

Static computational budget optimization with stochastic simulations

[arXiv:2301.08385]

PAPER • OPEN ACCESS

Computational budget optimization for Bayesian parameter estimation in heavy-ion collisions

Brandon Weiss¹ , Jean-François Paquet^{1,2}  and Steffen A Bass¹ 

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Jean-François Paquet

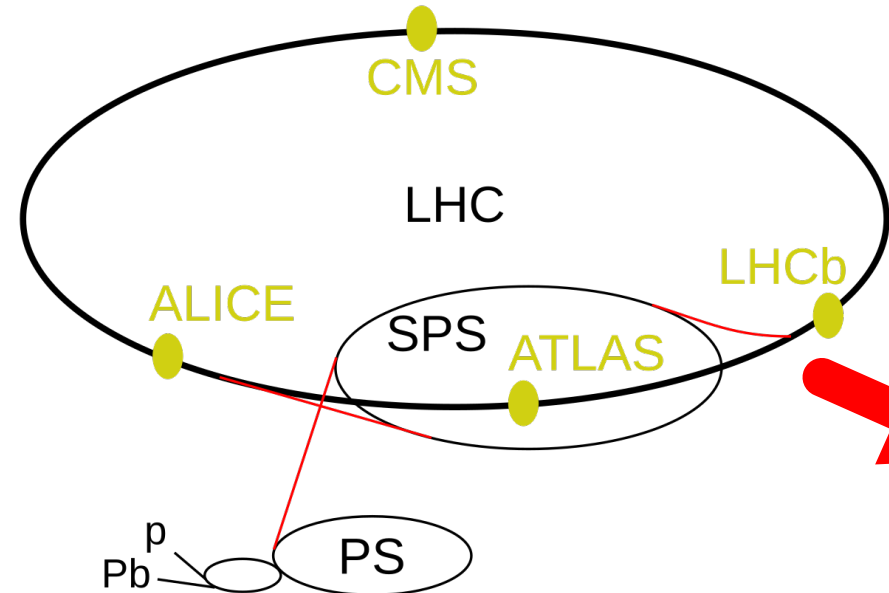
July 8, 2024



“Inverse Problems and Uncertainty Quantification in Nuclear Physics” Workshop



Ultrarelativistic heavy-ion collisions

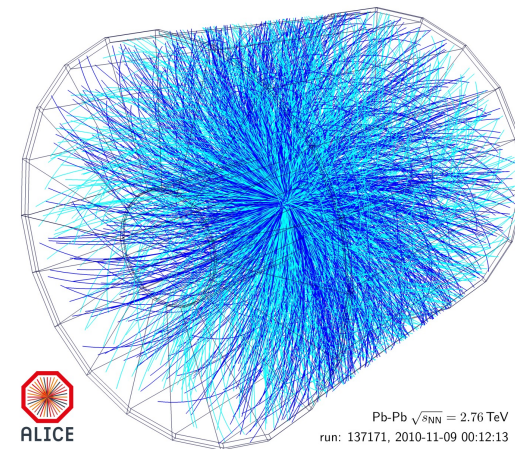
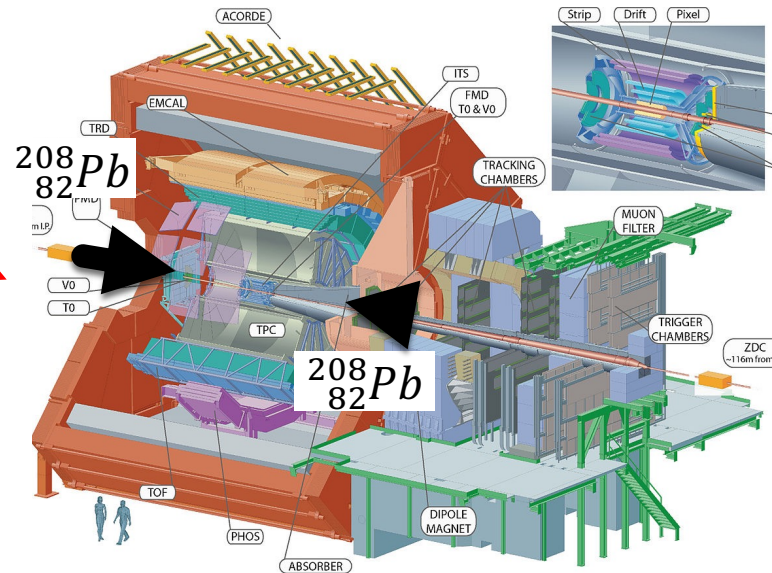


LHC complex

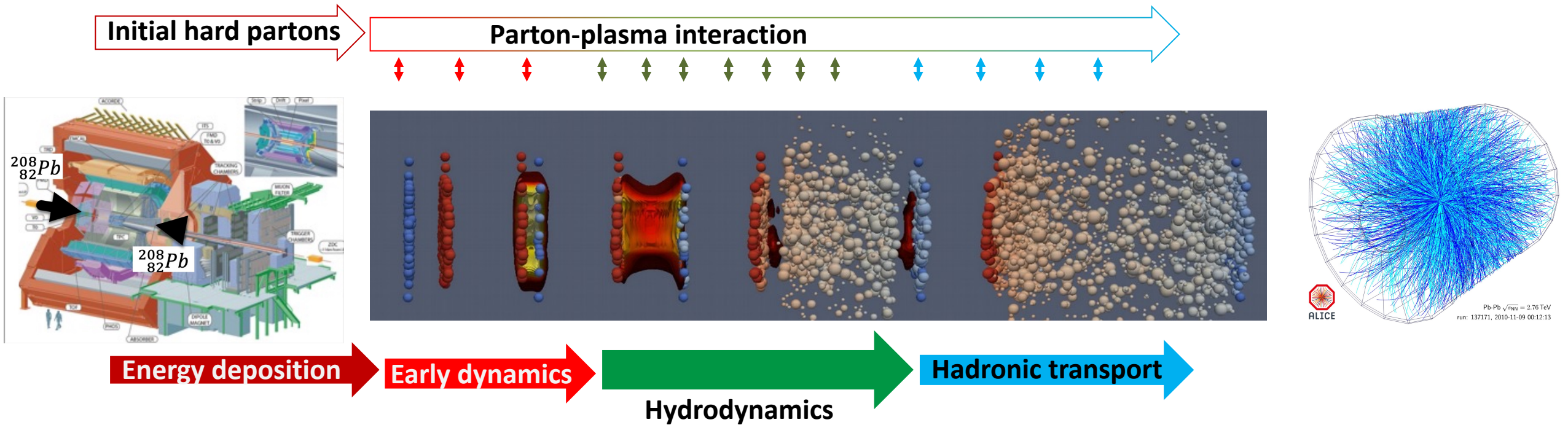
$$\frac{\sqrt{s}}{\text{nucleon}} \sim \text{TeV}$$

Ref.: ALICE, CERN

ALICE detector

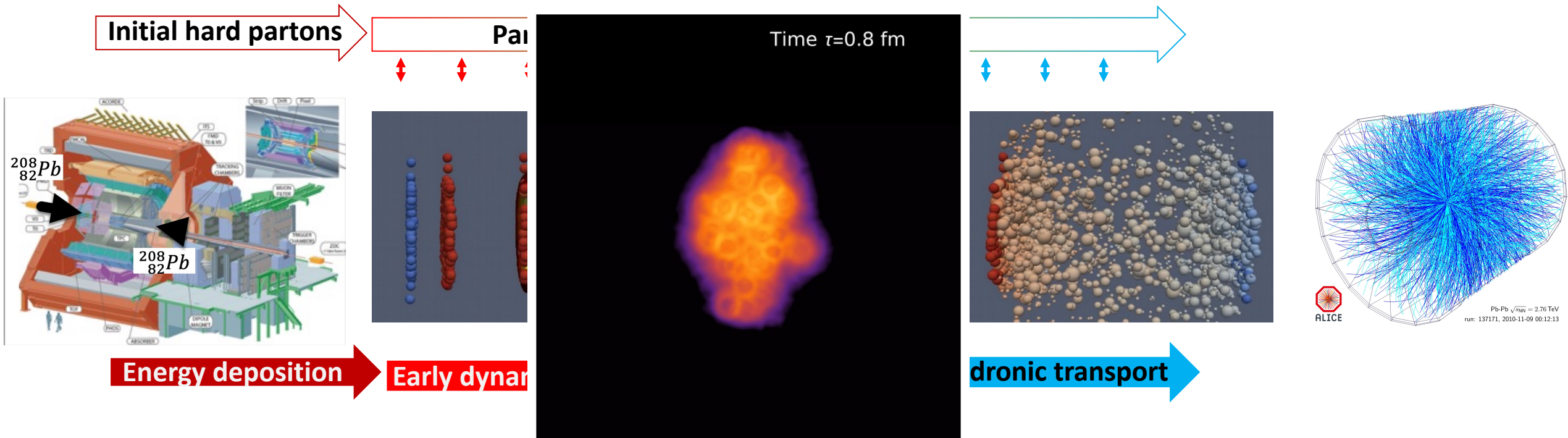


Pb-Pb $\sqrt{s_{NN}} = 2.76 \text{ TeV}$
run: 137171, 2010-11-09 00:12:13



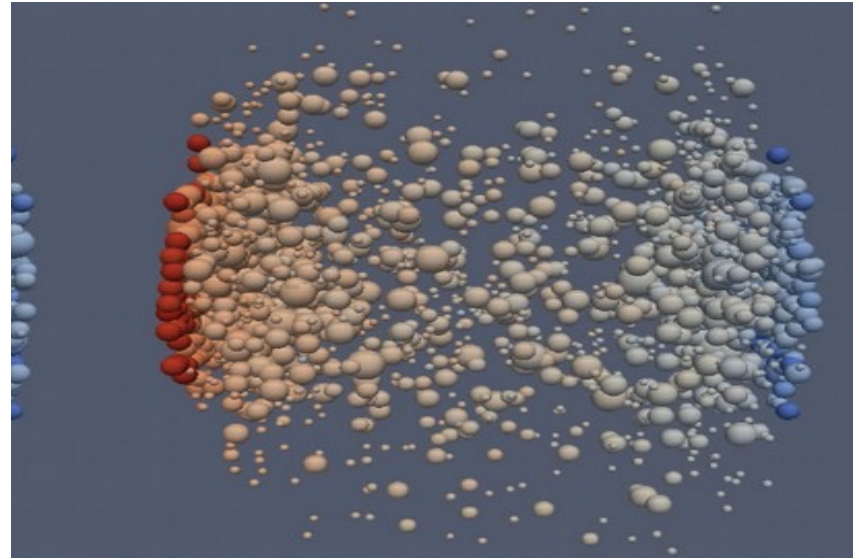
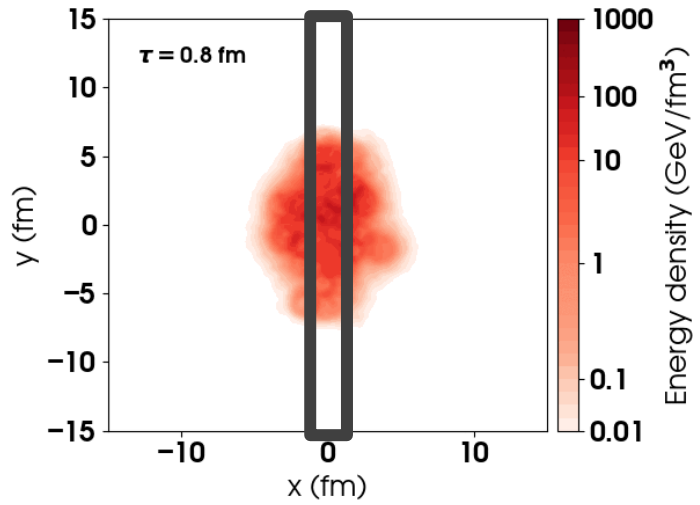
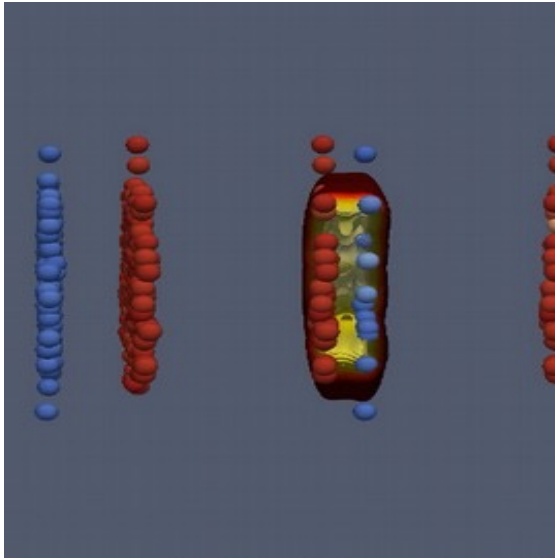
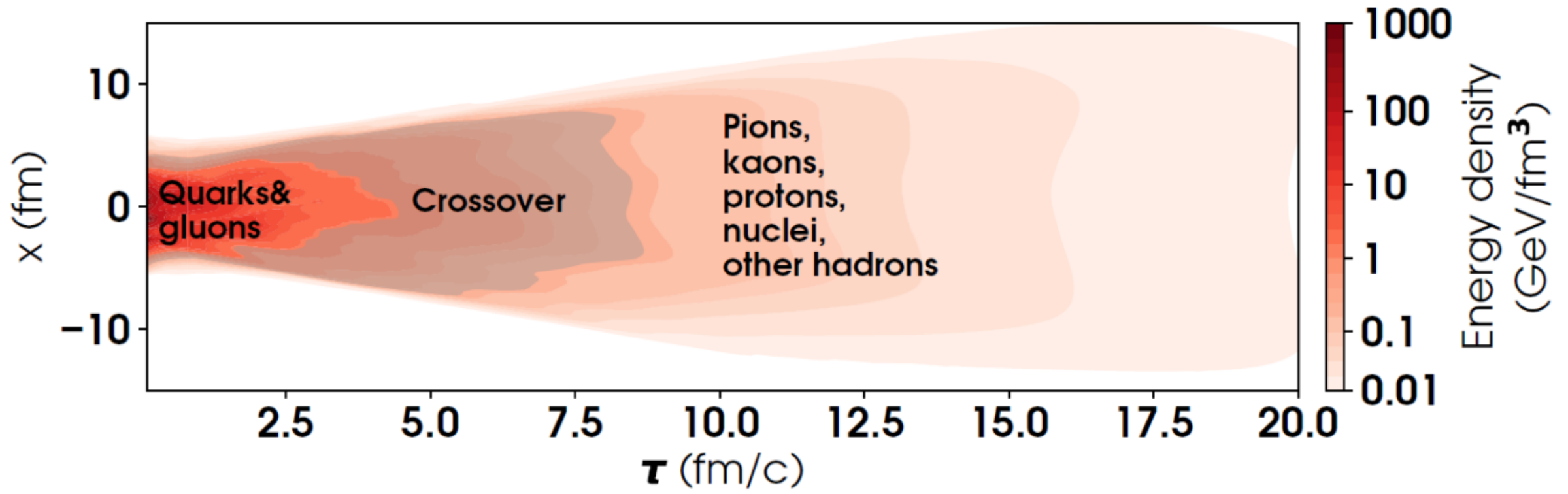
- Energy-momentum tensor of plasma: $T^{\mu\nu} = \epsilon u^\mu u^\nu - (P(\epsilon) + \Pi)(g^{\mu\nu} - u^\mu u^\nu) + \pi^{\mu\nu}$
- Conservation of energy and momentum: $\partial_\nu T^{\mu\nu} = 0$
- Transient relativistic viscous hydrodynamics

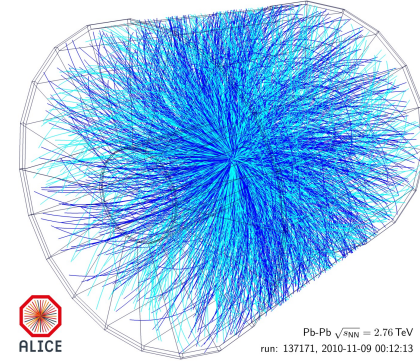
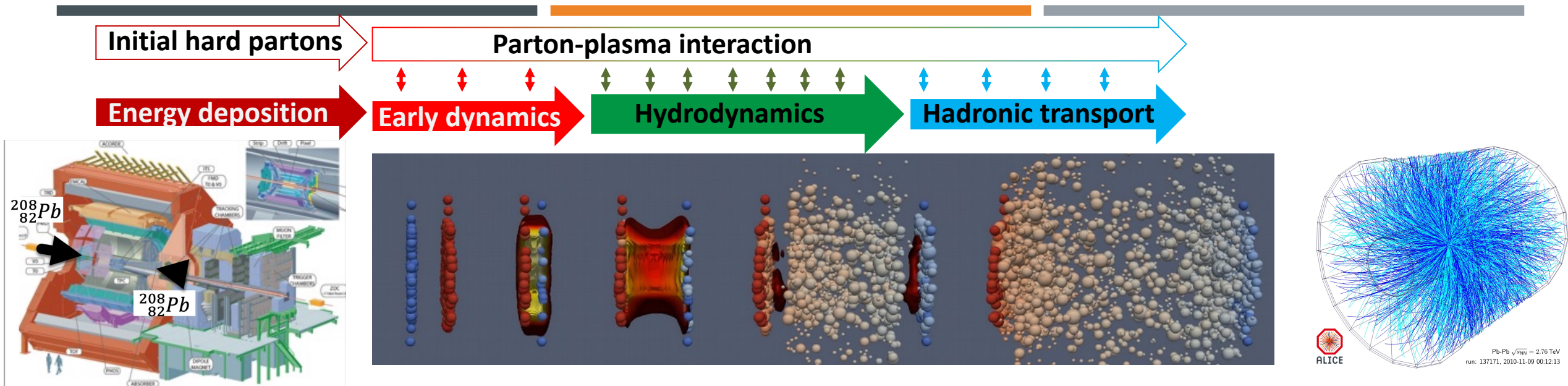
$$\tau_\pi \Delta^{\mu\nu}_{\alpha\beta} \dot{\pi}^{\alpha\beta} + \pi^{\mu\nu} = 2 \eta(T) (\partial^\mu u^\nu + \dots) + (2^{\text{nd}} \text{ order}); \quad \tau_\Pi \dot{\Pi} + \Pi = -\zeta(T) \partial_\mu u^\mu + (2^{\text{nd}} \text{ order});$$



- Energy-momentum tensor of plasma: $T^{\mu\nu} = \epsilon u^\mu u^\nu - (P(\epsilon) + \Pi)(g^{\mu\nu} - u^\mu u^\nu) + \pi^{\mu\nu}$
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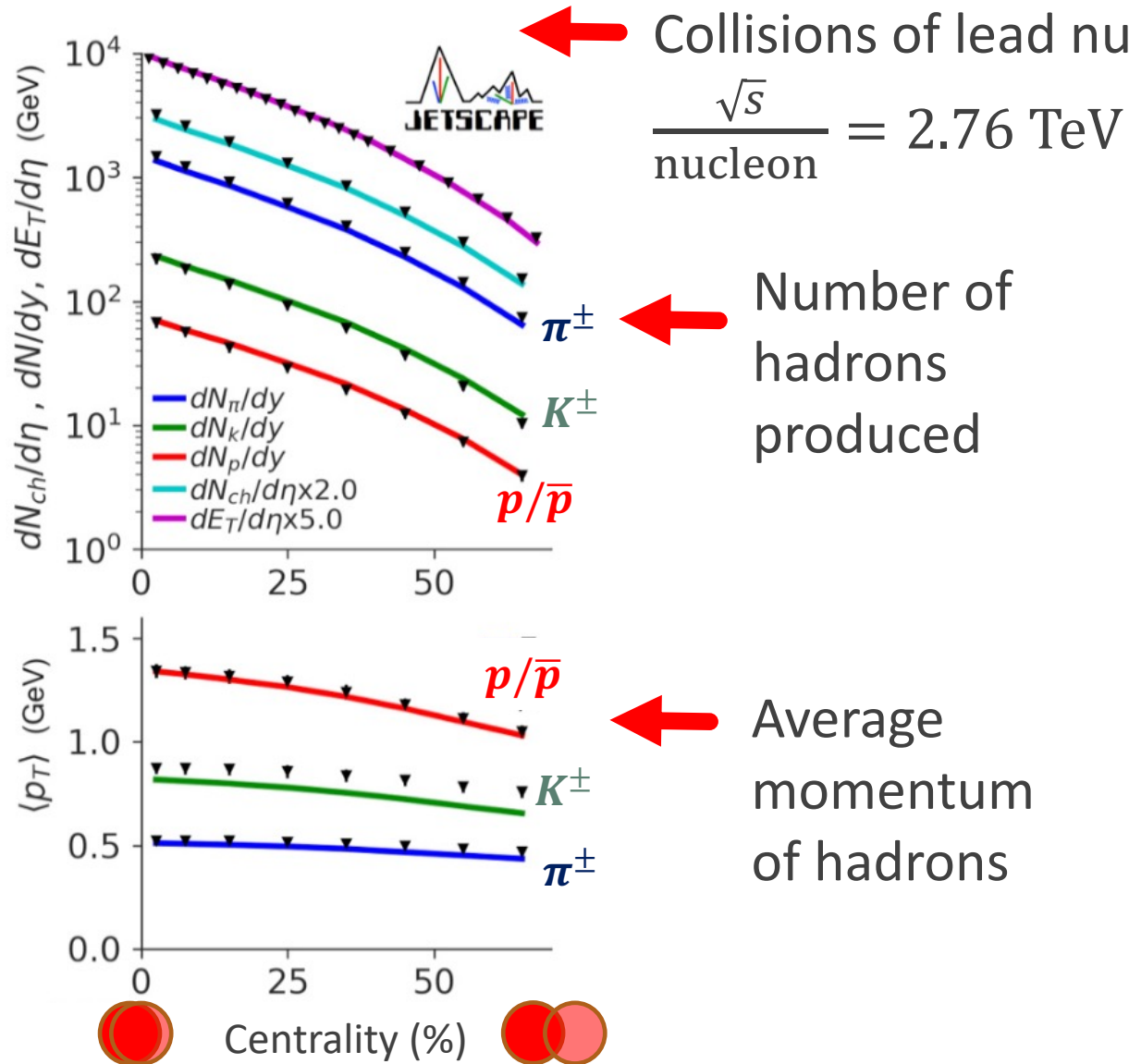
$$\tau_\pi \Delta^{\mu\nu}_{\alpha\beta} \dot{\pi}^{\alpha\beta} + \pi^{\mu\nu} = 2 \eta(T) (\partial^\mu u^\nu + \dots) + (2^{\text{nd}} \text{ order}); \quad \tau_\Pi \dot{\Pi} + \Pi = -\zeta(T) \partial_\mu u^\mu + (2^{\text{nd}} \text{ order});$$





- Functional description of the physics of heavy-ion collisions using: lattice QCD, relativistic hydrodynamics&transport, perturbative QCD, ...
- Model parameters: unknown or uncertain quantities
 - Shear&bulk viscosity of the plasma
 - Perhaps equation of state
 - Many parameters in the "initial stage" and in transition between stages

Model-data comparison



- Data available for handful of nuclei and \sqrt{s} (e.g. Au-Au $\sqrt{s_{NN}} = 0.2 \text{ TeV}$, Pb-Pb $\sqrt{s_{NN}} = 2.76 \text{ TeV}$)
- Large number of measured observables
 - Many energy/momentum bins
 - Many centrality bins
- Percent-level precision is common

Model-data comparison

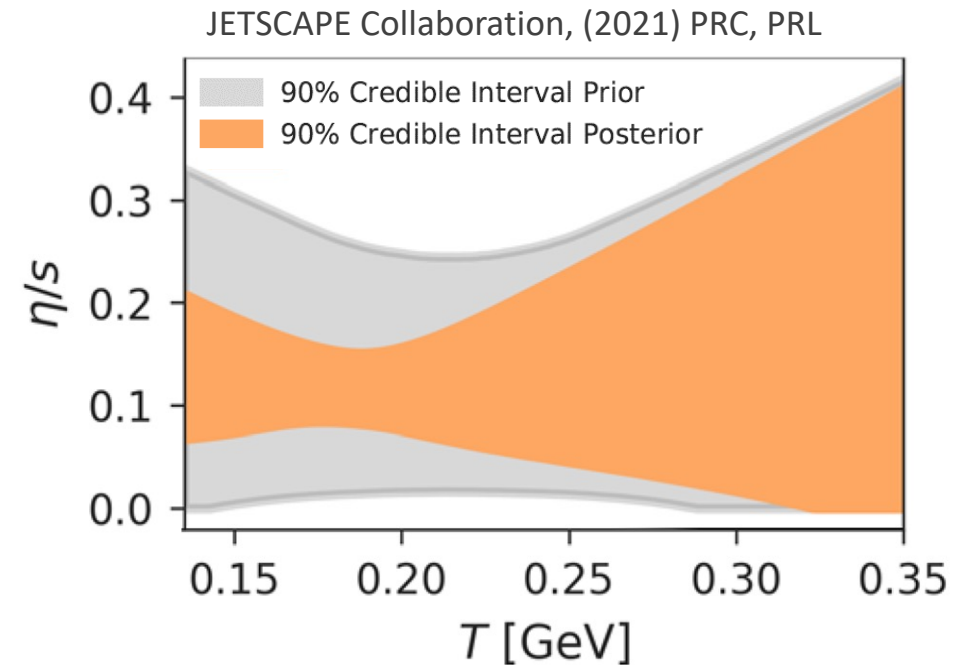
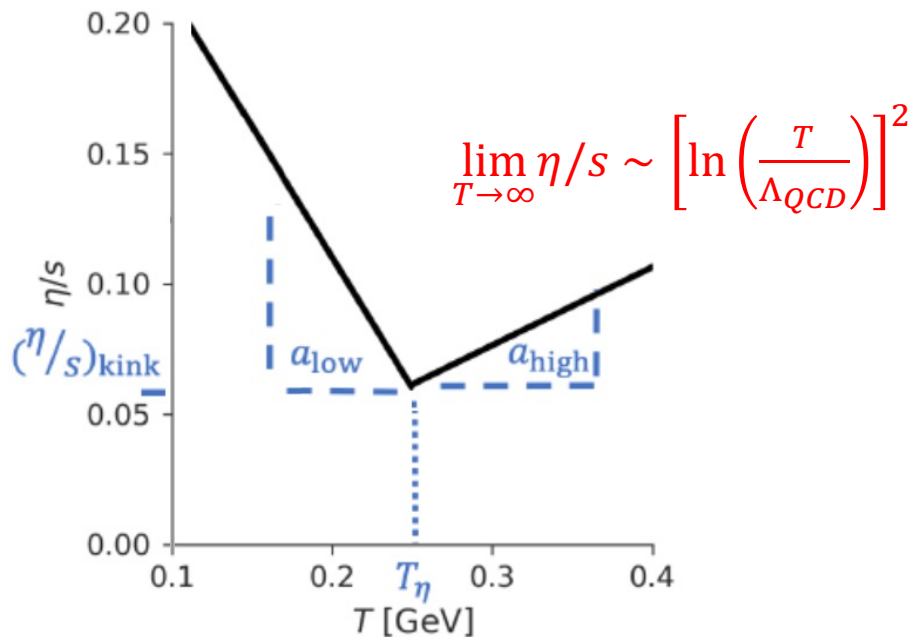
- Constraints from Bayesian inference:

$$\text{posterior}(\mathit{param}) \propto \exp\left(-\frac{1}{2} \sum_{\text{observables}} \frac{(\text{model}(\mathit{param}) - \text{data})^2}{(\text{uncertainty})^2}\right)$$

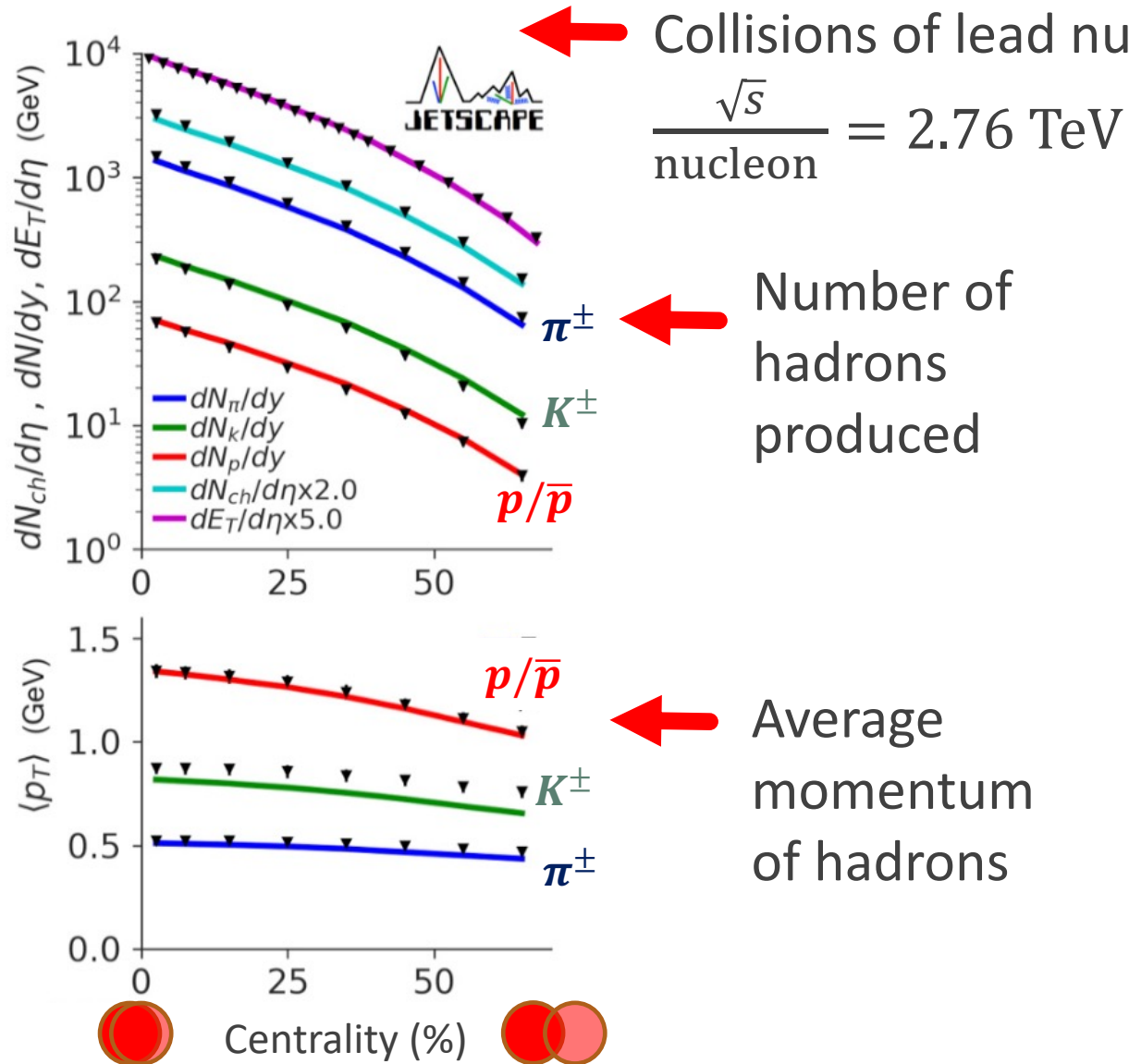
↑
Constraints on
parameters

Model prediction for given set of model parameters

- Challenge:
many parameters
(~10-20)



Model-data comparison



- For one choice of model parameters:

- Simulate 10^3 - 10^4 collisions (expt: 10^6) [model is stochastic]
- Simulation: a few core-minute/collision
- = ~ 100 - 1000 core-hours per param
- 1k param samples $\rightarrow \sim 10^5$ - 10^6 core-hour
- 10k param samples $\rightarrow \sim 10^6$ - 10^7 core-hour

Model-data comparison

MODEL TRAINING & OBTAINING DATA

A 20-dimensional model parameter space with 1,000 training points

Au+Au	Hydro events per design	Avg. hadronic events per hydro
200 GeV	1,000	1,000
19.6 GeV	2,000	4,000
7.7 GeV	2,000	8,000

 Open Science Grid delivered 5 million CPU hours for the data generation

- For one choice of model parameters:
 - Simulate 10^3 - 10^4 collisions (expt: 10^6) [model is stochastic]
 - Simulation: a few core-minute/collision
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- 10k param samples $\rightarrow \sim 10^6$ - 10^7 core-hour

Emulation

$$\text{posterior}(\overrightarrow{\text{param}}) \propto \text{prior}(\overrightarrow{\text{param}}) \times \exp\left(-\frac{1}{2}(\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{\text{D}})^T \text{Covar}^{-1}(\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{\text{D}})\right)$$

- Posterior is high-dimensional: expensive to sample
- Solution (that we use): replace model by emulators (Gaussian processes)
- Emulator covariance kernel:

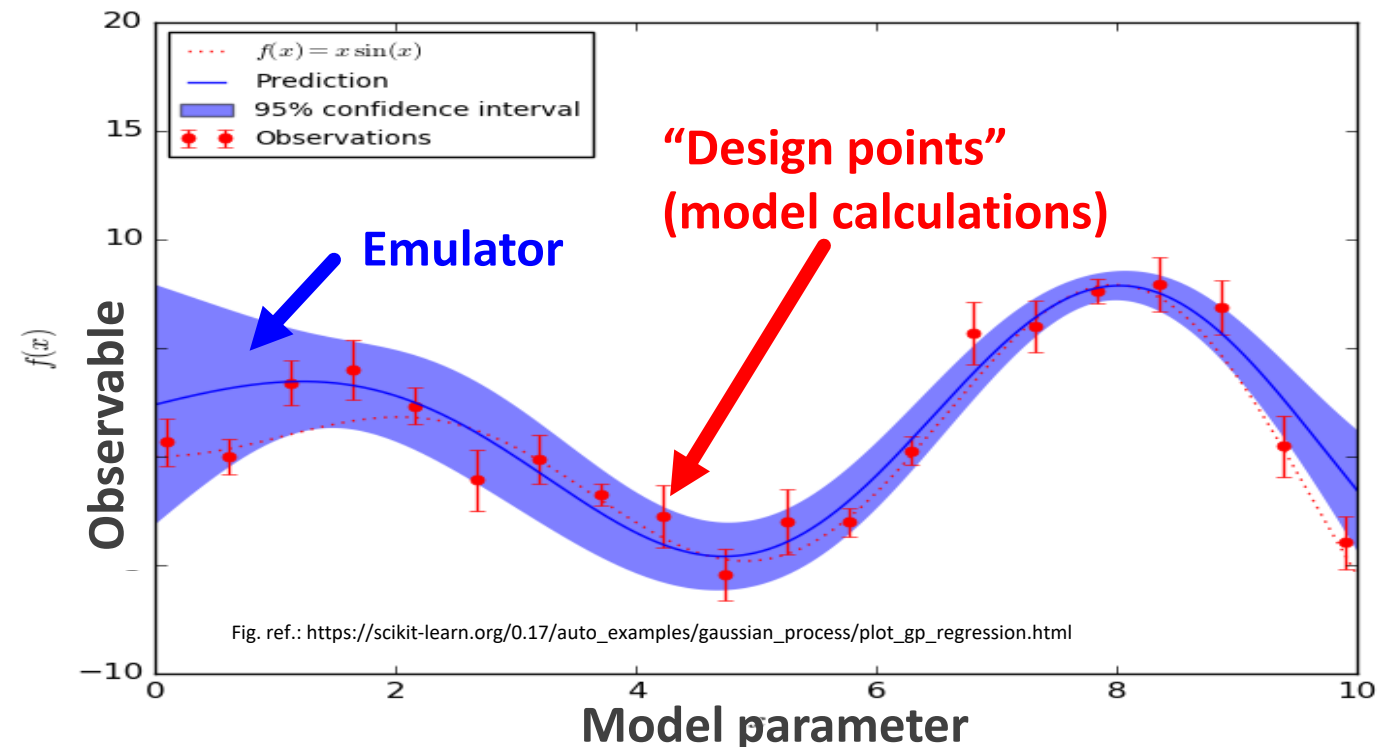
$$k(\mathbf{x}_p, \mathbf{x}_q) = k_{\text{exp}}(\mathbf{x}_p, \mathbf{x}_q) + k_{\text{noise}}(\mathbf{x}_p, \mathbf{x}_q)$$

”Interpolation component”:

$$k_{\text{exp}}(\mathbf{x}_p, \mathbf{x}_q) = C^2 \exp\left(-\frac{1}{2} \sum_{i=1}^s \frac{|x_{p,i} - x_{q,i}|^2}{l_i^2}\right)$$

”Statistical component”:

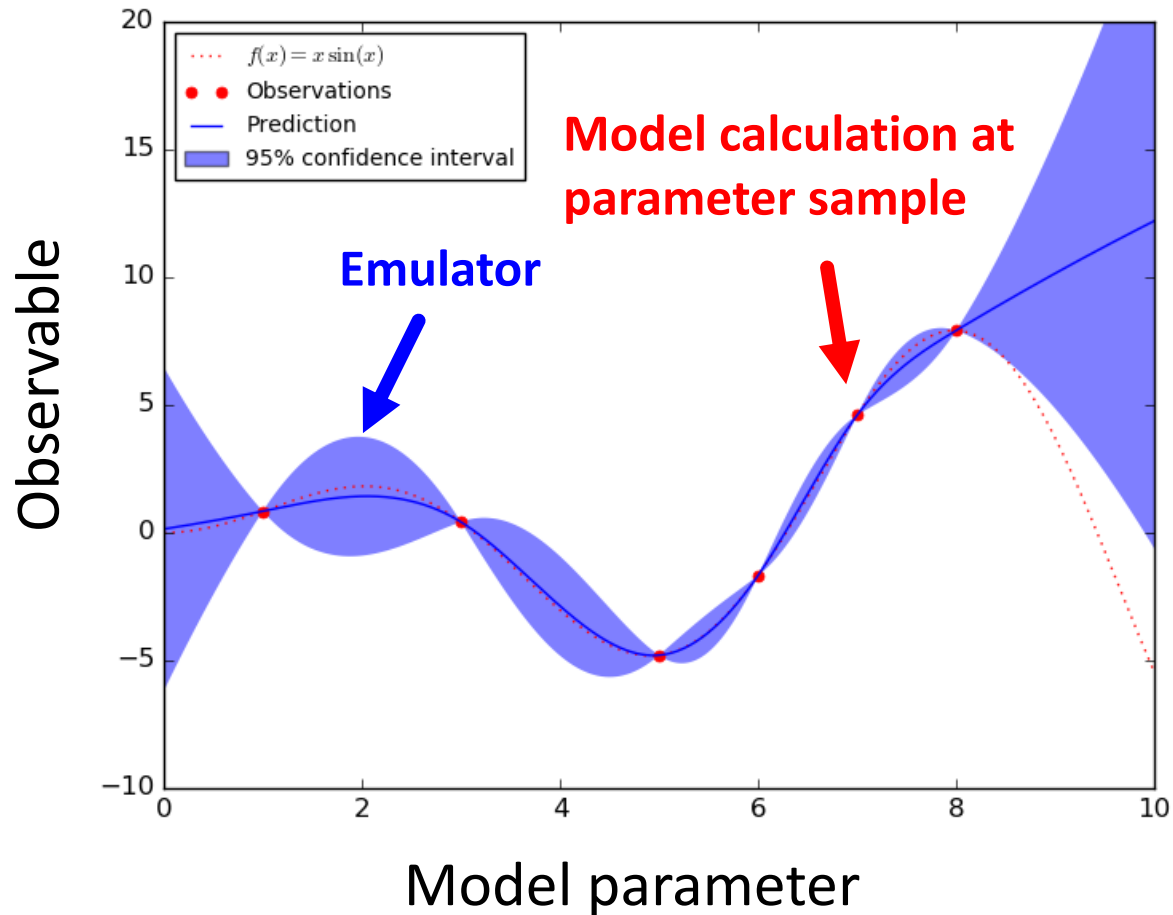
$$k_{\text{noise}}(\mathbf{x}_p, \mathbf{x}_q) = \sigma_{\text{noise}}^2 \delta_{p,q}$$



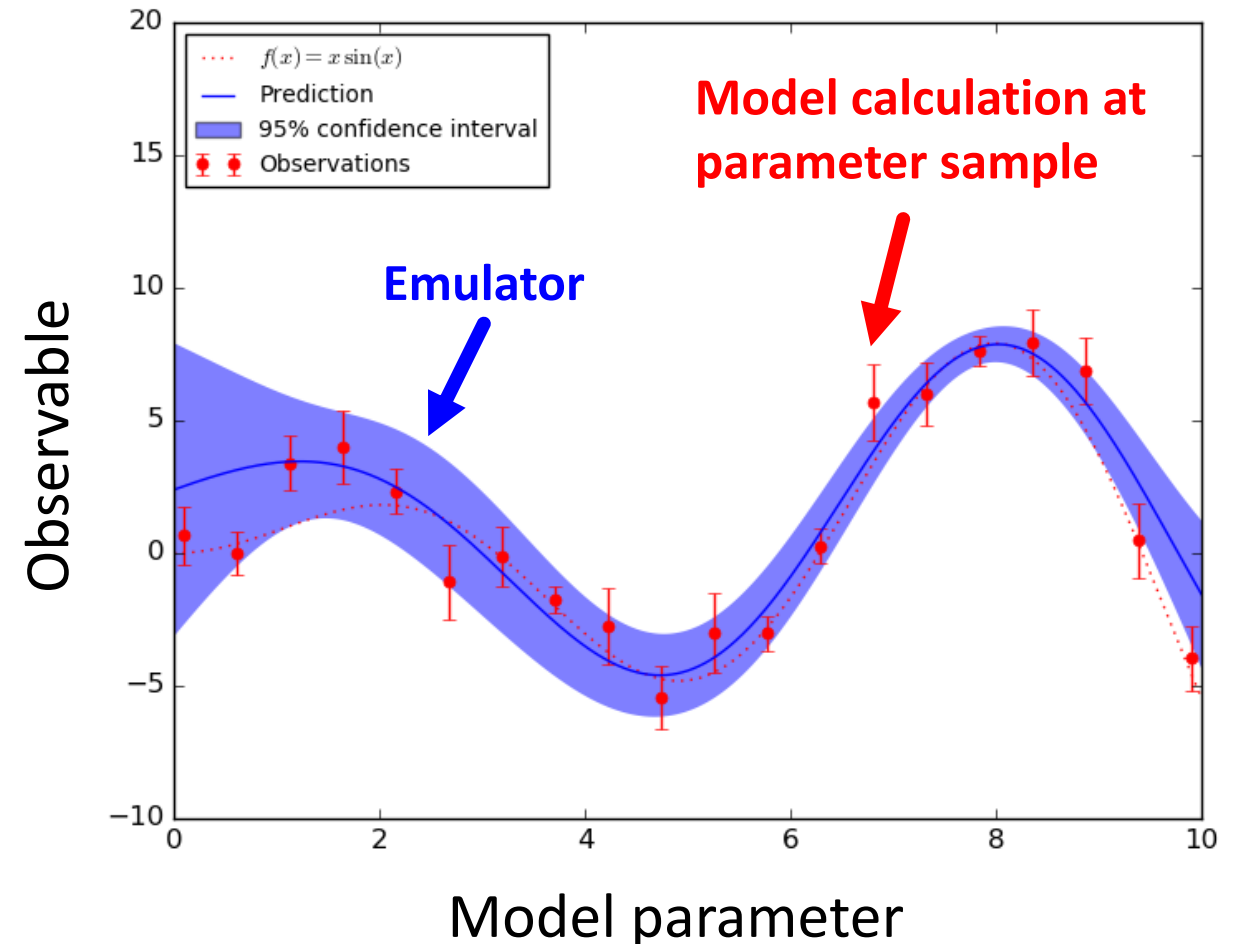
Emulation with stochastic simulations

Fig. ref.: https://scikit-learn.org/0.17/auto_examples/gaussian_process/plot_gp_regression.html

Smaller stat. uncertainty

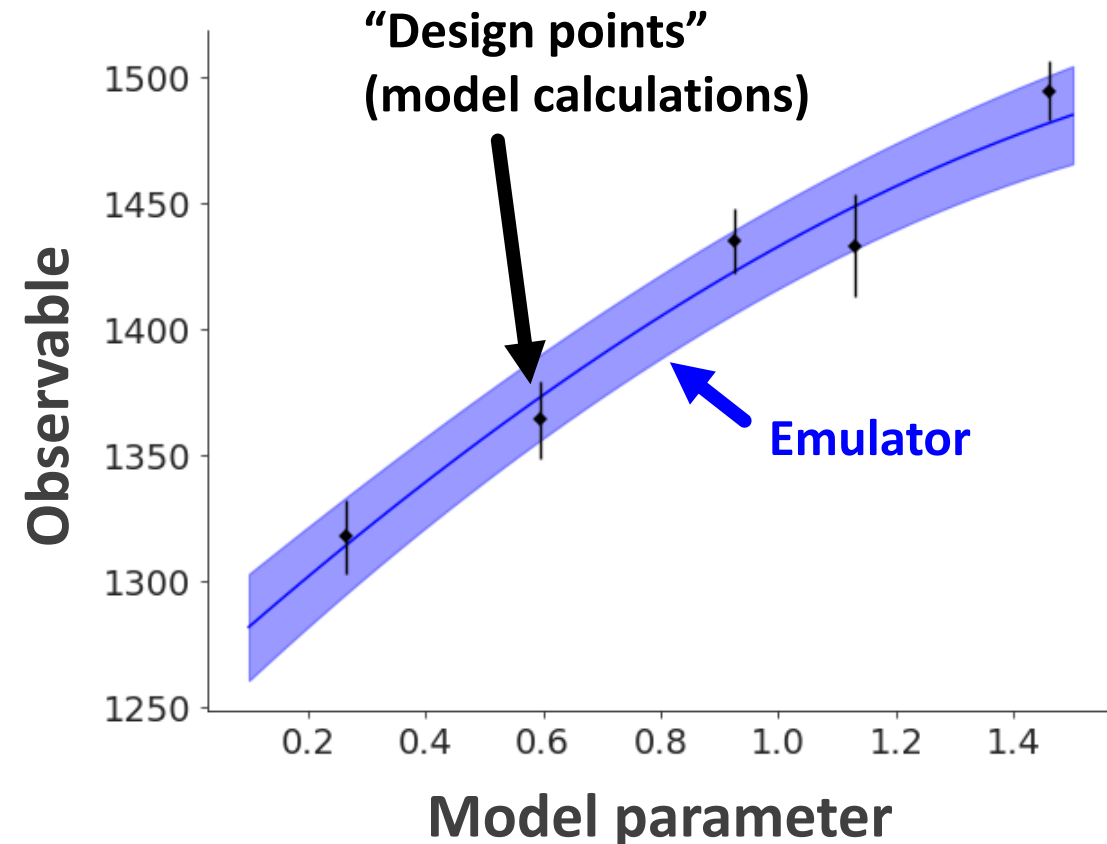


Larger stat. uncertainty



Trade-off in emulation

- Given computational budget:
 - M_{event} = collisions per parameter sample
 - $N_{param\ samples}$ = number of parameter samples
 - Budget = $M_{event} \times N_{param\ samples}$

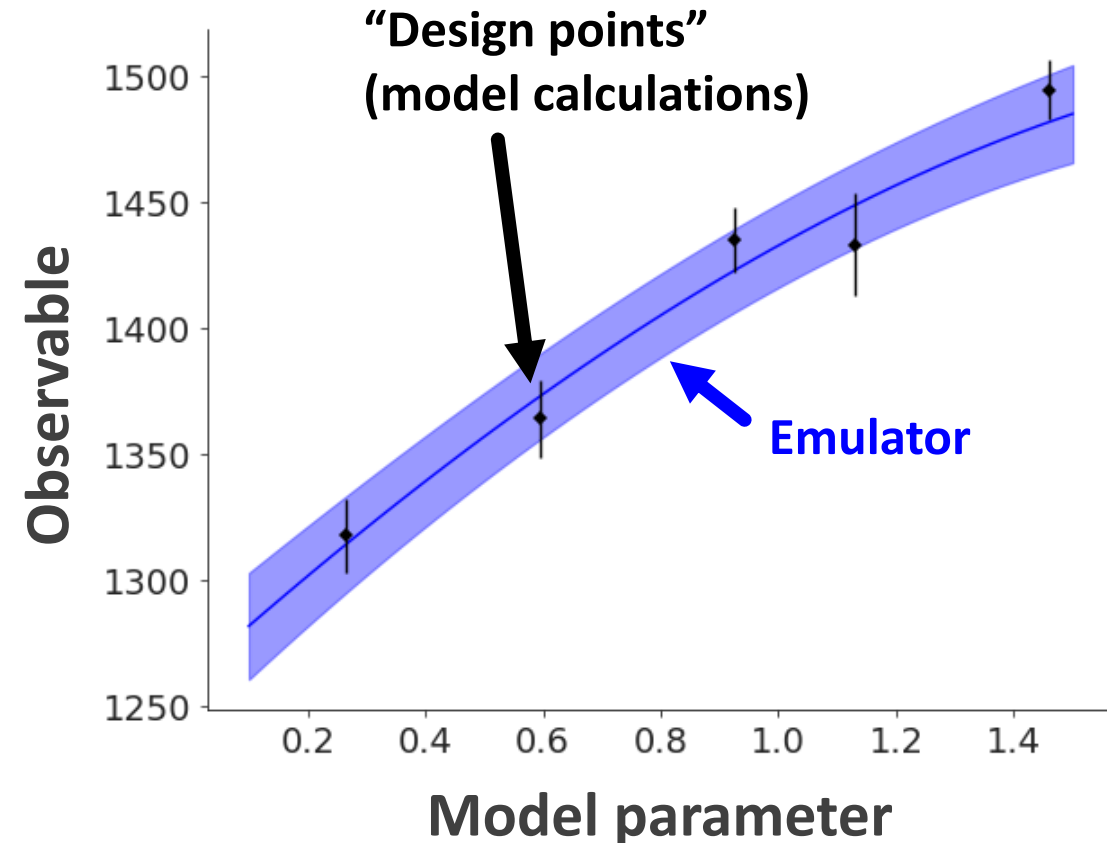


Trade-off in emulation

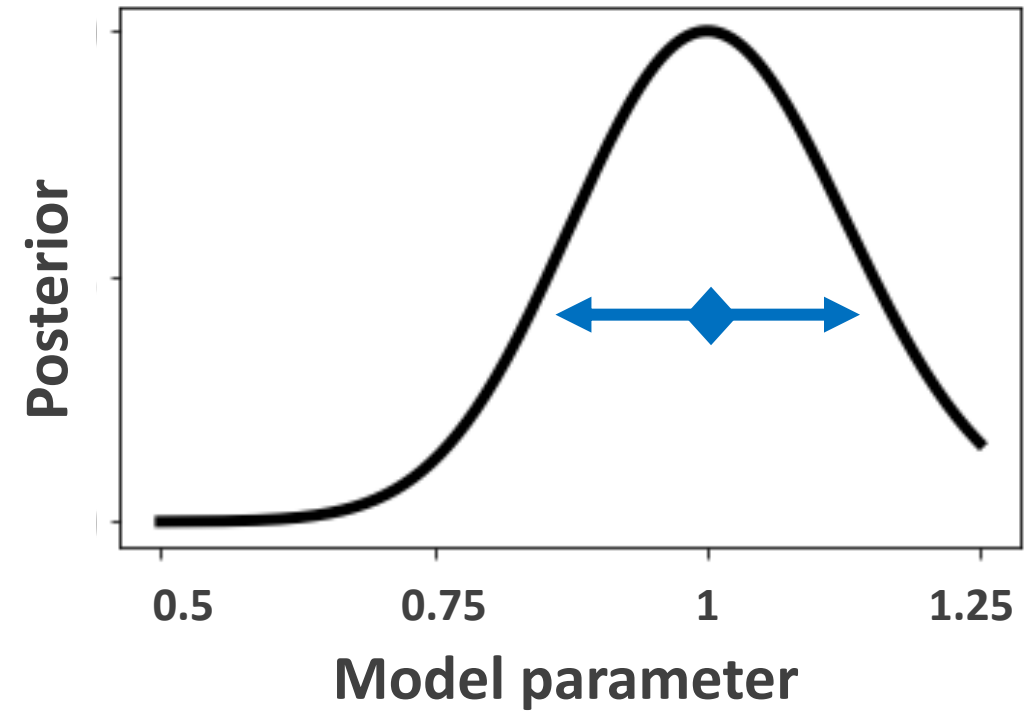
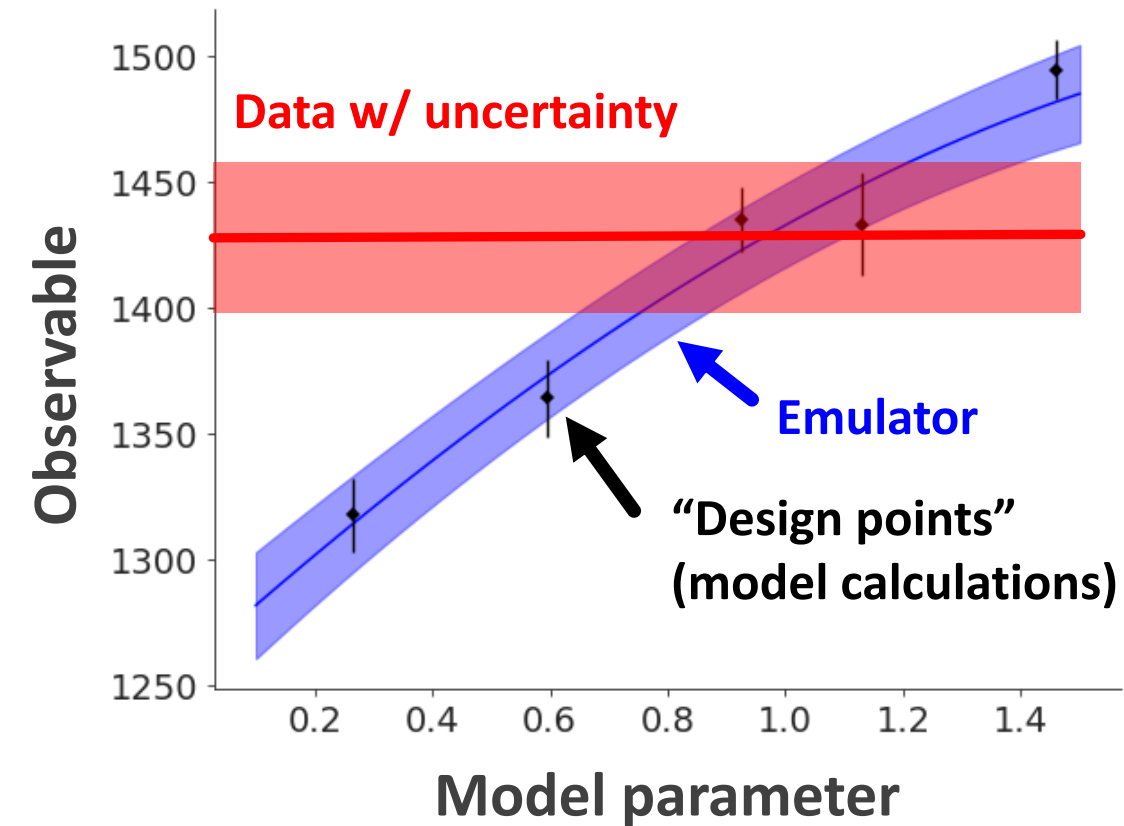
- Given computational budget:
 - M_{event} = collisions per parameter sample
 - $N_{param\ samples}$ = number of parameter samples
 - Budget = $M_{event} \times N_{param\ samples}$

- For given budget, what is the optimal M_{event} and $N_{param\ samples}$?
 - Optimal = minimizes uncertainty on parameters

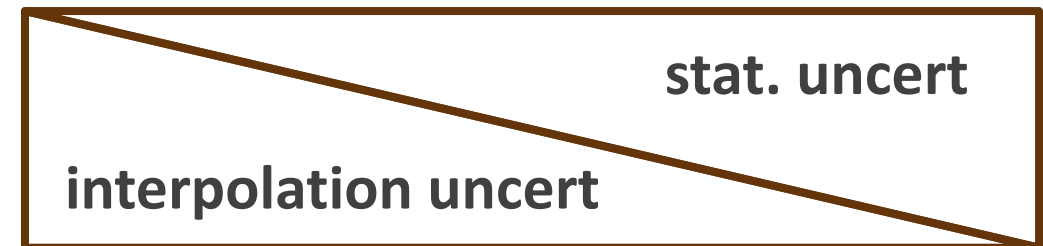
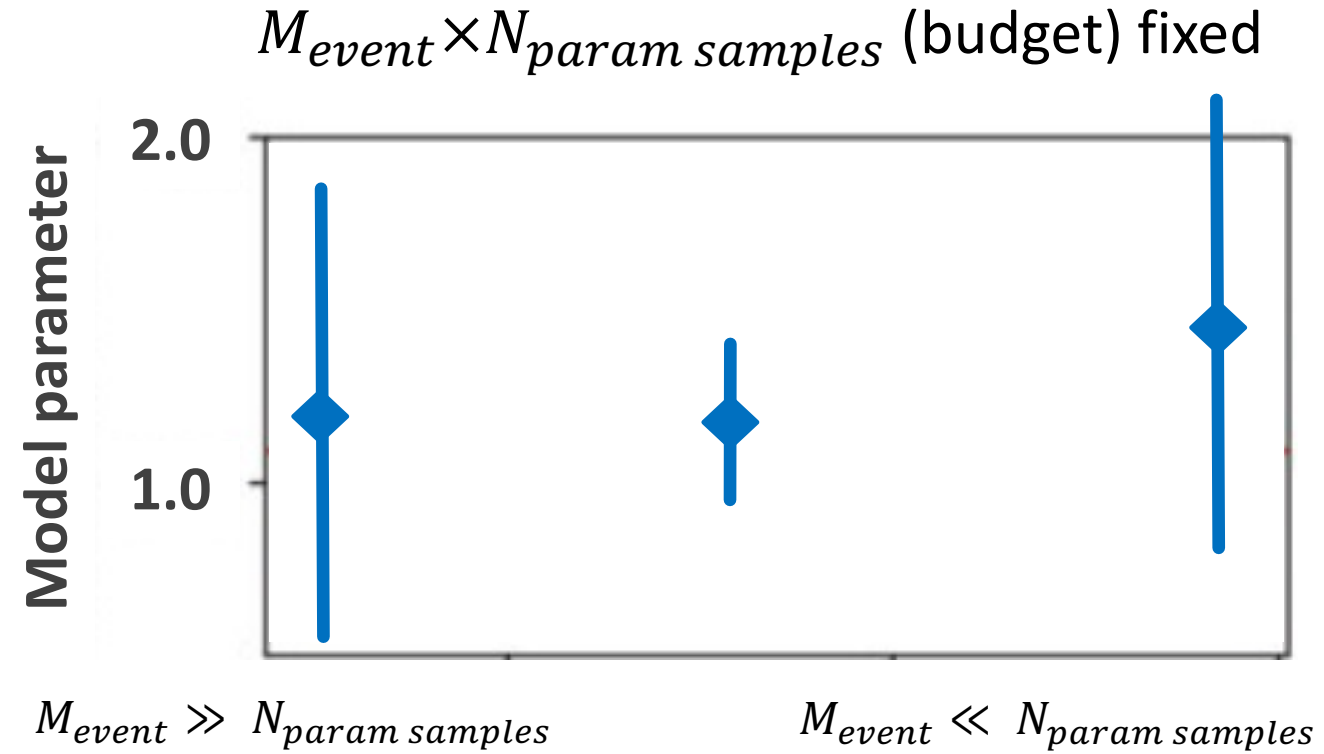
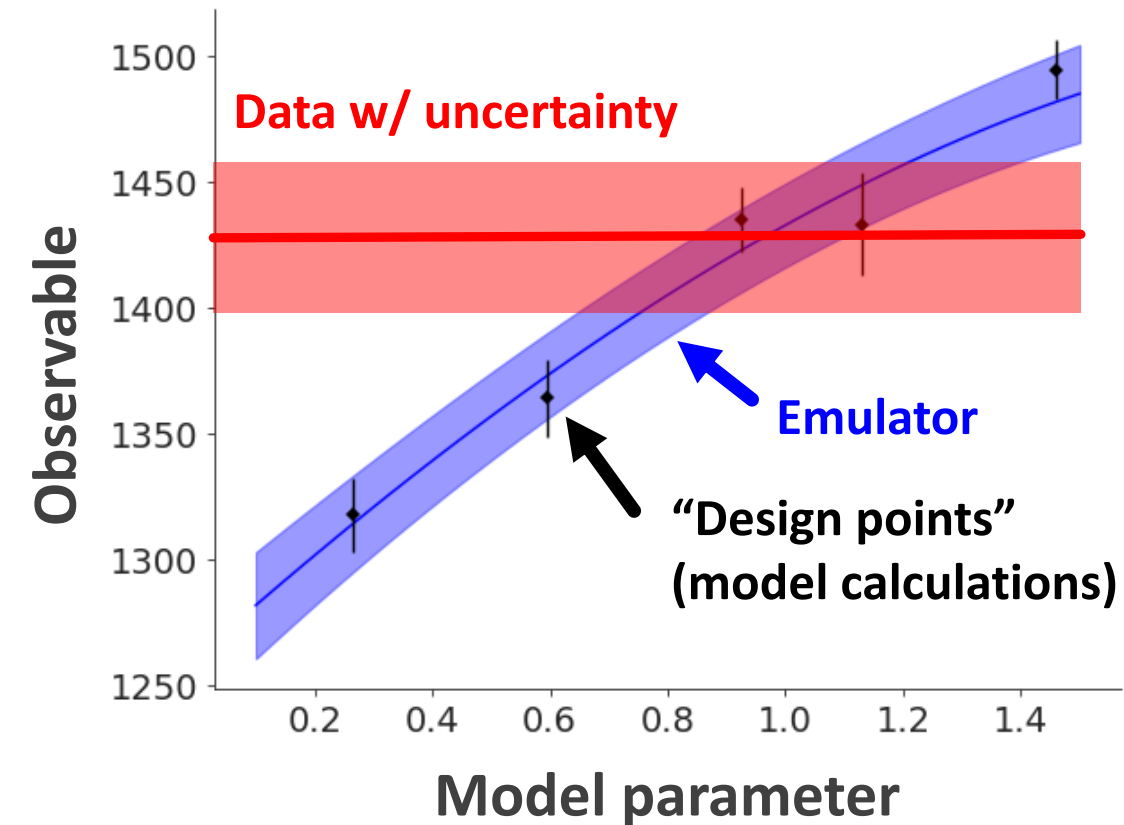
- “Rule of thumb”?:
 - $N_{param\ samples} \sim 10 \times (\text{number of model parameters})$



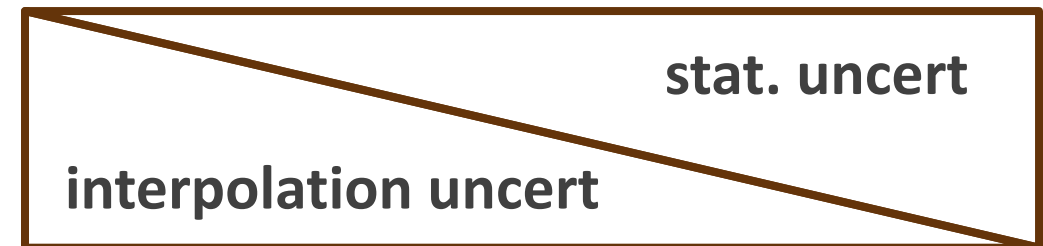
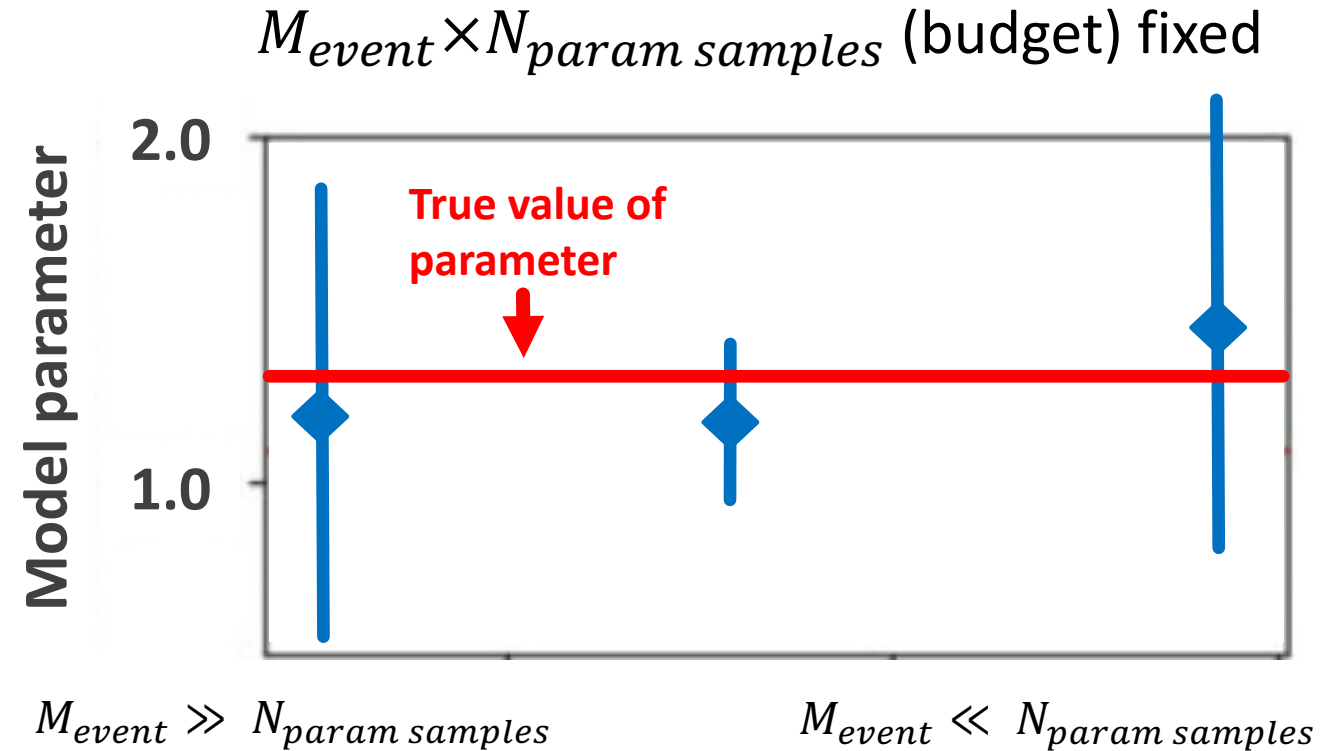
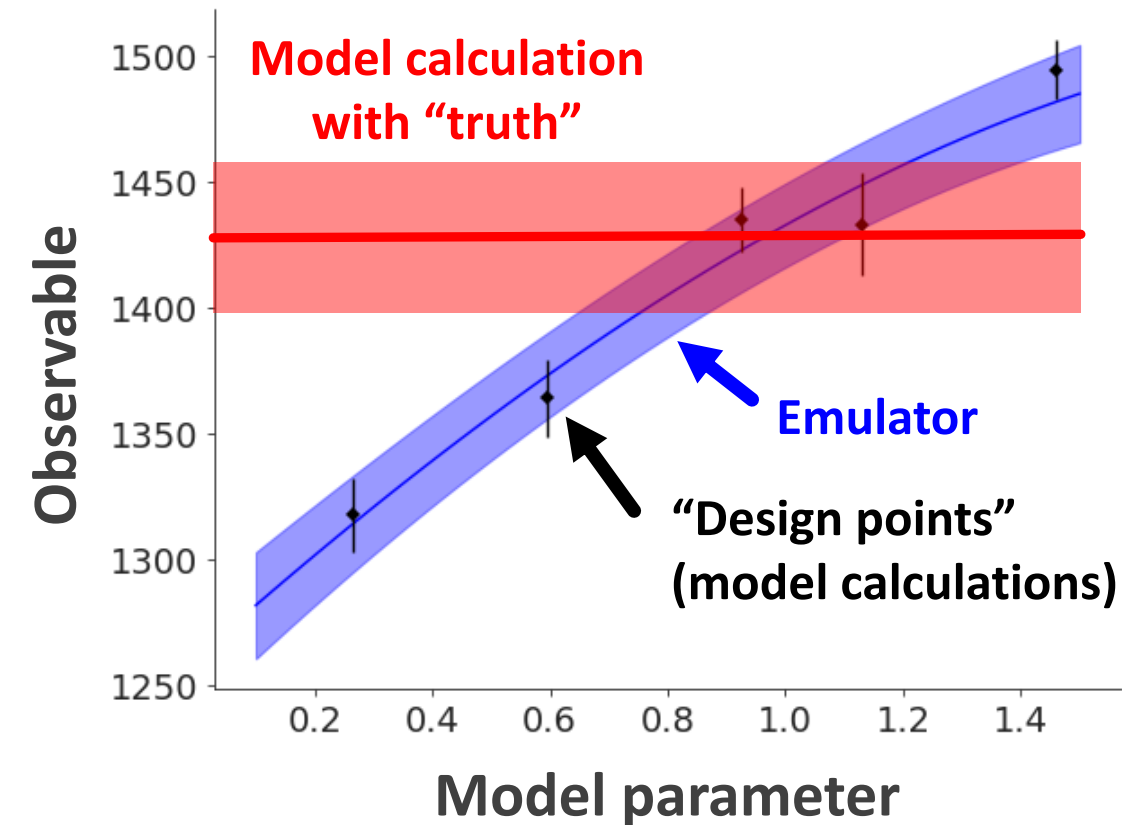
Trade-off in emulation



Trade-off in emulation

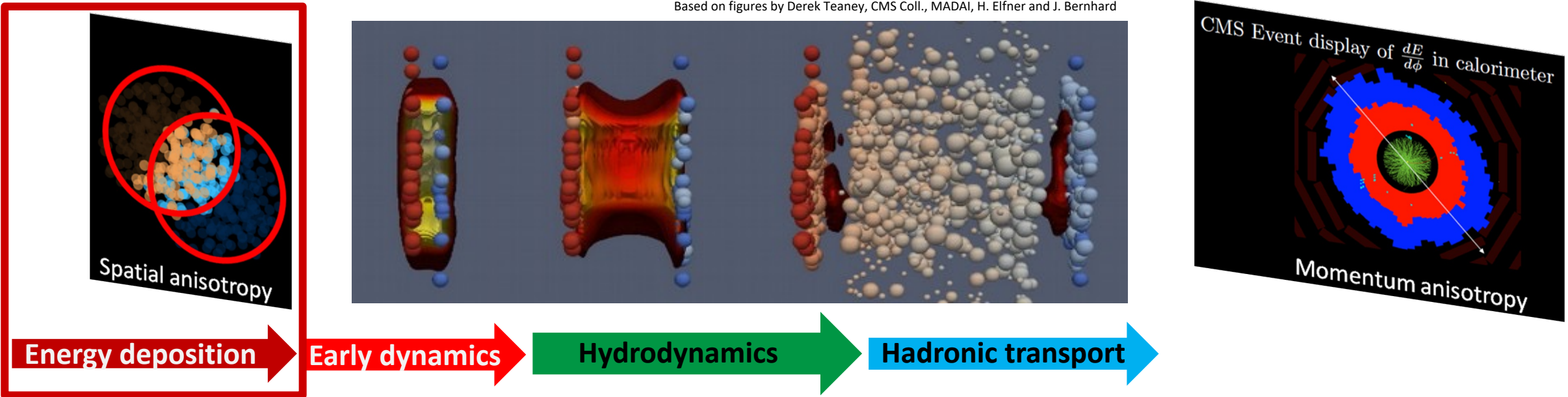


Trade-off in emulation with closure tests



Observable: transverse anisotropy

Based on figures by Derek Teaney, CMS Coll., MADAI, H. Elfner and J. Bernhard



Transverse initial energy density:

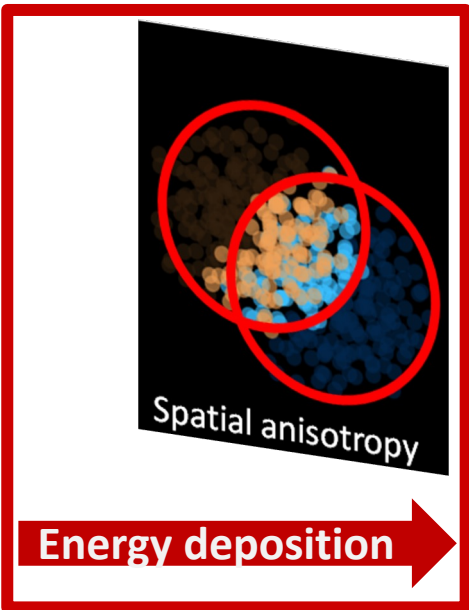
$$\varepsilon_n e^{in\Phi_n} = \frac{\int_0^\infty dr r \int_0^{2\pi} d\phi r^n \varepsilon(r, \phi) e^{in\phi}}{\int_0^\infty dr r \int_0^{2\pi} d\phi r^n \varepsilon(r, \phi)}$$

$$\langle \varepsilon_n \rangle = \frac{1}{M_{\text{ev}}} \sum_{j=1}^{M_{\text{ev}}} \varepsilon_n \{\text{event } j\}$$

Transverse momentum distribution of hadrons:

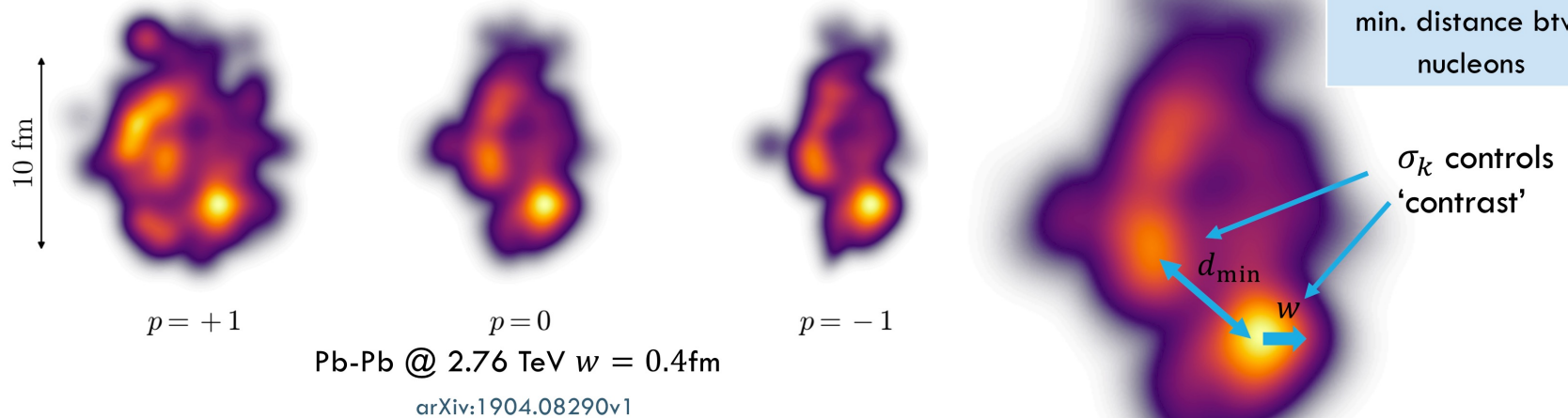
$$\frac{dN}{d\phi} = \frac{N}{2\pi} \left[1 + 2 \sum_n v_n \cos(n(\phi - \Phi_n)) \right]$$

Observable: transverse anisotropy



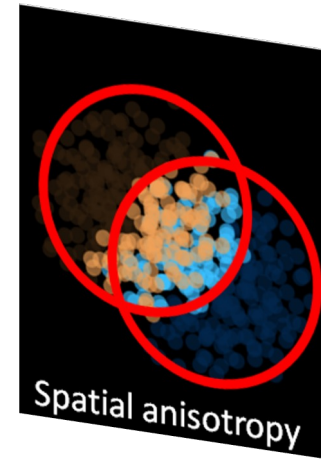
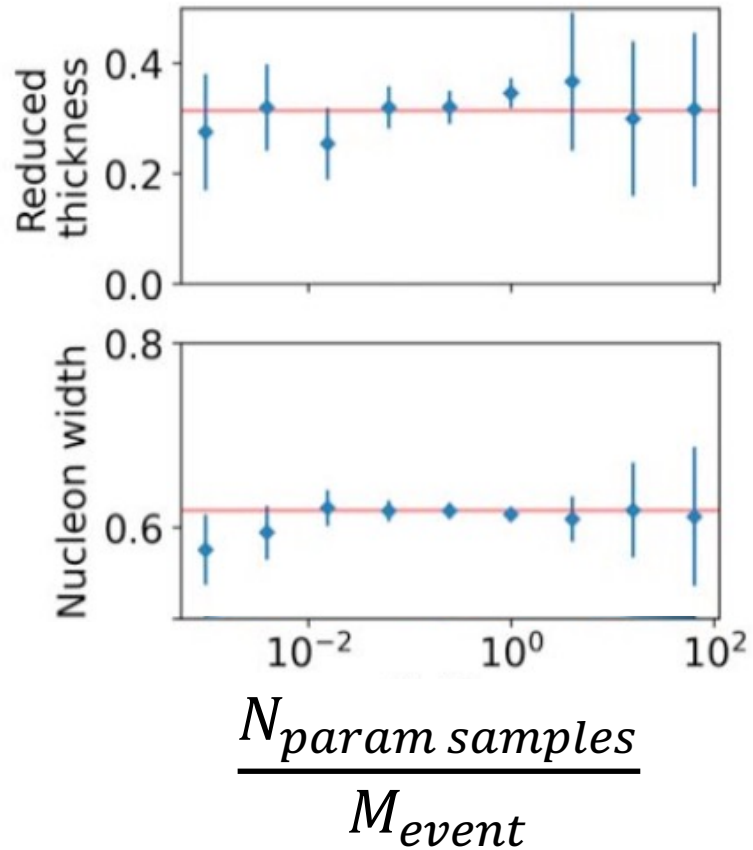
INITIAL ENERGY DEPOSITION (TRENTO)

Parameterization for energy deposition at $\tau = 0^+$



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

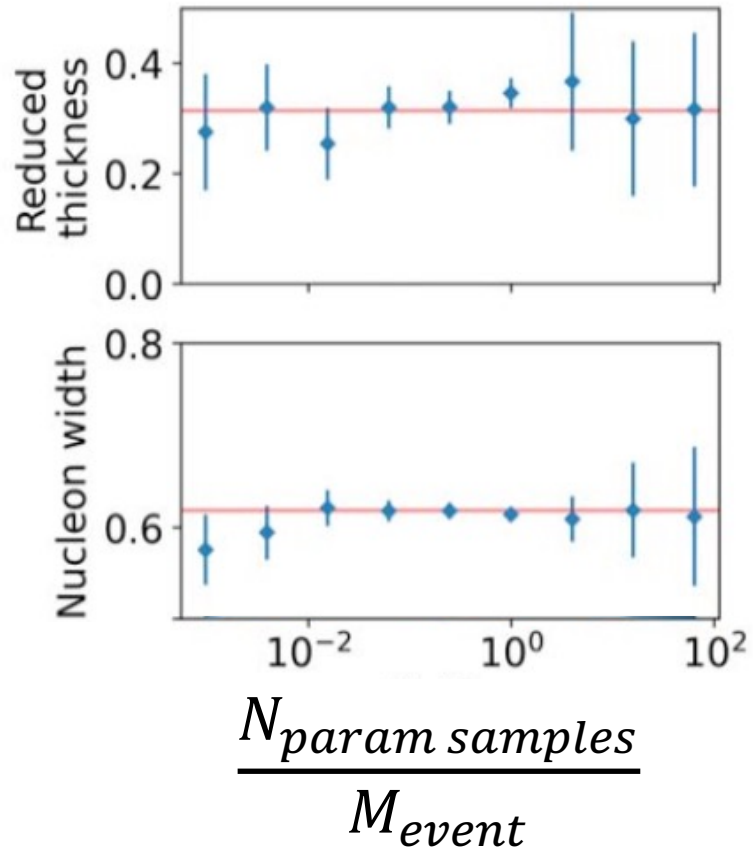
Results with two observables and two parameters



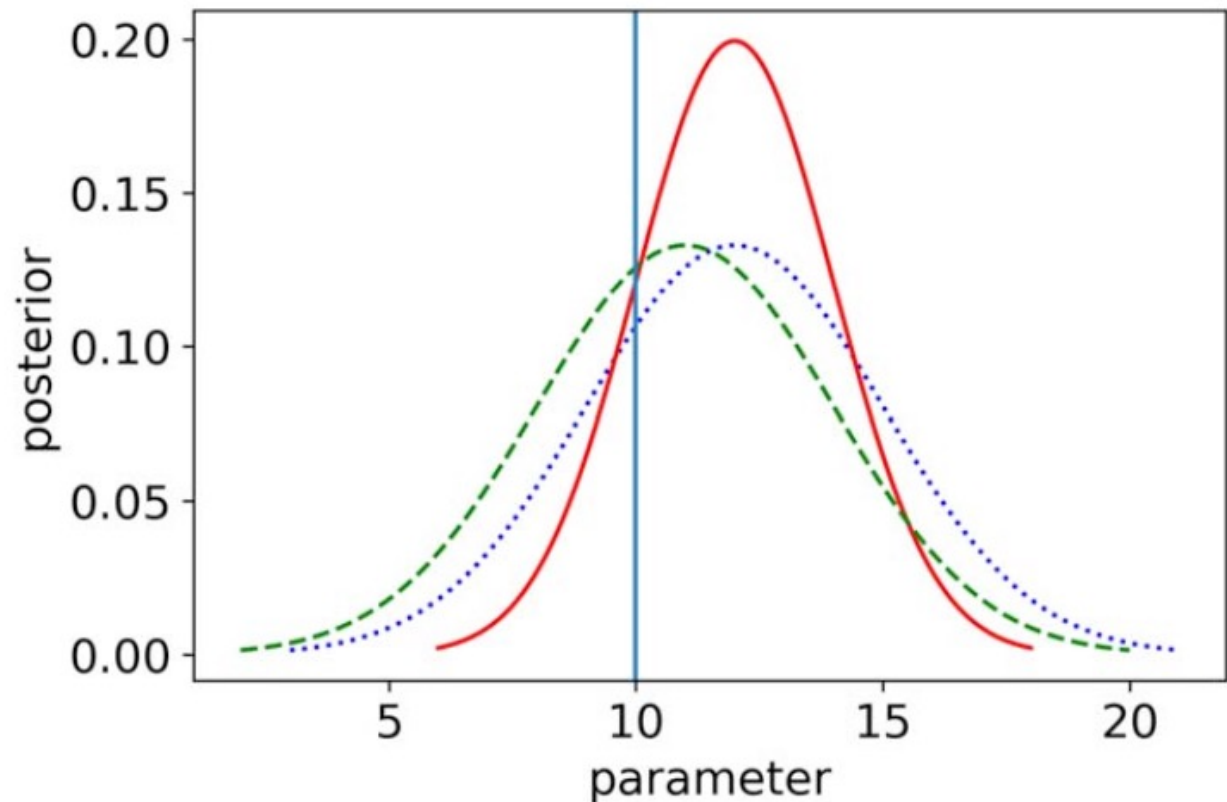
$$\varepsilon_n e^{in\Phi_n} = \frac{\int_0^\infty dr r \int_0^{2\pi} d\phi r^n \varepsilon(r, \phi) e^{in\phi}}{\int_0^\infty dr r \int_0^{2\pi} d\phi r^n \varepsilon(r, \phi)}$$

$$\langle \varepsilon_n \rangle = \frac{1}{M_{ev}} \sum_{j=1}^{M_{ev}} \varepsilon_n \{ \text{event } j \}$$

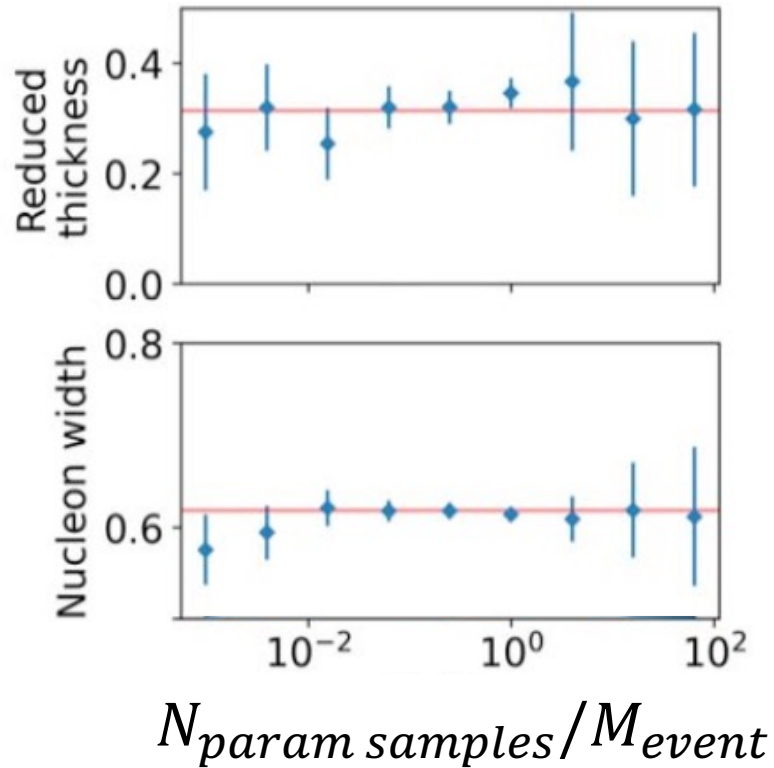
Results with two observables and two parameters



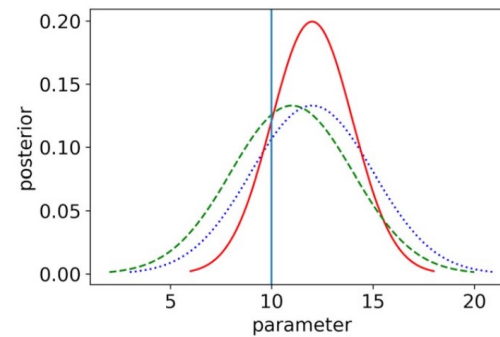
- Quantifying closure:
 - Value of posterior at true value of parameters



Results with two observables and two parameters

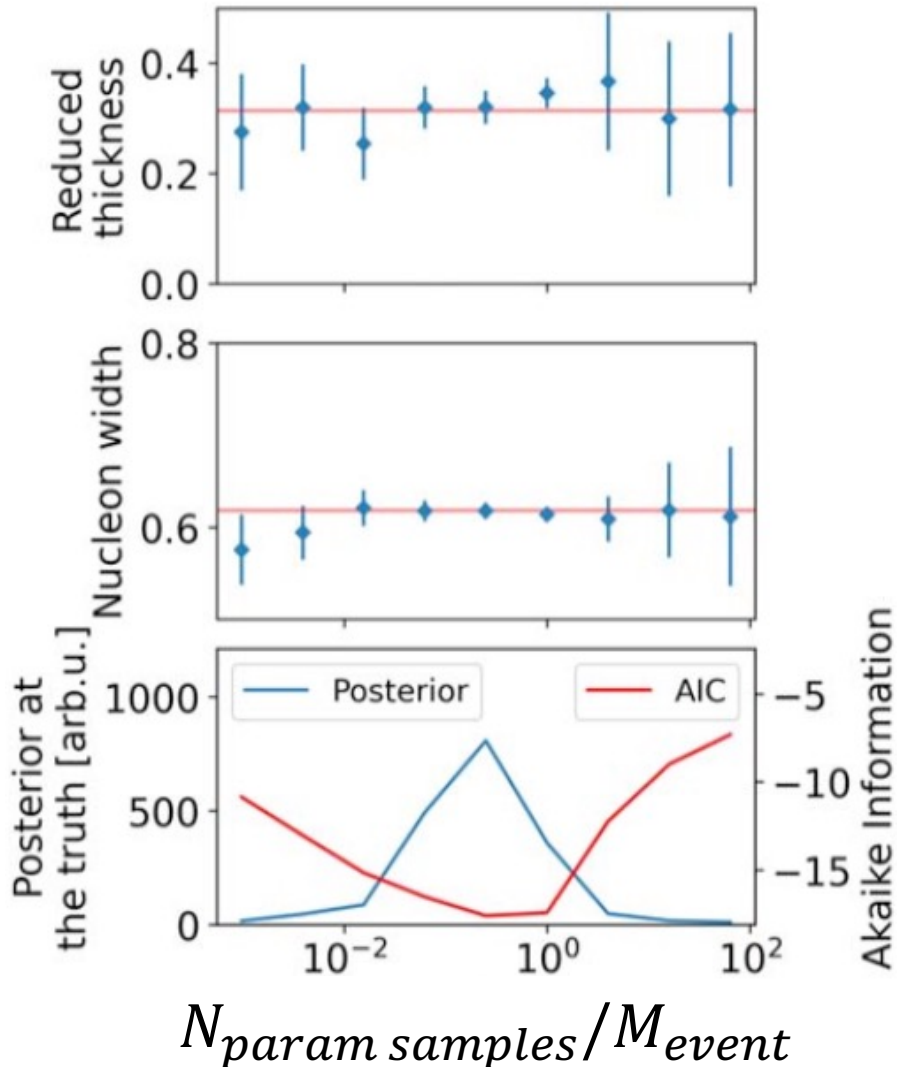


- Quantifying closure:
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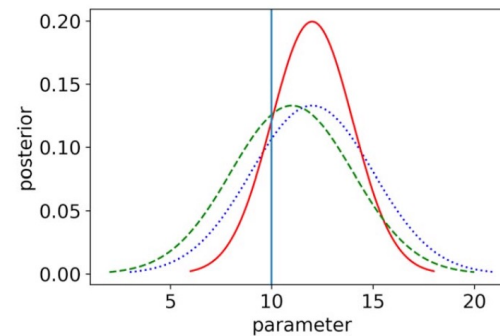


- Akaike information criterion
 - $= -2 \ln \text{Likelihood}_{max} + 2$ (number of model parameters)
 - Used for model comparison

Results with two observables and two parameters



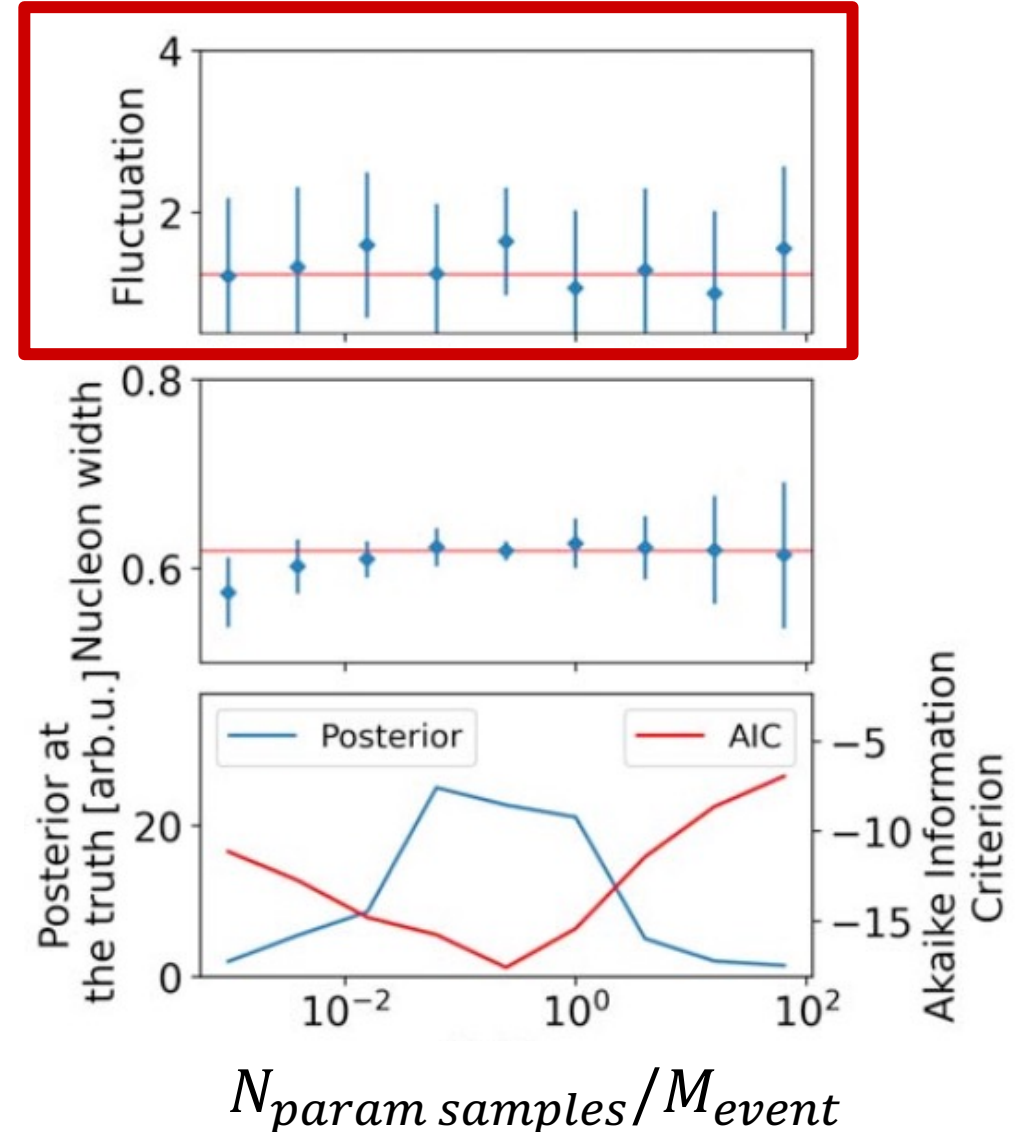
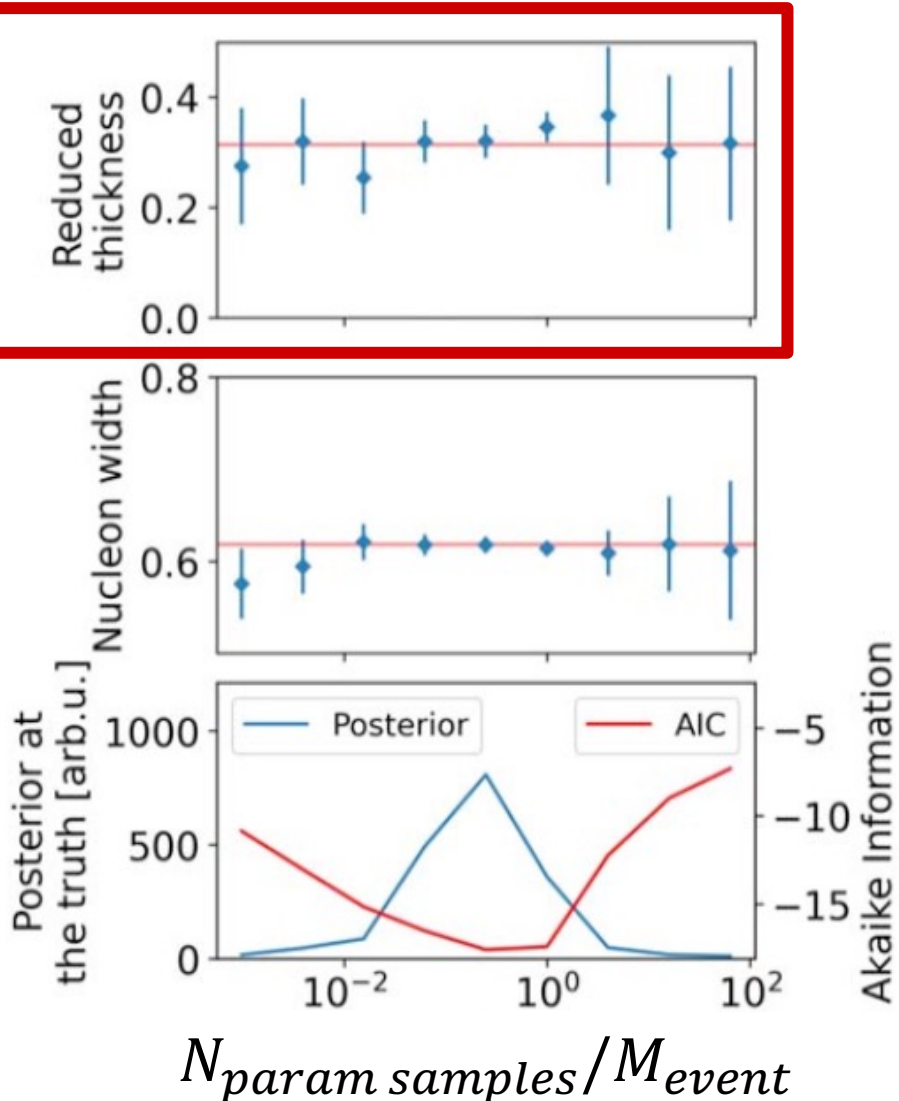
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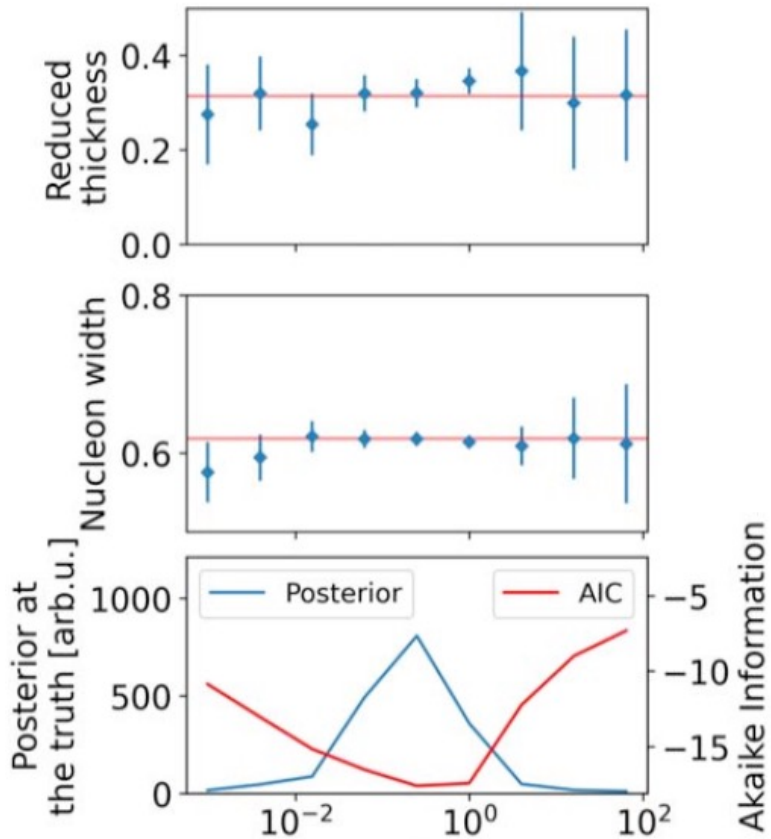
- Akaike information criterion
 - $= -2 \ln L_{max} + 2$ (*number of model parameters*)
 - Used for model comparison

Best use of budget (best constraints) when
 $N_{param\ samples}/M_{event} \sim 0.1 - 1$

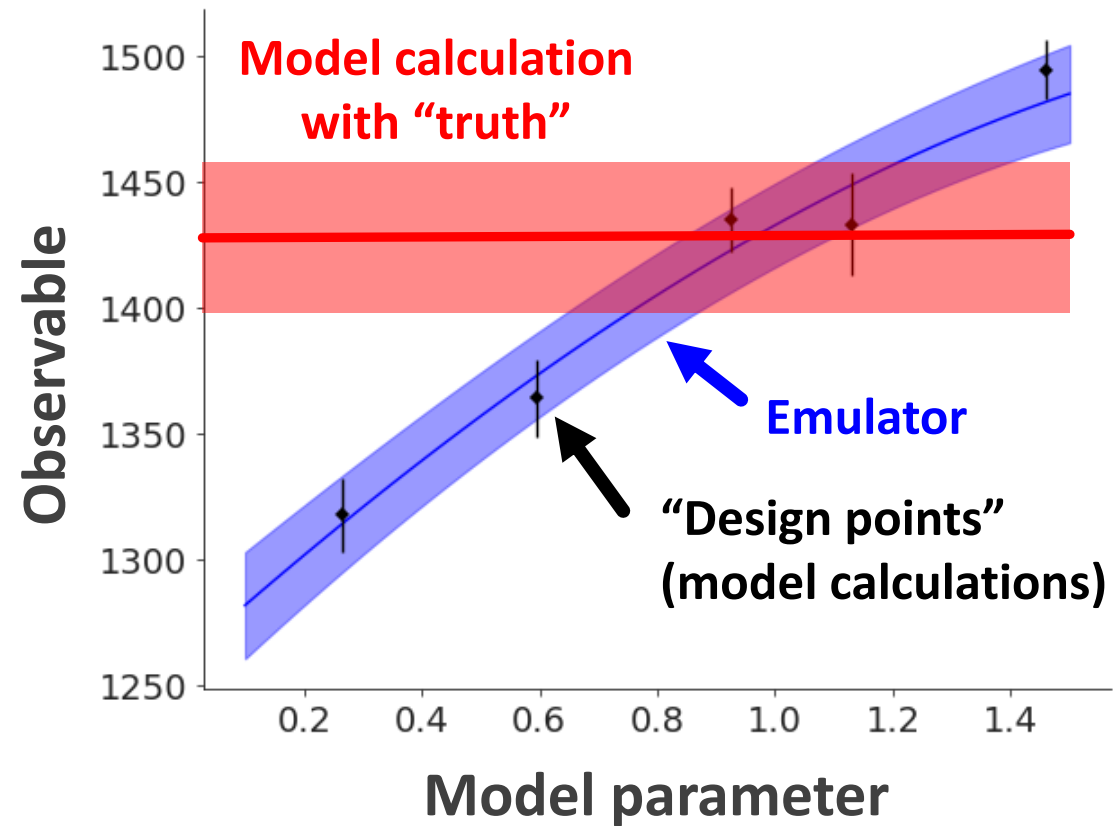
2 observables, 2 parameters (changing params)



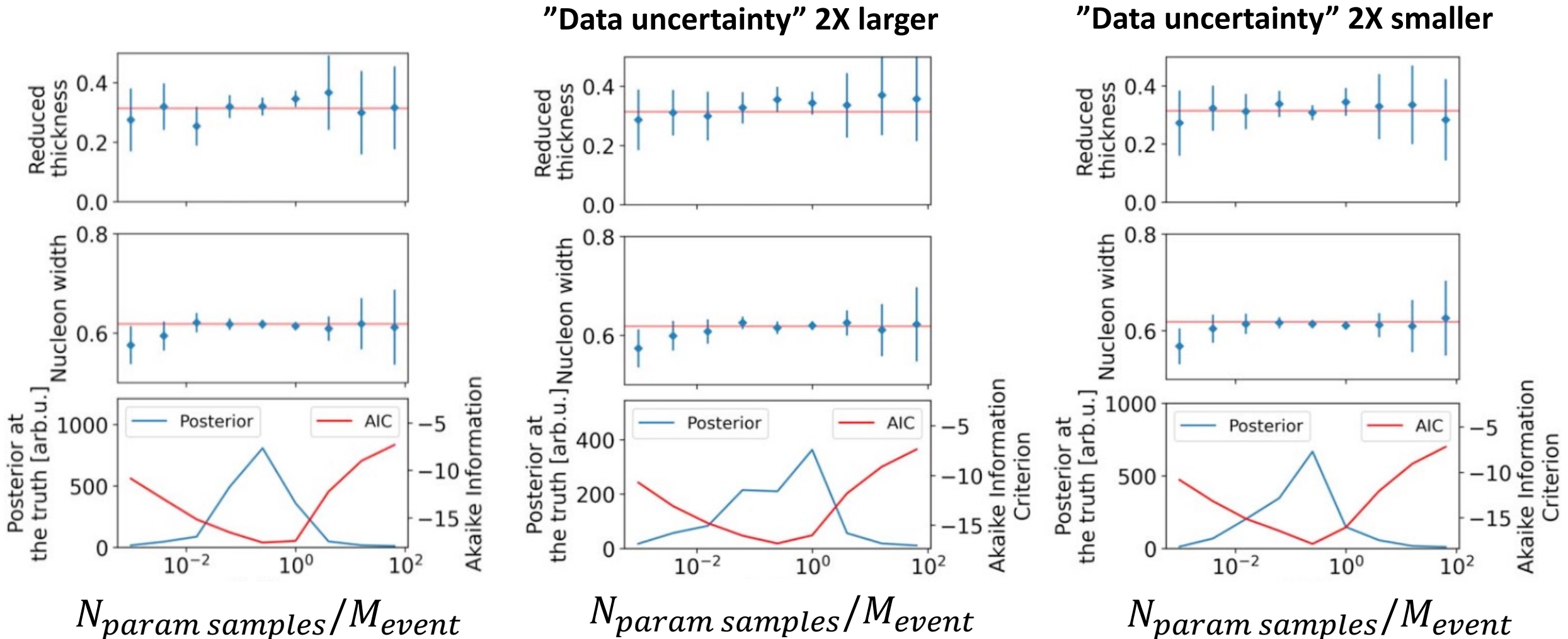
2 observables, 2 params (changing uncert. of “data”)



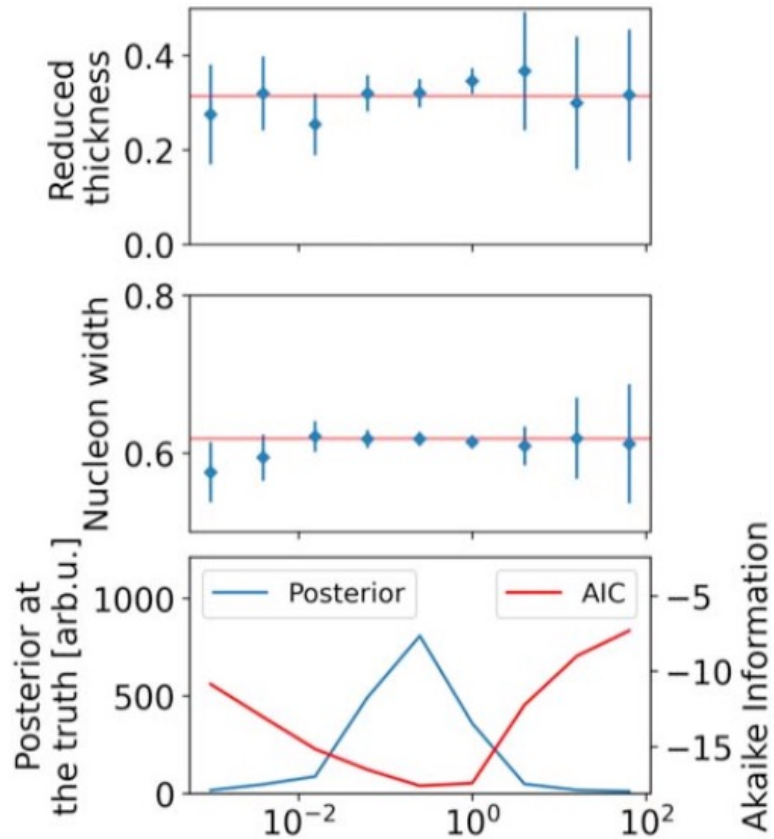
$N_{param\ samples} / M_{event}$



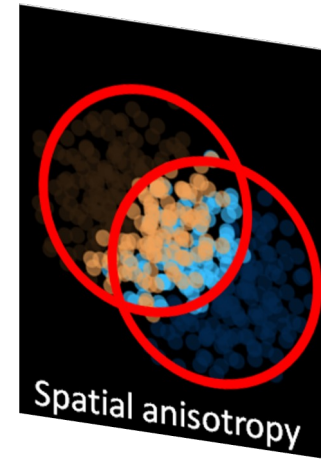
2 observables, 2 params (changing uncert. of “data”)



2/3/4 observables, 2 params (changing # of observables)



$N_{param\ samples} / M_{event}$

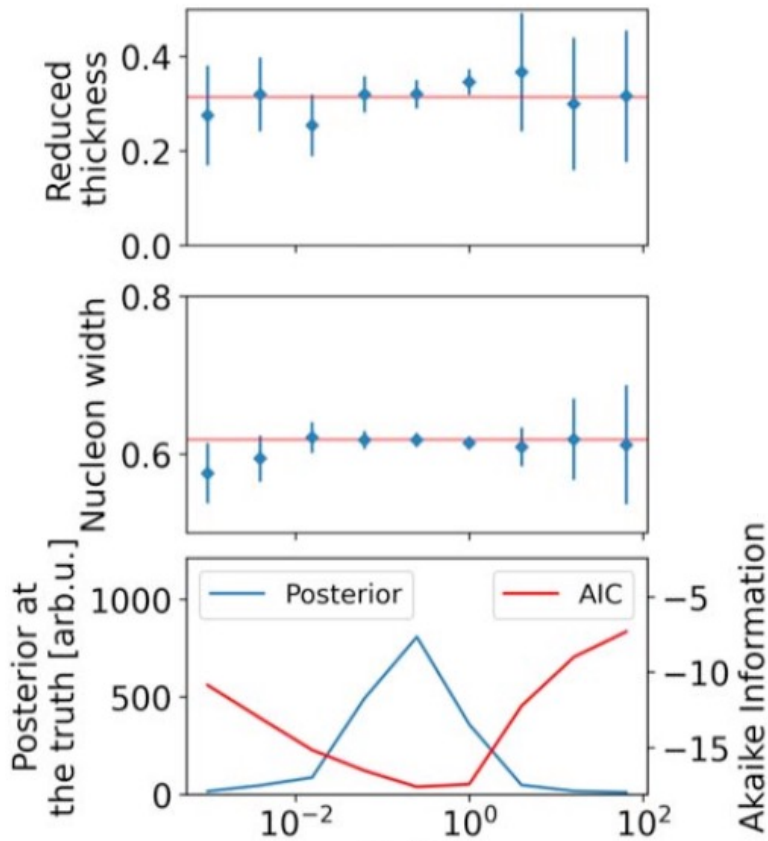


$$\varepsilon_n e^{in\Phi_n} = \frac{\int_0^\infty dr r \int_0^{2\pi} d\phi r^n \varepsilon(r, \phi) e^{in\phi}}{\int_0^\infty dr r \int_0^{2\pi} d\phi r^n \varepsilon(r, \phi)}$$

$$\langle \varepsilon_n \rangle = \frac{1}{M_{ev}} \sum_{j=1}^{M_{ev}} \varepsilon_n \{ \text{event } j \}$$

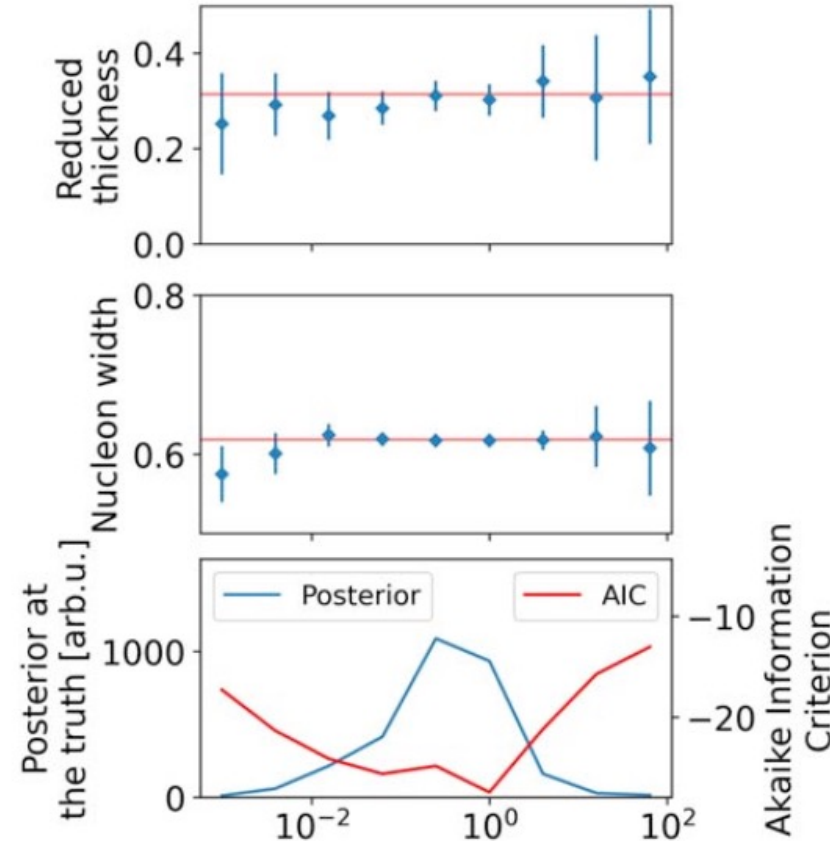
2/3/4 observables, 2 params (changing # of observables)

2 observables



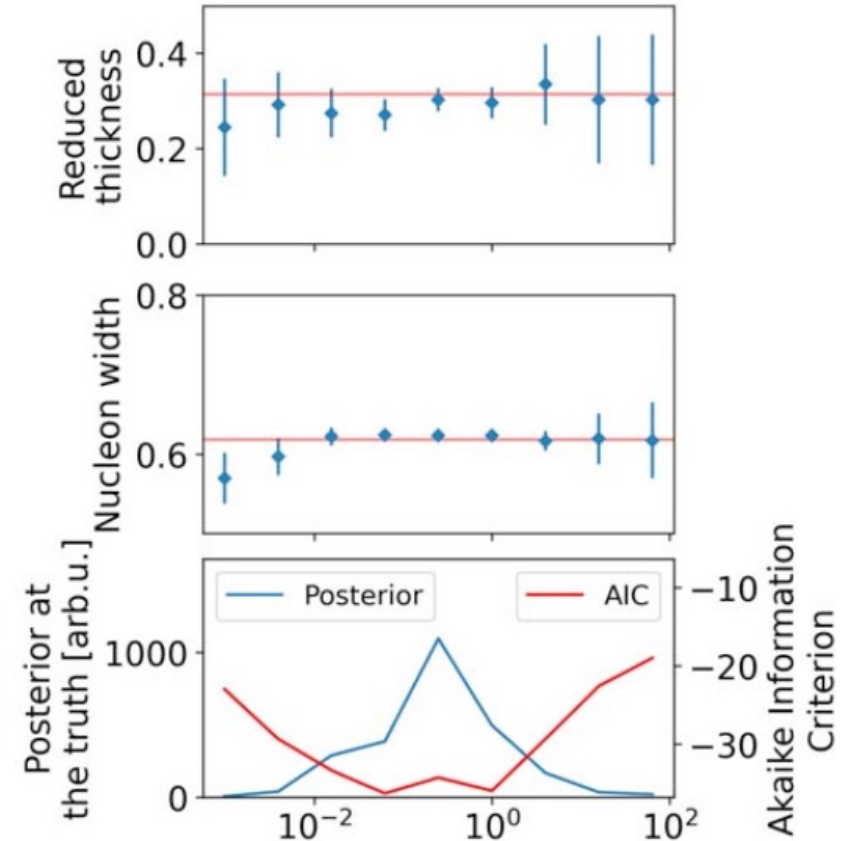
$N_{param\ samples} / M_{event}$

3 observables



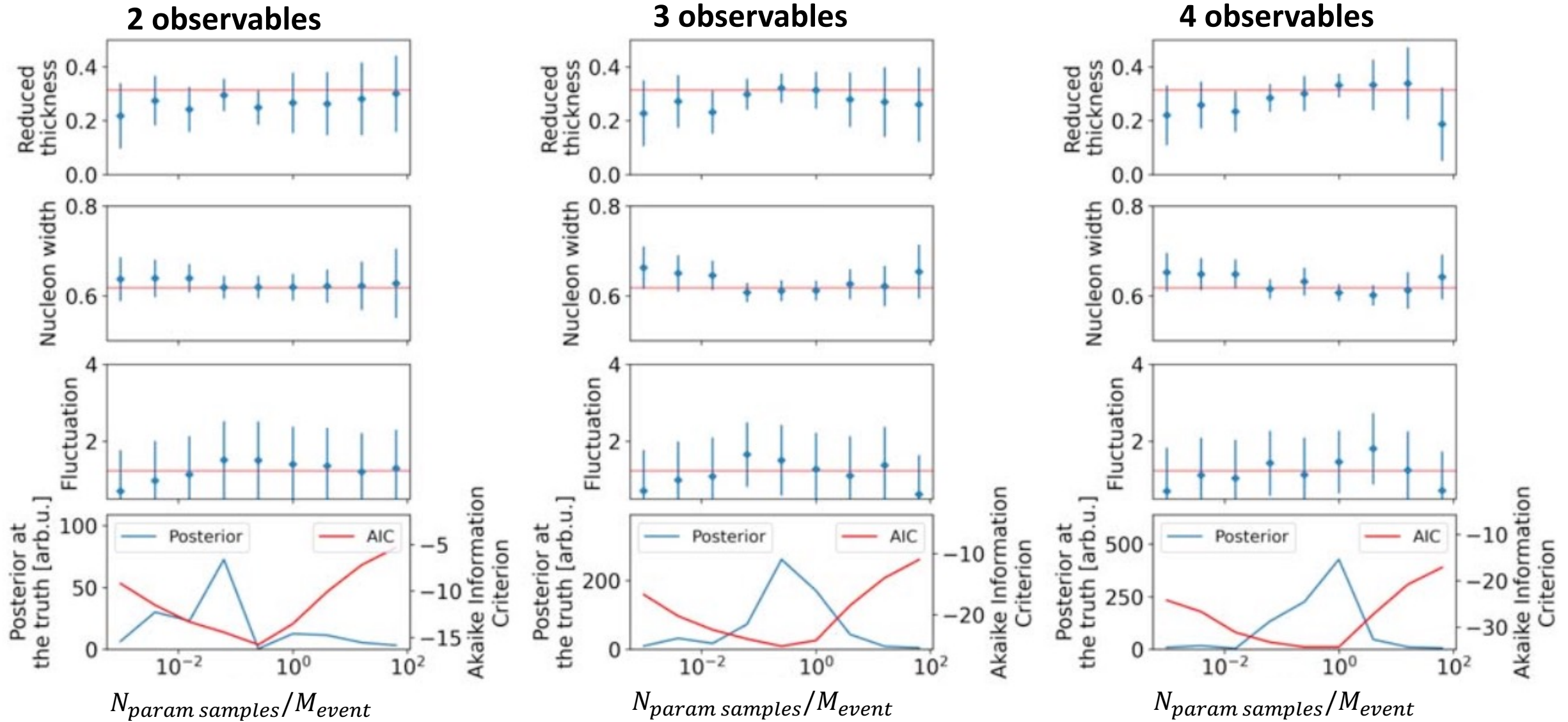
$N_{param\ samples} / M_{event}$

4 observables

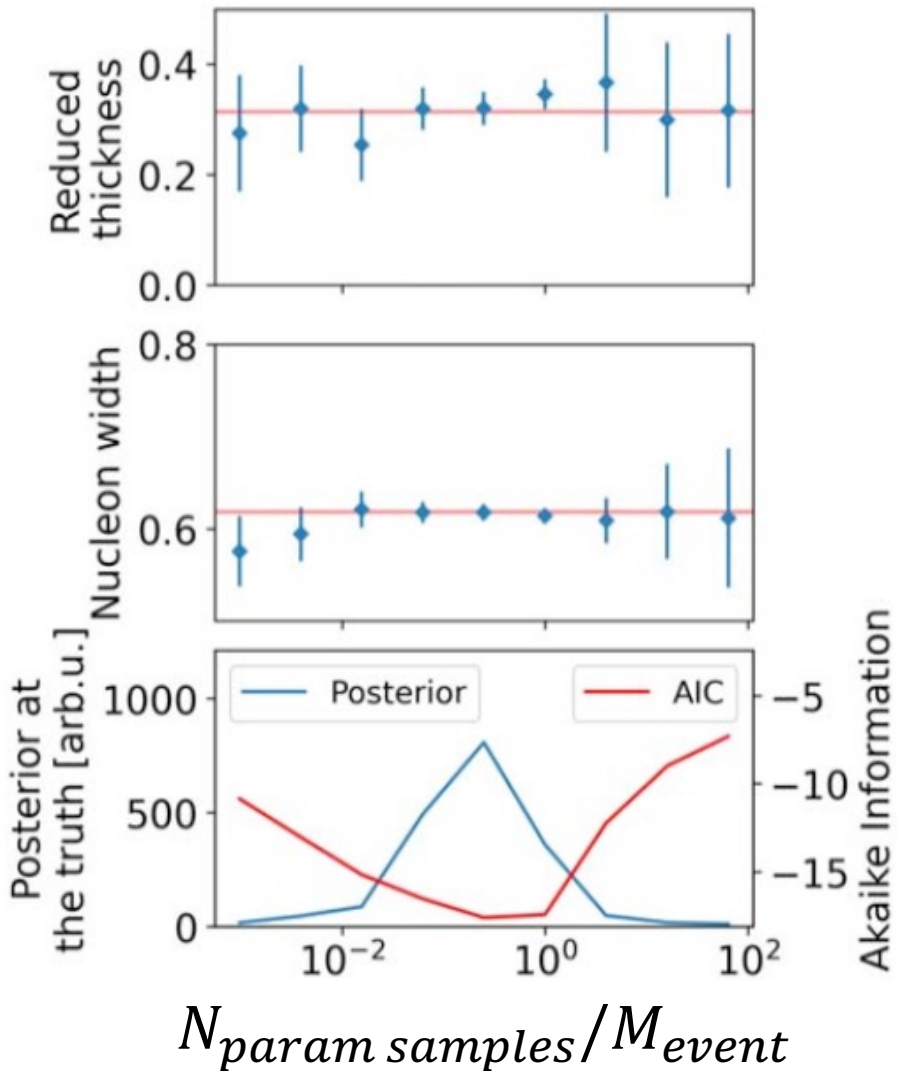


$N_{param\ samples} / M_{event}$

2/3/4 observables, 3 params (changing # of observables)



Analysis

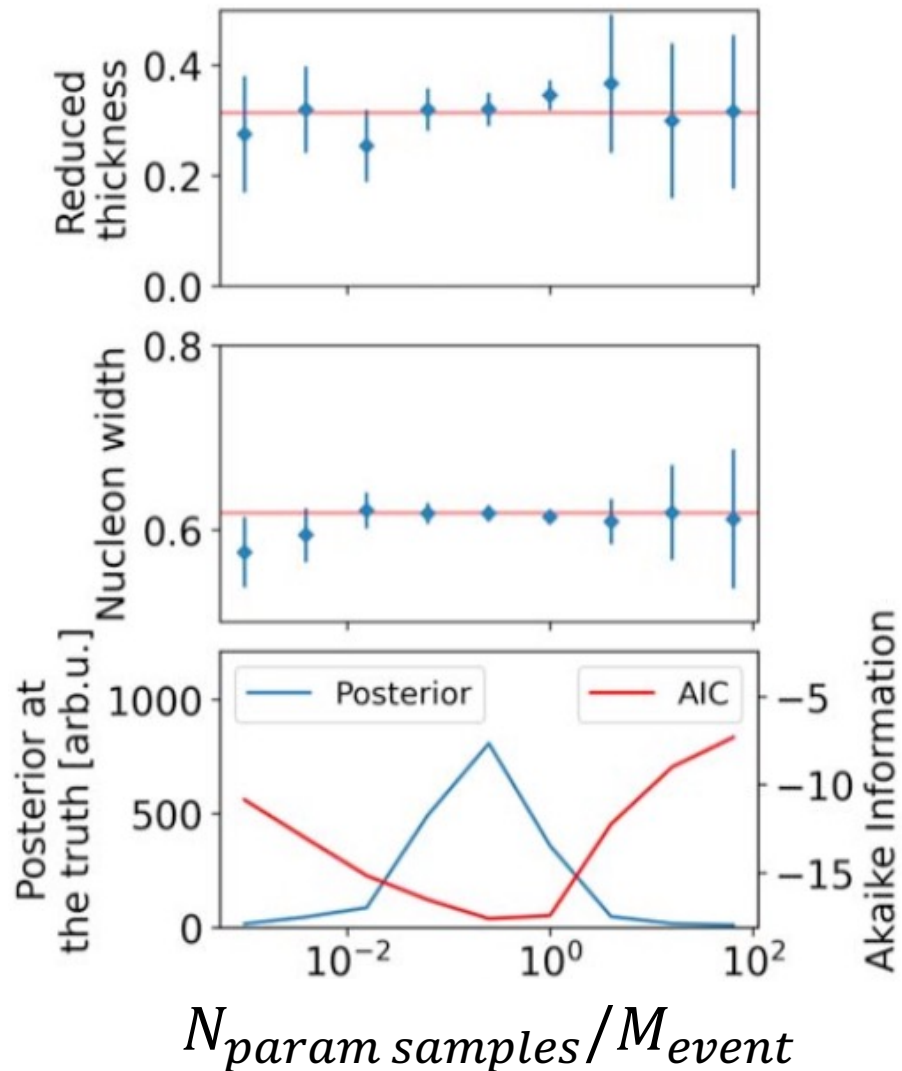


- Best use of budget (best constraints) when $N_{param\ samples}/M_{event} \sim 0.1 - 1$

or

$$N_{param\ samples}^{optimal?} \approx 0.25-1 \sqrt{\underbrace{M_{event} \times N_{param\ samples}}_{\text{Budget}}}$$

Analysis



- Best use of budget (best constraints) when $N_{param\ samples}/M_{event} \sim 0.1 - 1$

or

$$N_{param\ samples}^{optimal?} \approx 0.25-1 \sqrt{\underbrace{M_{event} \times N_{param\ samples}}_{\text{Budget}}}$$

- What had been used by contemporary publications?

- $N_{param\ samples} \sim 10^3$

- $M_{event} \sim 10^3 - 10^5$ (some 10^6)

- So $N_{param\ samples}/M_{event} \sim 0.01 - 1$

(overprioritizing statistical uncertainty over interpolation uncertainty?)

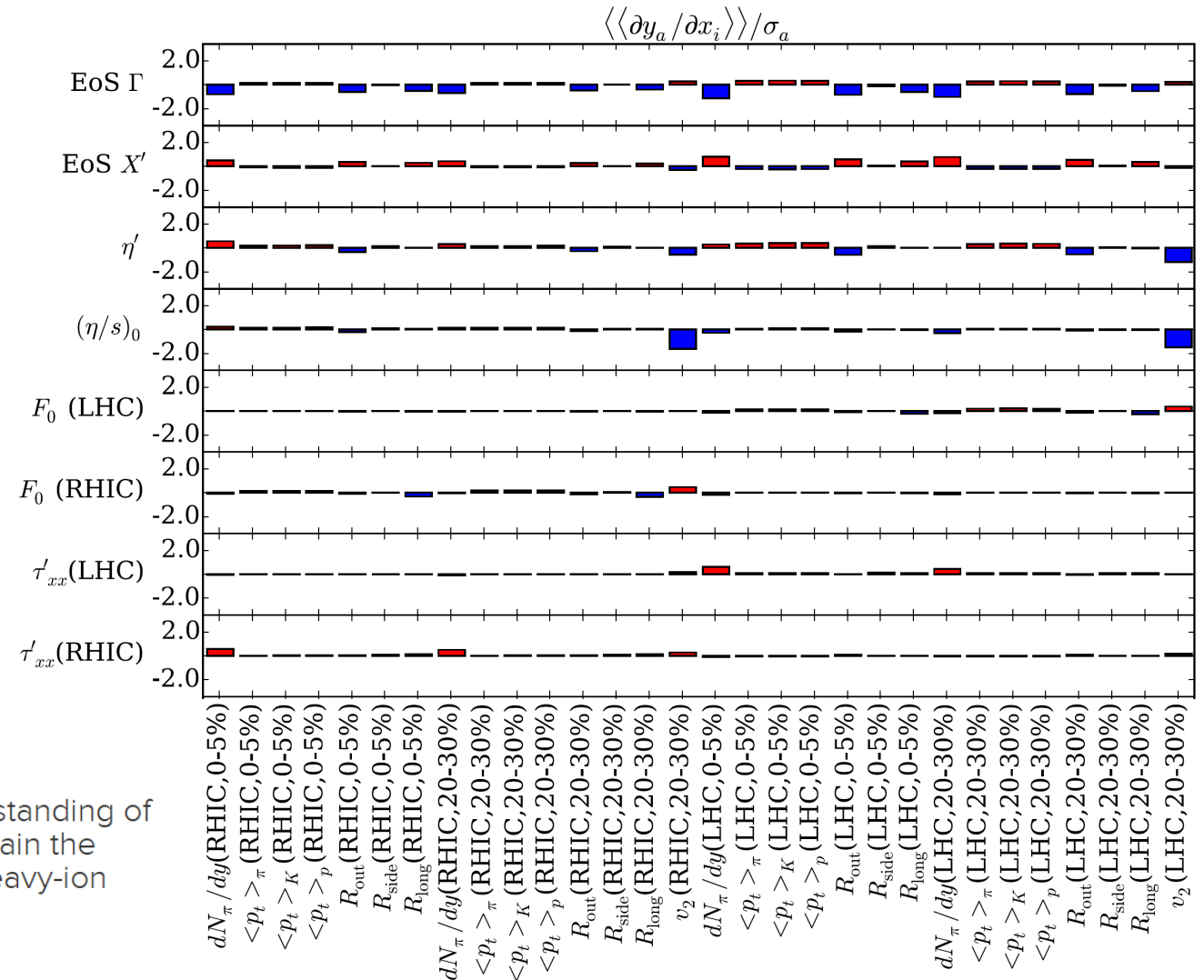
Analysis

- Does this generalize?

Depends on:

- Accuracy of data
- Sensitivity of observables to parameters

Model responses of an observable with respect to a given parameter



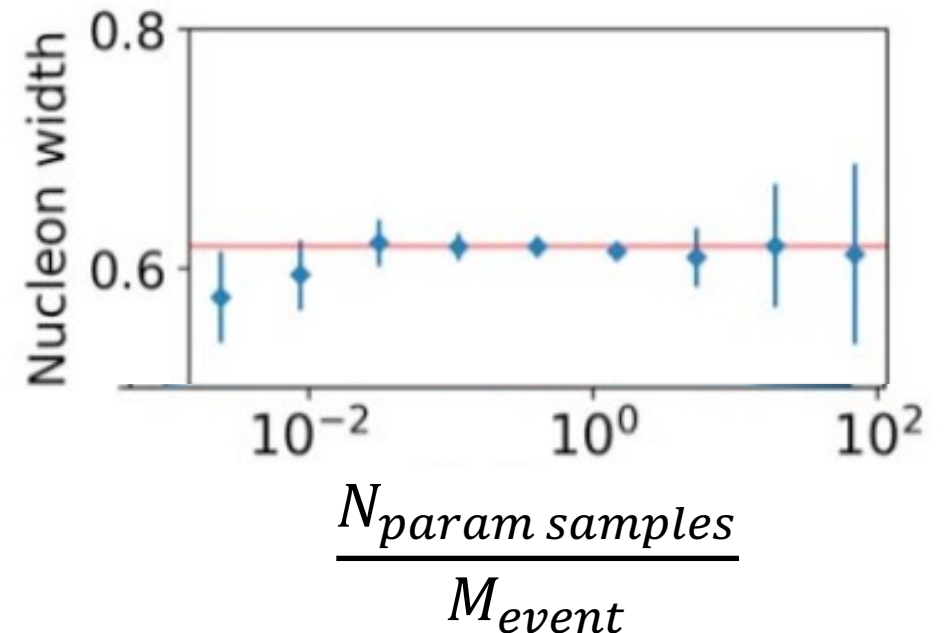
Toward a deeper understanding of how experiments constrain the underlying physics of heavy-ion collisions

Summary

- Stochastic simulations have additional trade-offs when optimizing analyses
- Depends on constraints provided by data on different parameters given model
- We used a simple model to study trade-offs

$$N_{param\ samples}^{optimal?} / M_{event} \sim 0.1 - 1$$

$$N_{param\ samples}^{optimal?} \approx 0.25-1 \sqrt{budget}$$



QUESTIONS?

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Computational budget optimization for Bayesian parameter estimation in heavy-ion collisions

Brandon Weiss¹ , Jean-François Paquet^{1,2}  and Steffen A Bass¹ 

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[arXiv:2301.08385]

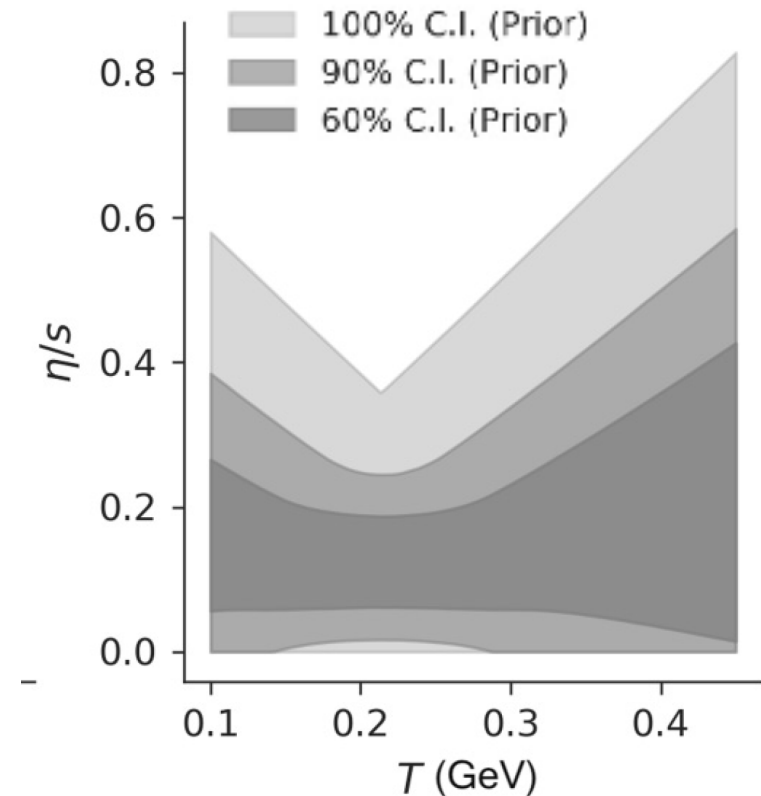
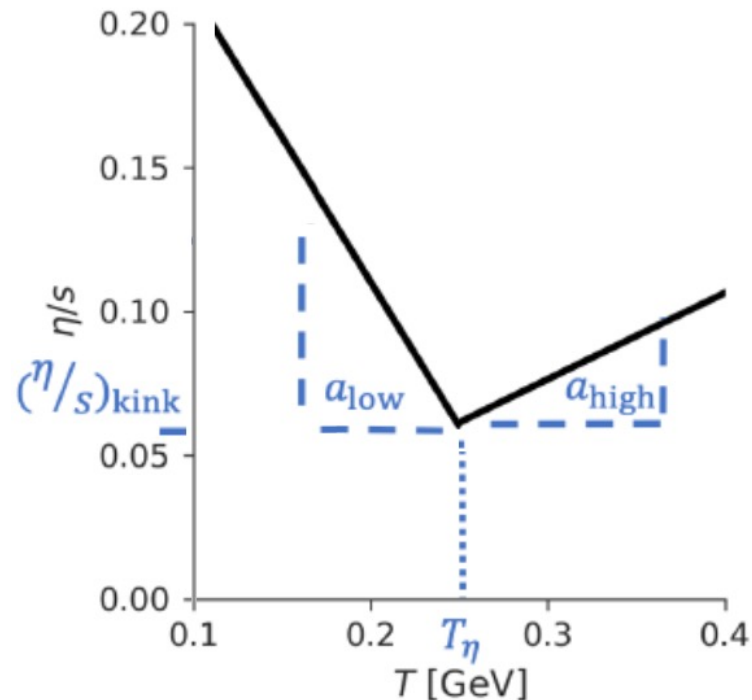


BACKUP



Prior: example for the shear viscosity $\eta/s(T)$

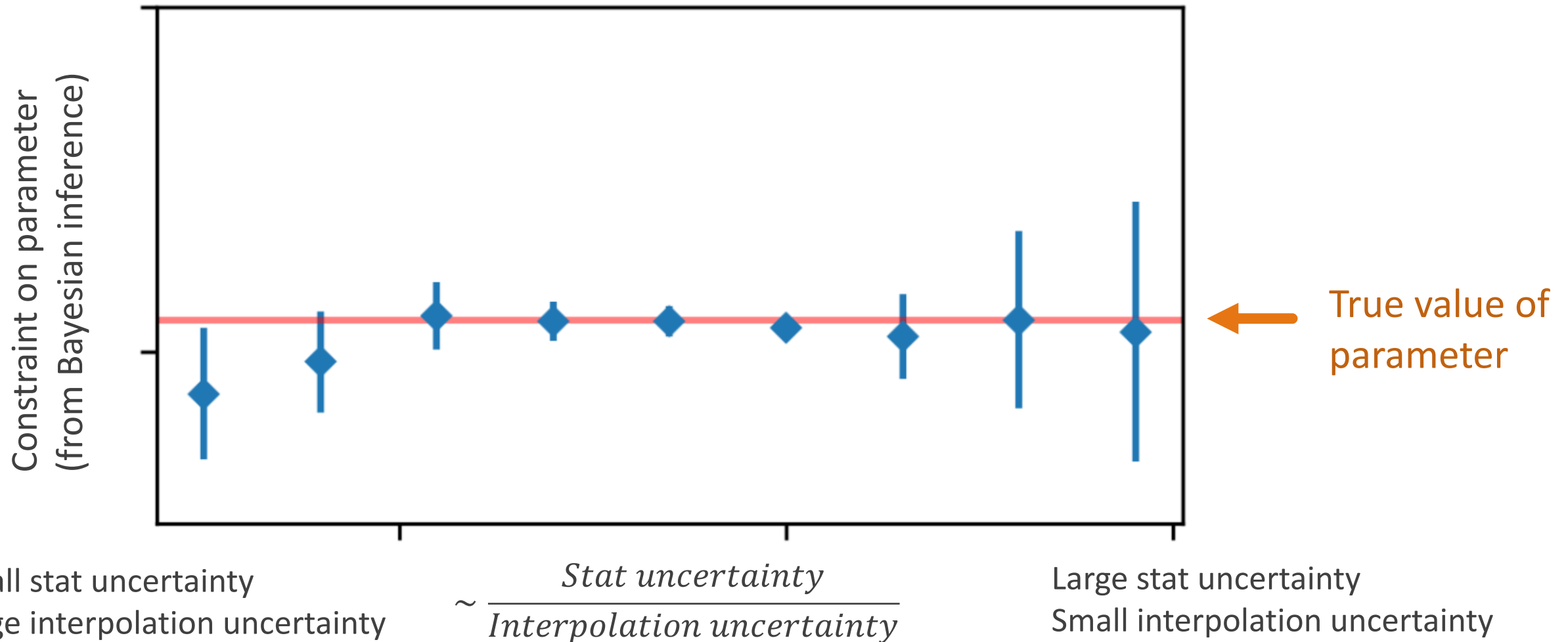
- Positive definite; continuous function of temperature T (at zero chemical potential)
- Large values may be excluded by model self-consistency, causality, ...
- Theoretical constraints? Self-consistency across model stages?
- Guidance from other substances (minimum near crossover)



Uncertainty optimization

Weiss et al (2023)
[arXiv:2301.08385]

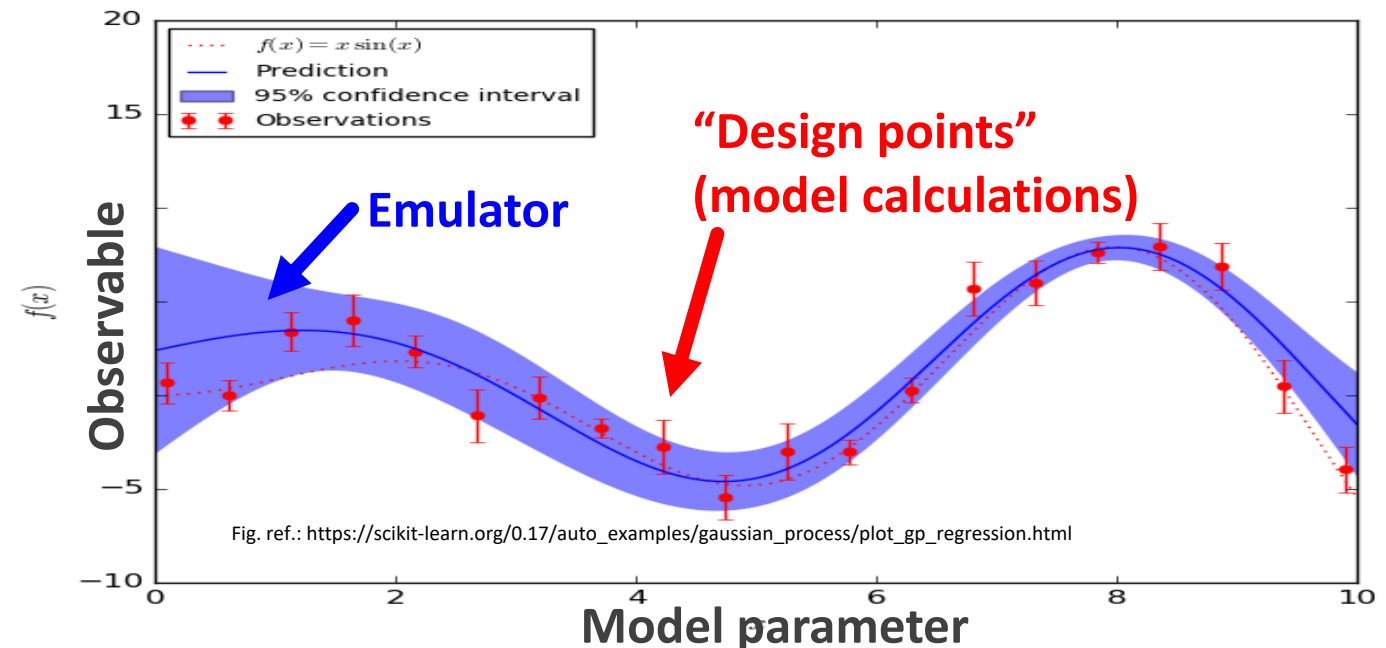
Model is stochastic (need to average over large number of collisions)



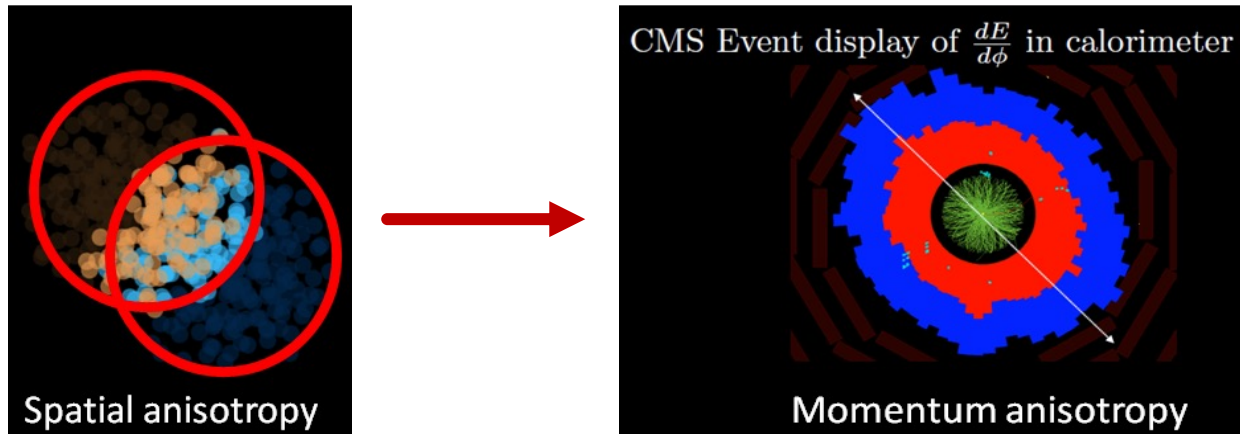
Emulation

$$\text{posterior}(\overrightarrow{\text{param}}) \propto \text{prior}(\overrightarrow{\text{param}}) \times \exp\left(-\frac{1}{2} (\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{\text{D}})^T \text{Covar}^{-1} (\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{\text{D}})\right)$$

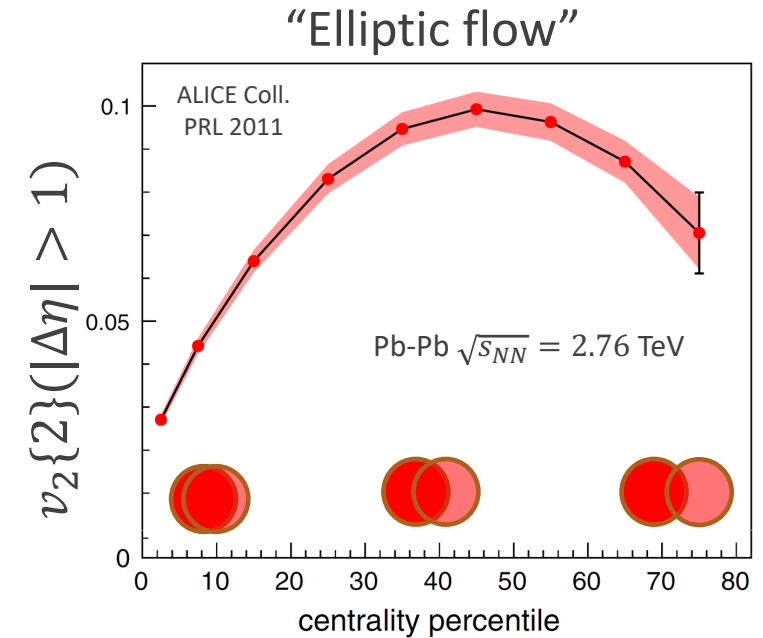
- Posterior is high-dimensional, and we cannot sample it easily for all values of the parameters
 - Option A: compute the posterior at a sample of model parameters and interpolate
 - Option B: compute the model's prediction at a sample of model parameters and interpolate



From impact geometry to momentum anisotropy



Based on figures by Derek Teaney, CMS Coll., MADAI, H. Elfner and J. Bernhard



- Spatial anisotropy from partial overlap of nuclei & fluctuation
- Interactions transfer spatial anisotropy into momentum one
- Rapid development of momentum anisotropies consistent with strongly-coupled system

Applications of emulation and Bayesian methods in heavy-ion physics

Jean-François Paquet

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Model-data comparison

- Experimental uncertainties lead to uncertainties on the model parameters
- Constraints from Bayesian inference:

$$\text{posterior}(\overrightarrow{\text{param}}) \propto \exp\left(-\frac{1}{2} \left(\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{D} \right)^T \text{Covariance}^{-1} \left(\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{D} \right)\right)$$

↑
Probabilistic constraints on parameters

↑
Prediction of model for given set of model parameters

↑
Covariance matrix (includes experimental uncertainties and their correlations)

↑
Mean value of data

If observables are uncorrelated:

$$\text{Covariance}^{-1} = \begin{bmatrix} \sigma_{d_1}^{-2} & 0 & 0 \\ 0 & \sigma_{d_2}^{-2} & 0 \\ 0 & 0 & \dots \end{bmatrix}$$

Bayes' theorem

- Experimental uncertainties lead to uncertainties on the model parameters
- Constraints from Bayesian inference:

$$\text{posterior}(\vec{\text{param}}) \propto \text{prior}(\vec{\text{param}}) \times \exp\left(-\frac{1}{2}(\vec{\text{Model}}(\vec{\text{param}}) - \vec{D})^T \text{Covar}^{-1}(\vec{\text{Model}}(\vec{\text{param}}) - \vec{D})\right)$$

Bayes theorem:

$$\text{prob}(d) \times \text{prob}(p|d) = \text{prob}(p, d) = \text{prob}(p) \times \text{prob}(d|p)$$

$$\text{Evidence} \times \text{Posterior} = \text{Joint} = \text{Prior} \times \text{Likelihood}$$

[how likely are
parameters given data]

[how likely are data
given parameters]

Note: Bayes' theorem says nothing about choice of likelihood function

Bayes' theorem, prior and iterative constraints

- Constraints from Bayesian inference:

$$\text{posterior}(\overrightarrow{\text{param}}) \propto \text{prior}(\overrightarrow{\text{param}}) \times \exp\left(-\frac{1}{2}(\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{\text{D}})^T \text{Covar}^{-1}(\overrightarrow{\text{Model}}(\overrightarrow{\text{param}}) - \overrightarrow{\text{D}})\right)$$

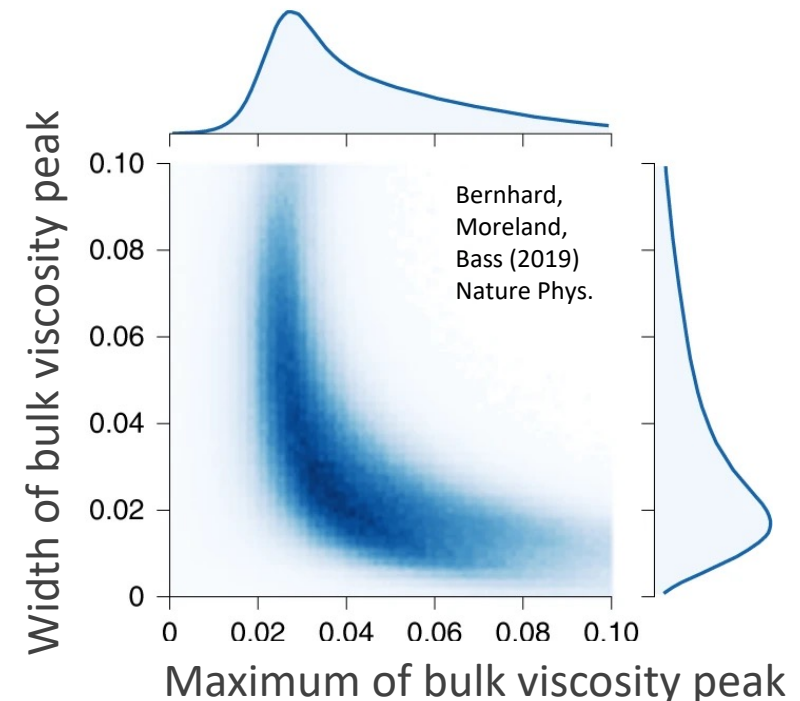
- In theory: posterior from one Bayesian inference (with data set #1) becomes prior for the next (with data set #2)
- In practice:
 - Models are being improved
 - Re-use of previous posteriors has been rare
- Note: prior should be independent of set of data currently being compared to

Model-data comparison

- Experimental uncertainties lead to uncertainties on the model parameters
- Constraints from Bayesian inference:

$$\text{posterior}(\vec{\text{param}}) \propto \text{prior}(\vec{\text{param}}) \times \exp\left(-\frac{1}{2}(\vec{\text{Model}}(\vec{\text{param}}) - \vec{D})^T \text{Covar}^{-1}(\vec{\text{Model}}(\vec{\text{param}}) - \vec{D})\right)$$

- Posterior has the dimension of the number of parameters
- Marginalized posterior: integrating posterior over all parameters except “n”



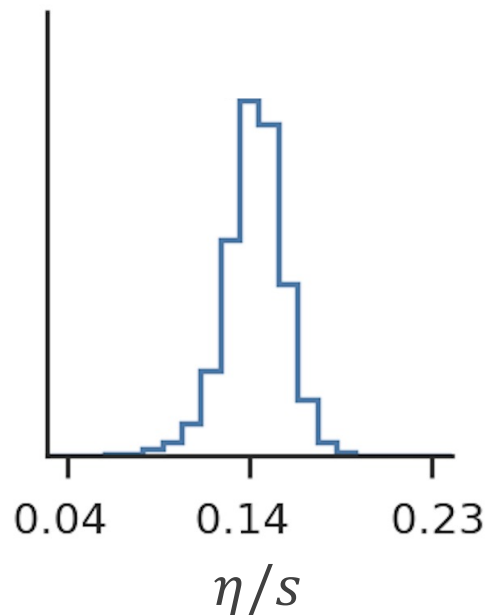
Model-data comparison

- Constraints from Bayesian inference:

$$\text{posterior}(\vec{\text{param}}) \propto \text{prior}(\vec{\text{param}}) \times \exp\left(-\frac{1}{2}(\vec{\text{Model}}(\vec{\text{param}}) - \vec{\text{D}})^T \text{Covar}^{-1}(\vec{\text{Model}}(\vec{\text{param}}) - \vec{\text{D}})\right)$$

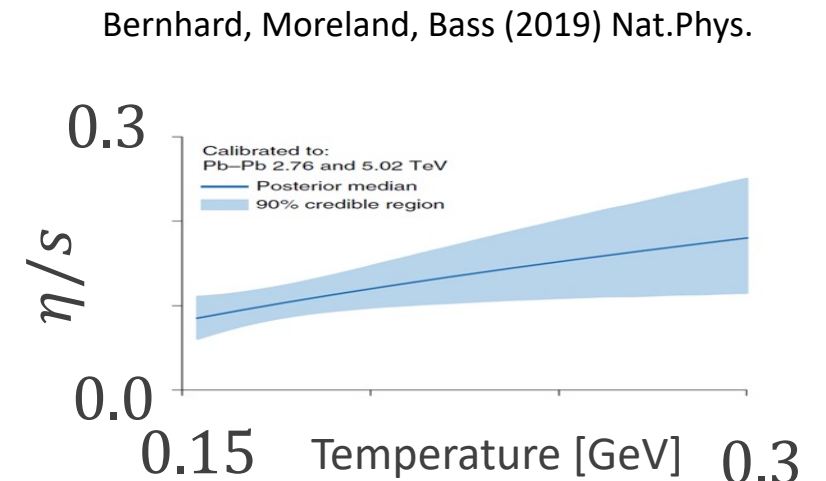
- Marginalized posterior: integrating posterior over all parameters except 1 or 2 or ...

$$\text{Marg. posterior}\left(\frac{\eta}{s}\right) = \int d(\text{initial cond. parameters})d(\text{bulk viscosity param})d(\dots) \text{posterior}(\vec{\text{param}})$$



←
If roughly
independent
of
temperature

→
If temperature
dependent



Different analyses = different constraints

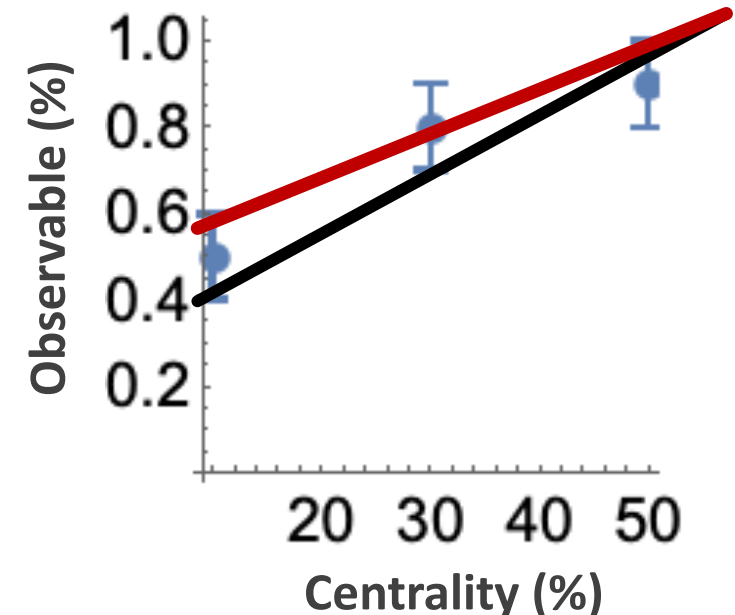
- Use different data sets
- Different modelling assumptions:
 - Hydrodynamics
 - Initial conditions
 - Cooper-Frye
 - Parameters and priors
- Treatment of correlations in experimental uncertainties

Experimental uncertainties and covariance matrix

$$\text{posterior}(\vec{\text{param}}) \propto \text{prior}(\vec{\text{param}}) \times \exp \left(-\frac{1}{2} \underbrace{\left(\text{Model}(\vec{\text{param}}) - \vec{D} \right)^T \text{Covar}^{-1} \left(\text{Model}(\vec{\text{param}}) - \vec{D} \right)}_{\text{Covariance matrix}} \right)$$

$$\begin{bmatrix} (y_1(\vec{p}) - y_1^{\text{expt}}) & (y_2(\vec{p}) - y_2^{\text{expt}}) \end{bmatrix} \underbrace{\left(\text{Covariance matrix} \right)^{-1}}_{\text{Covariance matrix}} \begin{bmatrix} (y_1(\vec{p}) - y_1^{\text{expt}}) \\ (y_2(\vec{p}) - y_2^{\text{expt}}) \end{bmatrix}$$

- Uncorrelated uncertainties: (stat. uncert.?) $\text{Cov} = \begin{bmatrix} (\sigma_1^{\text{expt}})^2 & 0 \\ 0 & (\sigma_2^{\text{expt}})^2 \end{bmatrix}$
- Fully-correlated uncertainties: (normalization uncert.?) $\text{Cov} = (\sigma^{\text{expt}})^2 \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$
- Partly-correlated uncertainties: (systematic uncert.?) $\text{Cov} = \begin{bmatrix} (\sigma_1^{\text{expt}})^2 & \text{Cov}(1,2) \\ \text{Cov}(2,1) & (\sigma_2^{\text{expt}})^2 \end{bmatrix}$



Uncertainties and covariance matrix

$$\text{posterior}(\vec{\text{param}}) \propto \text{prior}(\vec{\text{param}}) \times \exp\left(-\frac{1}{2} \underbrace{(\vec{\text{Model}}(\vec{\text{param}}) - \vec{\text{D}})^T \text{Covar}^{-1} (\vec{\text{Model}}(\vec{\text{param}}) - \vec{\text{D}})}\right)$$

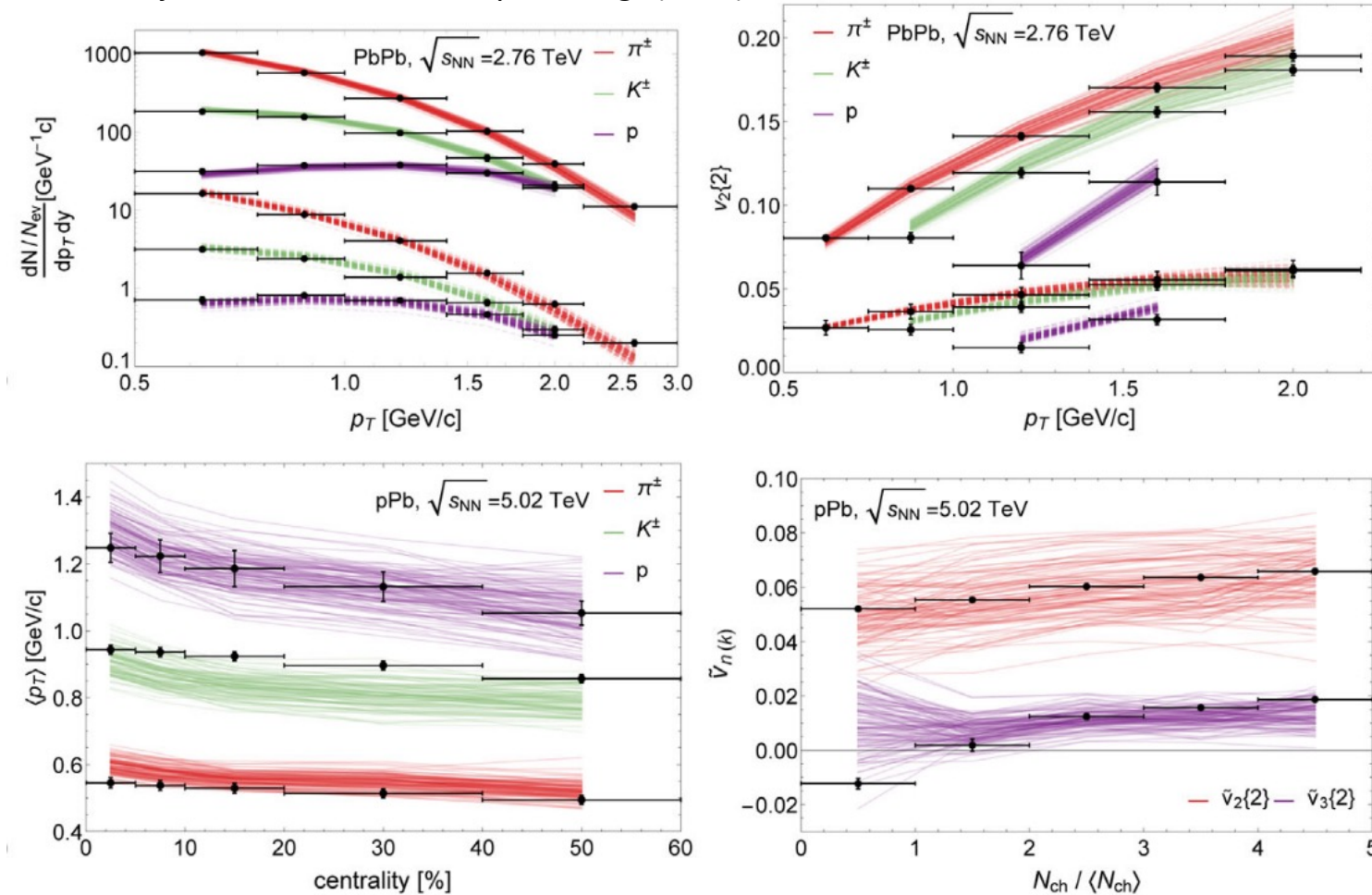
$$\begin{bmatrix} (y_1(\vec{p}) - y_1^{\text{expt}}) & (y_2(\vec{p}) - y_2^{\text{expt}}) \end{bmatrix} \underbrace{(\text{Covariance matrix})^{-1}} \begin{bmatrix} (y_1(\vec{p}) - y_1^{\text{expt}}) \\ (y_2(\vec{p}) - y_2^{\text{expt}}) \end{bmatrix}$$

$$\begin{aligned} \text{Covariance matrix} = & \begin{bmatrix} (\sigma_1^{\text{expt,uncorr}})^2 & 0 \\ 0 & (\sigma_2^{\text{expt,uncorr}})^2 \end{bmatrix} + (\sigma^{\text{expt,fully corr}})^2 \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} + \\ & \begin{bmatrix} (\sigma_1^{\text{expt,corr}})^2 & \text{cov}(1,2) \\ \text{cov}(2,1) & (\sigma_2^{\text{expt,corr}})^2 \end{bmatrix} + \\ & (\text{emulator covariance}) + (\text{model statistical uncertainty}) \end{aligned}$$

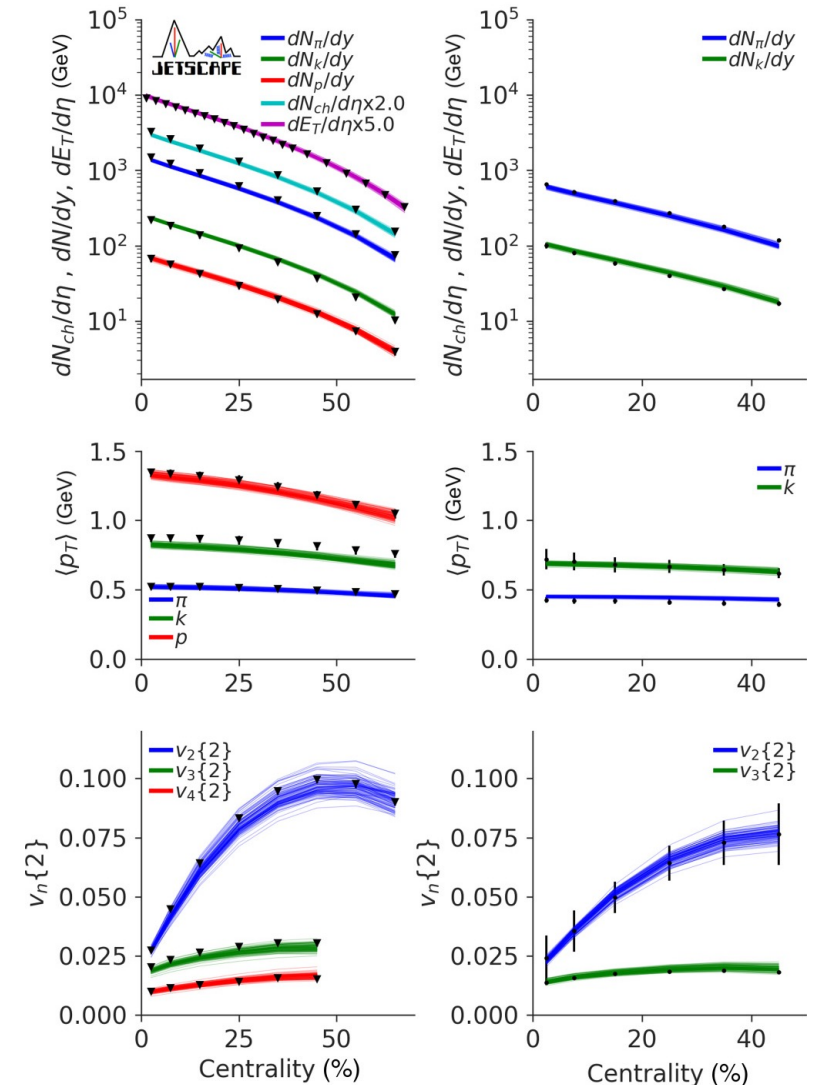
Hydrodynamic-based simulations of heavy ion collisions

- Successful in describing broad sets of measurements

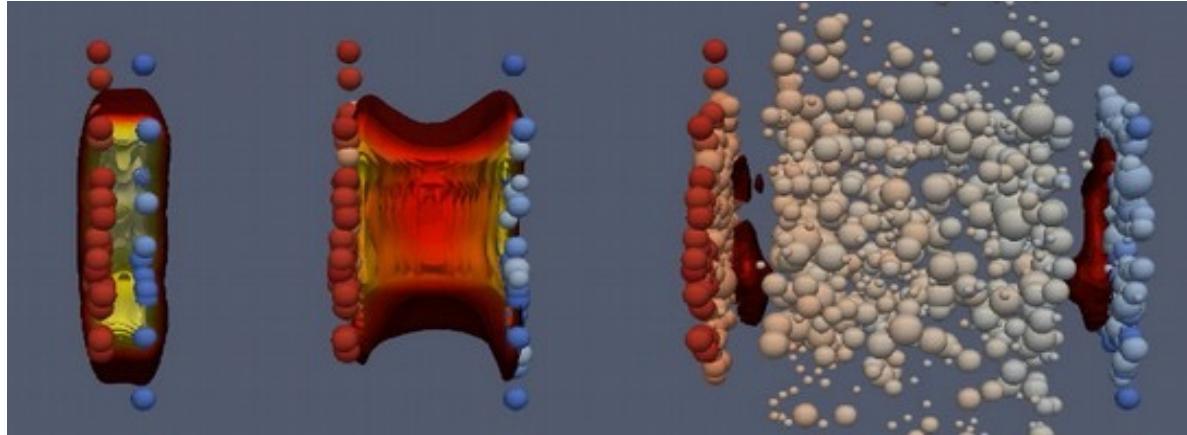
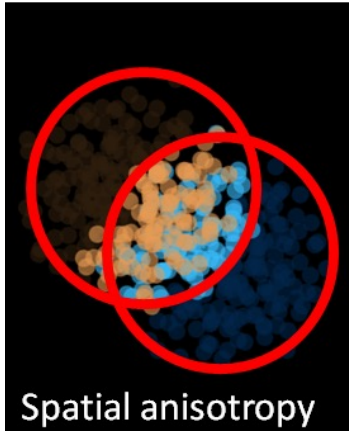
Nijs, van der Schee, Gürsoy, Snellings (2021) PRC, PRL



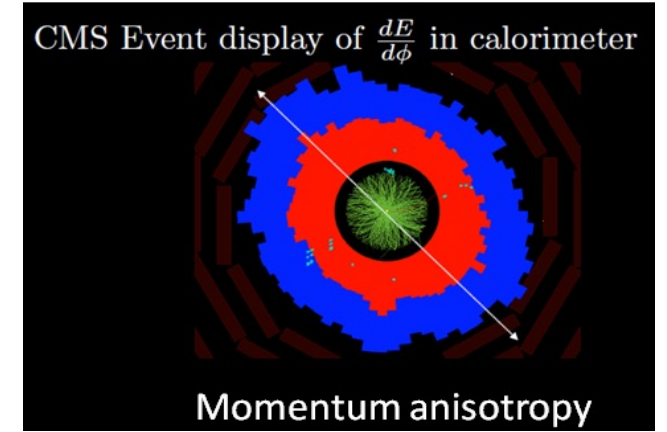
JETSCAPE Collaboration, (2021) PRC, PRL



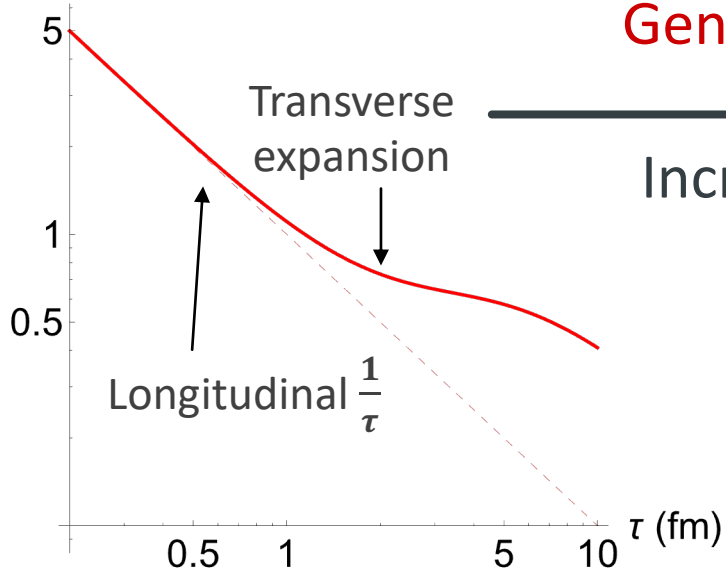
Interaction and expansion



Based on figures by Derek Teaney, CMS Coll., MADAI, H. Elfner and J. Bernhard



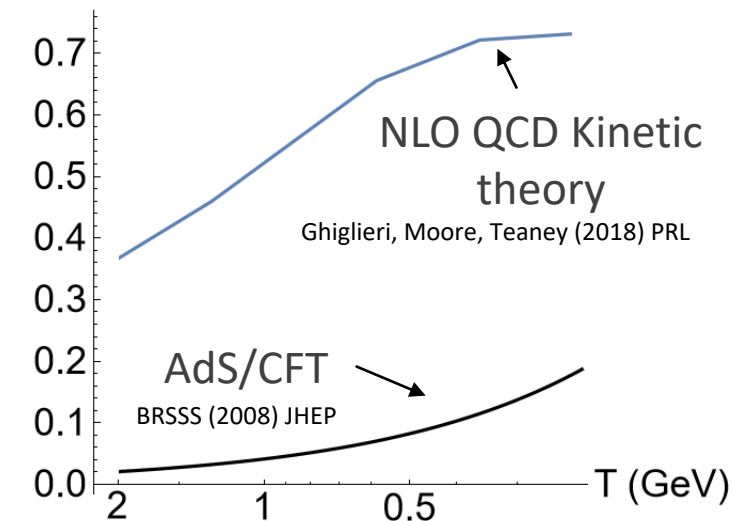
$$\theta = \partial_\nu u^\nu \text{ (1/fm)}$$



General decrease in expansion rate

Increase in local equilibration time (relaxation time)

$$\tau_R \sim (\eta/s)/T \text{ (fm)}$$



Parametrization of the viscosities

