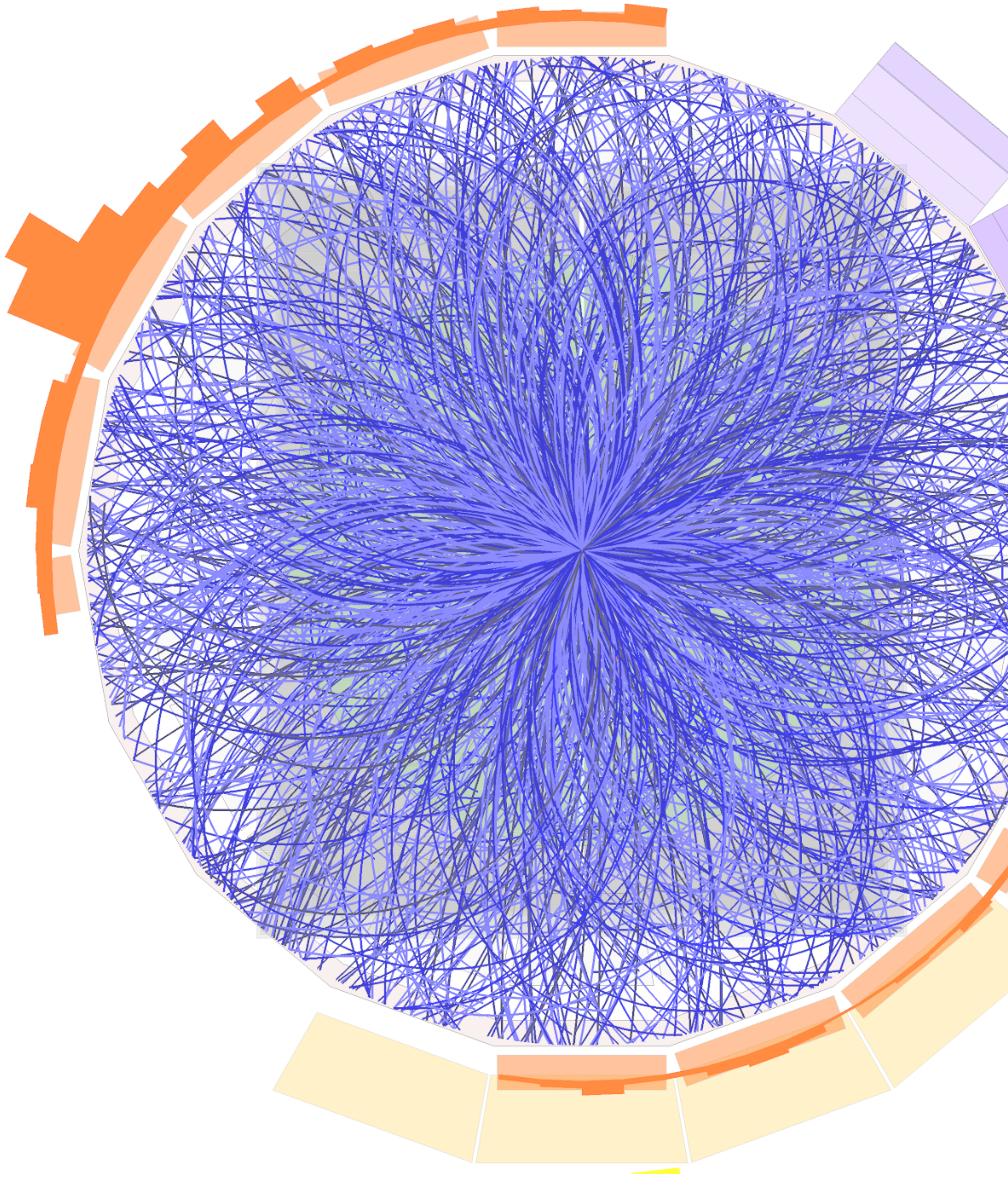
VarP–GP: cost-efficient Bayesian emulation of quark-gluon plasma modeling with variable statistical precision



Raymond Ehlers[1] Simon Mak[2]

Bayesian UQ meeting, 25 February 2026

In collaboration with Irene Ji and Peter Jacobs
Paper in preparation, arXiv:2602.xxxxx

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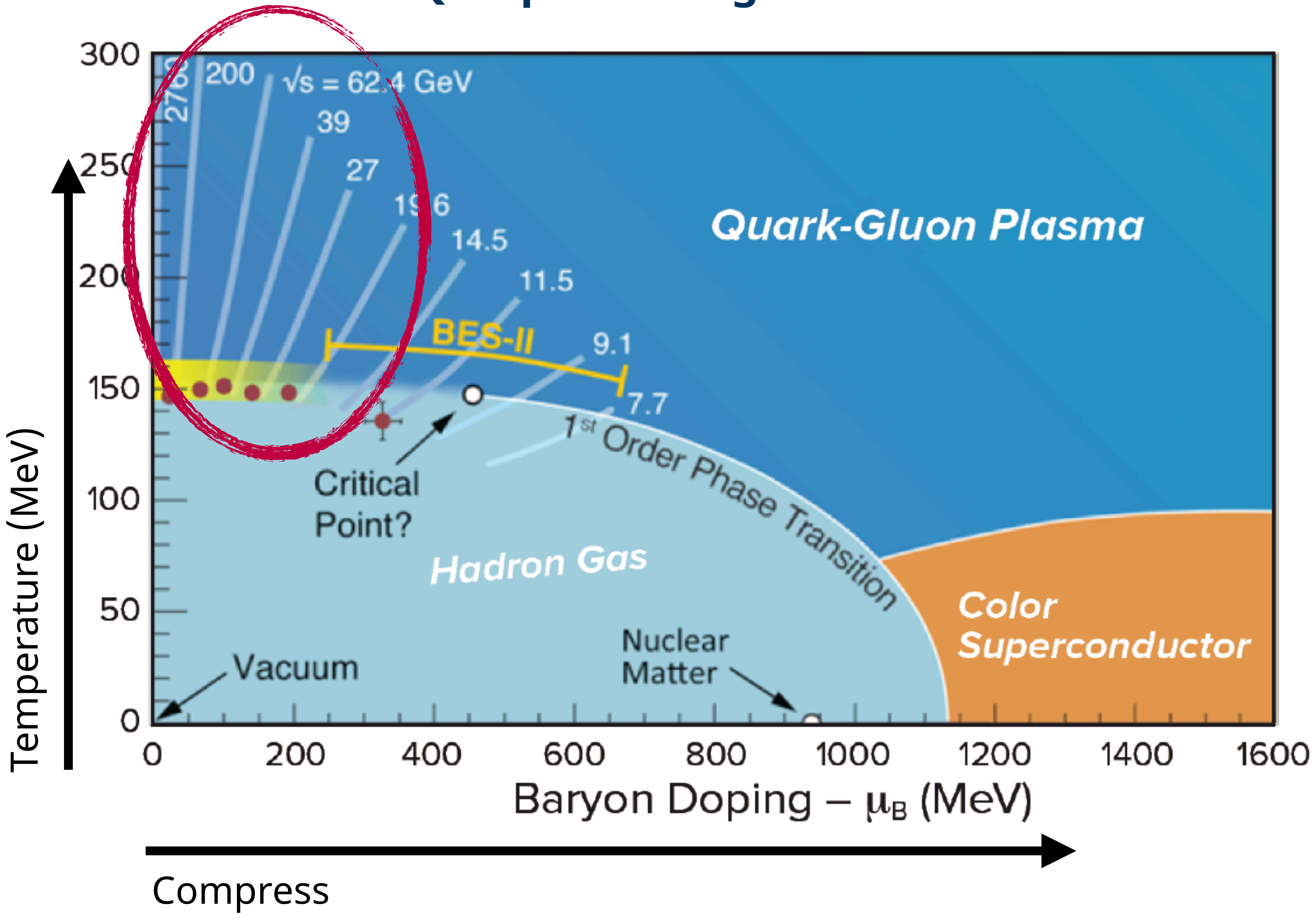
[2]Duke University

BERKELEY LAB Berkeley UNIVERSITY OF CALIFORNIA

Many-body dynamics and QCD matter

QCD phase diagram



For ensembles of many particles, we observe **complex, emergent behavior**

not derivable from elementary interactions

Dynamics of a heavy-ion collision

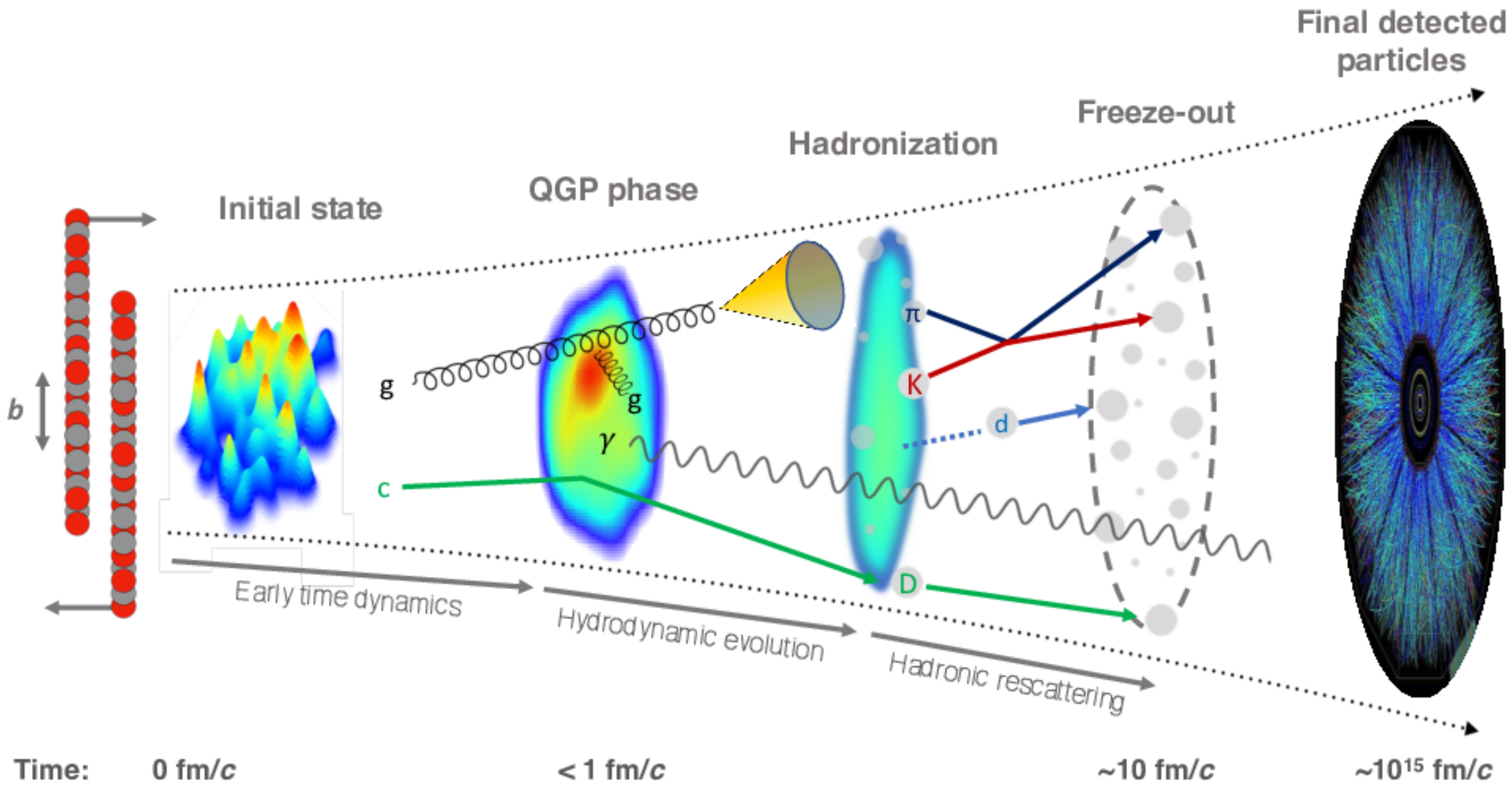


Illustration: ALICE, EPJC 84 (2024) 8, 813

Dynamics of a heavy-ion collision

Simulations (e.g. the forward model) are **calculated using Monte Carlo methods**

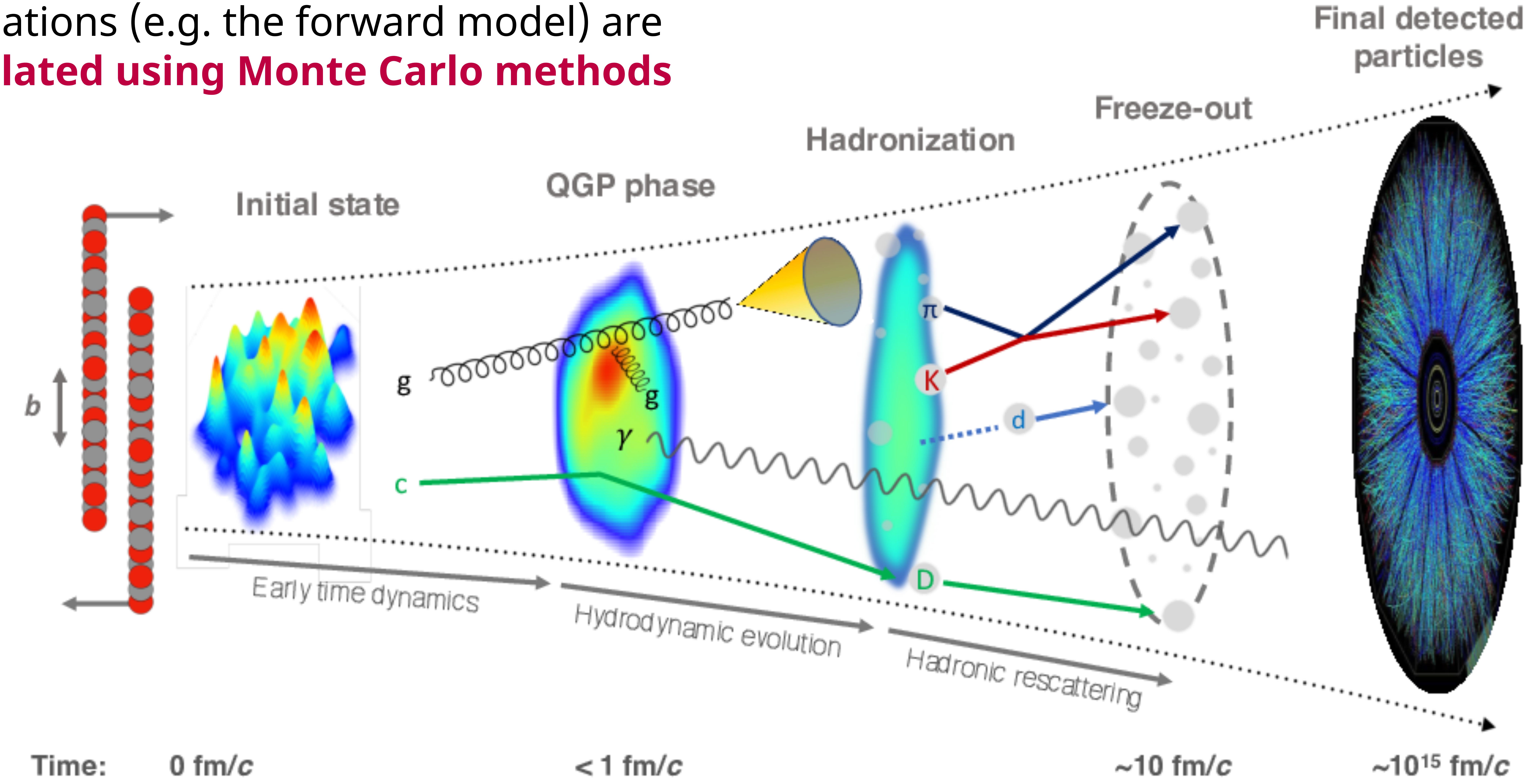


Illustration: ALICE, EPJC 84 (2024) 8, 813

Simulating dynamics of a heavy-ion collision

Typical simulation:
- 2+1D (“simple”): 40m/event
- 3+1D (“complex”): 15hr/event

“Soft-sector” dynamics

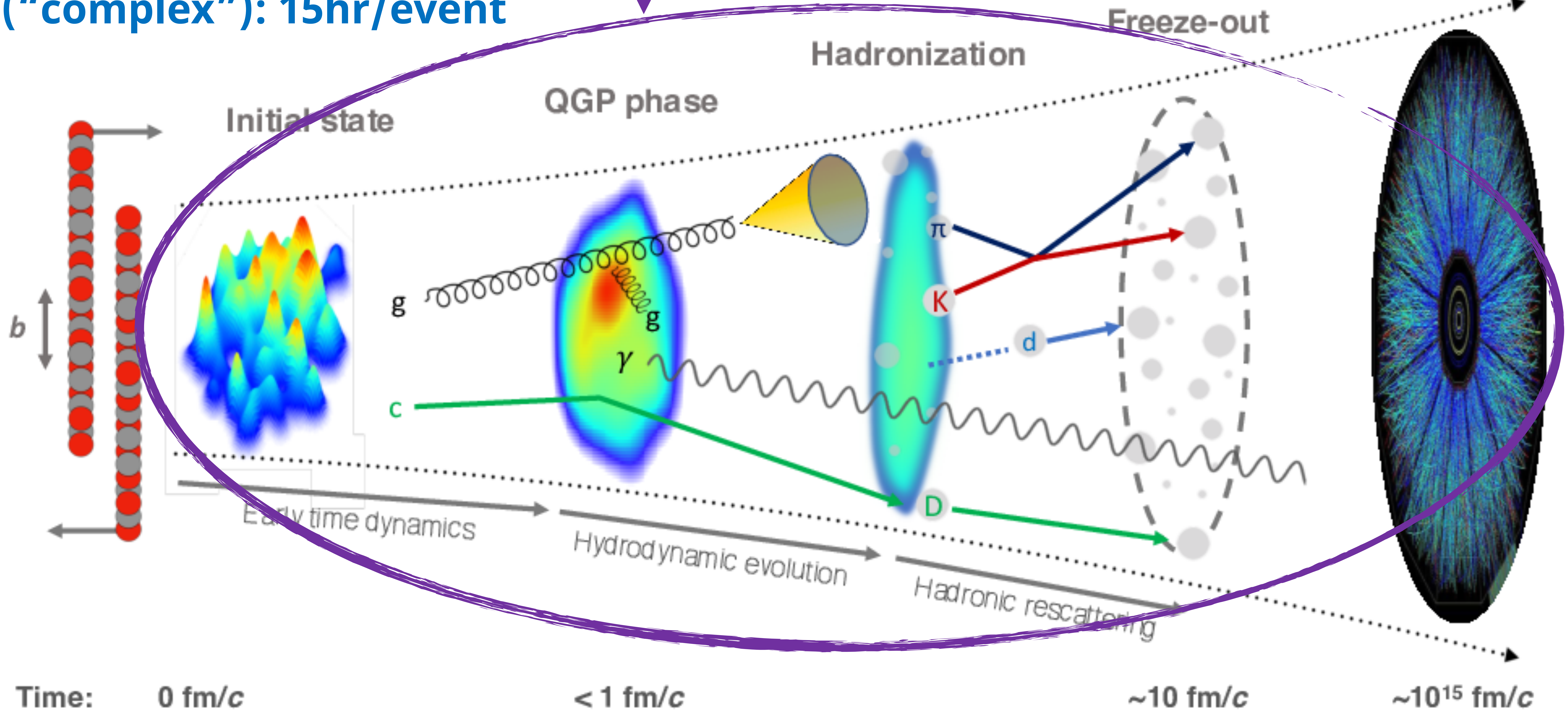


Illustration: ALICE, EPJC 84 (2024) 8, 813

Simulating dynamics of a heavy-ion collision

Hard-sector ("jet") dynamics (self-generated probe)

Typical simulation:
- 12 s/event

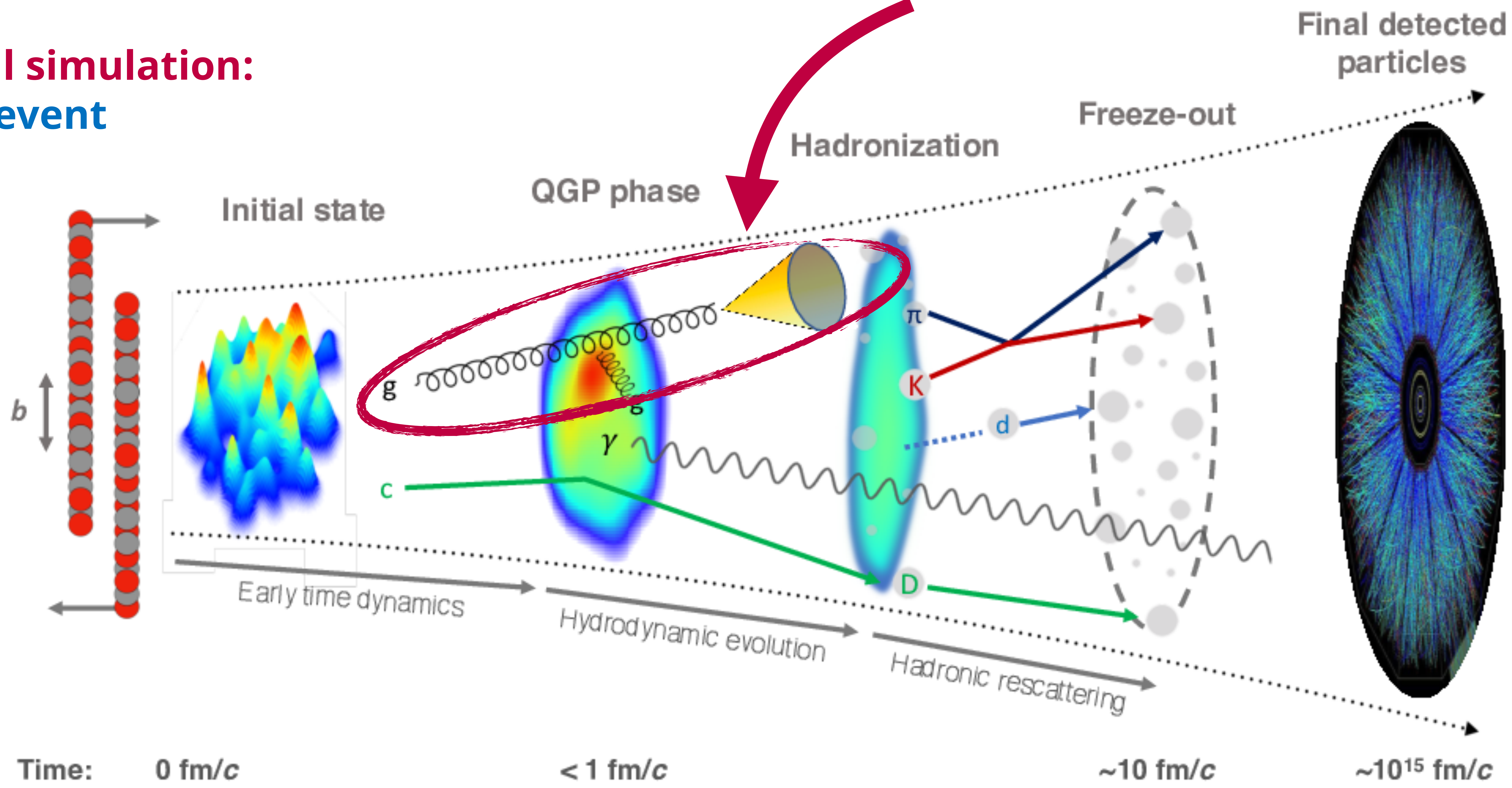


Illustration: ALICE, EPJC 84 (2024) 8, 813

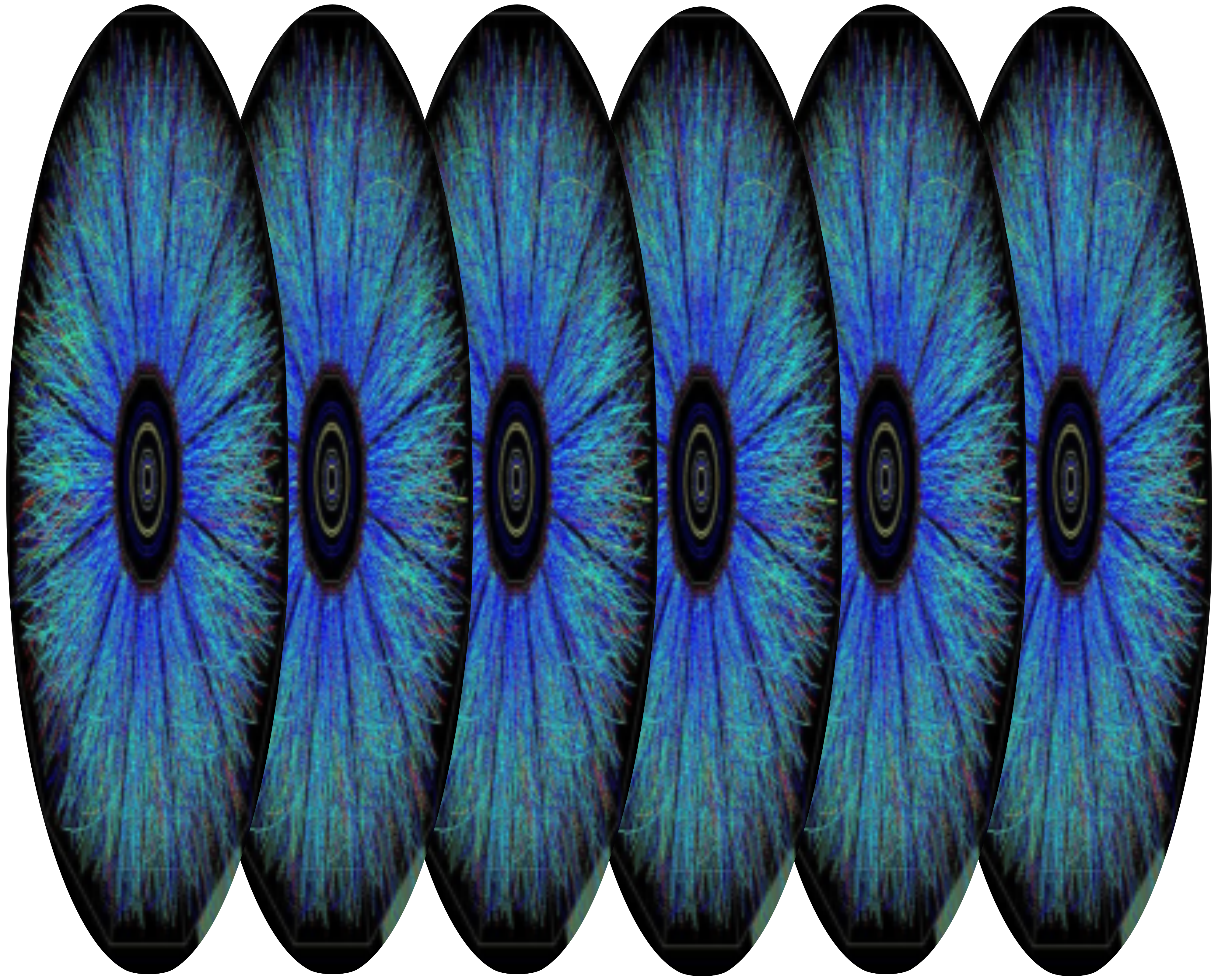
Simulating heavy-ion collisions

Soft-sector simulation:
- 2+1D ("simple"): 40m/event
- 3+1D ("complex"): 15hr/event

Require **> 1k events / design point**

Hard-sector simulation:
- 12 s/event

Require **> 1M events / design point**



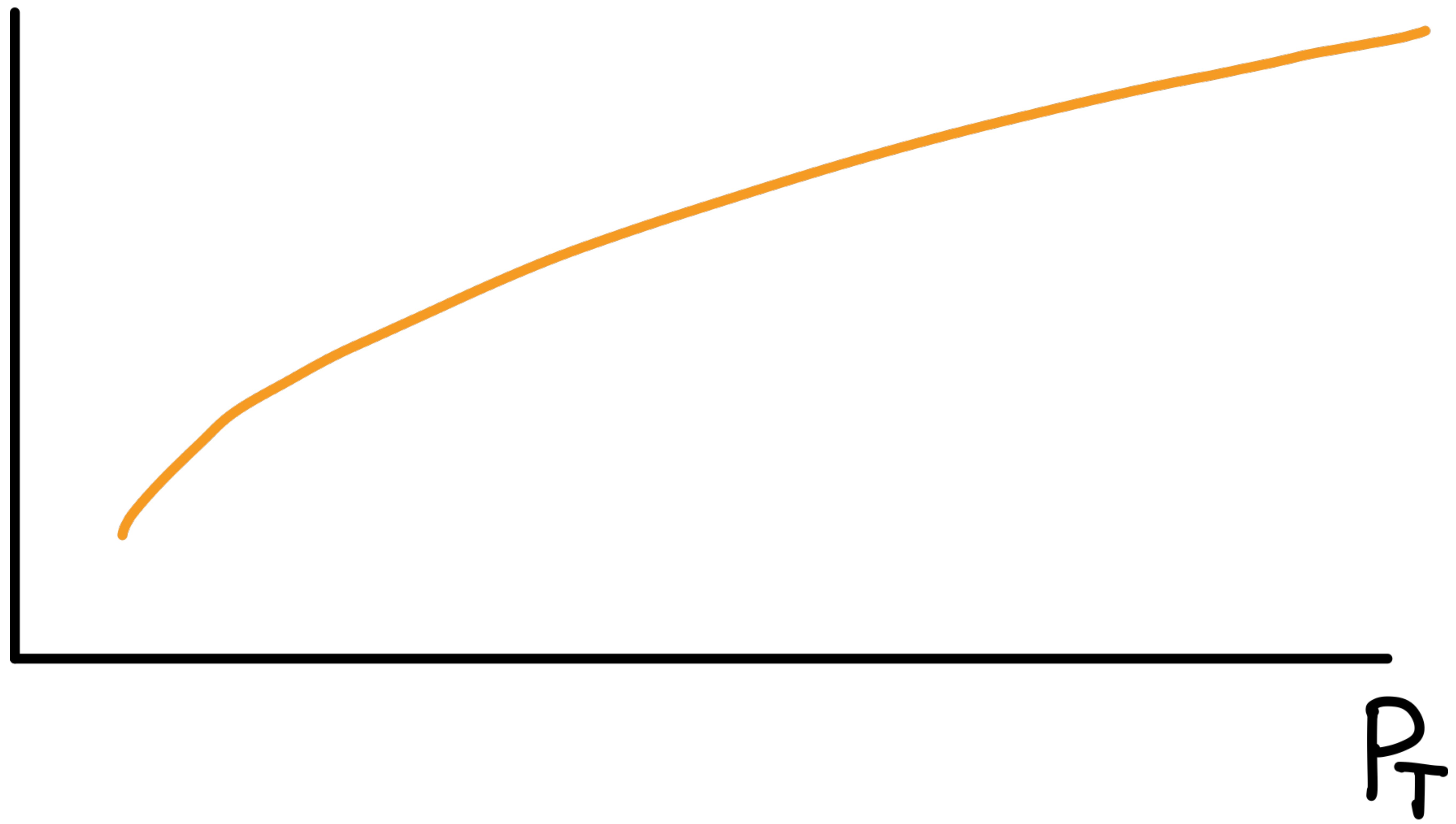
…

Opportunity:
MC simulations → specify statistical precision → measure of fidelity

Precision of MC sampled simulations

Opportunity:

MC simulations → specify statistical precision → measure of fidelity



Truth

Low precision

Medium precision

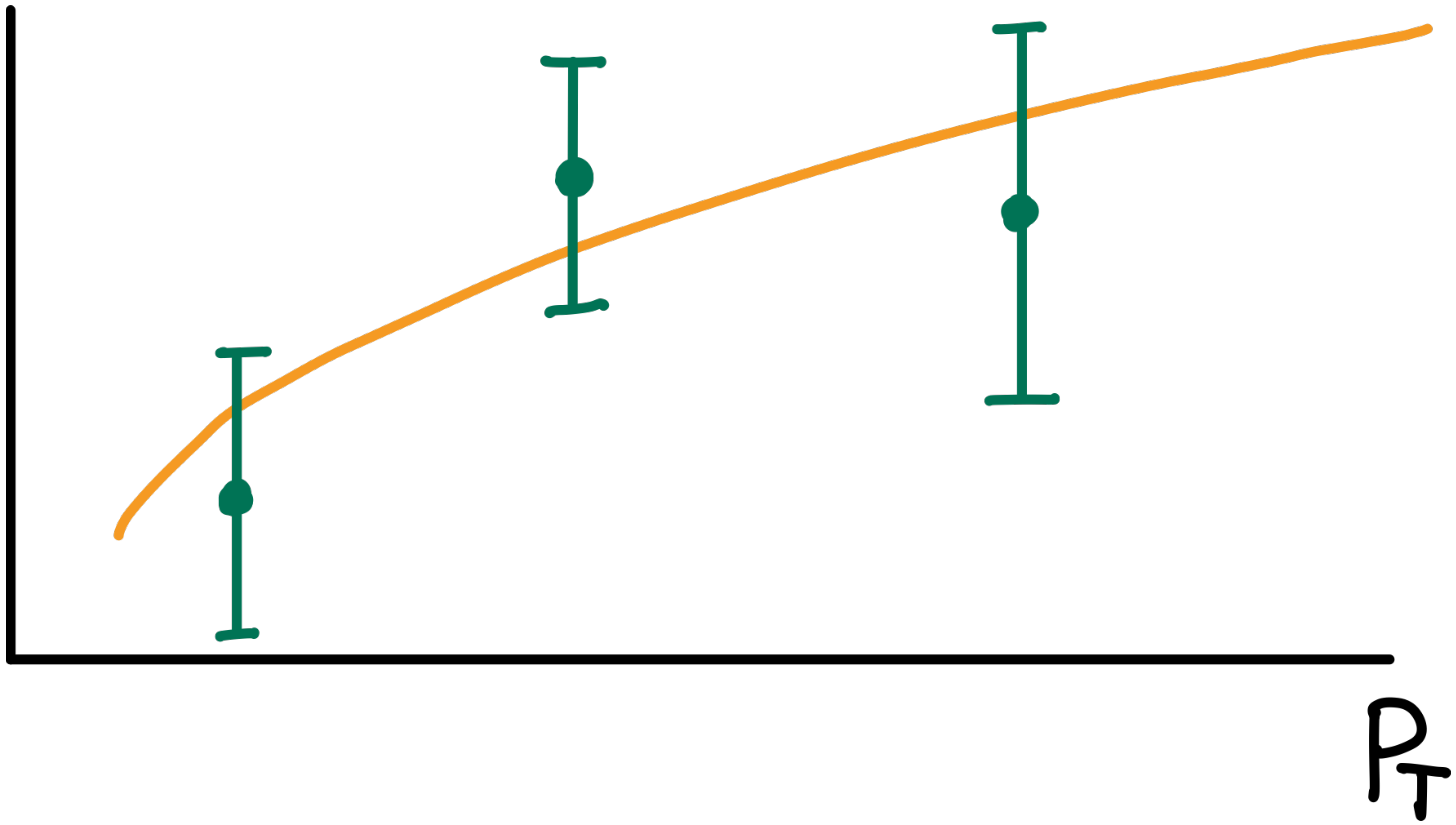
High precision

n.b. applies to any calculation with statistical precision

Precision of MC sampled simulations

Opportunity:

MC simulations → specify statistical precision → measure of fidelity



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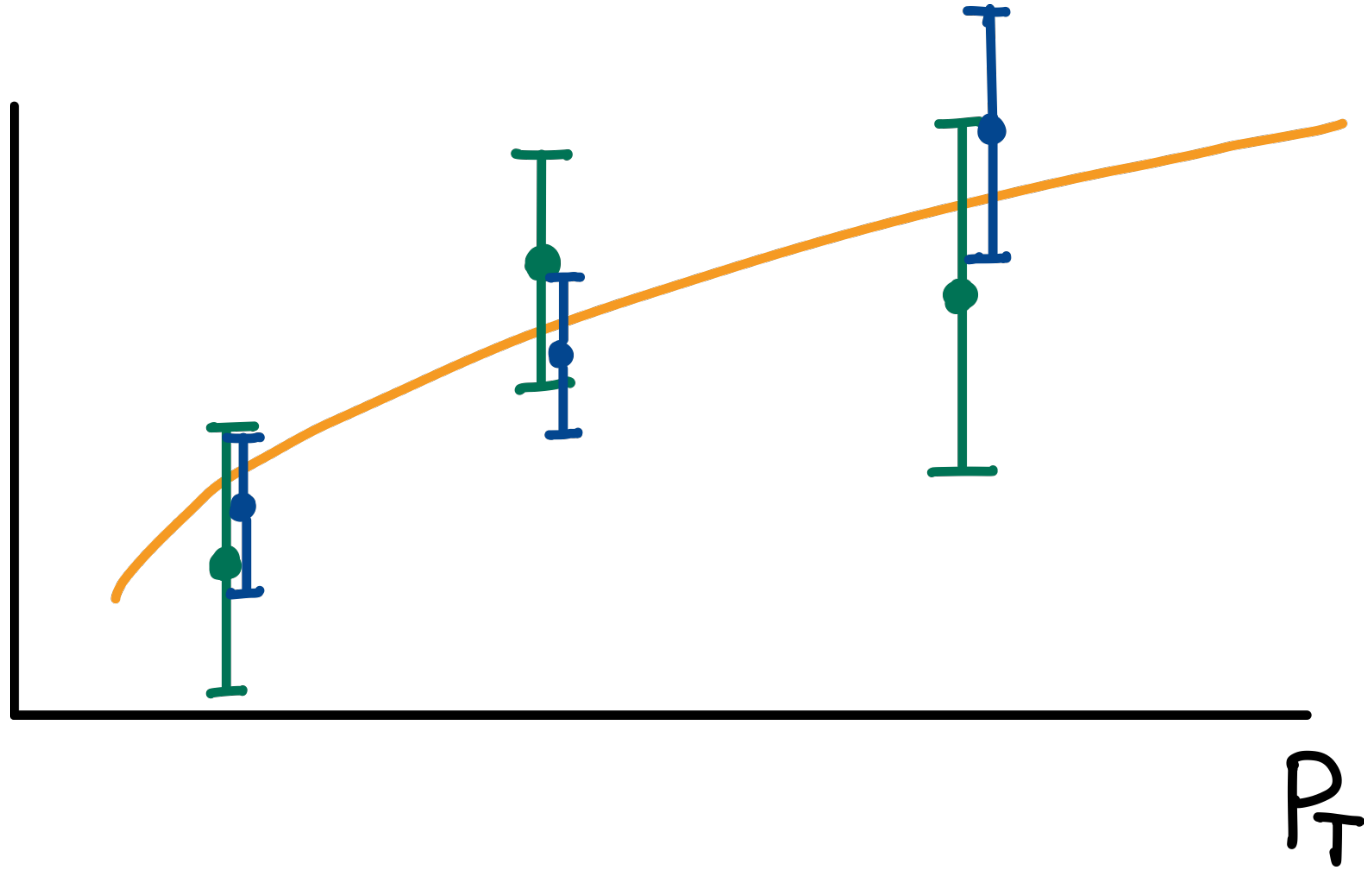

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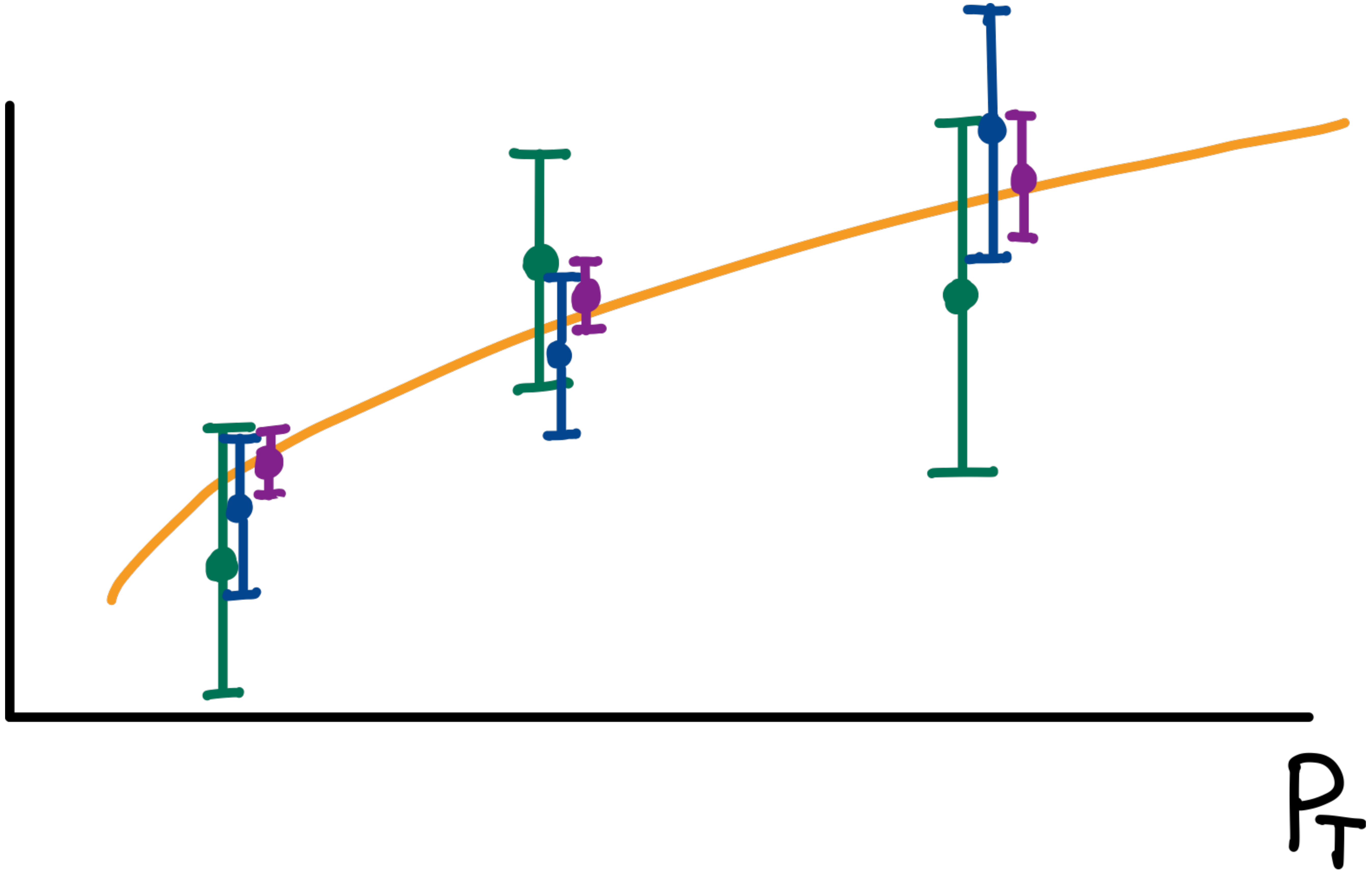

Truth
Low precision
Medium precision
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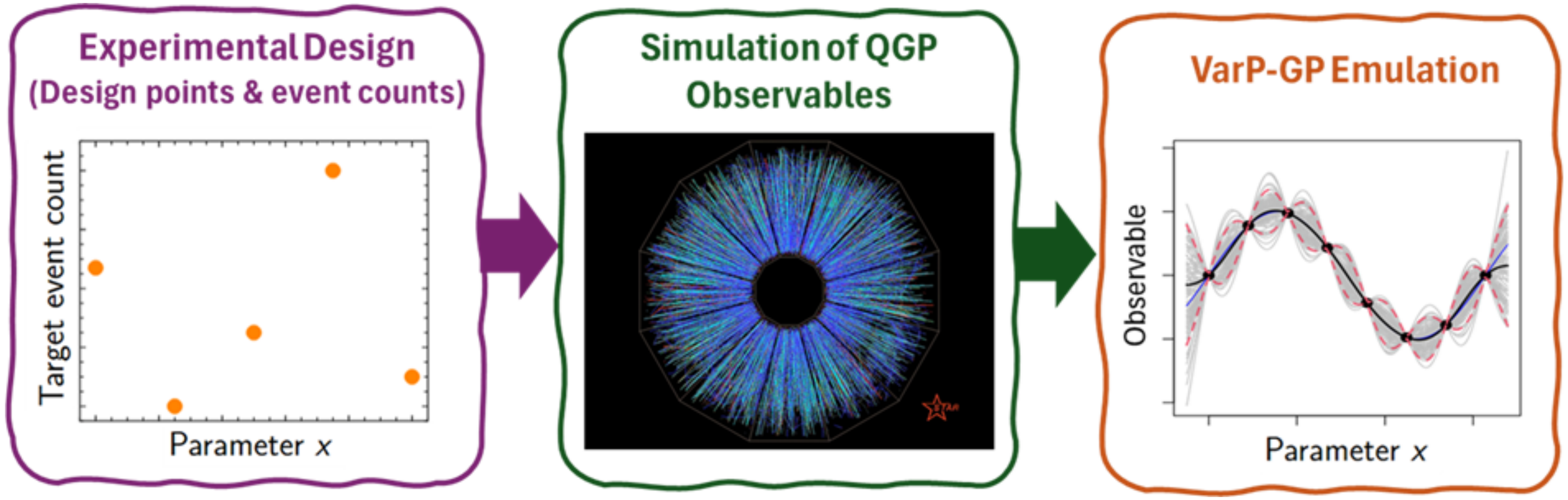
VarP-GP: Variable Precision Gaussian Process

VarP-GP: New **heteroskedastic GP emulator** that is trained on **calculations that have variable statistical precision** across the parameter design space



Two interacting GP models jointly learn the mean observable response and its varying statistical precision

RJE, IJ, SM, PMJ, arXiv:2602.xxxxx

Coupled Gaussian Processes

Standard (homoskedastic) GP

$$y_i = f(\mathbf{x}_i) + \epsilon_i, \quad \epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, 1/p).$$

Variance $s^2 = 1/p$, where p is constant statistical noise

$$f(\cdot) \sim \text{GP}\{\mu, k(\cdot, \cdot)\}$$

Predict new points:

$$[f(\mathbf{x}_{\text{new}})|\mathbf{y}] \sim \mathcal{N}\{\mu(\mathbf{x}_{\text{new}}), \sigma^2(\mathbf{x}_{\text{new}})\},$$

where:

$$\mu(\mathbf{x}) = \mu + \mathbf{k}(\mathbf{x})^\top(\mathbf{K} + p^{-1}\mathbf{I}_{n\times n})^{-1}(\mathbf{y} - \mu\mathbf{1}_n),$$
$$\sigma^2(\mathbf{x}) = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})^\top(\mathbf{K} + p^{-1}\mathbf{I}_{n\times n})^{-1}\mathbf{k}(\mathbf{x}).$$

VarP-GP (heteroskedastic)

$$y_i = f(\mathbf{x}_i) + \epsilon_i, \quad \epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}\left\{0, \frac{s^2(\mathbf{x}_i)}{m_i}\right\}.$$

$p_i = m_i/s^2(\mathbf{x}_i)$, where m_i is the event count

$$f(\cdot) \sim \text{GP}\{\mu_f, k_f(\cdot, \cdot)\}, \ \log s^2(\cdot) \sim \text{GP}\{\mu_s, k_s(\cdot, \cdot)\}.$$

Predict new points:

$$[f(\mathbf{x}_{\text{new}})|\mathbf{y}, \mathbf{p}] \sim \mathcal{N}\{\mu_f(\mathbf{x}_{\text{new}}), \sigma_f^2(\mathbf{x}_{\text{new}})\},$$

where:

$$\mu_f(\mathbf{x}) = \mu_f + \mathbf{k}_f(\mathbf{x})^\top(\mathbf{K}_f + \mathbf{P}^{-1})^{-1}(\mathbf{y} - \mu_f\mathbf{1}_n),$$
$$\sigma_f^2(\mathbf{x}) = k_f(\mathbf{x}, \mathbf{x}) - \mathbf{k}_f(\mathbf{x})^\top(\mathbf{K}_f + \mathbf{P}^{-1})^{-1}\mathbf{k}_f(\mathbf{x}).$$

→ **Coupled GP design pools information across design points**

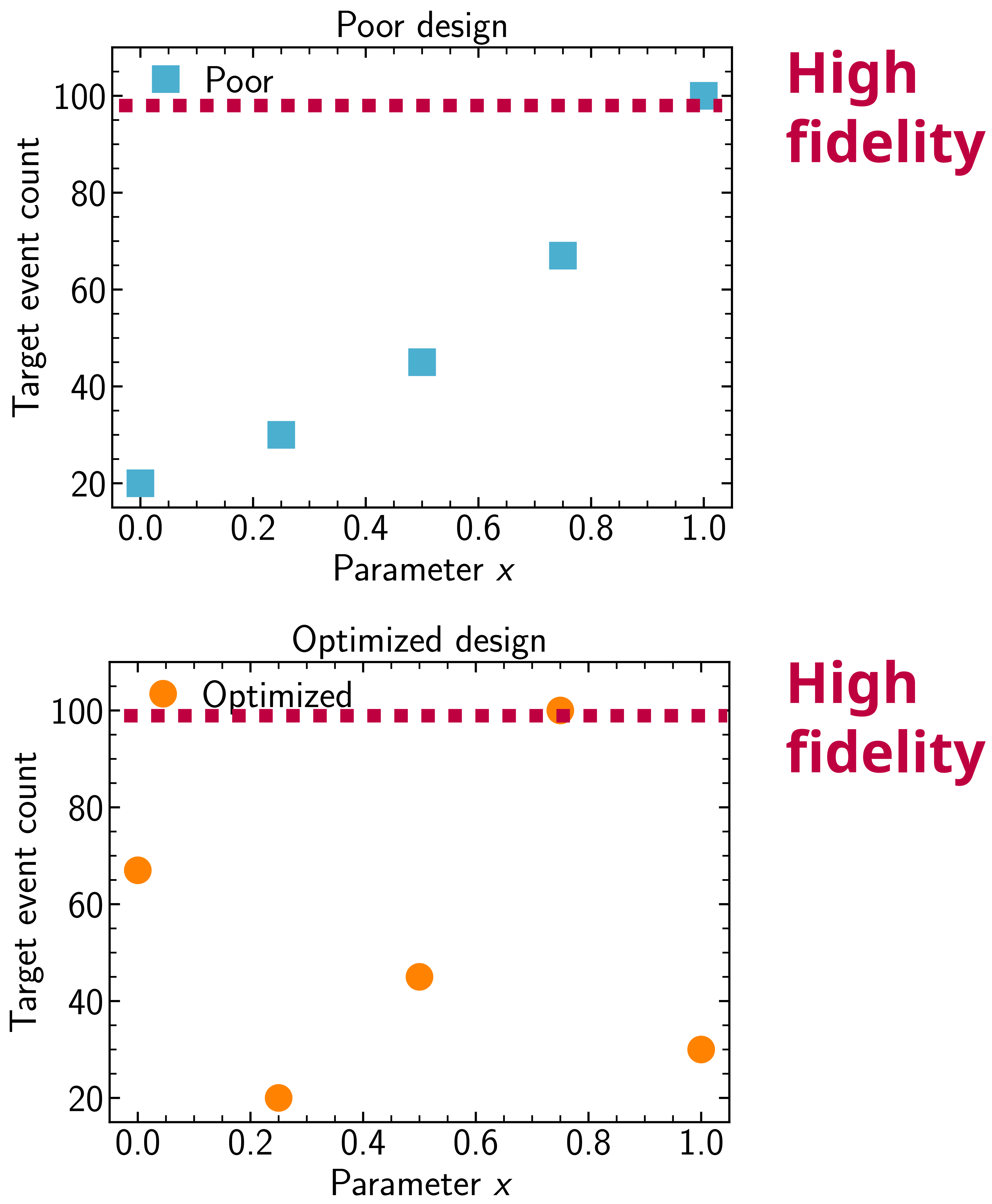
Experimental design

- Method to allocate design points + their precision
- Design based on multi-mesh method:
  Yuchi et al, Journal of Mechanical Design, 2023
- Two key developments:
  - For a fixed computing budget, **determine optimal precision per design point**

$$\mathscr{M} = \left\{ m : m = \underline{m} \left(\frac{\overline{m}}{\underline{m}} \right)^u, u = \frac{i-1}{n-1}, i = 1, \cdots, n \right\}.$$

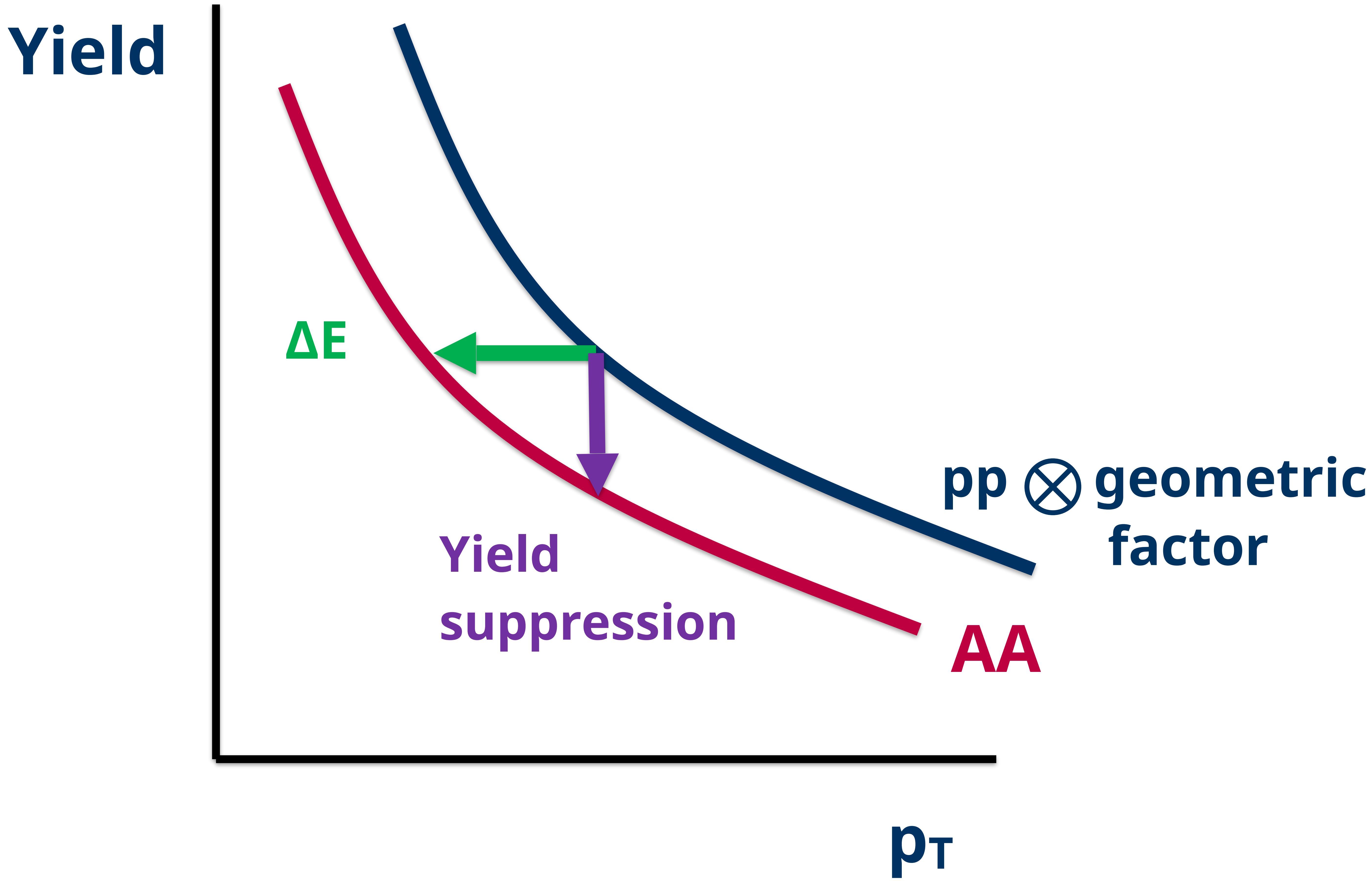
  - Assign precision to design points such that **close design points have different precision**

$$\underset{m_1,\cdots,m_n \in \mathscr{M}}{\text{argmax}} \min_{\substack{i,j=1,\cdots,n \\ i \neq j}} \|\mathbf{x}_i - \mathbf{x}_j\|_2 \cdot |m_i - m_j|.$$



RJE, IJ, SM, PMJ, arXiv:2602.xxxxx

Medium-induced modification of hard probes



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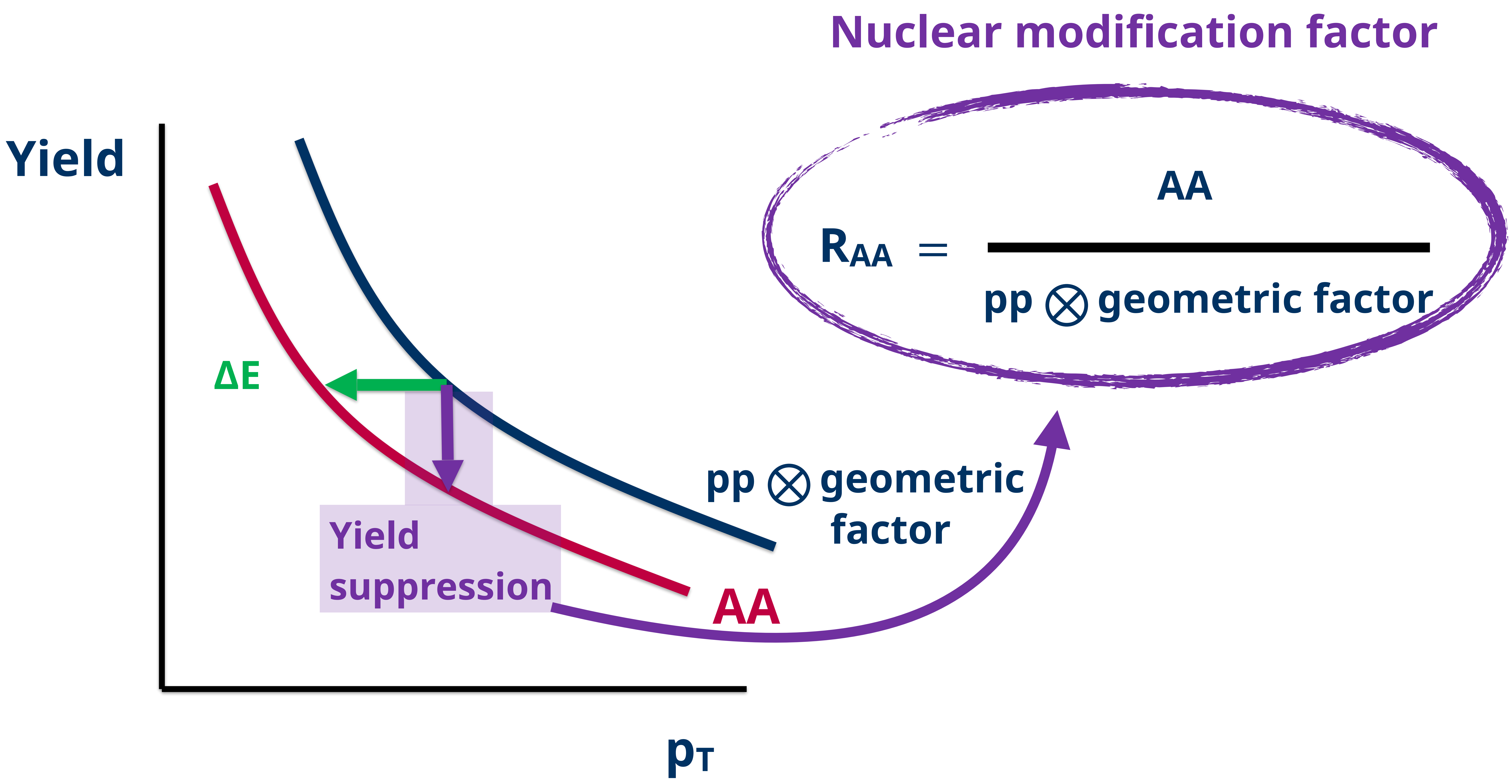

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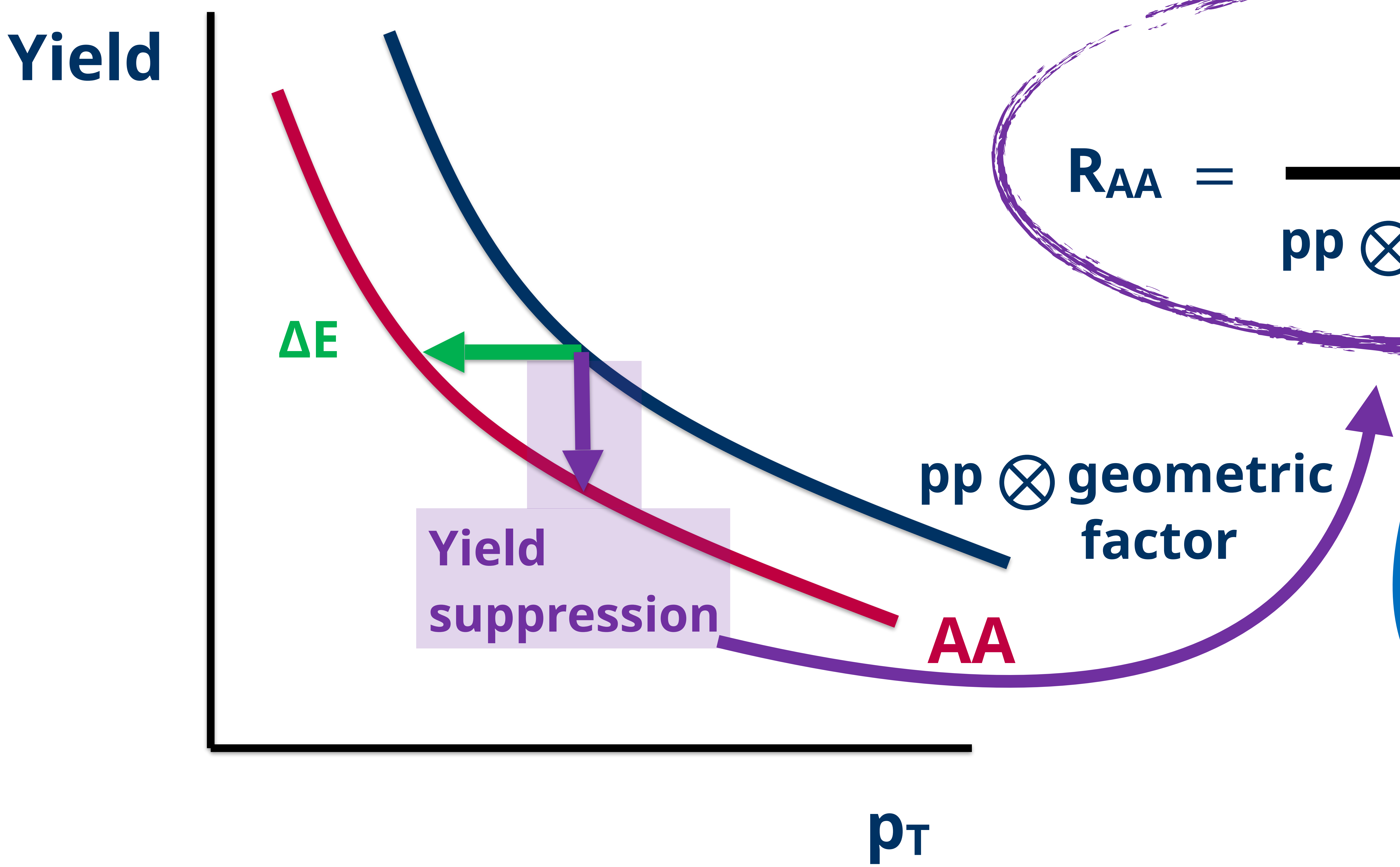
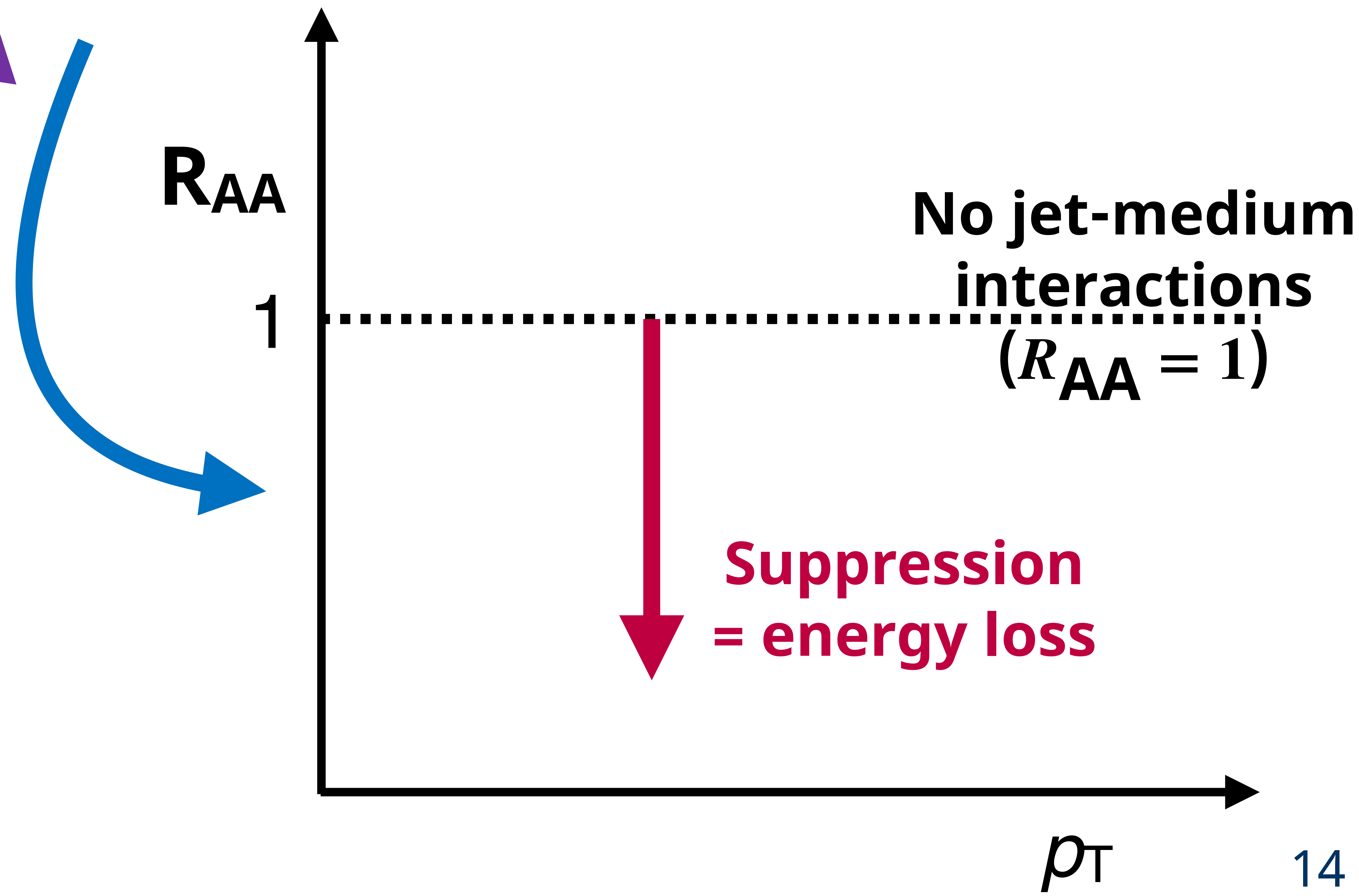


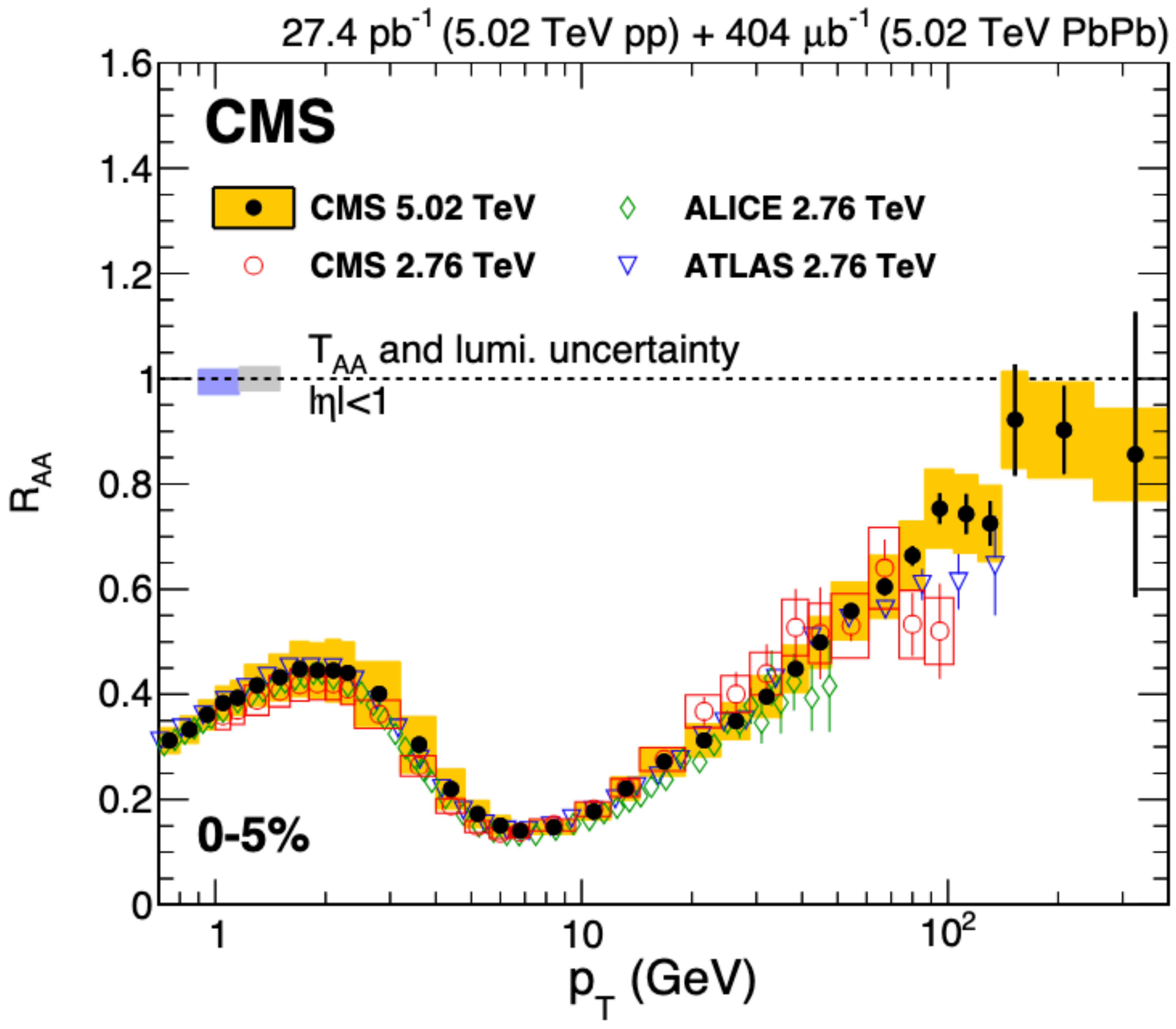
Nuclear modification factor

$$R_{AA} = \frac{AA}{pp \otimes \text{geometric factor}}$$

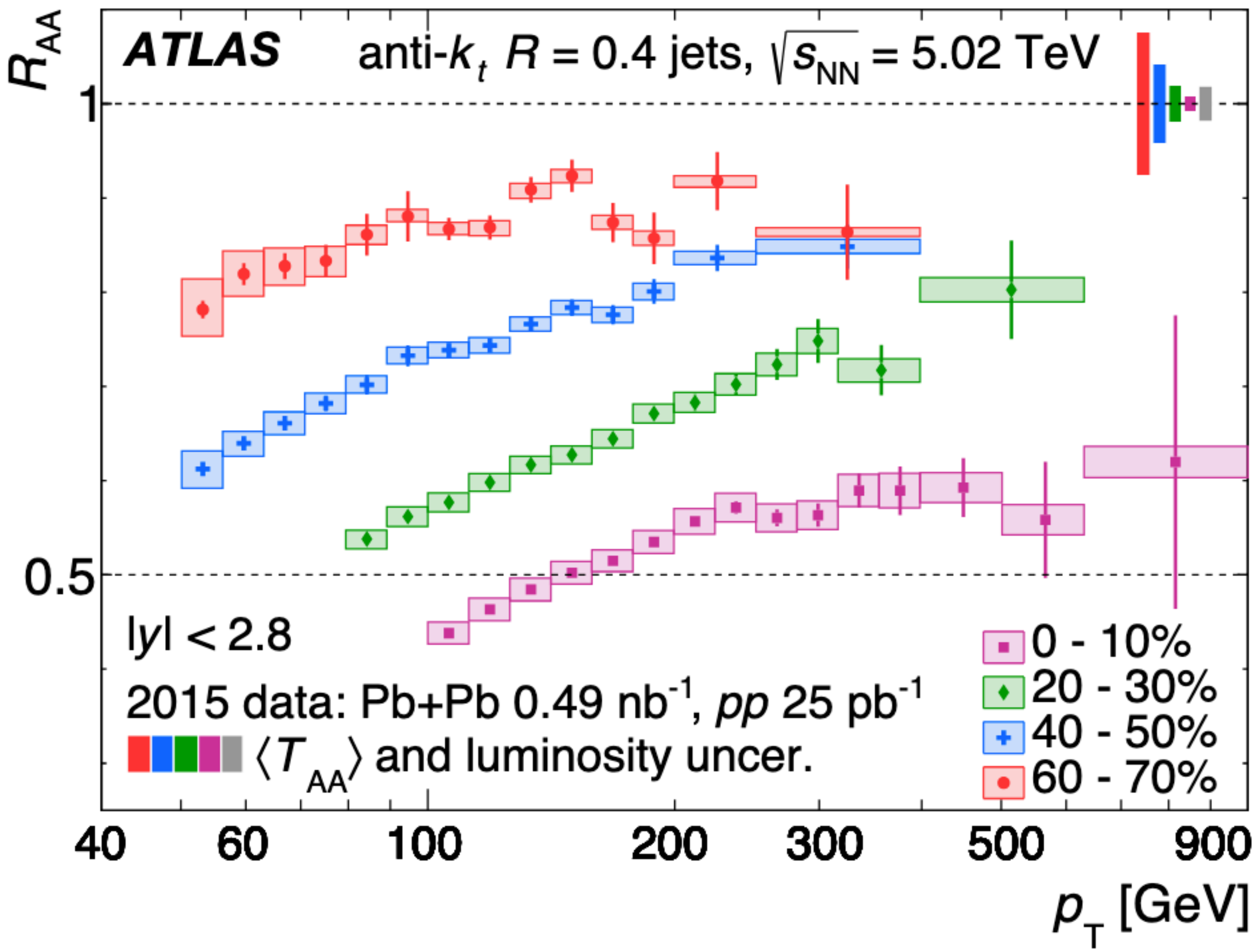


Measured yield modification

CMS, Hadron RAA



ATLAS, Jet RAA



CMS, JHEP 04 (2017) 039
ATLAS, PLB 790 (2019) 108-128

Measured yield modification

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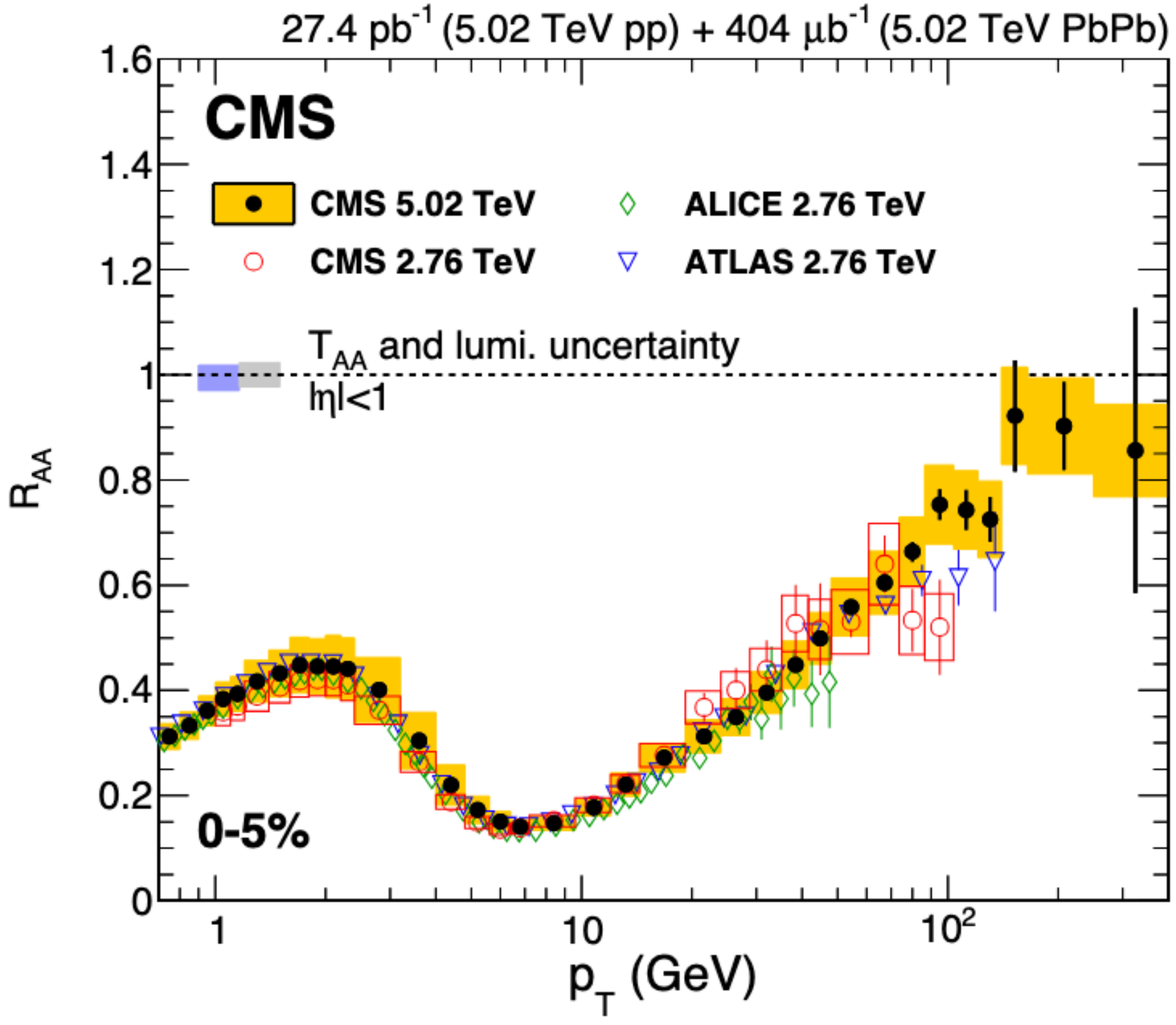

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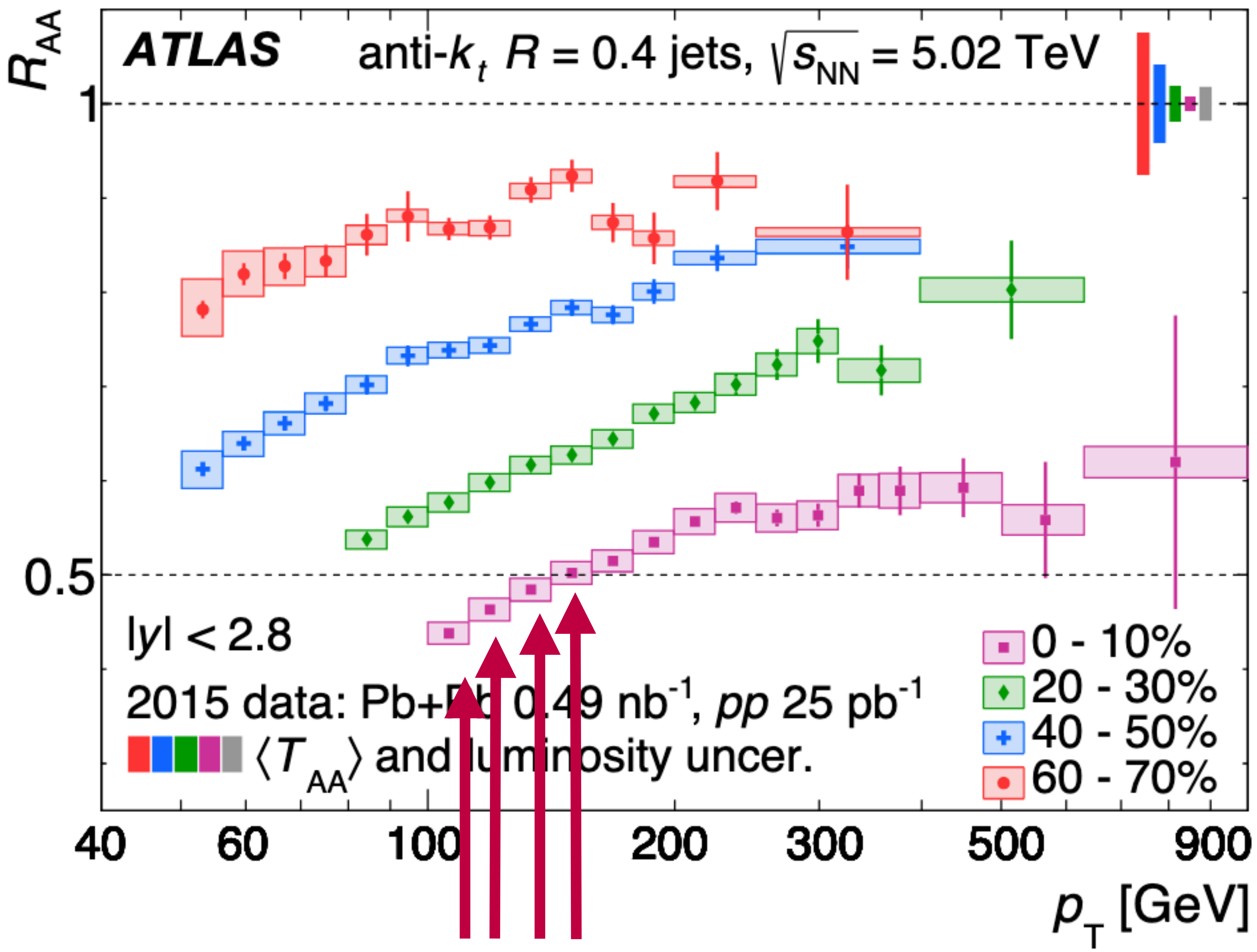
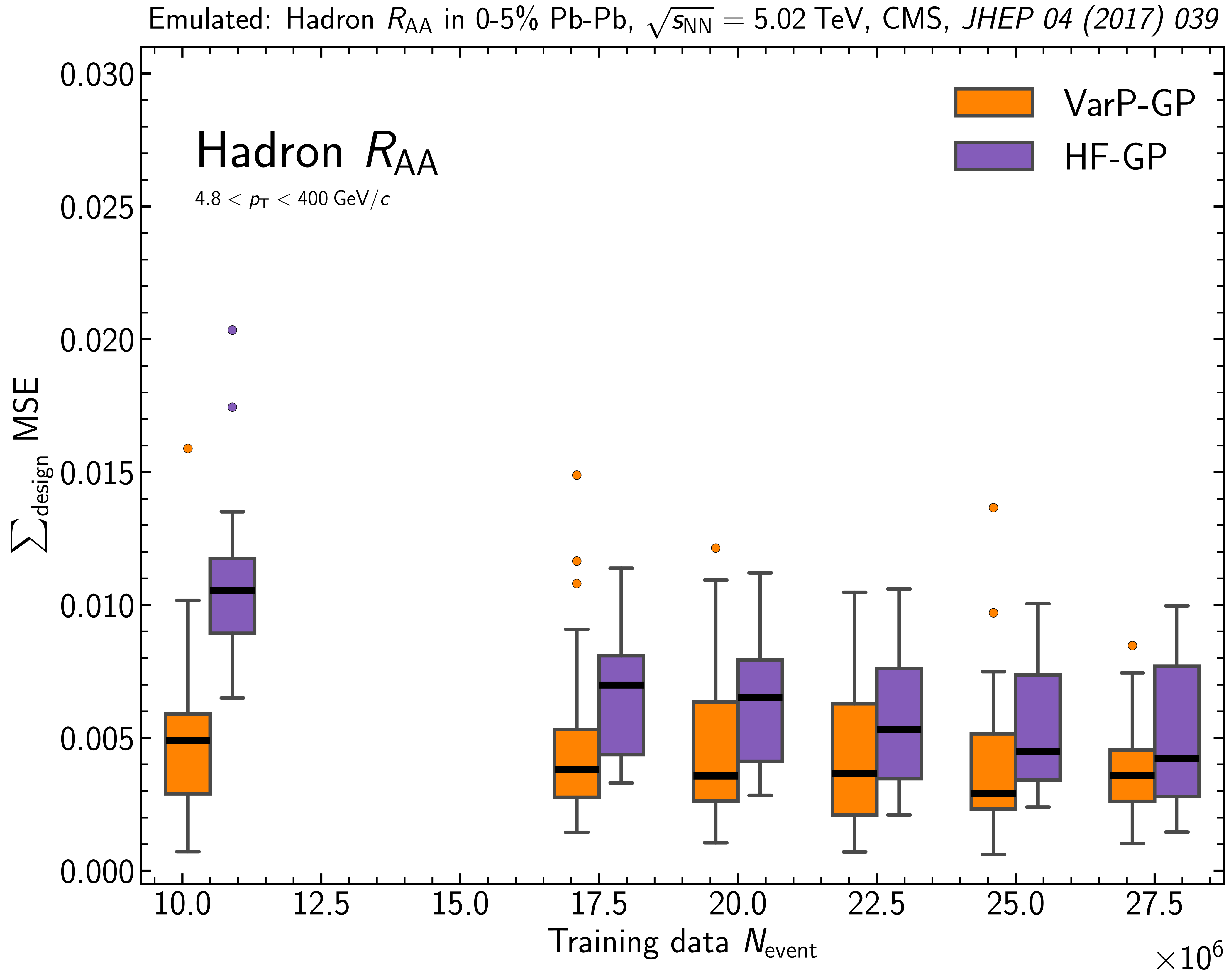


Emulator per bin

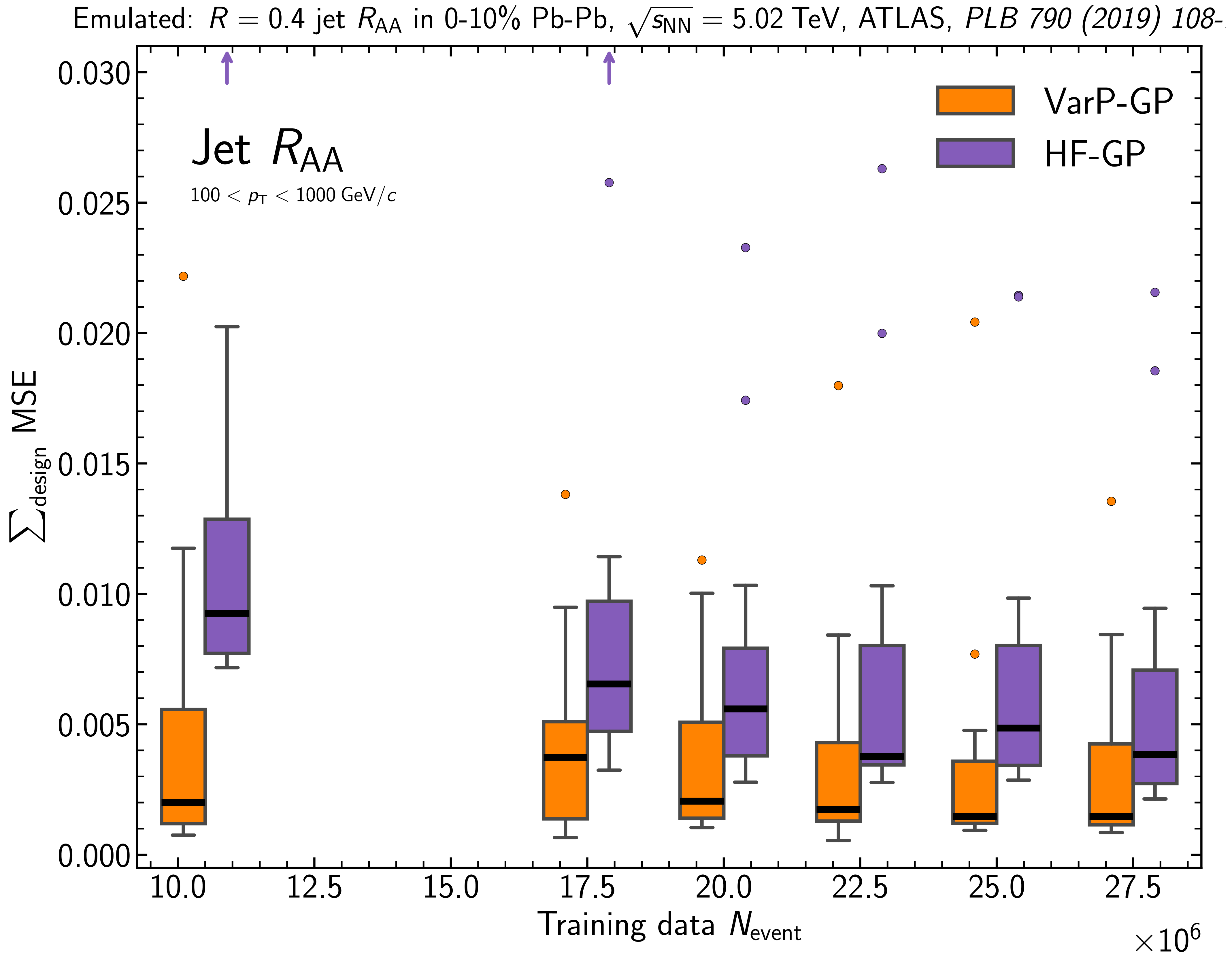
CMS, JHEP 04 (2017) 039
ATLAS, PLB 790 (2019) 108-128

Emulator uncertainty: MSE per pt bin

Hadron RAA



Jet RAA

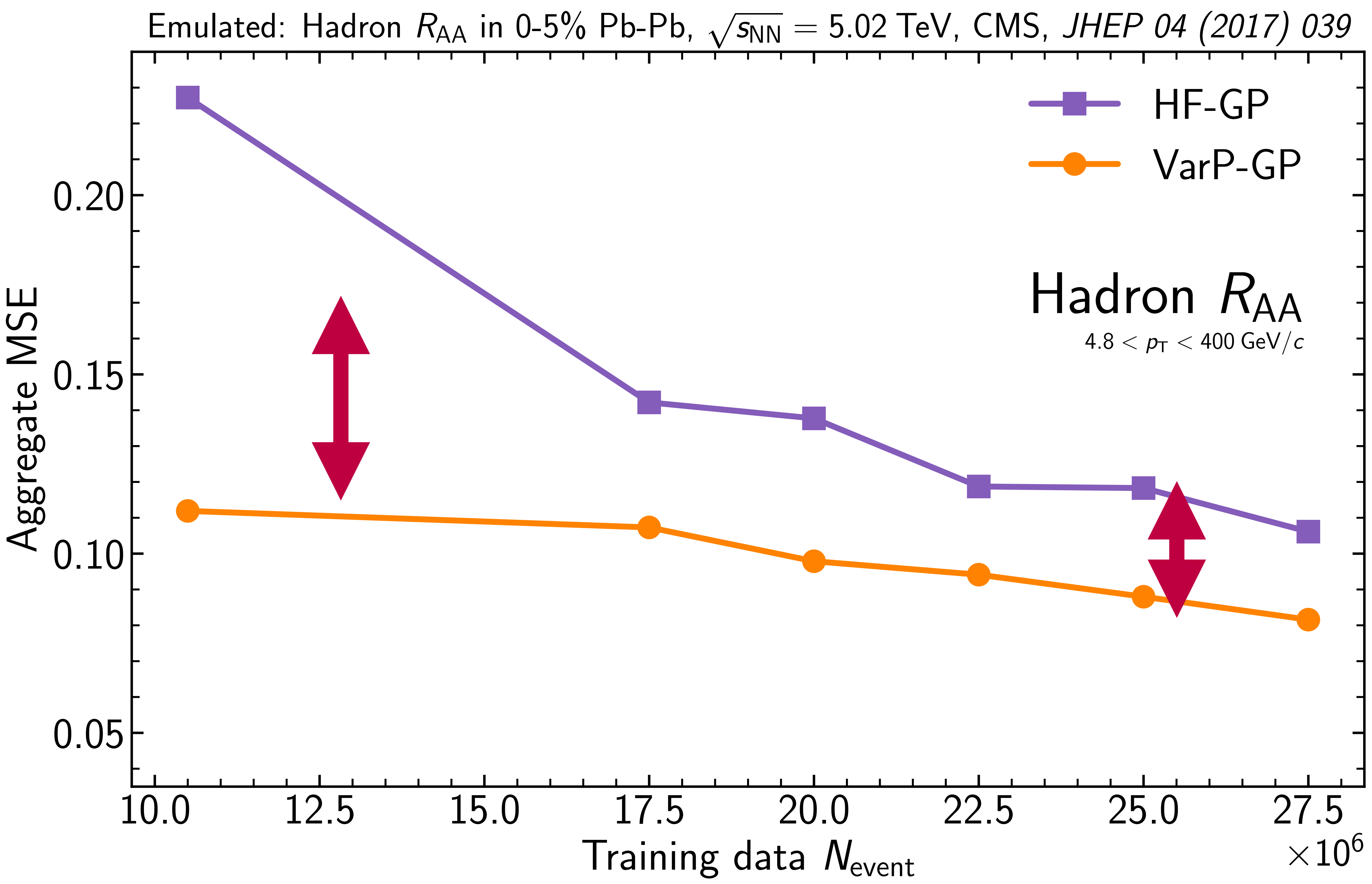


Smaller MSE, smaller variance

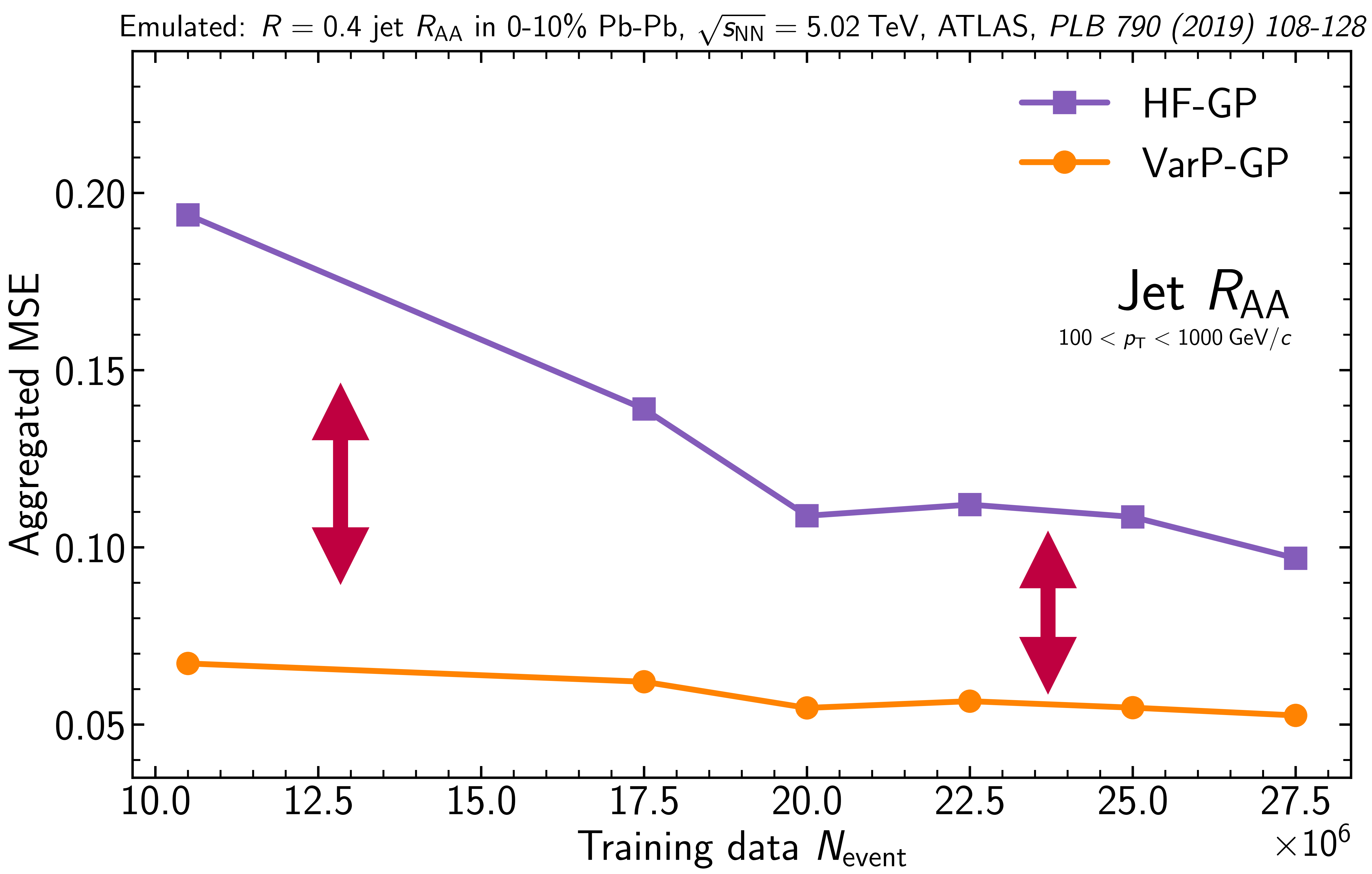
RJE, IJ, SM, PMJ, arXiv:2602.xxxxx

Emulator uncertainty: aggregated MSE

Hadron RAA



Jet RAA



➡ **Information across the parameter space is more important than limited high fidelity points**

RJE, IJ, SM, PMJ, arXiv:2602.xxxxx

Model parameter sensitivity

Total-effect: Direct variation and correlation with other parameters

Normalized total-effect Sobol' index

$$S_{T_l} = \frac{\mathbb{E}_{\mathbf{X}_{\sim l}}[\mathrm{Var}_{X_l}\{f(\mathbf{X})|\mathbf{X}_{\sim l}\}]}{\mathrm{Var}_{\mathbf{X}}\{f(\mathbf{X})\}}$$

$$S_{T_l(\mathrm{norm})} = \frac{S_{T_l}}{\sum_{l=1}^{d} S_{T_l}}, \qquad l = 1, \cdots, d.$$

Normalized over all sensitivity

Model parameters

- α_s (denoted α_s^{fix} in Eq. 4 in Ref. [21]), the coupling at the soft scale, ranging from $0.1 \leq \alpha_s \leq 0.5$.
- Q_0, the transition scale between the higher (MATTER) and lower (LBT) virtuality stages of the simulation, ranging from 1 GeV $\leq Q_0 \leq$ 10 GeV.
- τ_0, the start time of jet modification, ranging from $0 \leq \tau_0 \leq 1.5$ fm/c.
- Parameters c_1, c_2, c_3, which control the modification of $\hat{q}$ with increasing virtuality, ranging from $-5 \leq \log(c_{1,2}) \leq \log(10)$ and $-3 \leq \log(c_3) \leq \log(100)$.

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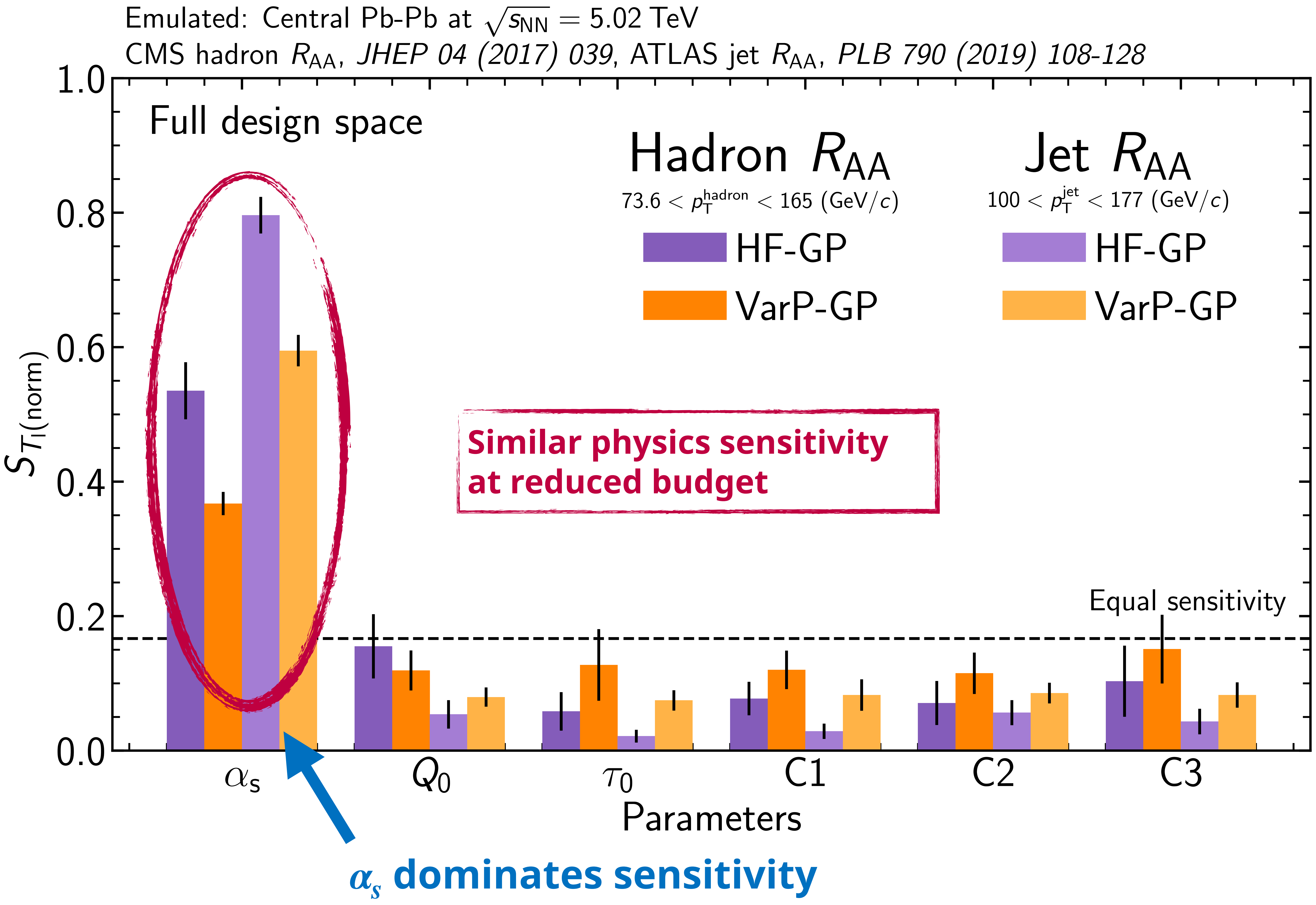
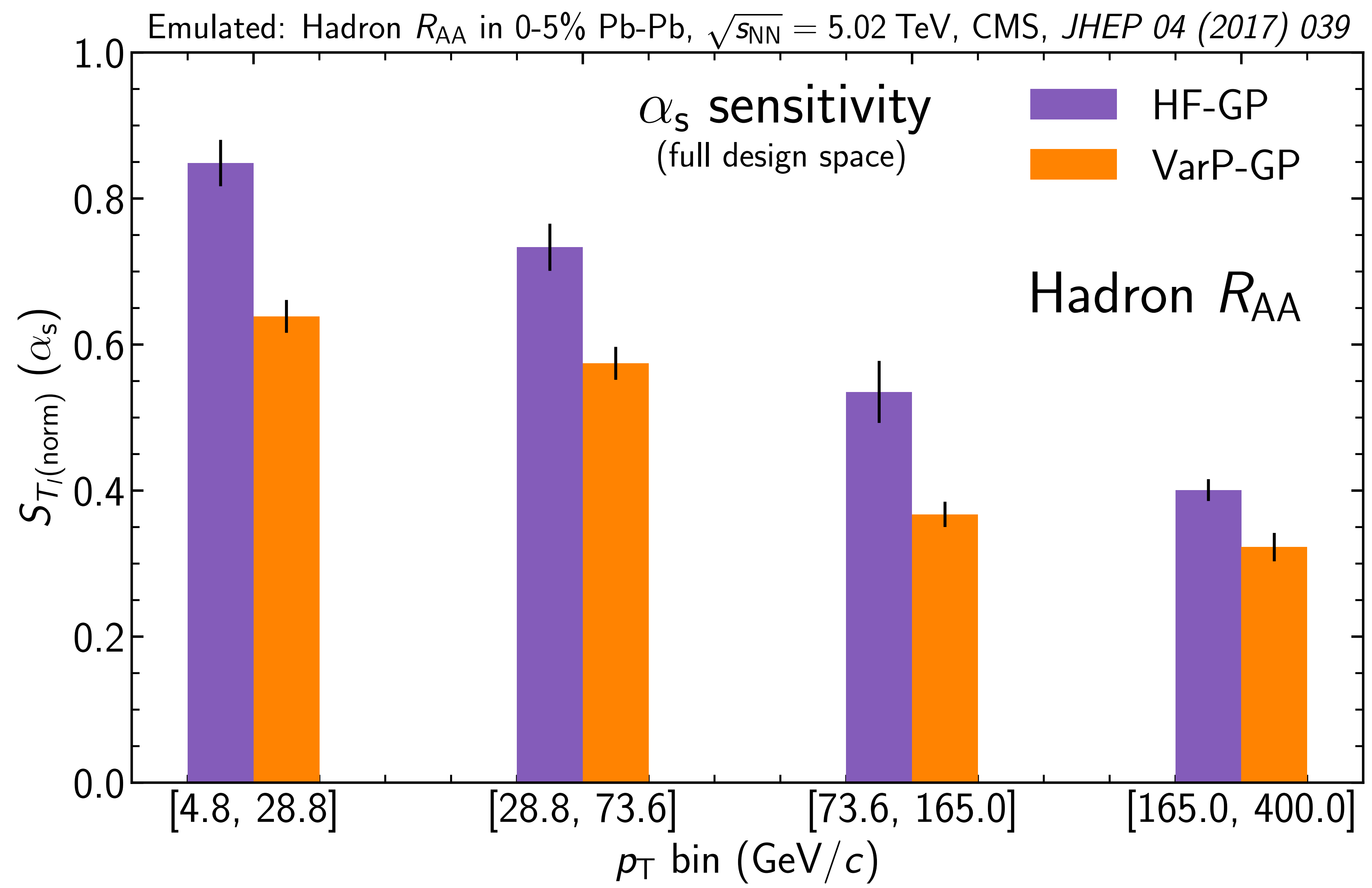
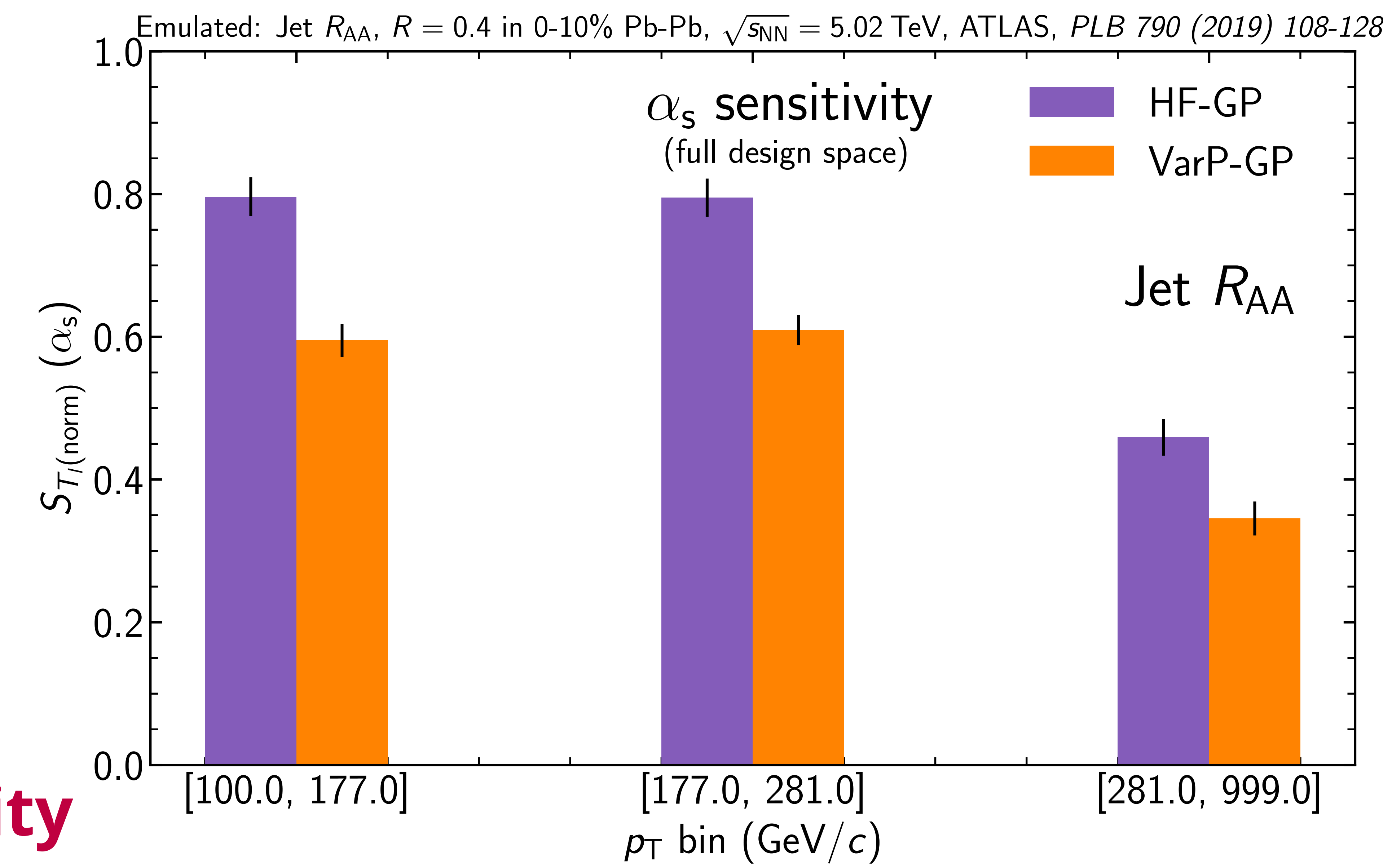


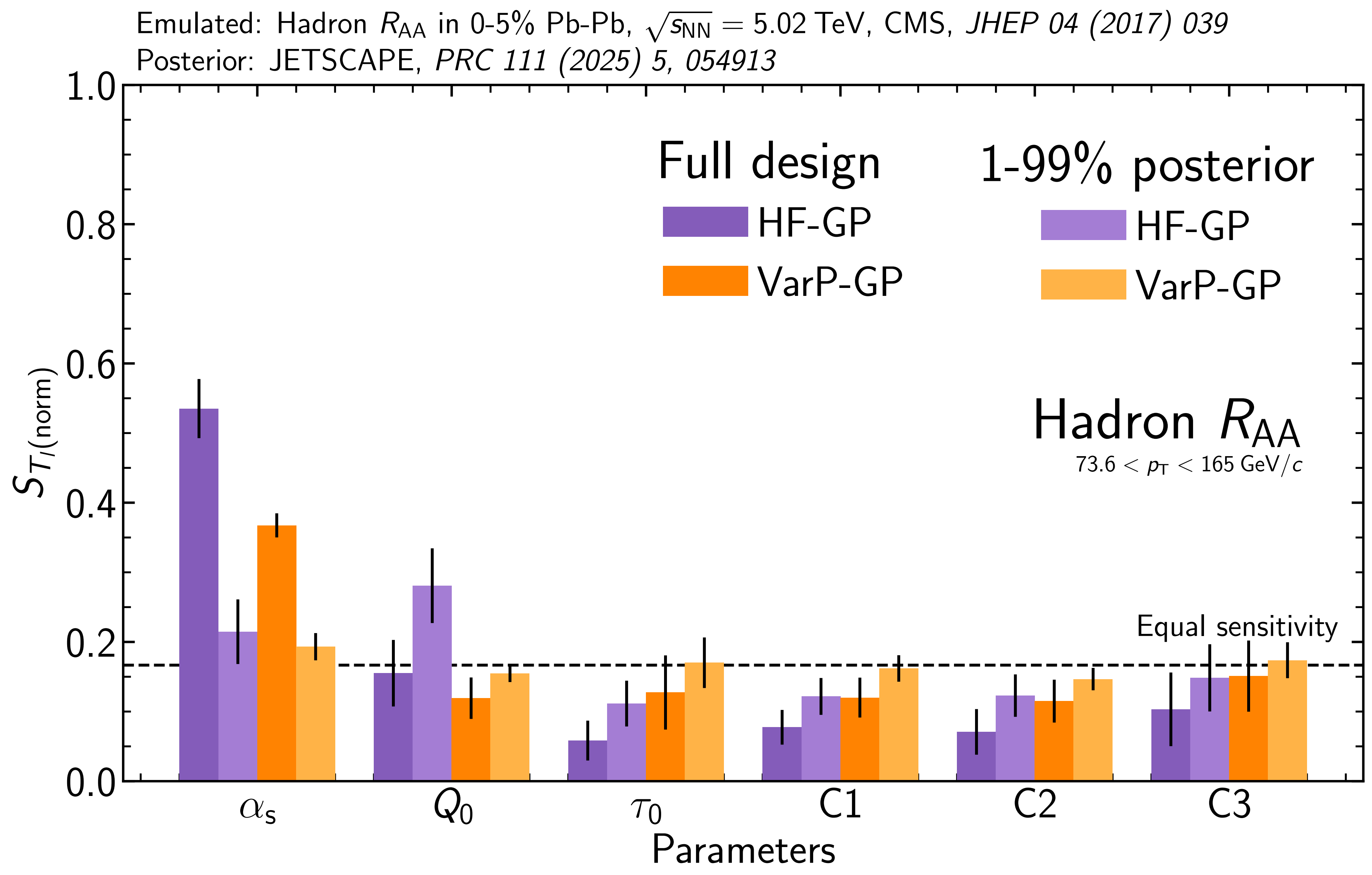
Model parameter sensitivity/2

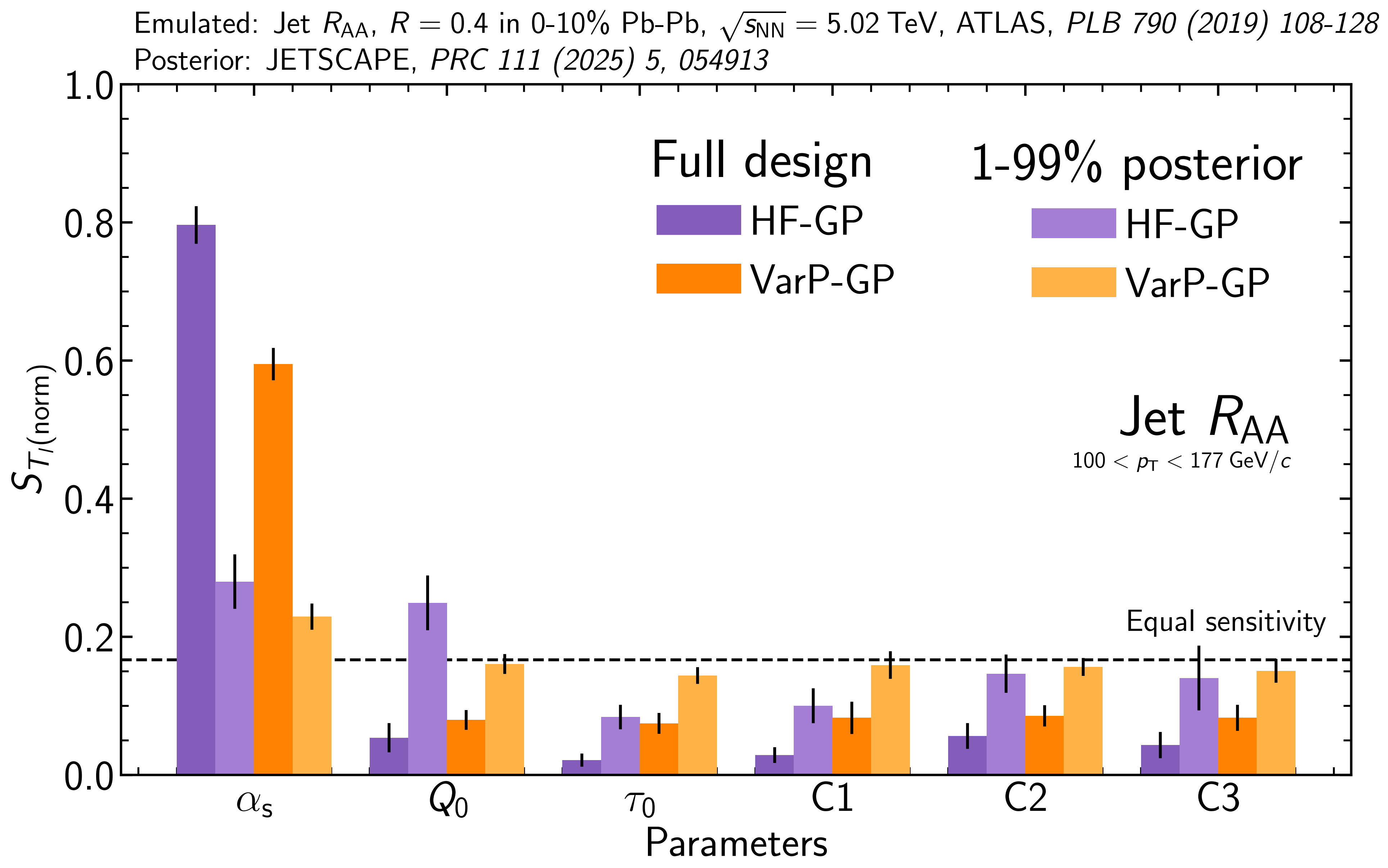




α_s sensitivity

Local vs global

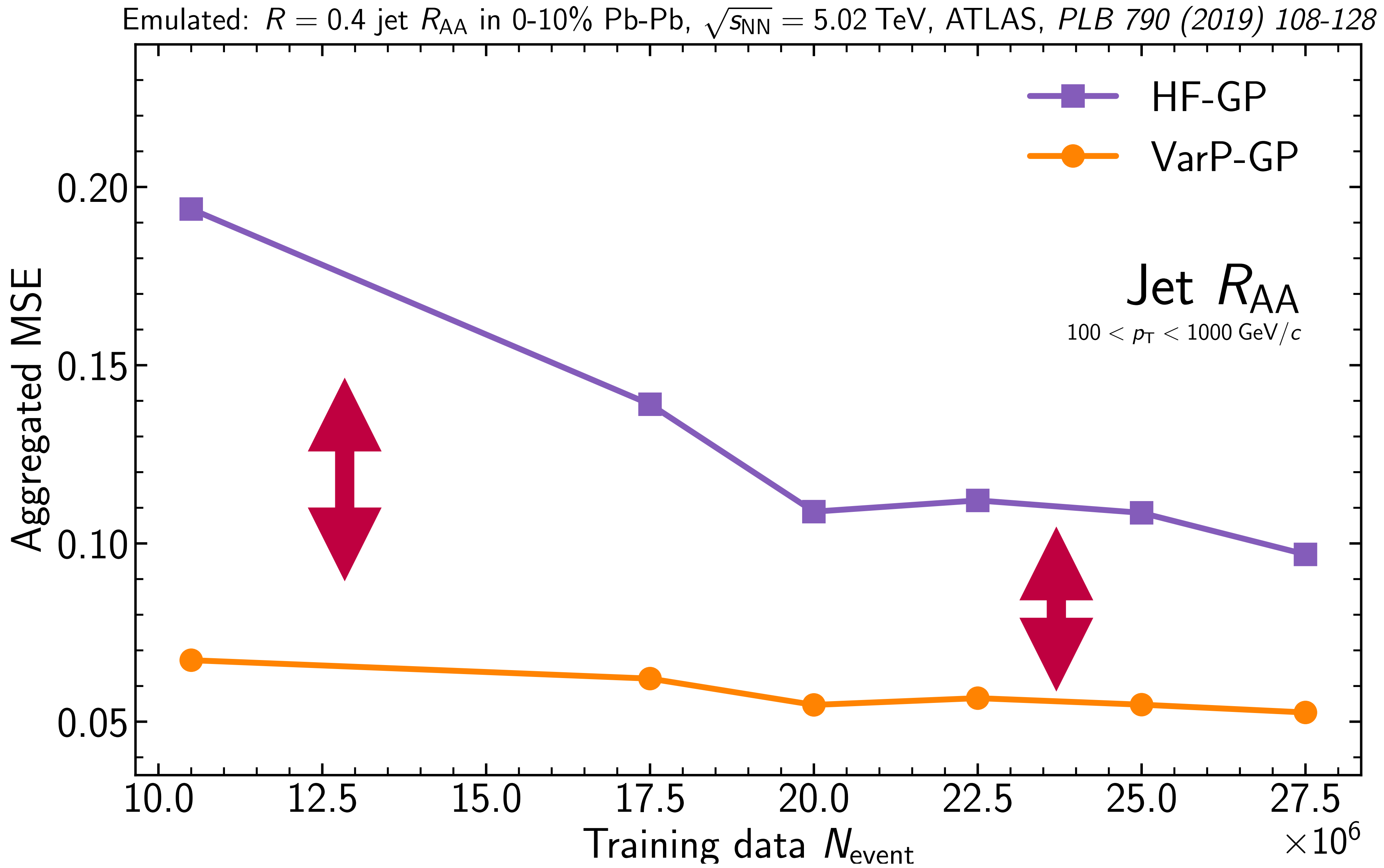


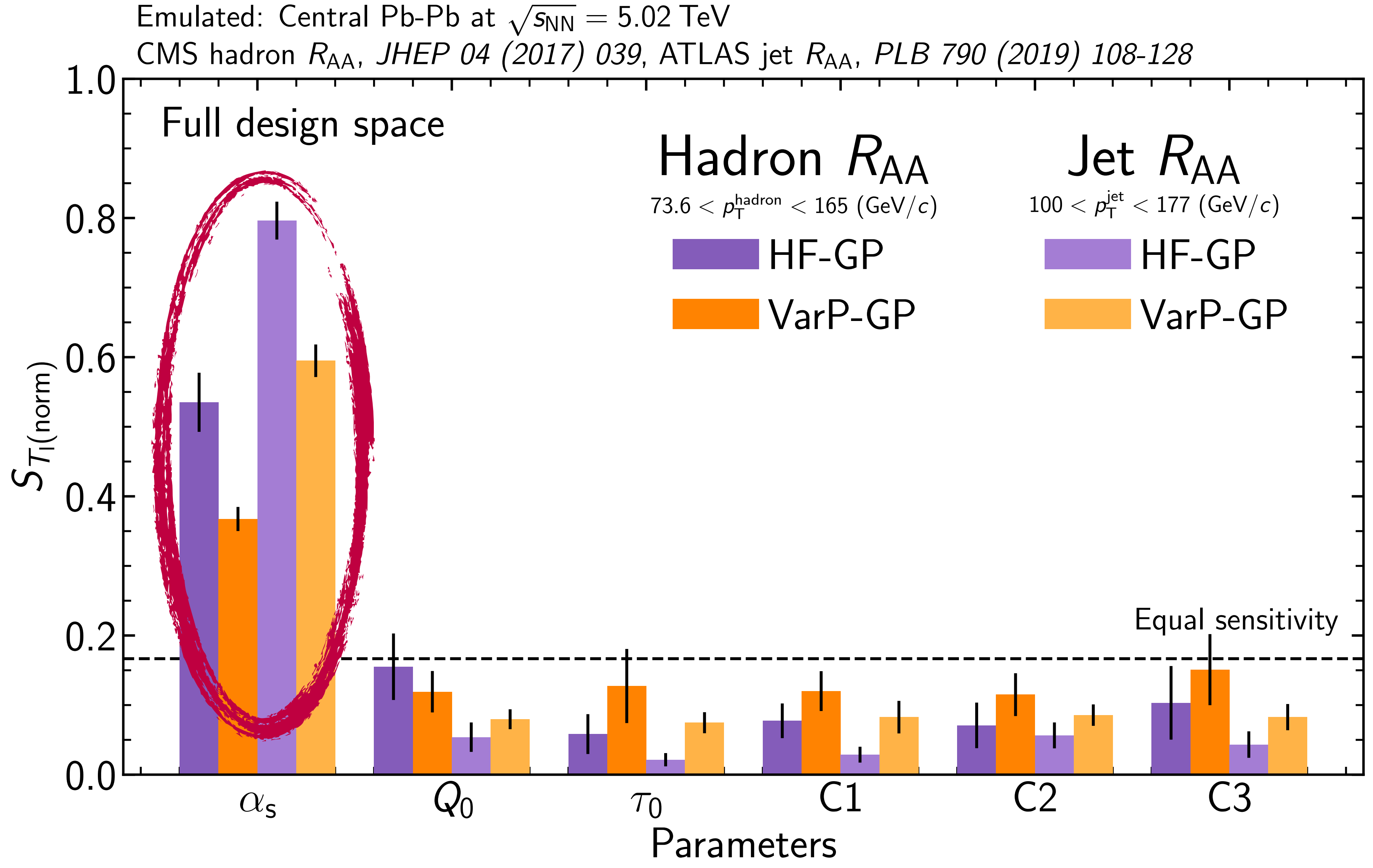


RJE, IJ, SM, PMJ, arXiv:2602.xxxxx

Summary

- **VarP-GP: Variable Precision GP**
  - New **heteroskedastic GP emulator** trained on calculations with **variable statistical precision across the parameter design space**
- Two novel developments:
  - Method to **efficiently distribute varied precision over design space**
  - Coupled GPs predict **mean and uncertainty**
- **Pools information across design space to provide better predictions at fixed computational budget**
  - Improved performance vs high fidelity GP
- **First sensitivity studies** for hard-sector observables





RJE, IJ, SM, PMJ, arXiv:2602.xxxxx

Backup

Bayesian inference: QGP

Legend

Hendrik, Lipei, Raymond, Oct 2024

Bayesian inference: QGP

Legend

...sterior | Applications | Assessments | Codes

models (expensive)
~5-30 parameters

training data

Experimental data

posterior

predictions

experimental design

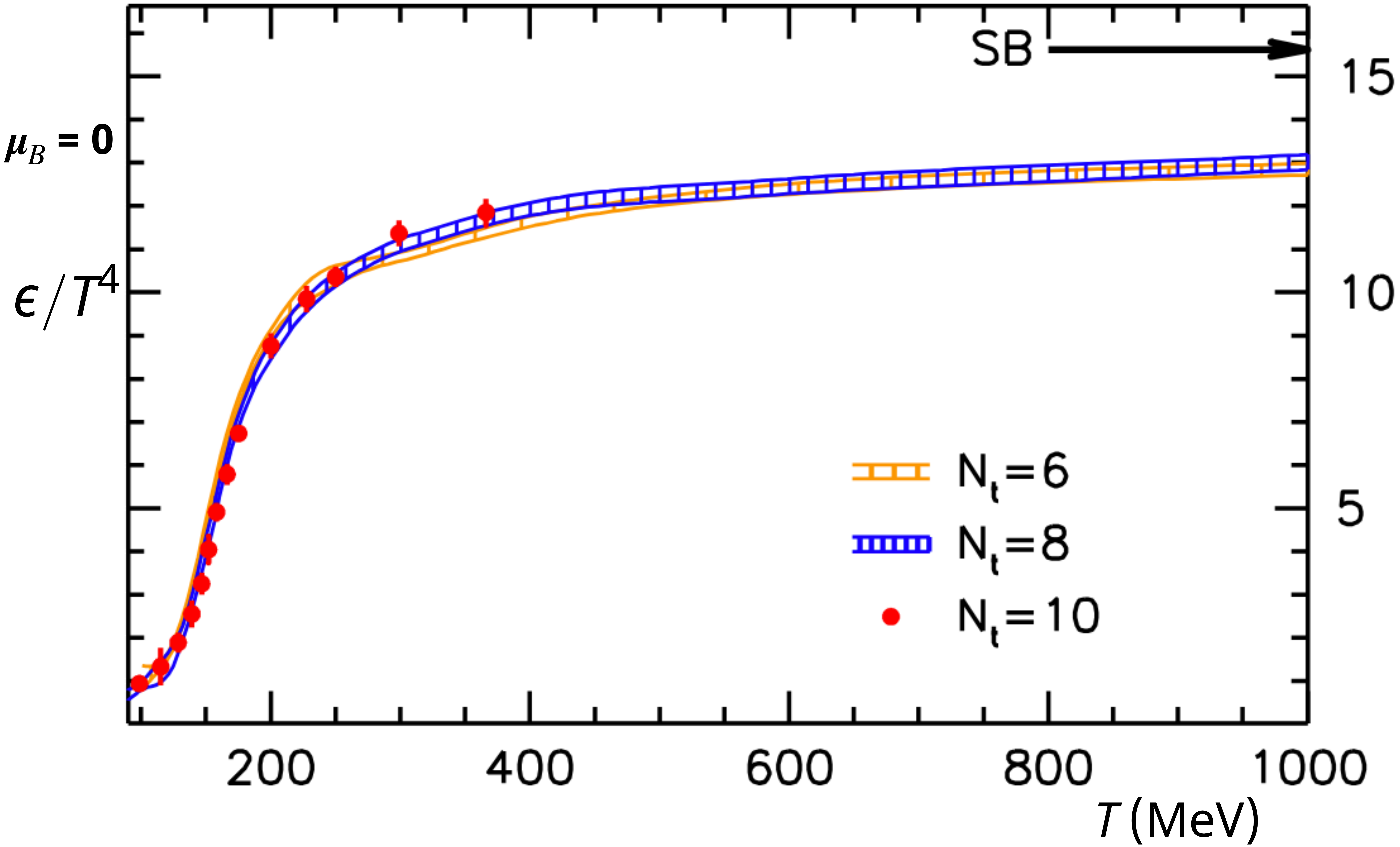
posterior analysis:
- ML: use posteriors as new priors
- clustering for multimodal posteriors

Bayes factor (model selection)

- Forward model **cost depend on physics processes** of interest
- **Expensive**: Usually **O(millions) core-hours over entire design parameter space**
- **~5-30 parameters, all of interest** (i.e. not nuisance parameters)
- Critical: **selection of design points**

Lattice QCD and the quark-gluon plasma

Lattice QCD
calculations at μ_B **= 0**



S. Borsanyi et al, JHEP 11 (2010) 077

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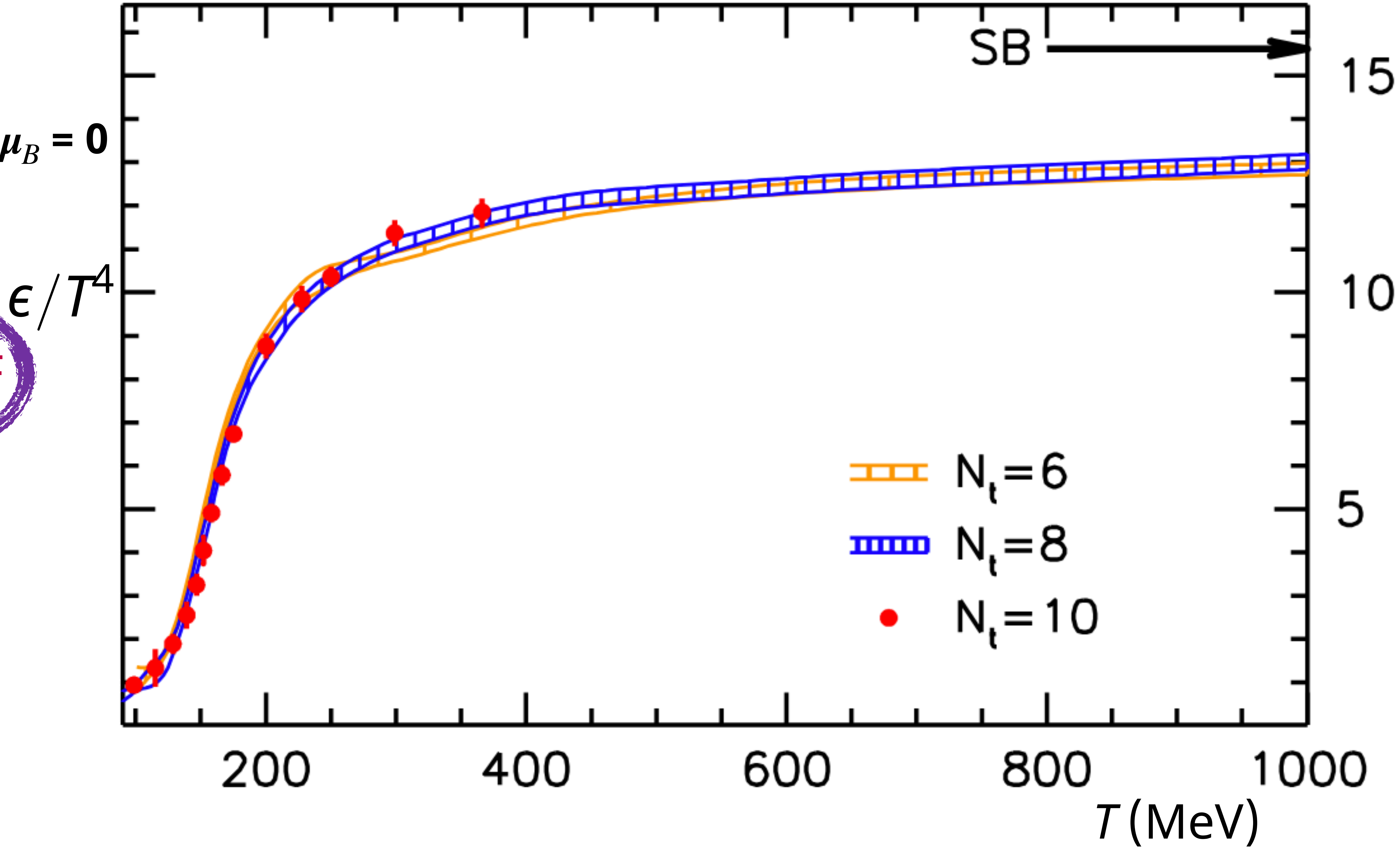
$\epsilon/T^4 \sim$ DOF



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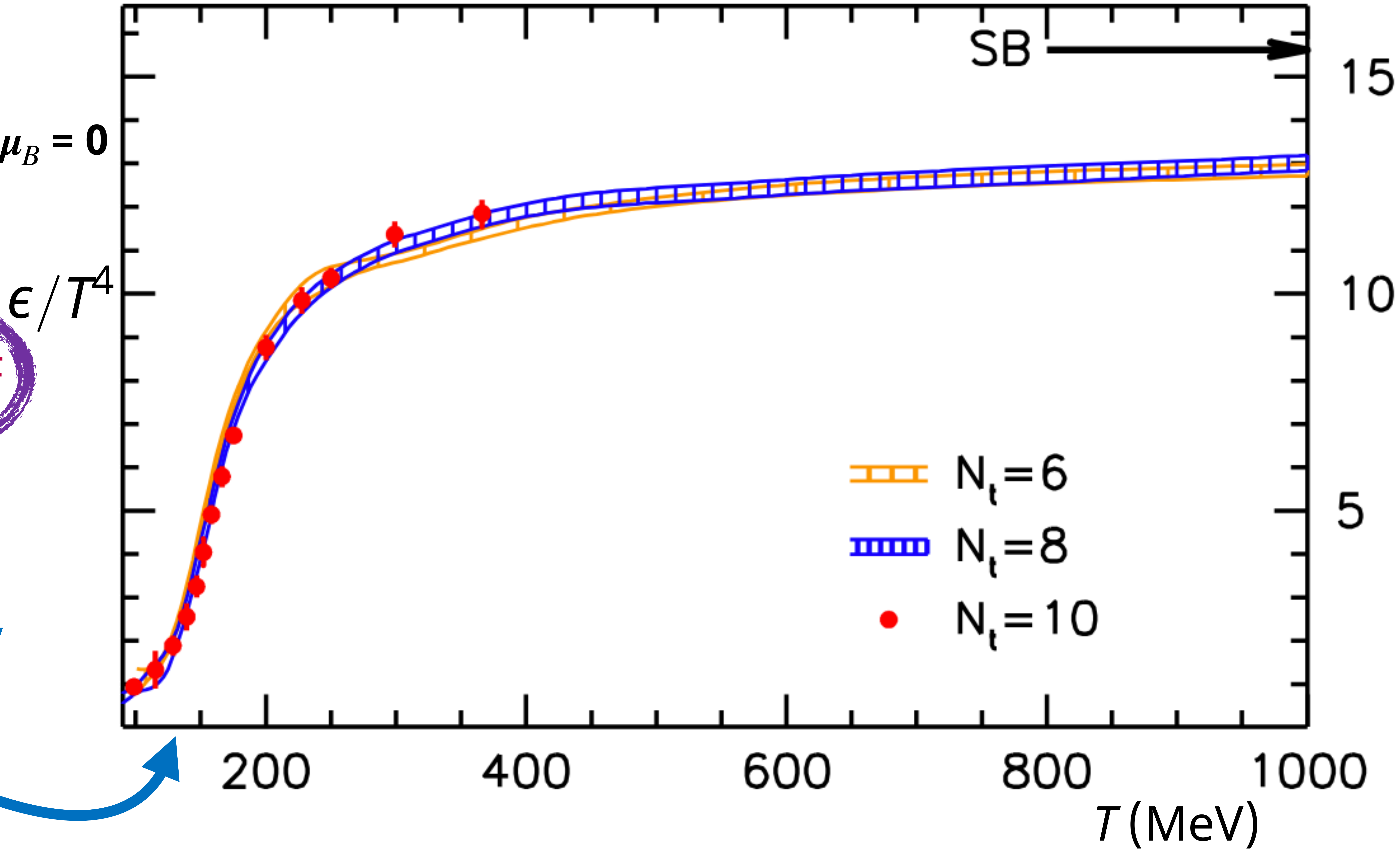
Predict **phase transition** at $T_C \sim$ **155 MeV**



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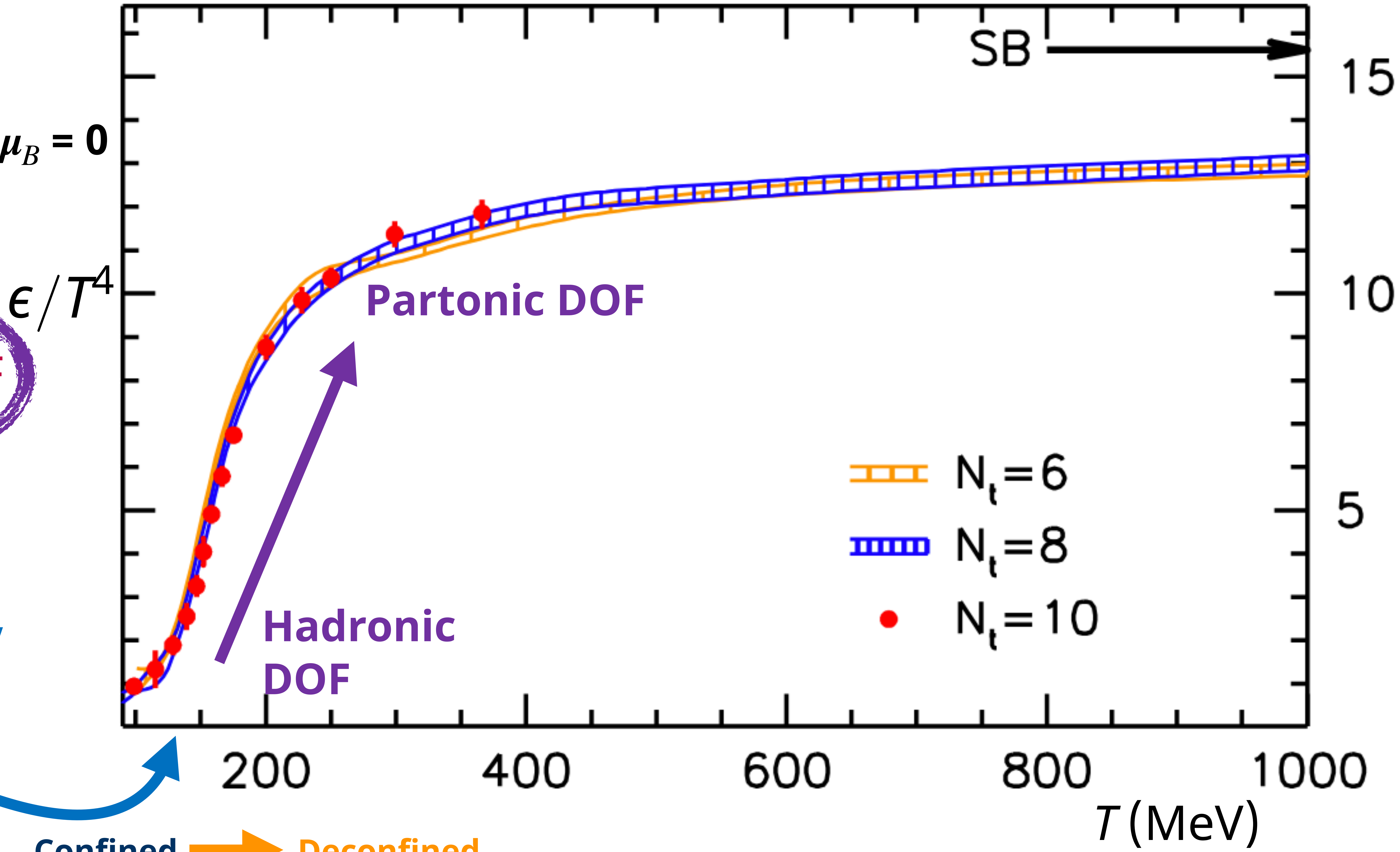

Confined → **Deconfined**

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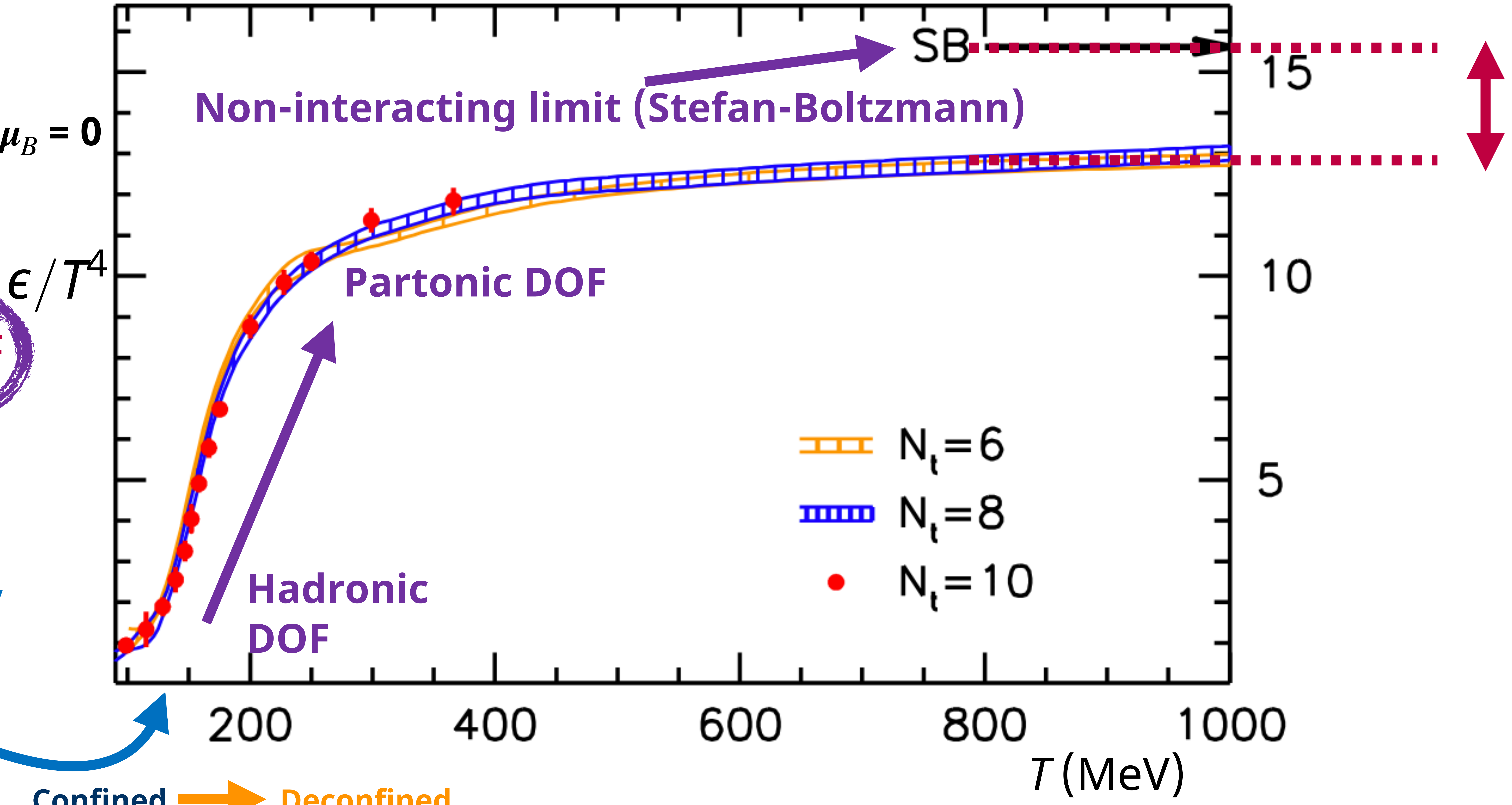

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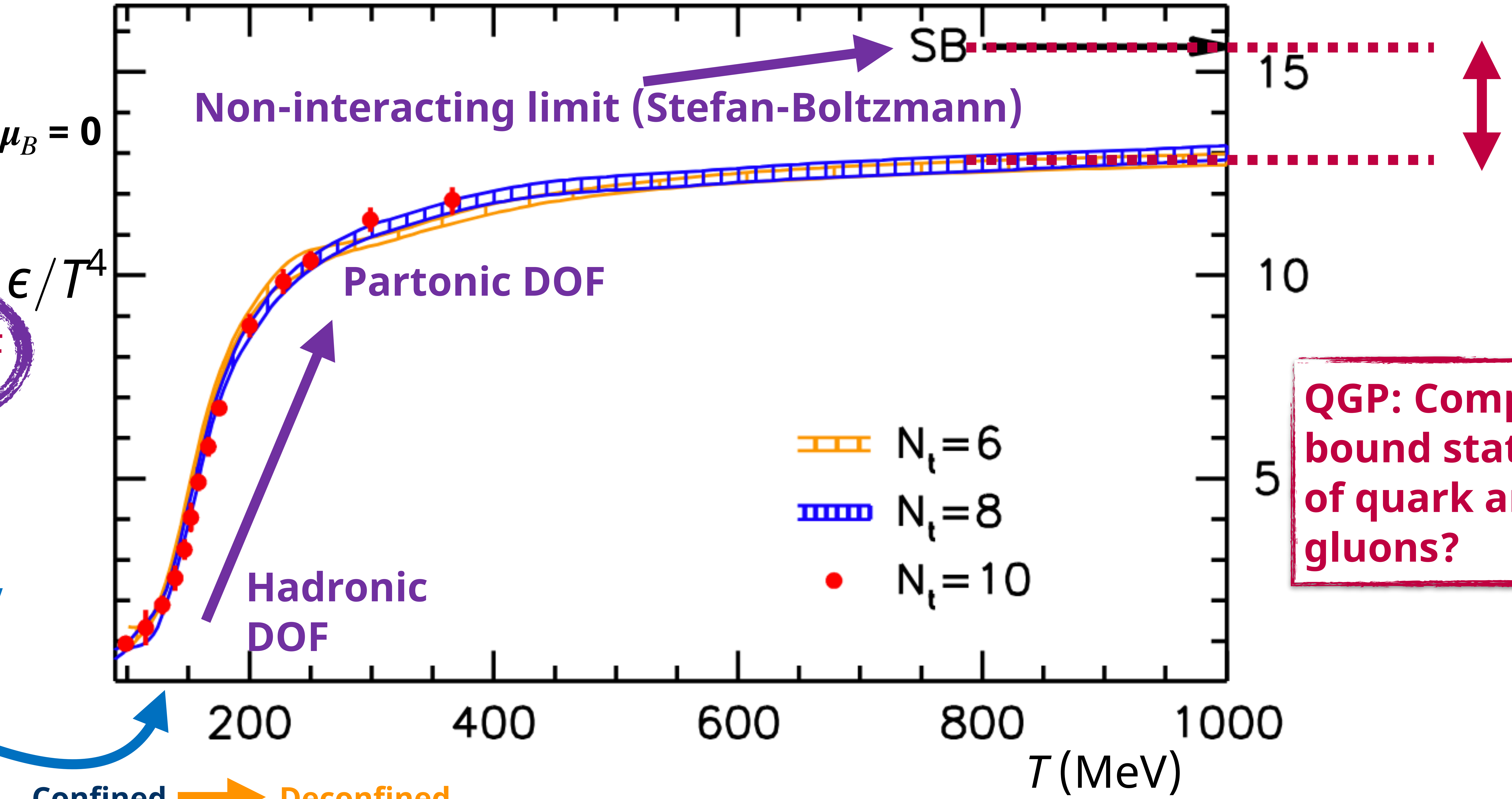


Confined → **Deconfined**

QGP: Complex bound states of quark and gluons?

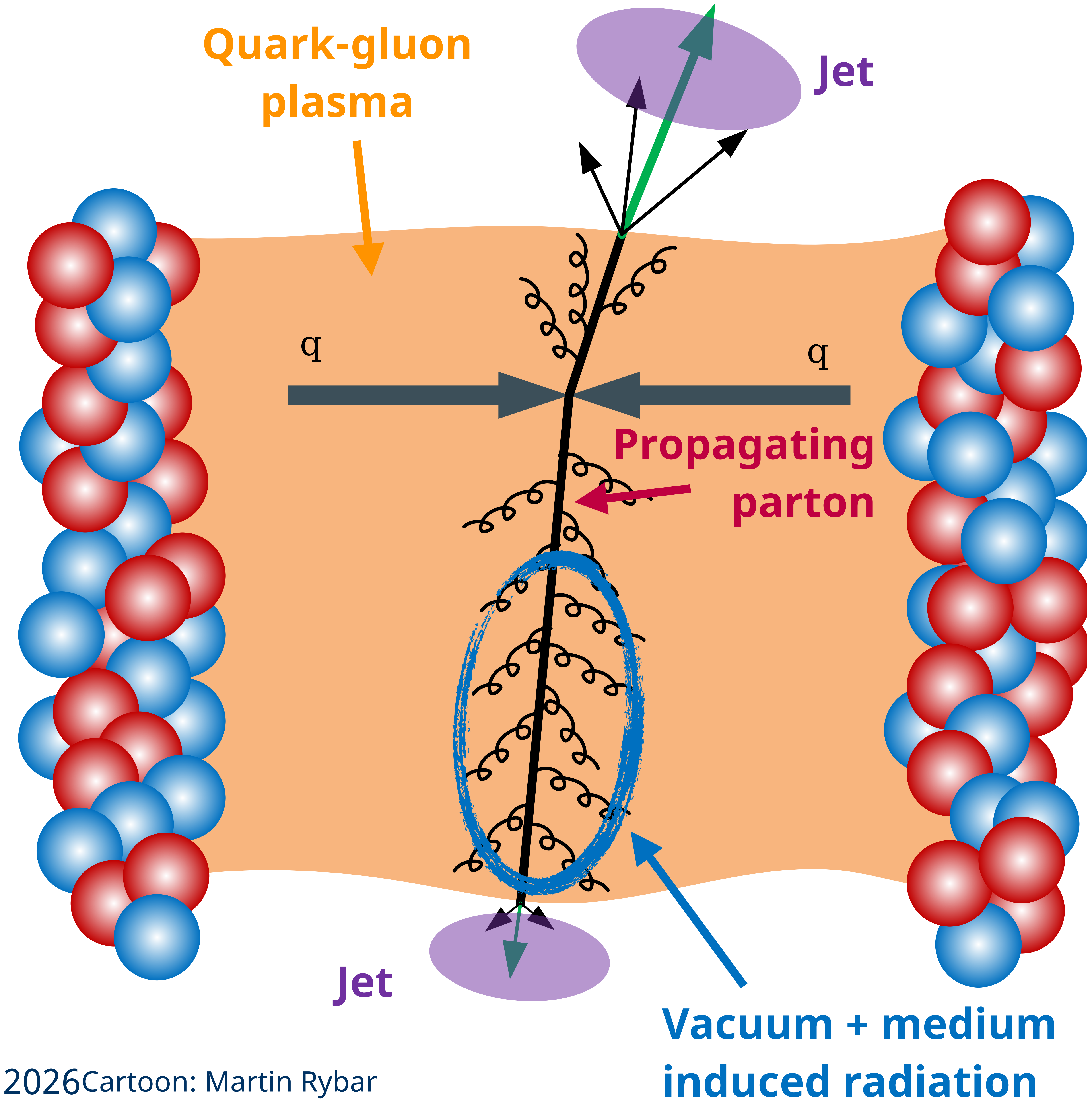
S. Borsanyi et al, JHEP 11 (2010) 077

Jets in the quark-gluon plasma: jet quenching

Jets produced early,
evolve with and
interact with medium

Interactions between parton
and medium: “jet quenching”

High momentum
→ resolve short distance scales
→ probe QGP microstructure



Cartoon: Martin Rybar

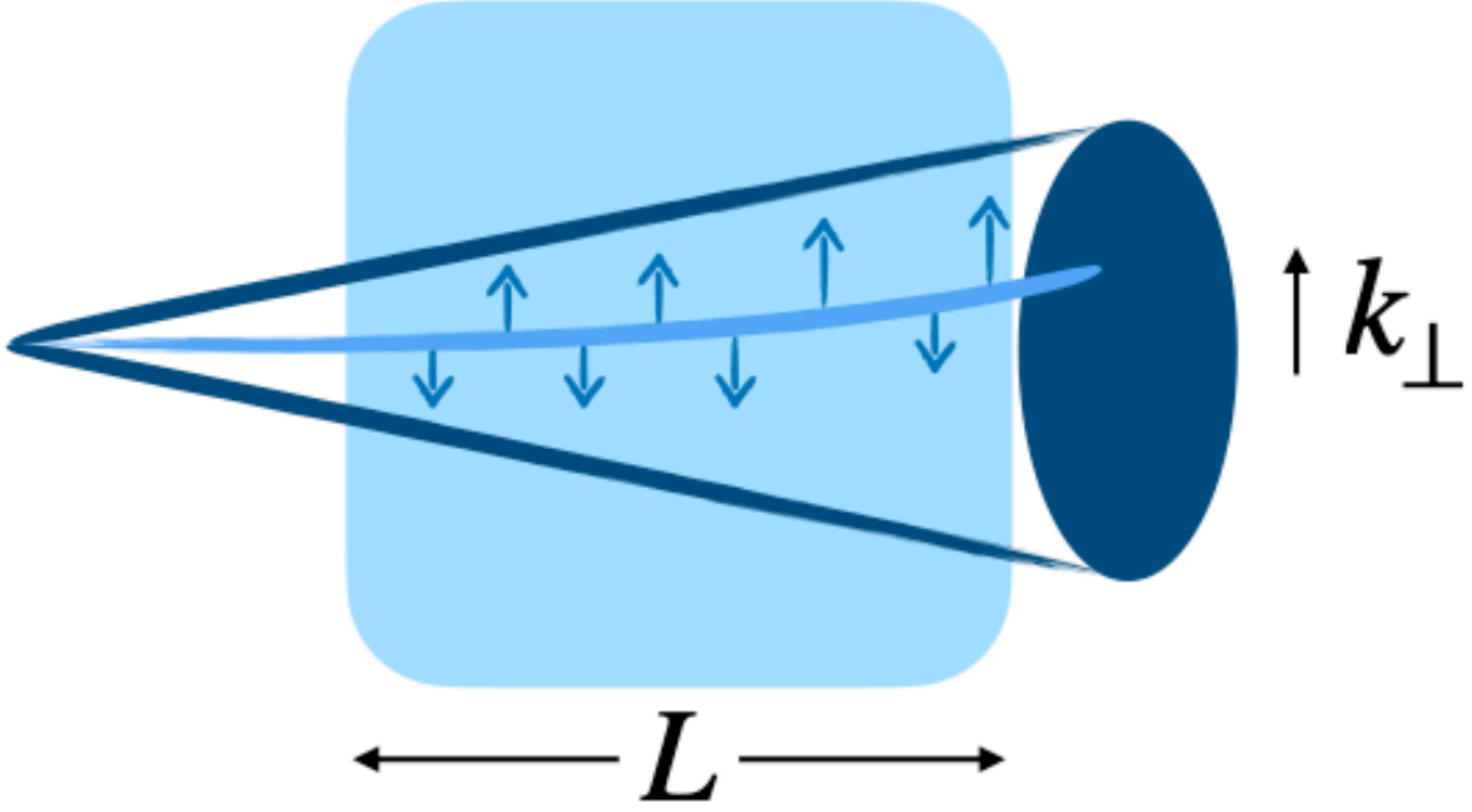
Bayesian analysis: Model

Analysis | **Model** | Data

- Ex: **Energy loss in QCD** matter characterized by **jet transport coefficient** $\hat{q}$
  - Path length L, momentum transfer k

$$\hat{q} \equiv \frac{\langle k_T^2 \rangle}{L} \sim \int k^2 C(k) \mathrm{d}^2 k$$

- **How to select functional form of $\hat{q}$?**



Bayesian analysis: Connecting models and data

Analysis | Model | Data

- **For a given model, which parameters are most compatible with exp. measurements**?
- Given data $\vec{x}$ and parameters $\vec{\theta}$, we can apply **Bayes' theorem**

$$P(\theta|x) = \frac{P(x|\theta)P(\theta)}{P(x)}$$

For further details, see: RJE @ Hard Probes 2024, arXiv:2507.22288
Matt Luzum, IS 2025

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- $P(\theta)$: **prior** distribution for θ
  - Choice makes assumptions explicit

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$$P(\theta|x) = \frac{P(x|\theta)P(\theta)}{P(x)}$$

- $P(x|\theta)$: **likelihood**
  x is described by θ
  - Depends on covariance, **data + theory uncert.**
- $P(\theta)$: **prior**
  distribution for θ
  - Choice makes assumptions explicit

For further details, see: RJE @ Hard Probes 2024, arXiv:2507.22288
Matt Luzum, IS 2025

Bayesian analysis: Connecting models and data

Analysis | Model | Data

- **For a given model, which parameters are most compatible with exp. measurements**?
- Given data $\vec{x}$ and parameters $\vec{\theta}$, we can apply **Bayes' theorem**

$$P(\theta|x) = \frac{P(x|\theta)P(\theta)}{P(x)}$$

- $P(\theta|x)$: **posterior dist.:** prob of θ given x
  - Most prob. value → **best description** of data
- $P(x|\theta)$: **likelihood** x is described by θ
  - Depends on covariance, **data + theory uncert.**
- $P(\theta)$: **prior** distribution for θ
  - Choice makes assumptions explicit

→ **Posterior encodes everything we want to learn**

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- **Extracting QGP properties is important, but not the only goal!**
- **Broad consistency of model and data**?
  - Search for **regions of tension, areas for improvement**
- **Sensitivity studies + experimental design**
  - **What should we measure next?**

- $P(\theta|x)$: **posterior dist.:** prob of θ given x
  - Most prob. value → **best description** of data

data + theory uncert.

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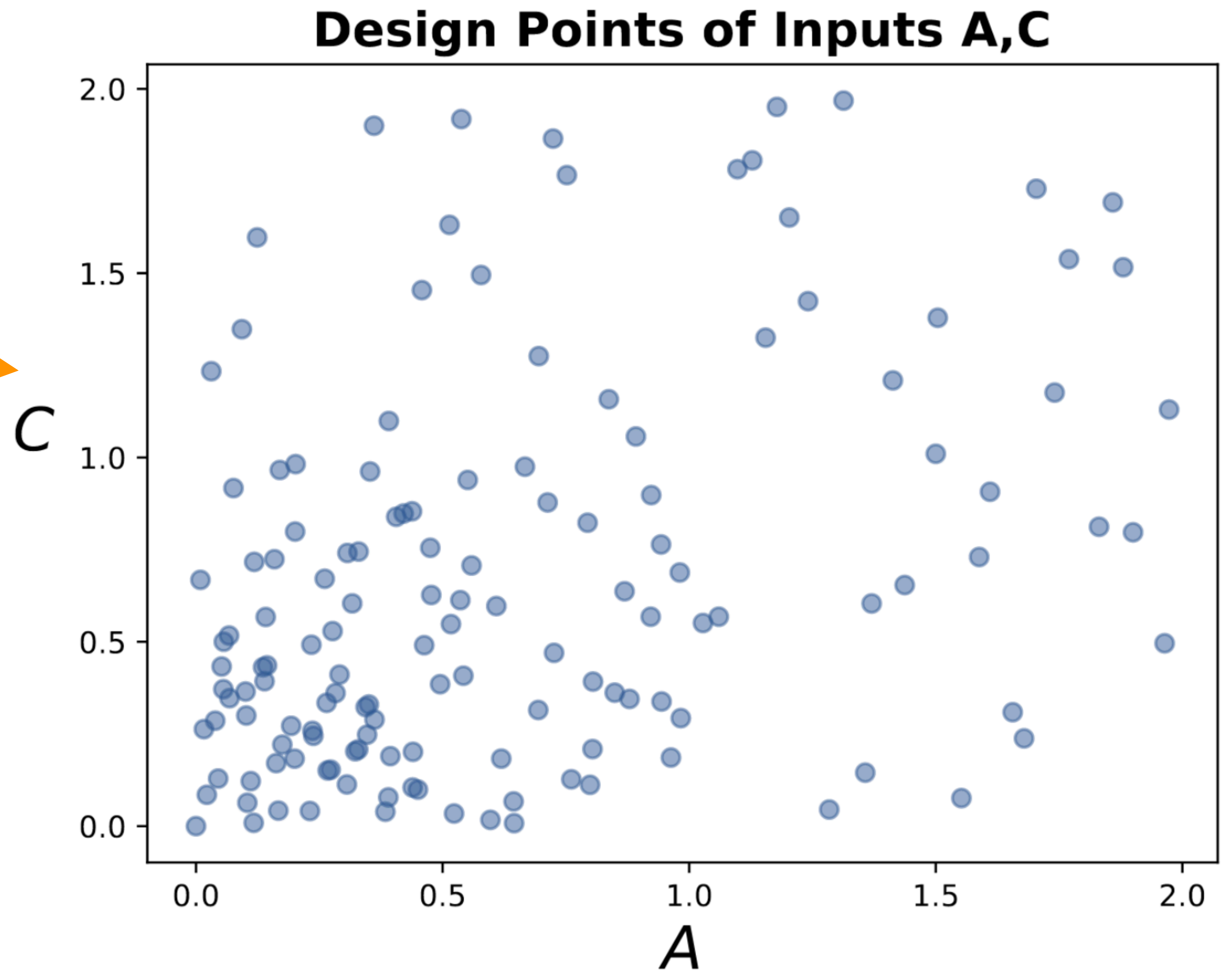
Bayesian analysis: In practice

Analysis | Model | Data

Simplified procedure

1. **Implement parameters to control model (a "parametrization")**
2. **Explore parameter space (w/ bounds from prior)**



- Approach enables **computationally tractable procedure** to extract parameters
  - Calculate limited number of points
  - Interpolate to cover phase space
- **Parameterization + prior choices matter, intertwined with model**

*: Model not necessarily formulated in terms of $\hat{q}$

Bayesian analysis: In practice

Analysis | Model | Data

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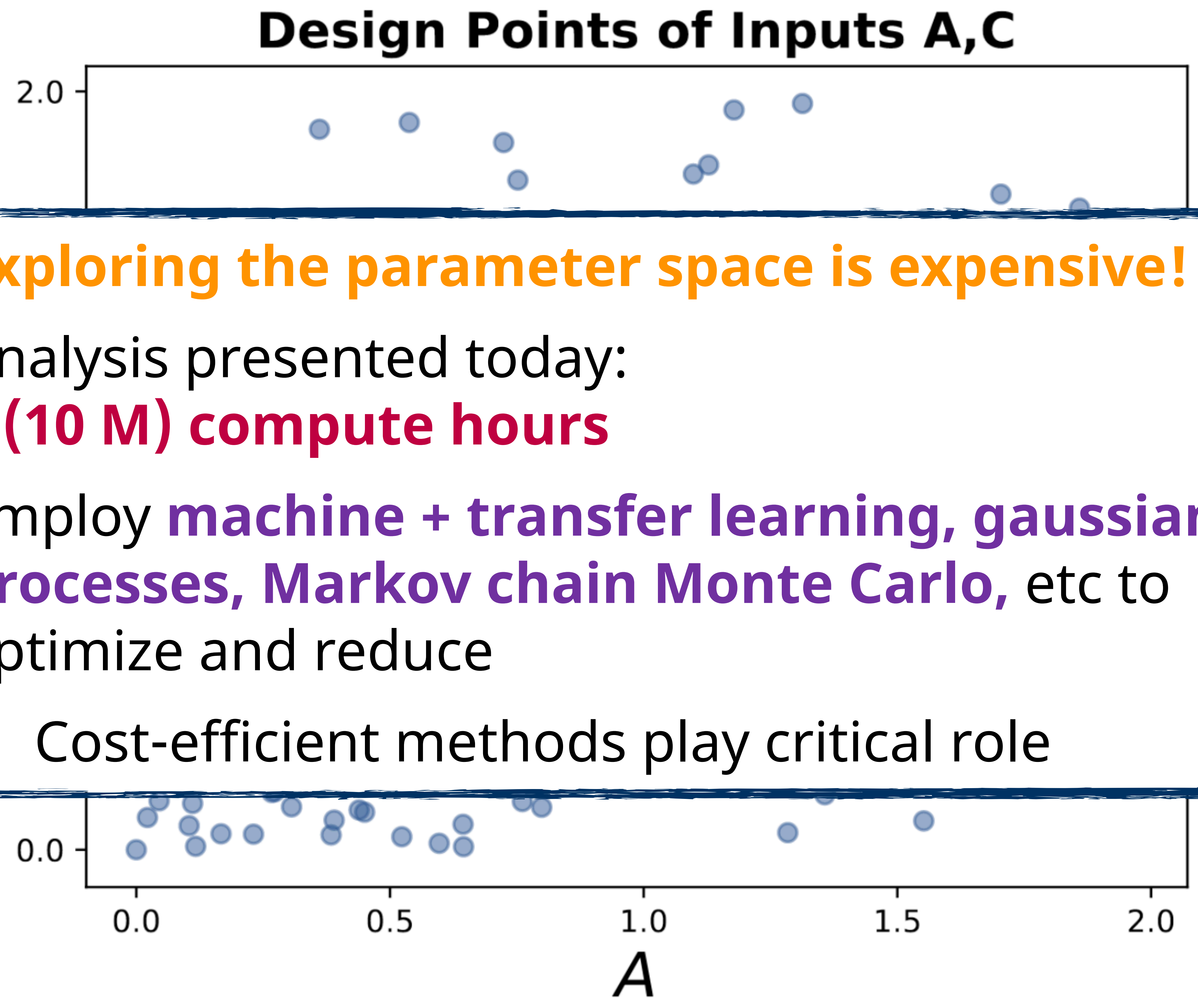


- **Exploring the parameter space is expensive!**
- Analysis presented today:
  O(10 M) compute hours
- Employ **machine + transfer learning, gaussian processes, Markov chain Monte Carlo**, etc to optimize and reduce
  - Cost-efficient methods play critical role

*: Model not necessarily formulated in terms of $\hat{q}$

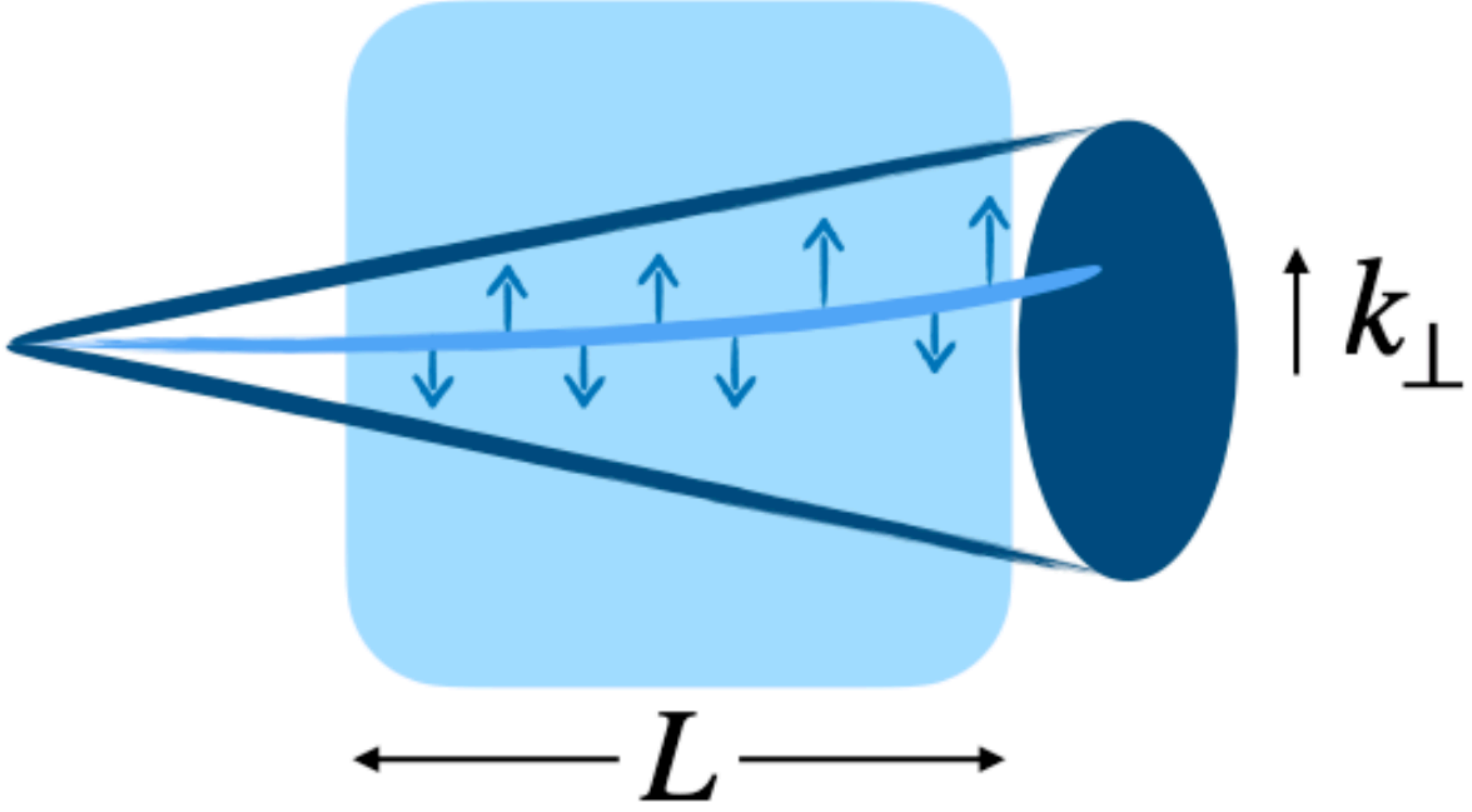
Bayesian analysis: Model*

Analysis | **Model** | Data

- **Pick your favorite Monte Carlo:**
  CUJET, DREENA, Hybrid,
  JETSCAPE (MATTER+LBT), (Co)LBT, LIDO,
  MATTER, MARTINI, pQCD based, …
  - Explore parameter space of these models
- **Model choices matter!**
- **Conclusions may be more general**

- Ex: **Energy loss in QCD** matter characterized by **jet transport coefficient** $\hat{q}$
  - Path length L, momentum transfer k

$$\hat{q} \equiv \frac{\langle k_T^2 \rangle}{L} \sim \int k^2 C(k) \mathrm{d}^2 k$$



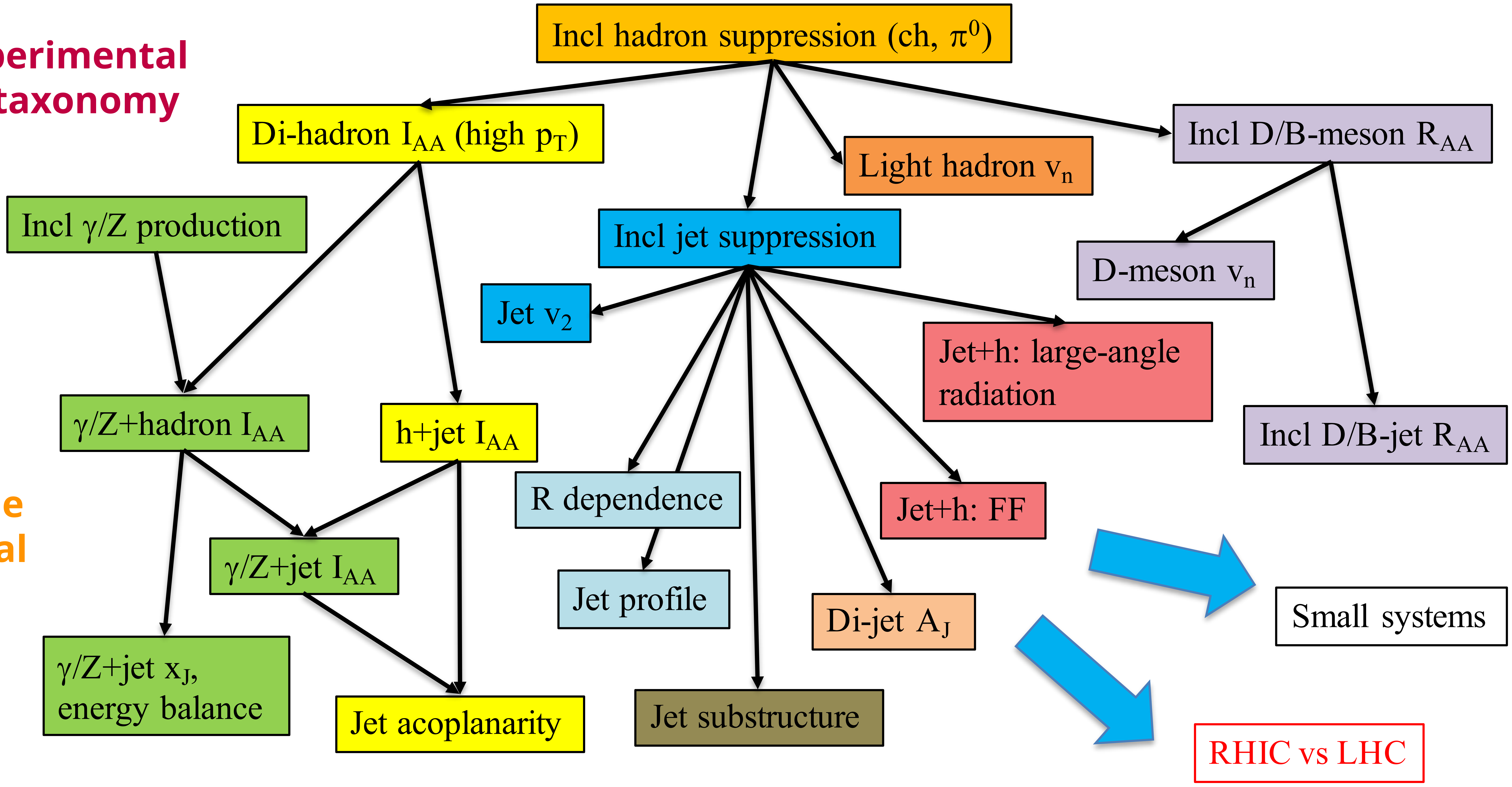
*: focusing on the hard sector

Bayesian analysis: Data

Analysis | Model | **Data**

Possible experimental observable taxonomy

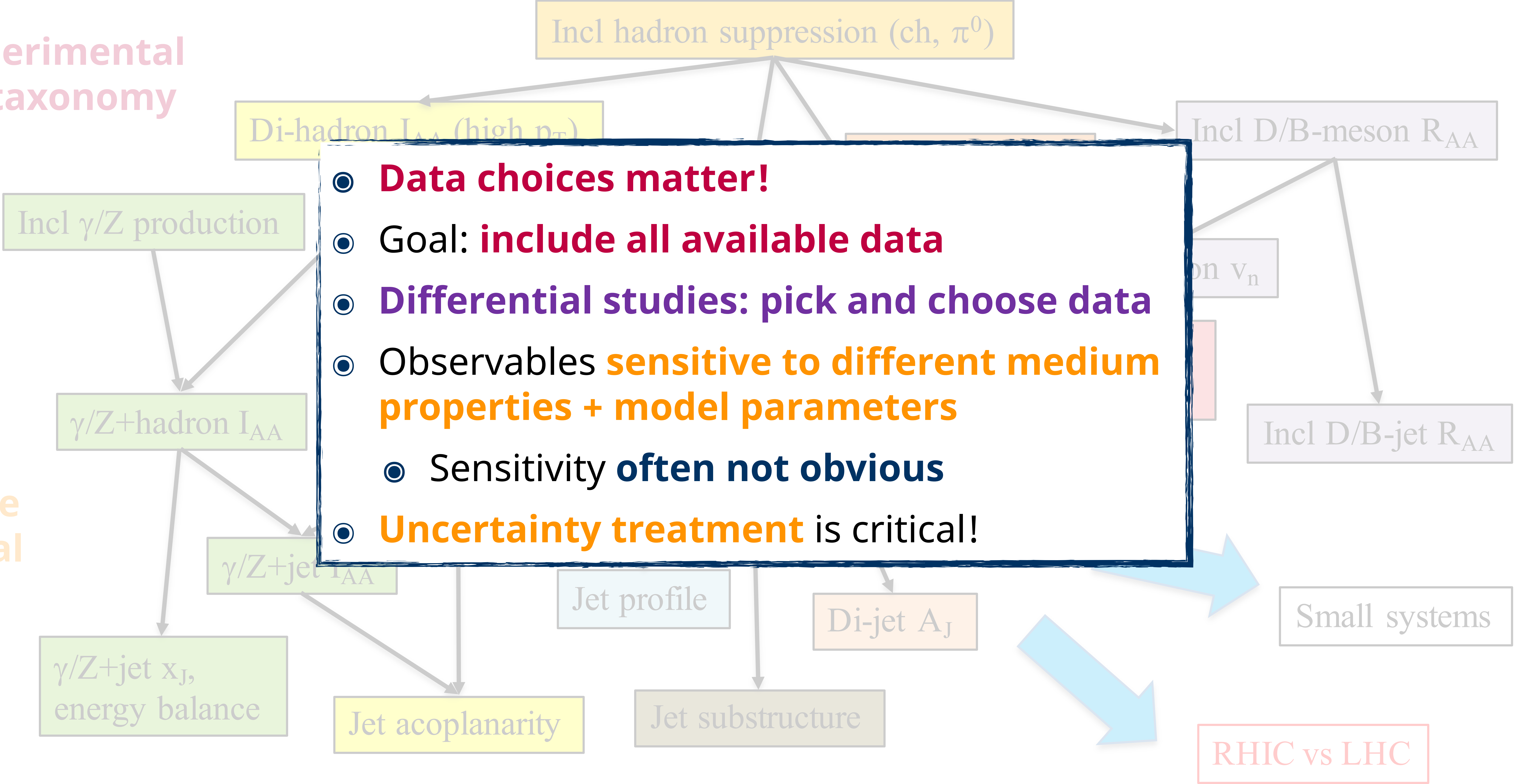
Line adds **one experimental element**



Bayesian analysis: Data

Analysis | Model | **Data**

Possible experimental observable taxonomy



- **Data choices matter!**
- Goal: **include all available data**
- **Differential studies: pick and choose data**
- Observables **sensitive to different medium properties + model parameters**
  - Sensitivity **often not obvious**
- **Uncertainty treatment** is critical!

Line adds **one experimental element**

Inclusive hadron and jet R_{AA} data

Analysis | Model | **Data**

- **Inclusive hadron and jet R_{AA} data**
- We adopt an **agnostic approach**: all qualified dataset by a cutoff time (Feb 2022) are included[1]
  - "Qualified" = right category, in target phase space, possible to compare rigorously
- In total **729 data points** used, jump up from previous iteration of analysis of similar nature
- Treat experimental **uncertainty correlations where possible** (incl. source-by-source info)

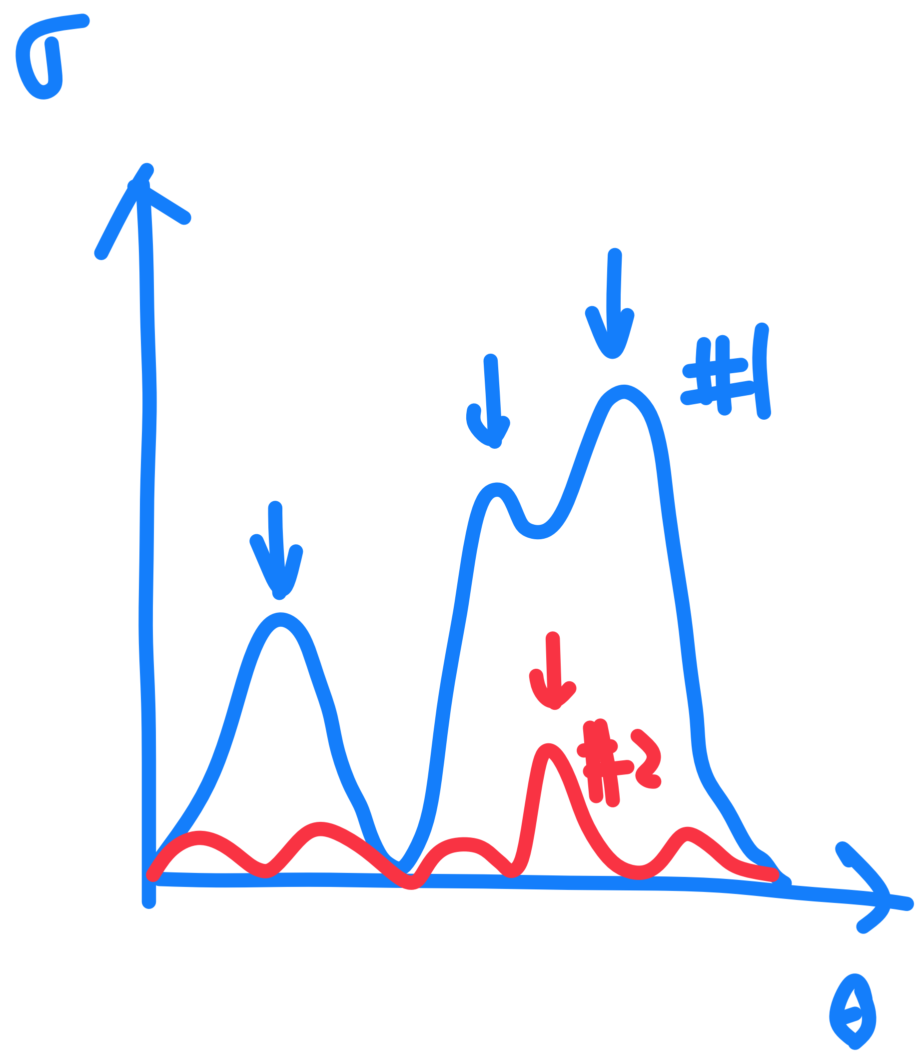
Inclusive hadron R_{AA}					
Collab./ref.	System; $\sqrt{s_{NN}}$ [TeV]	Species	Accept.	centr. %	p_T range [GeV/c]
STAR [101]	Au–Au; 0.2	charged	$\|\eta\| < 0.5$	[0,40]	[9,12]
ALICE [102]	Pb–Pb; 2.76, 5.02	charged	$\|\eta\| < 0.8$	[0,50]	[9,50]
ATLAS [99]	Pb–Pb; 2.76	charged	$\|\eta\| < 2$	[0,40]	[9,150]
CMS [103]	Pb–Pb; 2.76	charged	$\|\eta\| < 1.0$	[0,50]	[9,100]
CMS [100]	Pb–Pb; 5.02	charged	$\|\eta\| < 1.0$	[0,50]	[9,400]
PHENIX [104]	Au–Au; 0.2	π^0	$\|\eta\| < 0.35$	[0,50]	[9,20]
ALICE [105, 106]	Pb–Pb; 2.76	π^0	$\|\eta\| < 0.7$	[0,50]	[9,20]
ALICE [107, 108]	Pb–Pb; 2.76	$\pi^\pm$	$\|\eta\| < 0.8$	[0,40]	[9,20]
ALICE [109]	Pb–Pb; 5.02	$\pi^\pm$	$\|\eta\| < 0.8$	[0,50]	[9,20]

Inclusive jet R_{AA}						
Collab./ref.	System; $\sqrt{s_{NN}}$ [TeV]	type	R	Accept.	centr. %	p_T range [GeV/c]
STAR [110]	Au–Au; 0.2	charged	[0.2,0.4]	$\|\eta\| < 1 - R$	[0,10]	[15,30]
ALICE [111]	Pb–Pb; 2.76	full	0.2	$\|\eta\| < 0.5$	[0,30]	[30,100]
ALICE [22]	Pb–Pb; 5.02	full	0.2,0.4	$\|\eta\| < 0.5$	[0,10]	[40,140]
ATLAS [112]	Pb–Pb; 2.76	full	0.4	$\|\eta\| < 2.1$	[0,50]	[32,500]
ATLAS [113]	Pb–Pb; 5.02	full	0.4	$\|\eta\| < 2.8$	[0,50]	[50,1000]
CMS [114]	Pb–Pb; 2.76	full	[0.2,0.4]	$\|\eta\| < 2.0$	[0,50]	[70,300]
CMS [115]	Pb–Pb; 5.02	full	[0.2,1.0]	$\|\eta\| < 2.0$	[0,50]	[200,1000]

[1]: ATLAS Hadron R_{AA} @ 5.02 TeV after cutoff date

Active learning design points

- First batch (40): Latin Hypercube → Train emulators → Final set of design points (230)
- Train emulators → Predictive error across phase space → Pick next batch (20-40 points) → Train emulators



Analysis
Model
Data

Prioritize **reducing predictive error across the full space**

Do not look at experimental data during this process

RJE, JETSCAPE, arXiv:2408.08247

Model and $\hat{q}$ parametrization

Analysis | **Model** | Data

JETSCAPE multi-stage model: MATTER+LBT

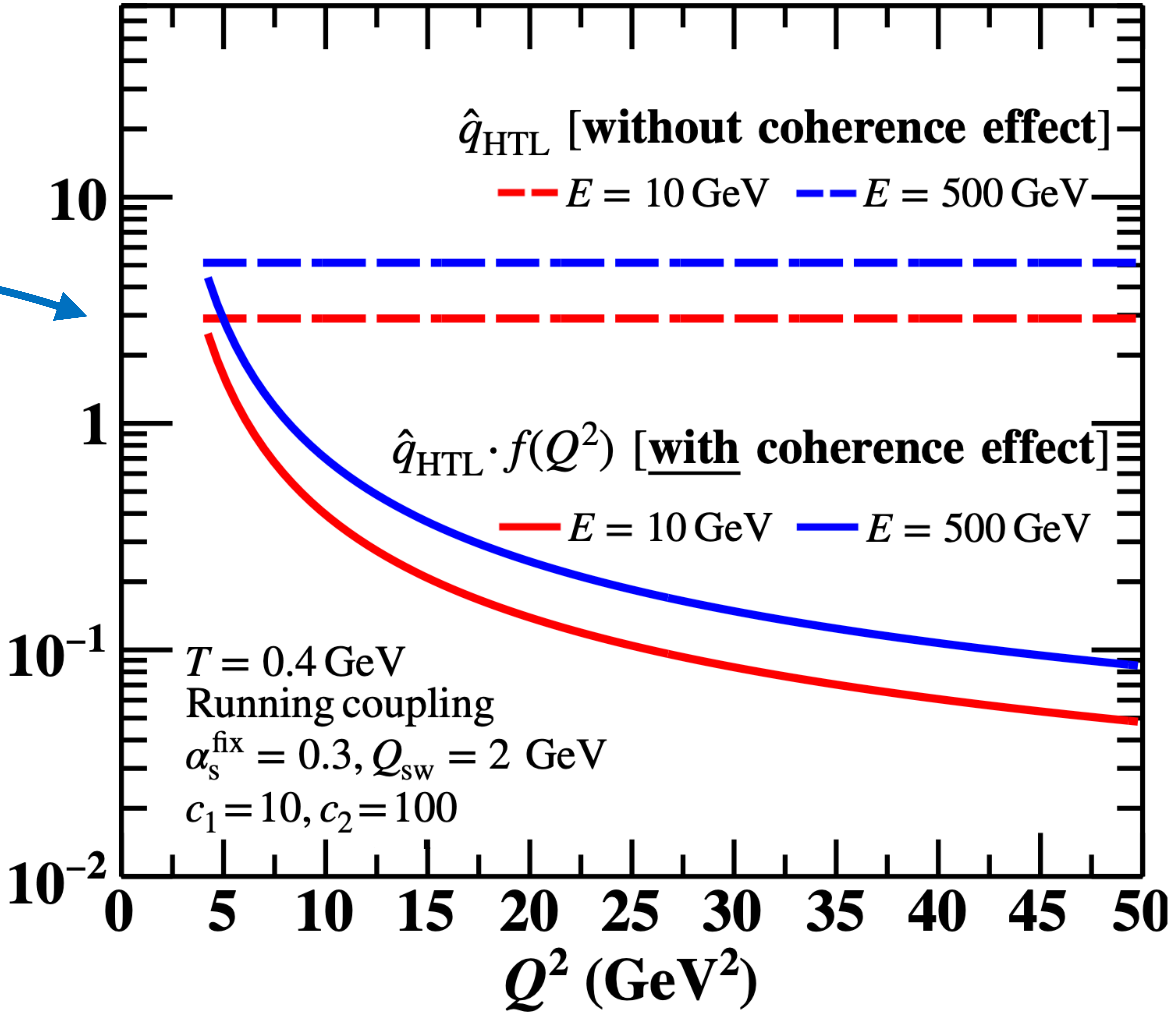
$$\hat{q}(E,T,Q) = \hat{q}^{\text{run}}_{\text{HTL}} \times f(Q^2)$$

$$\hat{q}^{\text{run}}_{\text{HTL}} = \alpha_{s,\text{fix}} \times \alpha_s(\mu^2) C_a \frac{42\zeta(3)}{\pi} T^3 \log\left(\frac{\mu^2}{6\pi T^2 \alpha_{s,\text{fix}}}\right)$$

$$f(Q^2) = \left.\frac{N(\exp(c_3(1-x_B))-1)}{1 + c_1 \ln(Q^2/\Lambda^2_{\text{QCD}}) + c_2 \ln^2(Q^2/\Lambda^2_{\text{QCD}})}\right|_{Q \geq Q_0}$$

- 6 total parameters:
  - α_s
  - c_1, c_2, c_3
  - Q_0 (switching virtuality)
  - τ_0 (start time)

◉ Propagated through **calibrated 2+1D hydro**



JETSCAPE, *Phys.Rev.C* 107 (2023) 3, 034911
JETSCAPE, *Phys.Rev.C* 110 (2024) 4, 044907

Model and $\hat{q}$ parametrization

Analysis | **Model** | Data

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$$f(Q^2) = \frac{N(\exp(c_3(1 - \ldots}{1 + c_1 \ln(Q^2/\Lambda^2_{\text{QCD}}) + \ldots}$$

- 6 total parameters:
  - α_s
  - c_1, c_2, c_3
  - Q_0 (switching virtuality)
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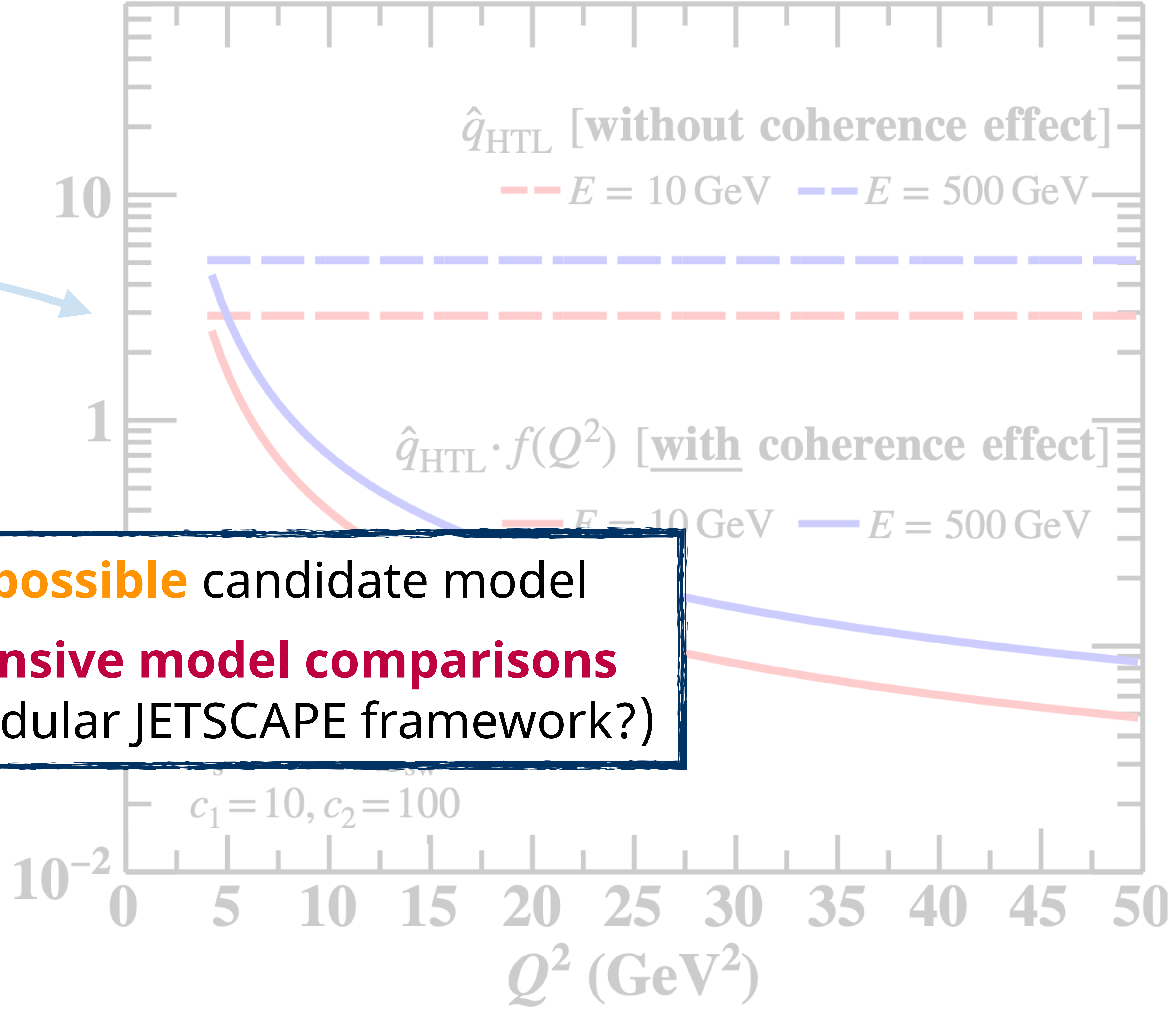
- Propagated through **calibrated 2+1D hydro**



JETSCAPE, *Phys.Rev.C* 107 (2023) 3, 034911
JETSCAPE, *Phys.Rev.C* 110 (2024) 4, 044907

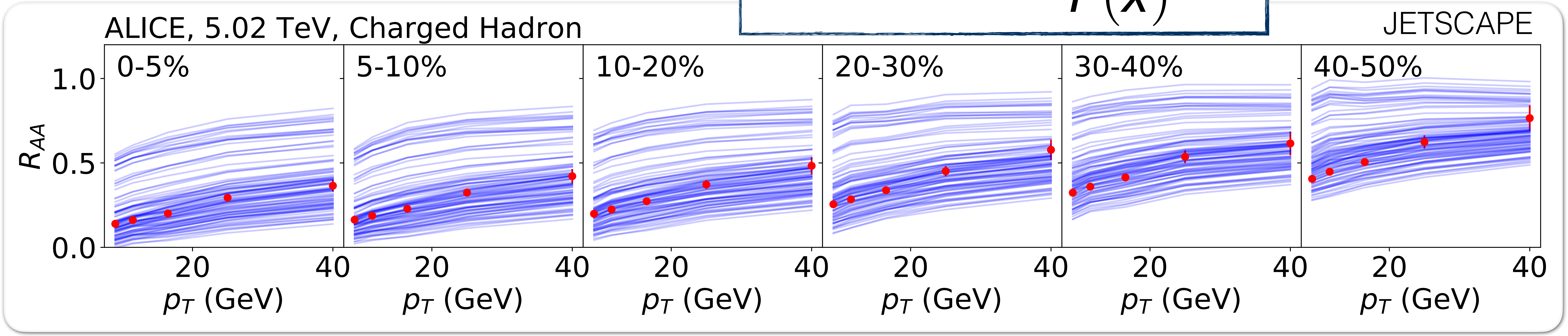
- Today: Taken as one **possible** candidate model

➡ **Later: comprehensive model comparisons**
(advantage of modular JETSCAPE framework?)

From Prior to Posterior

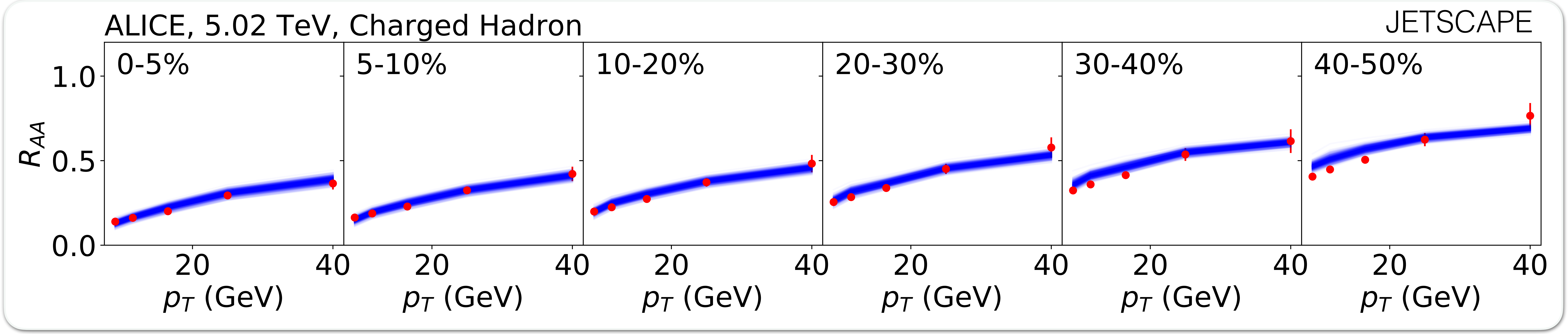
$$P(\theta|x) = \frac{P(x|\theta)P(\theta)}{P(x)}$$

Data
Prior



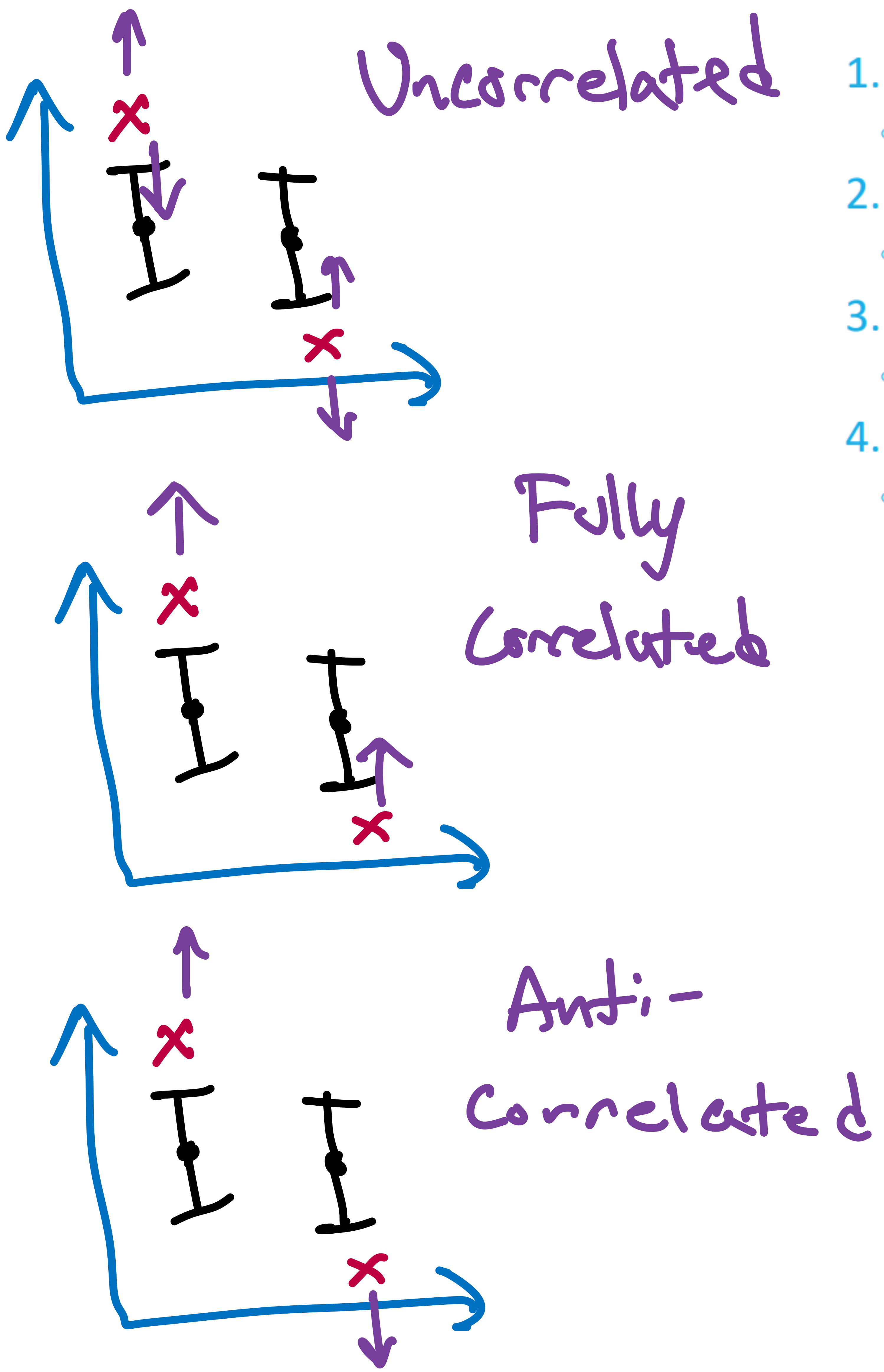
↓ Analysis

Data
Posterior



RJE, JETSCAPE, arXiv:2408.08247

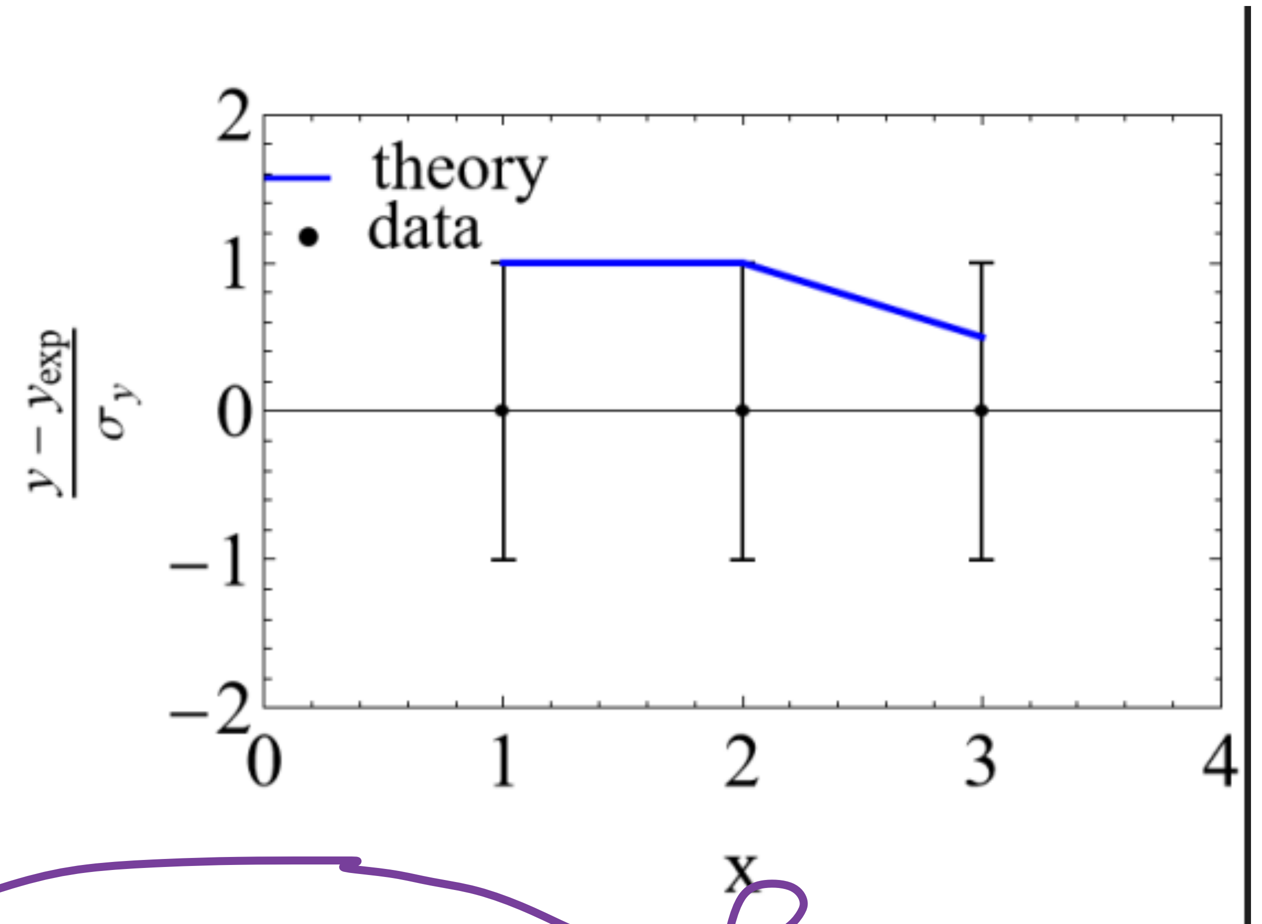
Measurement uncertainties and correlations

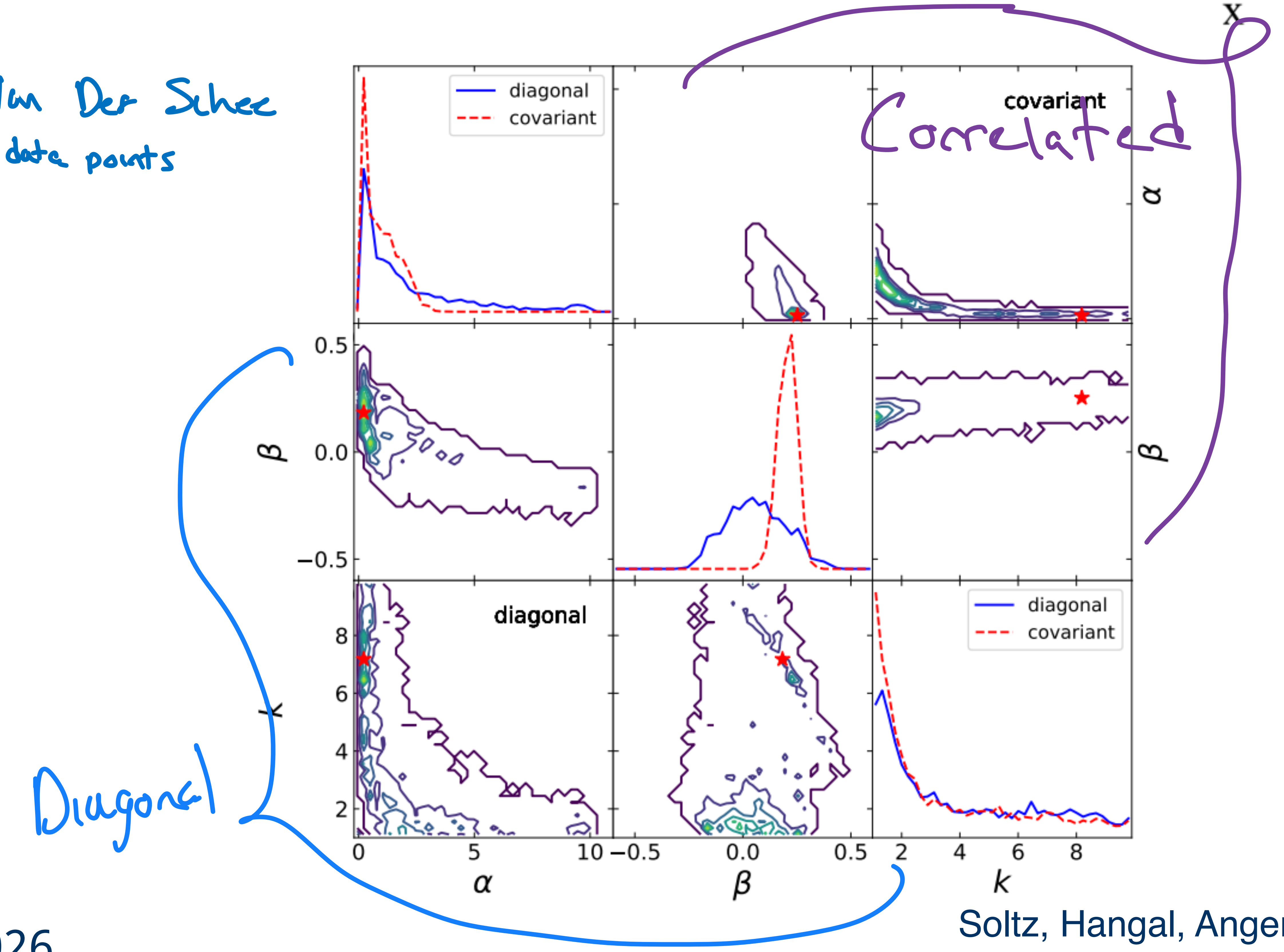


1. For uncorrelated uncertainties?
   - 0.325
2. If 1 & 2 are fully correlated?
   - Ill defined / infinity
3. If 1 & 3 are fully correlated?
   - Ill defined / zero
4. For a realistic covariance matrix?
   - 1.439

Example from Van Der Schee for liklihood w/ 3 data points

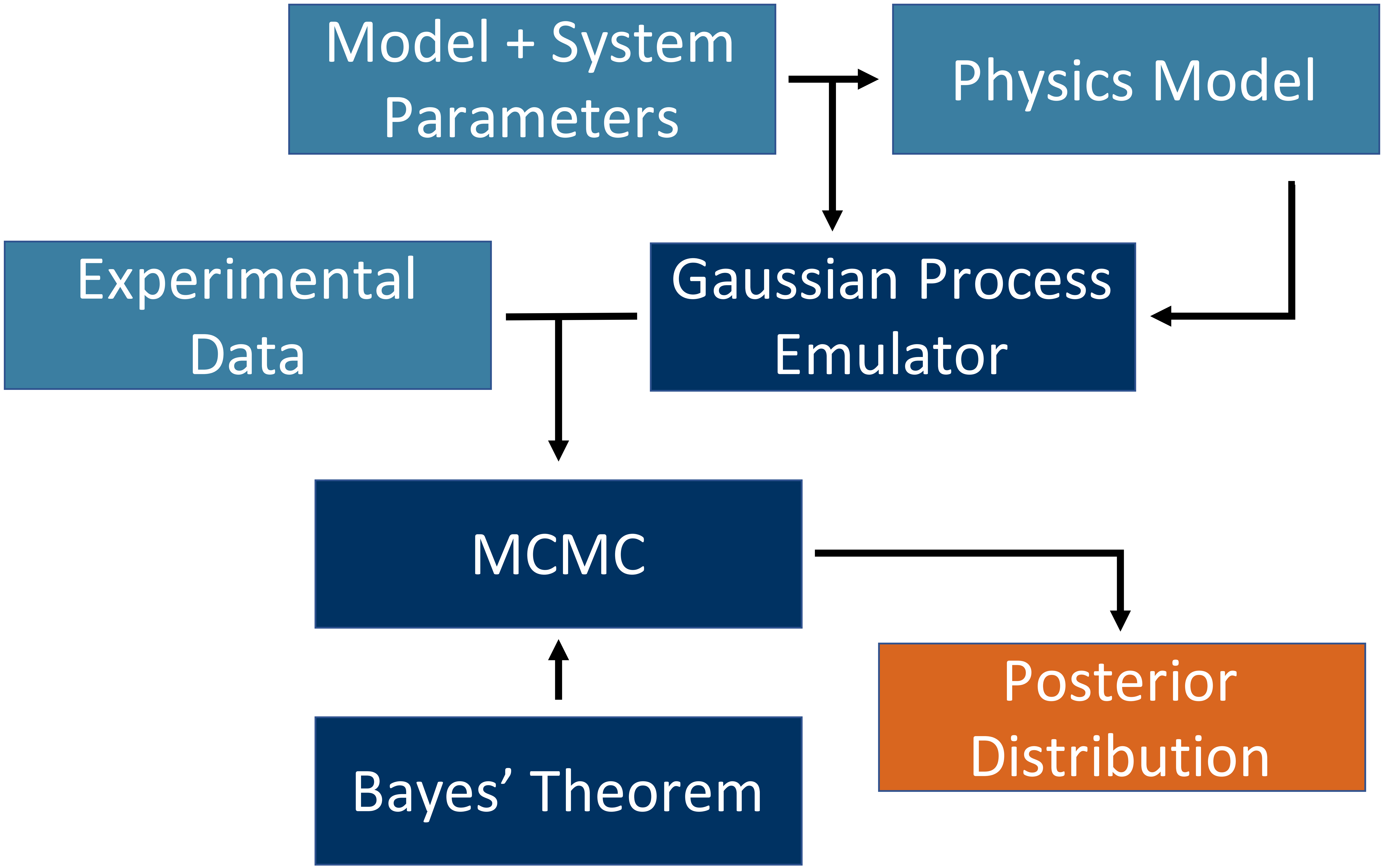
```
Σ = ( 1   0.8 0.6
      0.8 1   0.8
      0.6 0.8 1   );
δy = {1, 1, 0.5};

Δ2 = δy.Inverse[Σ].δy
likelihood = e^(-Δ2/2) / √Det[Σ]
1.32813

1.43879
```





Soltz, Hangal, Angerami, arXiv:2412.03724

Bayesian inference workflow



JETSCAPE Framework

- **MC event generator package for heavy ion collisions**
  - General, modular and extensible
  - Communication between modules
  - Available on GitHub github.com/JETSCAPE