New Perspectives Conference 2021

FERMILAB-SLIDES-21-090-ND

Fitting NOvA cross-section parameters with Markov Chain Monte Carlo

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for the NOvA collaboration

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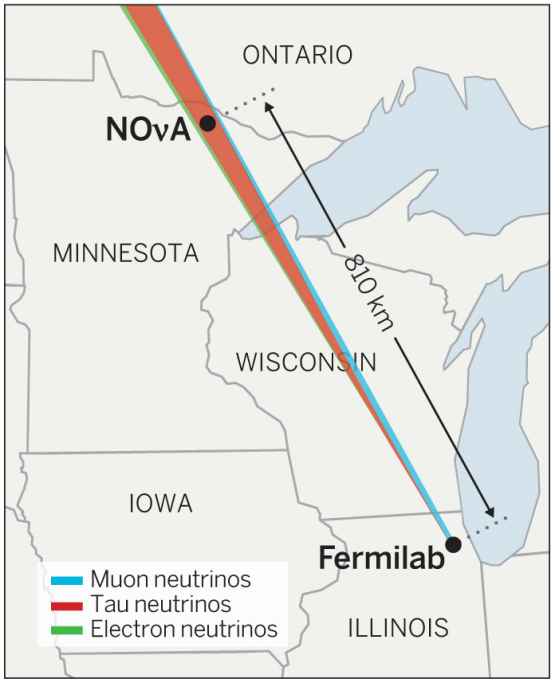
Motivation of the MCMC fit

- NuMI Off-Axis ν_e Appearance (NOvA) Experiment observes neutrino interactions to measure oscillation parameters.
- Contains a Near Detector (ND) at Fermilab & Far Detector (FD) 810 km away in Minnesota.
- Primary physics goals: (1) the mass ordering and value of Δm^2_{23}, (2) CP-violation (δ_{CP}), (3) the mixing angle θ_{23}.



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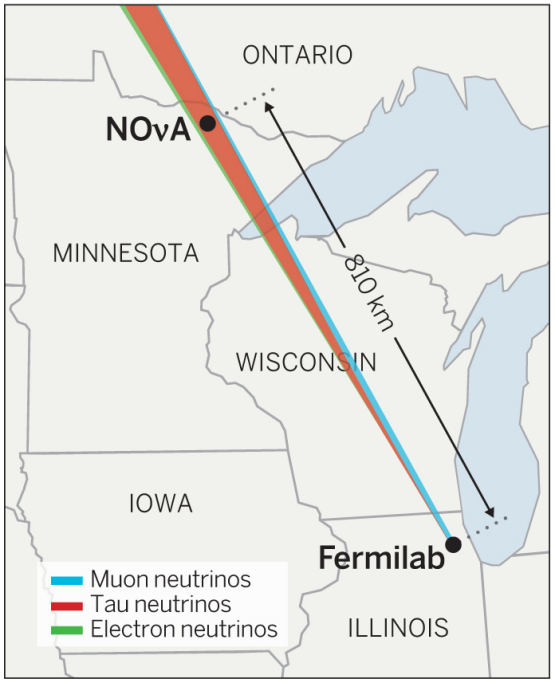

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- Primary physics goals: (1) the mass ordering and value of Δm^2_{23}, (2) CP-violation (δ_{CP}), (3) the mixing angle θ_{23}.
- The long-term goal of this MCMC work is to...

  ...fit the neutrino oscillation ($sin^2(\theta_{23})$, Δm^2_{23}, and δ_{CP}) and NOvA's physics model parameters...

  ...simultaneously to the NOvA ND + FD data...

  ...with MCMC.

- This talk demonstrates the principle of MCMC fitting.
  - Fit a set of NOvA physics model parameters to fake data.

What is MCMC?

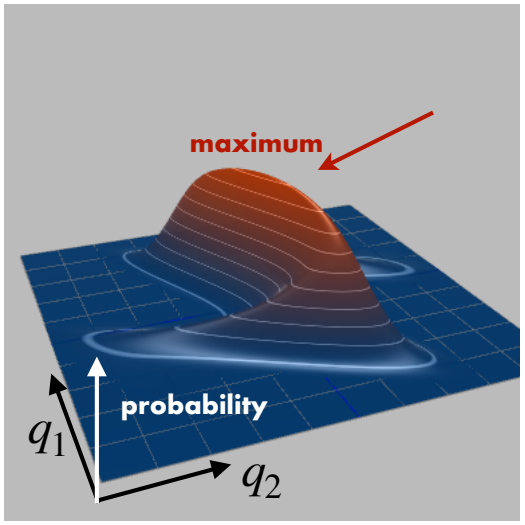
- MCMC is a Bayesian inference parameter estimation tool.
- In Bayes' theorem, we seek to locate the maximum of the posterior probability distribution.
  - Posterior is complex: N parameters → N dimensions ($dim(\vec{q})$ = 16, in this talk).

Bayes Theorem:

$$P(\vec{q}\,|\,data) \propto P(data\,|\,\vec{q}) \times P(\vec{q})$$

posterior ∝ **likelihood** × **prior**

2D example posterior distribution



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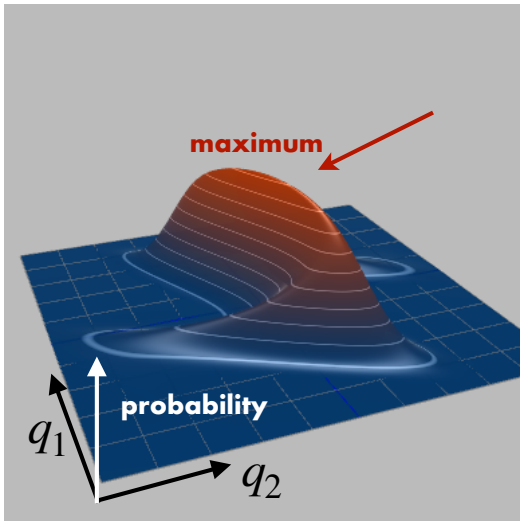

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- Explore space by a Markov transition (i.e. a conditional prob.) – $T(\vec{q}'|\vec{q})$.
- Use Hamiltonian Monte Carlo (HMC) to explore posterior Efficiently & Repeatedly:
  - Include conjugate variable: $\vec{p}$, so $(\vec{q}) \rightarrow (\vec{q},\vec{p})$.
  - $pdf(\vec{q},\vec{p}) \equiv \mathrm{H}(\vec{q},\vec{p}) = \mathrm{KE}(\vec{q},\vec{p}) + \mathrm{V}(\vec{q})$.
  - In 2D, ball in a gravitational field analogy:
    - Efficiently: if $\mathrm{V}(\vec{q}) \downarrow$, then probability $\uparrow$.
    - Repeatedly: "Drop" ball from different locations – each "drop" is known as a sample.

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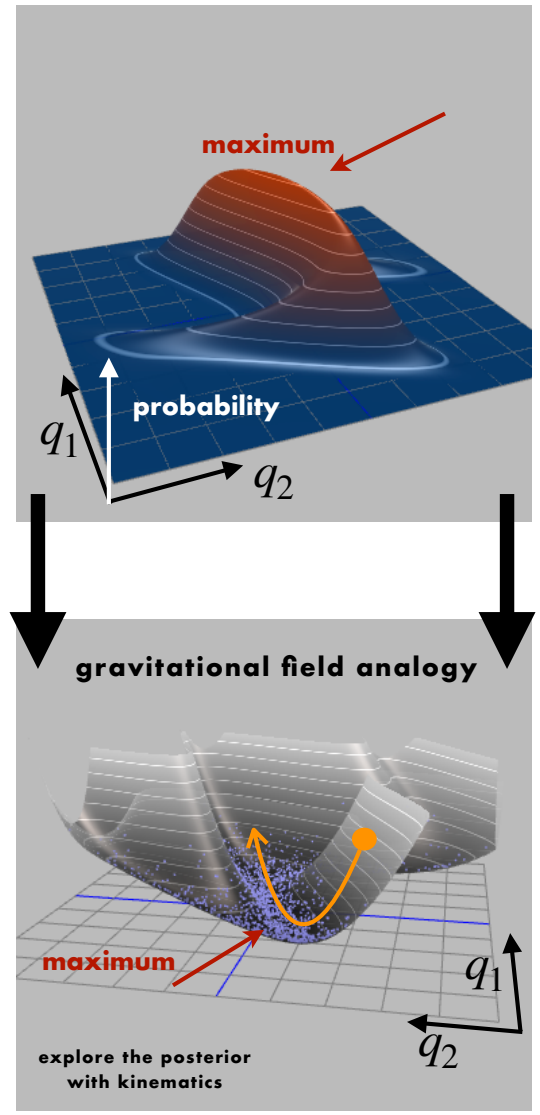
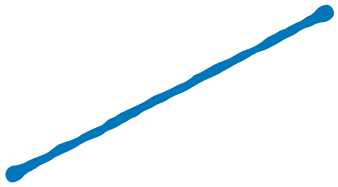
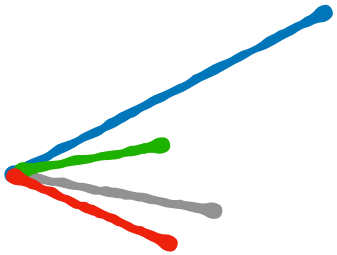


Divide the ND predictions into topologies

Muon

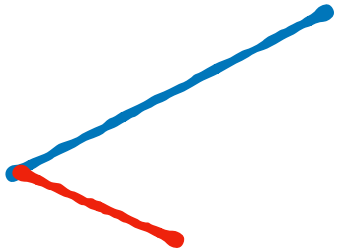


Muon + Pion + other

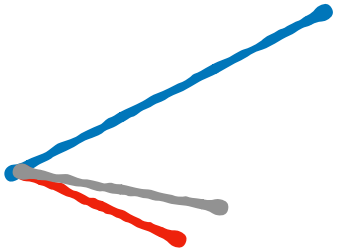


- Split ν & $\bar{\nu}$ ND interactions into five topologies in two variables: E_{had}^{vis} & $Reco|\vec{q}_3|$.
  - E_{had}^{vis} – energy deposited in the detector.
- Will focus on ν and E_{had}^{vis}.

Muon + Proton

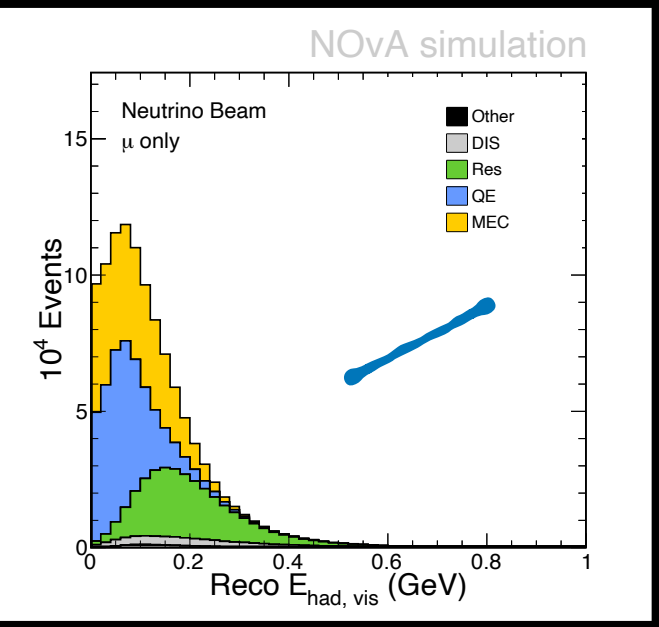


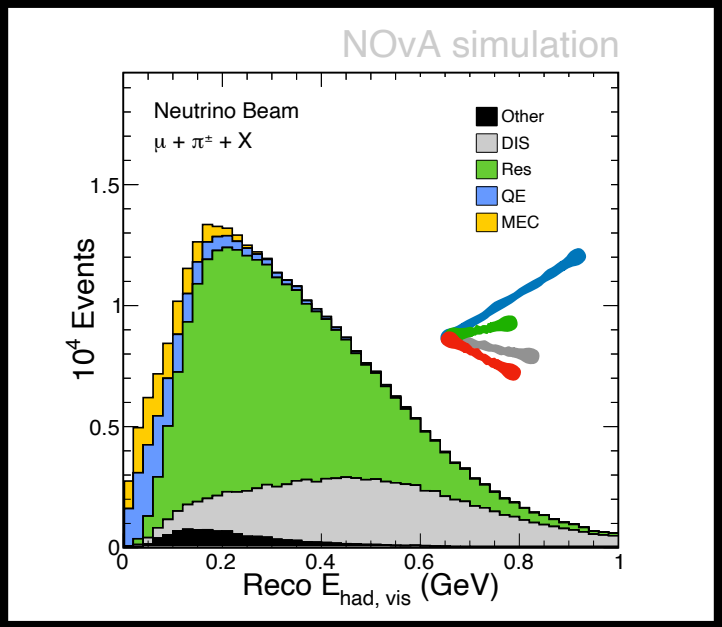
Muon + Proton + other



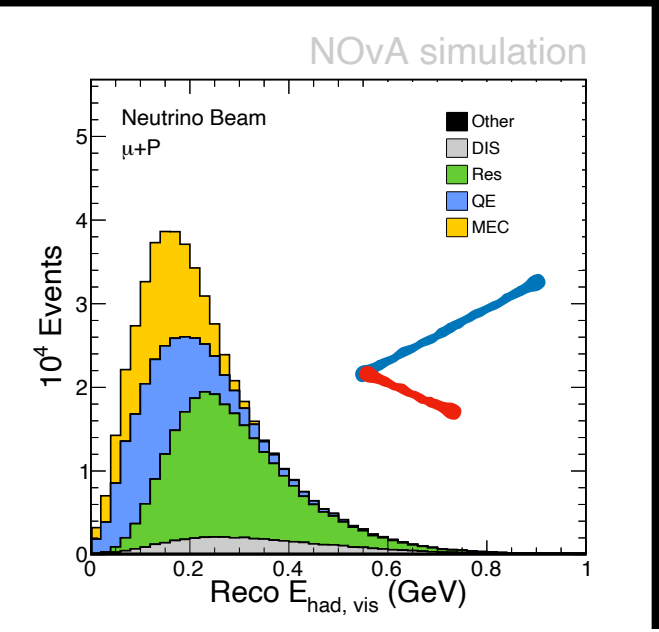
Remaining

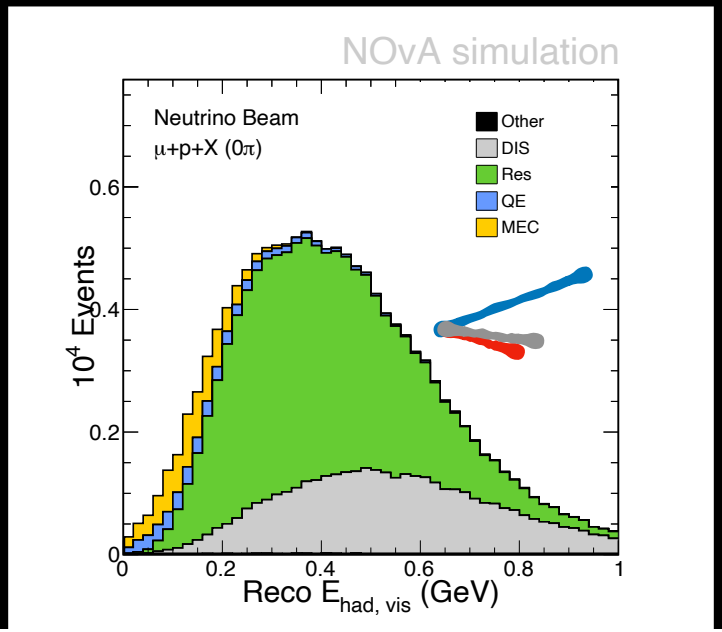
Divide the ND predictions into topologies: ν in *Reco* $E_{had,\ vis}$

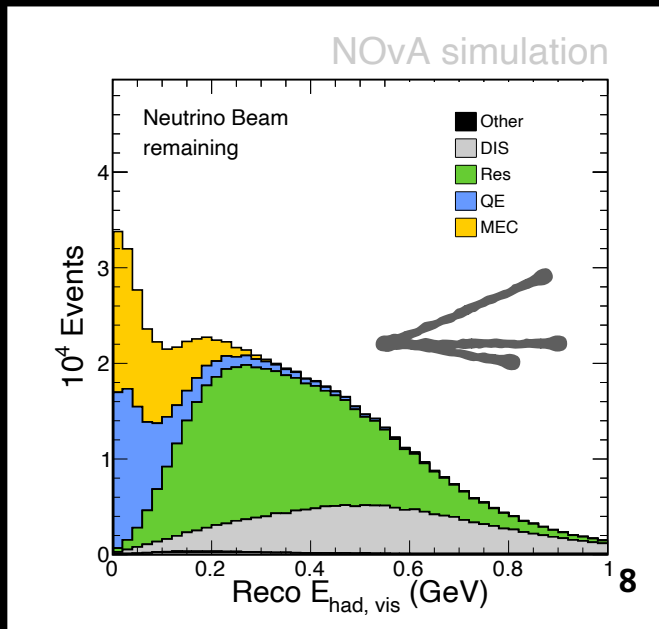




- GENIE v3 simulation of the five ND topologies in E_{had}^{vis}.
  - *Reco* $|\vec{q}_3|$ in backup slide.
- Next is to create ND fake data in these topologies...







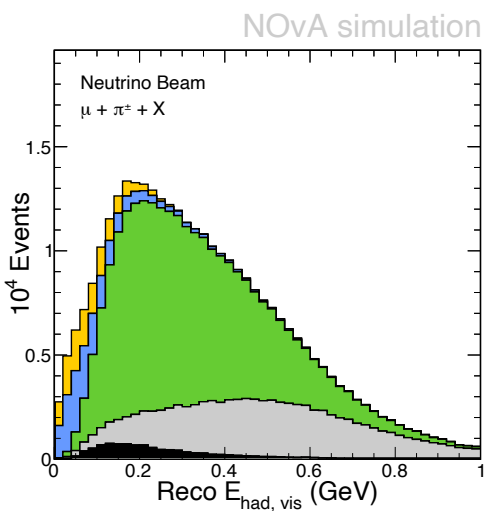
Creating Fake Data

Parameters:	Shift
1. ————	0 σ
2. ————	0 σ
3. ————	0 σ
4. ————	0 σ
5. ————	0 σ
...	...

- Identify the parameters from NOvA's systematic uncertainties to fit.
- Apply a random shift to each parameter (from a Gaussian).

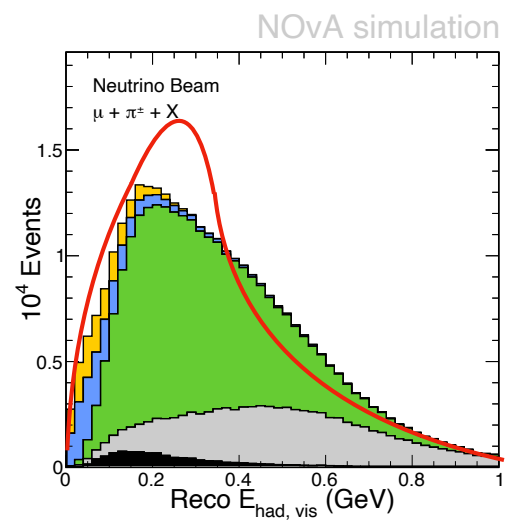
Shift
-0.7 σ
1.5 σ
0.3 σ
-0.2 σ
-0.4 σ
...

nominal prediction



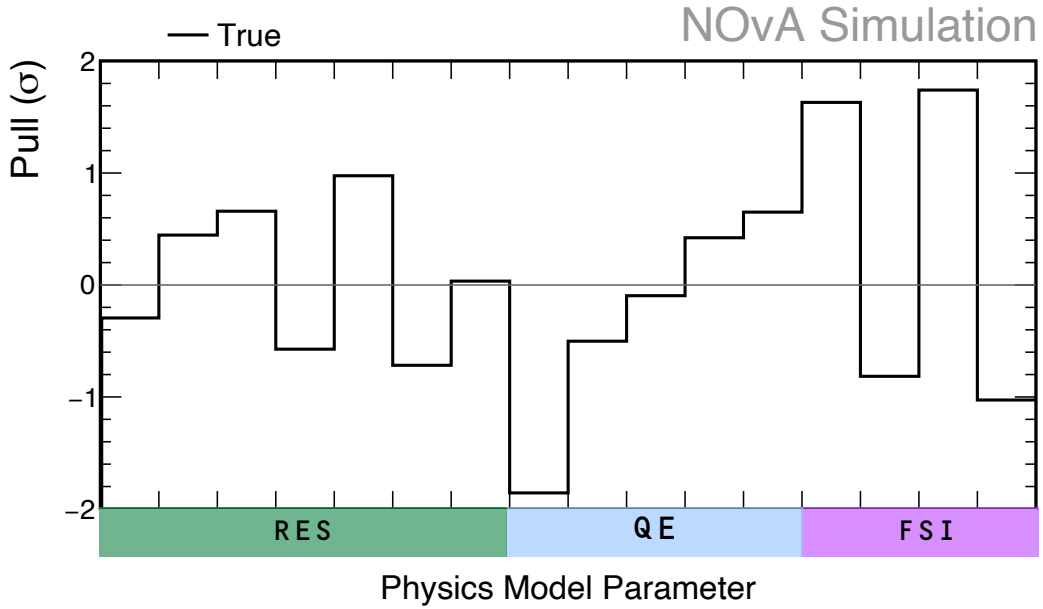
- Apply these shifts to the nominal simulation...
- ...to get a new, distorted distribution: the fake data.
- Repeat for each topology.

fake data



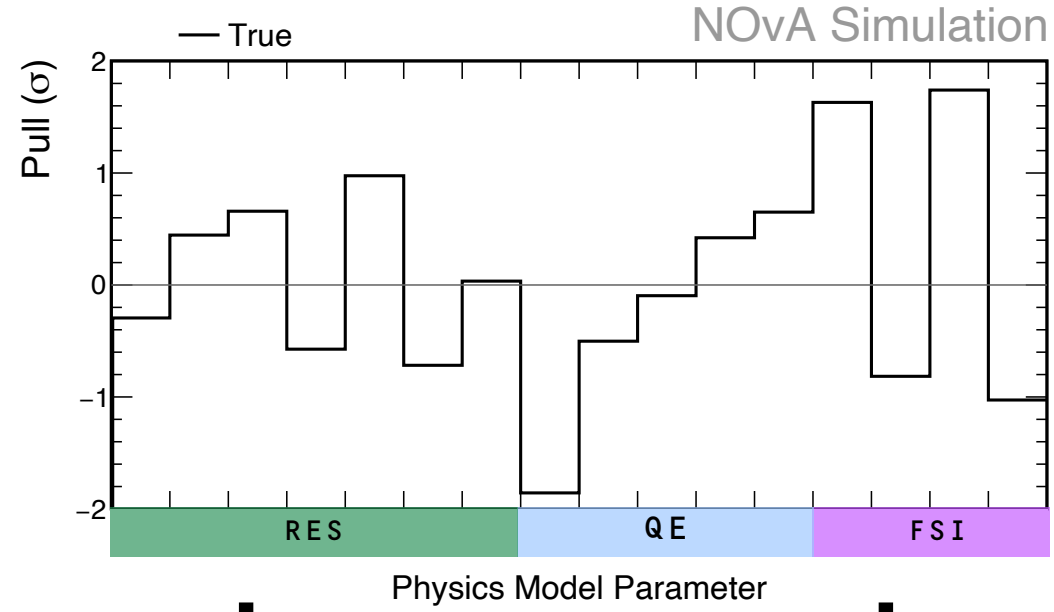
Fake Data Fitting

- In a perfect fit, many MCMC samples will identically match the true pull values...

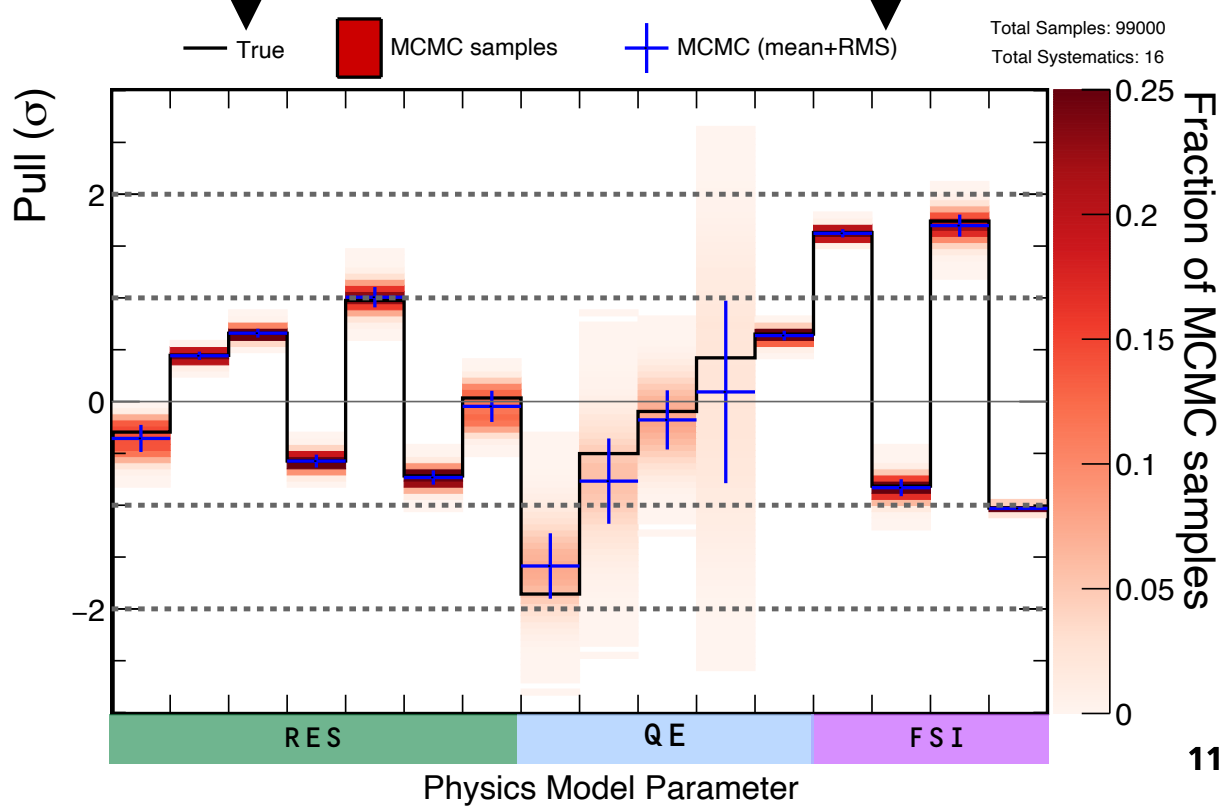


Fake Data Fitting

- In a perfect fit, many MCMC **samples** will identically match the true pull values...
- RES & FSI parameters: a perfect fit – nearly all (dark red) samples overlap the true pull (**black**).

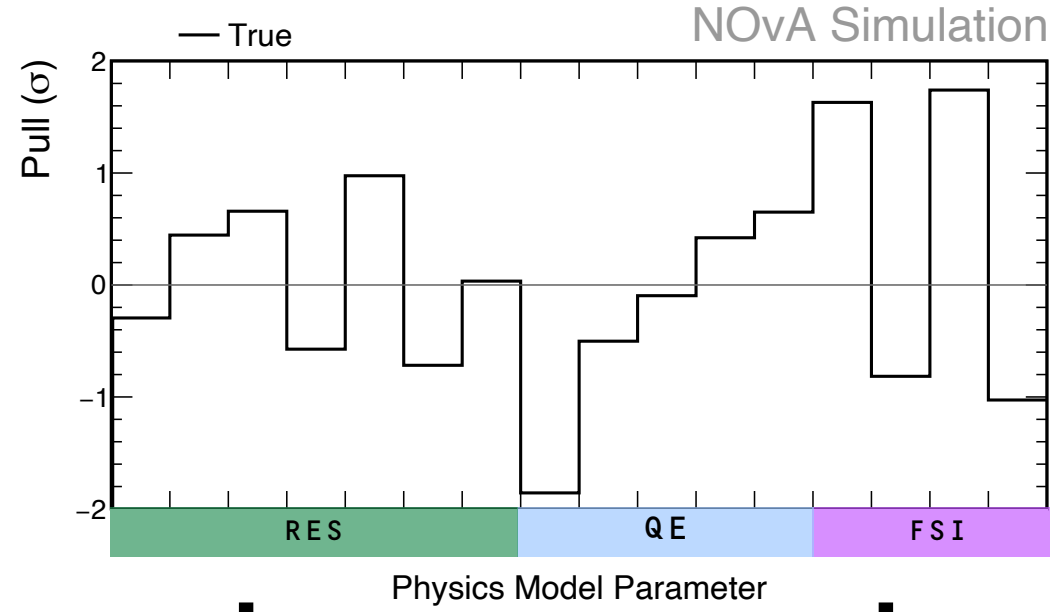


Fit Parameters with MCMC



Fake Data Fitting

- In a perfect fit, many MCMC **samples** will identically match the true pull values...
- RES & FSI parameters: a perfect fit – nearly all (dark red) samples overlap the true pull (**black**).
- QE: samples produce a wide spread of pull values (pink).
  - MCMC tells us about parameters that are not well constrained.



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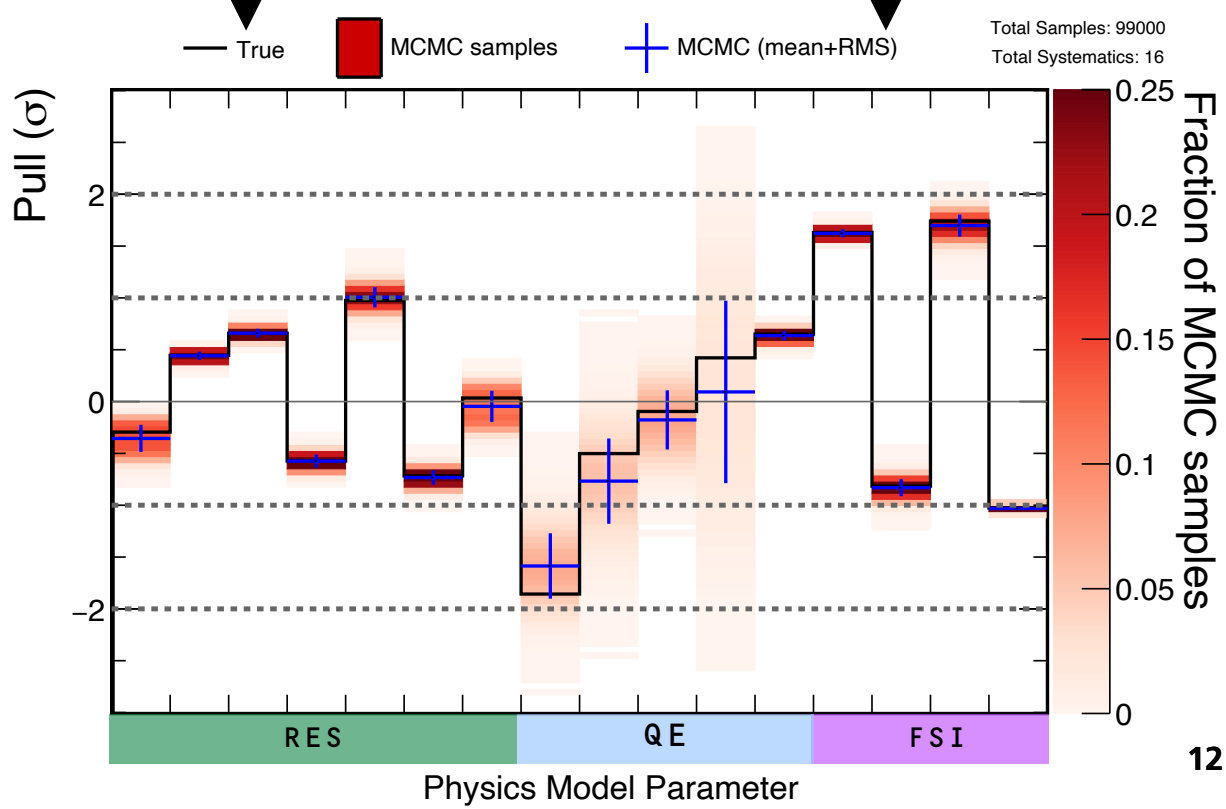
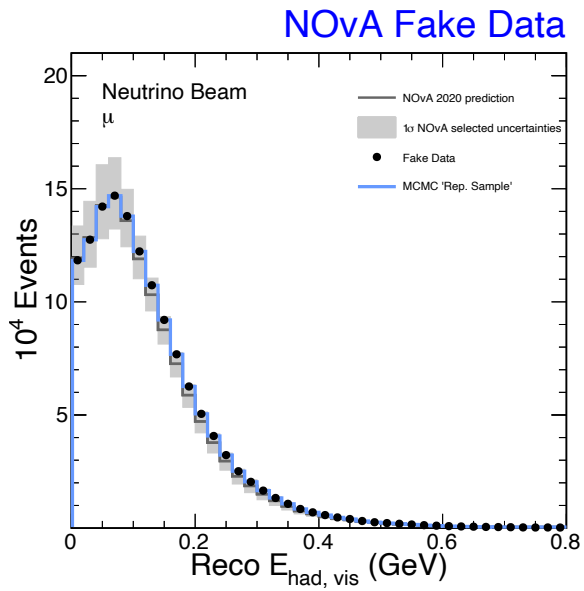
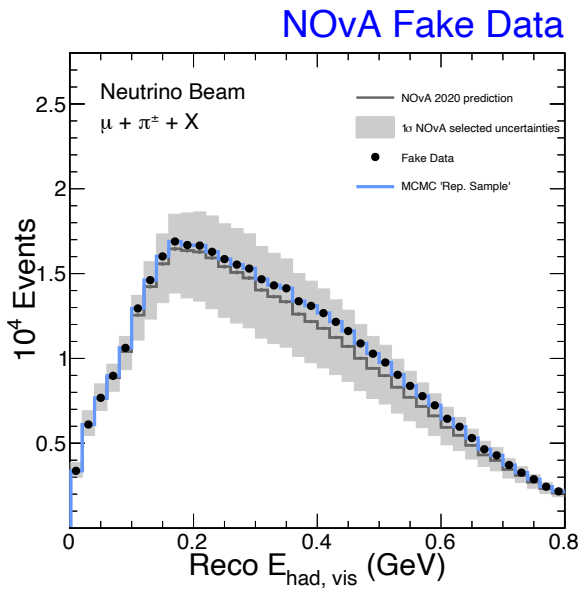
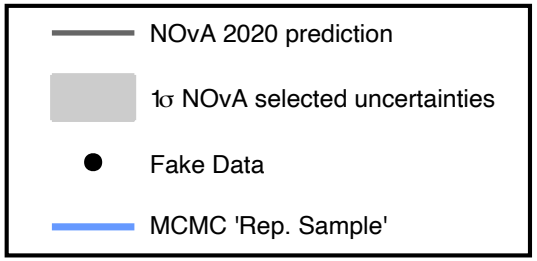


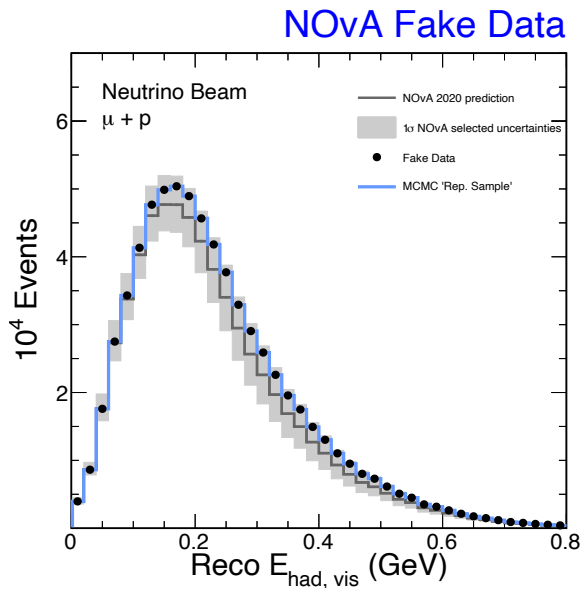
Fitted ND topological distributions: ν in $E_{had,\ vis}$

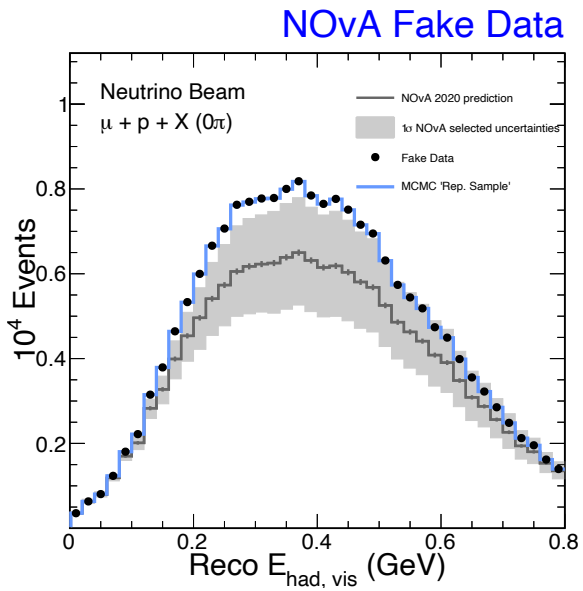


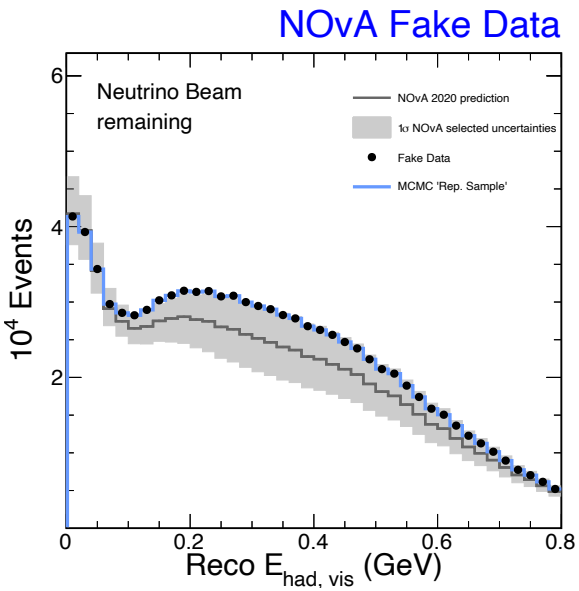




- MCMC fit is strong: 'Rep Sample' (min χ^2) from posterior agrees with the fake data (black) for all topologies.

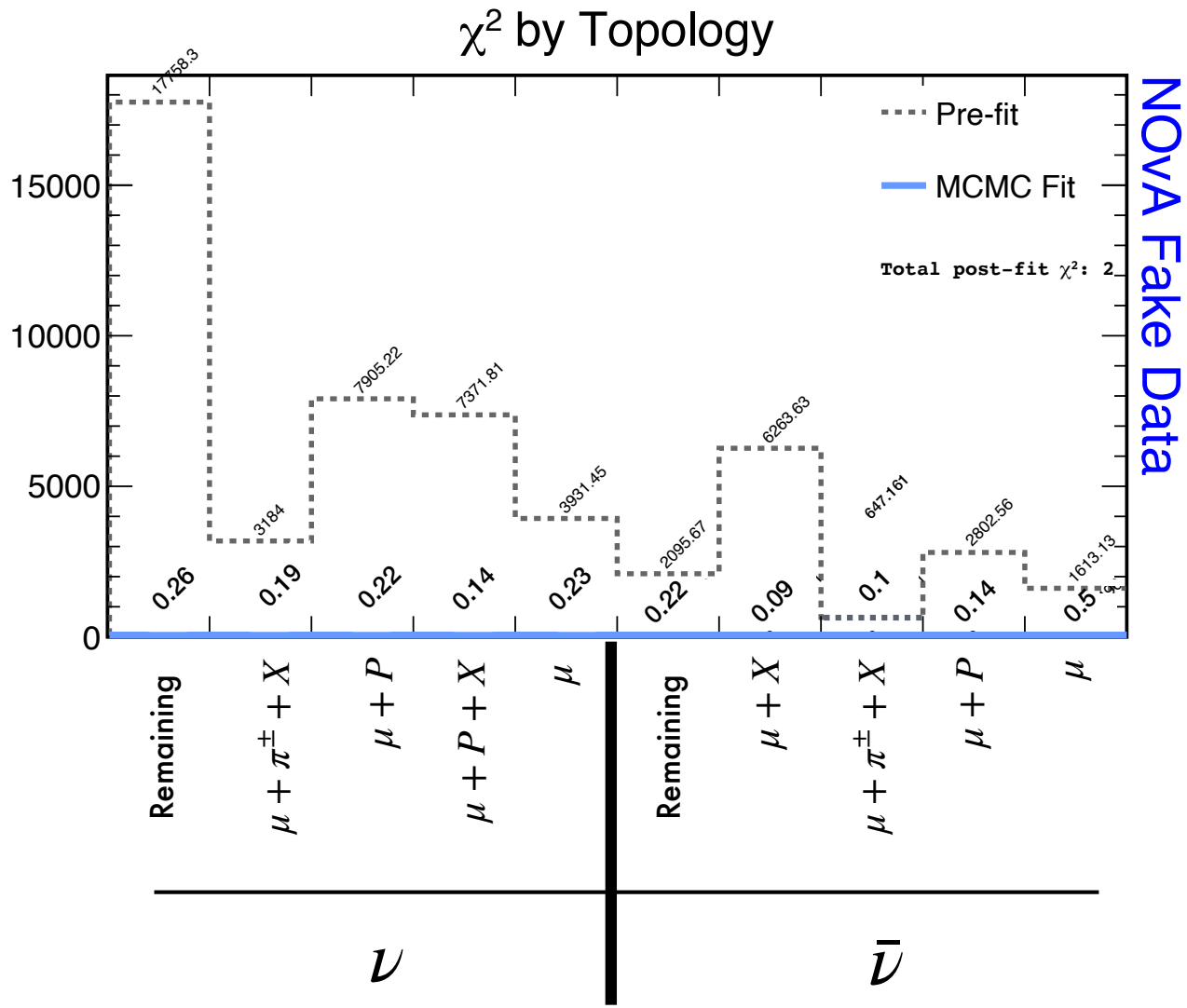






Assessing the Fake Data fit

- Use a quantitative metric to evaluate MCMC, the χ^2 – plotted for each topology.
- $\chi^2 \approx 0$ for all topologies:
  - MCMC fit agrees almost identically to the fake data.
- MCMC can successfully fit NOvA physics model parameters.

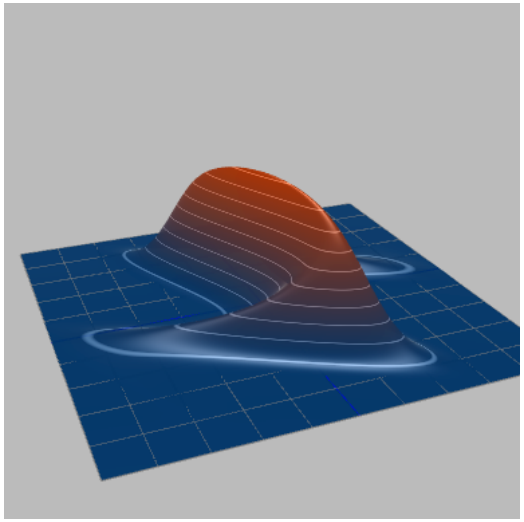


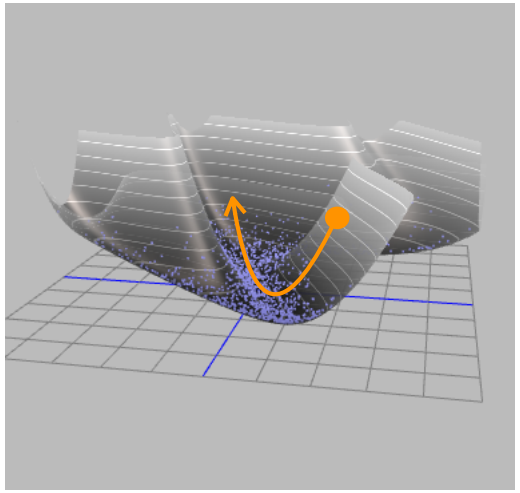
Conclusions

- Markov Chain Monte Carlo is a Bayesian inference parameter fitting tool.
- This talk is a demonstration of the fitting procedure:
  - MCMC successfully fits NOvA physics model parameters to fake data.
- Future directions:
  - fit all physics model parameters to ND data.
  - simultaneously fit ND & FD data to all NOvA systematic uncertainties.
- I would like to acknowledge the support of:
  - DOE Office of Science Tufts University grant: DE-SC0019032
  - URA Visiting Scholars Program Award #20-F-05

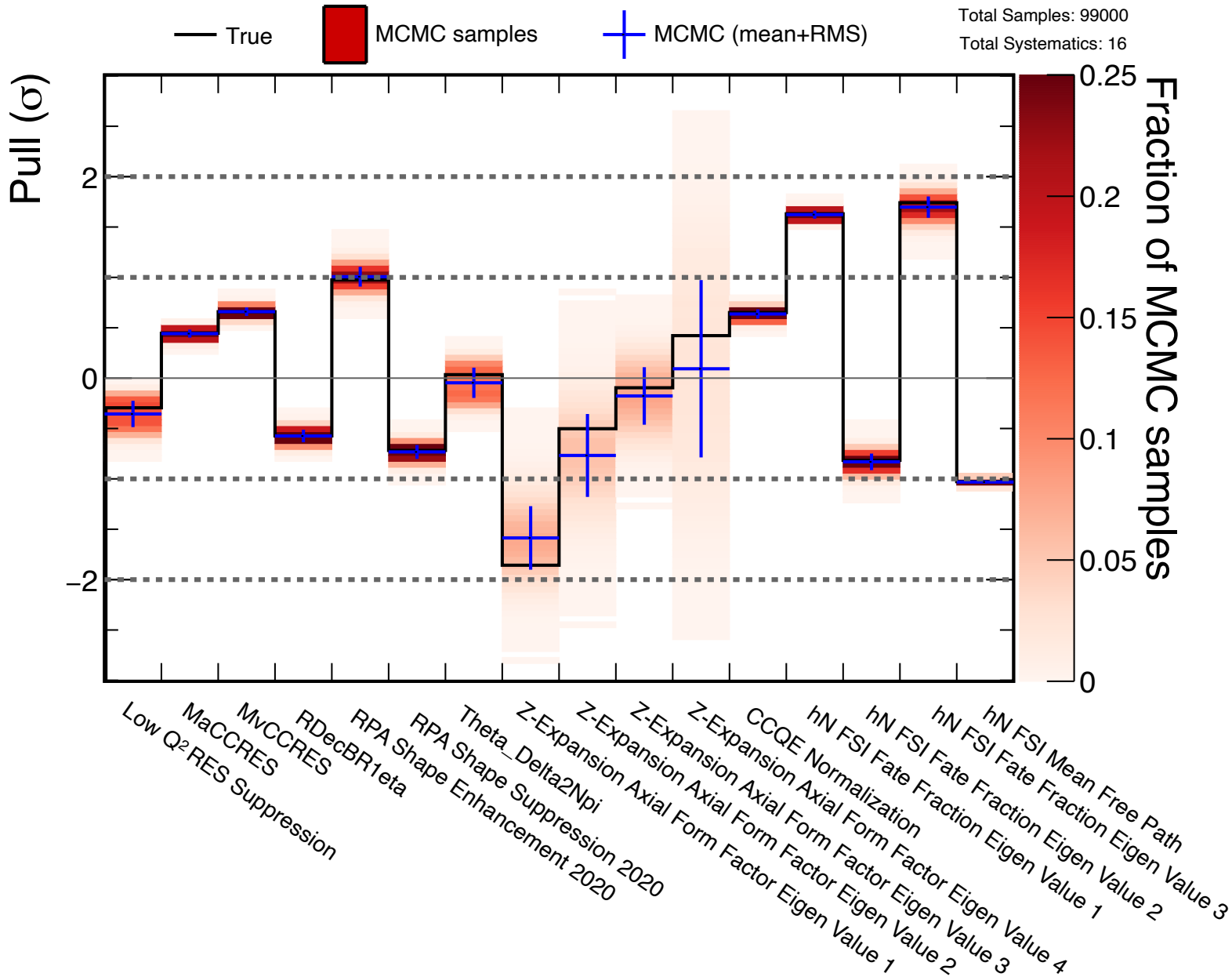
http://novaexperiment.fnal.gov

Back up

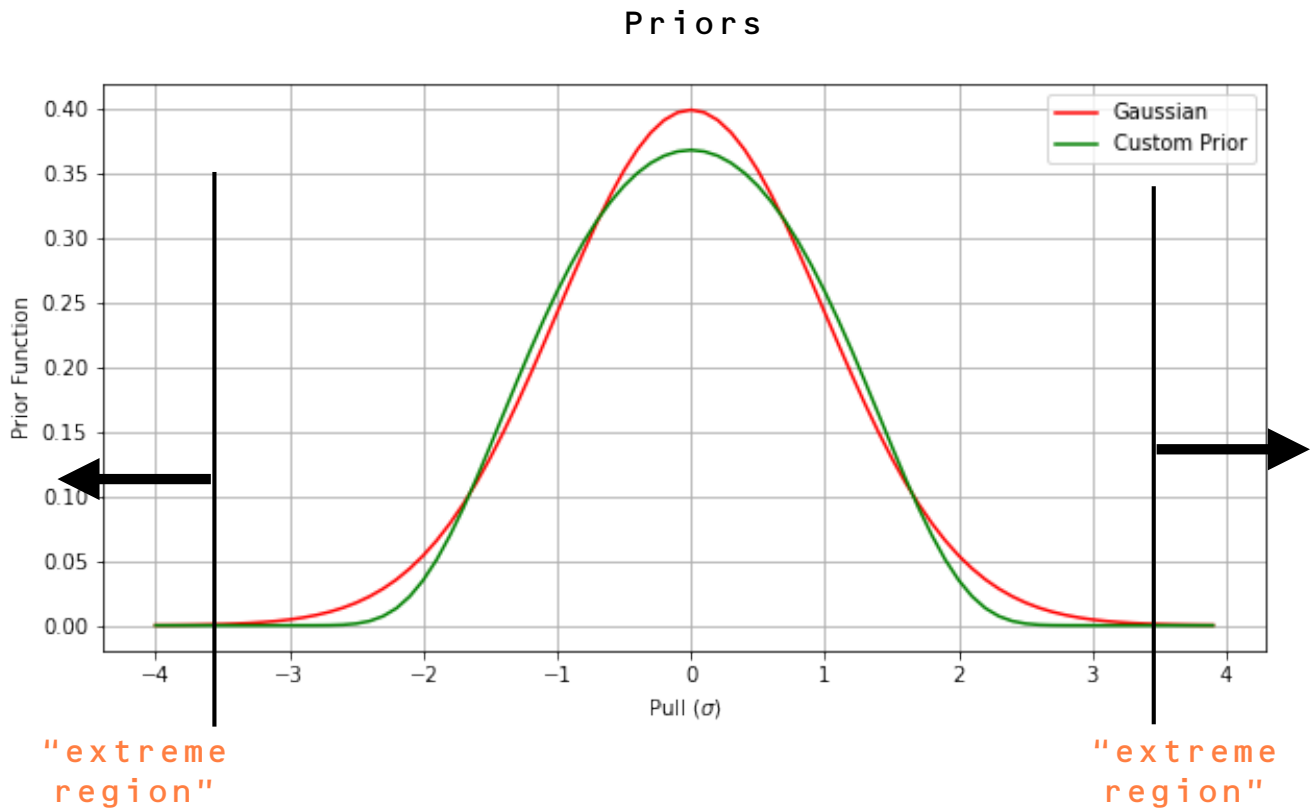




Fitting Fake Data



MCMC Prior Choice

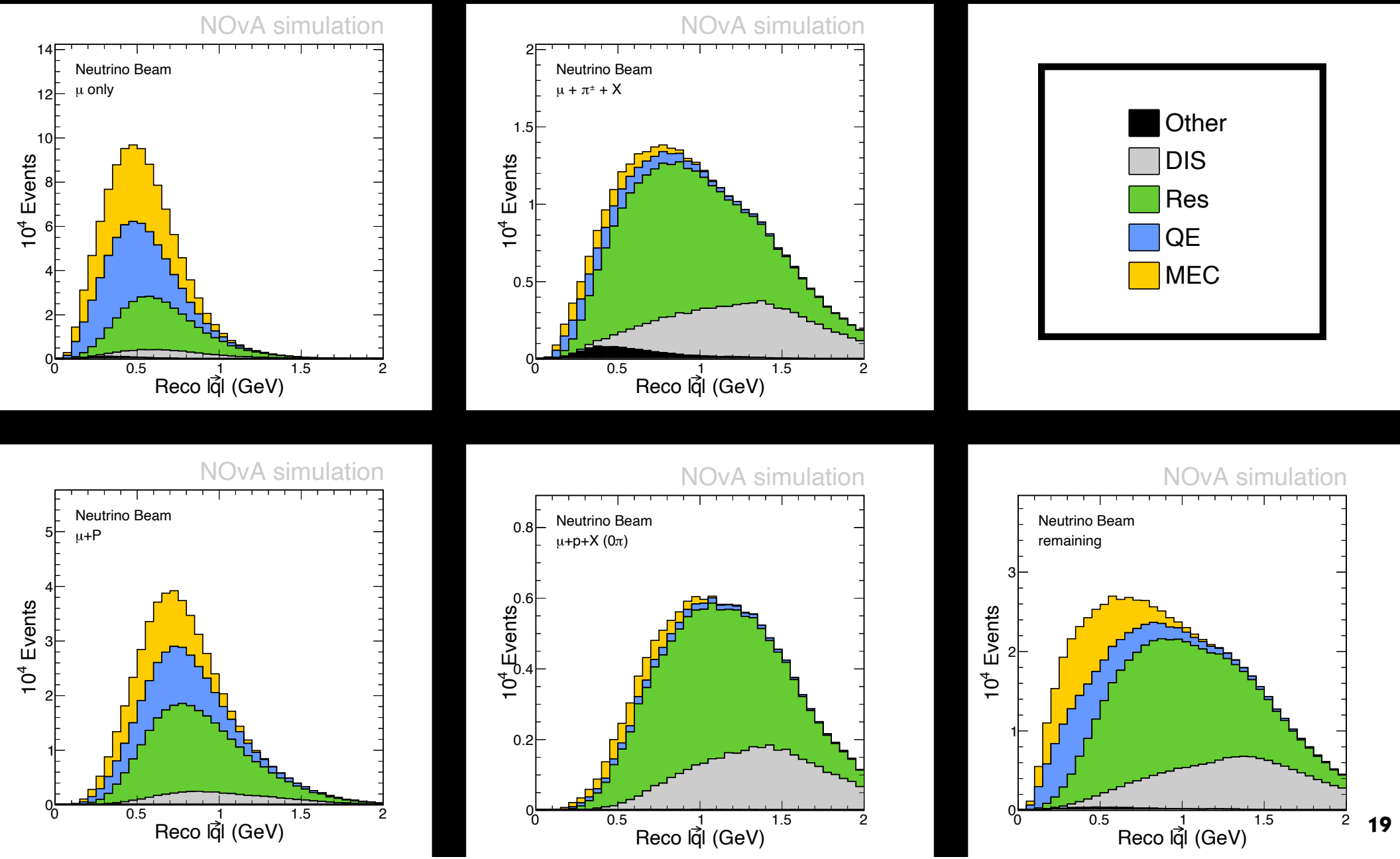


- We believe any pull beyond $\pm 3\sigma$ does not have a solid physical meaning – "extreme region".
- We use a narrow, Gaussian-like prior to prevent pulls in the "extreme region".

Custom Prior: $p(x) = e^{-e^{0.3025x^2}}$

ND Topological distributions:

ν in $Reco\ |\vec{q}_3|$



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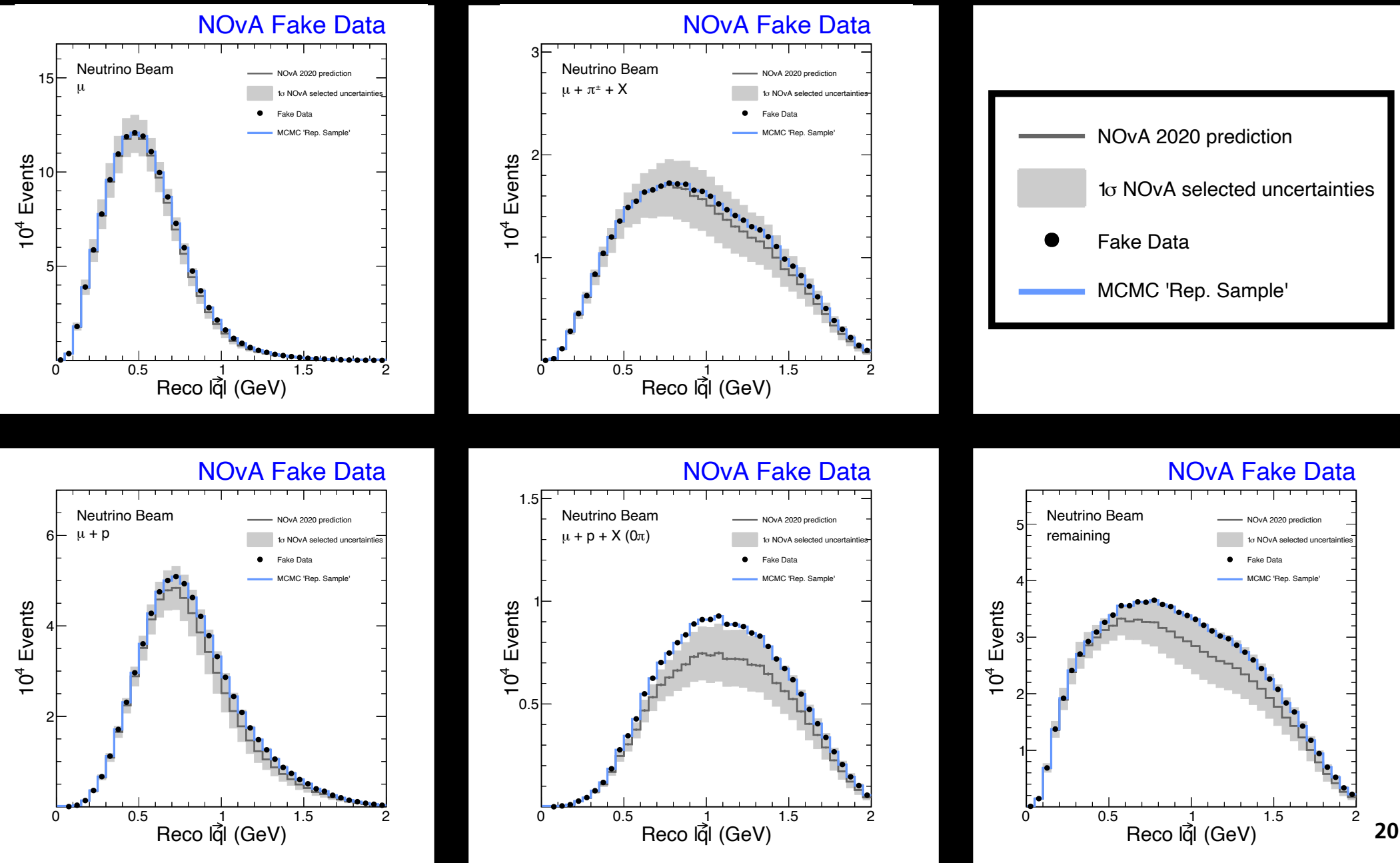
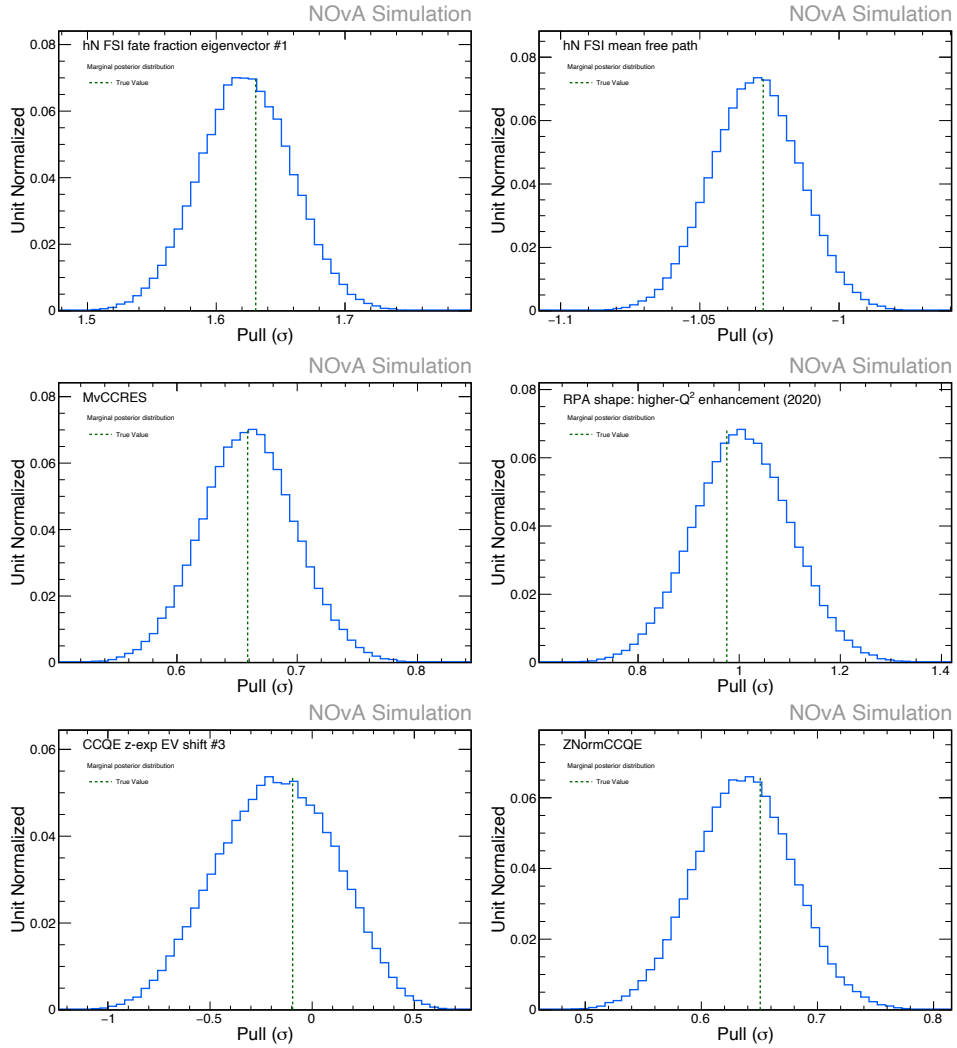


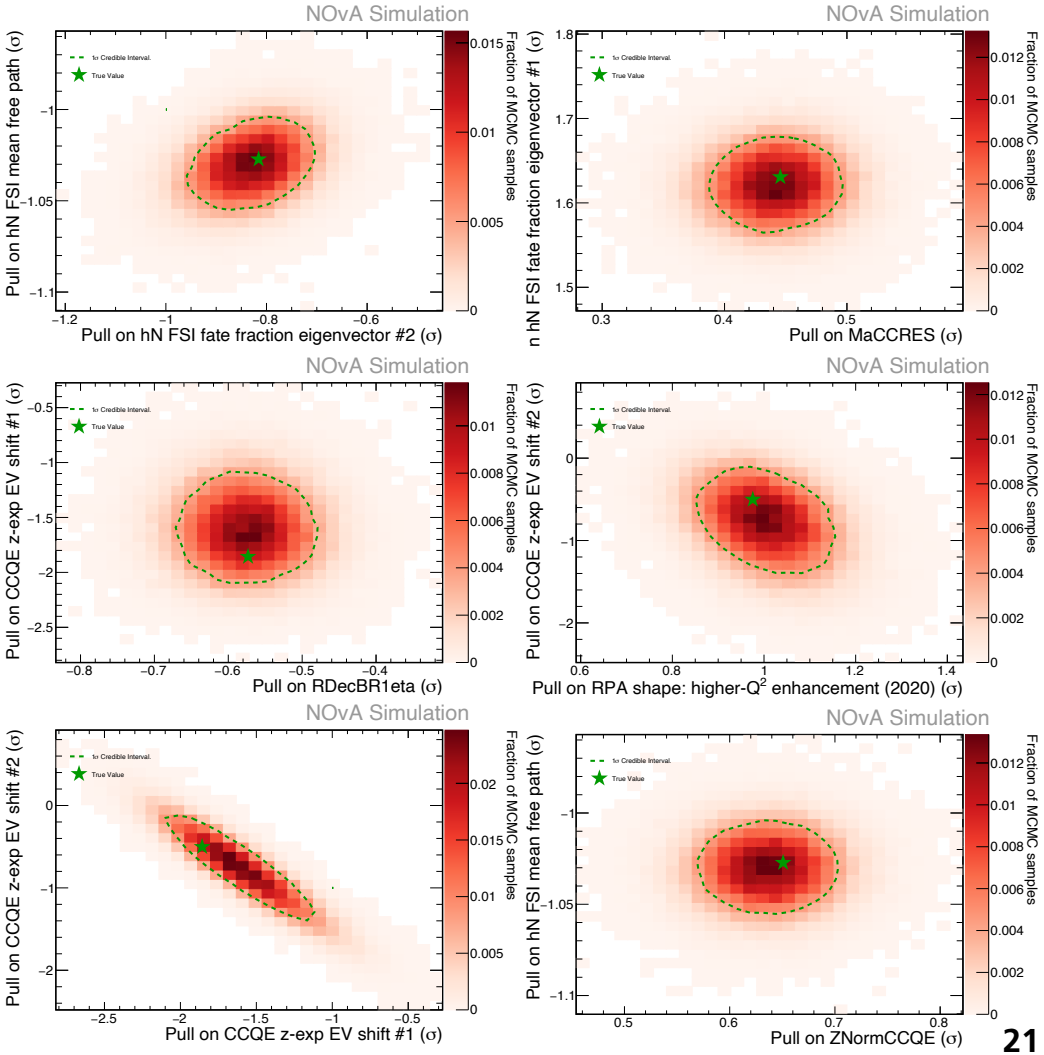
Examining marginal distributions

- One advantage of Bayesian inference is the ability to marginalize over undesired parameters to examine the probability distributions for desired parameters.

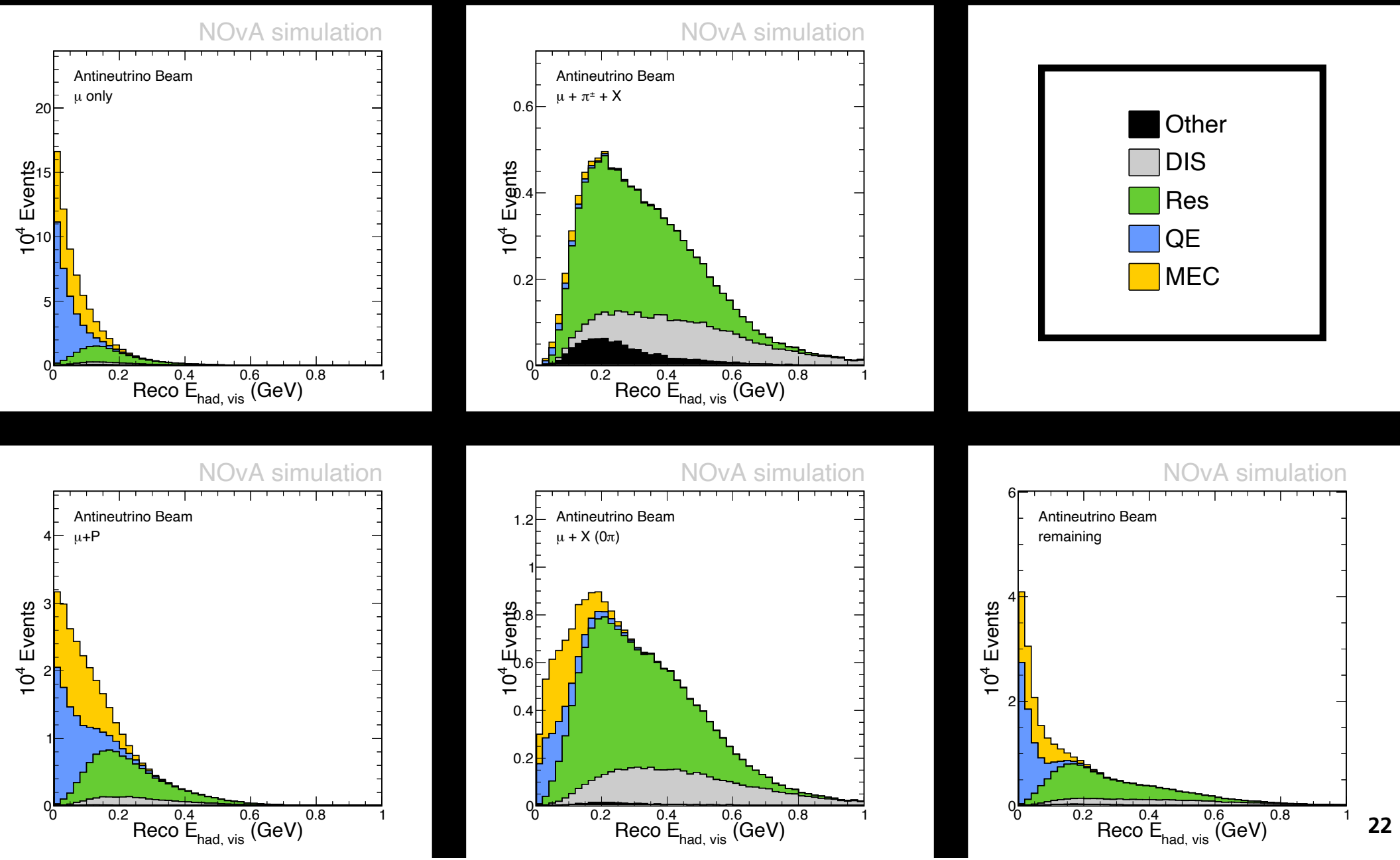
1D marginals



2D marginals



ND Topological distributions: $\bar{\nu}$ in *Reco* $E_{had,\ vis}$



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