

Inferring the composition of Ultra-High Energy Cosmic Rays

Michele Tammaro

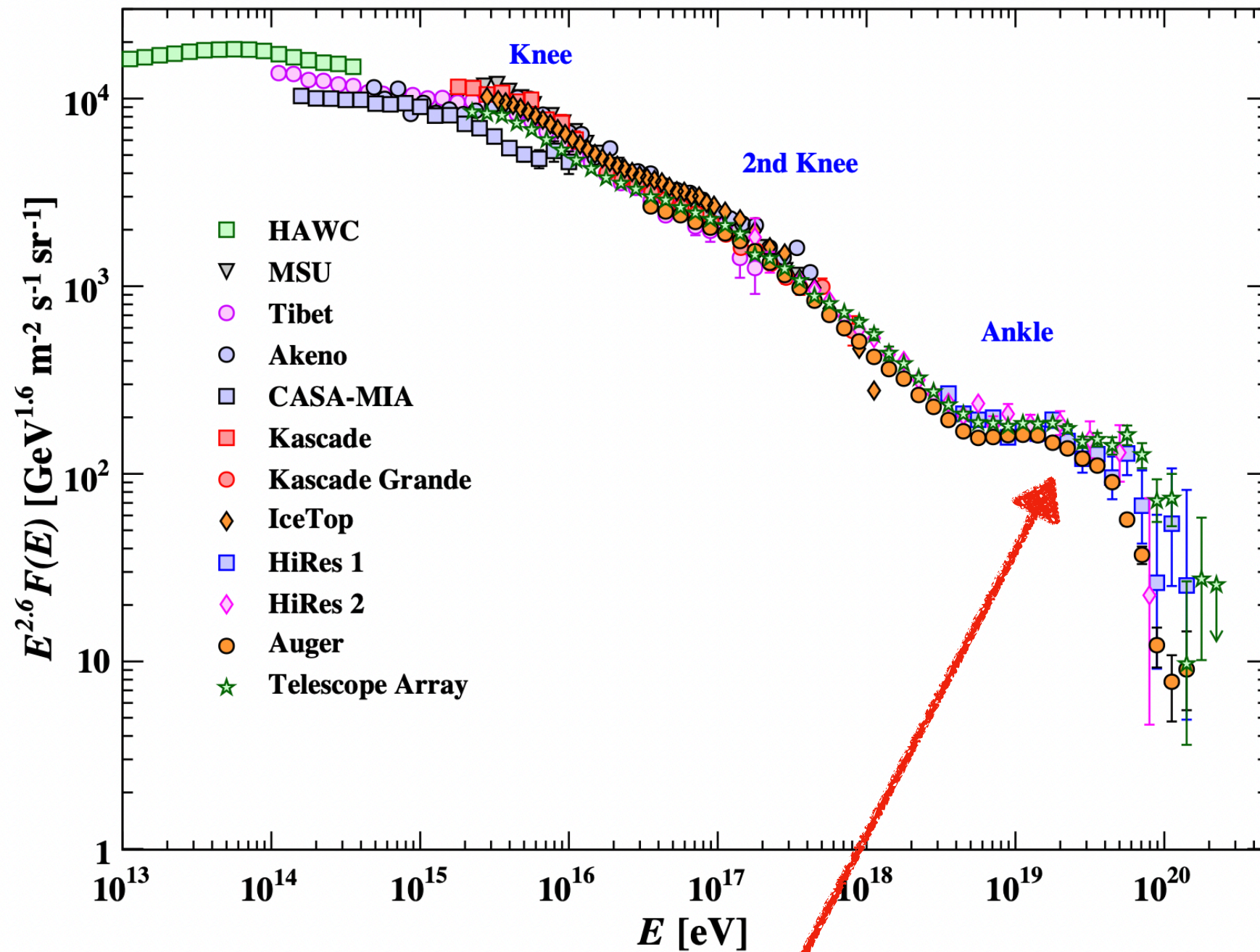
@ Re[Incontri] di Fisica Partenopea, 20/12/2023

with B. Bortolato and J.F. Kamenik (2212.04760, 2304.11197 and more to come...)



Istituto Nazionale di Fisica Nucleare
SEZIONE DI FIRENZE

Ultra High-Energy Cosmic Rays (UHECR)



$$\phi \sim 10^{-2} \text{ km}^{-2} \text{ yr}^{-1}$$

Where?

Astrophysical sources of UHECR

How?

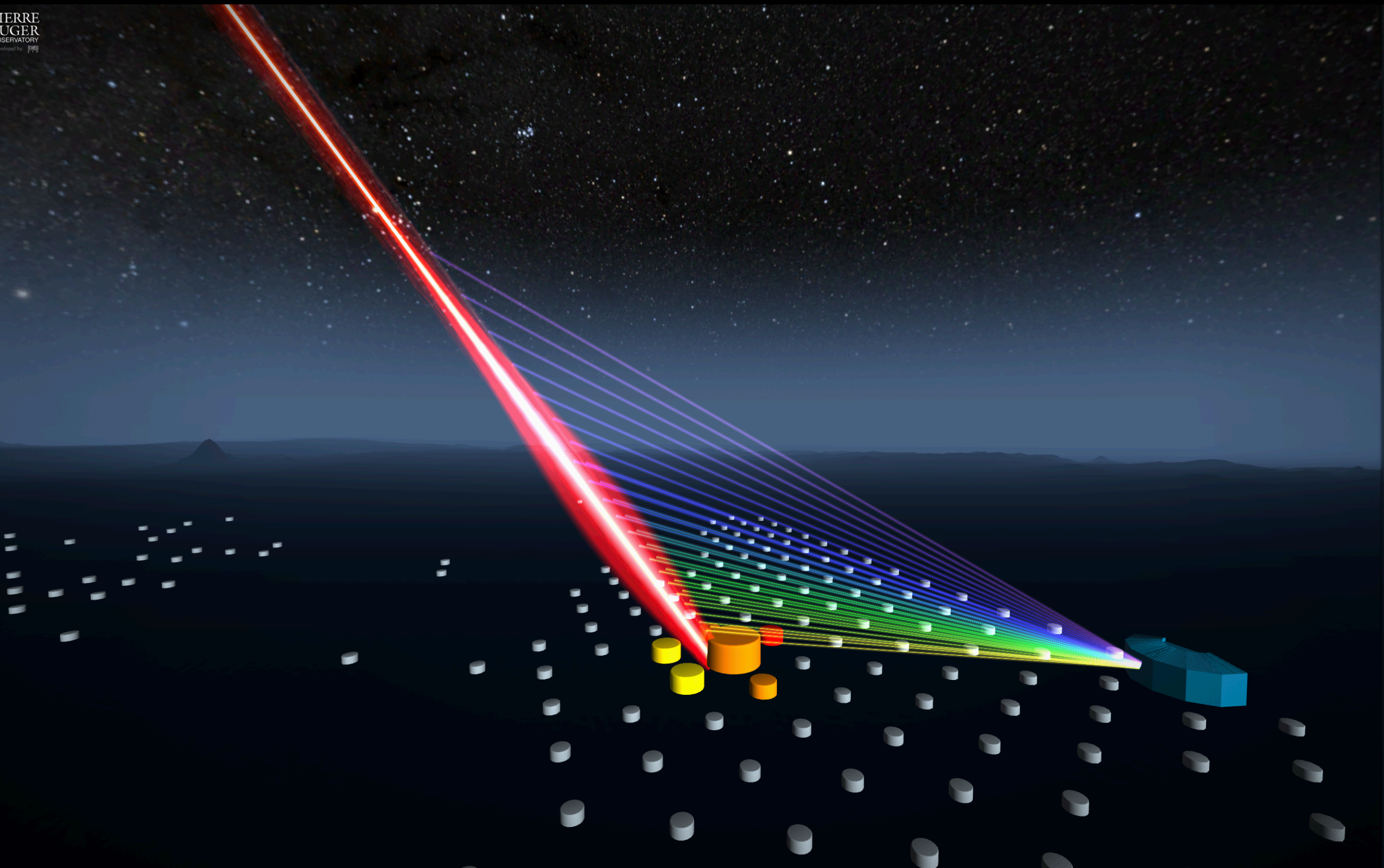
Acceleration mechanisms

What?

Mass composition

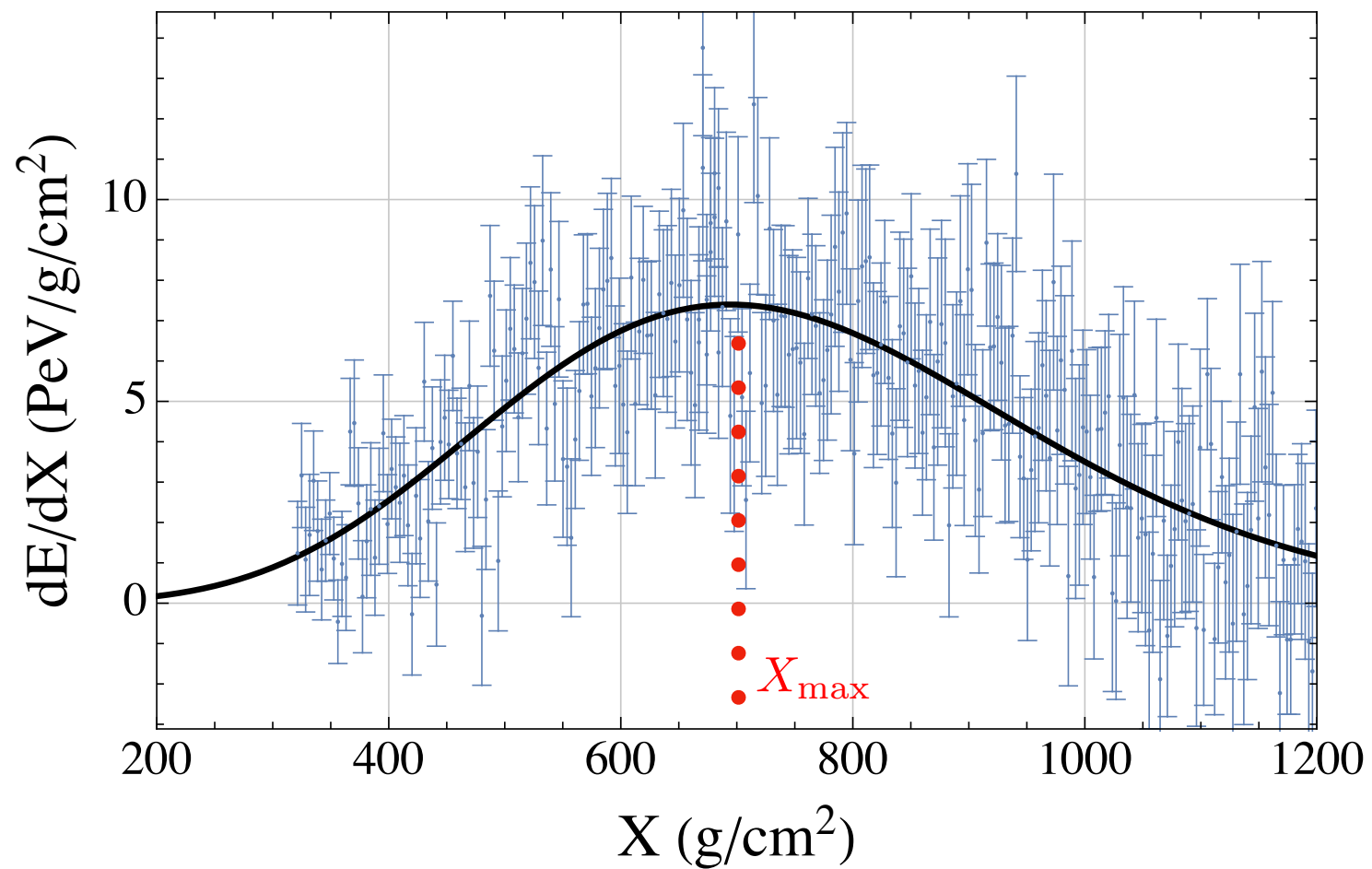
Hybrid Showers

TERRE
UGER
SERVATORY
developed by: 

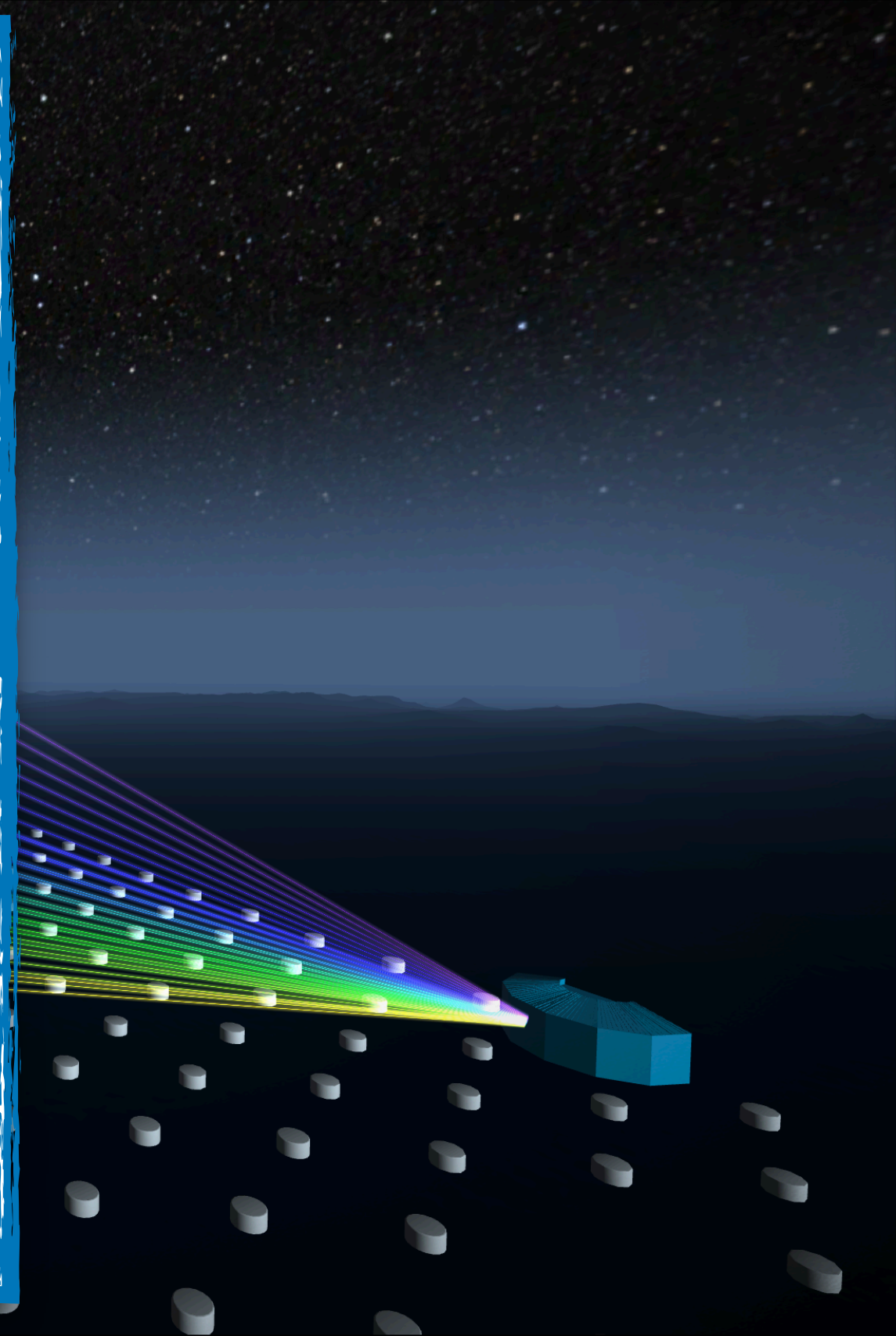


Hybrid Showers

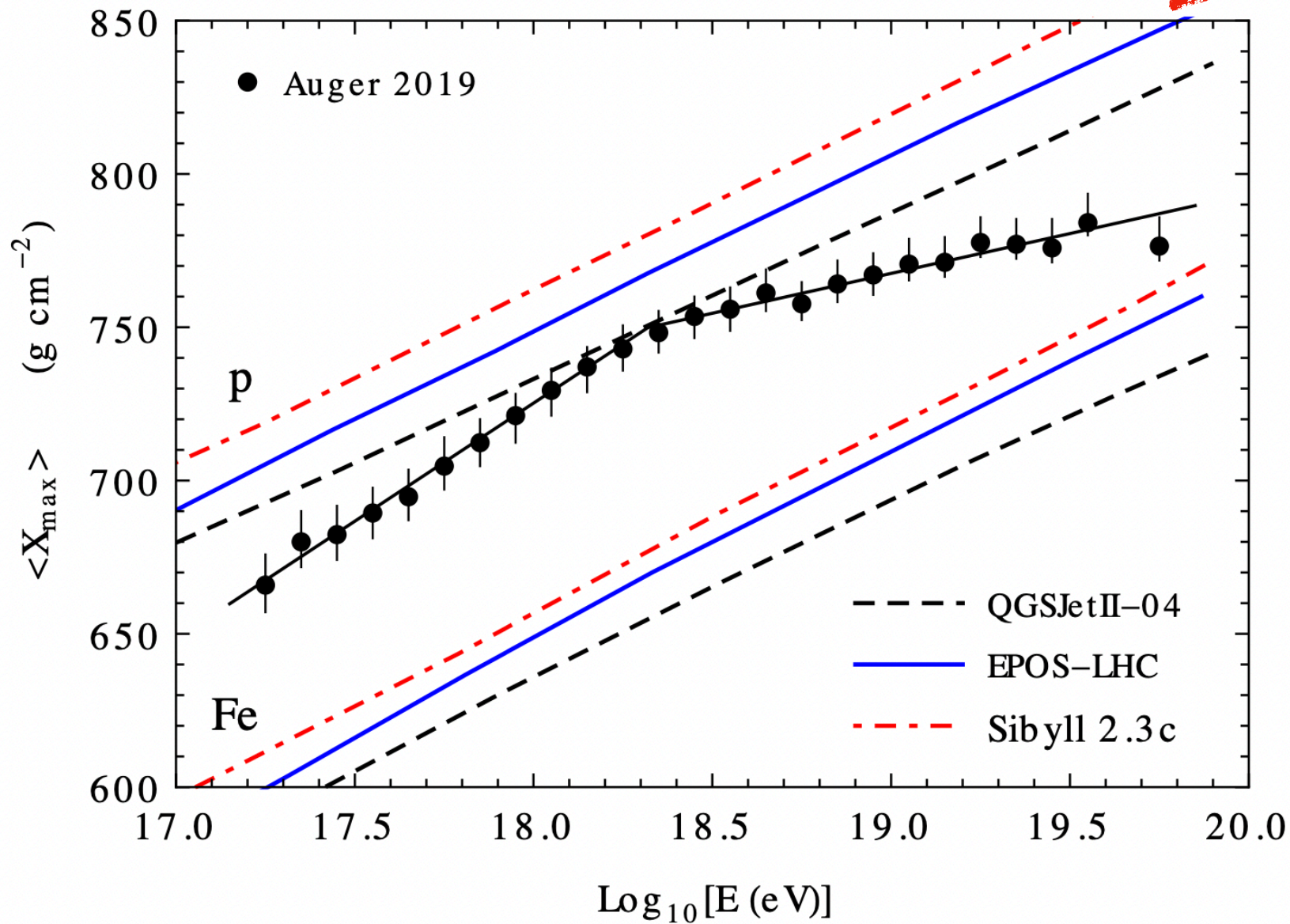
$$X_{\text{ground}} \sim 1200 \text{ g/cm}^2$$



$$\langle X_{\text{max}} \rangle \propto \log E - \log A$$



(Lipari: 2012.06861)



Different models, which one to use?
(Not in this talk, but interesting problem)

Simulations performed with
CORSIKA
(<https://www.iap.kit.edu/corsika/>)

Auger data seems to indicate heavier primaries at higher energies

What has been done

Fit X_{\max} distribution with mixture

(p, He, N, Fe)

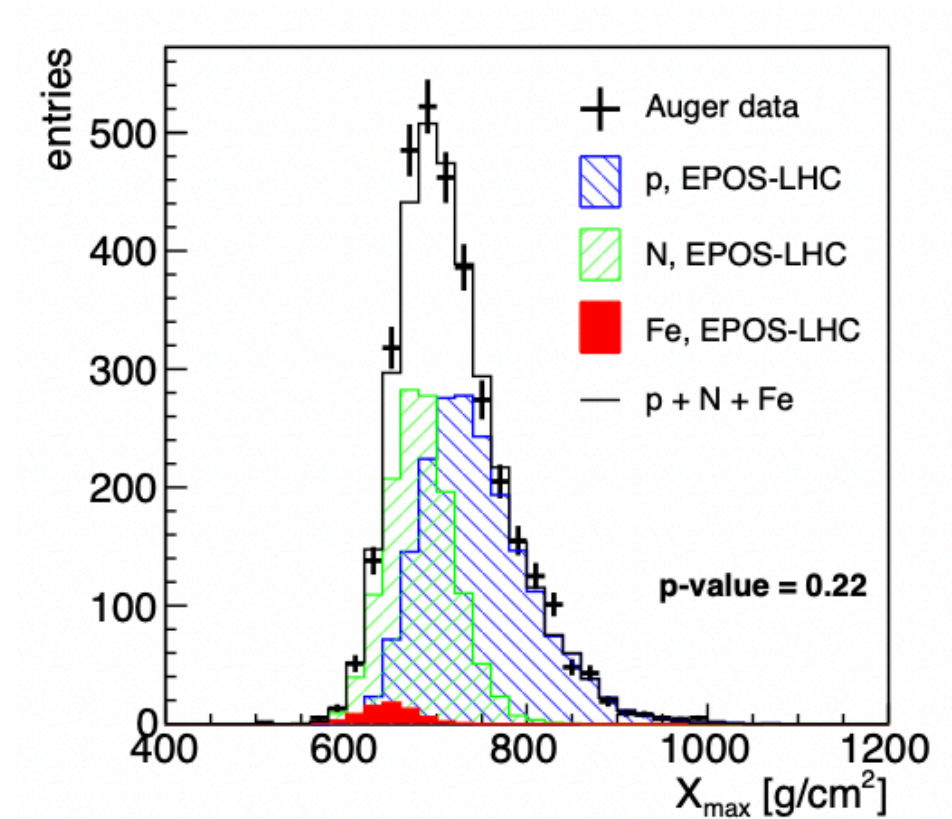
Bin and count

(Arsene, Sima: 2001.02667)

(Auger Coll.: 1409.5083)

(Lipari: 2012.06861)

$p \sim 65\%$, $N \sim 35\%$



What we propose

$$w = (w_p, w_{He}, \dots, w_{Fe}) \quad \sum_i^{26} w_i = 1$$

25 free parameters

Decompose distribution in moments \longrightarrow Unbinned likelihood

Faster computation with Nested Sampling

What has been done

Fit X_{\max} distribution with mixture

(p, He, N, Fe)

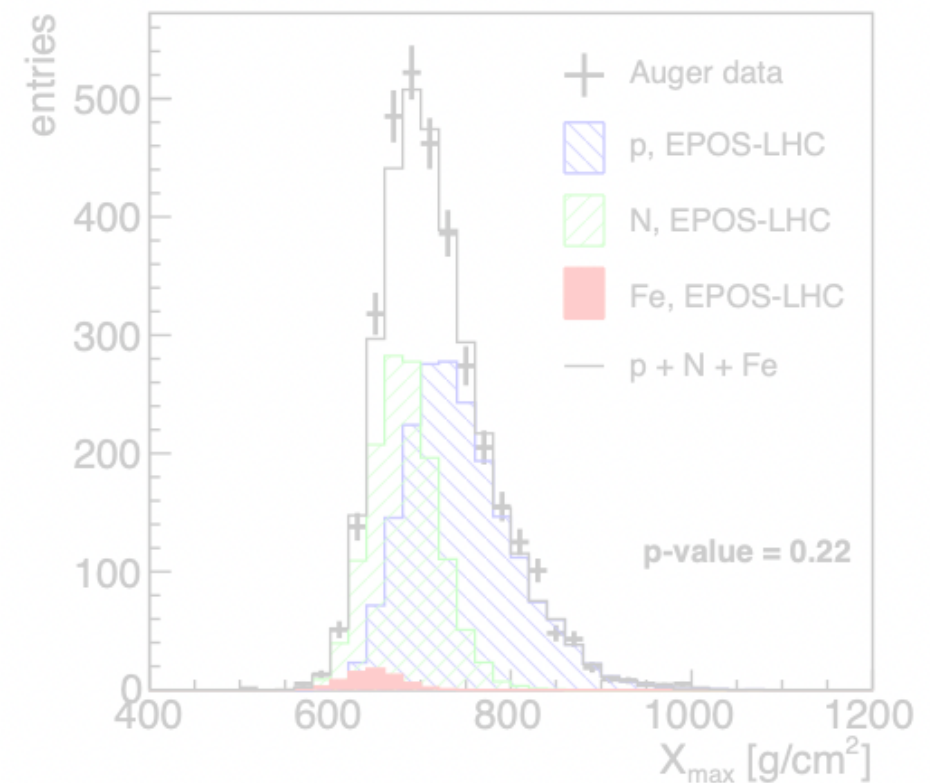
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$$w = (w_p, w_{He}, \dots, w_{Fe})$$

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25 free parameters

Decompose distribution in moments



Unbinned likelihood

Faster computation with Nested Sampling

Problem is reduced to fit vector of moments

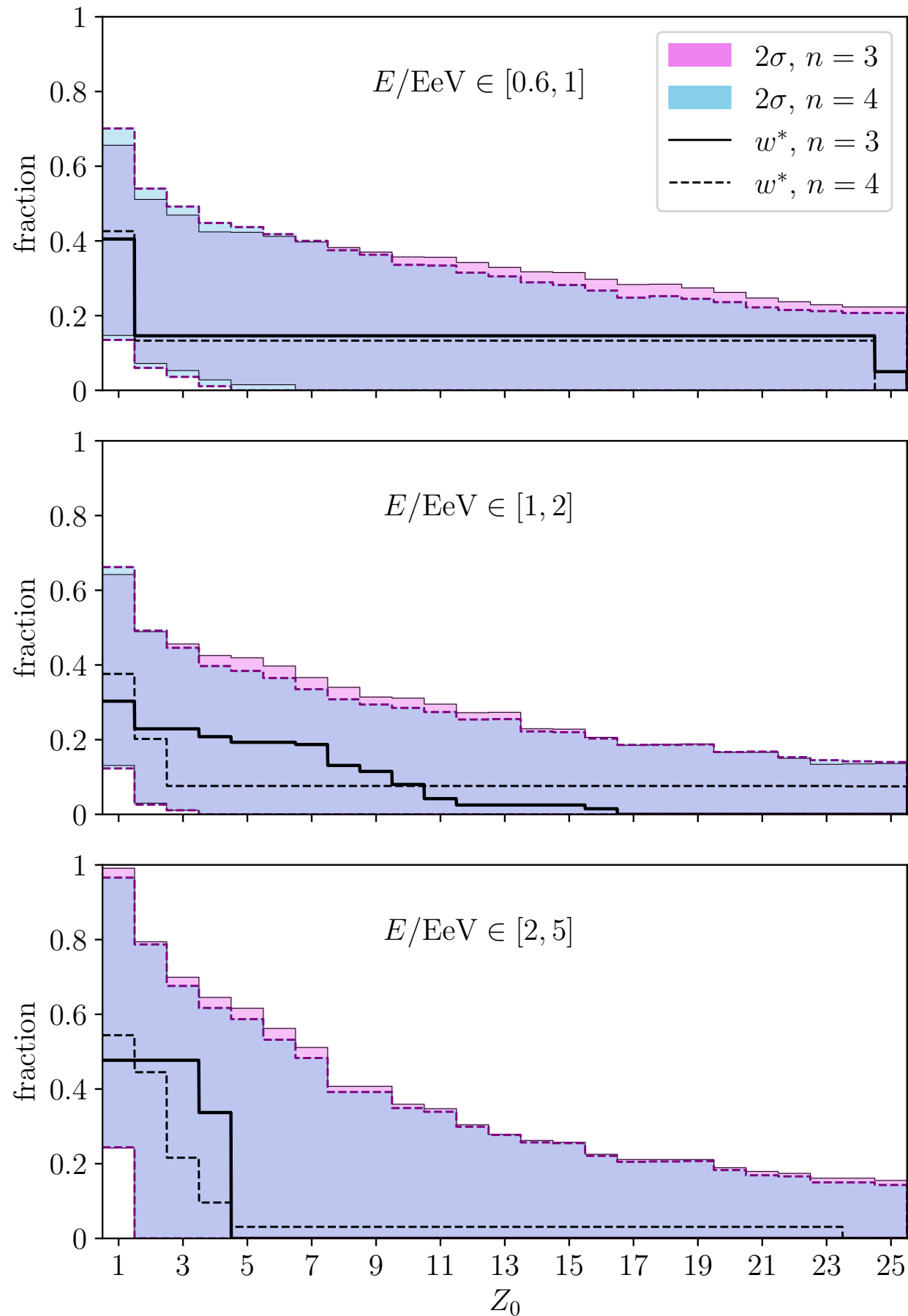
$$\tilde{\mathcal{L}}(z, w) = \overset{\text{Data}}{\mathcal{N}_n(z \mid \tilde{\mu}, \tilde{\Sigma})} \times \overset{\text{Simulations}}{\mathcal{N}_n(z \mid \mu_w, \Sigma_w)}$$

$$\mathcal{L}(w) = \int \tilde{\mathcal{L}}(z, w) \, d^n z$$

Assume a flat prior (Dirichlet distribution) and Maximize log-likelihood

$$\mathcal{P}(w) = \frac{\mathcal{L}(w) \text{Dir}(w, \alpha)}{\int \mathcal{L}(w) \text{Dir}(w, \alpha) \, d^D w}$$

EPOS



Full (cumulative) composition - EPOS

Fraction of elements heavier than Z_0

Can exclude 100% proton compositions

Results are unchanged increasing the number of features

N.B.: publicly available data is very limited (few hundreds of events)

Including ground data

Hybrid

$$(x_i, y_i)_{i=1, \dots, N}$$

FD

SD

$$\text{Correlation } \rho(x, y) = \frac{\text{Cov}(x, y)}{\sigma(x)\sigma(y)}$$

Non-Hybrid

$$(\hat{x}(\hat{y}_j), \hat{y}_j)_{j=1, \dots, M}$$

How much information is added?

Assumption:
the underlying distribution of events
is the same for both sets

Including ground data

$$\mathcal{X}_\ell = \{(x_i, y_i)\}_{i=1, \dots, B}$$

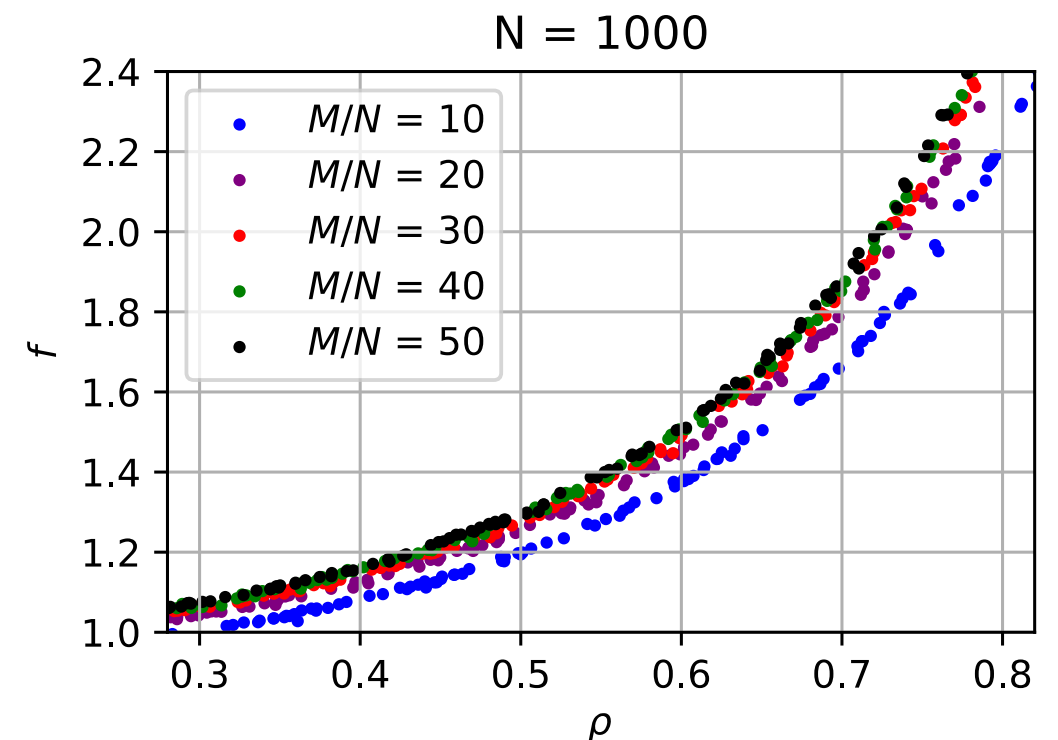
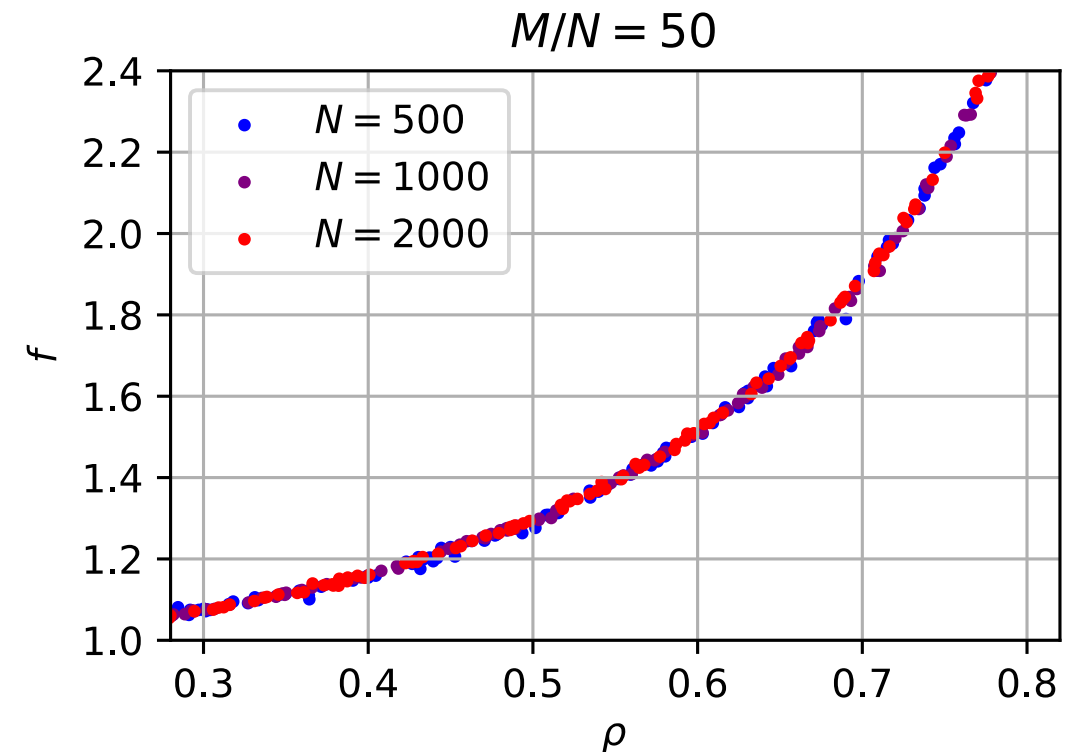
B = number of bootstrapping samples

Get joint distributions $P_\ell(x, y)$

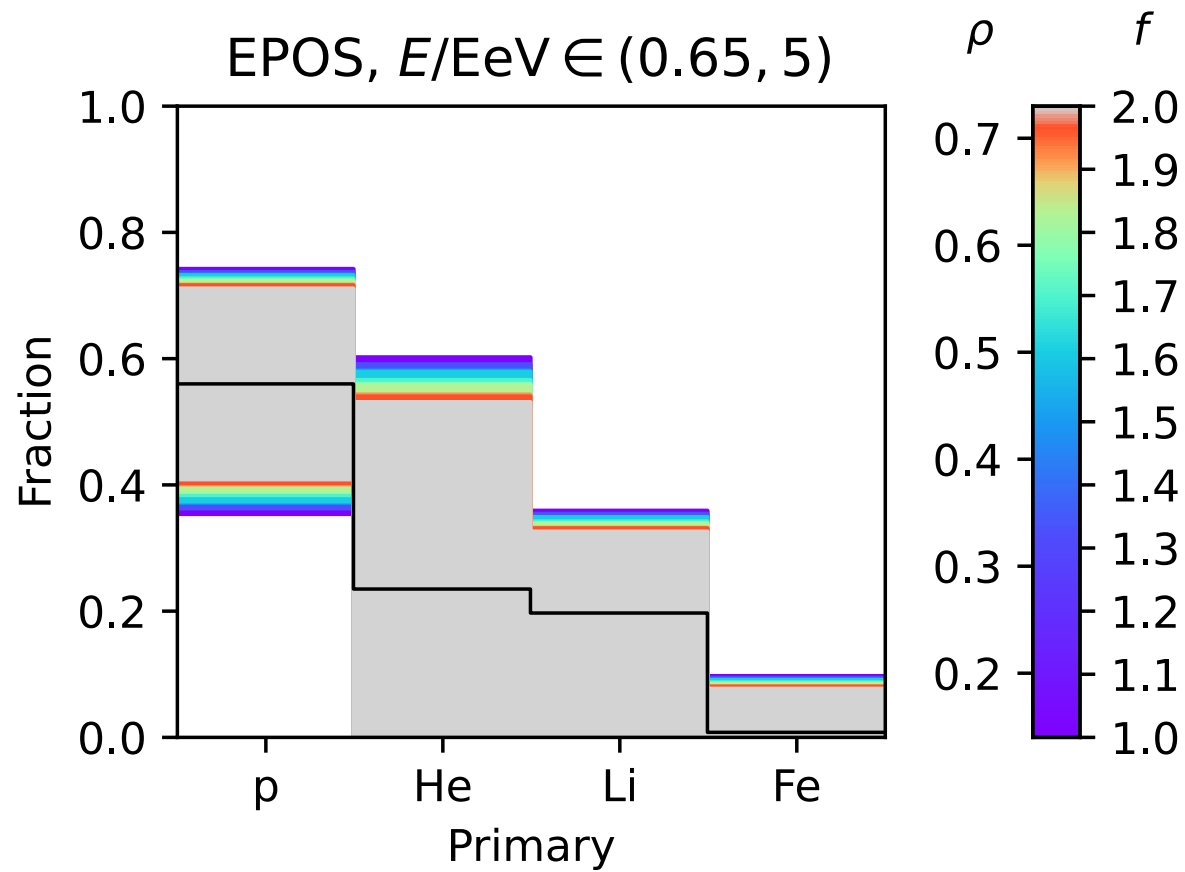
$$\mathcal{X}_\ell^{\text{inf}} = \{(\hat{x}(\hat{y}_j), \hat{y}_j)\}_{j=1, \dots, B}$$

$$\mathcal{X}_\ell^{\text{comb}} = \mathcal{X}_\ell \cup \mathcal{X}_\ell^{\text{inf}} = \{(X, Y)\}_\ell$$

$$f \equiv \frac{\text{Var}(\bar{x})}{\text{Var}(\bar{X})} \quad \text{Effective factor of included events}$$



Including ground data



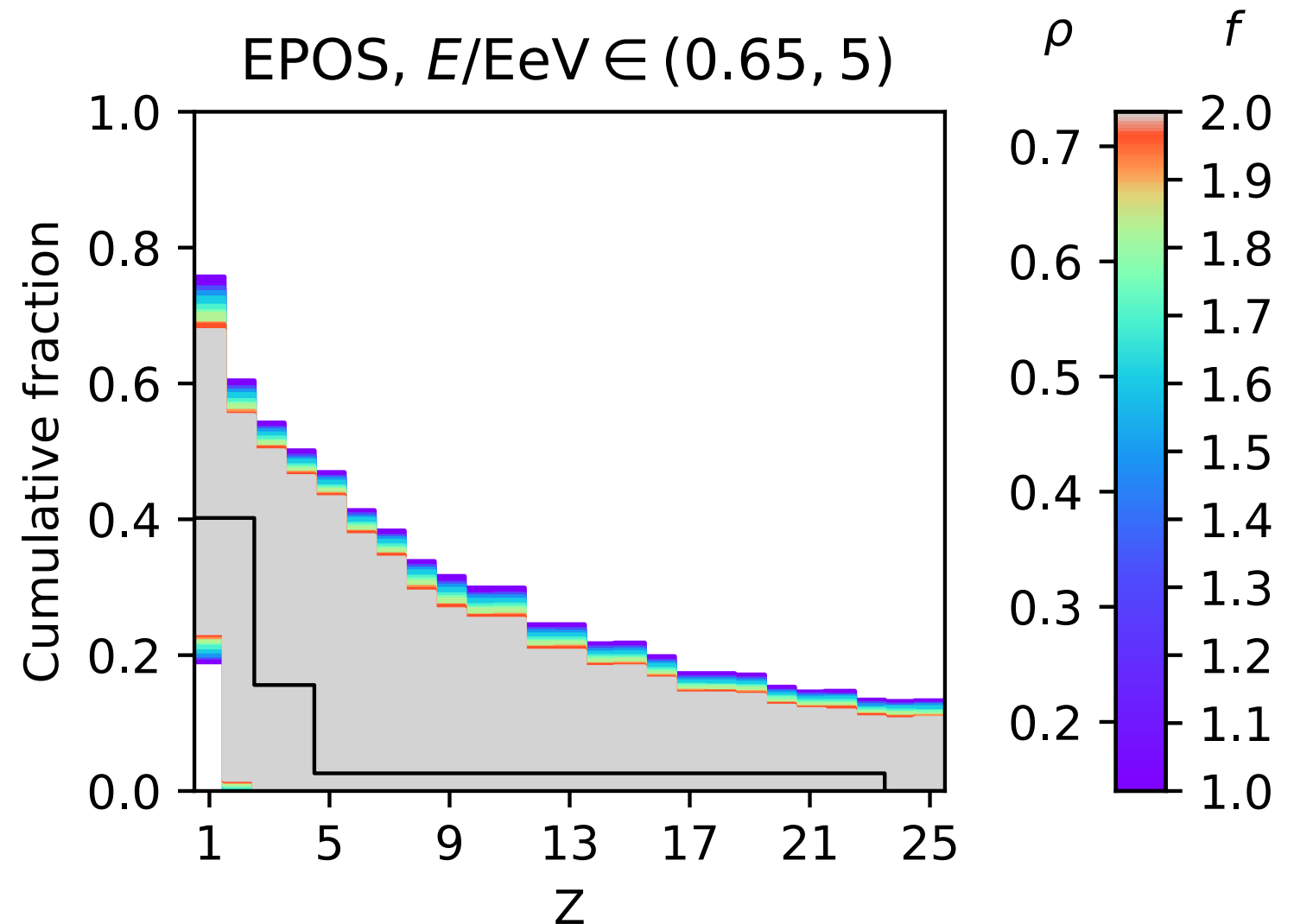
With $\sim 70\%$ correlation we can effectively double the statistical power

$\rho \sim 30\%$ with (non)-linear fits

(Auger Coll.: 1710.07249)

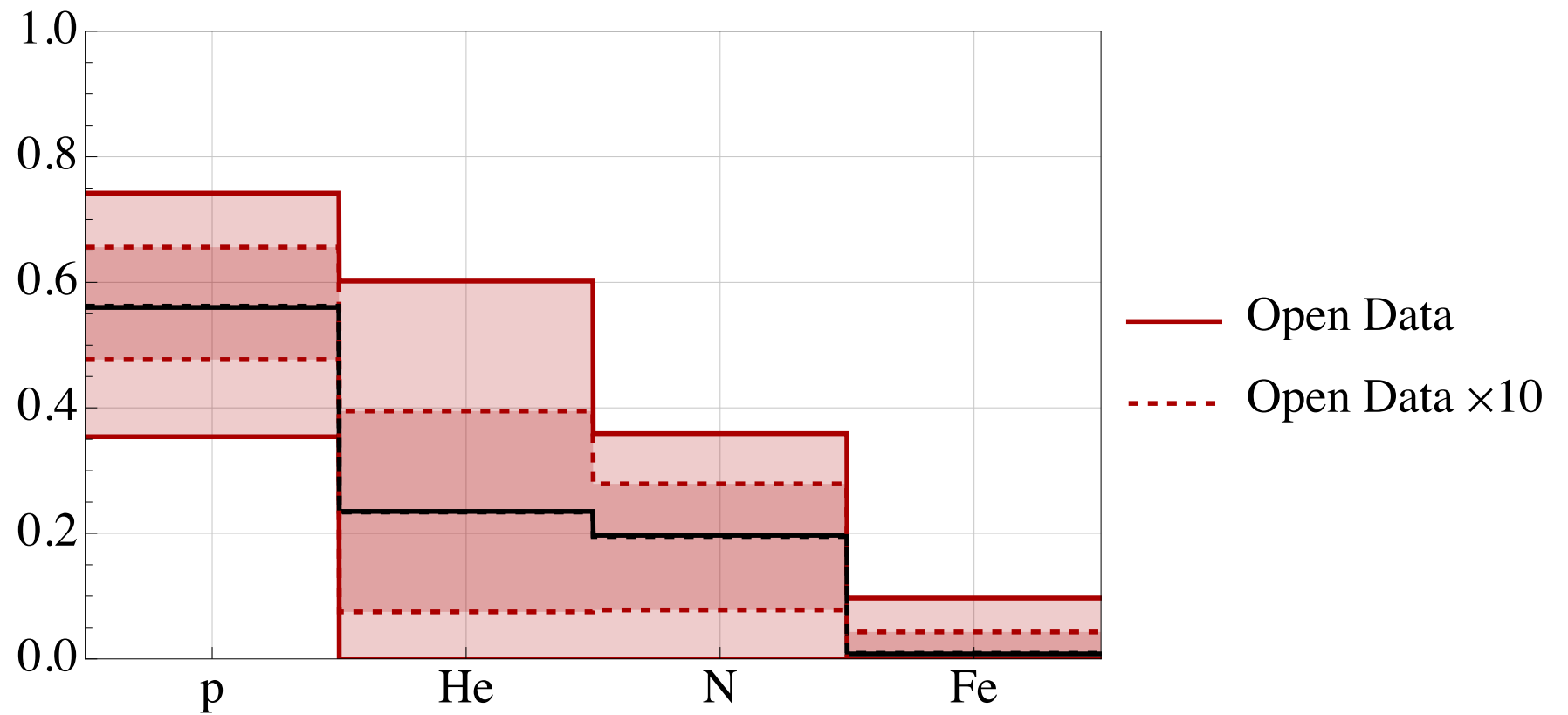
$\rho \sim 70\%$ with Deep Neural Network

(Auger Coll.: 2101.02946)



Including ground data

Projecting for larger datasets (but still a small fraction of the full)

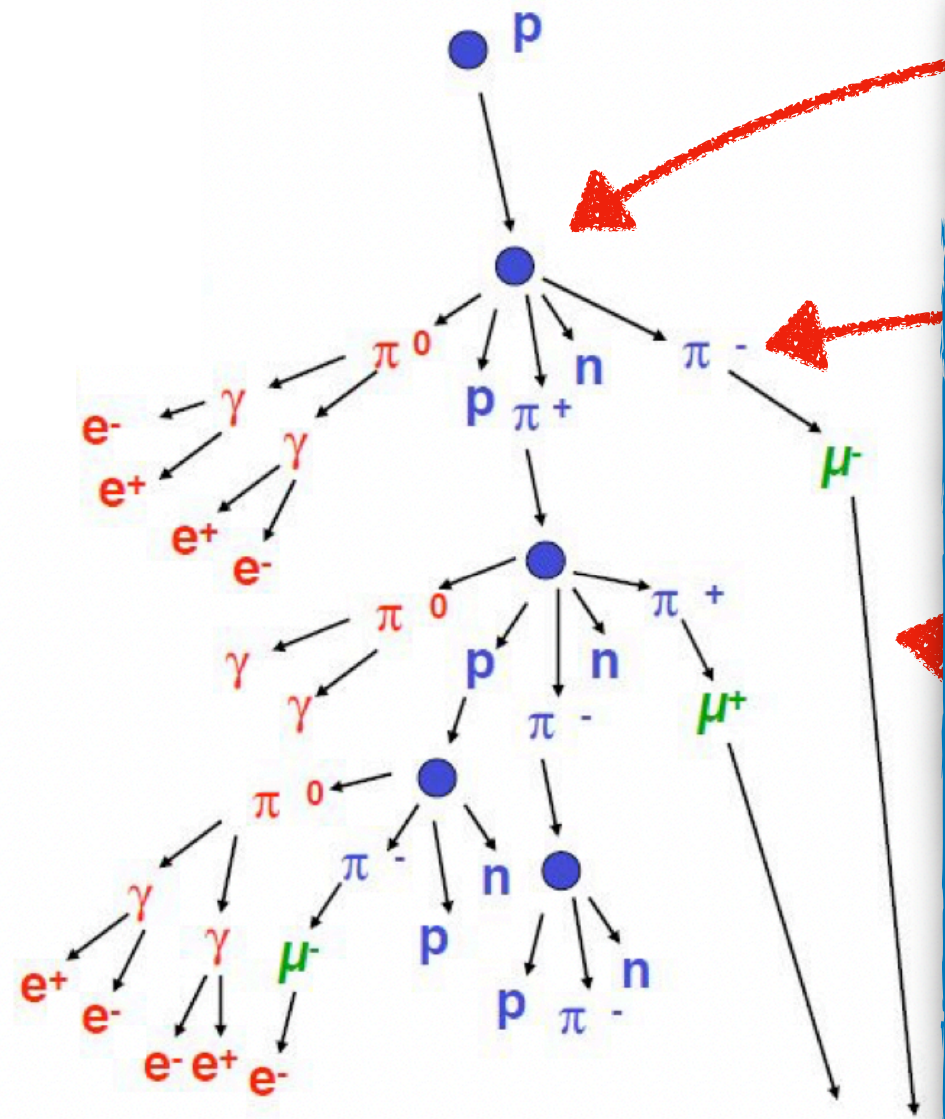


Summary

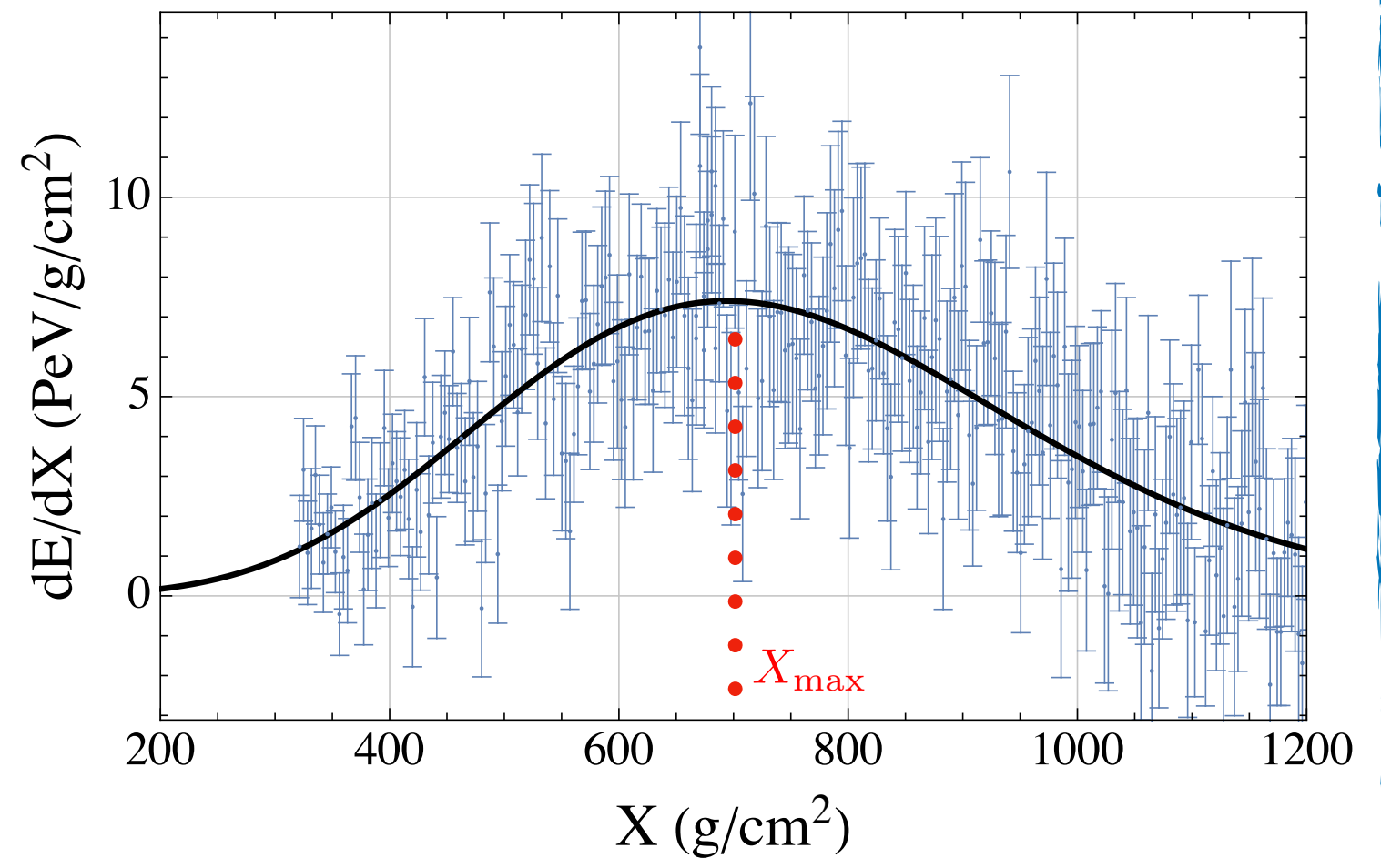
- We build a simple framework for inference of UHECR mass composition
- $n = 3$ moments are good discriminating features
- Limited by very low statistics
- Many ideas for improvements

Backup slides

Extensive Air Showers (EAS)

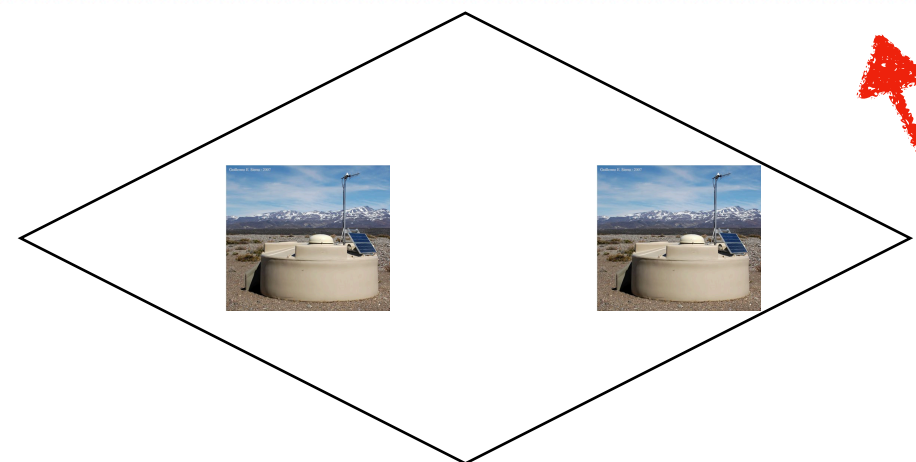


$$X_{\text{ground}} \sim 1200 \text{ g/cm}^2$$



(Gaisser, Hillas, '77)

$$f_{GH}(X) = \left(\frac{dE}{dX}\right)_{\text{max}} \left(\frac{X-X_0}{X_{\text{max}}-X_0}\right)^{\frac{X_{\text{max}}-X_0}{\lambda}} \exp\left(-\frac{X_{\text{max}}-X}{\lambda}\right)$$



Cherenkov detectors

Interlude: Bayesian inference

$\mathbf{X} = x_1, \dots, x_n$ data sample

θ parameters, $x \sim p(x|\theta)$

The diagram illustrates the Bayesian inference equation with red arrows pointing to its components:

- Likelihood**: Points to $P(\mathbf{X}|\theta)$ in the numerator of the first fraction.
- Prior distribution**: Points to $P(\theta)$ in the numerator of the second fraction.
- Evidence**: Points to $P(\mathbf{X})$ in the denominator of the first fraction and $\int \mathcal{L}(\theta|\mathbf{X})P(\theta)d\theta$ in the denominator of the second fraction.
- Posterior distribution**: Points to $P(\theta|\mathbf{X})$ on the left side of the equation.

$$P(\theta|\mathbf{X}) = \frac{P(\mathbf{X}|\theta)P(\theta)}{P(\mathbf{X})} = \frac{\mathcal{L}(\theta|\mathbf{X})P(\theta)}{\int \mathcal{L}(\theta|\mathbf{X})P(\theta)d\theta}$$

Maximum Likelihood Estimate (MLE): select θ that maximize \mathcal{L}

Maximum a Posteriori Estimation (MPE) for Bayesian people

Interlude: Bayesian inference

$\mathbf{X} = x_1, \dots, x_n$ data sample

θ parameters, $x \sim p(x|\theta)$

$\mathbf{X} \equiv X_{\max}$

$\theta \equiv w = (w_p, w_{\text{He}}, \dots, w_{\text{Fe}})$ $\sum_i w_i = 1$

$\mathcal{L}(\theta|\mathbf{X})$ from simulations

The diagram illustrates the Bayesian inference equation:
$$P(\theta|\mathbf{X}) = \frac{P(\mathbf{X}|\theta)P(\theta)}{P(\mathbf{X})} = \frac{\mathcal{L}(\theta|\mathbf{X})P(\theta)}{\int \mathcal{L}(\theta|\mathbf{X})P(\theta)d\theta}$$
 Red arrows point from the terms 'Likelihood' and 'Prior distribution' to the numerator of the first fraction. A red arrow points from 'Evidence' to the denominator of the second fraction. A red arrow points from the entire equation to the label 'Posterior distribution'.

Maximum Likelihood Estimate (MLE): select θ that maximize \mathcal{L}

Maximum a Posteriori Estimation (MPE) for Bayesian people

Interlude: Bayesian inference

$\mathbf{X} = x_1, \dots, x_n$ data sample

θ parameters, $x \sim p(x|\theta)$

$\mathbf{X} \equiv X_{\max}$

$\theta \equiv w = (w_p, w_{He}, \dots, w_{Fe}) \quad \sum_i w_i = 1$

Likelihood Prior distribution

$$P(\theta|\mathbf{X}) = \frac{P(\mathbf{X}|\theta)P(\theta)}{P(\mathbf{X})} = \frac{\mathcal{L}(\theta|\mathbf{X})P(\theta)}{\int \mathcal{L}(\theta|\mathbf{X})P(\theta)d\theta}$$

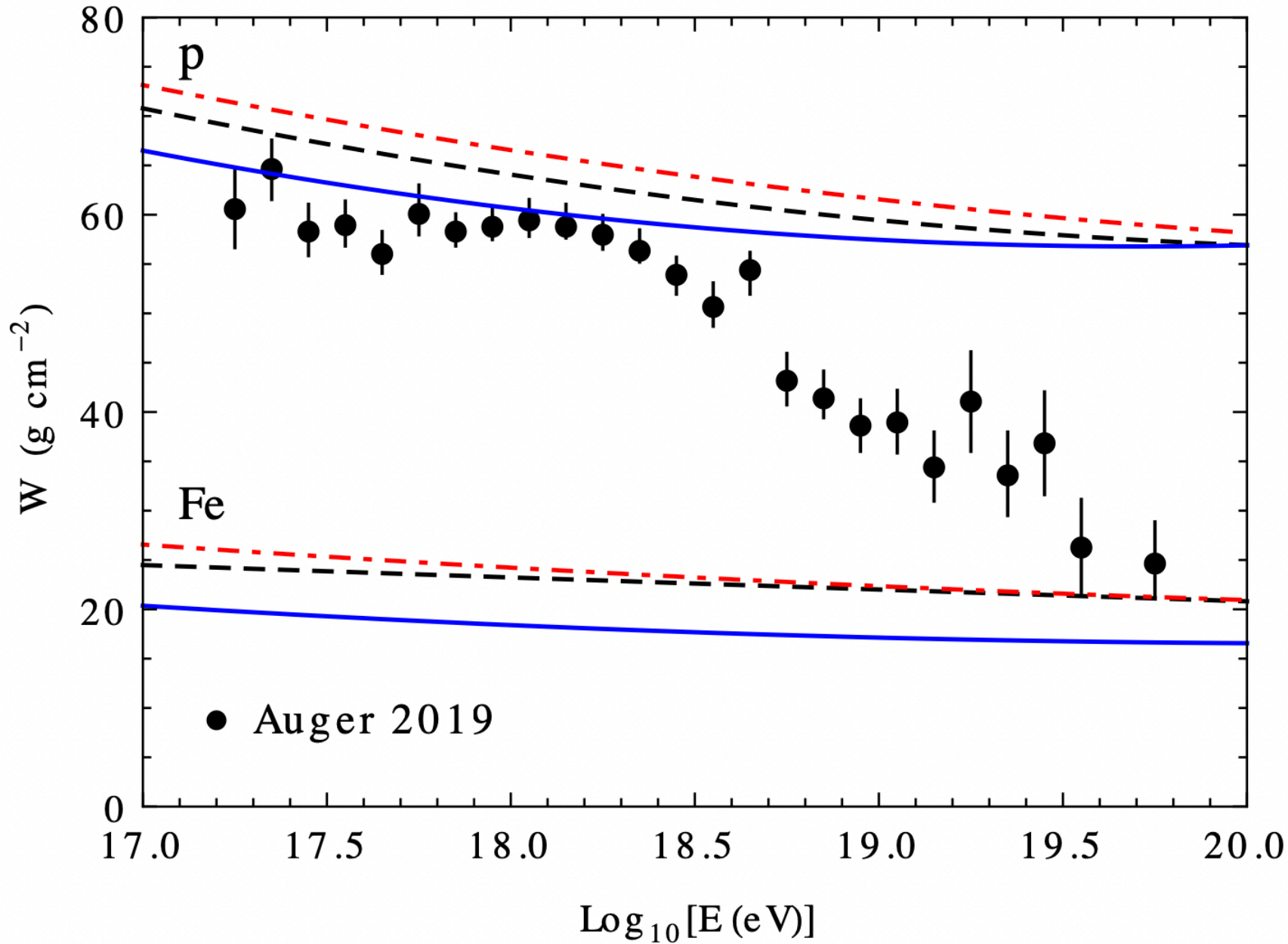
Posterior distribution Evidence

Maximum Likelihood Estimate (MLE): select θ that maximize \mathcal{L}

Maximum a Posteriori Estimation (MPE) for Bayesian people

(Lipari: 2012.06861)

$$W = \left(\langle X_{\max}^2 \rangle - \langle X_{\max} \rangle^2 \right)^{1/2}$$

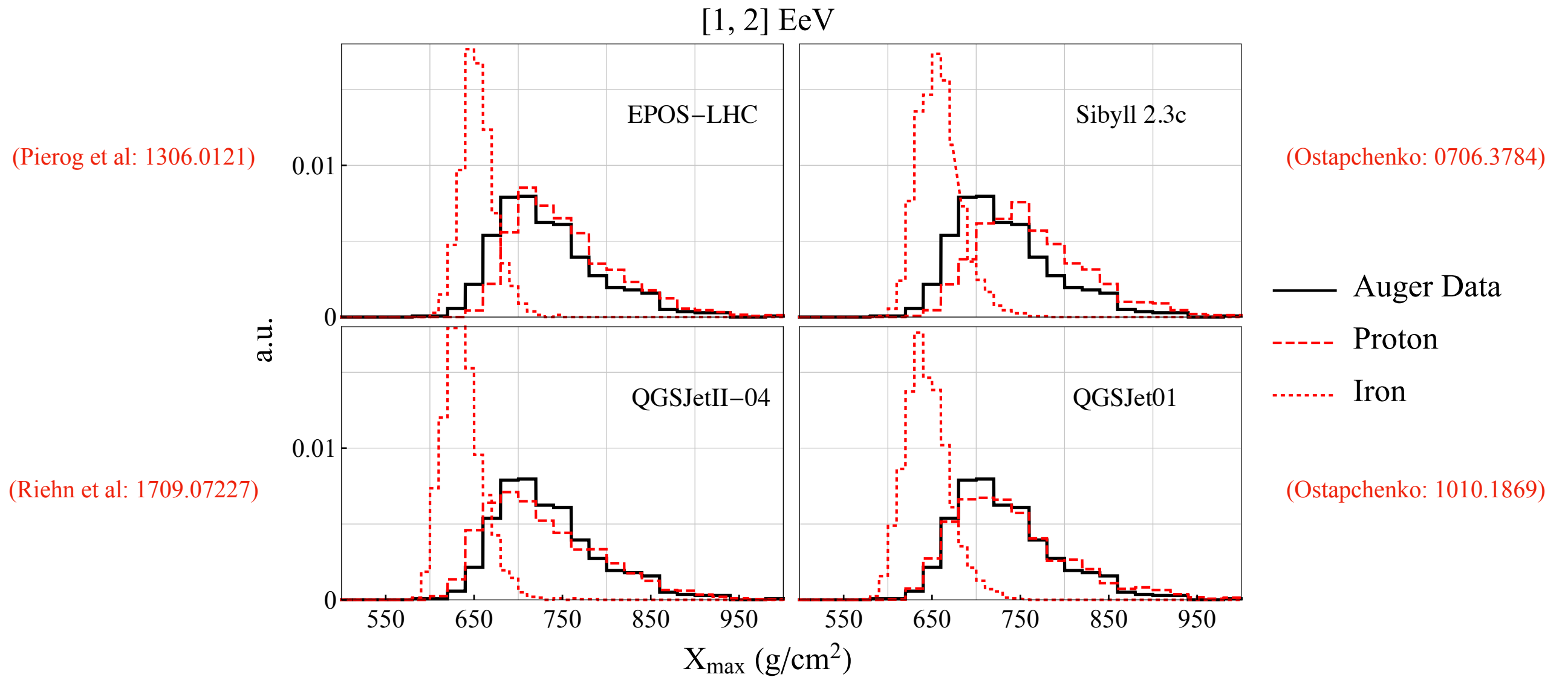


Simulations performed with
CORSIKA
(<https://www.iap.kit.edu/corsika/>)

Single or two-element mixture cannot reproduce the data

(depending on the model...)

The results will be model-dependent



Data

Pierre Auger Open Data 2021

- $\sim 10\%$ of total data
- 1602 hybrid showers in $E \in [0.6, 60]$ EeV
- Split in three bins: $E \in [0.6, 1]$, $[1, 2]$, $[2, 5]$ EeV
- ~ 500 events per bin

$$P_{\text{Aug}}(X_{\text{max}}|E)$$

Simulations with CORSIKA

- 4 hadronic models
- 26 primaries from p to Fe
- 2000 shower per element/bin/model
- 624000 simulations

$$P_{\text{sim}}(X_{\text{max}}|Z, E)$$

Convolute all with detector effects

(Auger Coll.: 1409.5083)

Bonus achievement: get complaints from both IJS and CERN clusters

Probability Distribution Function (PDF)

Each data/simulation point is given as $(X_{\max}, \delta X_{\max})$

Data

$$P_{\text{Aug}}(X_{\max}|E) = \frac{1}{N} \sum_{j=1}^N \mathcal{N}(X_{\max} | X_{\max}^j, \delta X_{\max}^j)$$

Simulations

Set of inputs

Detector effects

$$P_{\text{sim}}(X_{\max} | S = \{E, Z, H\}) = \frac{1}{\tilde{N}} \sum_j \int d\tilde{X} \mathcal{N}(\tilde{X} | X_{\max}^j, \delta X_{\max}^j) \times R(X_{\max} - \tilde{X}) \times \epsilon(\tilde{X})$$

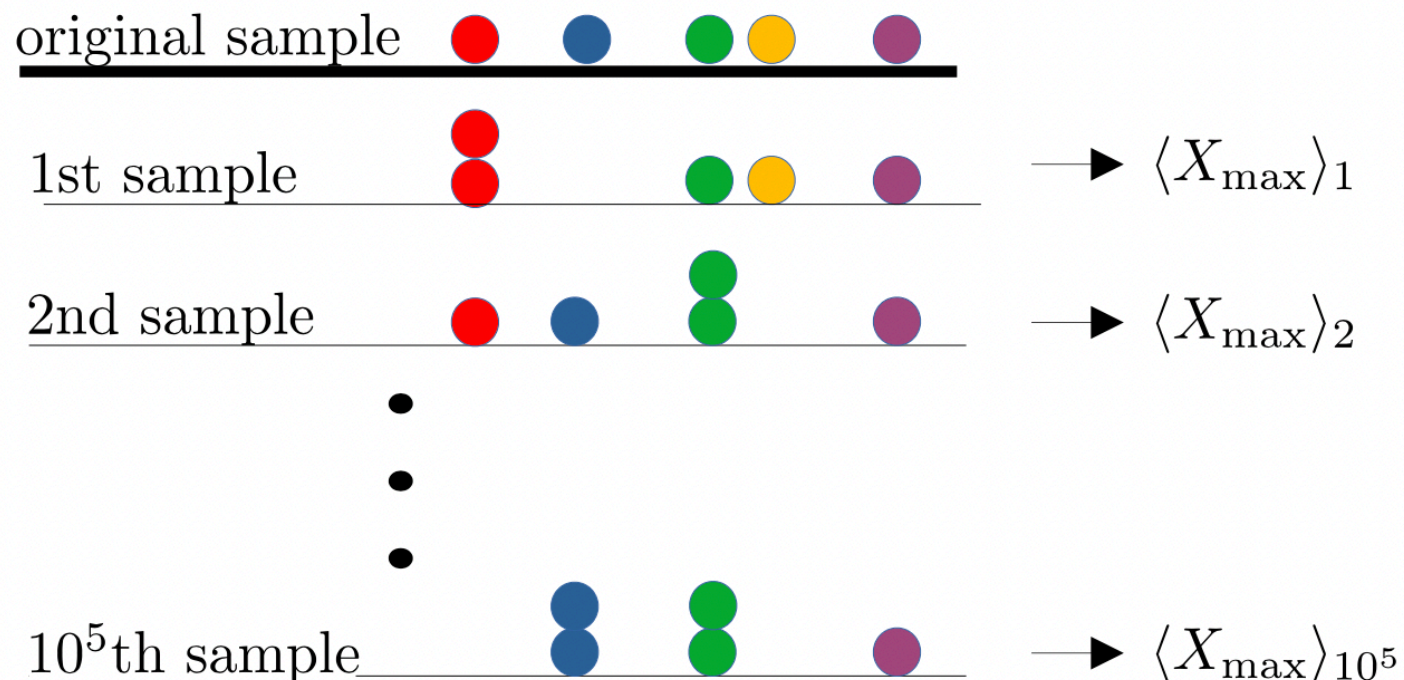
Moments

$$\langle X_{\max}^n \rangle_Z = \frac{\int P(X_{\max} | Z) X_{\max}^n dX_{\max}}{\int P(X_{\max} | Z) dX_{\max}}$$

$$\langle X_{\max}^n \rangle(w) = \frac{\sum_Z \langle X_{\max}^n \rangle_Z w_Z}{\sum_Z w_Z}$$

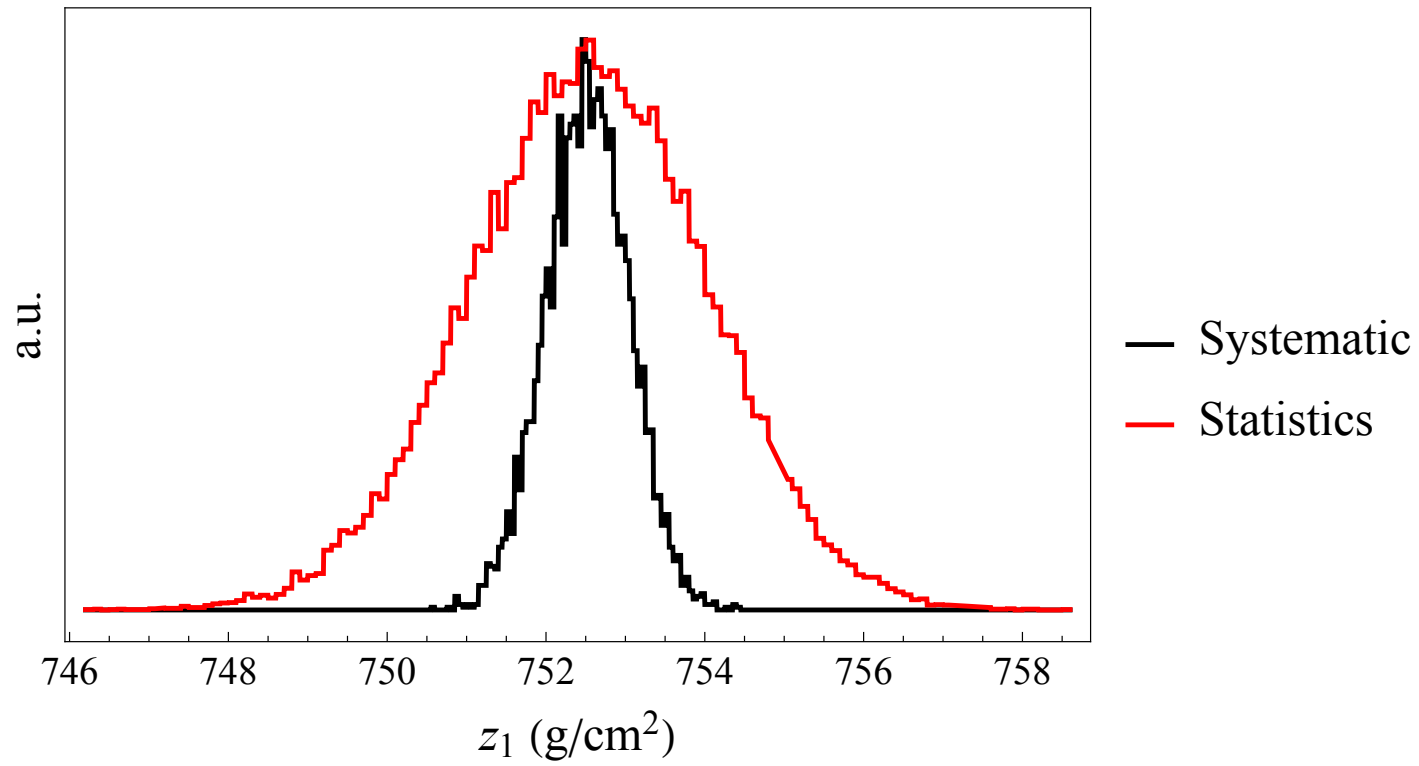
All systematic uncertainties are included

Bootstrapping



Include statistical uncertainties
(data and simulation)
by Bootstrapping

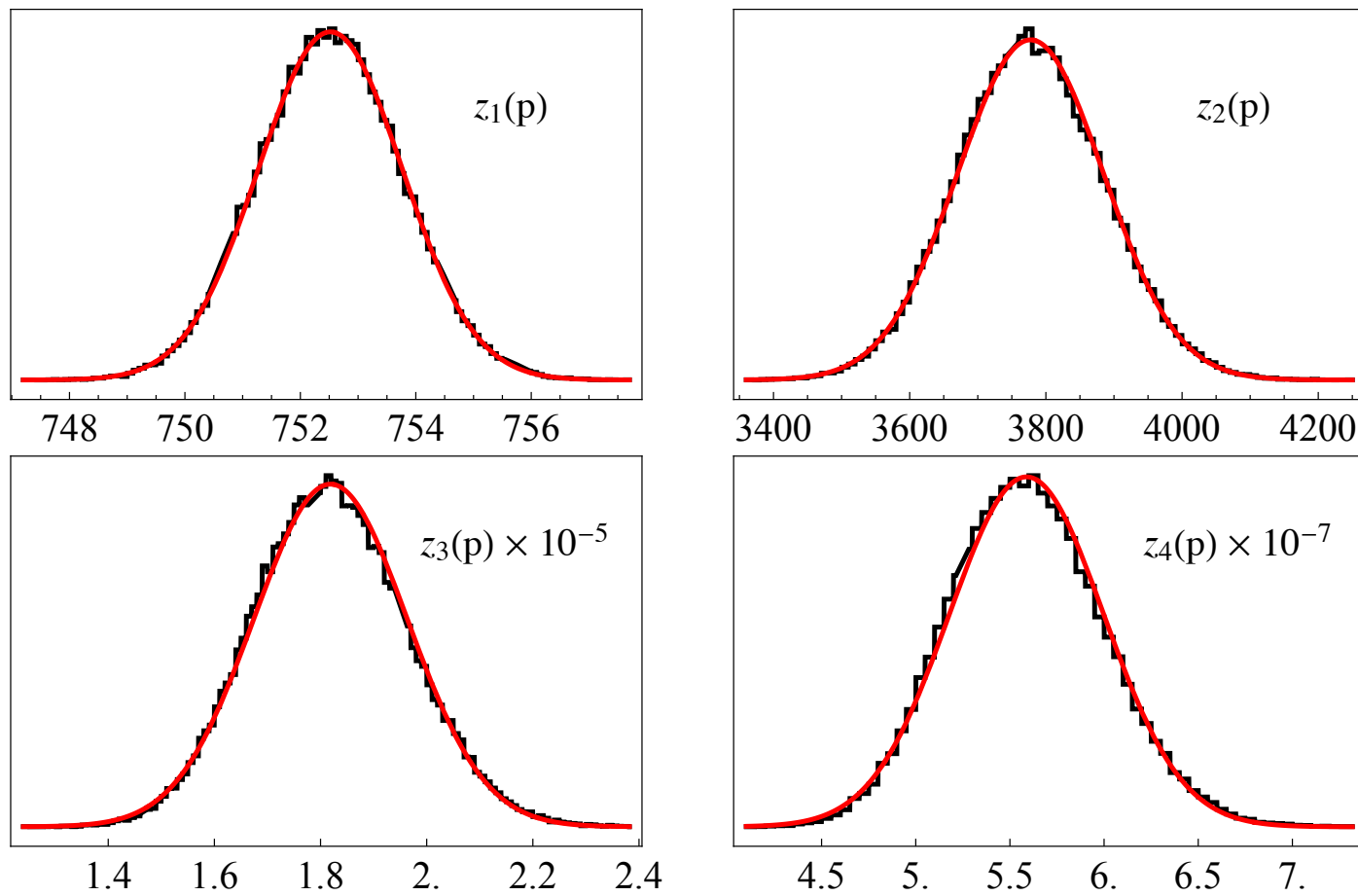
p, EPOS, [1,2] EeV



Simulations

$$z(w) \sim \mathcal{N}_n \left(z \mid \mu(w), \Sigma(w) \right)$$

p, EPOS, [1, 2] EeV



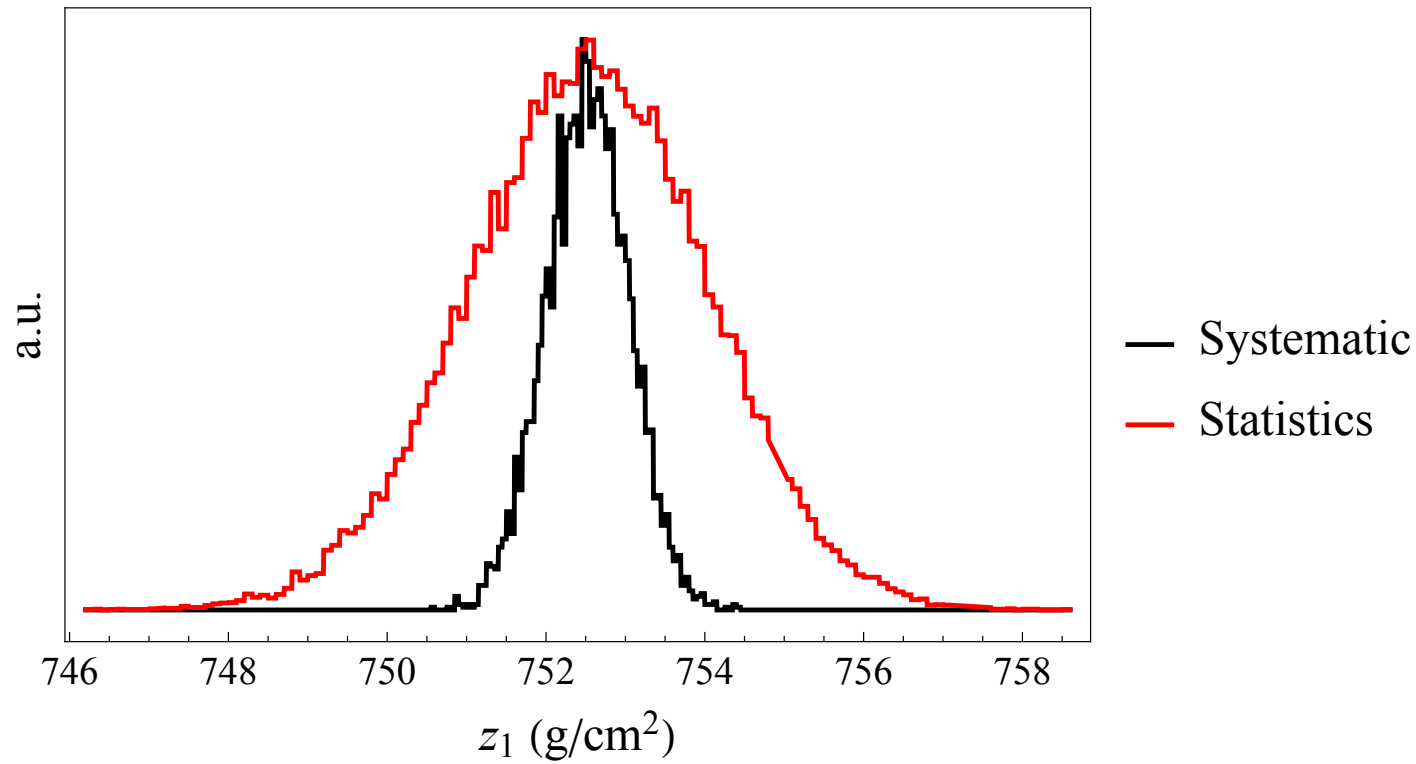
Data

$$\tilde{z} \sim \mathcal{N}_n \left(z \mid \tilde{\mu}, \tilde{\Sigma} \right)$$

— Bootstrap

— Normal

p, EPOS, [1,2] EeV



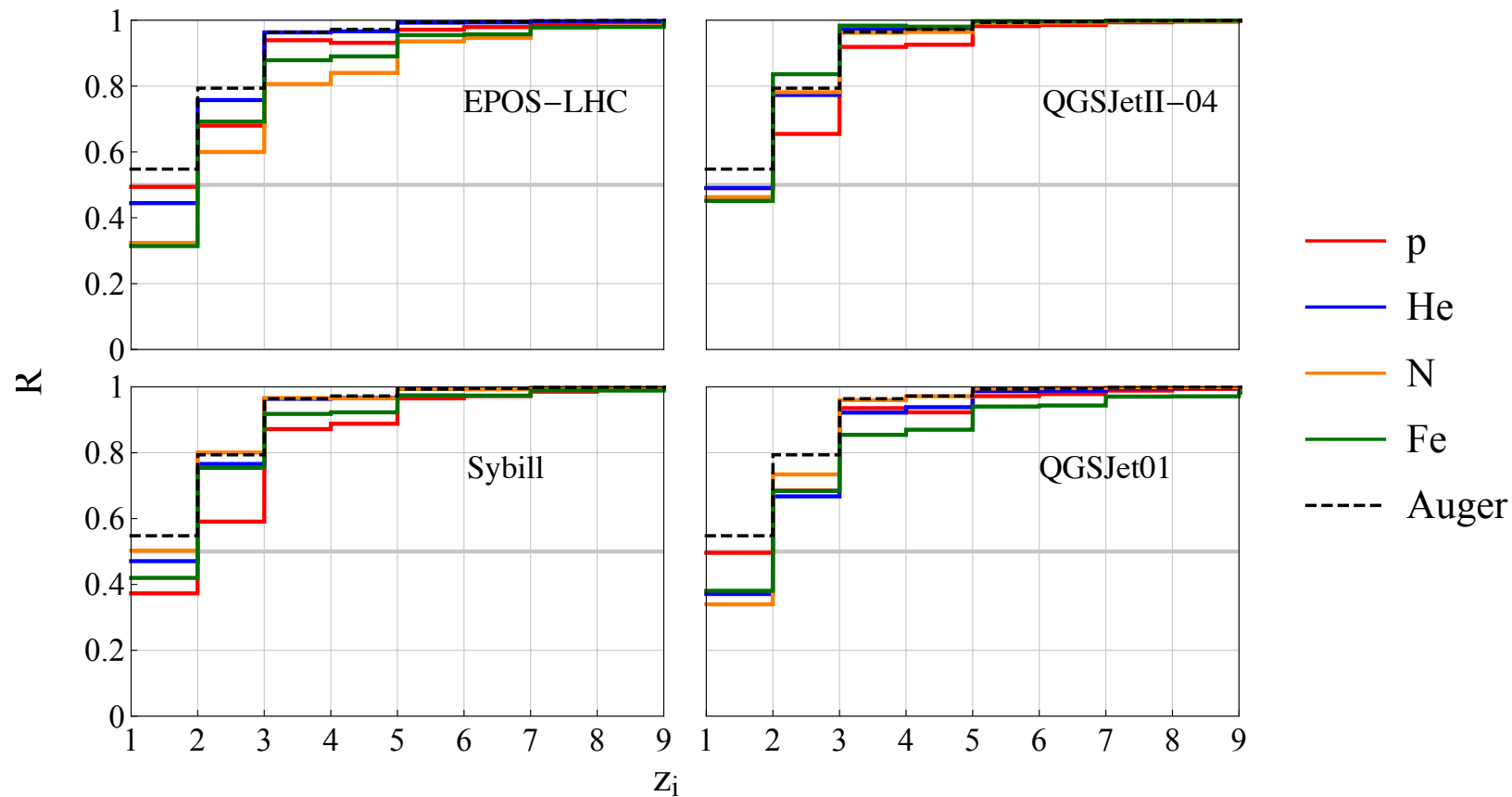
Simulations

$$z(w) \sim \mathcal{N}_n \left(z \mid \mu(w), \Sigma(w) \right)$$

Data

$$\tilde{z} \sim \mathcal{N}_n \left(z \mid \tilde{\mu}, \tilde{\Sigma} \right)$$

[1, 2] EeV



Higher moments are strongly correlated

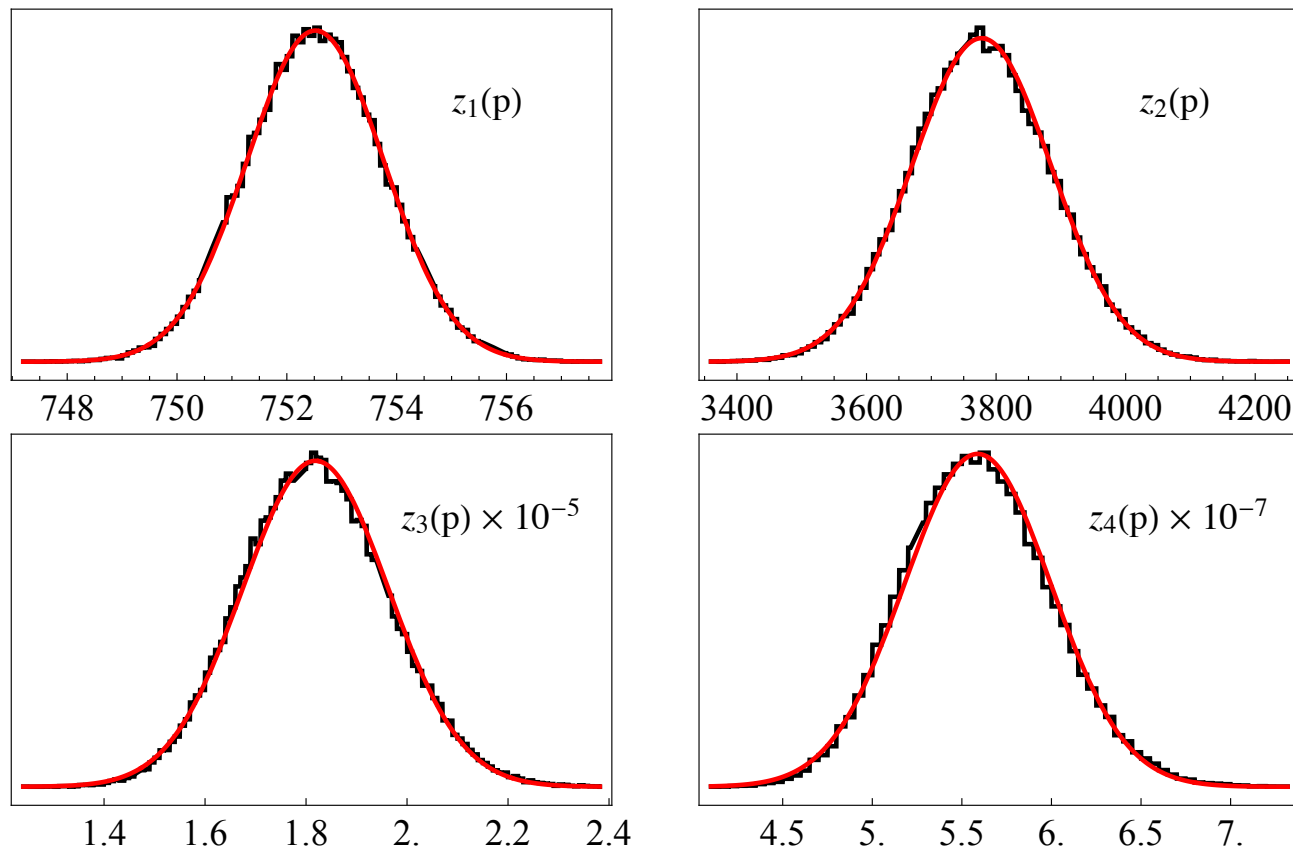
Moments

$$\langle X_{\max}^n \rangle_Z = \frac{\int P(X_{\max} | Z) X_{\max}^n dX_{\max}}{\int P(X_{\max} | Z) dX_{\max}}$$

$$\langle X_{\max}^n \rangle(w) = \frac{\sum_Z \langle X_{\max}^n \rangle_Z w_Z}{\sum_Z w_Z}$$

All systematic uncertainties are included

p, EPOS, [1, 2] EeV



— Bootstrap
— Normal

Include statistical uncertainties
(data and simulation)
by Bootstrapping

Simulations


$$z(w) \sim \mathcal{N}_n(z | \mu(w), \Sigma(w))$$

Data

$$\tilde{z} \sim \mathcal{N}_n(z | \tilde{\mu}, \tilde{\Sigma})$$

Nested Sampling

Evidence $Z = \int \mathcal{L}(w) \text{Dir}(w) d^D w = \int_0^1 \mathcal{L}(X) dX,$

- at step $k = 1$, sample N_{live} points (compositions)
- select w_1 with lowest likelihood L_1 ; w_1 is a dead point
- at step $k > 1$, sample a new live point w from prior, with constraint $\mathcal{L}(w) > L_{k-1}$
- Find the dead point w_k , with likelihood L_k Can be estimated with Beta distributions
- calculate volume of prior region with $L_{k-1} < \mathcal{L}(w) \leq L_k$ 
- calculate evidence shift $\delta Z_k = L_k \delta X_k$

Output is a set of w_k with weights $u_k = \delta Z_k / Z$

$$\text{CL}(\mathcal{L}_0) = \sum_{(w_k, u_k) \mid \mathcal{L}(w) \geq \mathcal{L}_0} u_k$$

Nested Sampling

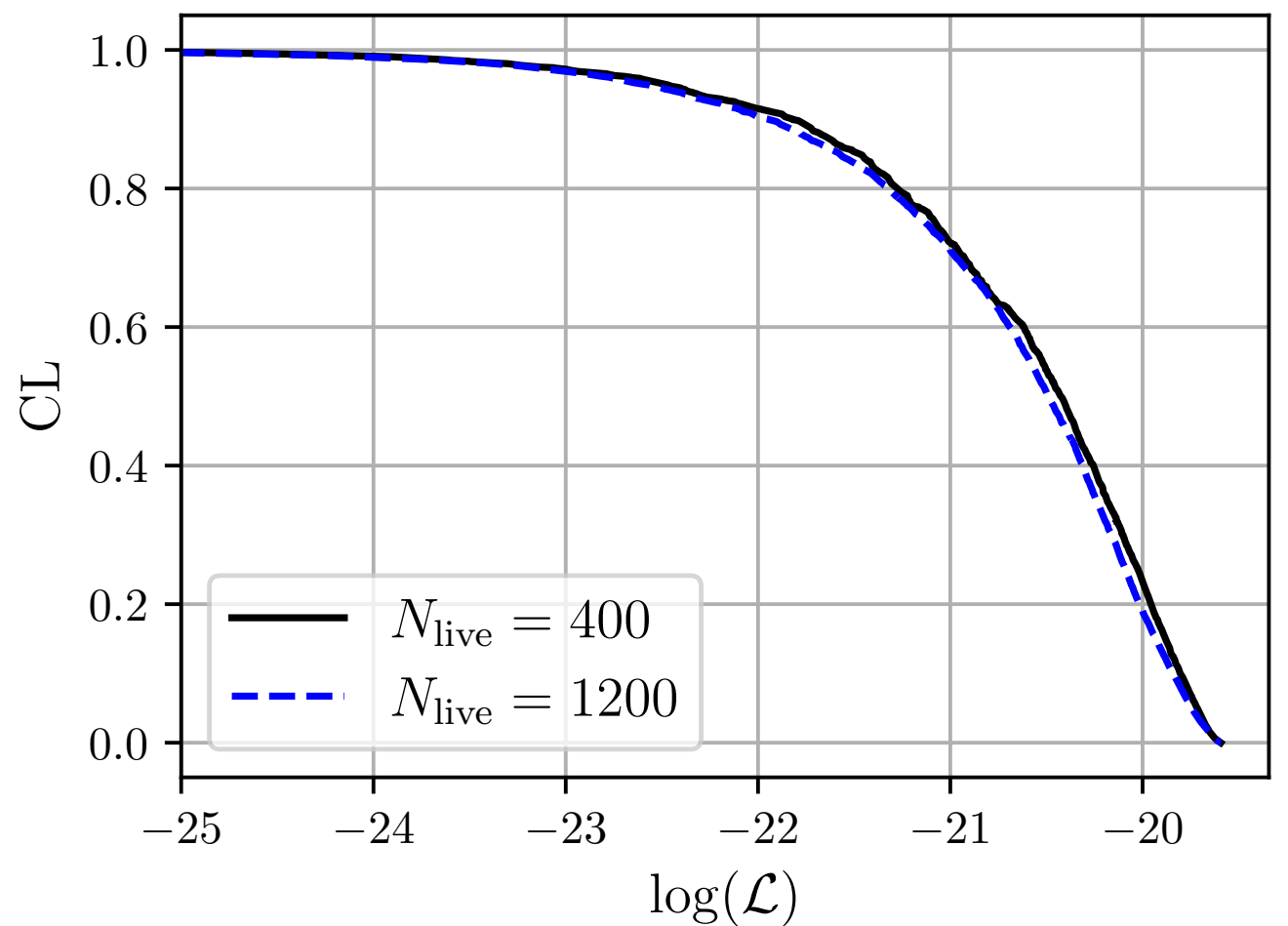
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- at step $k = 1$, sample N_{live} points (compositions)
- select w_1 with lowest likelihood
- at step $k > 1$, sample a new point w_k with $\mathcal{L}(w) > L_{k-1}$
- Find the dead point w_k , with $\mathcal{L}(w_k) = L_{k-1}$
- calculate volume of prior region V_k
- calculate evidence shift δZ_k

Output is a set of w_k with weights

$$\text{CL}(\mathcal{L}_0) =$$

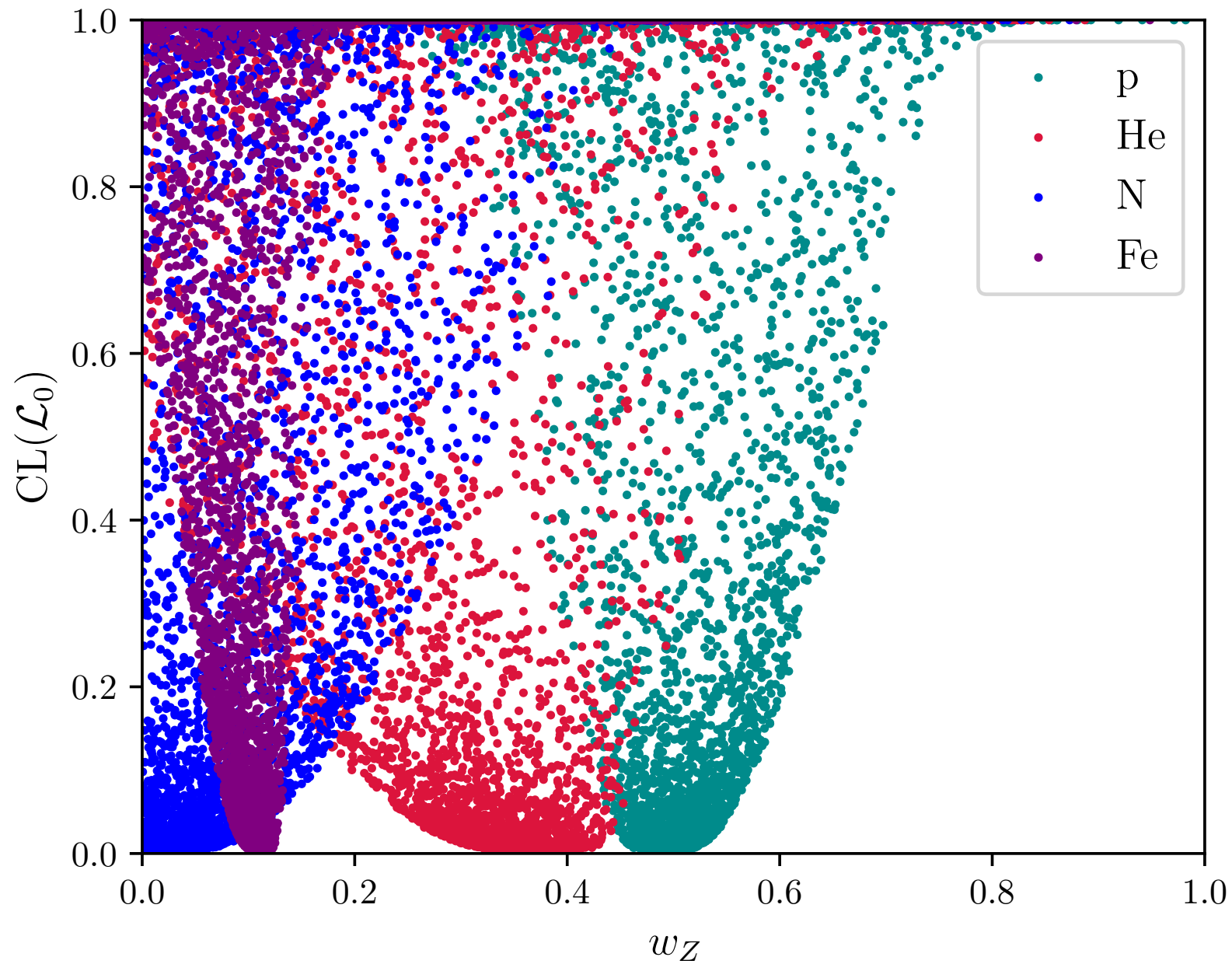
$$(w_k, u_k) \mid \mathcal{L}(w) \geq \mathcal{L}_0$$



Full likelihood form

$$\begin{aligned} \mathcal{L} = & (2\pi)^{-\frac{D}{2}} \det \left(\Sigma_w + \tilde{\Sigma} \right)^{-\frac{1}{2}} \exp \left[-\frac{1}{2} \left(\mu_w^T \Sigma_w \mu_w + \tilde{\mu}^T \tilde{\Sigma} \tilde{\mu} \right) \right. \\ & \left. + \frac{1}{2} \left(\mu_w^T \Sigma_w^{-1} + \tilde{\mu}^T \tilde{\Sigma}^{-1} \right) \left(\Sigma_w^{-1} + \tilde{\Sigma}^{-1} \right)^{-1} \left(\Sigma_w \mu_w + \tilde{\Sigma} \tilde{\mu} \right) \right] \end{aligned}$$

4 primary mixture

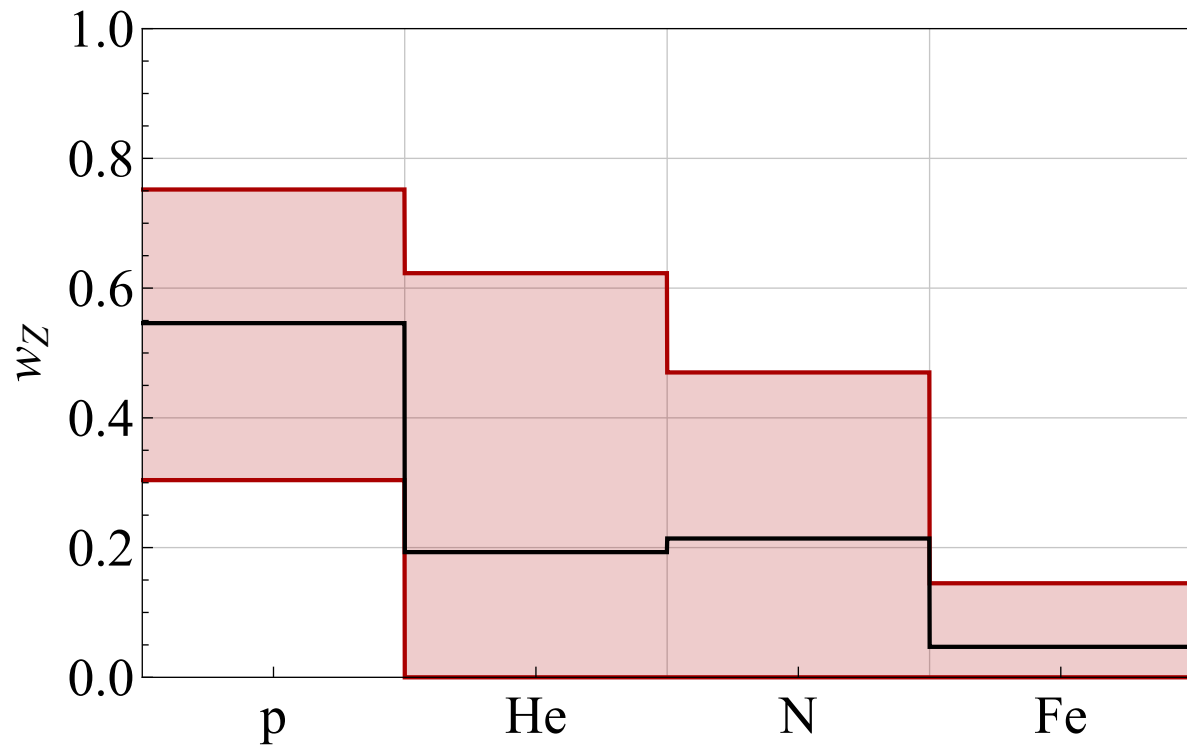


Projections of 4D log-likelihood

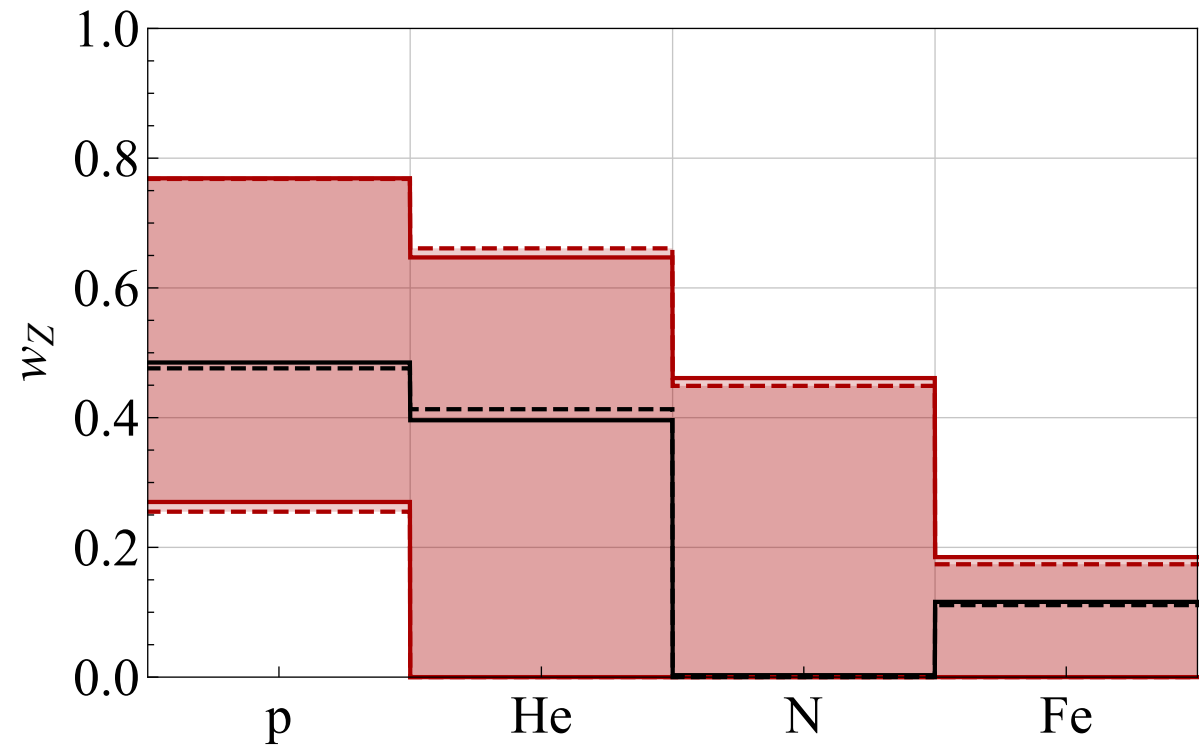
NS allows to efficiently sample the likelihood and find the Confidence Levels (CL)

4 primary mixture

Binned, EPOS, $\log_{10}E \in [17.9, 18.0]$

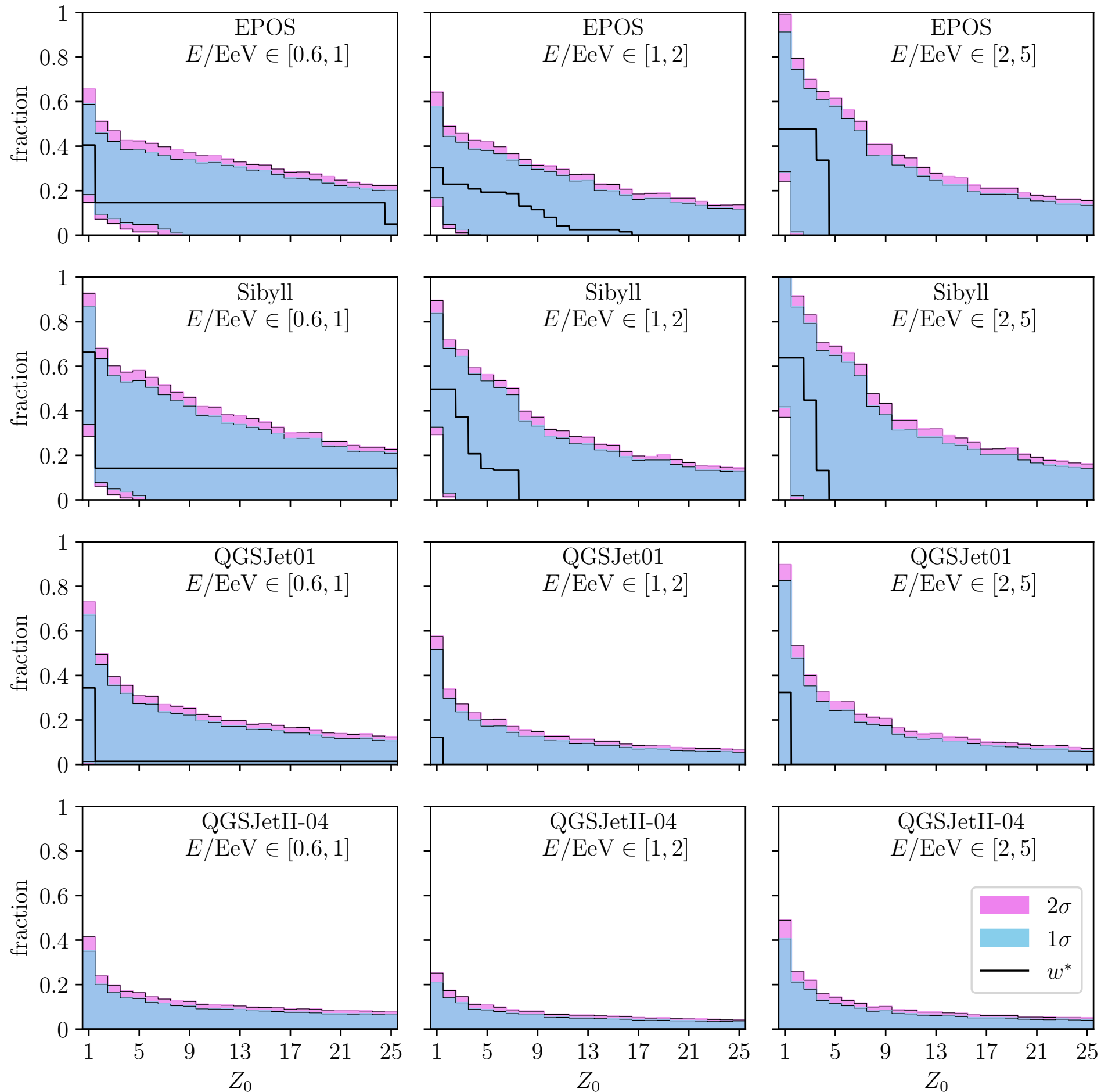


Unbinned, EPOS, $\log_{10}E \in [17.9, 18.0]$



Consistent with results from 2001.02667

Results are unchanged increasing
the number of features



EPOS and Sibyll (LHC-based) exclude 100% proton and can give bounds on heavy elements

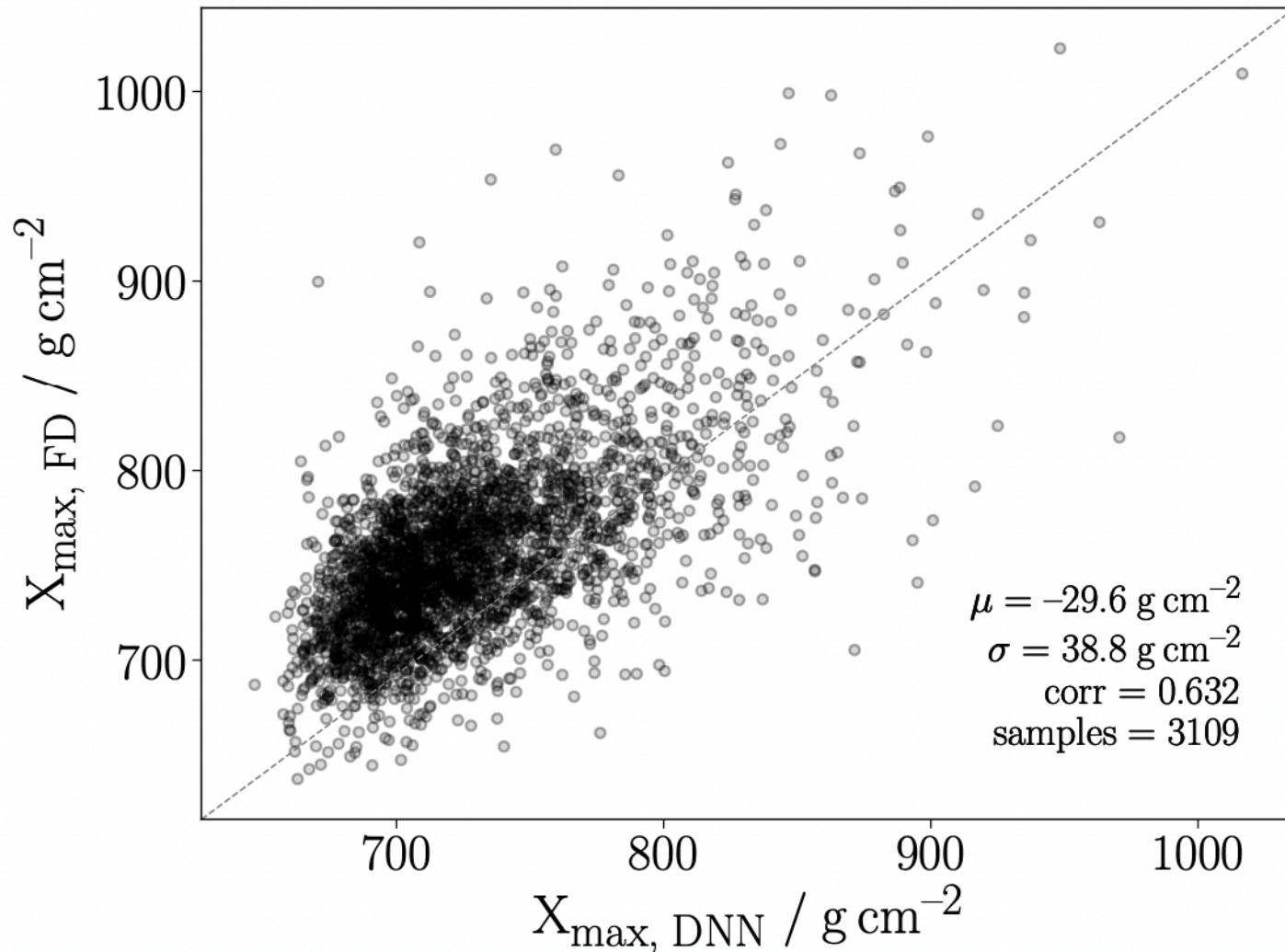
QGS models are consistent with 100% proton composition

SD to FD

Build a map from Surface Detector data to Fluorescent Detector data (X_{\max})

(Auger Coll.: 2101.02946)

Train Deep Neural Network (DNN)
on simulated data



Shows strong correlations



As good as simulations (ground
data sims are ~wrong)



Trained with 4 primaries

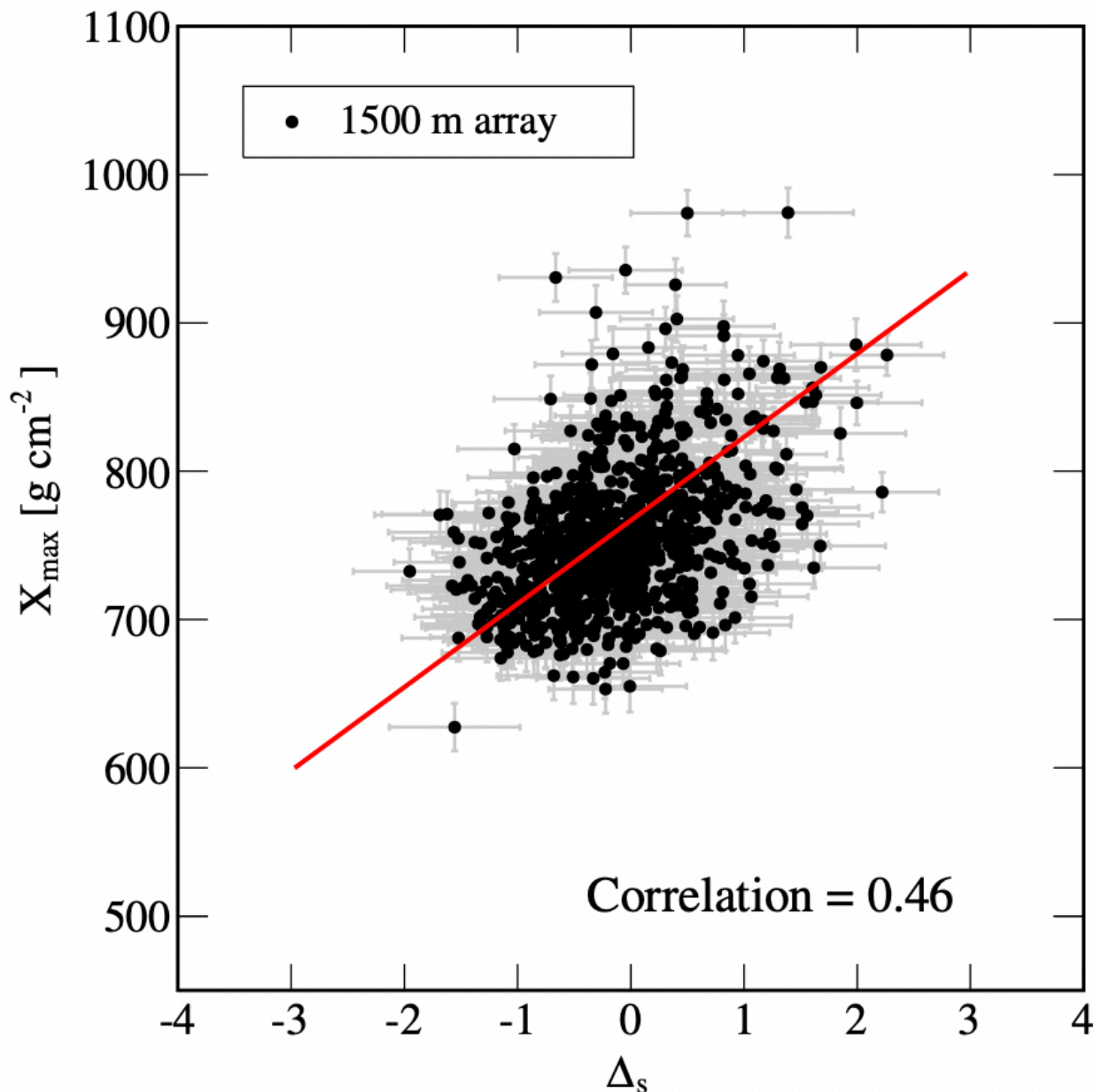


We do not have access to this
DNN

SD to FD

Build a map from Surface Detector data to Fluorescent Detector data (X_{\max})

(Auger Coll.: 1710.07249)



Build simple observable that correlates with FD

— Weaker correlation and large uncertainties

— Some quantities are given fits

✓ We can reproduce and use this

✓ We can (try to) improve on this