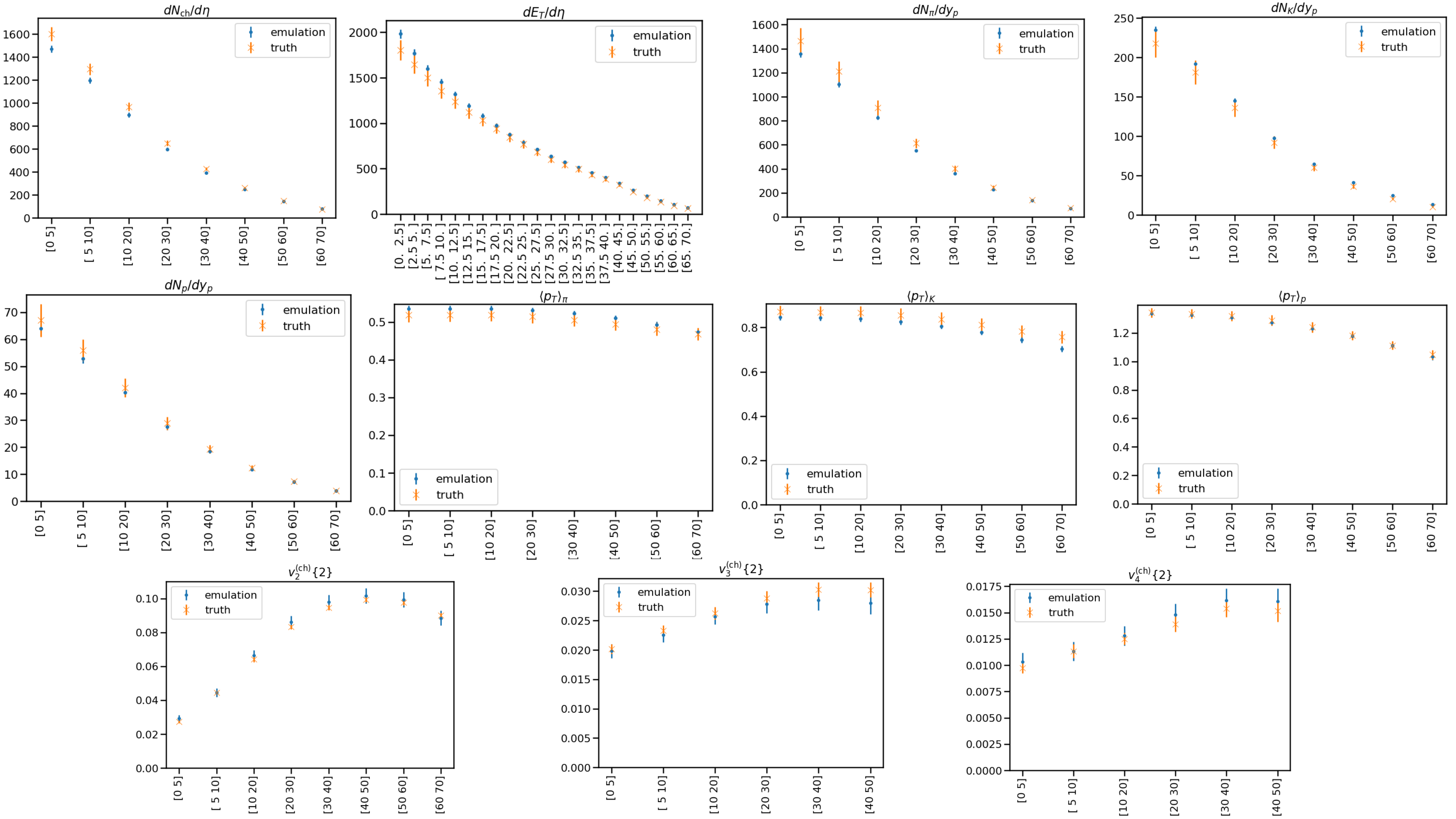
Closure Tests



Specific Shear Viscosity



Specific Bulk Viscosity

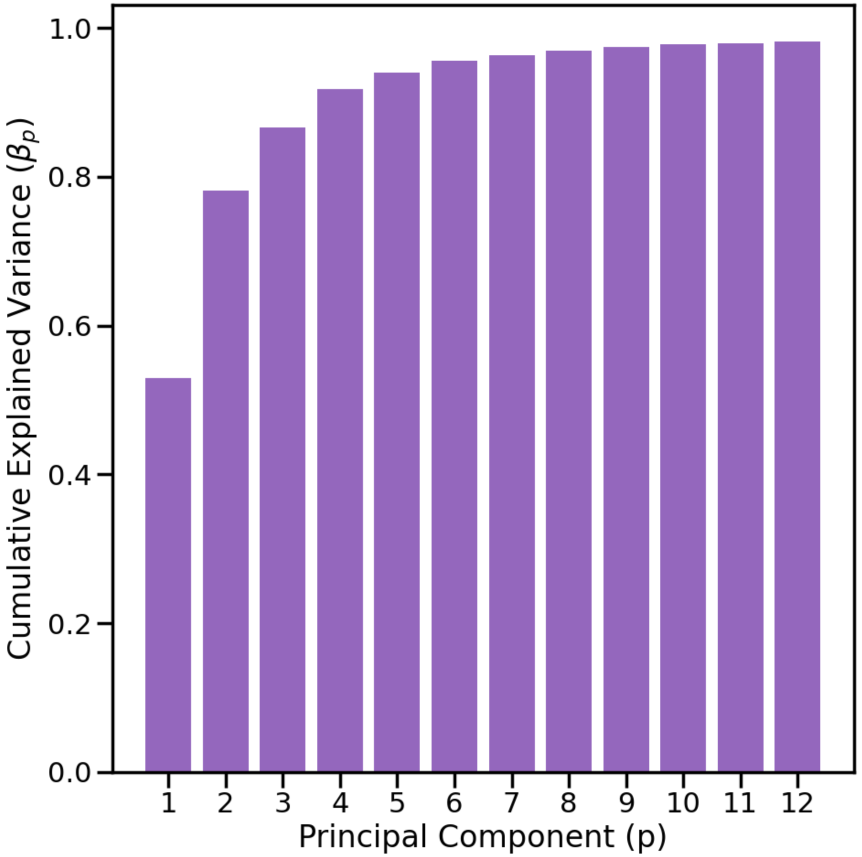


$dN_{ch}/d\eta$
$dE_T/d\eta$
dN_π/dy_p
dN_K/dy_p
dN_p/dy_p
$\langle p_T \rangle_\pi$
$\langle p_T \rangle_K$
$\langle p_T \rangle_p$
$v_2^{(ch)}\{2\}$
$v_3^{(ch)}\{2\}$
$v_4^{(ch)}\{2\}$
emulation
truth
[0 5]
[5 10]
[10 20]
[20 30]
[30 40]
[40 50]
[50 60]
[60 70]

MCMC

```
args={'sampler': 'PTMC',
      'nburnin' : '1000',
      'ndim' : '15',
      'niterations' : '5000' ,
      'ntemps' : '500',
      'nthin' : '10',
      'nwalkers' : '100' ,
      'nthreads' : '28',
      'Tmax' : '1000'},
```

PC



Cumulative Explained Variance (β_p)
0.0
0.2
0.4
0.6
0.8
1.0
1
2
3
4
5
6
7
8
9
10
11
12
Principal Component (p)