Improved heavy-ion model emulators and Bayesian framework to model theoretical uncertainties

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Bayesian Analysis of Nuclear Dynamics

Hydrodynamics and related observables in heavy-ion collisions
Subatech / IMT-Atlantique, Nantes

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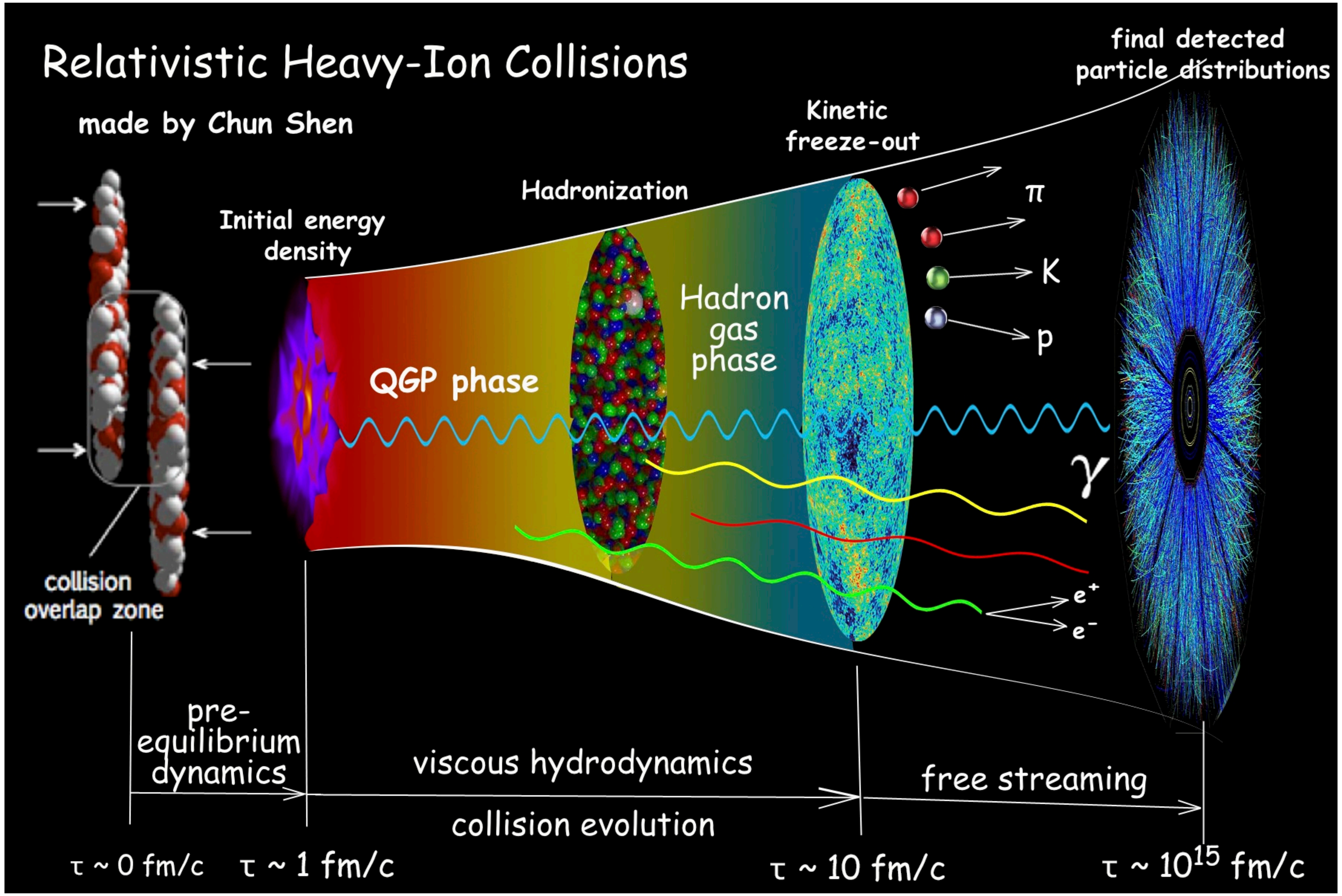
Overview

- Introduction: Heavy-ion collisions and multi-stage physics models
- Part 1 : Emulators
  - Model emulators using Gaussian Processes
  - Existing emulators: PCGP, PCSK. New emulators: LCGP and AKSGP

    In collaboration with Moses Chan, Richard Furnstahl, Ulrich Heinz, and Matthew Pratola
- Part 2 : Quantifying theoretical uncertainties
  - Tensions between extracted specific viscosities in different heavy-ion studies.
  - Quantifying theoretical uncertainties: Model discrepancy

    In collaboration with Richard Furnstahl, Ulrich Heinz, Matthew Pratola
  - Example: Ball drop experiment
- Summary

Heavy-ion collisions



Quark Gluon Plasma (QGP) phase:
Signs of "fluid" formation.
Two decades of research.

- Equation of state? $P(T,\mu),\ \epsilon(T,\mu)$
  Hydro input taken from lattice QCD.

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

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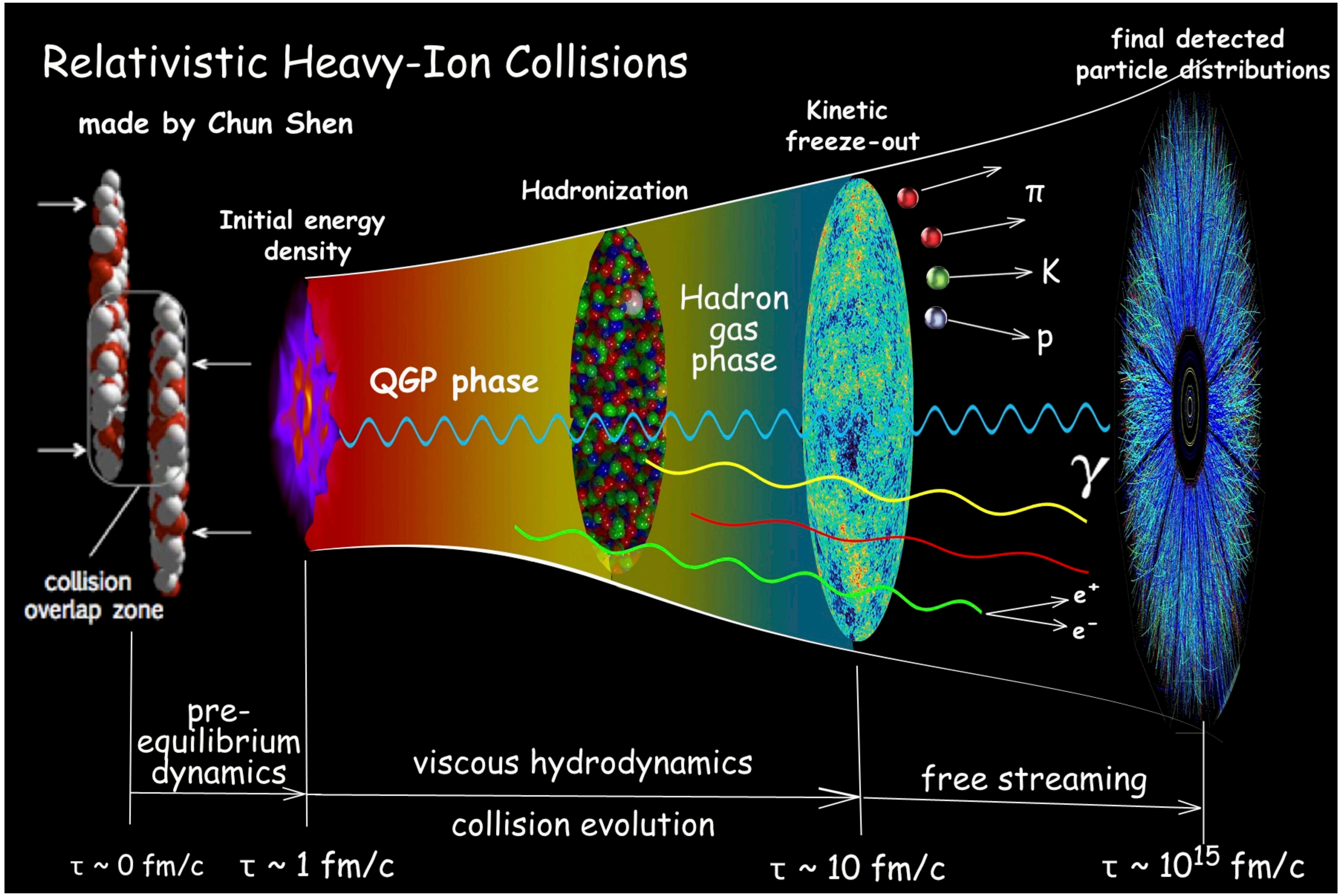

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Challenges: models are multi-stage, uncertain, and expensive

Measurements (in transverse plane at midrapidity)

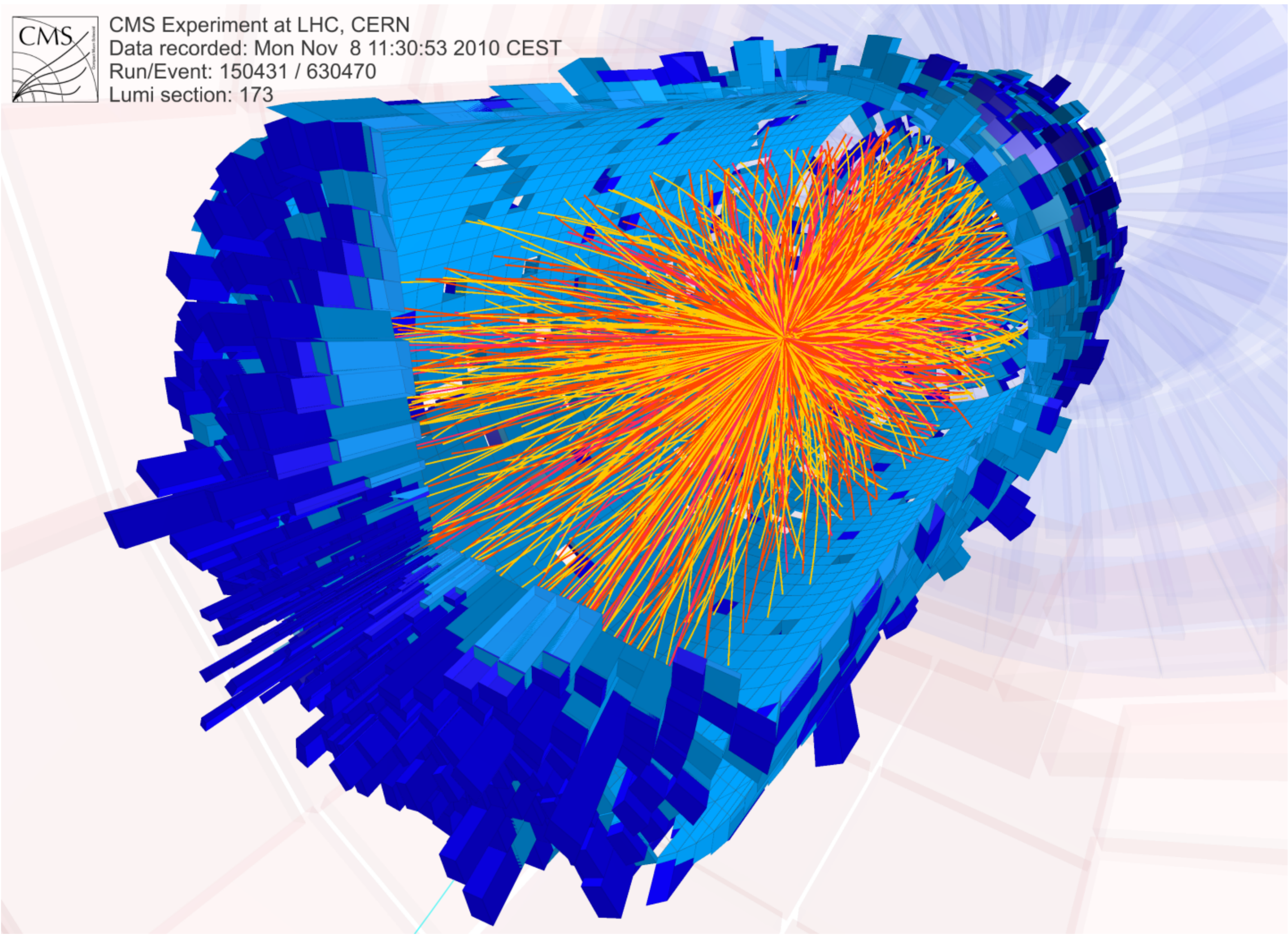
Particle yields for kaons, pions and protons:
$\frac{dN_\pi}{dy}, \frac{dN_K}{dy}, \frac{dN_p}{dy}$

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

Mean transverse energy:
$dE_T/d\eta$

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

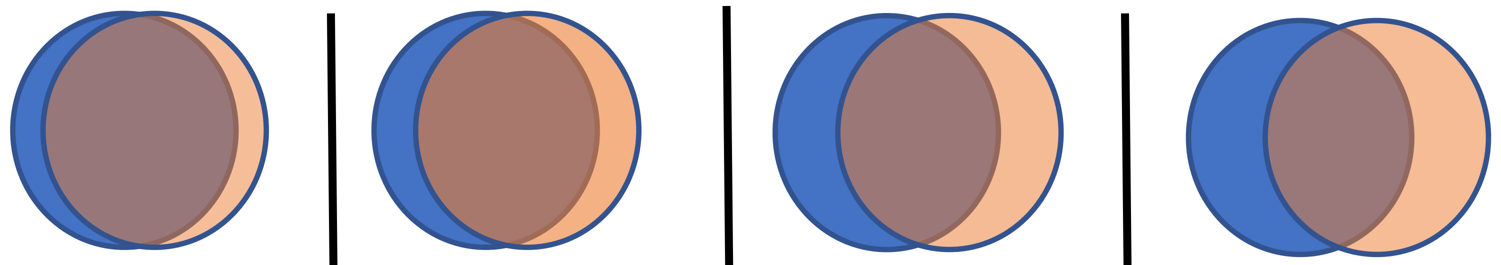
Mean transverse momentum fluctuations:
$\frac{\delta p_T}{< p_T >}$



Mean transverse momenta of kaons, pions, protons:
$\langle p_T \rangle_\pi,\ \langle p_T \rangle_K,\ \langle p_T \rangle_p$

Centrality

0-5 % | 5-10 % | 20-30 % | 40-50 %



Observables type

$dE_T/d\eta$

$dN_{ch}/d\eta$

$\frac{dN_i}{dy}$

$v_2^{ch}\{2\}$

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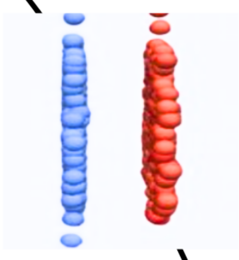
$\frac{\delta p_T}{\langle p_T \rangle}$

$< p_T >_i$

Observables
(≈ 100)

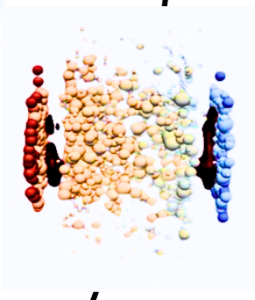
Simulation models



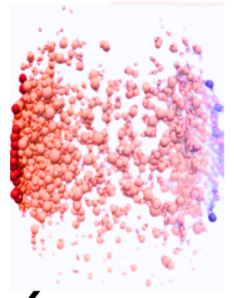
Initial conditions
- Trento
- IP-Glasma

Pre-Equilibrium
- Free Stream
- KoMPoST
- KTiSO

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



Particlization
- Grad
- CE
- PTB
- PTMA

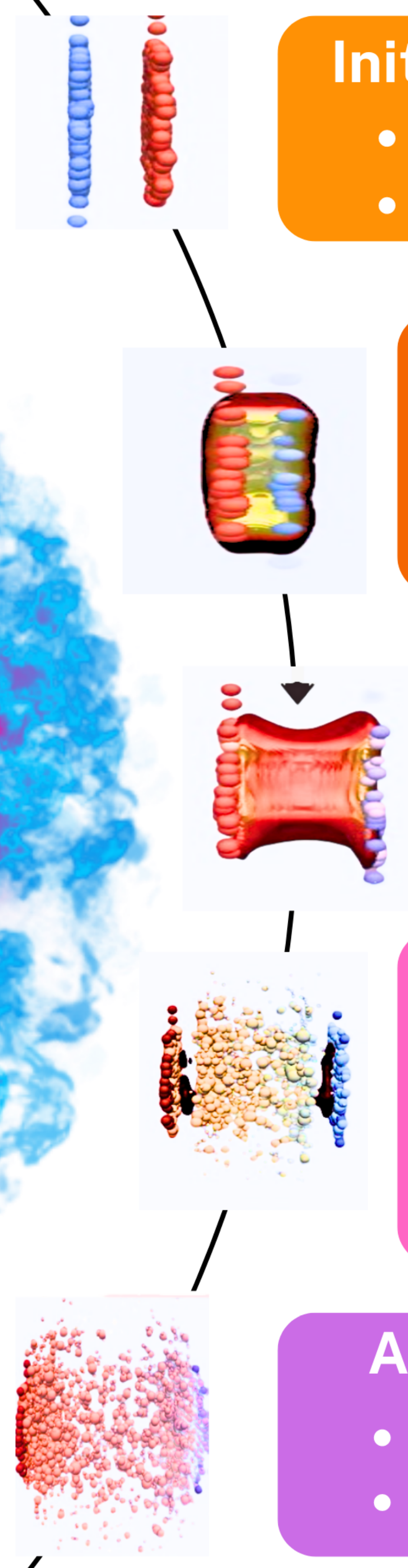


After Burner
- SMASH
- URQMD

multi-stage models

Slide adapted from D. Liyanage

Simulation models



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JETSCAPE SIMS calibration

D. Everett *et al.* 2010.03928, 2011.01430

Pb - Pb at 2.76 TeV
≈100 Observables

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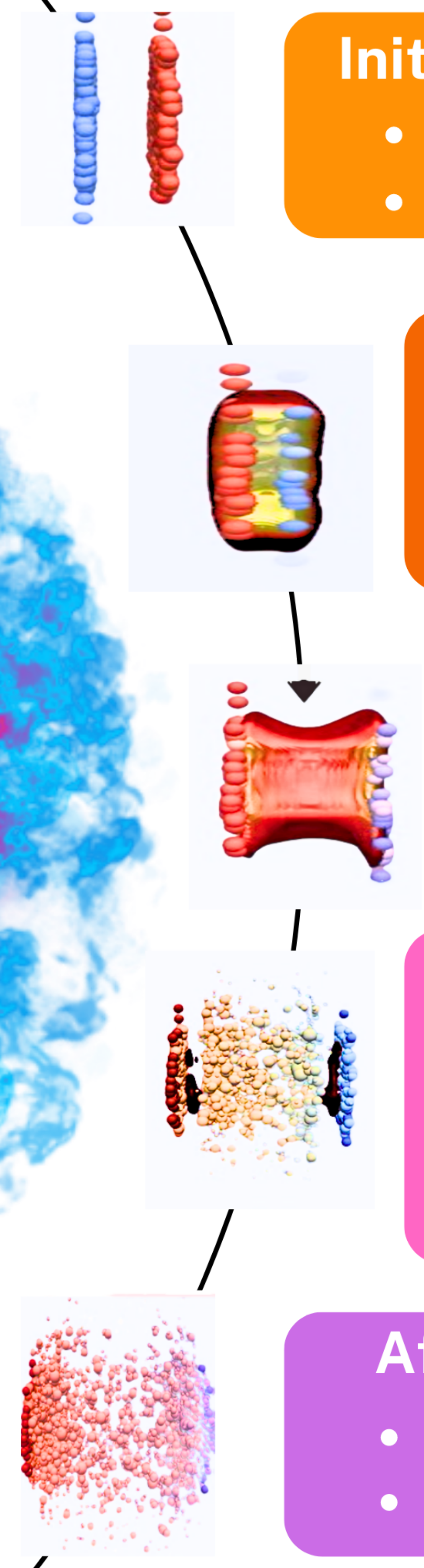
Simulation models



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Free-stream

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Viscous Anisotropic Hydrodynamics Model

M. McNelis *et al.* 2101.02827
D. Liyanage *et al.* 2302.14184

VAH

PTMA

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

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Model parameters

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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
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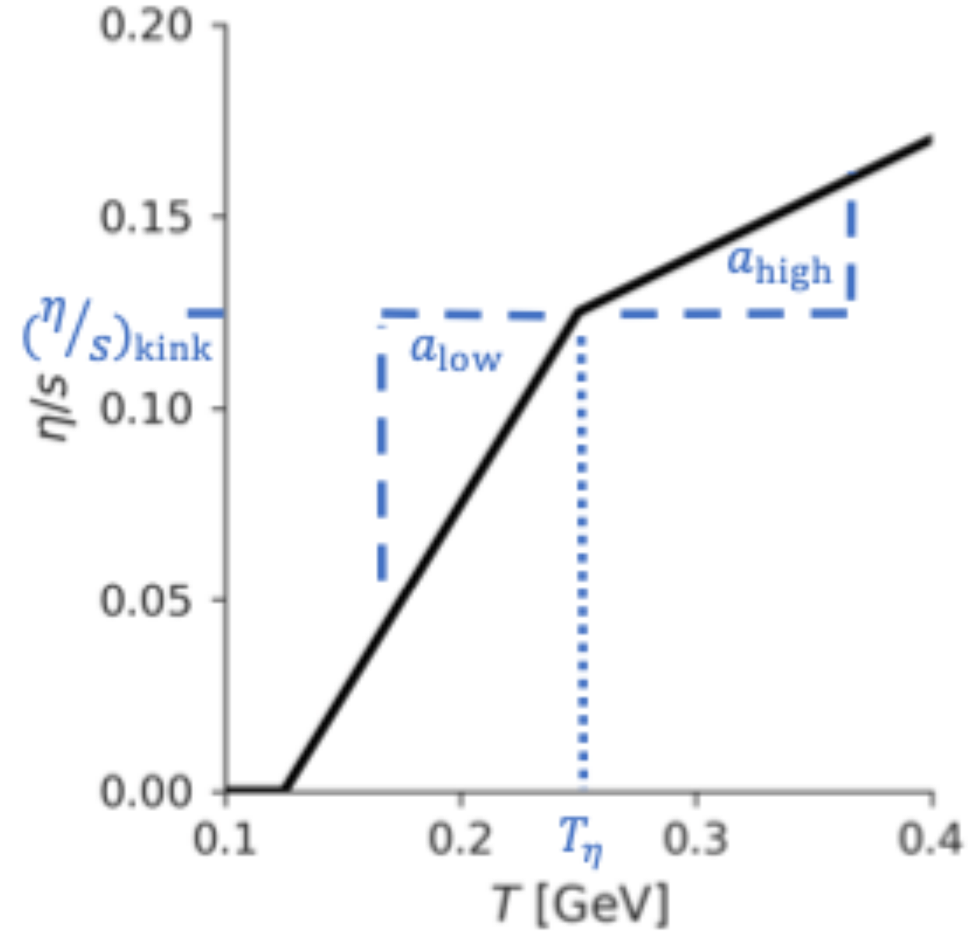
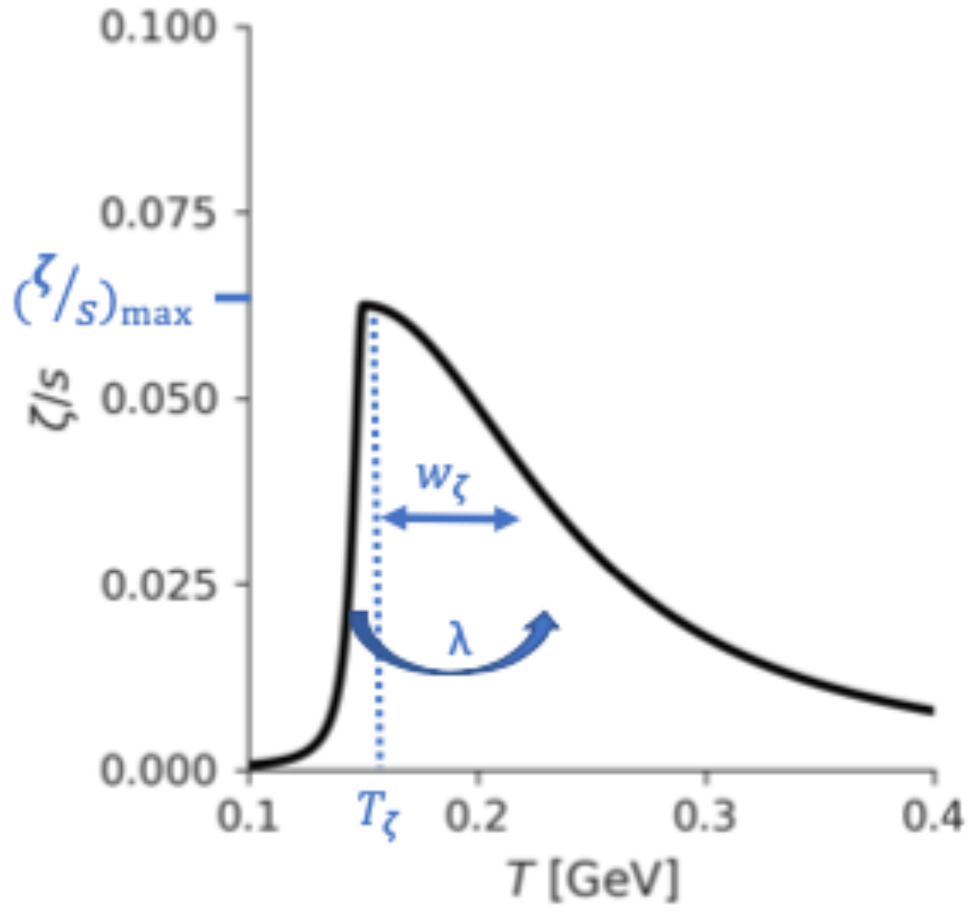
≈15 model parameters





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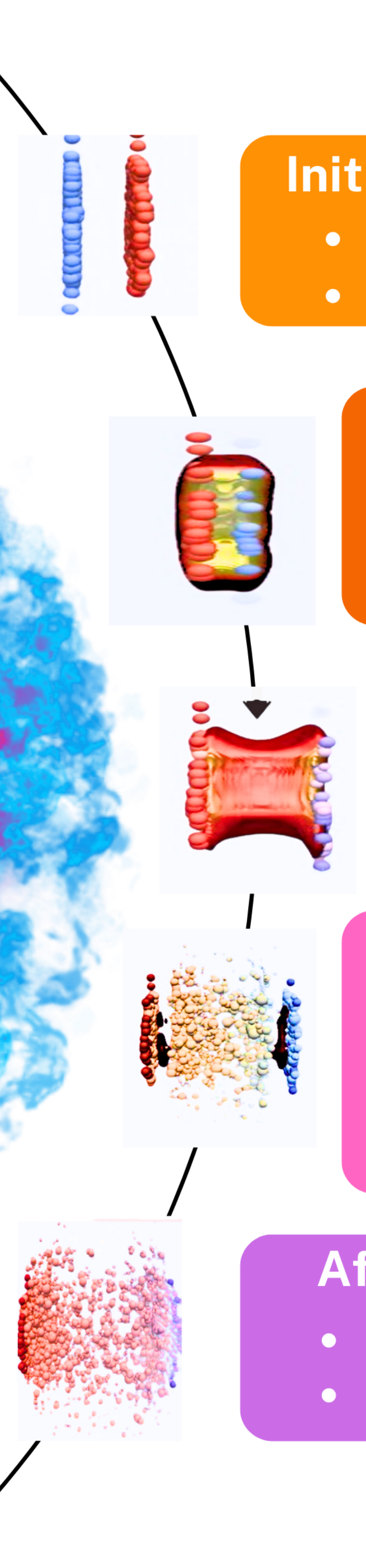

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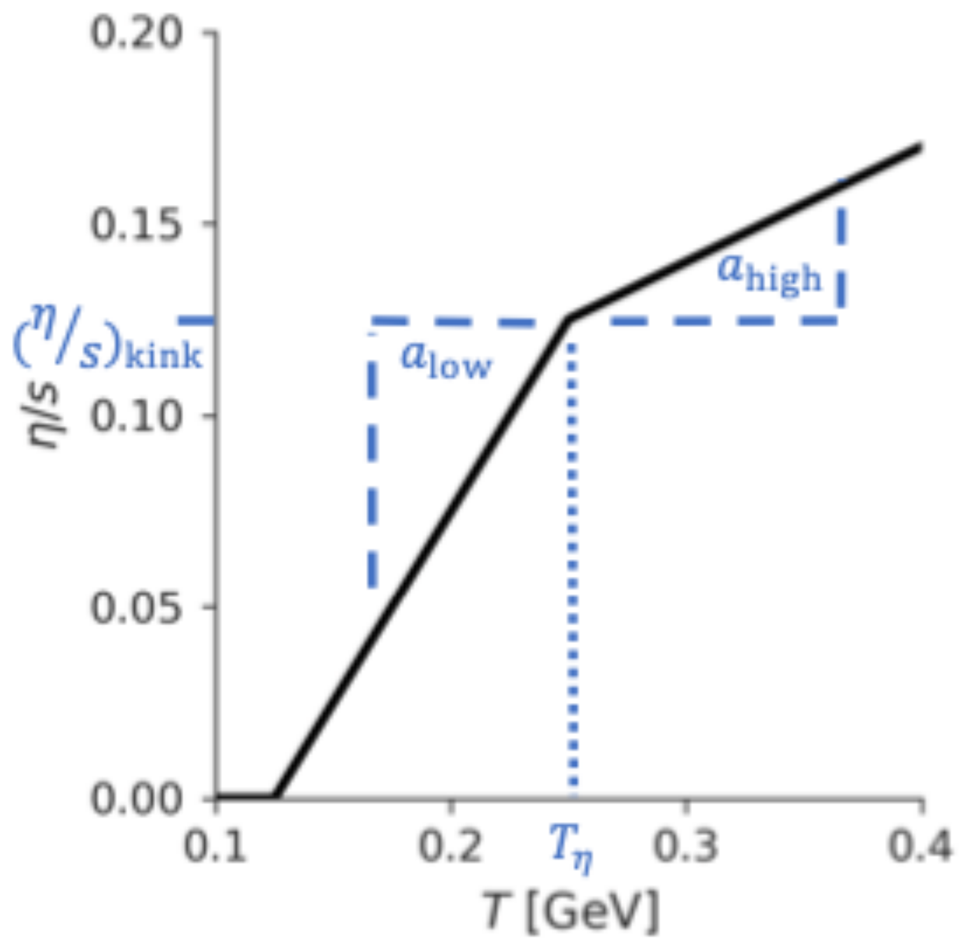

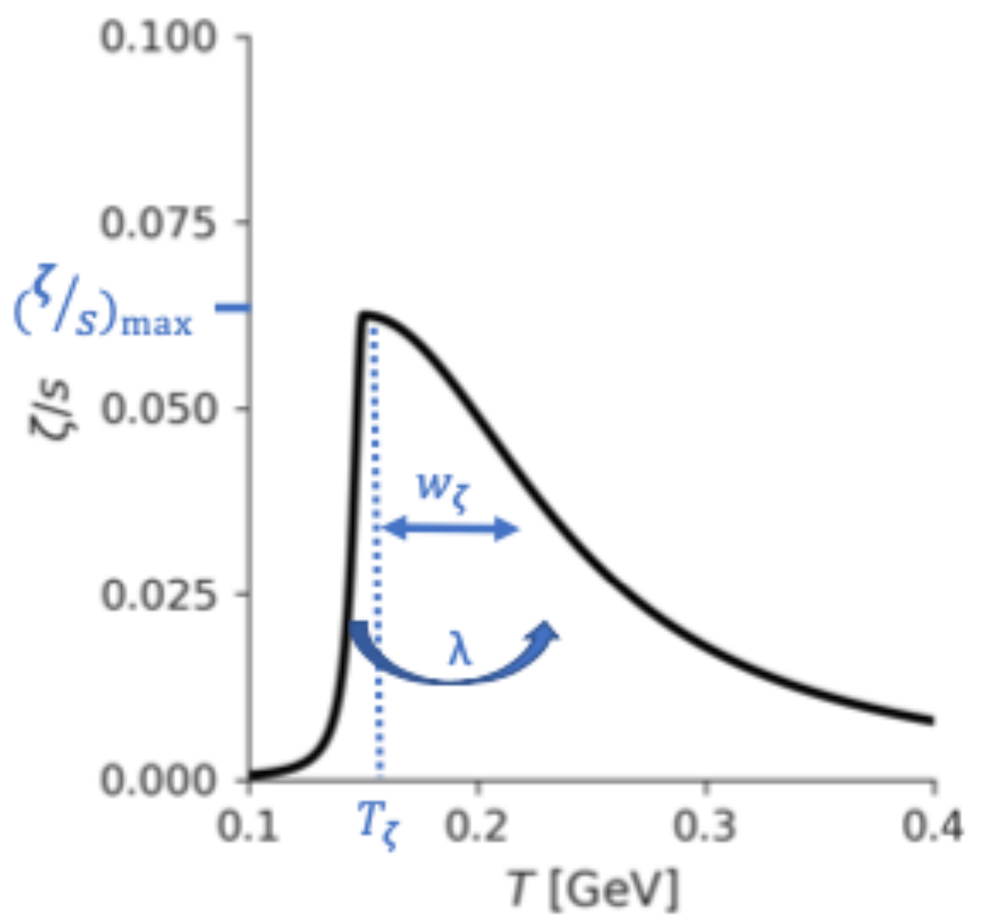

Bayesian studies require >10^9 CPU hours.
Need for fast and accurate model surrogates.

Slide adapted from D. Liyanage

Part 1 : Gaussian process Model emulators

Gaussian process

Formal definition: A Gaussian process (GP) is a collection of random variables, any finite number of which have a joint Gaussian distribution.

Intuitive explanation: A Gaussian process (GP) represents an infinite set of functions, all derived from a specific "generating" function (the covariance kernel). The distribution of values these functions take at any input point is Gaussian.

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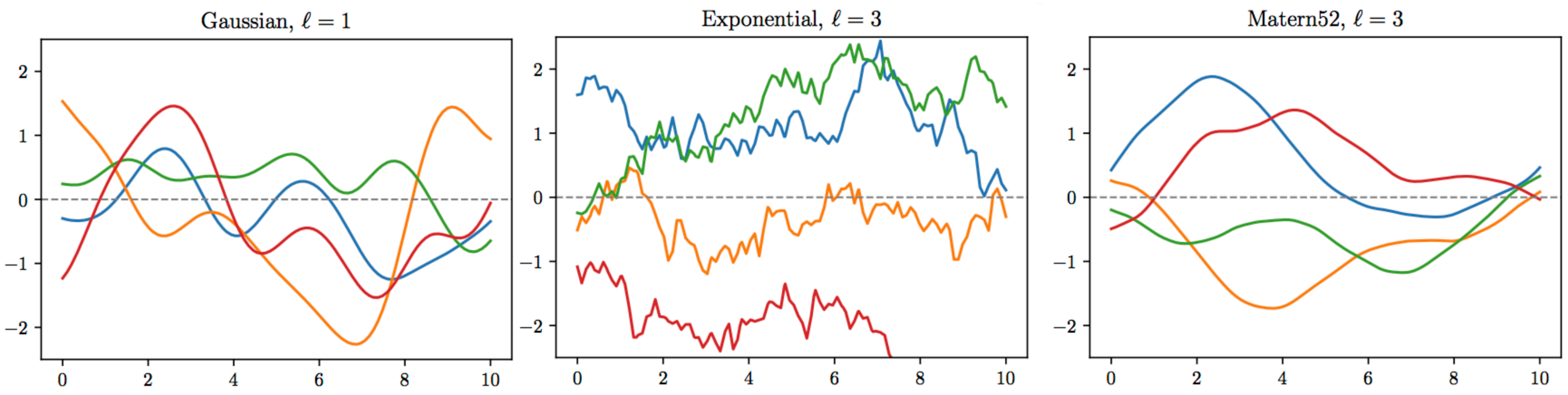
Some draws from a GP with different covariance kernel



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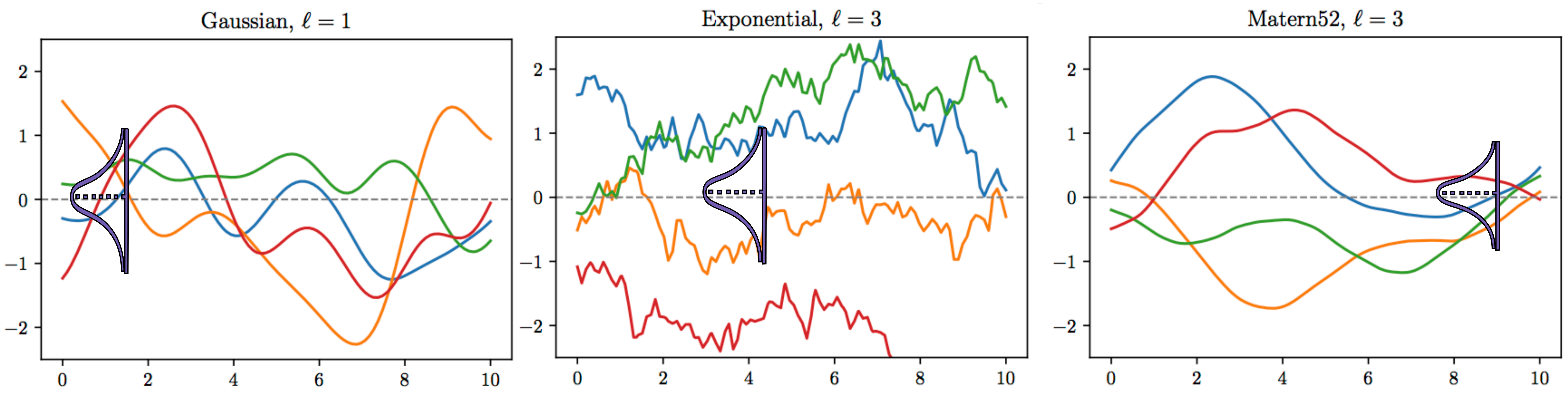

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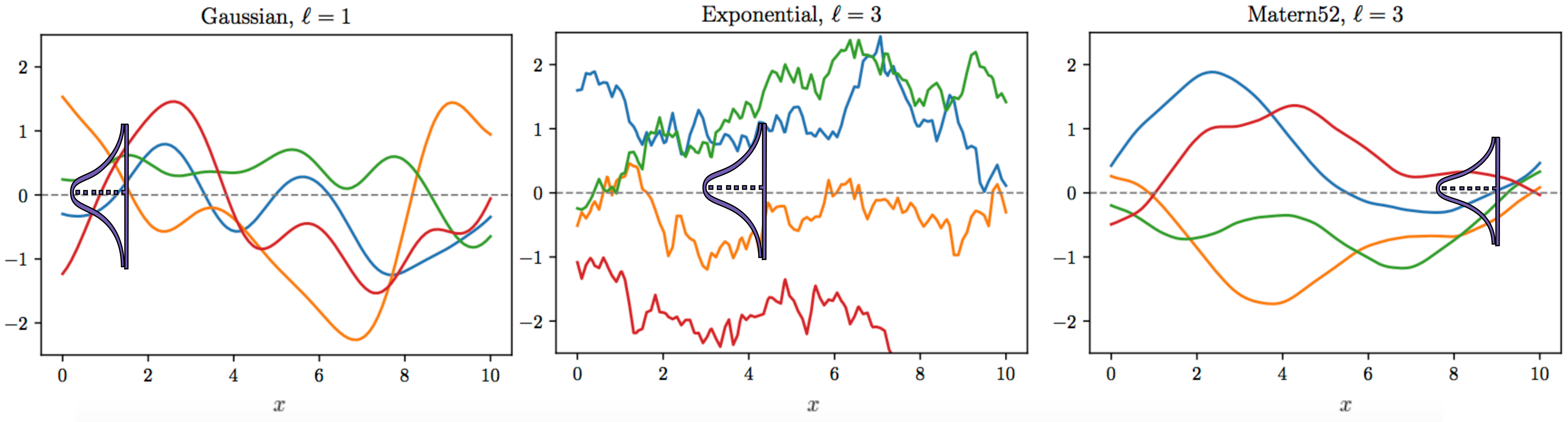
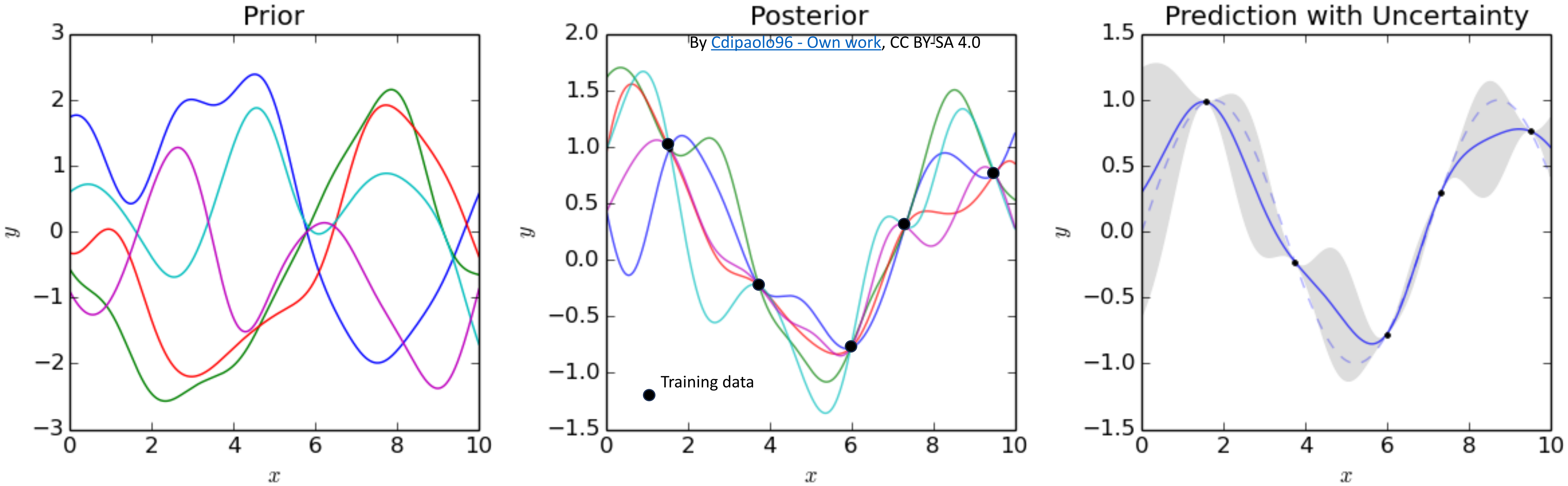


GP emulator training:
Before training (prior) —> Training on data (posterior): keep only the curves passing through the data and optimize the hyper-parameters of covariance function accordingly —> Predict with uncertainty.



Gaussian Process based model emulators

- Basis Representation Gaussian Process: Trains reduced number of GP's than number of observables.
  - **PCGP** : Principle component based Gaussian Process. Consider mean, but ignores variance of data from simulation.

Existing emulator

D. Hidden, et. al.
https://doi.org/10.1198/016214507000000888

  - **PCSK** : Principle component based Gaussian Process. Consider mean, but ignores variance of data from simulation during hyperparameter optimization. Considers variance in posterior predictive distribution.

Existing emulator

D. Liyanage, Ö. Sürer, M. Plumlee, W. Matthew, U. Heinz,
Phys. Rev. C. 108.054905

M. Plumlee, Ö. Sürer, S. Wild, M. Chan
BAND SURMISE package

  - **LCGP** : Transformation basis for data is estimated during GP training to allow variations in observable error. Adjusts mean and covariance from GP predictions according to variations in observable error.

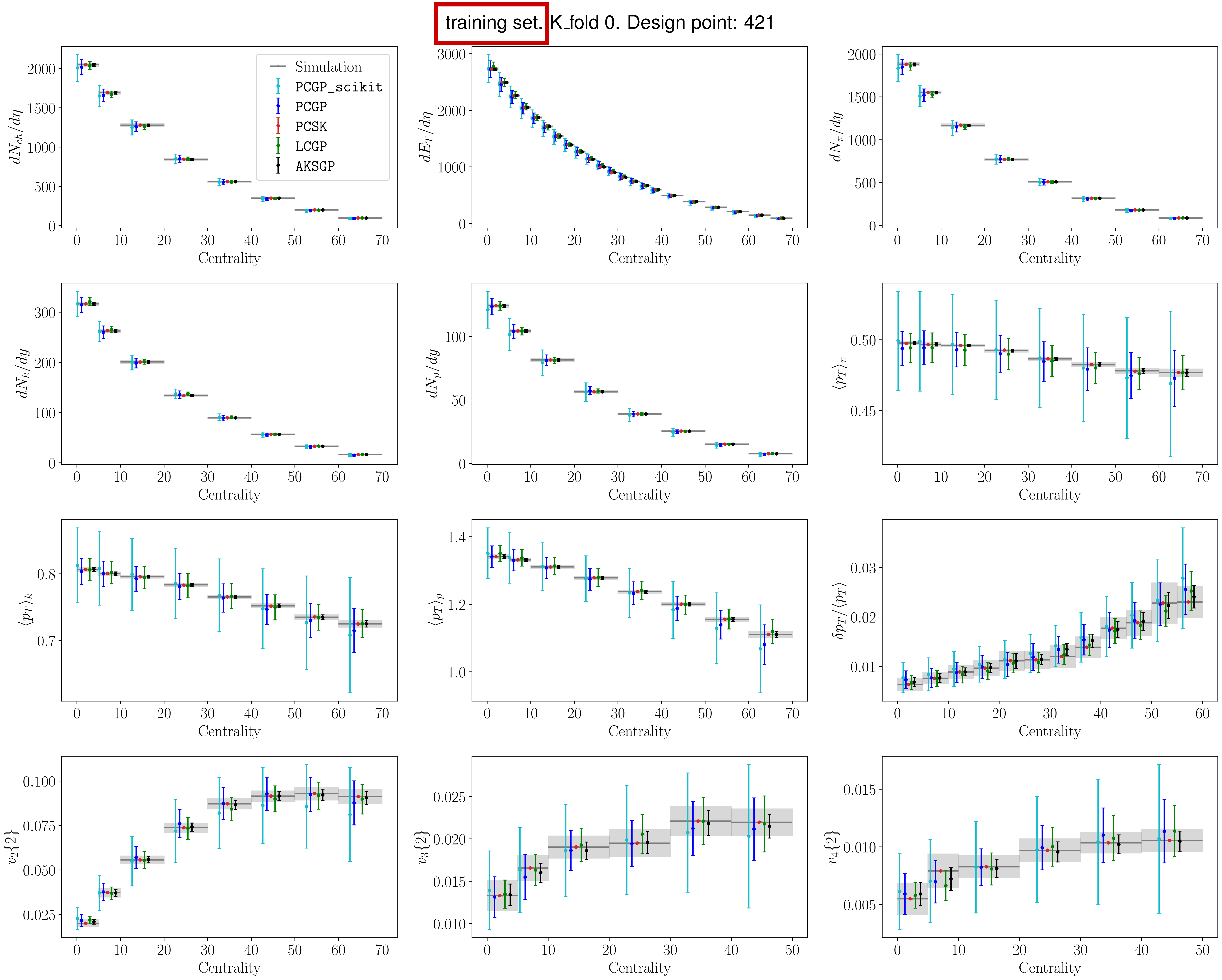
New emulator

M. Chan, PhD Thesis
High-Dimensional Gaussian Process Methods for Uncertainty Quantification

- Automatic kernel selection Gaussian Process (**AKSGP**): Trains independent GP's for each observable.
  - Account for both means and variances of data from simulation during GP training, ensuring that optimized hyperparameters are informed by both.
  - The appropriate covariance kernel is automatically selected from a predefined list of kernels.

New emulator

Predictions on training data



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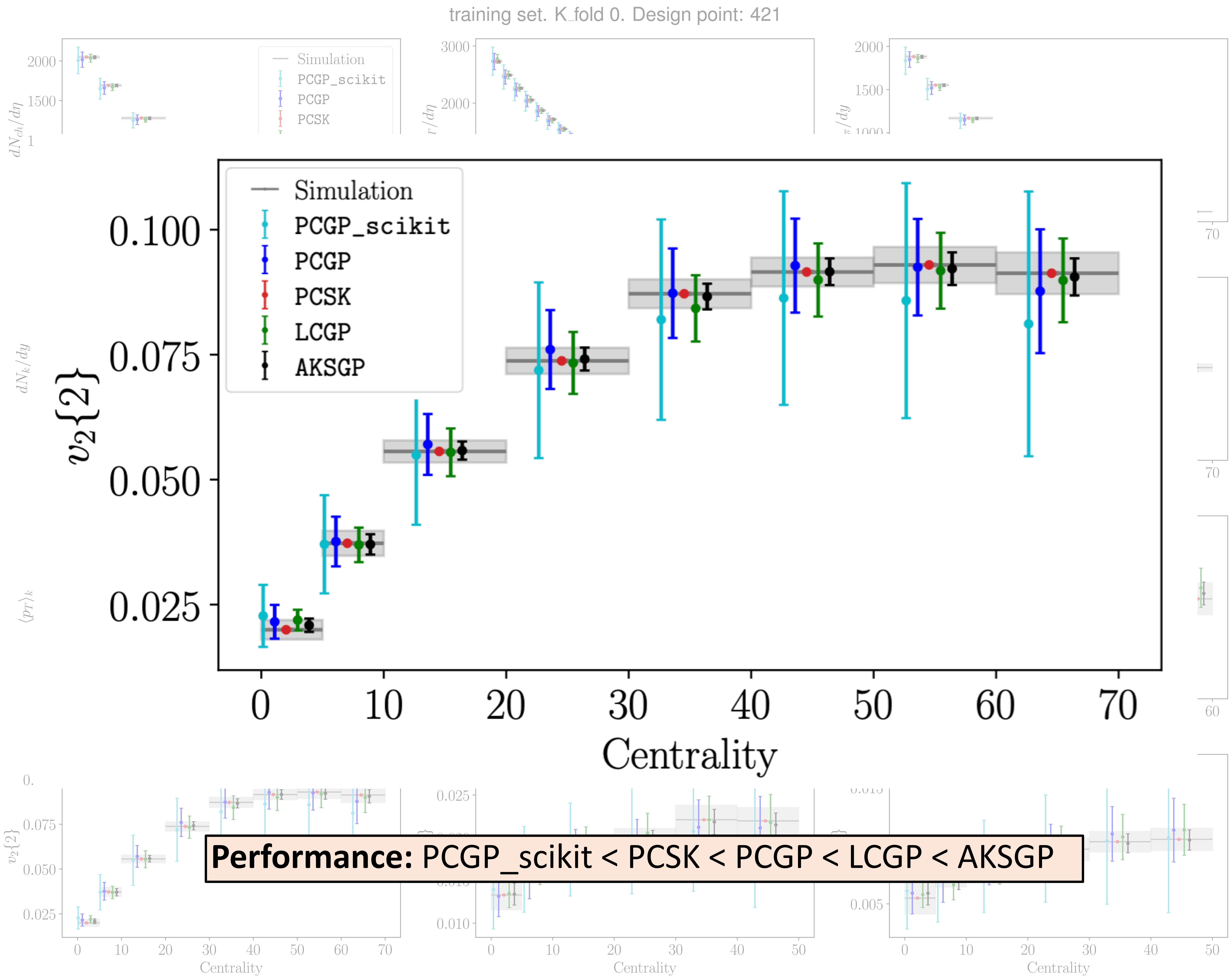
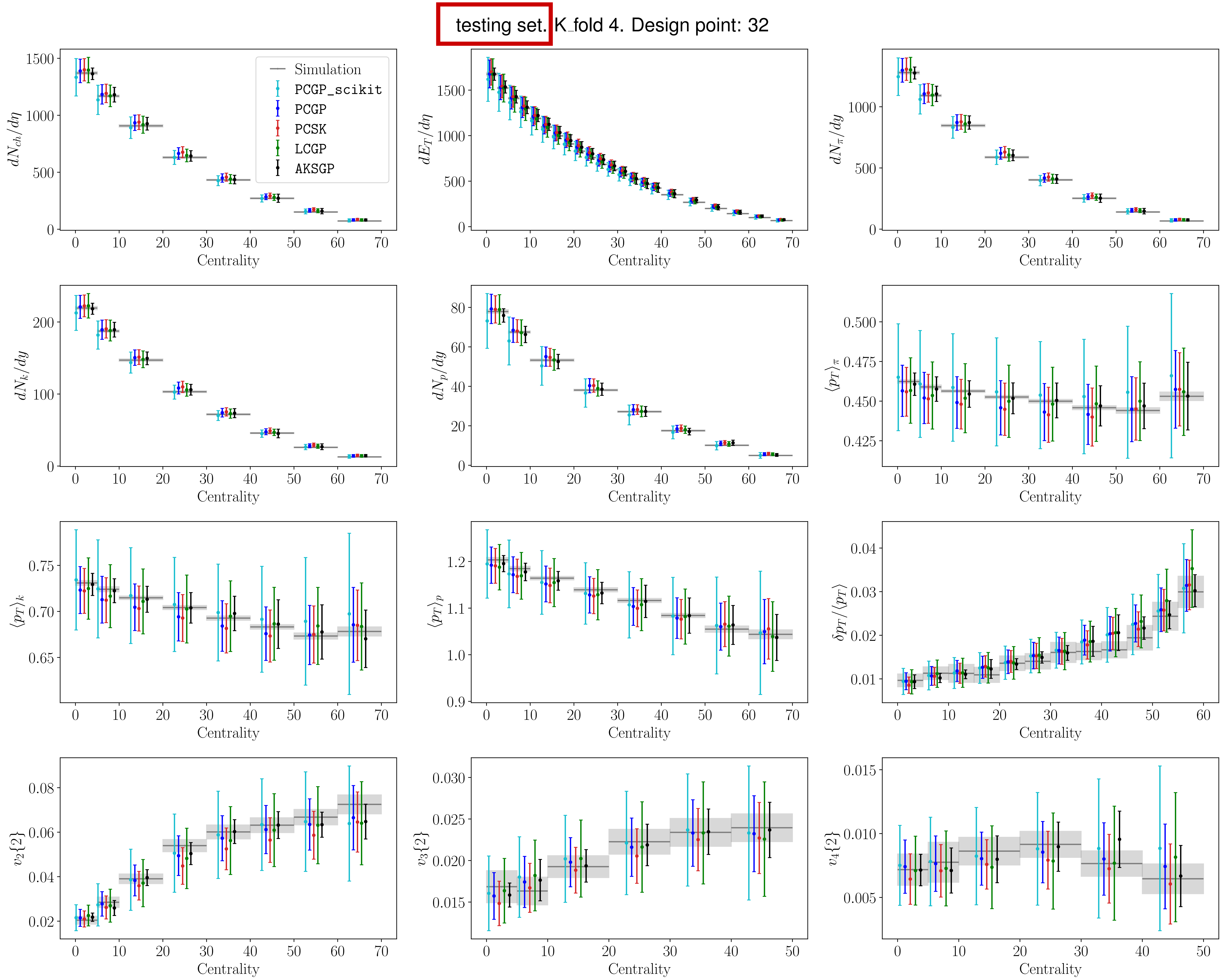


Performance: PCGP_scikit < PCSK < PCGP < LCGP < AKSGP

Predictions on test data



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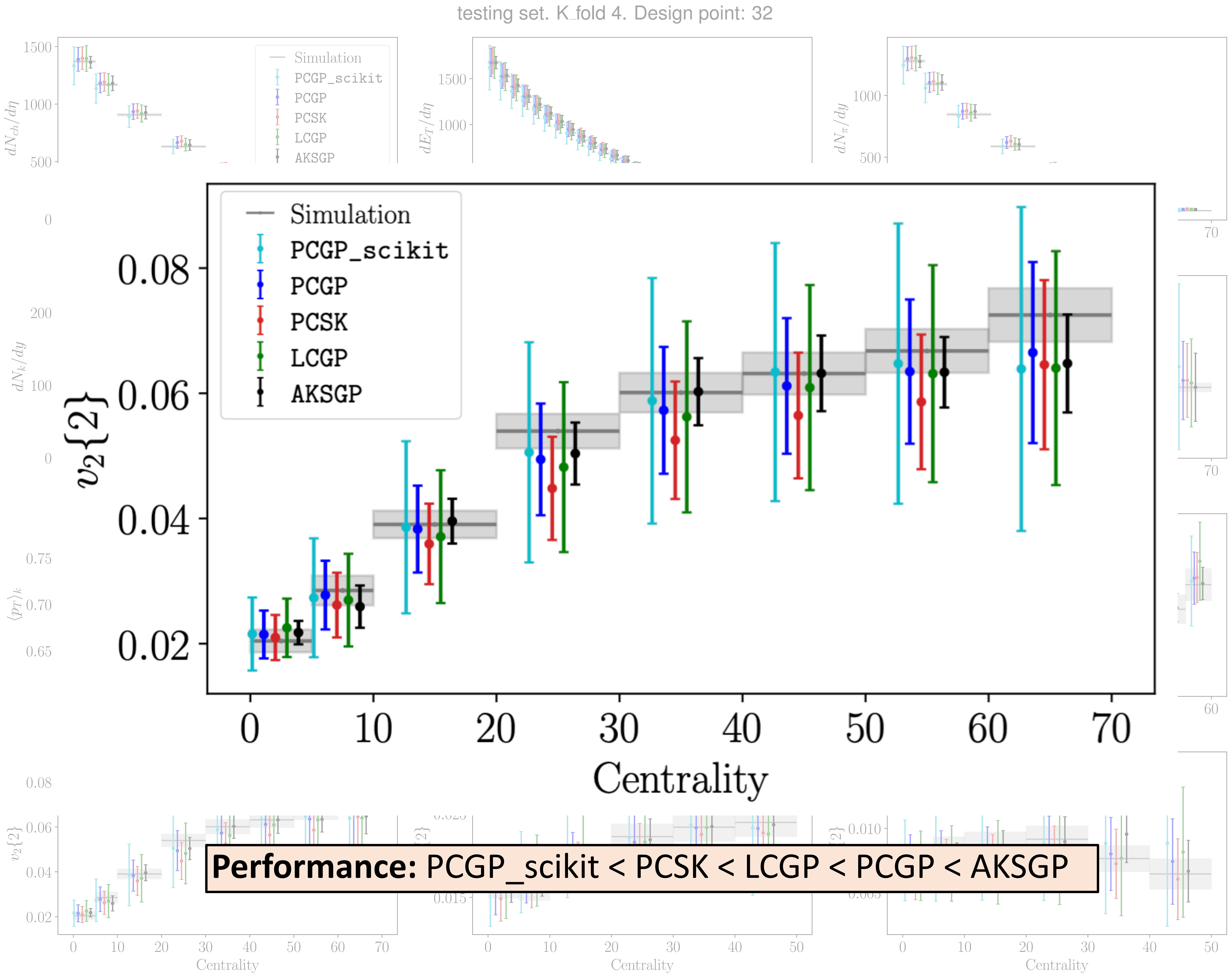


Performance: PCGP_scikit < PCSK < LCGP < PCGP < AKSGP

Different metrics for comparing Emulators

Mean (standard deviation) over 5-fold cross validation (split training and test data randomly 5 times)

	PCGP	PCGP_scikit	PCSK	LCGP	AKSGP	
RMSE	0.249 (0.009)	0.284 (0.012)	0.273 (0.010)	0.28 (0.009)	0.267 (0.003)	← 0 is best
95% Coverage	0.937 (0.007)	0.985 (0.004)	0.912 (0.008)	0.961 (0.006)	0.888 (0.006)	← 0.95 is best
KL Divergence	79.032 (5.801)	185.705 (17.342)	94.445 (5.998)	113.52 (7.317)	70.927 (6.555)	← 0 is best
Hellinger Distance	0.687 (0.004)	0.742 (0.004)	0.696 (0.004)	0.721 (0.004)	0.676 (0.003)	← 0 is best
Wasserstein Distance	0.270 (0.011)	0.422 (0.021)	0.290 (0.012)	0.345 (0.015)	0.258 (0.005)	← 0 is best

AKSGP kernel list: (RBF, Matern 1/2, Matern 3/2, Matern 5/2). Easily extendable to more kernels (non-stationary, anisotropic)

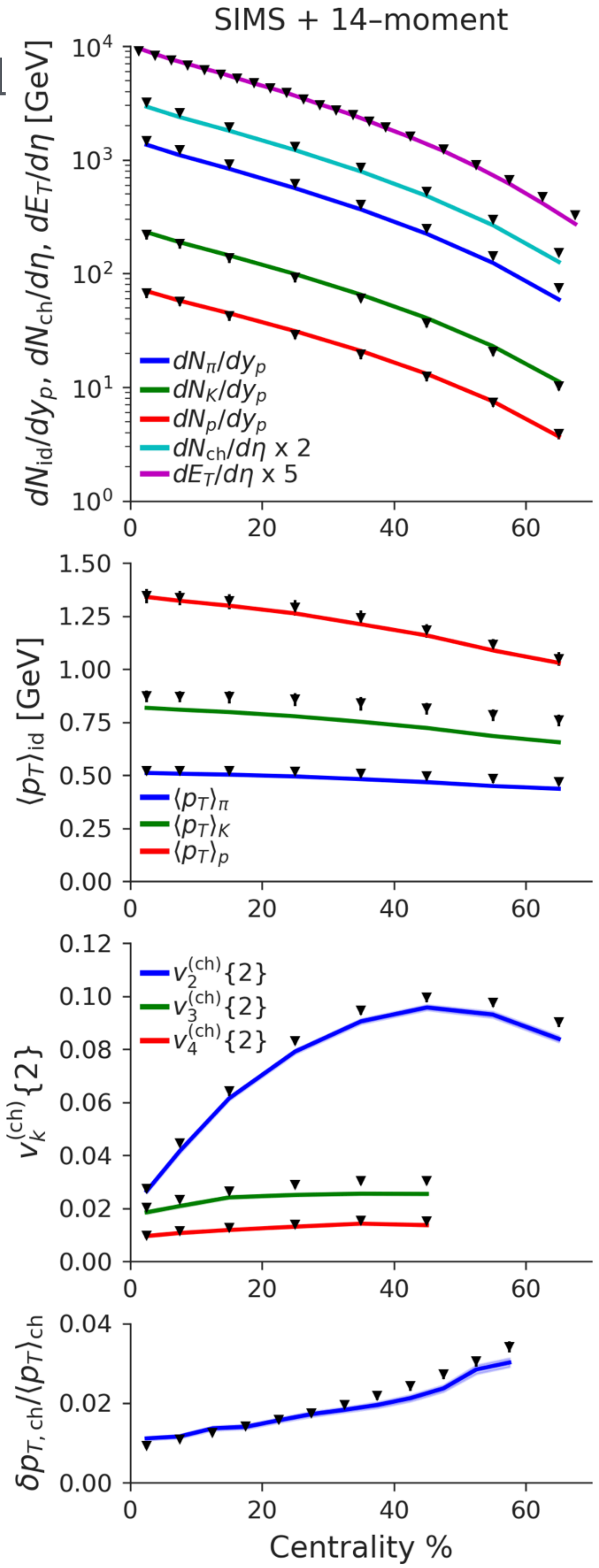
Ongoing work in collaboration with Moses Chan, Richard Furnstahl, Ulrich Heinz, and Matthew Pratola

Part 2 : Quantifying theoretical uncertainties

Model prediction

Scikit GP
RBF kernel

Best fit (MAP) output from the calibrated Models:



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

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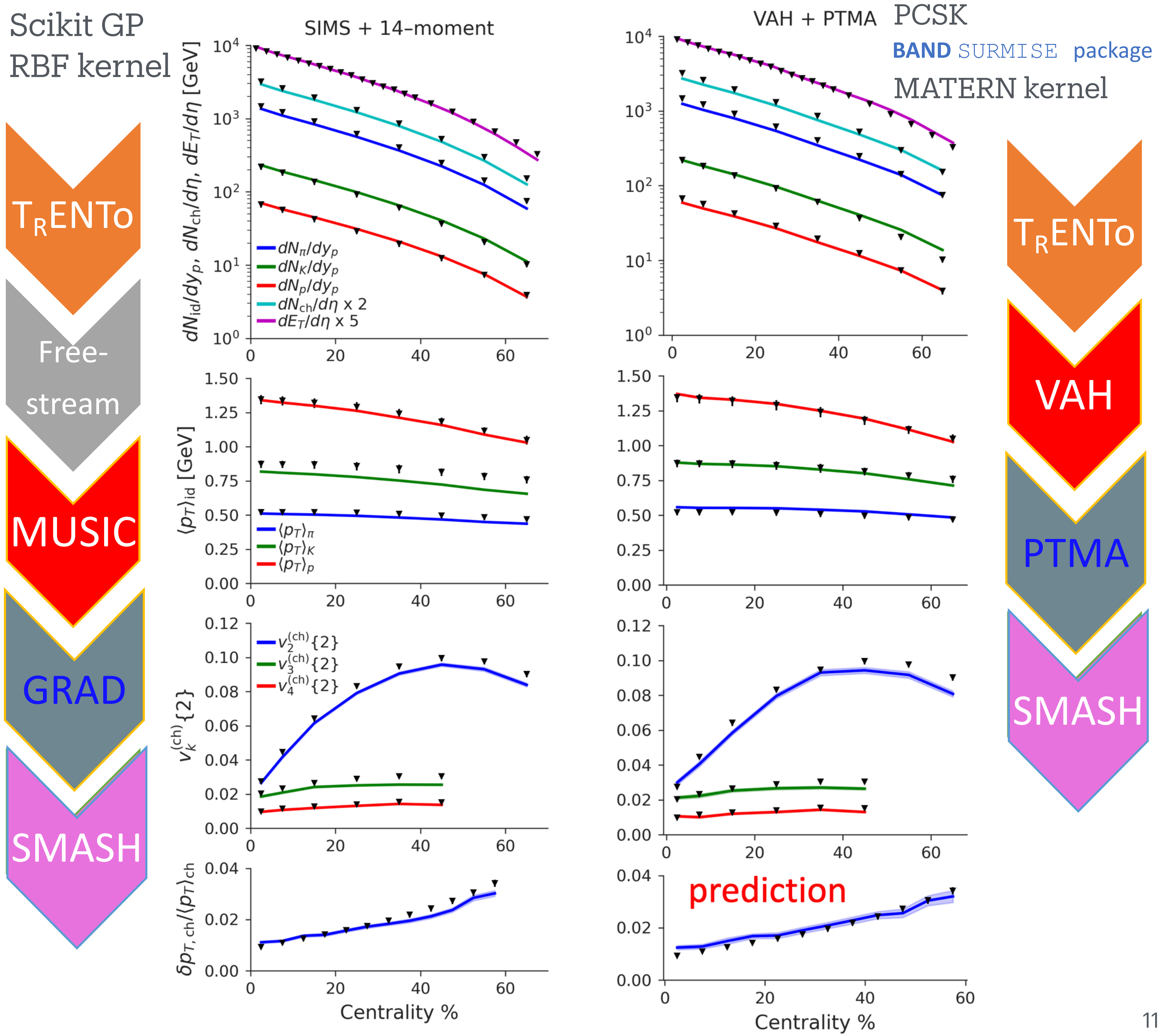

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D. Liyanage et al., 2302.14184

Model prediction

Best fit (MAP) output from the calibrated Models:

- MAP predictions for VAH+PTMA are in slightly better agreement with experimental data than SIMS+14-moment model.
- How to quantify the level of improvement? Are the inferred physical parameters statistically compatible? How to quantify their theory uncertainty?

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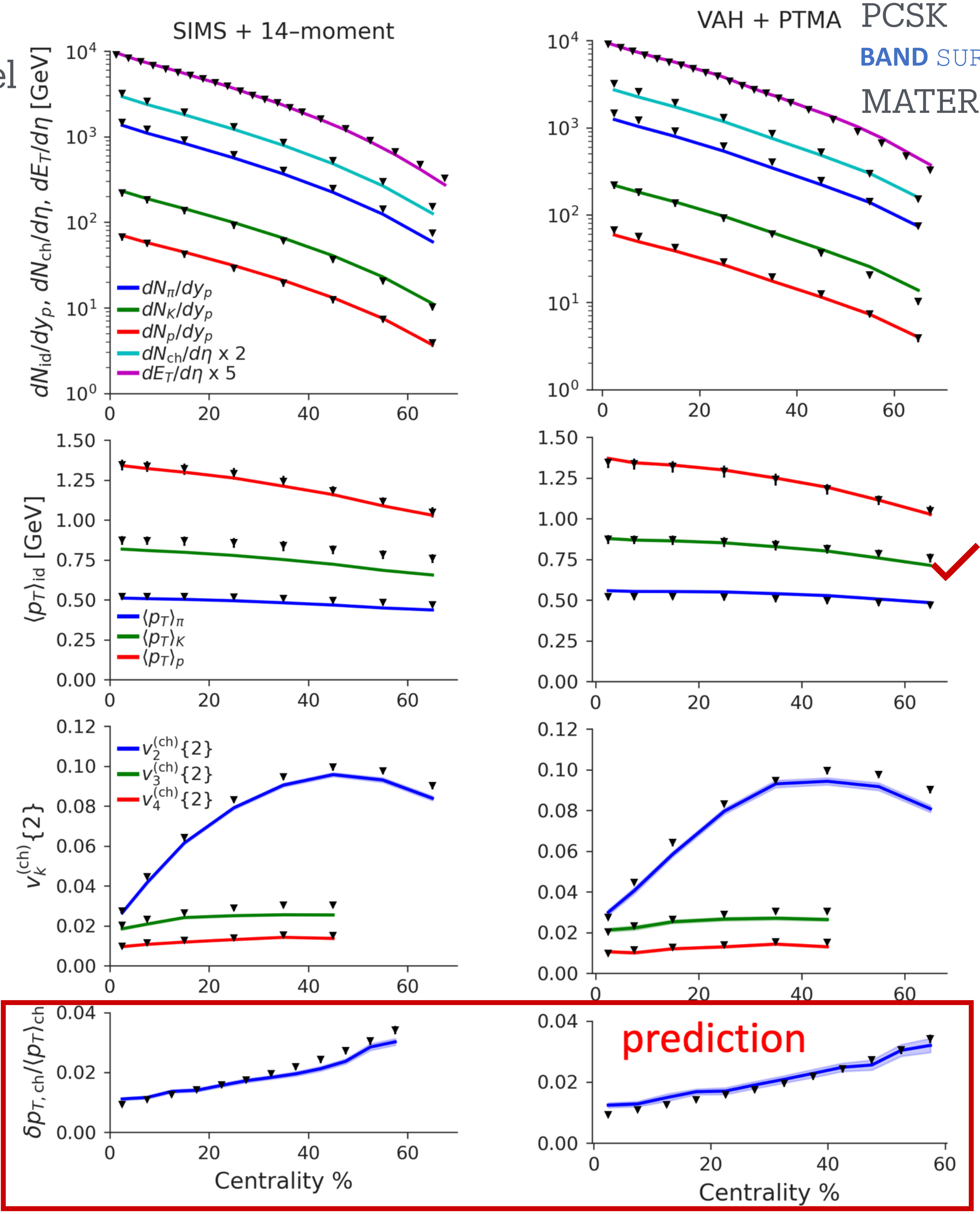

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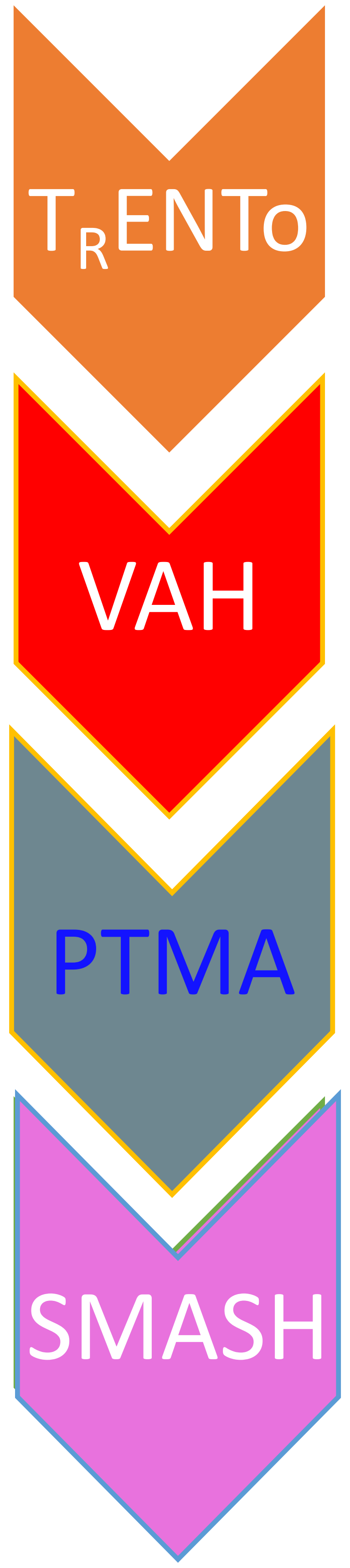
BAND SURMISE package
MATERN kernel



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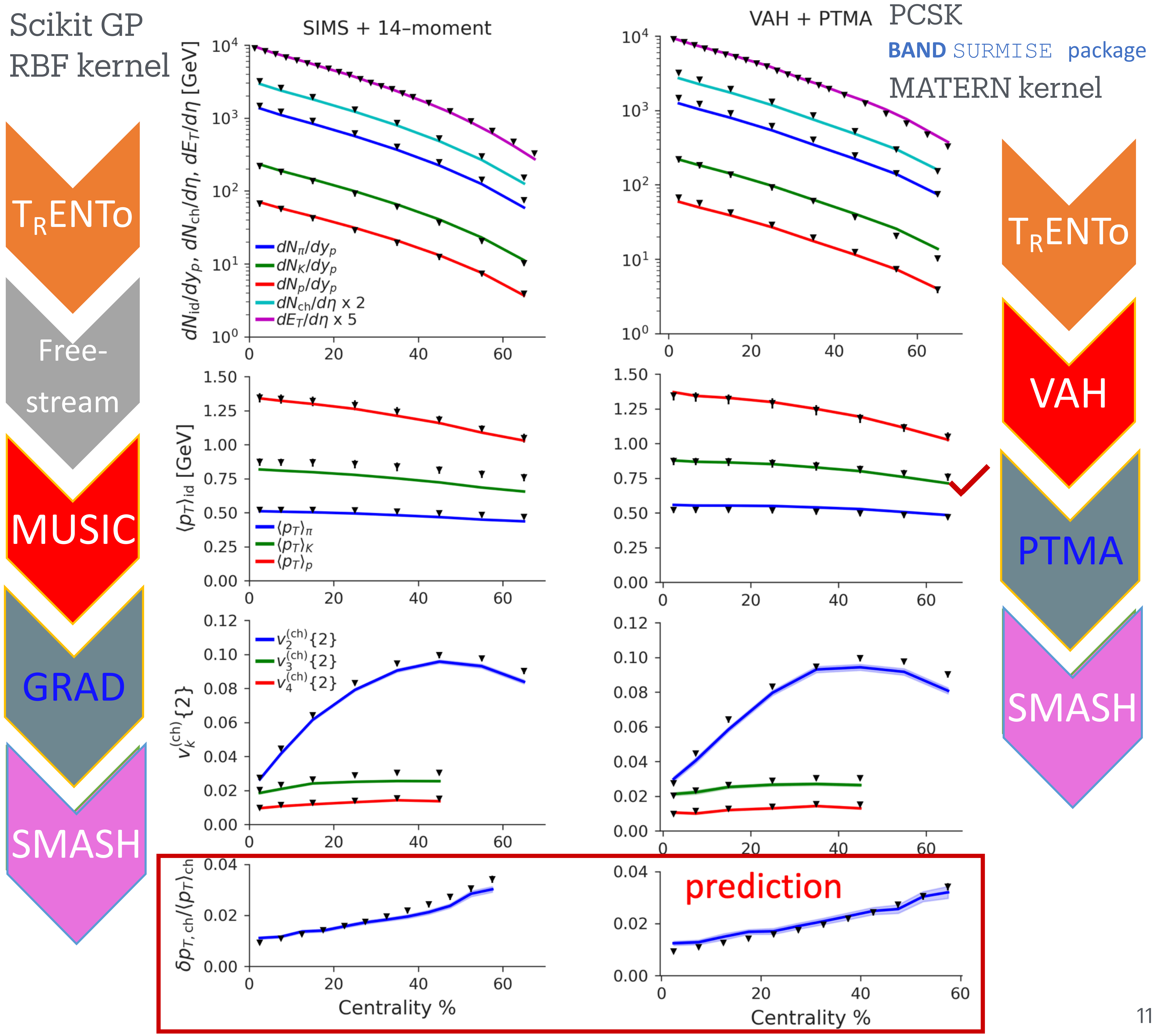
- Our aim — Correct inference of physical parameters.



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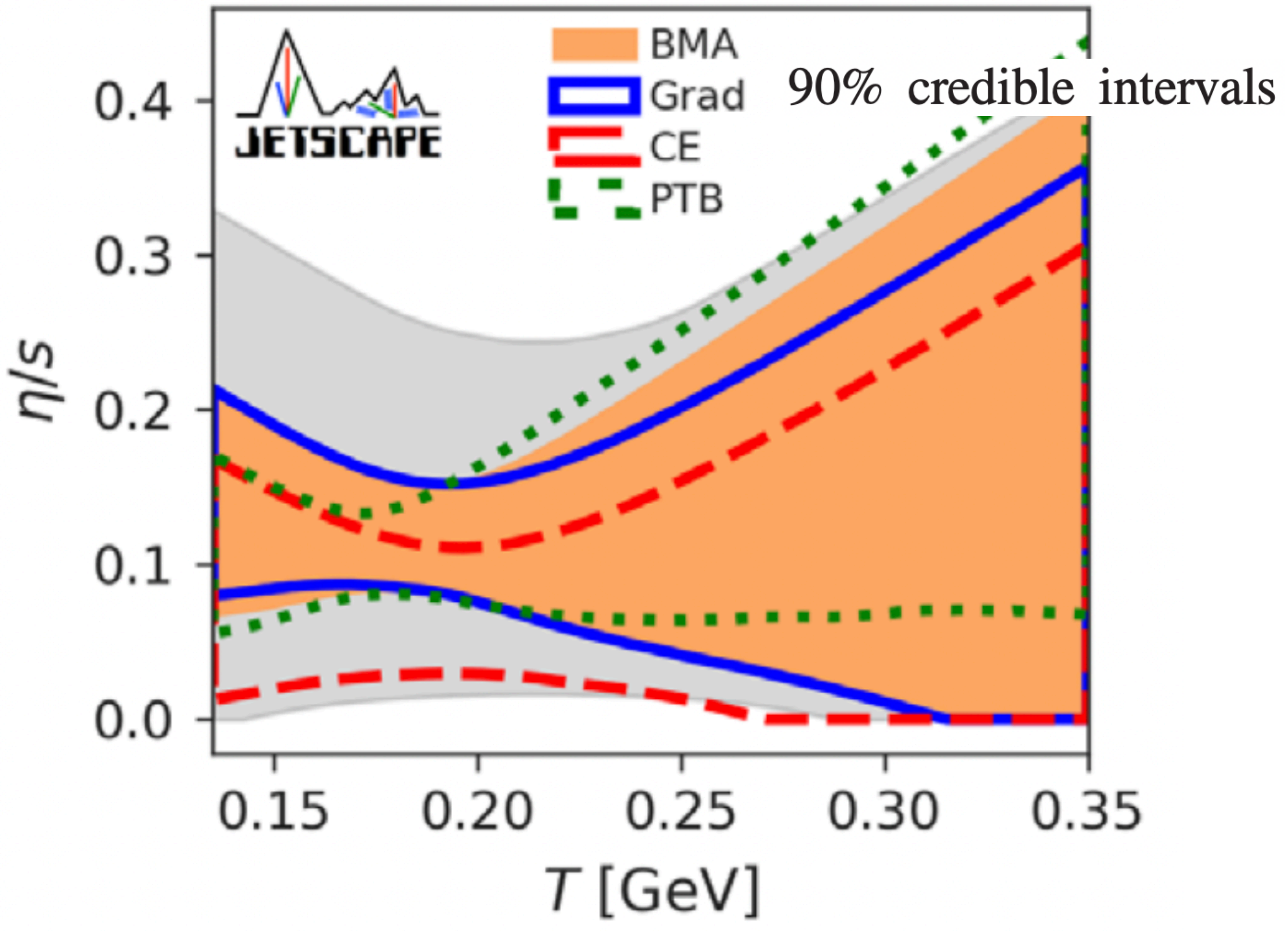
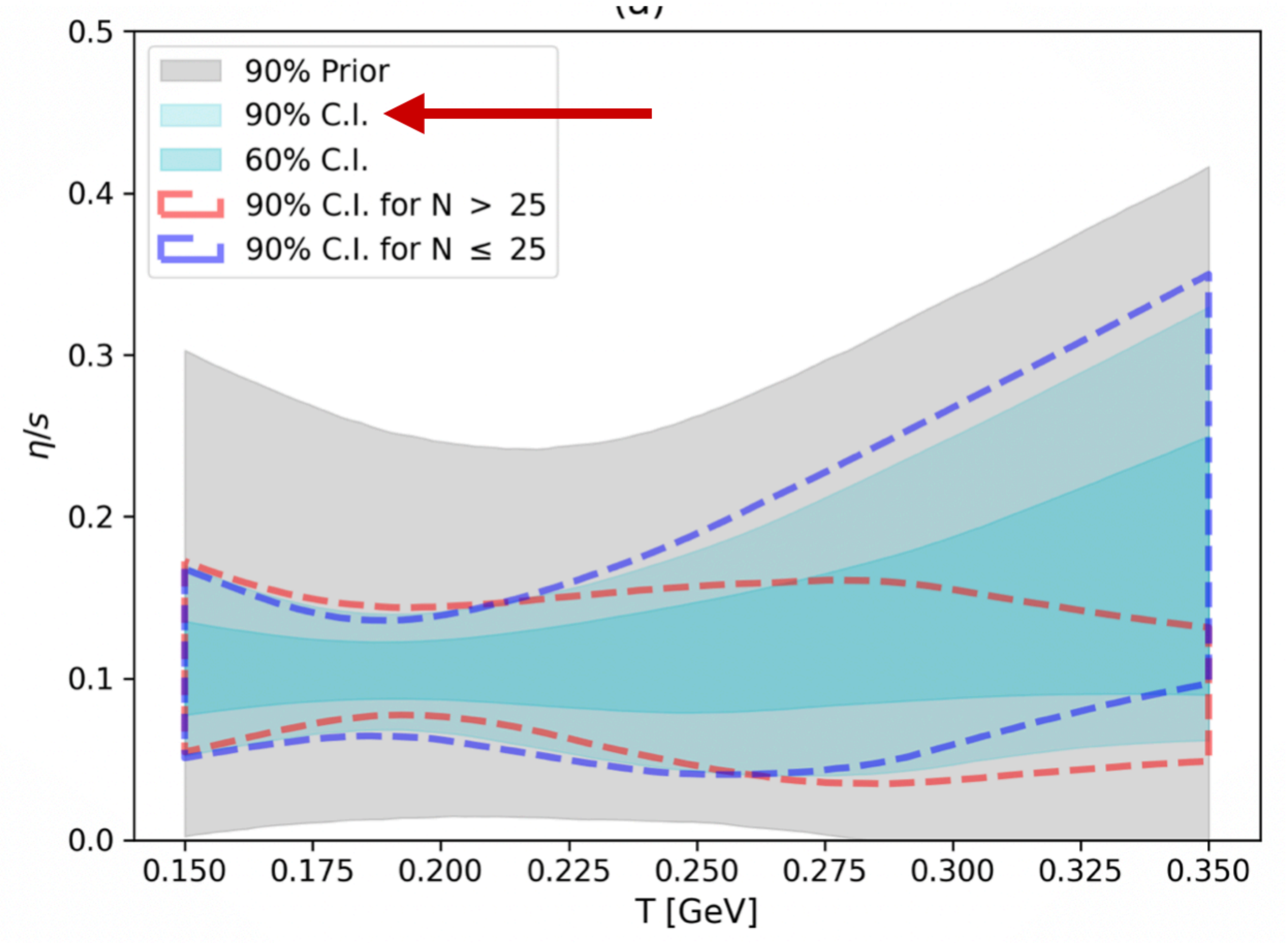
Tension between different studies

Coefficient of shear viscosity: η





JETSCAPE SIMS calibration

D. Everett *et al.* 2010.03928, 2011.01430

Three different models: Grad, CE, PTB

- Posterior distributions for η/s differ between models but are mutually statistically compatible.

Viscous Anisotropic Hydrodynamics Model

M. McNelis *et al.* 2101.02827

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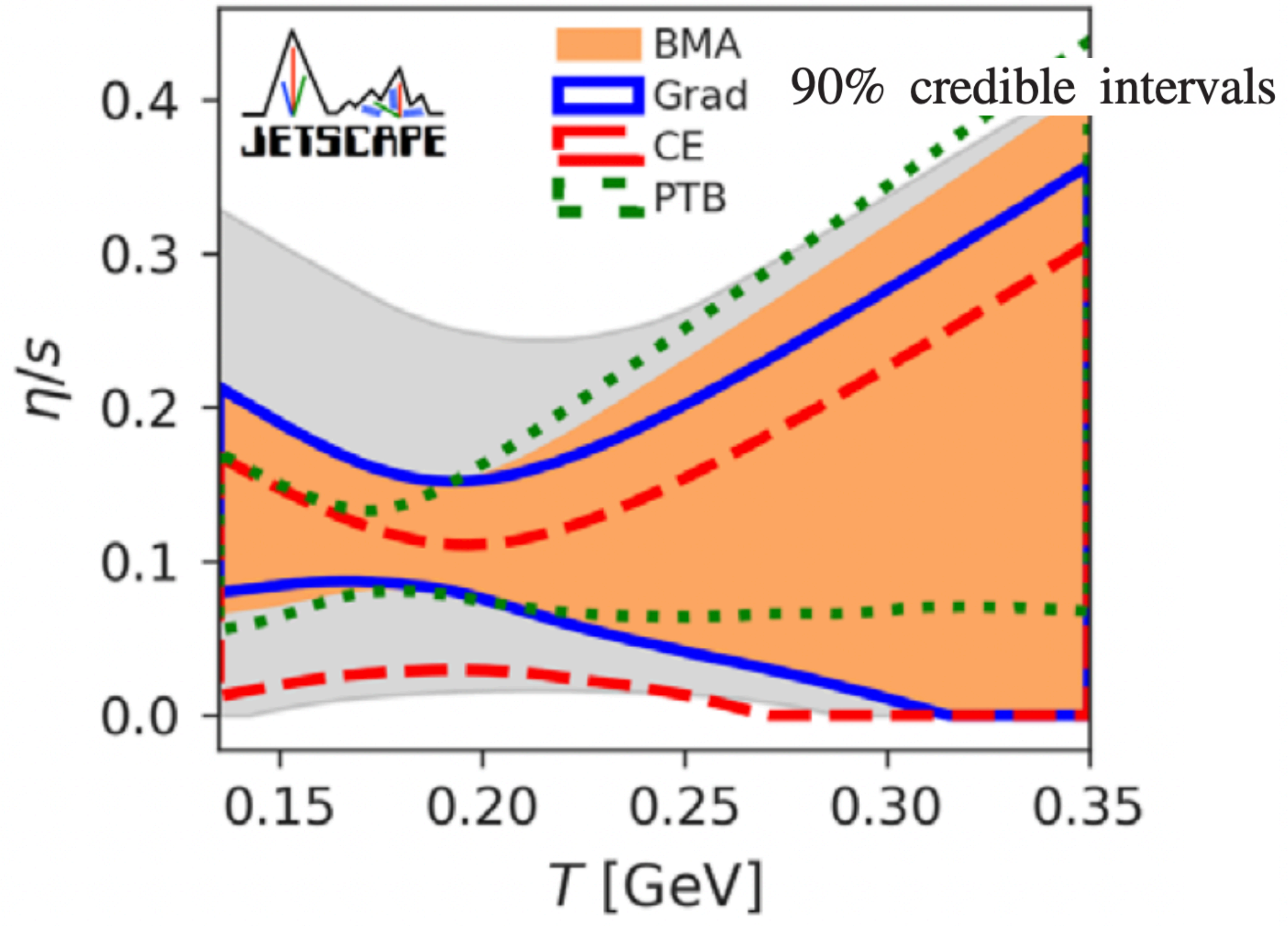

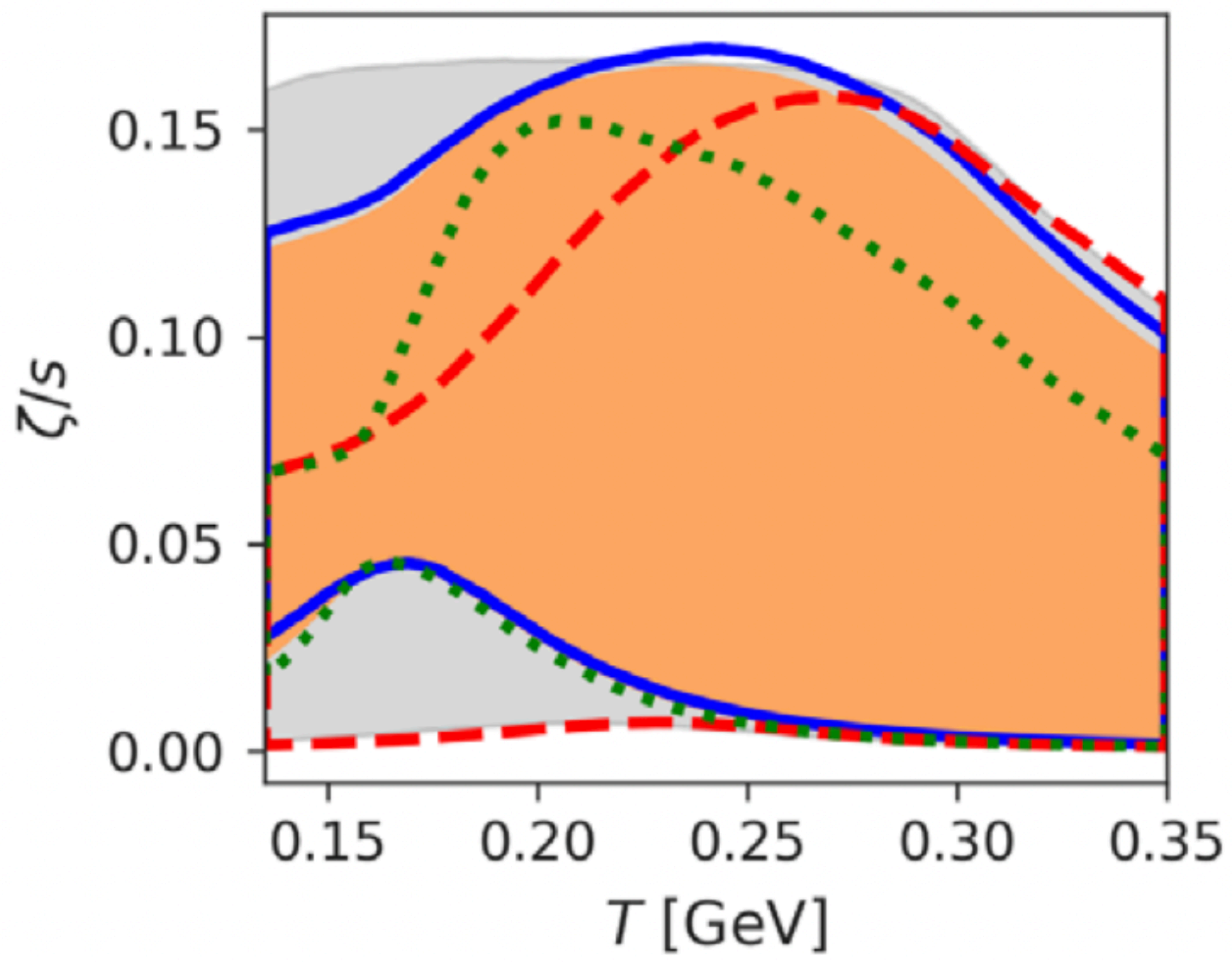

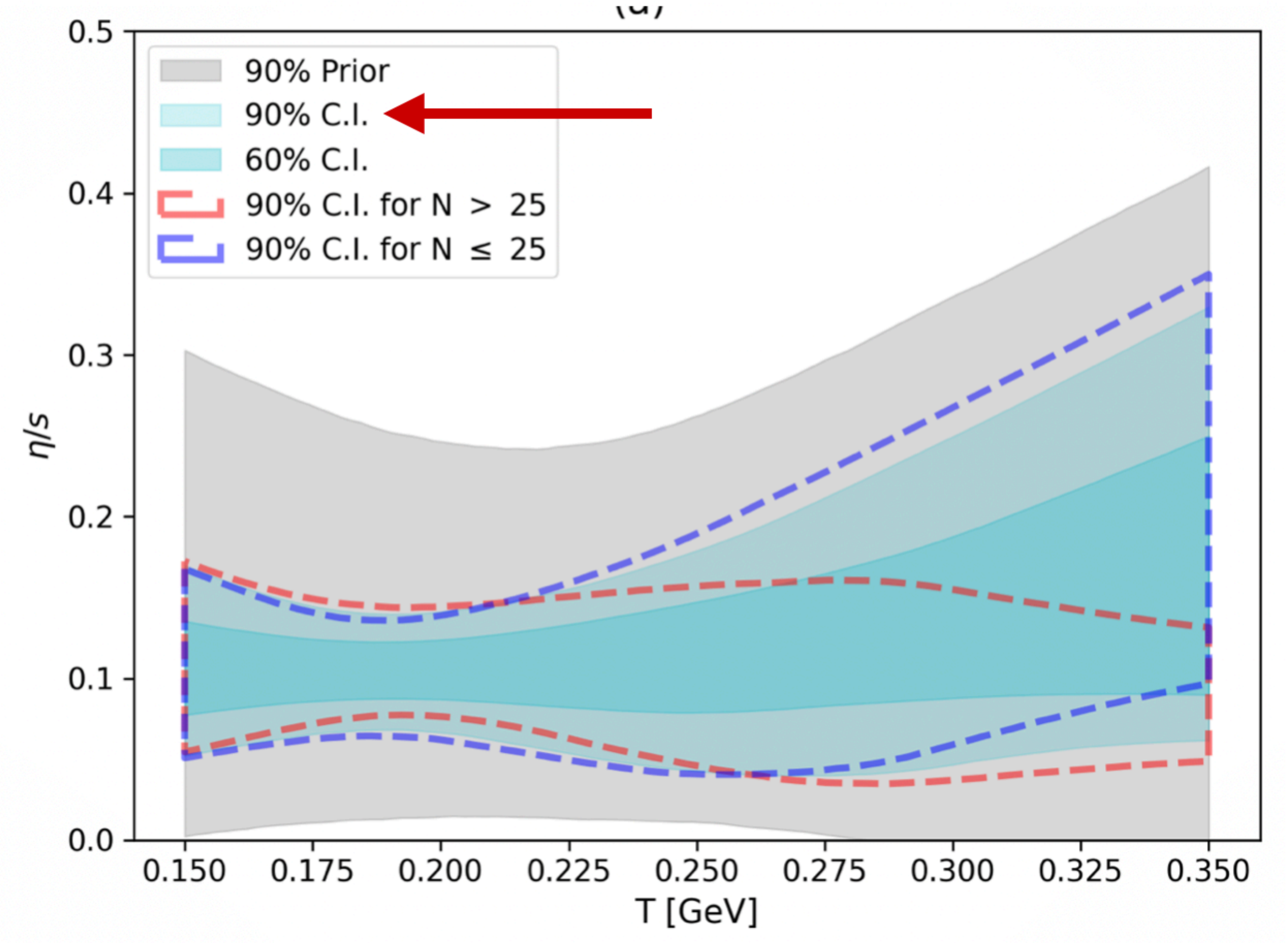

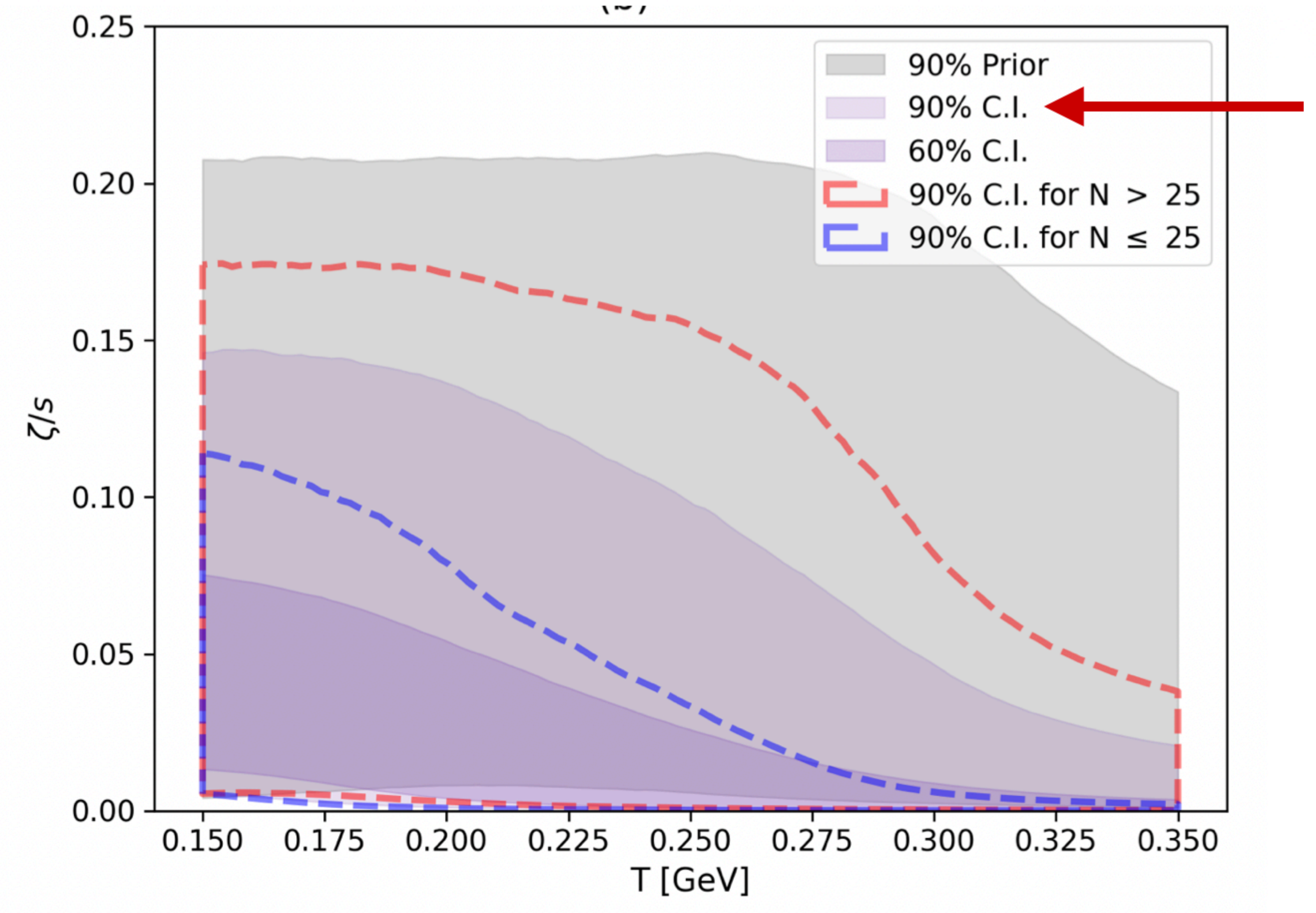

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Three different models: Grad, CE, PTB

- Posterior distributions for η/s differ between models but are mutually statistically compatible.
- Larger model differences seen in posterior distributions for ζ/s, but still statistically compatible.

Viscous Anisotropic Hydrodynamics Model

M. McNelis *et al.* 2101.02827

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Accounting for theoretical uncertainties: Model discrepancy

George Box: “All models are wrong, but some are useful”

Accounting for theoretical uncertainties: Model discrepancy

George Box: "All models are wrong, but some are useful"

- All theories are approximations of an underlying truth and should be applied only within their domains of validity. Extending a theory beyond its scope not only leads to incorrect parameter estimates, rendering them as mere fitting variables, but also reduces the utility of the data. Therefore, it is essential to account for the uncertainties in the theory.

- Consideration of theoretical uncertainties for the complex multi-stage heavy-ion models is beyond current theoretical capabilities. As a first step, we develop a statistical framework to model this uncertainty.

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

$$\underbrace{y(t_i)}_{\text{Physical observation}} = \underbrace{\zeta(t_i)}_{\text{Truth}} + \underbrace{\epsilon(t_i)}_{\text{Observation error}}$$

Statistical equation

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But truth may not be among the models considered

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George Box: "All models are wrong, but some are useful"

- All theories are approximations of an underlying truth and should be applied only within their domains of validity. Extending a theory beyond its scope not only leads to incorrect parameter estimates, rendering them as mere fitting variables, but also reduces the utility of the data. Therefore, it is essential to account for the uncertainties in the theory.

- Consideration of theoretical uncertainties for the complex multi-stage heavy-ion models is beyond current theoretical capabilities. As a first step, we develop a statistical framework to model this uncertainty.

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

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

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

J. Brynjarsdóttir and A. O'Hagan, https://iopscience.iop.org/article/10.1088/0266-5611/30/11/114007

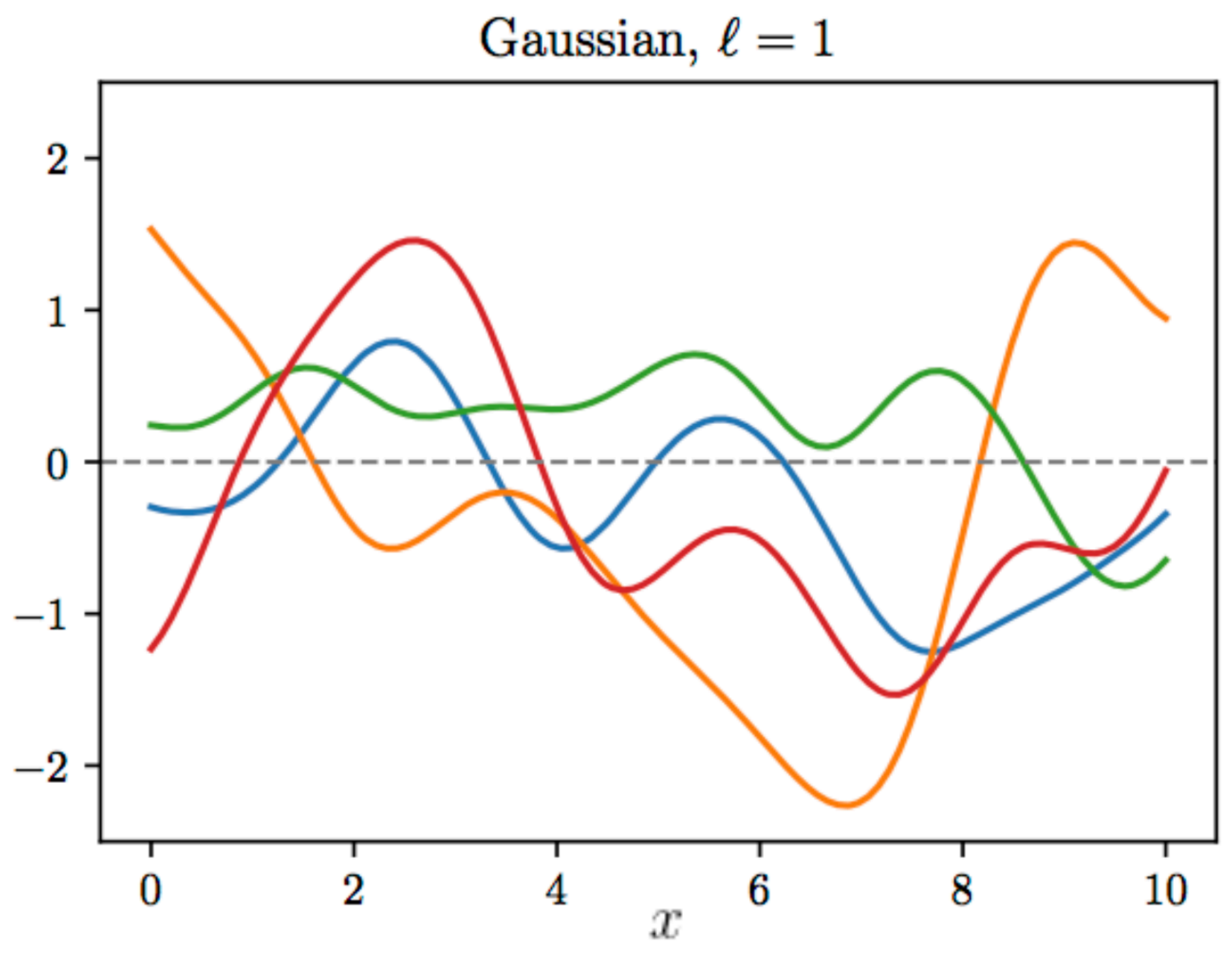
D. Higdon, M. Kennedy, *et. al.*, https://doi.org/10.1137/S1064827503426693

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

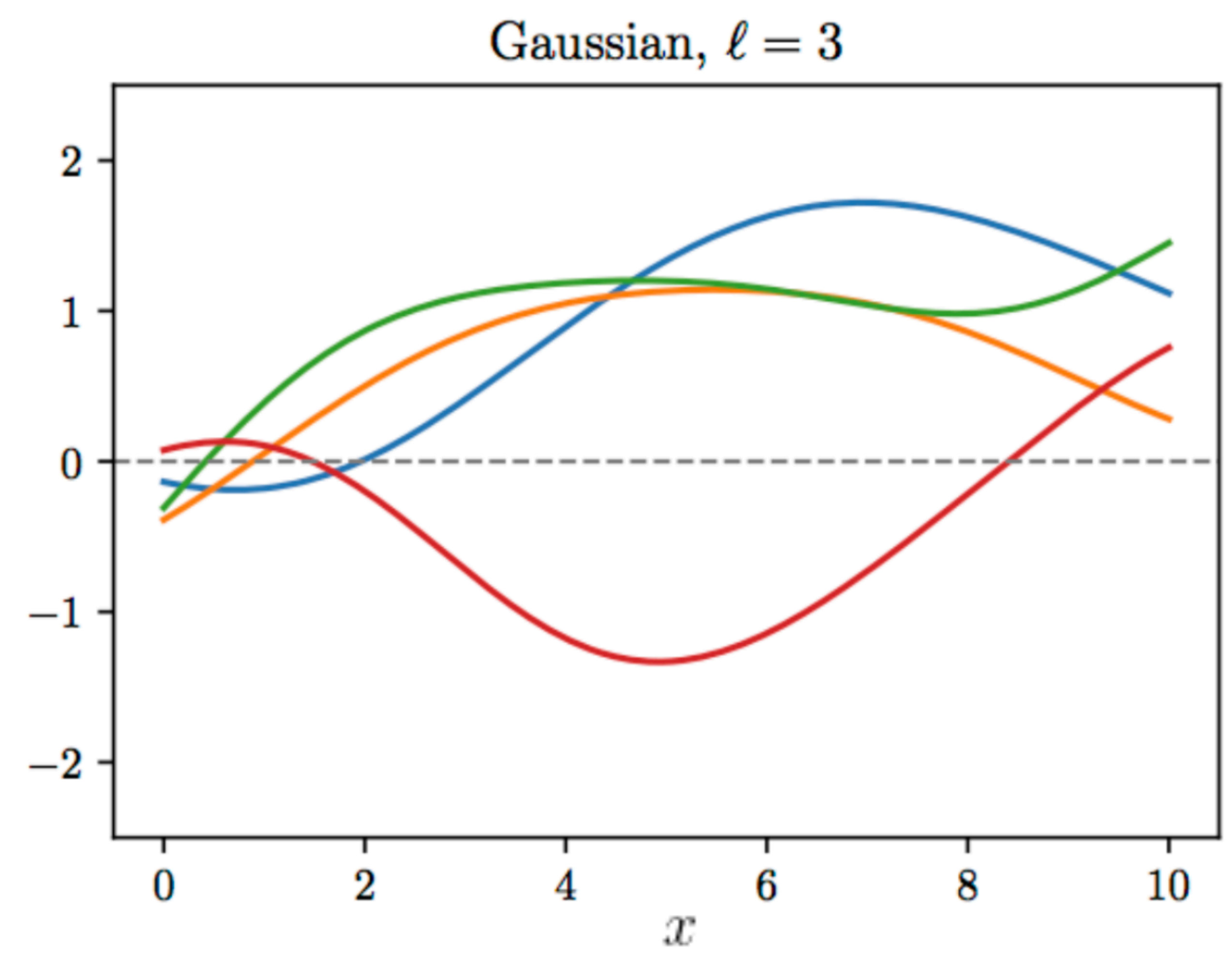
Gaussian process: flexible modeling

Gaussian kernel: $k(x_i, x_j) = \bar{c}^2 \exp\left(-\frac{d(x_i, x_j)^2}{2\ell^2}\right)$

Correlation length ℓ ->

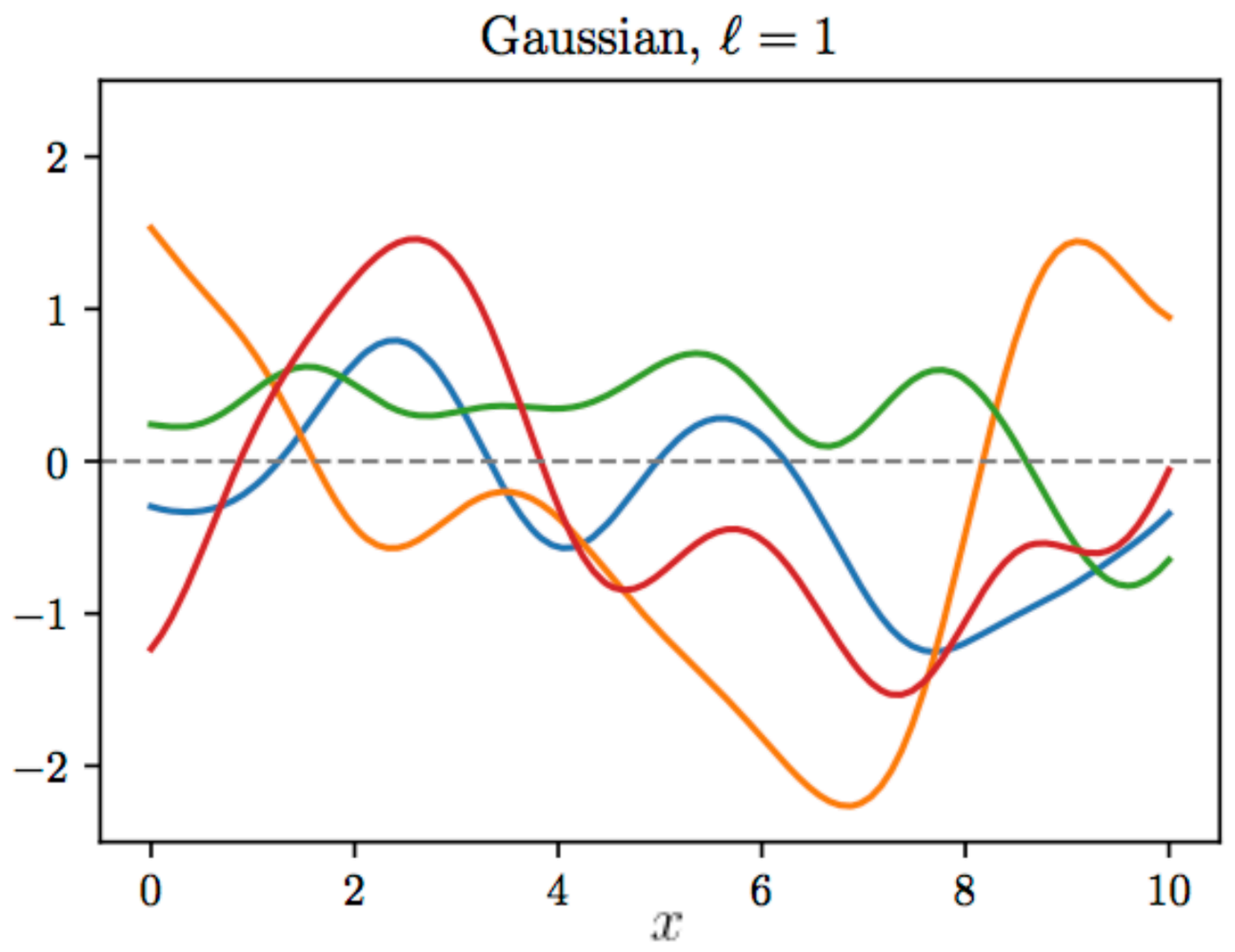


Variation over a length of 1

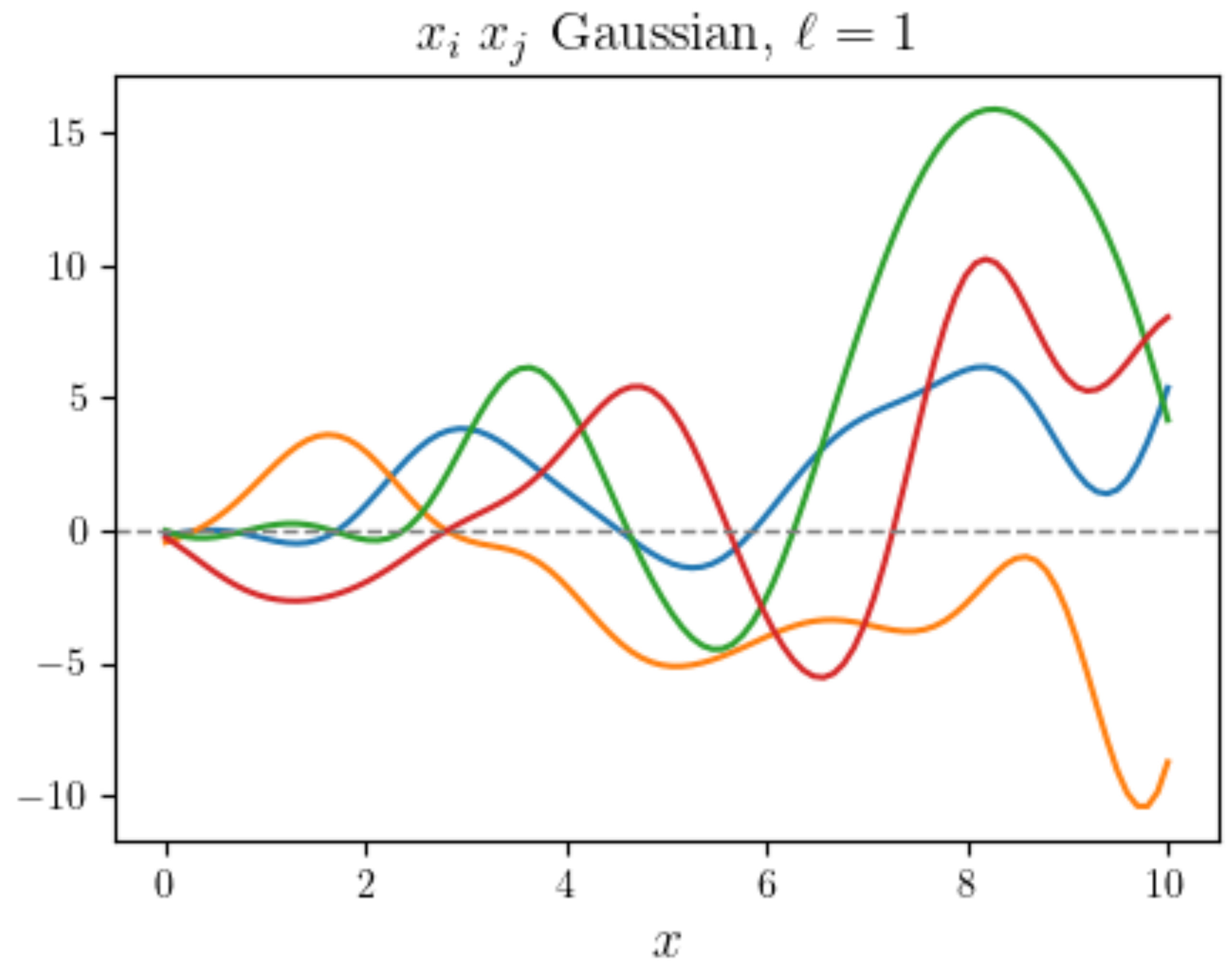


Variation over a length of 3

Stationary vs non-stationary kernel ->



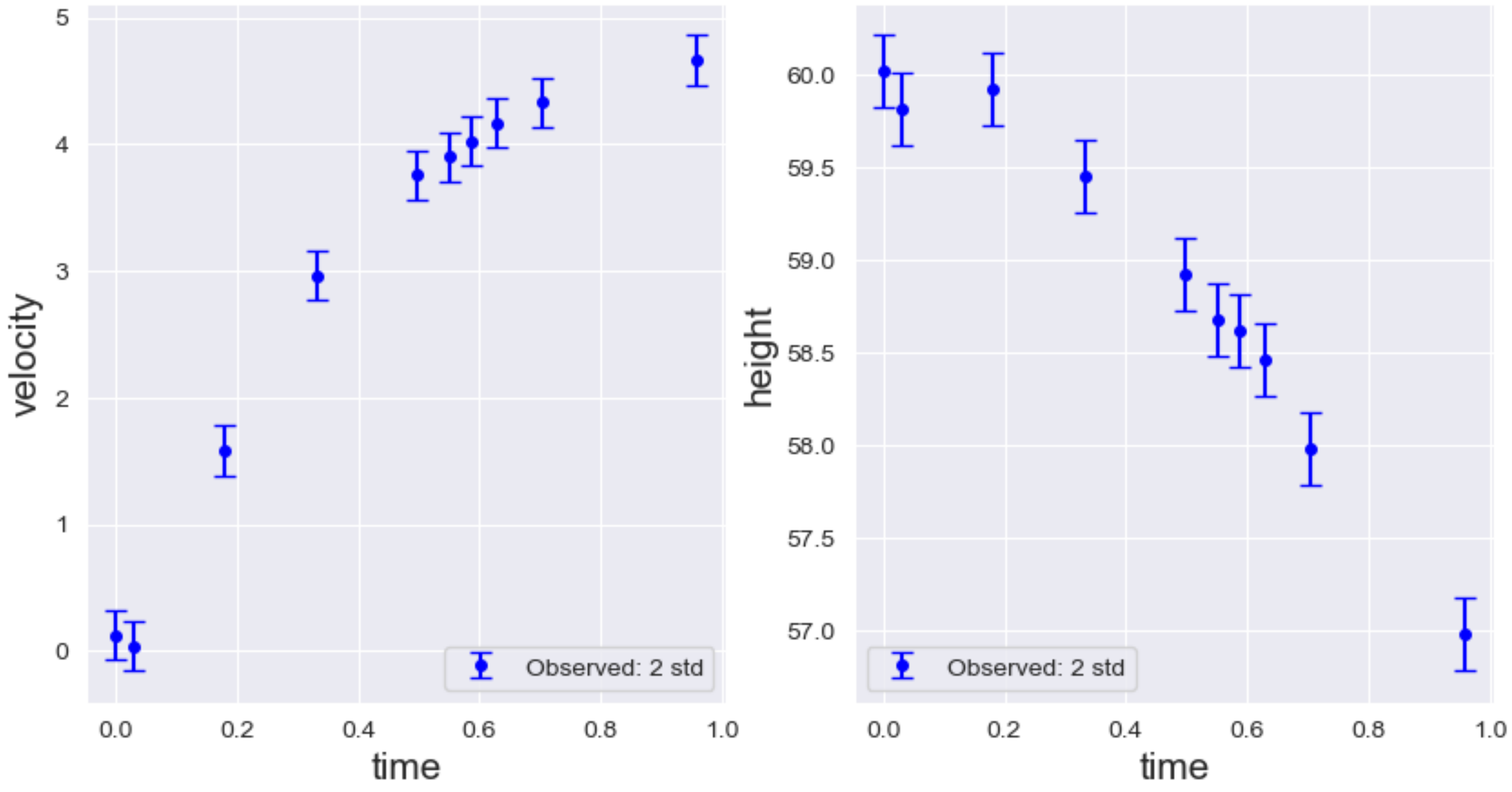
Stationary



Non-stationary

A simple example: ball drop experiment

- A ball is dropped from a tower of height 60 m
- Velocity and height are measured at different times. Measurements are uncertain.

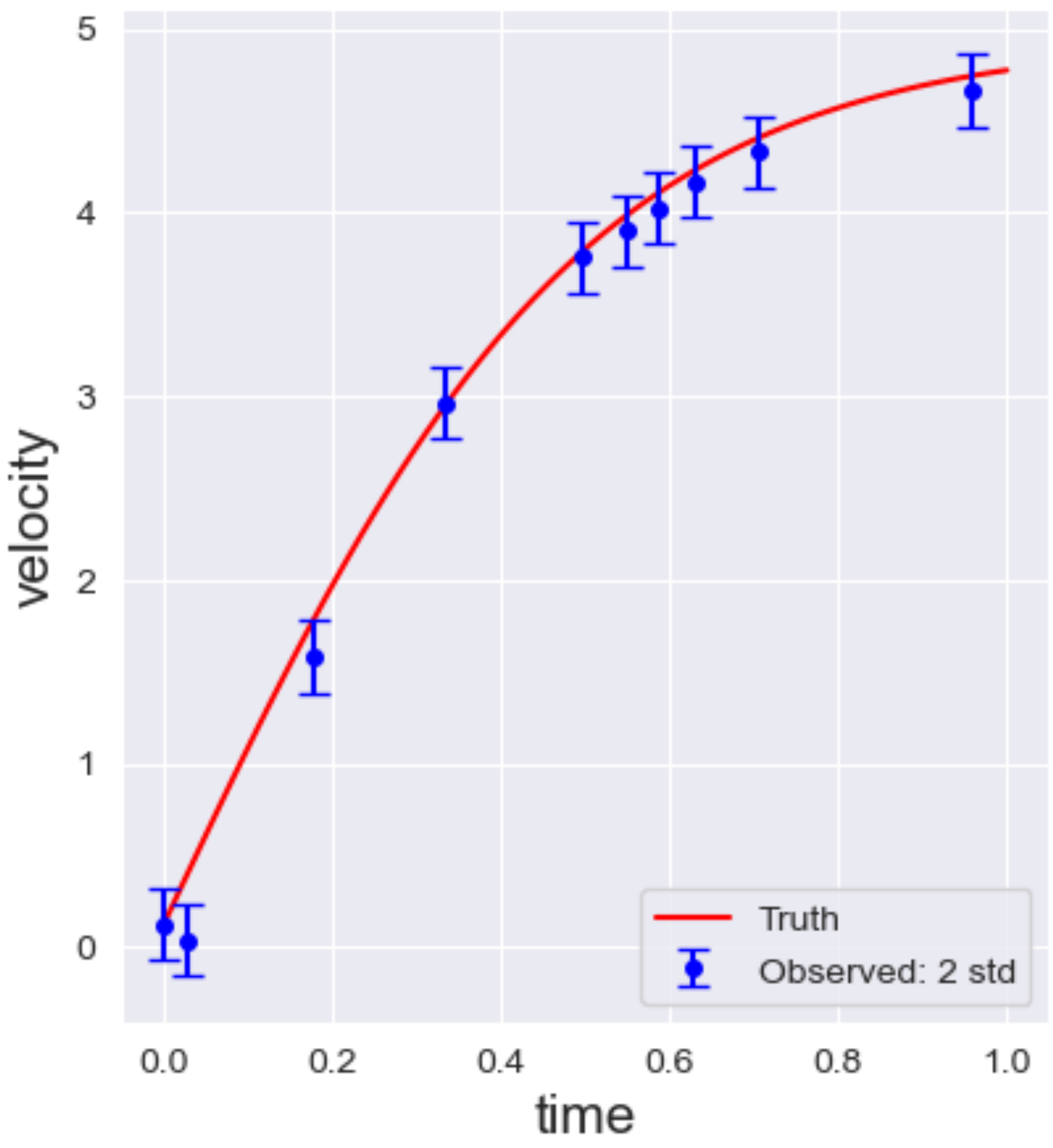


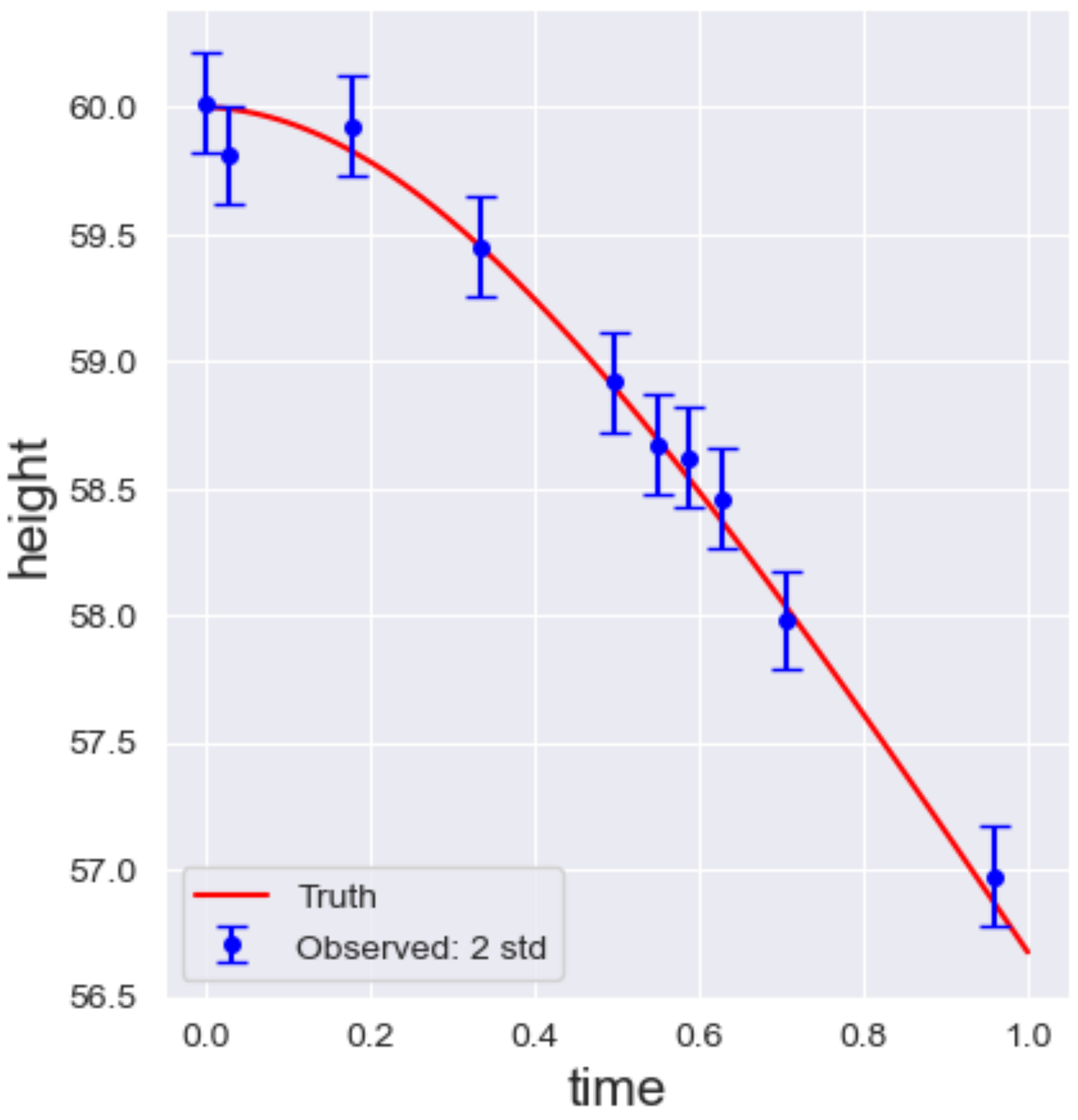
A simple example: ball drop experiment

- A ball is dropped from a tower of height 60 m
- Velocity and height are measured at different times. Measurements are uncertain.
- **Reality has air resistance.**

Drag force: $\mathbf{f}_D = -(bv + cv^2)\,\hat{\mathbf{v}}$

EoM: $m\dfrac{d\mathbf{v}}{dt} = m\mathbf{g} - b\mathbf{v} - cv^2\hat{\mathbf{v}}\,, \quad \dfrac{dh}{dt} = -v$





A simple example: ball drop experiment

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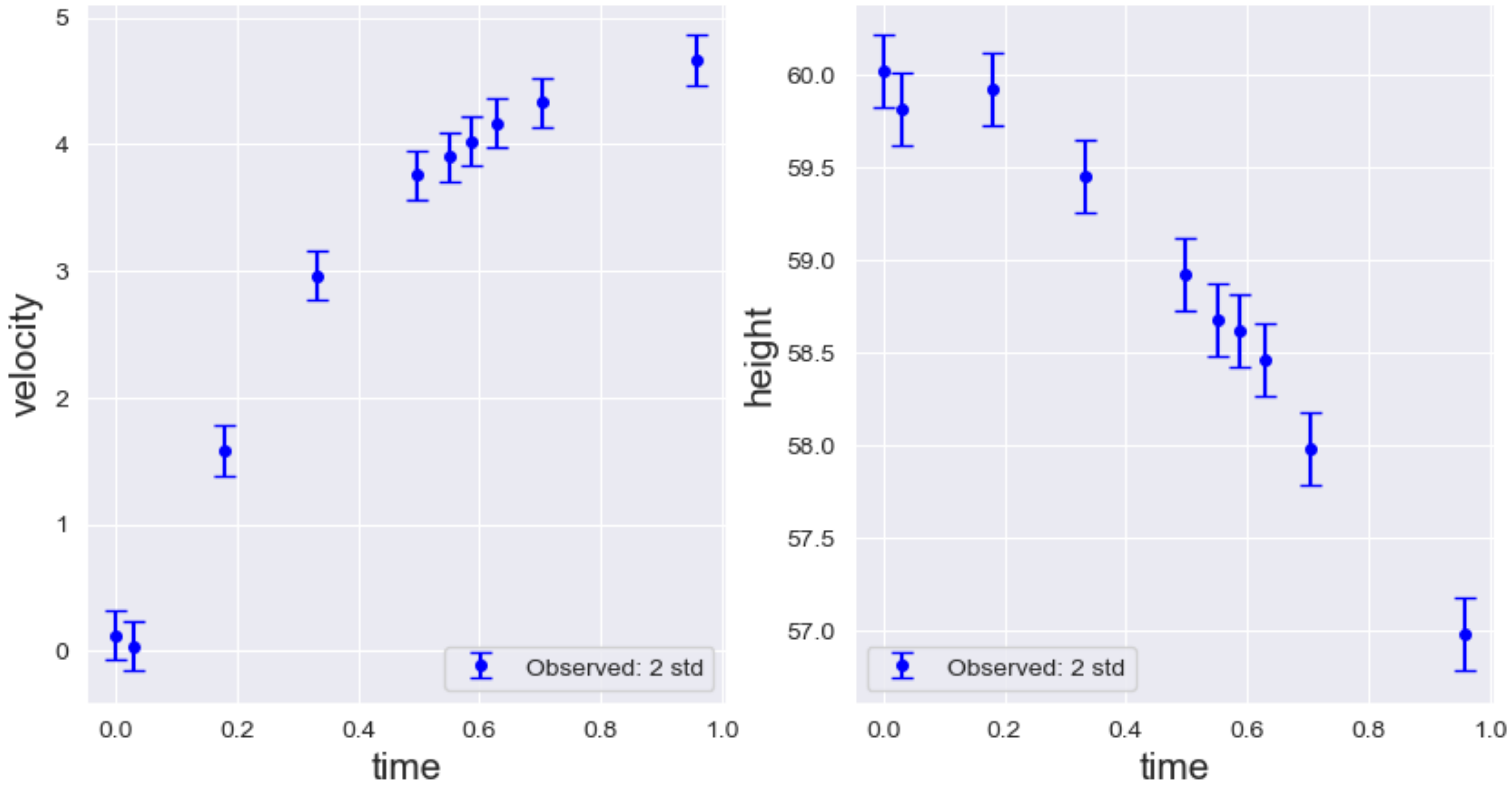


Goal is to measure the acceleration due to gravity g $(9.8\, m/s^2)$.

Physics model

- Physics theory considered ignores air resistance.

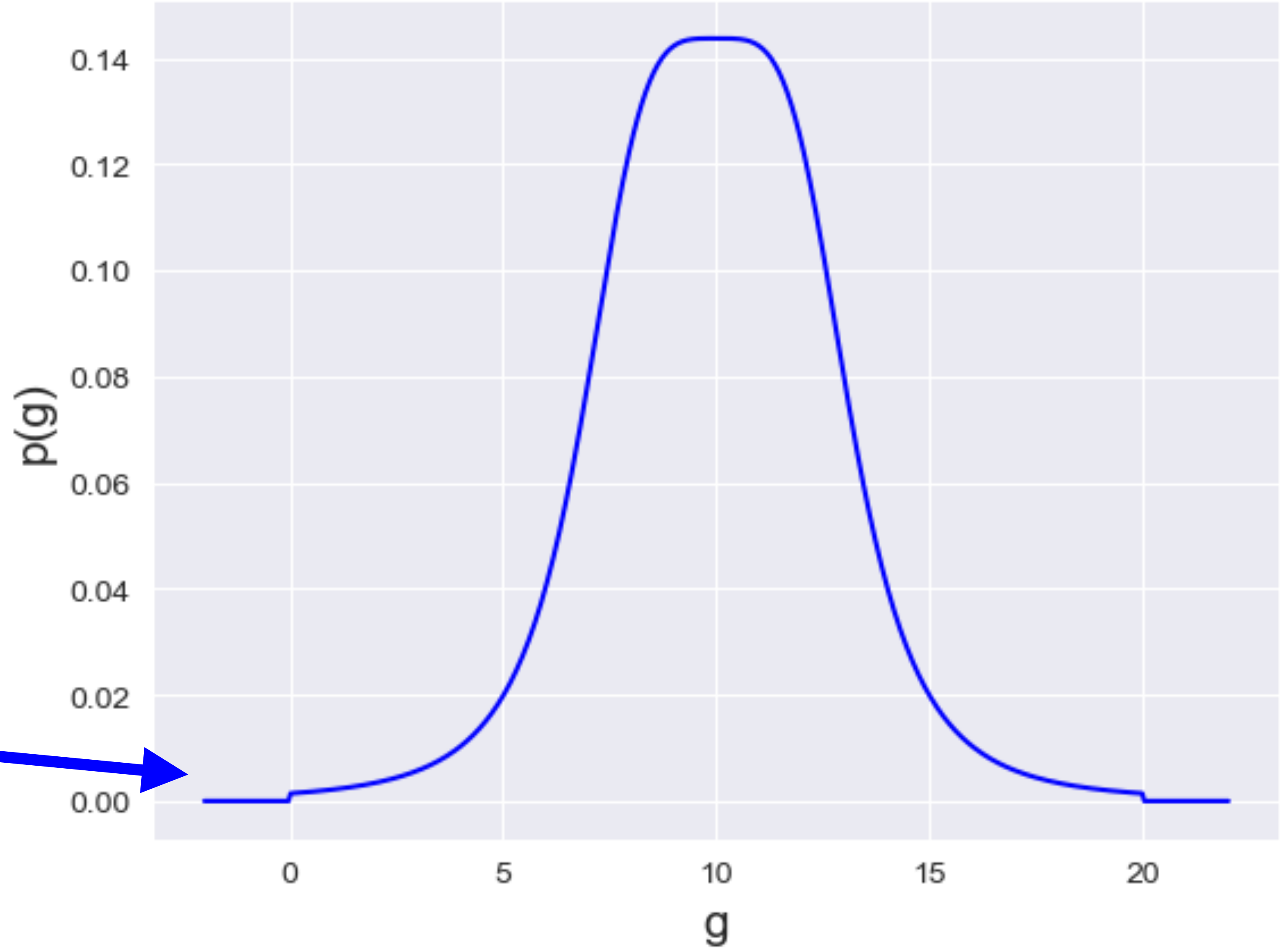
EoM: $v = v_0 + gt \quad h = h_0 - v_0 t - \frac{1}{2} g t^2$

- Bayesian inference considers the parameters g and v_0 to be random variables.

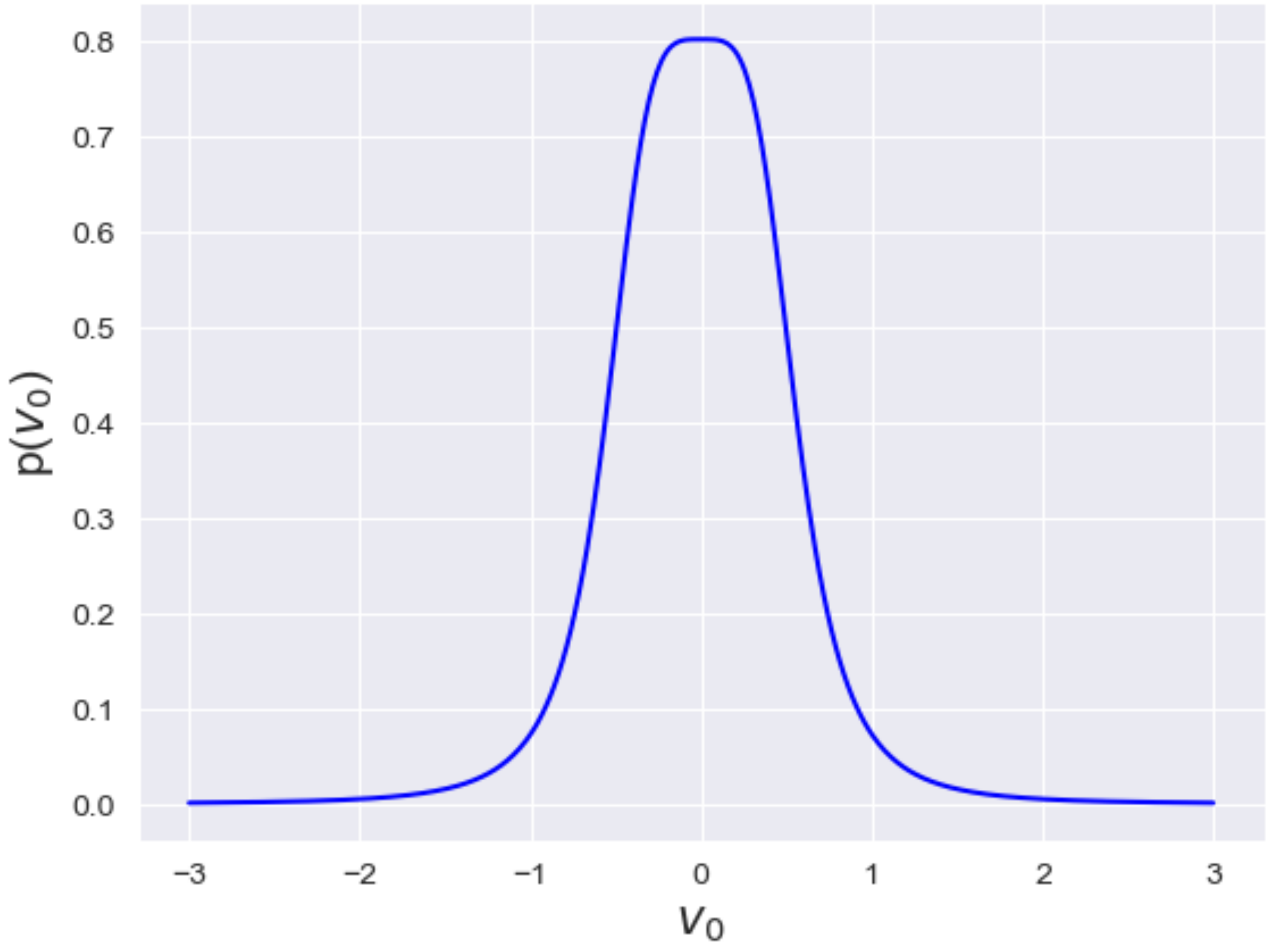
Bayesian updating of knowledge

$$\underbrace{\mathrm{pr}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}}, I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathbf{y}_{\mathrm{exp}}|\boldsymbol{\theta}, I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\boldsymbol{\theta}|I)}_{\text{prior}}$$

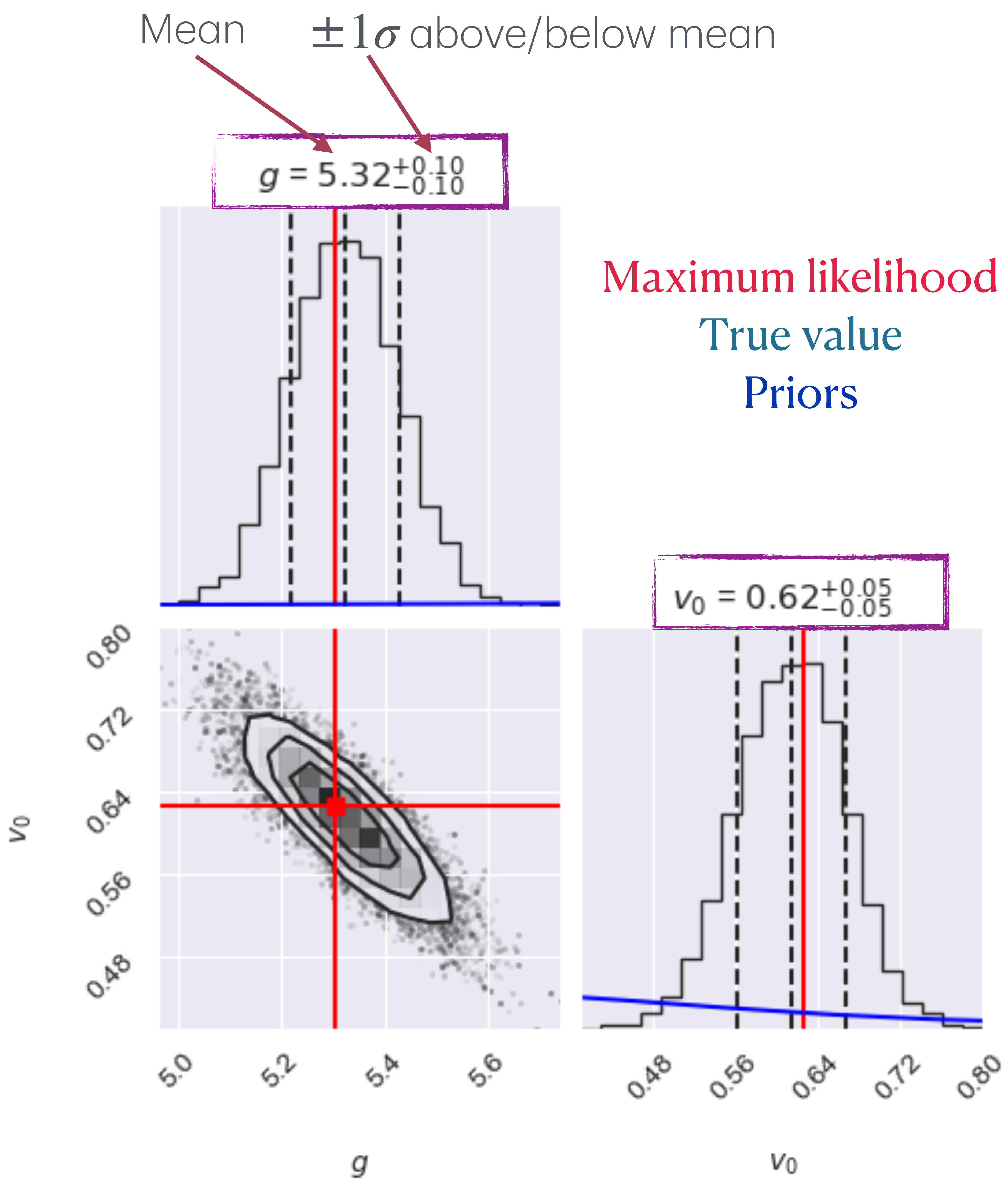
Priors



Physics input: g always positive

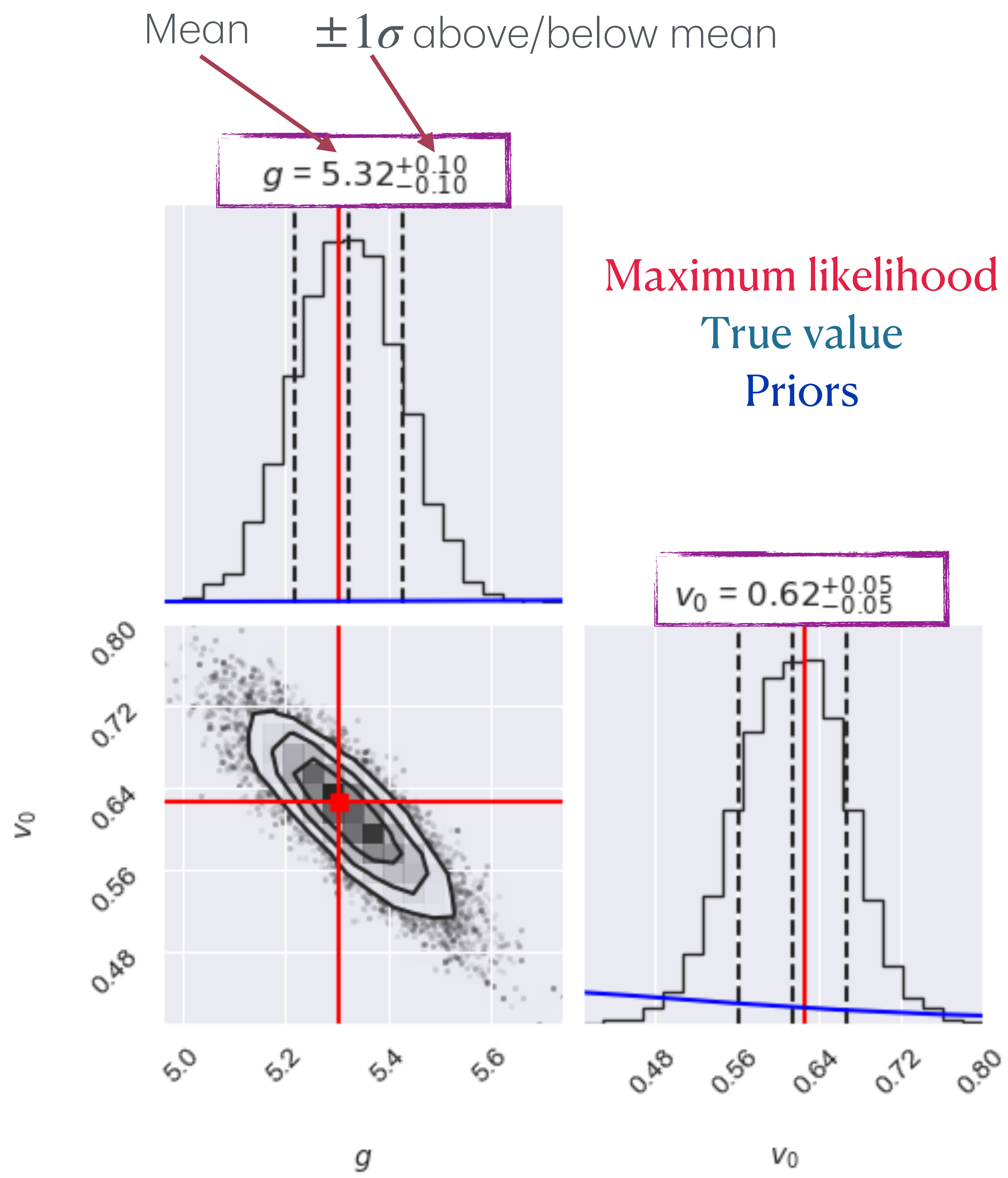


Bayesian inference without model discrepancy

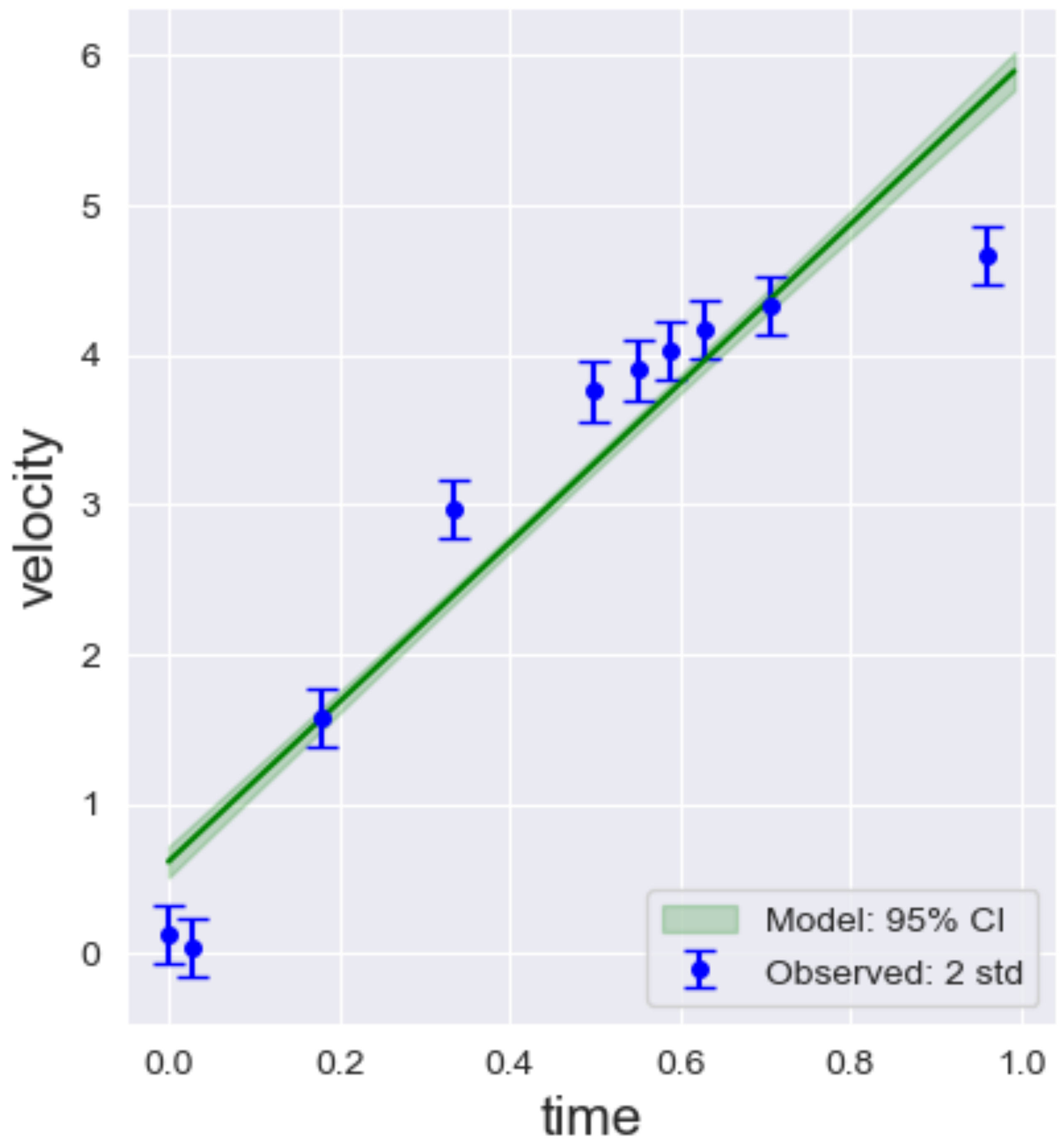


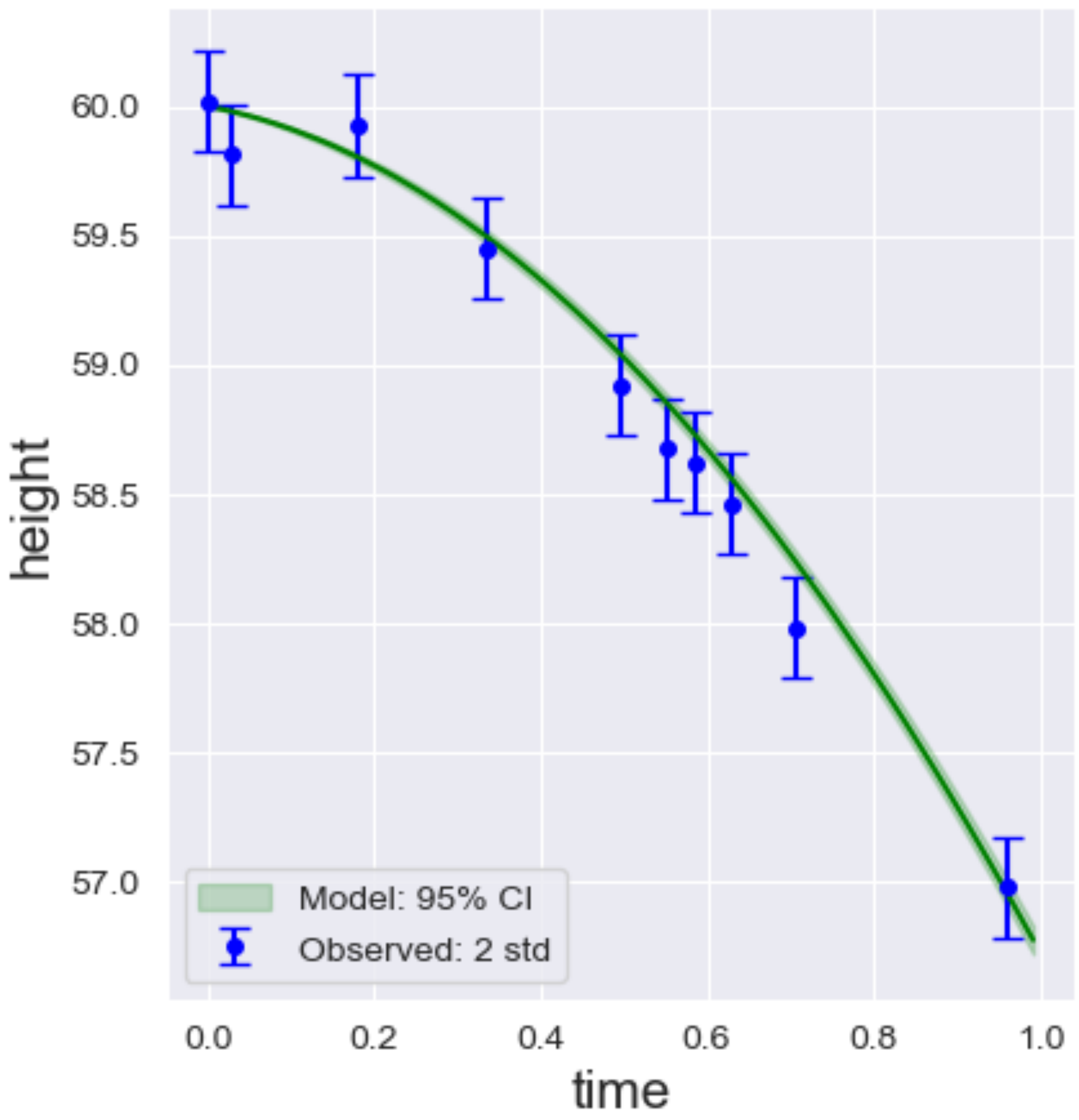
- Inferred values of parameters are far from truth : $g\,(9.8)$, $v_0\,(0)$
- Parameter inference incorrect and confident.

Bayesian inference without model discrepancy

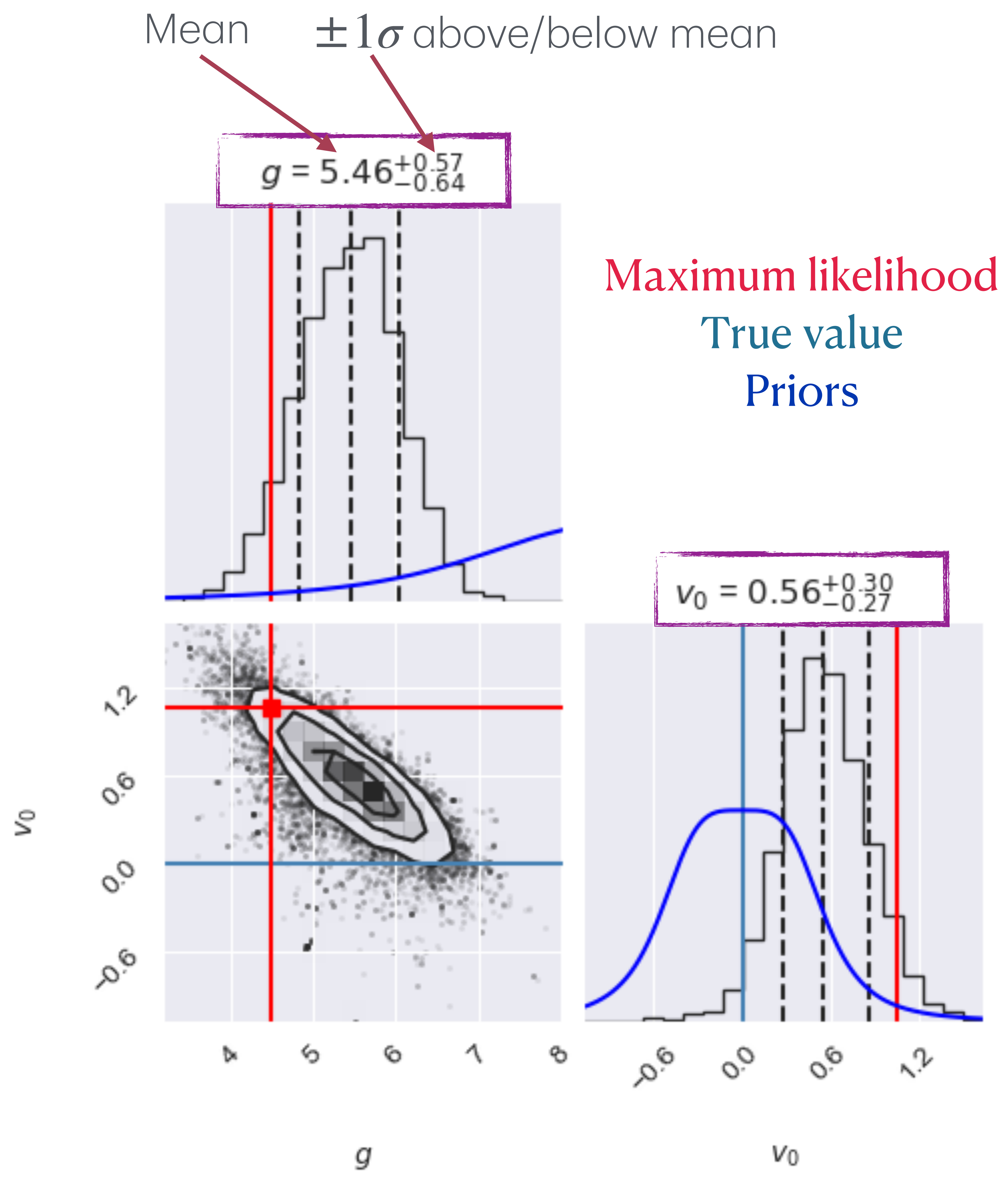


- Inferred values of parameters are far from truth : g (9.8), v_0 (0)
- Parameter inference incorrect and confident.
- Model prediction seems bad for velocity, but shows good agreement for height.

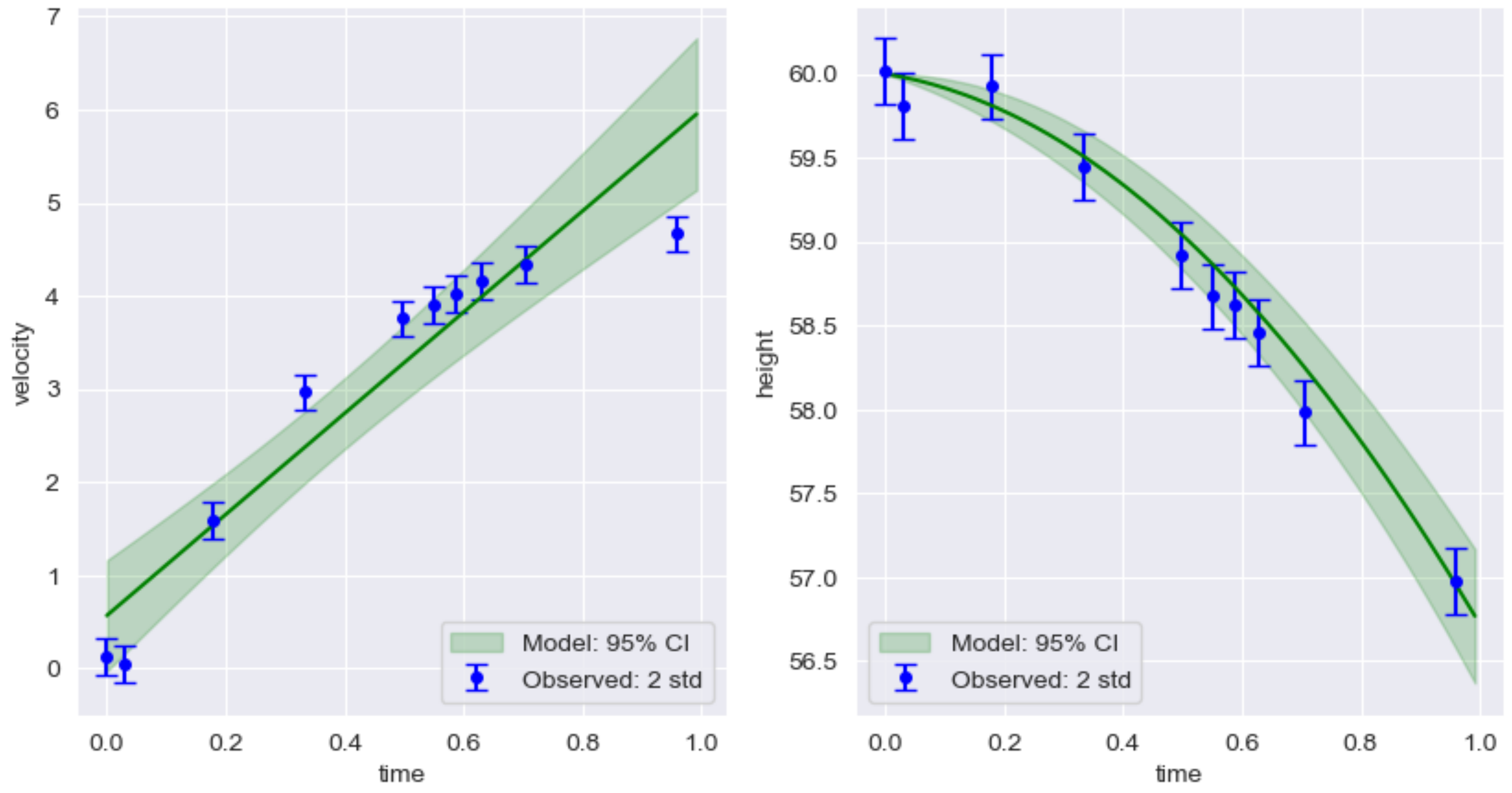




With model discrepancy (physics uninformed)



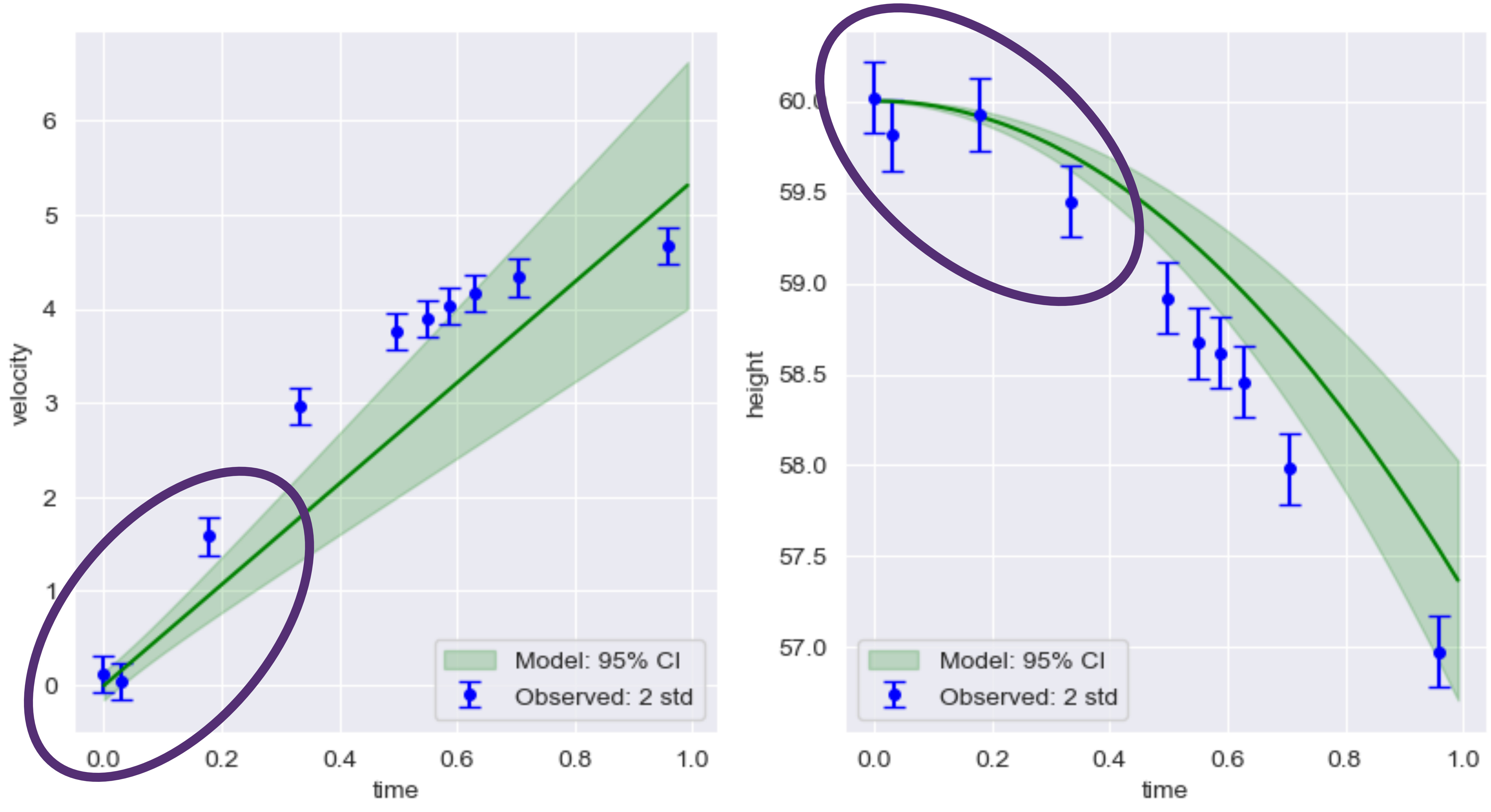
- Added discrepancy term $\delta(t_i)$.
  Stationary covariance (RBF kernel). $k(t_i, t_j) = \bar{c}^2 \exp\left(-\frac{d(t_i, t_j)^2}{2\ell^2}\right)$
- Parameter inference still incorrect but less confident.



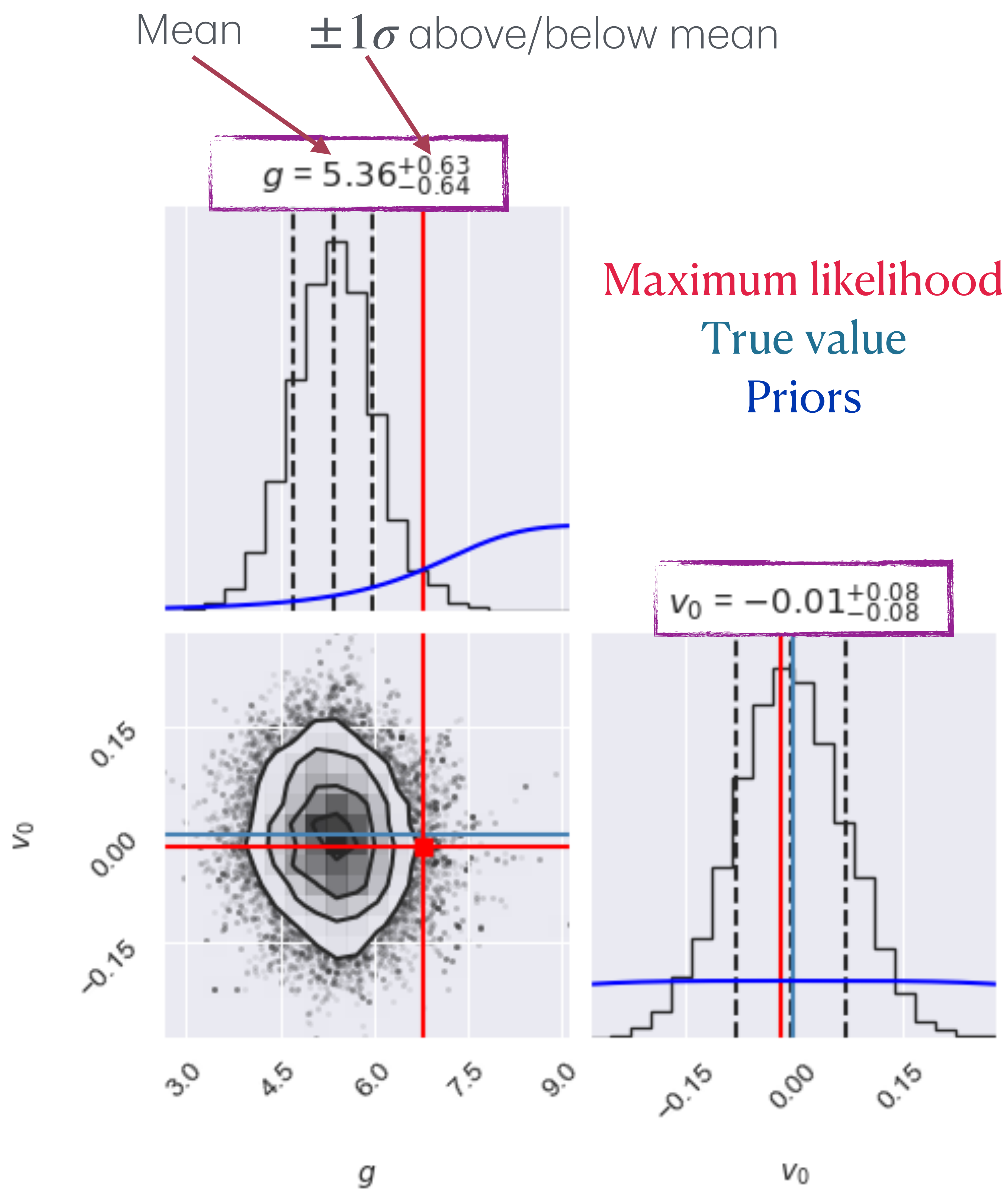
With model discrepancy (physics informed-I)

- We know model ignores air drag, so let variance of discrepancy GP increase with time. Non-stationary covariance.

$$k(t_i, t_j) = \bar{c}^2 t_i t_j \exp\left(-\frac{d(t_i, t_j)^2}{2\ell^2}\right)$$



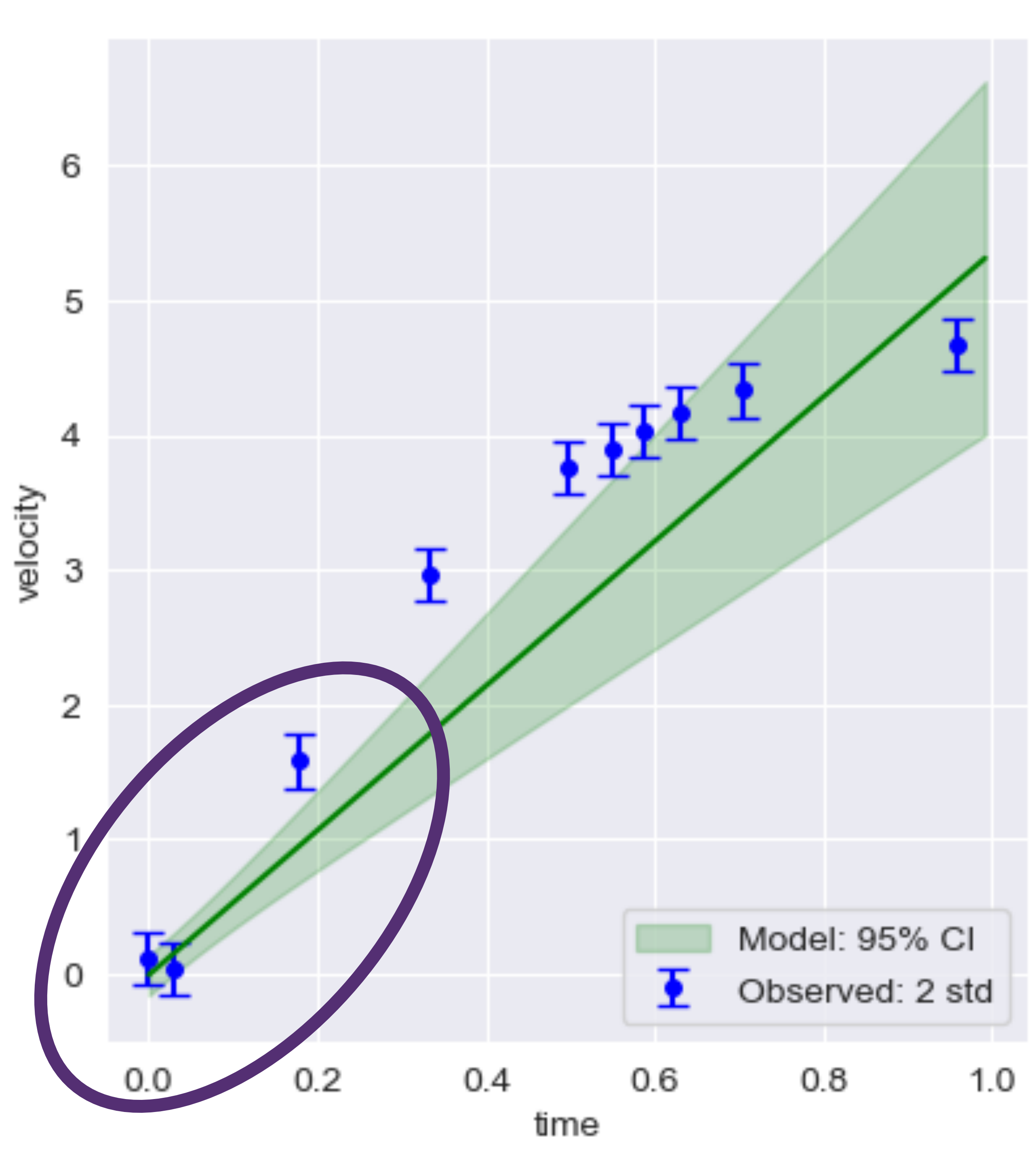
With model discrepancy (physics informed-I)

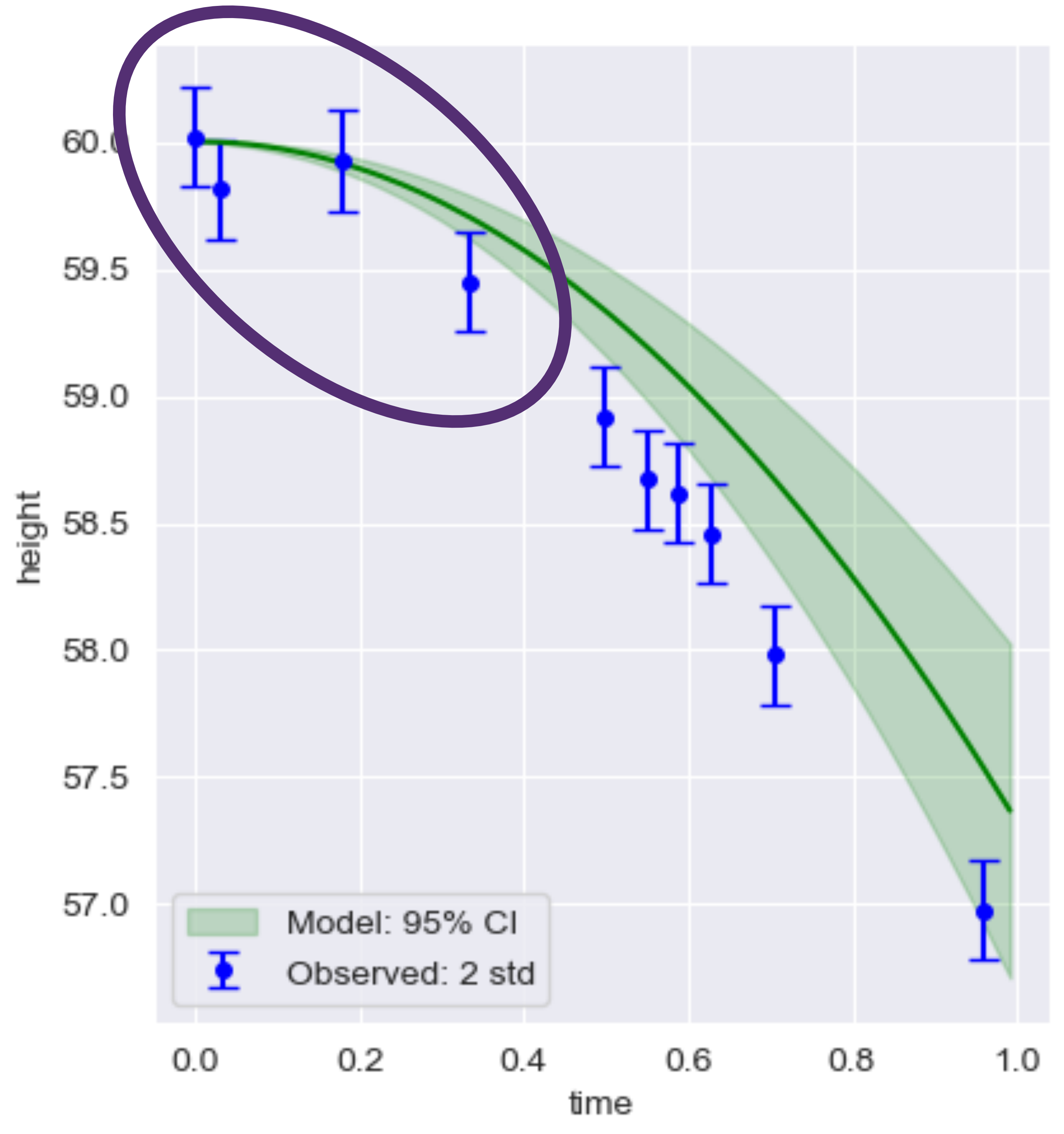


- We know model ignores air drag, so let variance of discrepancy GP increase with time. Non-stationary covariance.

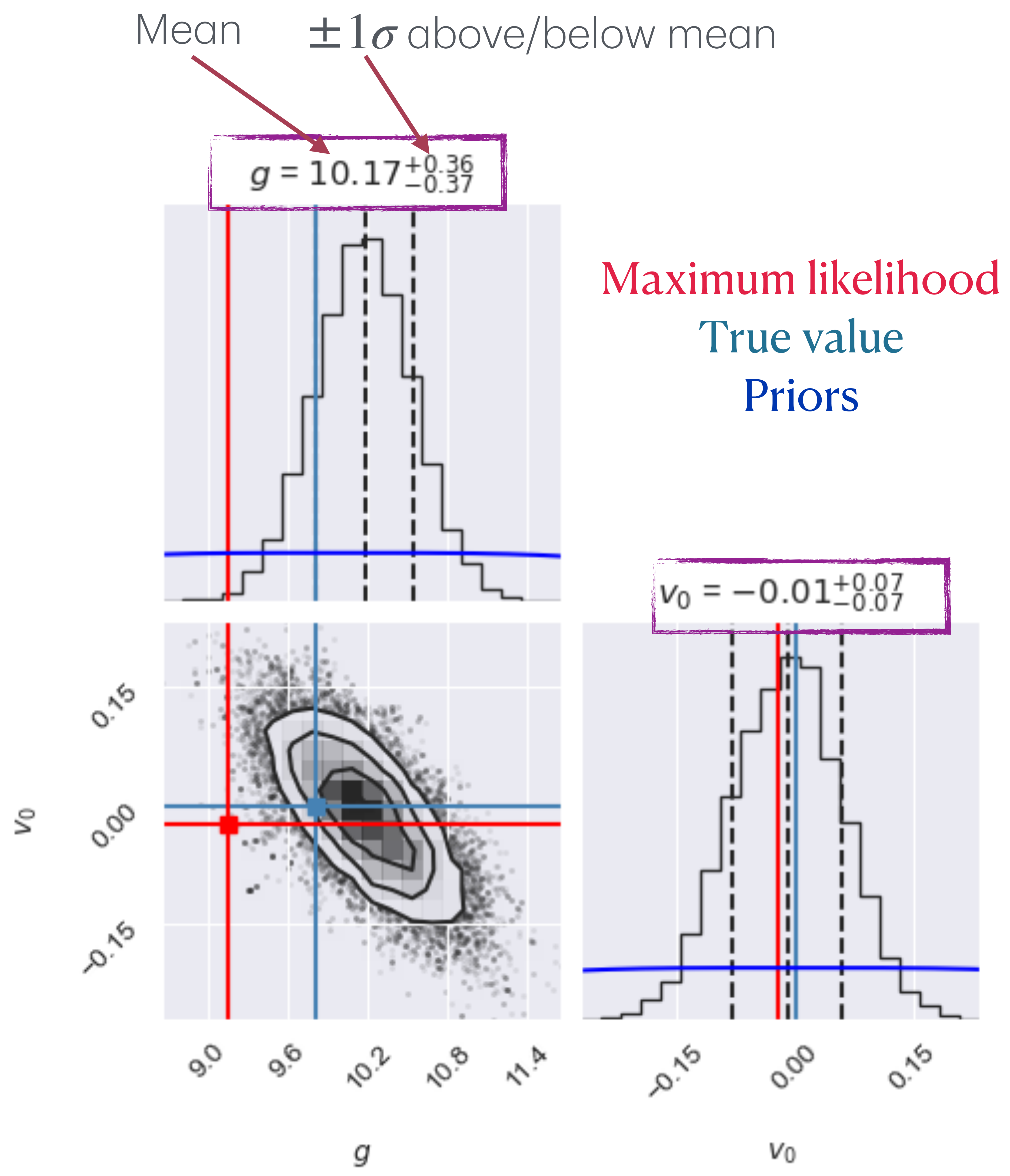
$$k(t_i, t_j) = \bar{c}^2 t_i t_j \exp\left(-\frac{d(t_i, t_j)^2}{2\ell^2}\right)$$

- Parameter inference more accurate and confident for v_0. Still incorrect but less confident for g.





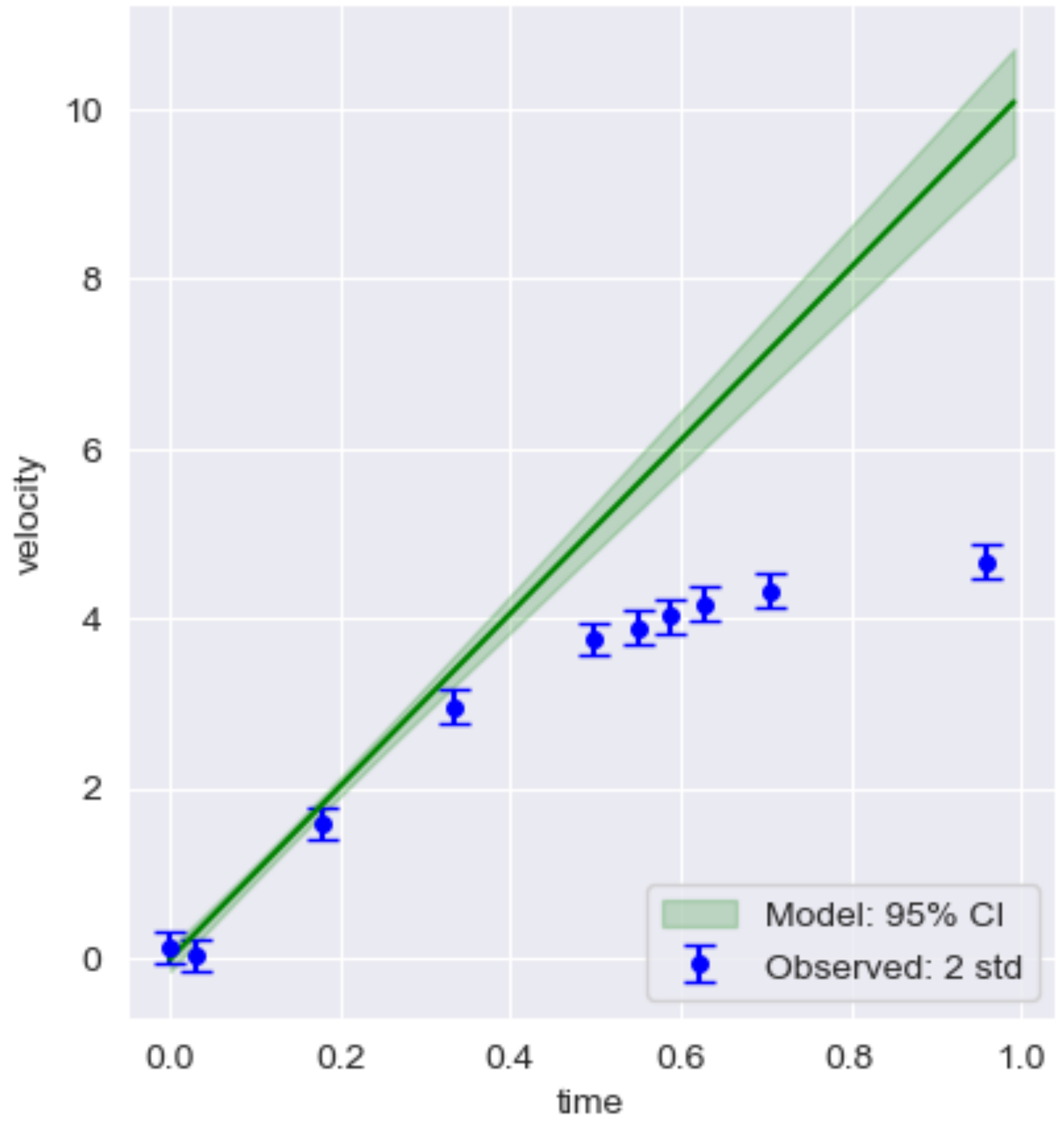
With model discrepancy (physics informed-II)

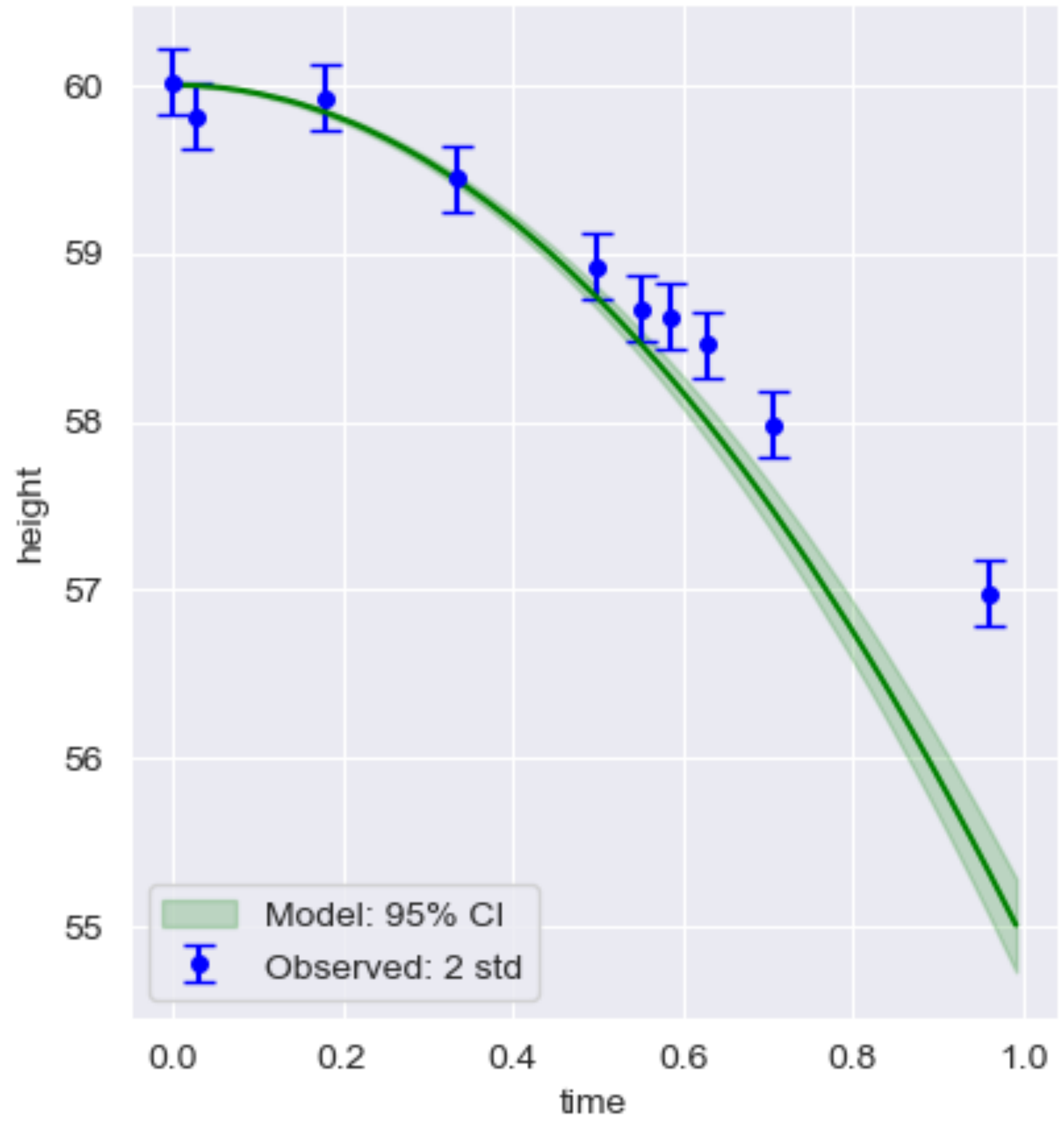


- We know model ignores air drag, so let variance of discrepancy GP increases with time. Non-stationary covariance.
- Additionally, say we know from physics that the rate at which the model deviates from truth in time is quadratic (this can be a parameter).

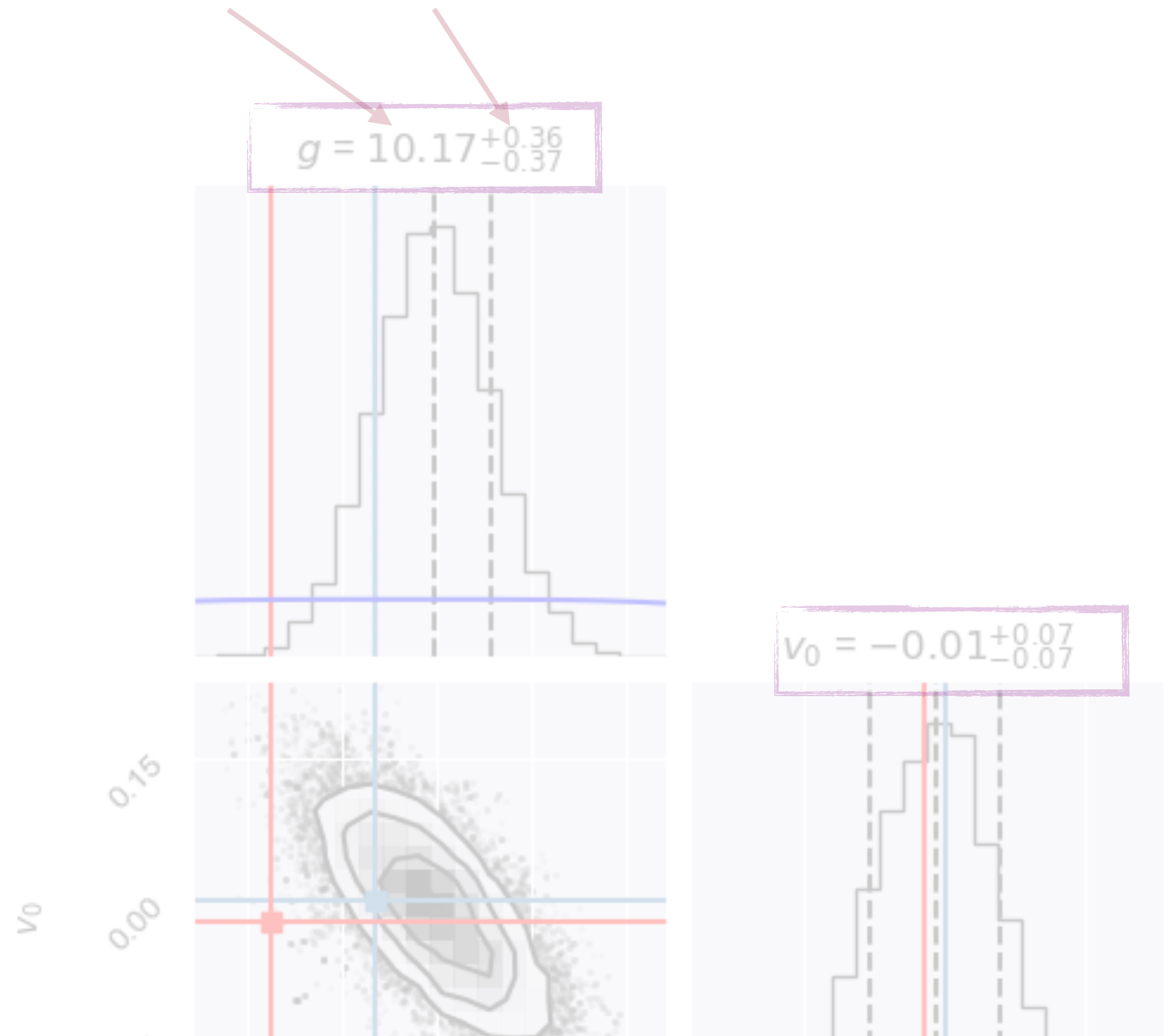
$$k(t_i, t_j) = \bar{c}^2 t_i^2 t_j^2 \exp\left(-\frac{d(t_i, t_j)^2}{2\ell^2}\right)$$

- Parameter inference more accurate and confident for v_0 and g.

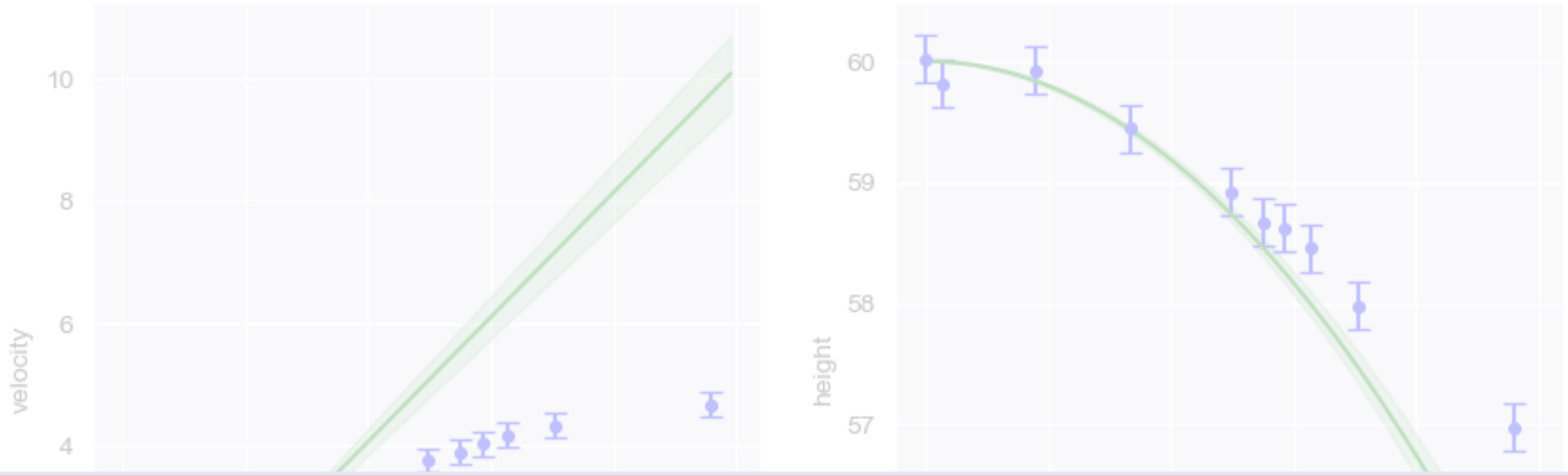




With model discrepancy (physics informed-II)



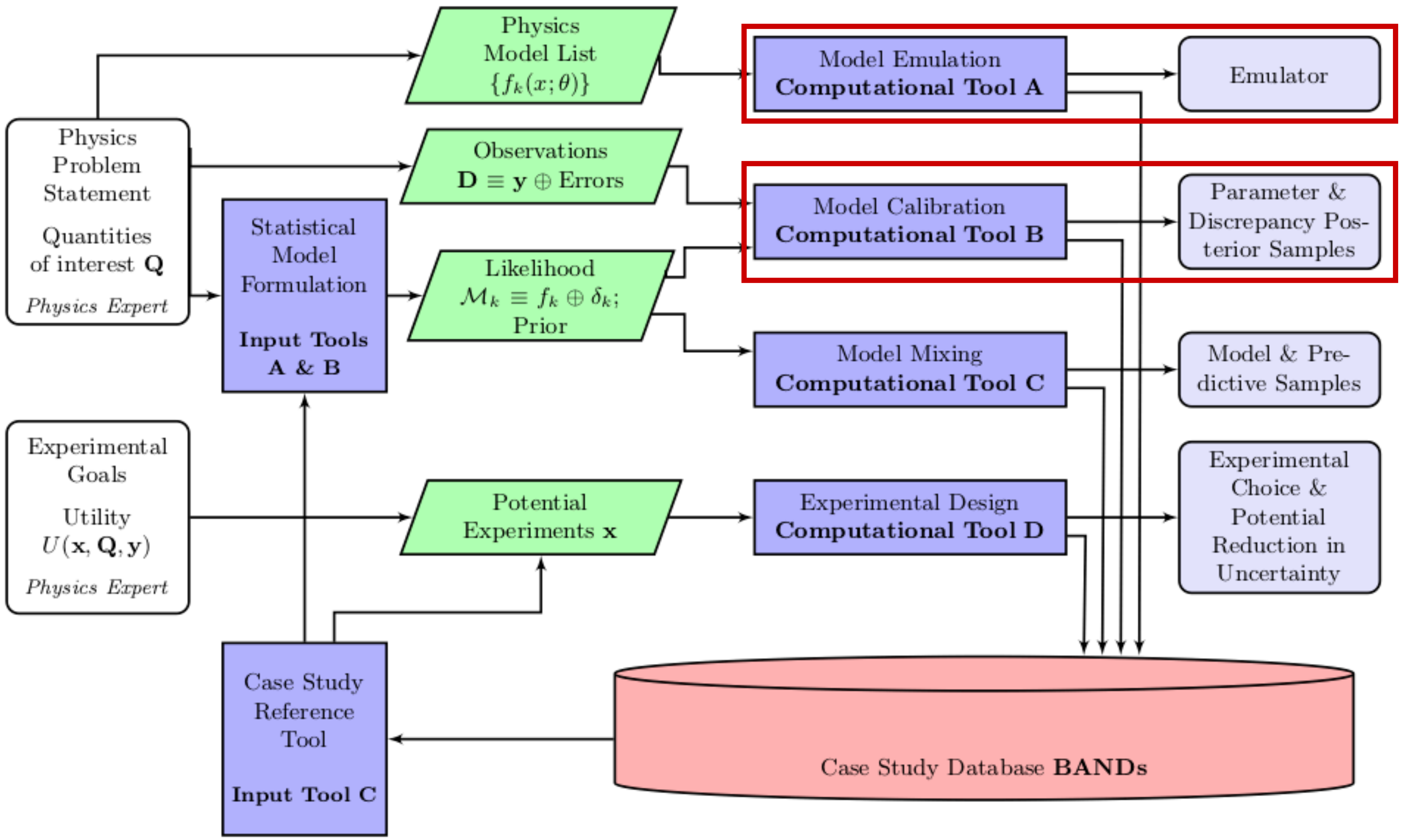
$$k(t_i, t_j) = \bar{c}^2 t_i^2 t_j^2 \exp\left(-\frac{d(t_i, t_j)^2}{2\ell^2}\right)$$



Revised George Box: “All models are wrong, but ~~some~~ models that *know* when they are wrong, are useful.”

Summary

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



Bayesian Analysis of Nuclear Dynamics

Summary

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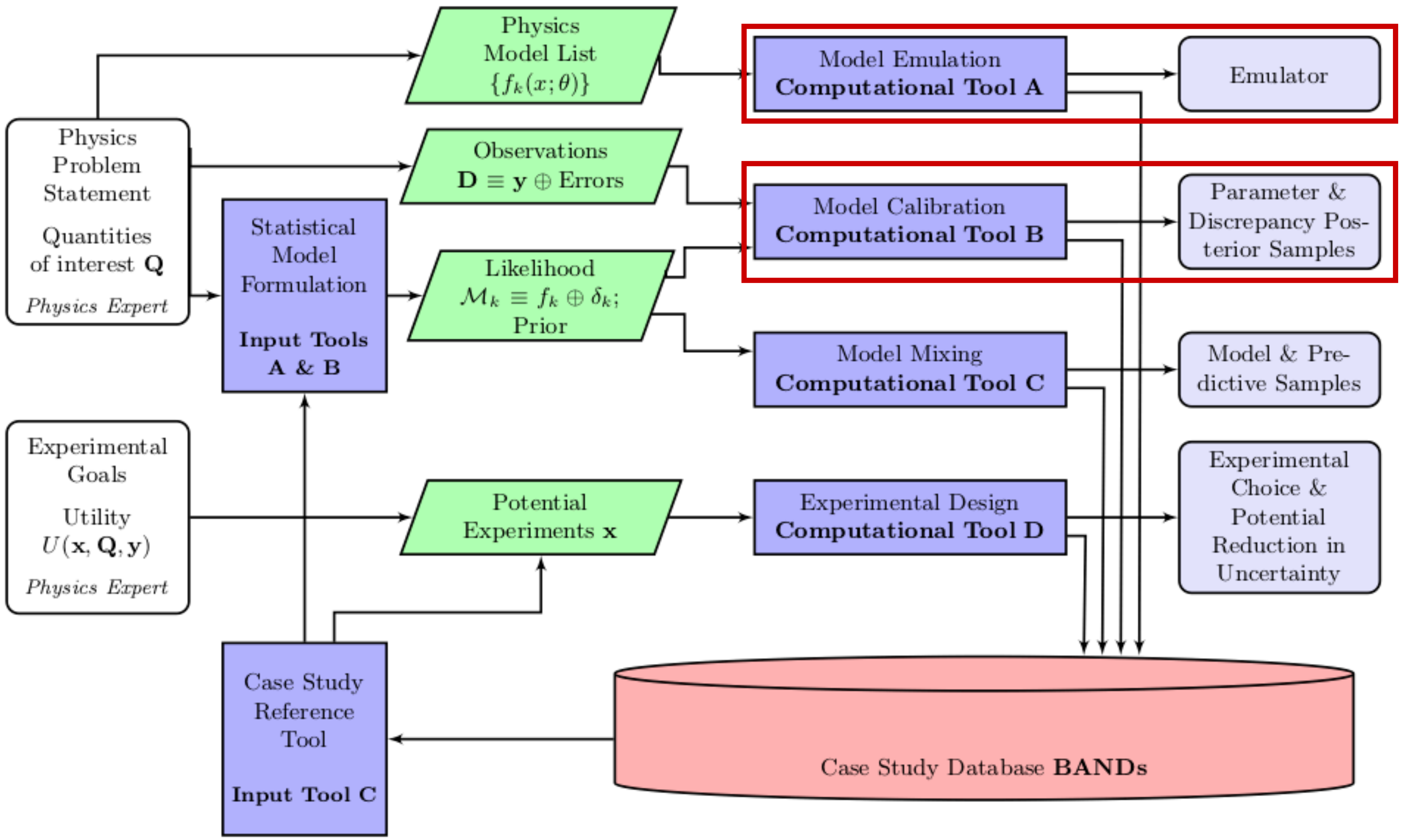
- Quantifying theoretical uncertainties is a *necessity* for correct parameter inference.

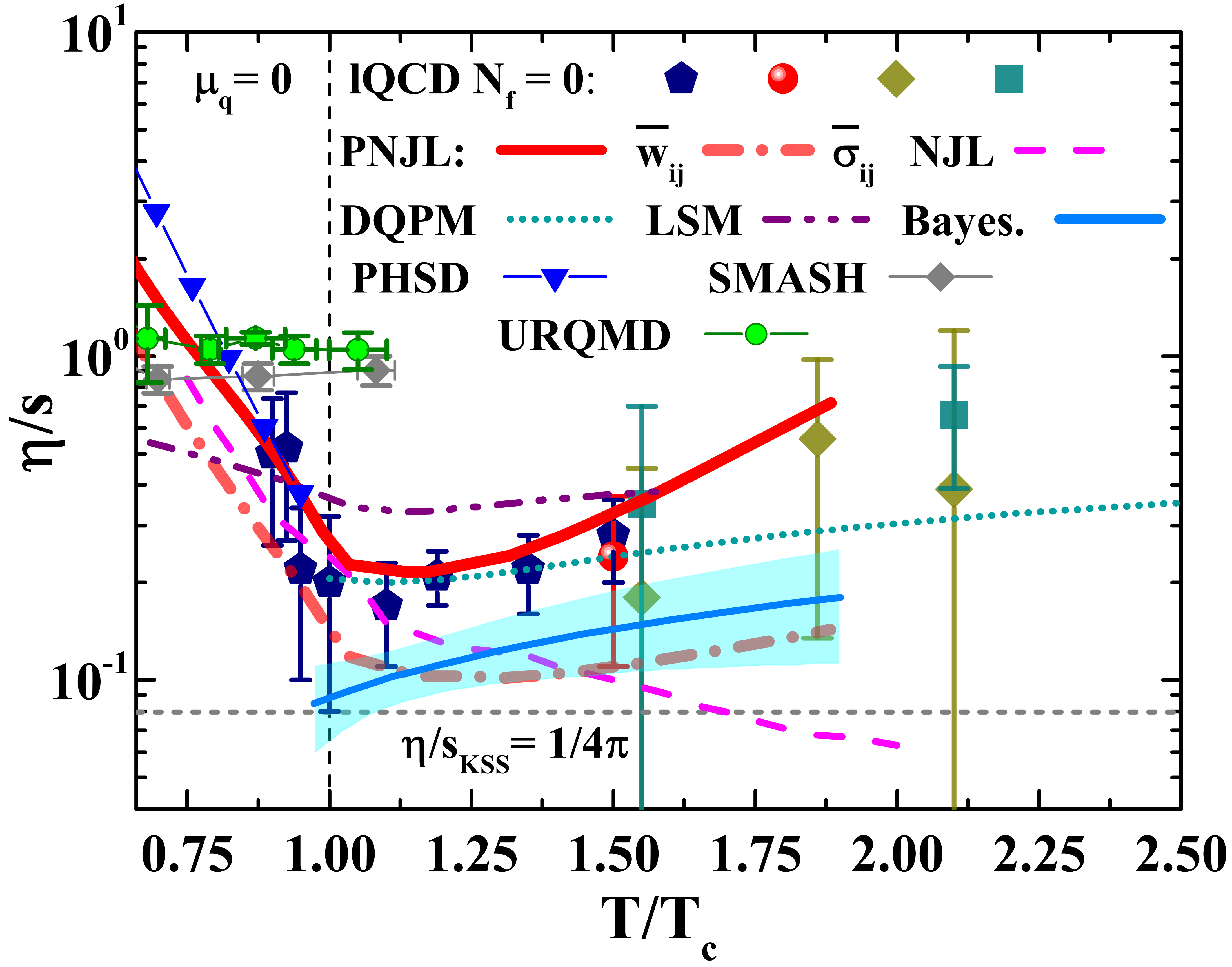


BAND
Bayesian Analysis of Nuclear Dynamics

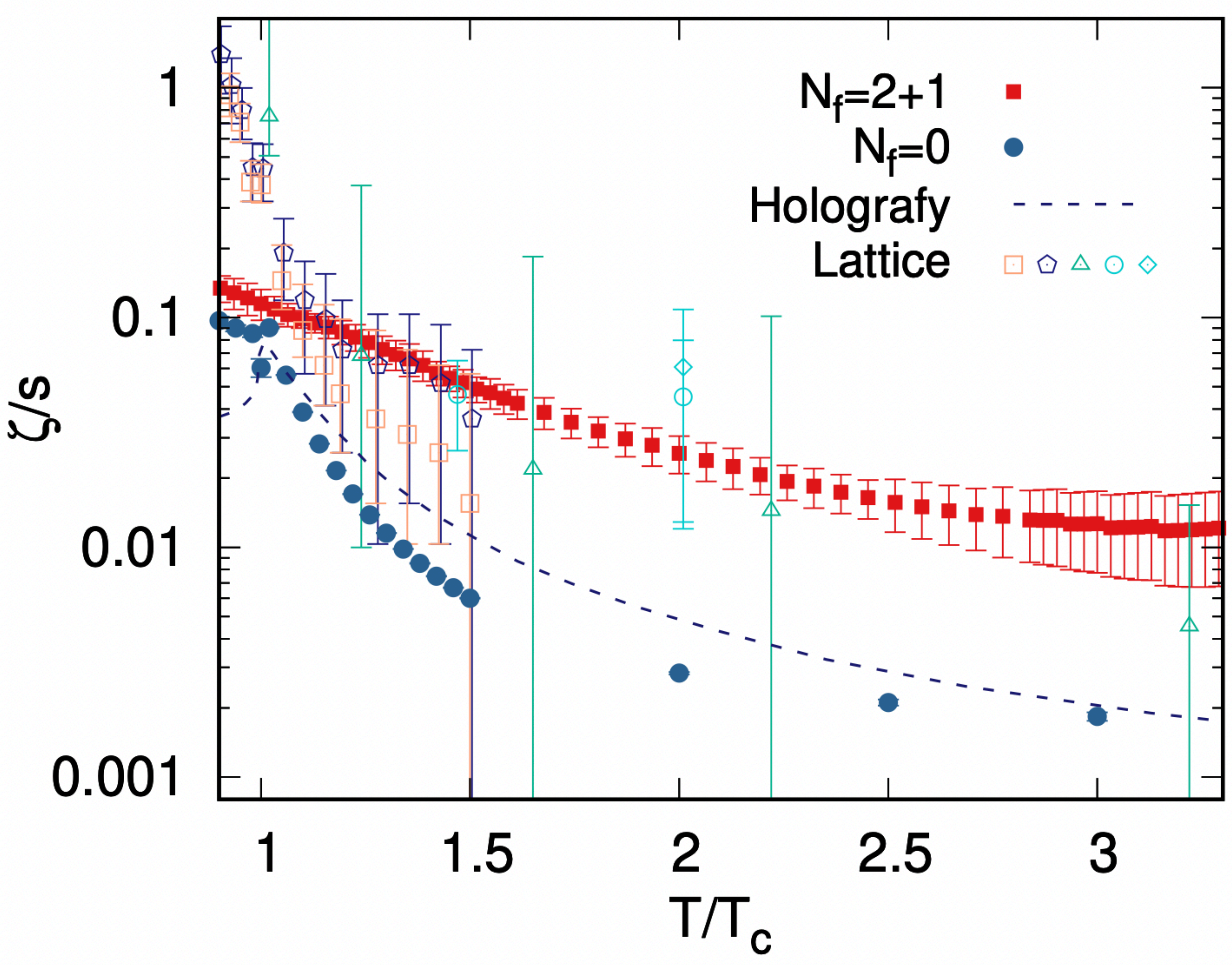
Thank You!

Backup

Transport coefficients from different calculations



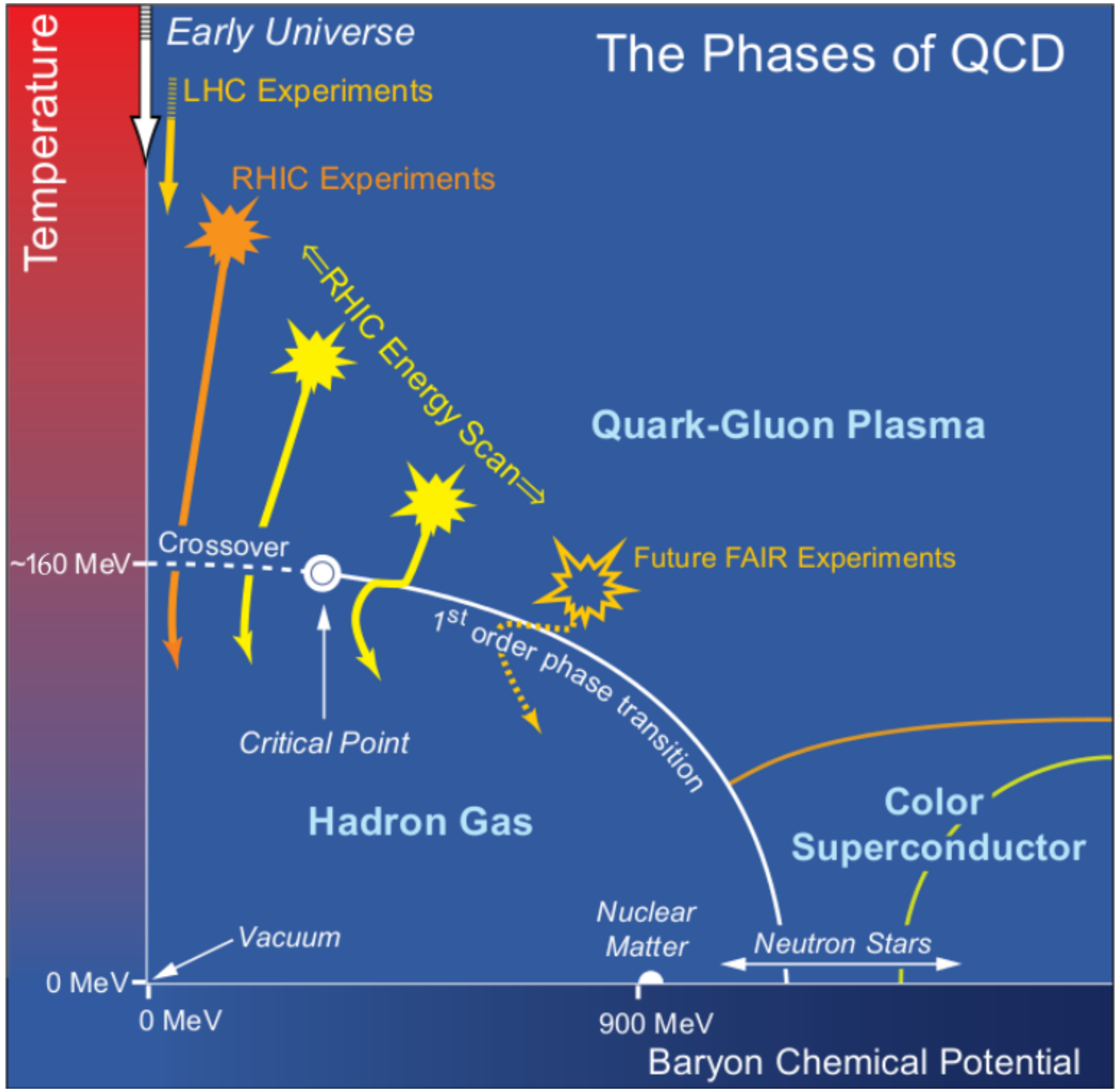
O. Soloveva, D. Fuseau, J. Aichelin, E. Bratkovskaya, 2011.03505



Valeriya Mykhaylova Thesis

Large Uncertainties

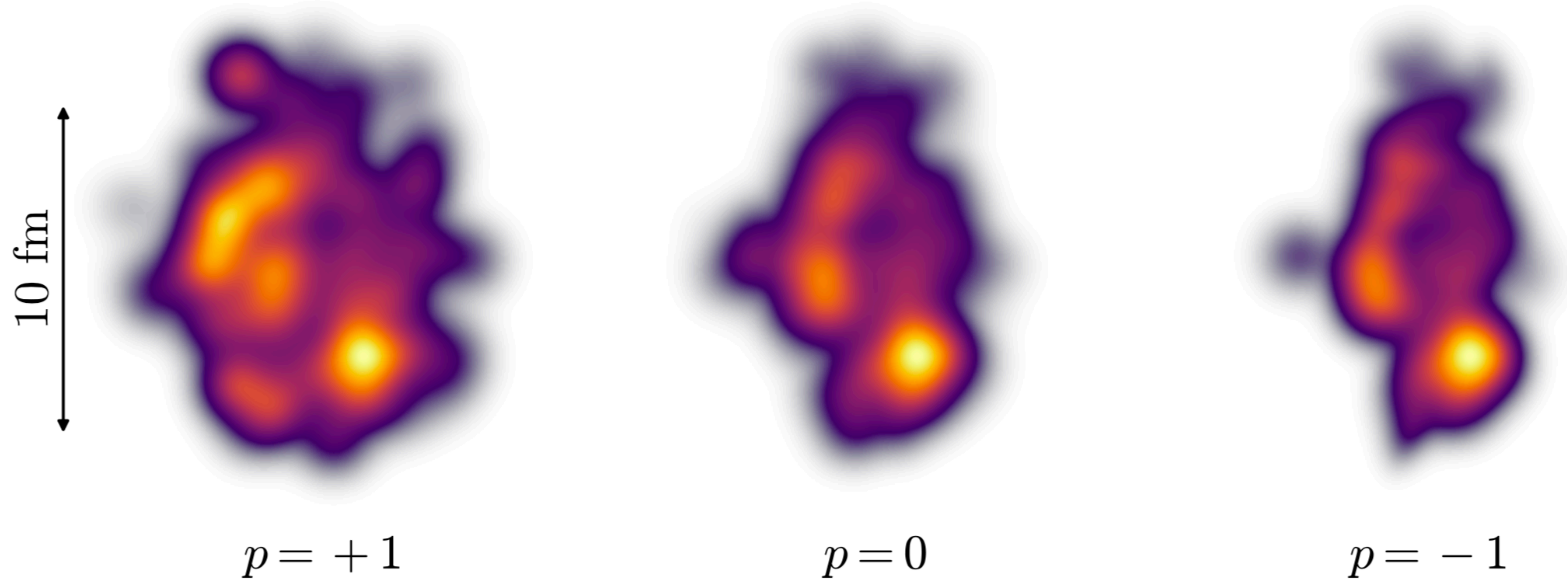
QCD phase diagram



Foka, Panagiota *et al* - arXiv:1702.07233

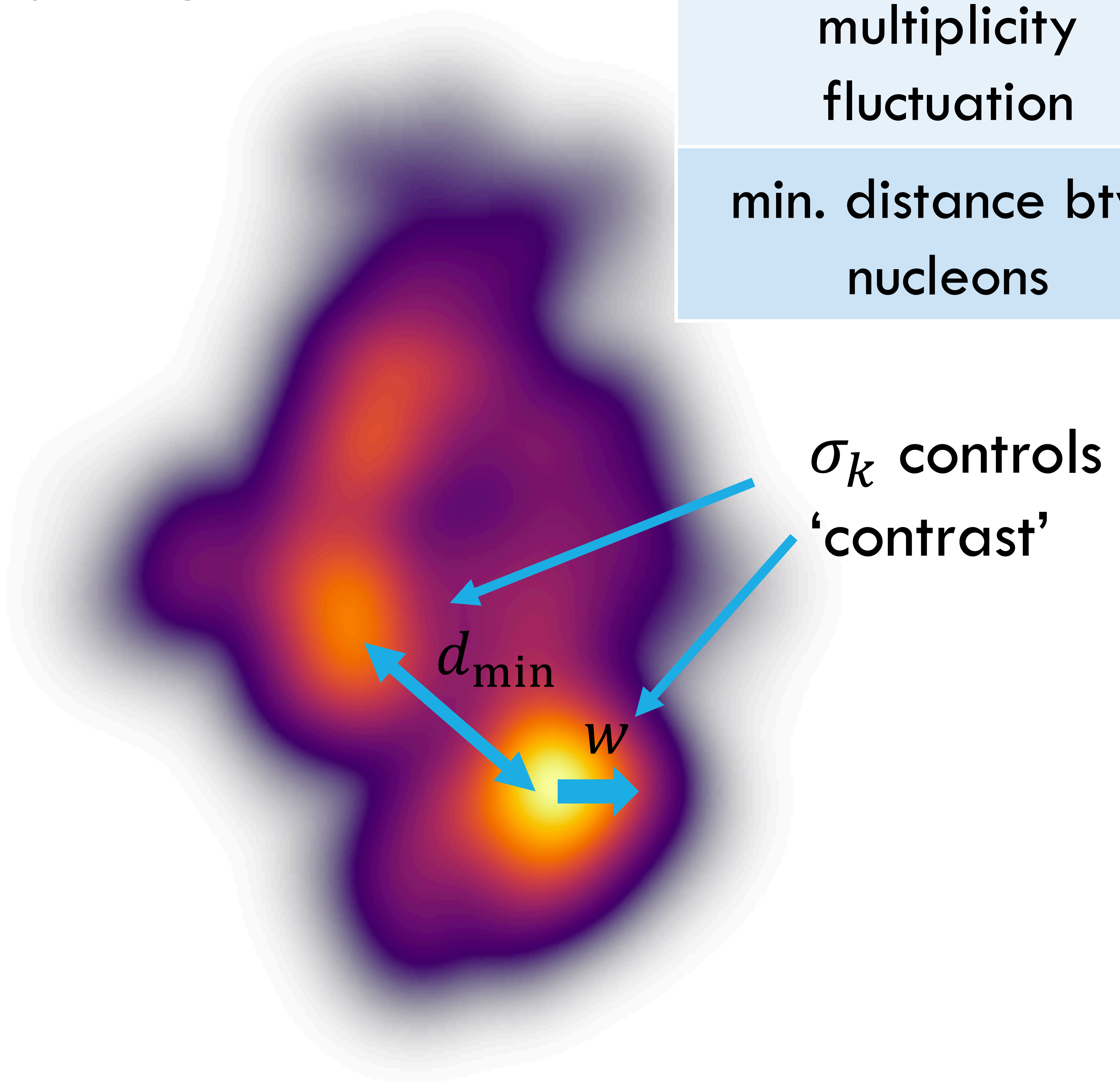
Initial Energy Deposition (TRENTO)

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



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

arXiv:1904.08290v1



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

Slide adapted from D. Everett

Pre-hydro (freestreaming)

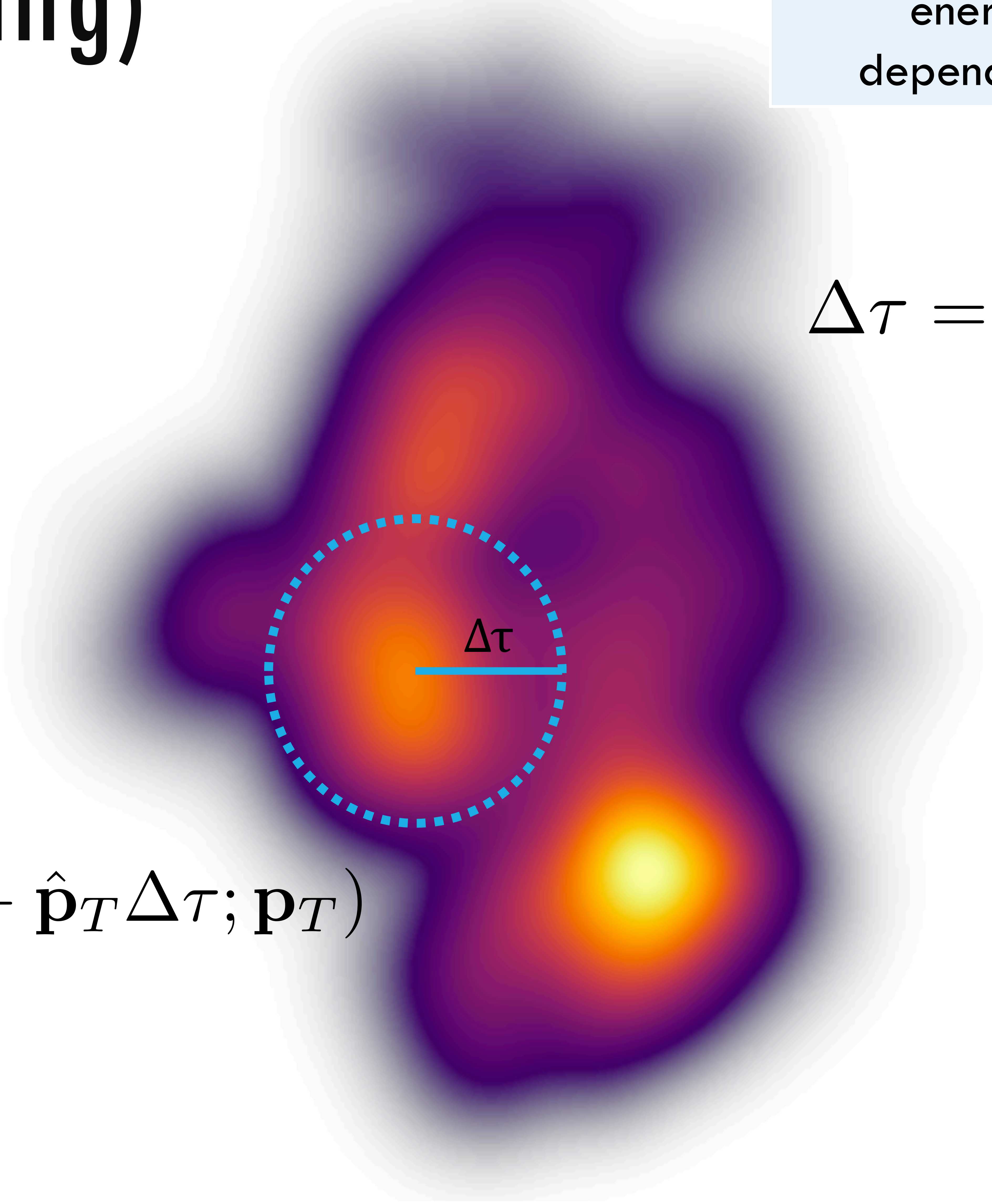
Parameter	Symbol
ref. proper time	τ_R
energy dependence	α

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

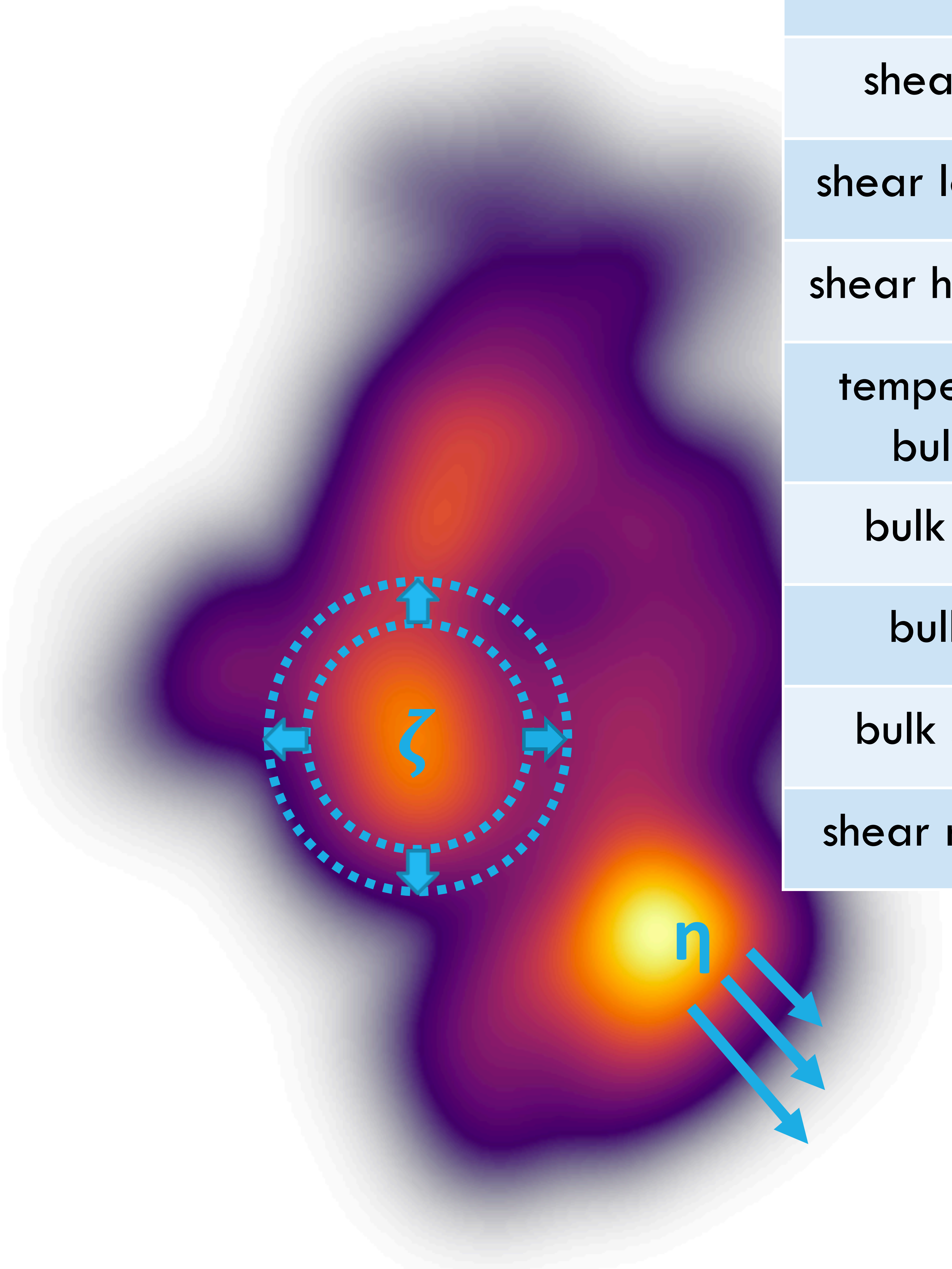
Viscous Hydro

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

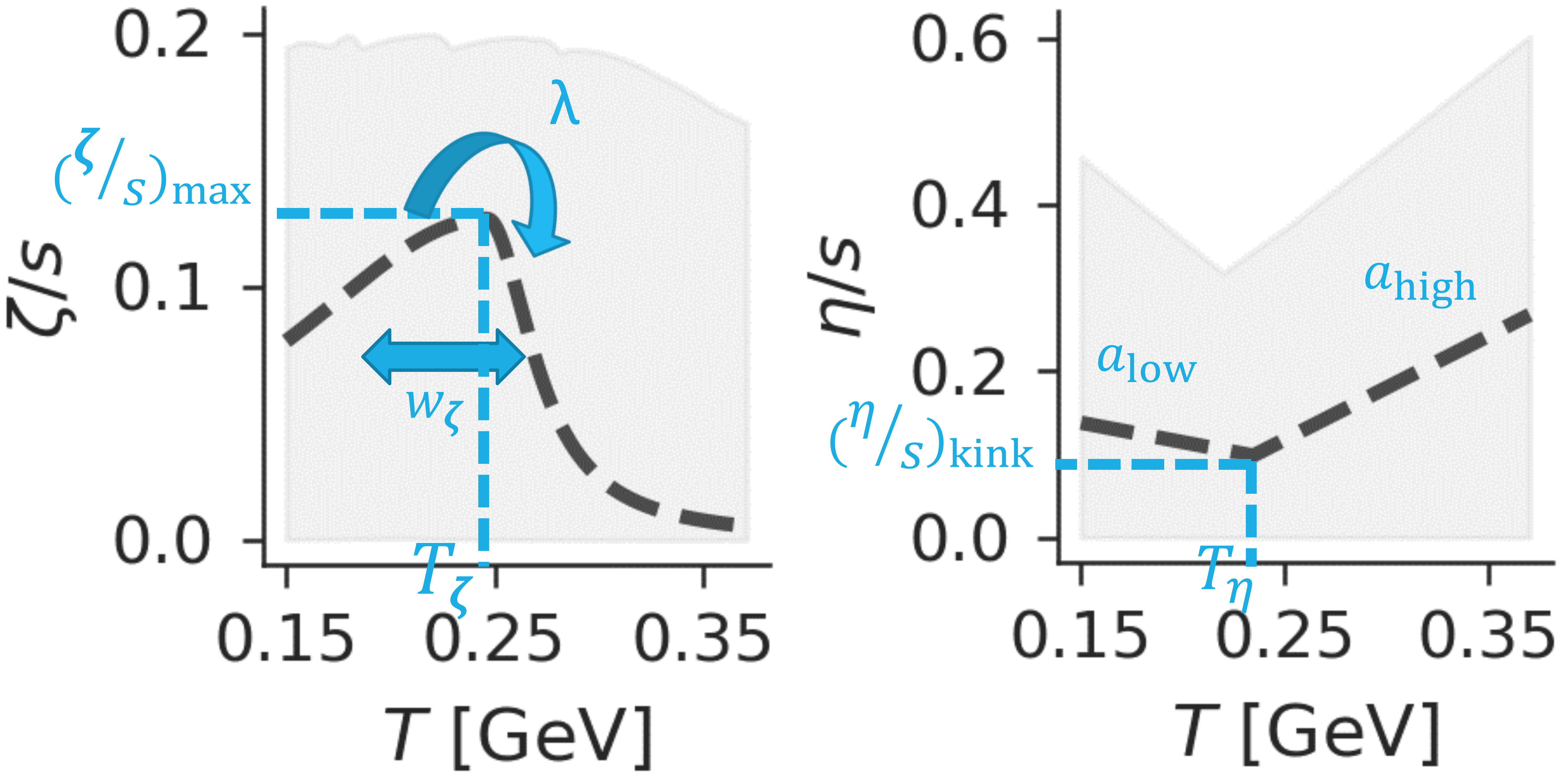


Parameter	Symbol
temperature of kink	T_η
shear at kink	$(\eta/s)_{\mathrm{kink}}$
shear low-T slope	a_{low}
shear high-T slope	a_{high}
temperature of bulk peak	T_ζ
bulk at peak	$(\zeta/s)_{\mathrm{max}}$
bulk width	w_ζ
bulk skewness	λ
shear relax. time	b_π

Slide adapted from D. Everett

Viscous Hydro

Viscosity parameterizations:



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bulk skewness	λ
shear relax. time	b_π

Slide adapted from D. Everett

Heavy-ion simulation

(JETSCAPE model for Pb-Pb collisions at $\sqrt{s_{NN}} = 2.76$ TeV)

- Simulation model takes parameter $\theta \in \mathbb{R}^d$ as input and produces $\mathbf{y}(\theta) \in \mathbb{R}^p$, $\mathbf{y}(\theta) = (y_1(\theta), \ldots, y_p(\theta))^T$ as outputs (observables). Number of model parameters $d = 17$, and number of outputs $p = 110$.

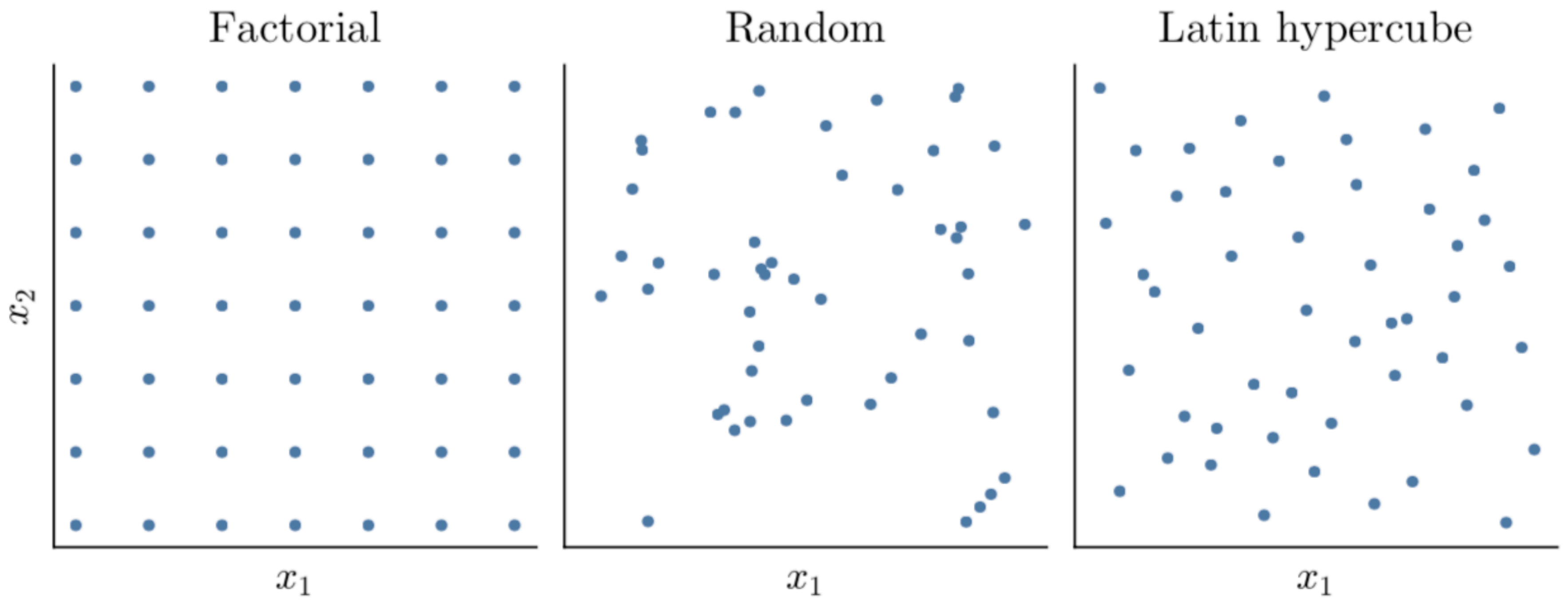
- The simulation model is stochastic: For a given θ, model can produce different outputs on each run (event). Physics model output is $p = 110$ distributions. **uncertain**

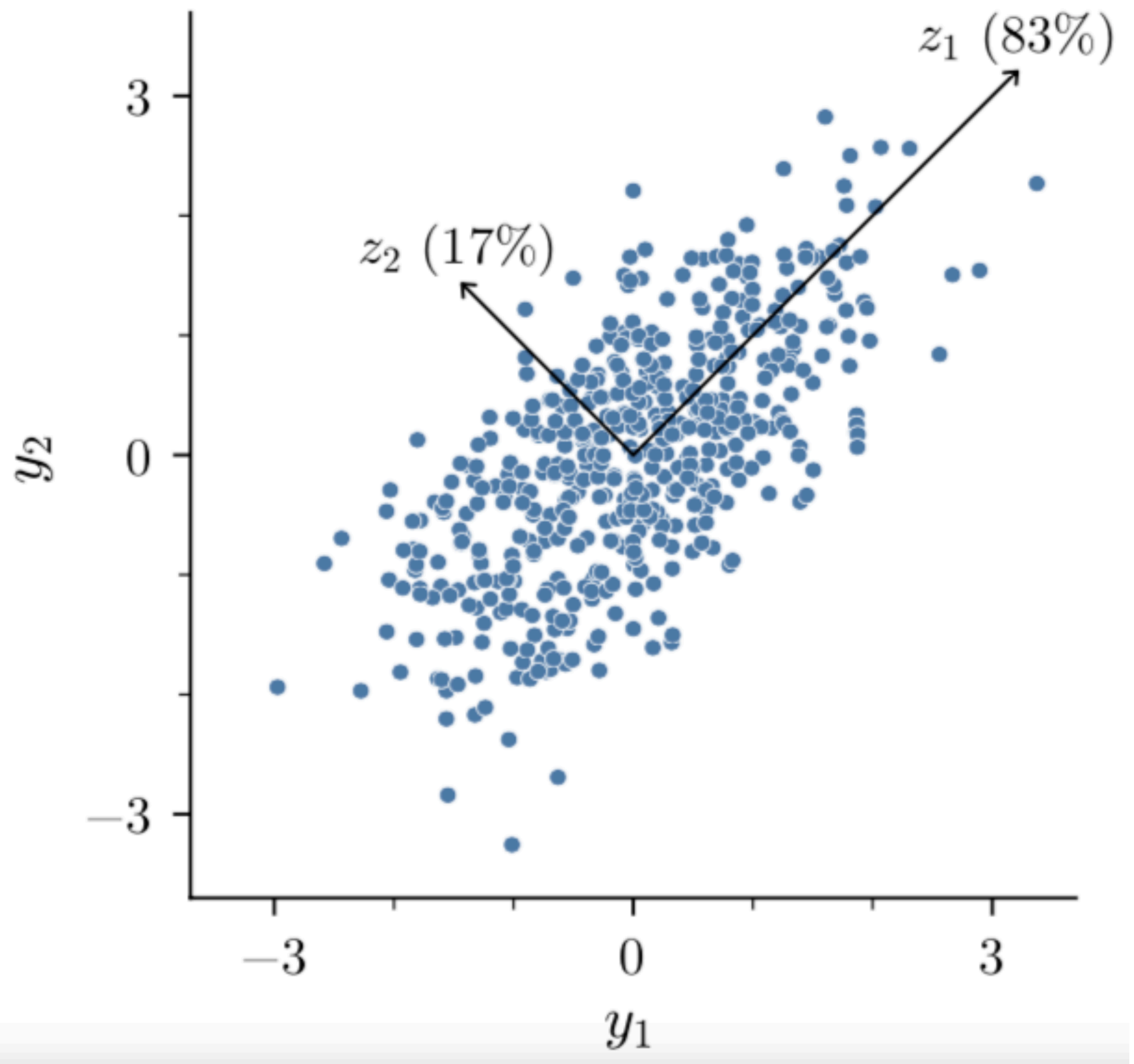
- Model is computationally expensive: ≈1000 CPU hours needed to run 2500 events at one parameter set θ. Bayesian posterior inference requires model simulations at $> 10^6$ samples of parameter space. >10^9 CPU hours required. Inference is out of reach without emulation. **expensive**

- Need for fast and accurate model surrogates to perform any Bayesian study.
Gaussian process based model emulators are used in heavy-ion studies.

Gaussian Process based model emulators

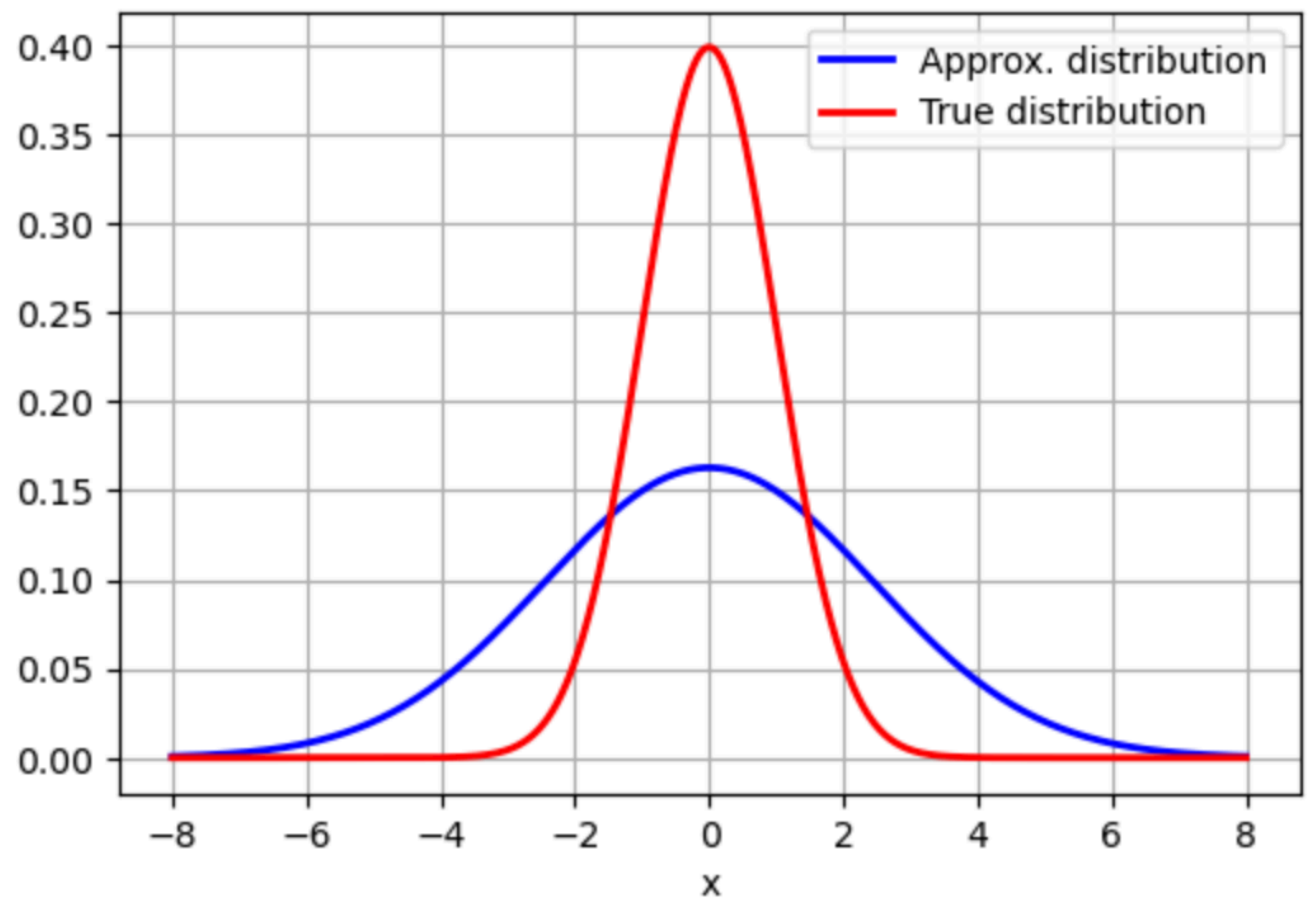
- We want emulators to "interpolate" in the d (=17) dimensional parameter space.
  - Consider the mean values of the p (=110) distributions for each θ_i : $\mathbf{y}(\theta_i)$.
  - For n (=500) training set $\{\theta_1, \ldots, \theta_n\}$ (Latin Hypercube Sampling), define a $n \times p$ matrix: $\mathbf{M} \equiv \{\mathbf{y}(\theta_1), \ldots, \mathbf{y}(\theta_n)\}$
  - Standardize dataset by removing mean and scaling to unit variance for all p-distributions: $\mathbf{M} \rightarrow \tilde{\mathbf{M}}$
  - Principal Component Analysis → Reduce dimensionality of dataset
  - Transform by doing PCA and keep $q < p$ principal components. In most applications, $q \ll p$ is sufficient to describe almost all the variance in the original dataset.
- Train q independent Gaussian process corresponding to the q reduced observables (means). Each Gaussian process is d dimensional.



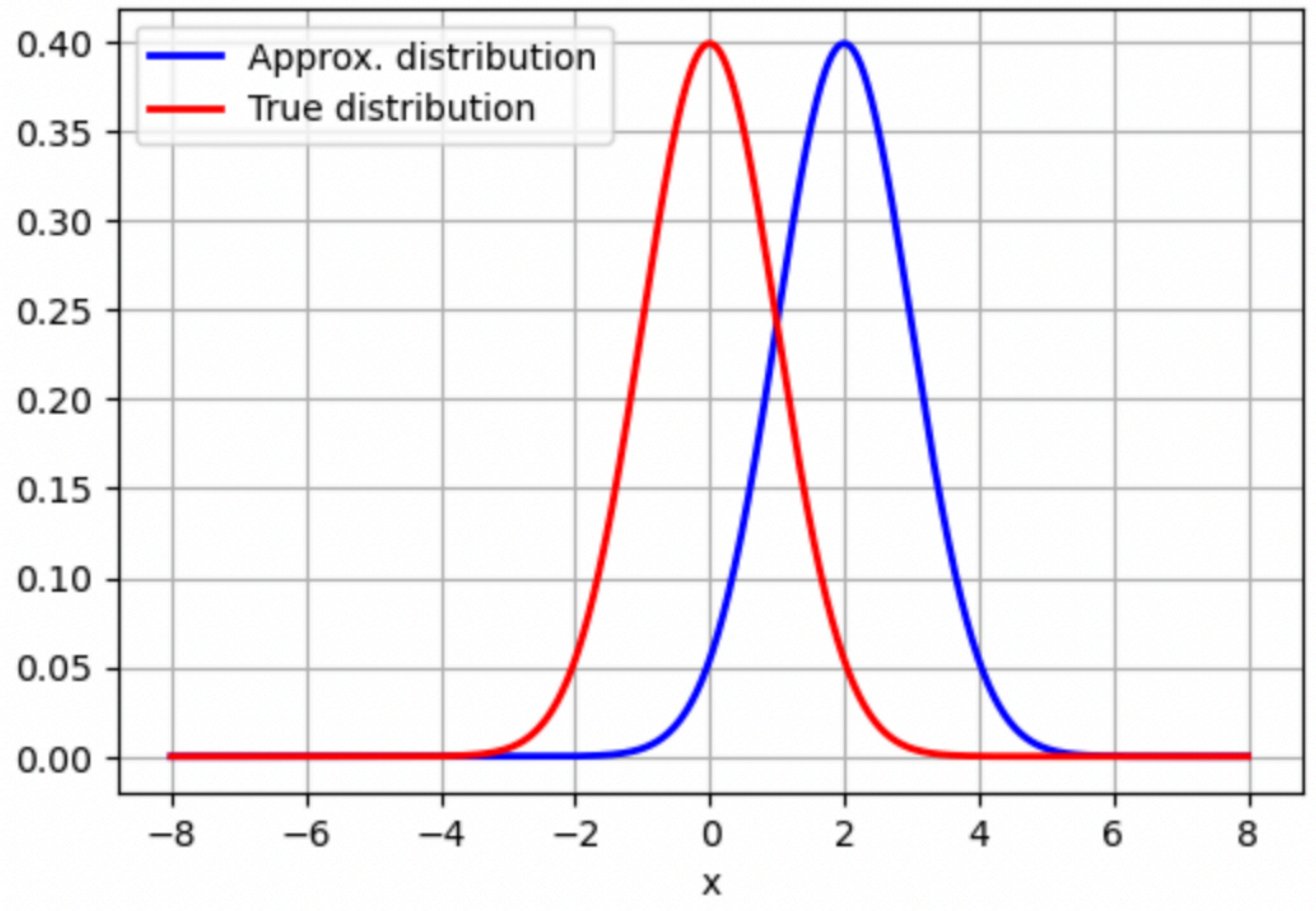


Metrics for comparing emulators

- **Root mean squared error (RMSE):** Compares mean of two distributions: square root of the mean squared error.
- **95 % Empirical coverage:** Measures how often the mean of true distribution P fall within the 95 % predicted confidence interval of the approximate distribution Q. Does not involve variance of the true distribution P.
- **Kullback–Leibler divergence:** Compares distributions. Expected excess "surprise" from using approximate distribution Q instead of true distribution P.
- **Hellinger distance:** Compares distributions. $\propto 1-$amount of overlap between two distributions.
- **Wasserstein distance:** Compares distributions. Amount of work required to turn one distribution into another.




```
Metric
-----------------------------------
RMSE                    0.000000
95% Coverage            1.000000
KL Divergence           1.604120
Hellinger Distance      0.404261
Wasserstein Distance    1.449490
-----------------------------------
```




```
Metric
-----------------------------------
RMSE                    2.000000
95% Coverage            0.000000
KL Divergence           2.000000
Hellinger Distance      0.627271
Wasserstein Distance    2.000000
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```

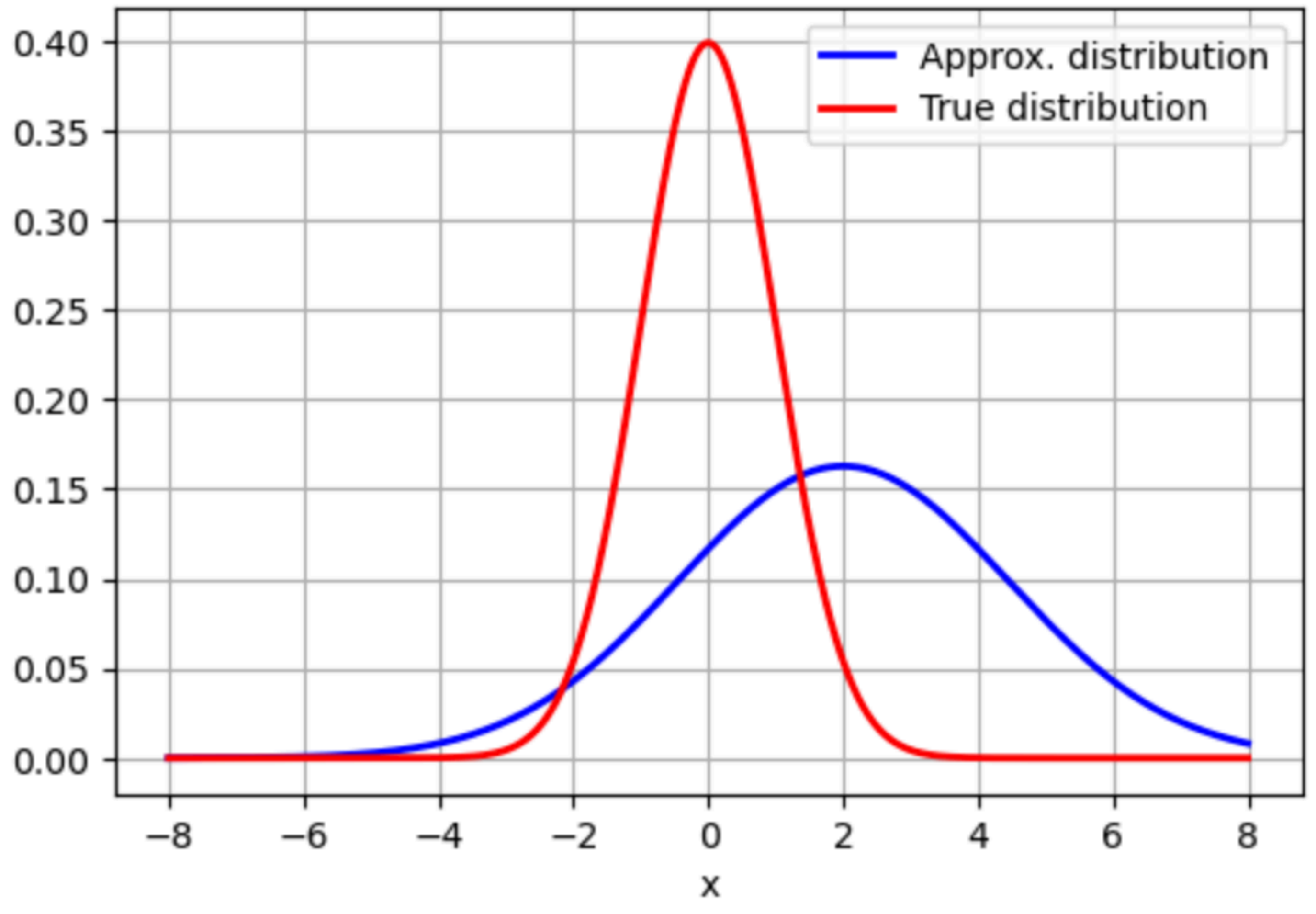


```
Metric
-----------------------------------
RMSE                    2.000000
95% Coverage            1.000000
KL Divergence           3.604120
Hellinger Distance      0.524207
Wasserstein Distance    2.470024
-----------------------------------
```