

Progress of a NOvA Near Detector Fit with MCMC

on the path towards a ND + FD joint fit with
Markov Chain Monte Carlo



Nov. 17, 2022

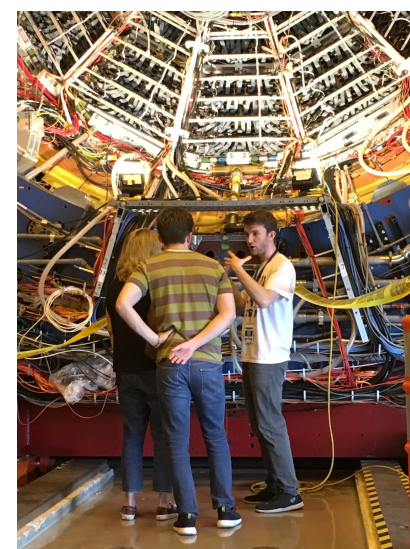
EDG Postdoc application

Michael Dolce (he/his)



Personal Background

- **2016 & 2017** — two summers at BNL as a SULI under-grad intern.
- **2017** — Graduated from the University at Albany.
- **2017** — Enrolled as a PhD student at Tufts.
- **2023** — Graduation from Tufts.



circa 2016

Outline

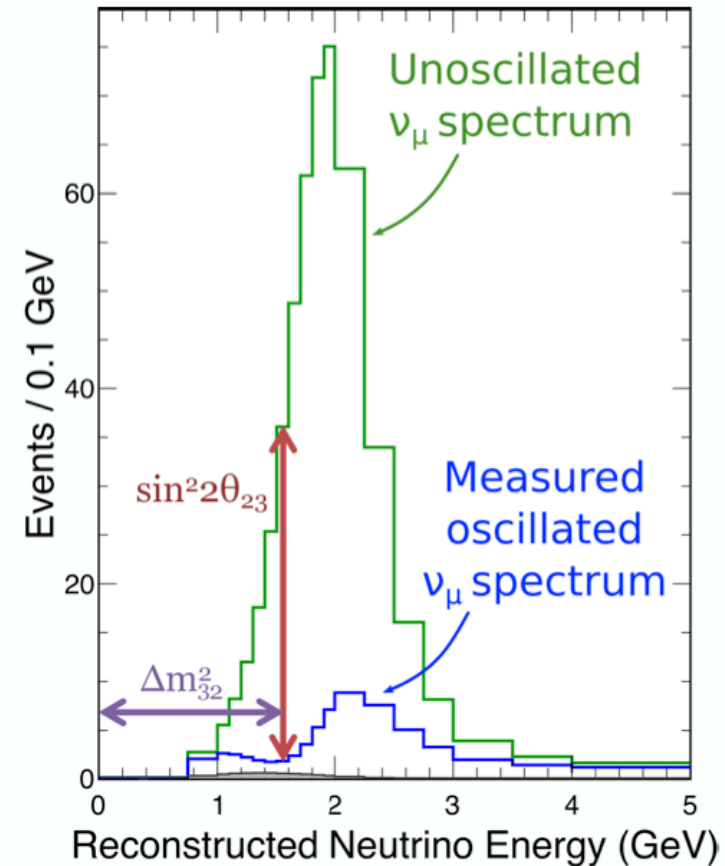
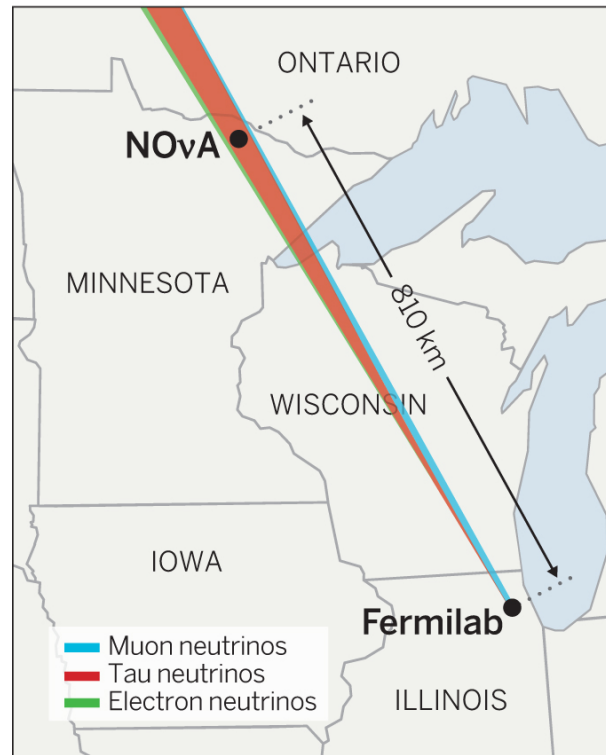
- Brief description of NOvA experiment.
- NOvA's Near Detector (ND) topological samples.
- Markov Chain Monte Carlo (MCMC).
- ND fake data fit.
- Improvements to the ND fit.
- ND fit with data.
- Summarize.

Some important takeaways

- Why a joint fit?
- Why MCMC over (traditional) Frequentist fit?
- What's wrong with GENIE?

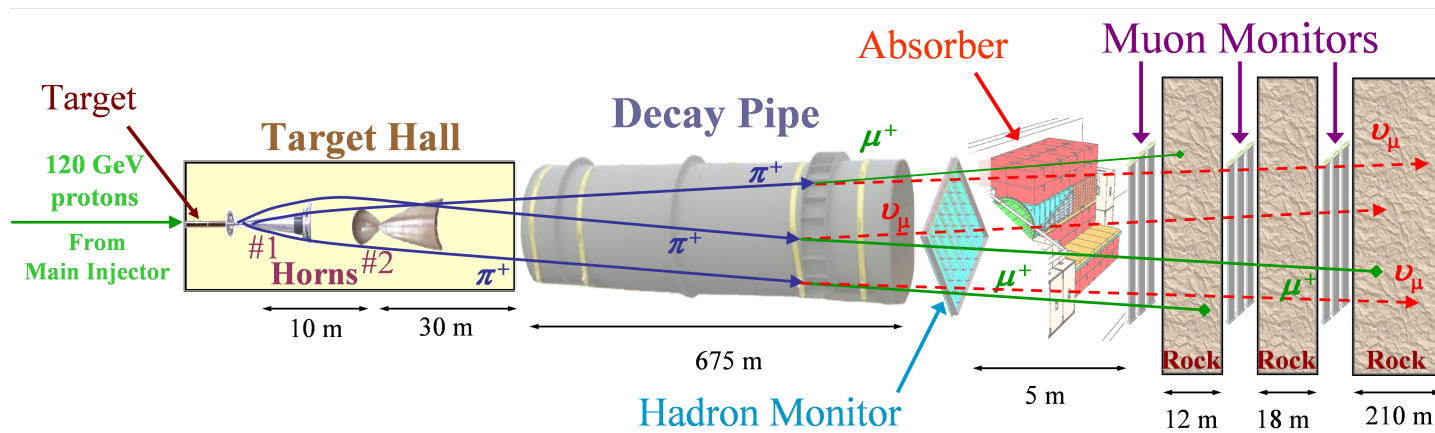
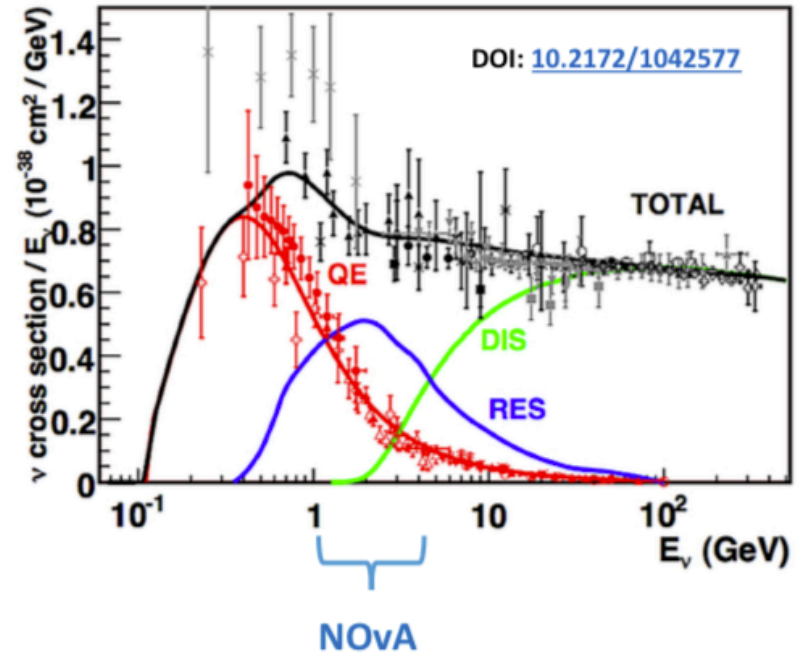
NOvA Experiment

- NOvA observes neutrino oscillations and measures PMNS matrix oscillation parameters:
 - θ_{23} — amplitude of the oscillation.
 - Δm_{32}^2 — the “dip” location.
 - δ_{CP} — asymmetry between ν_μ and $\bar{\nu}_\mu$ appearance.
- NOvA receives beam at $\langle E_\nu \rangle \sim 2$ GeV, 14 mrad off-axis.



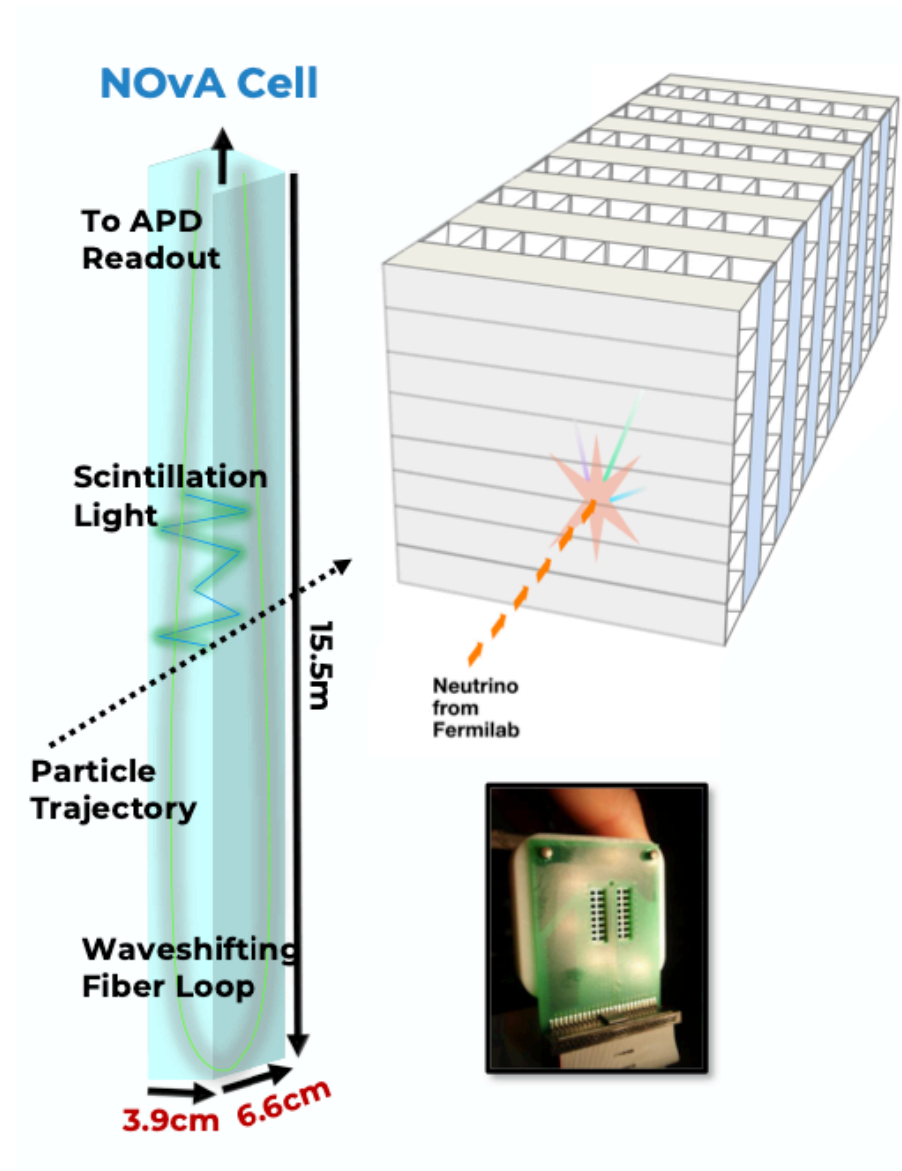
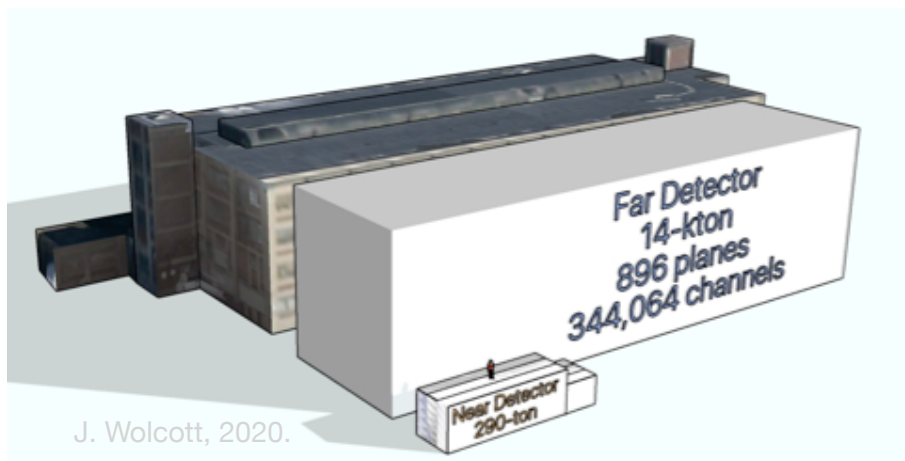
NOvA Experiment

- Receives neutrinos from the NuMI beamline at Fermilab.
- Designed for two configurations:
 - ν_μ — Forward Horn Current (**FHC**).
 - $\bar{\nu}_\mu$ — Reverse Horn Current (**RHC**).
- An array of neutrino interactions.

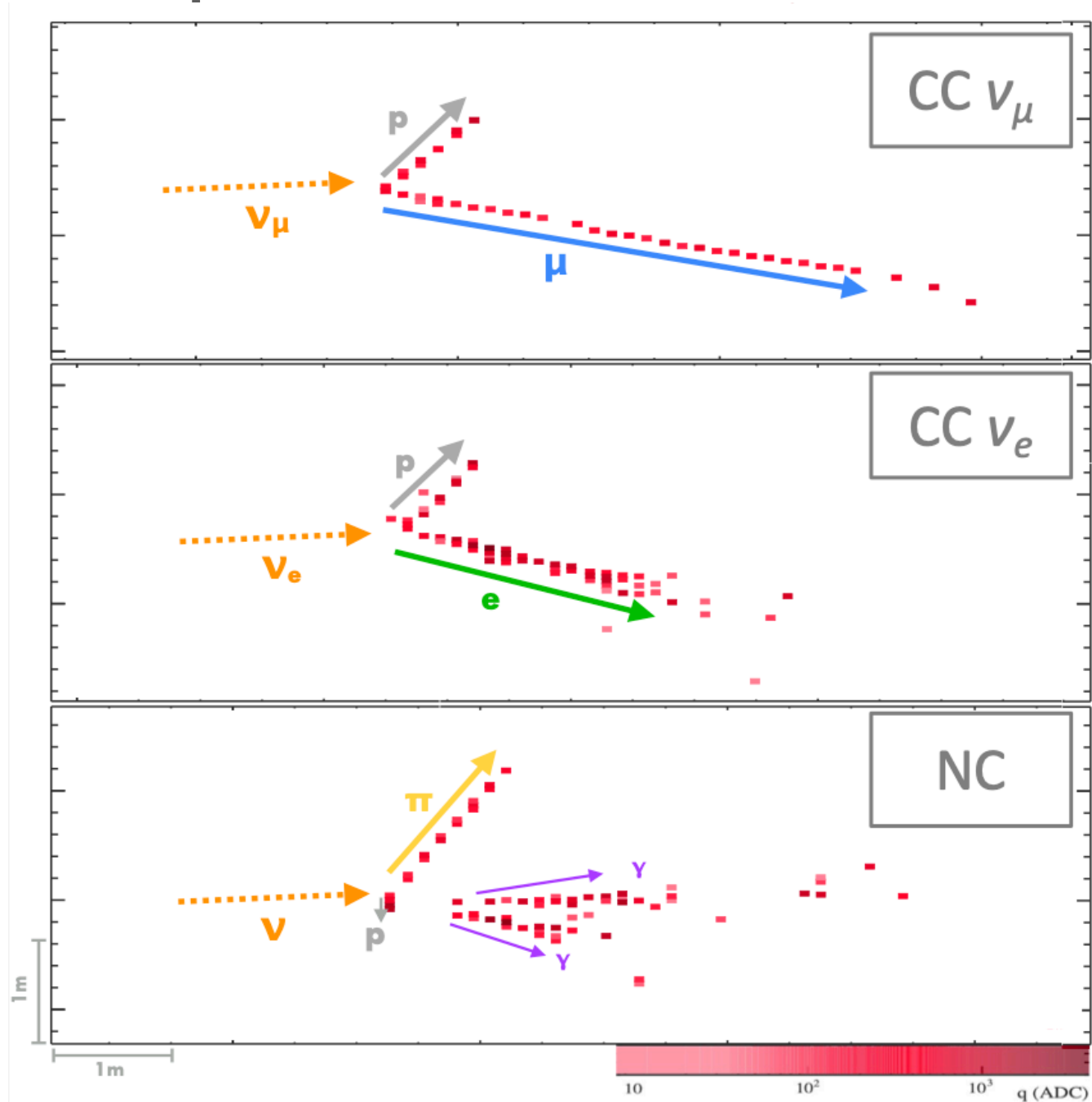


NOvA Experiment

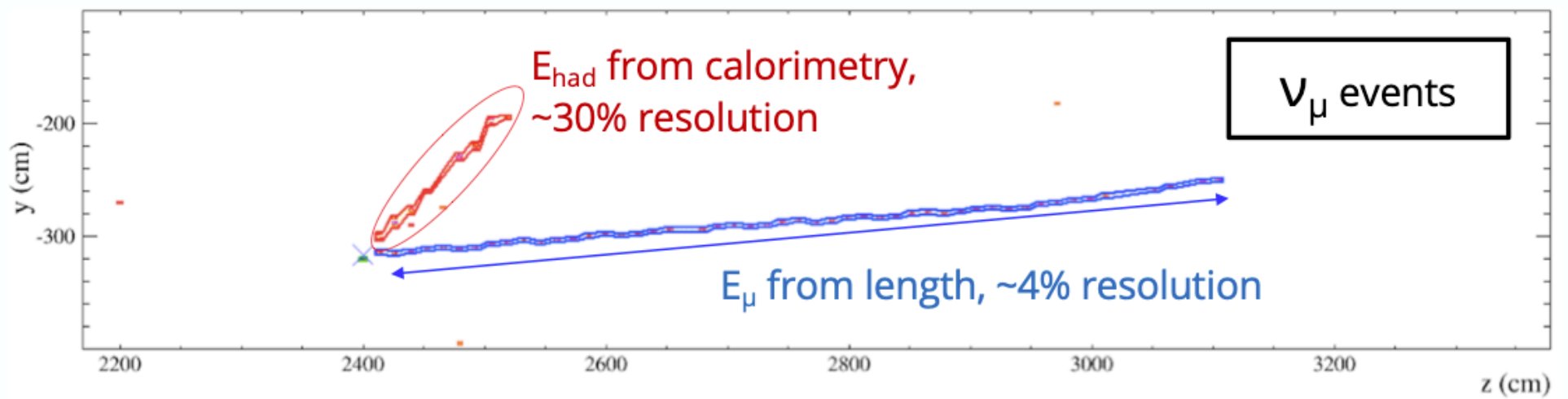
- The two detectors are active tracking calorimeters.
- PVC cells are filled with liquid scintillator.
 - arranged orthogonally.
 - wavelength shifting fiber fed to APD readout.
- Functionally equivalent.



NOvA Experiment



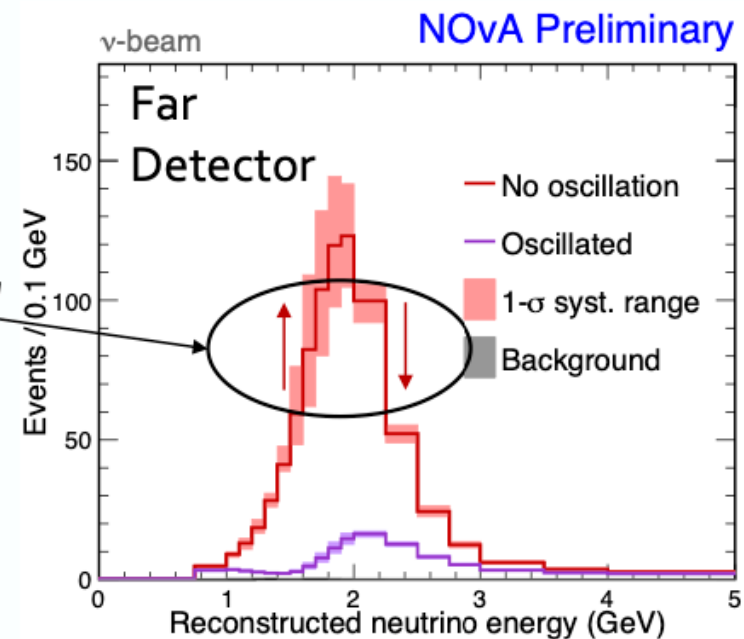
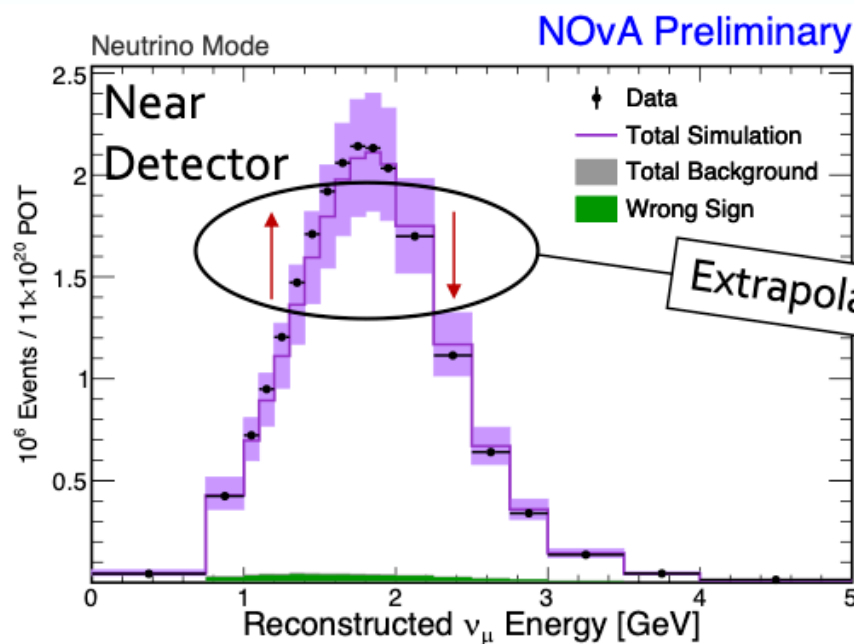
NOvA Experiment



E. Cataño-Mur, 2022.

Traditional NOvA analysis

- NOvA **extrapolation** procedure:
 - Near Detector Data/MC agreement as correction to the Far Detector MC.
 - Reduces flux + cross section uncertainties (at the cost of acceptance).
 - Performed with Frequentist statistics.
 - Oscillation parameter contours formed via Feldman-Cousins (FC) pseudo-experiments on NERSC supercomputer.



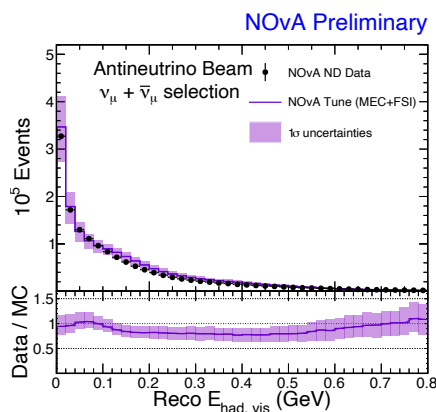
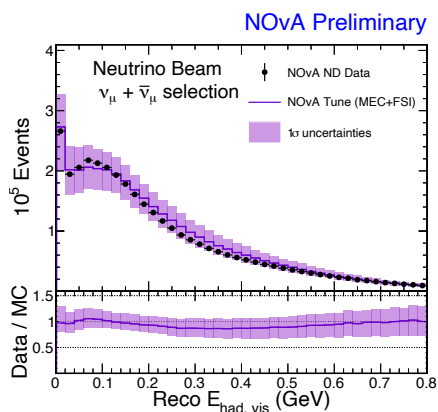
Takeaway: Why joint fit?

- My thesis will fit the NOvA Near and Far Detector data **simultaneously**.
 - constrain uncertainties **and** measure oscillation parameters.
- Performed with Markov Chain Monte Carlo (MCMC), using Stan software package.
- Maximize the statistical power of the NOvA ND data.
- Easier to interpret NOvA MC & model deficiencies.
- New means of interpreting NOvA data.

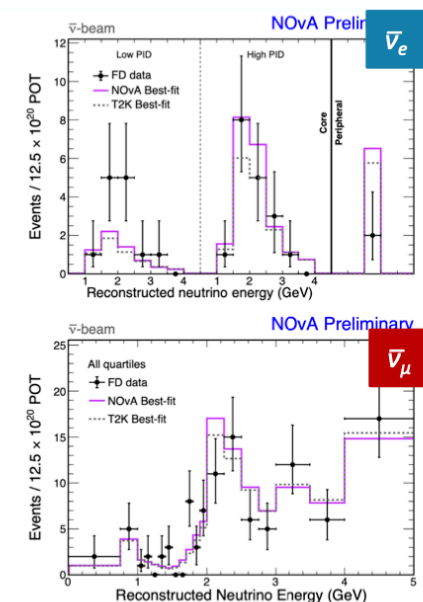
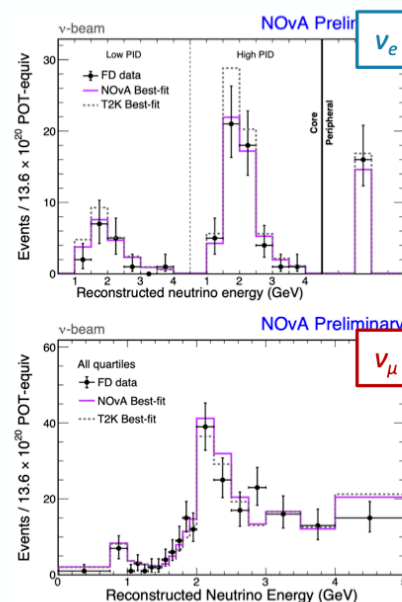
ND

+

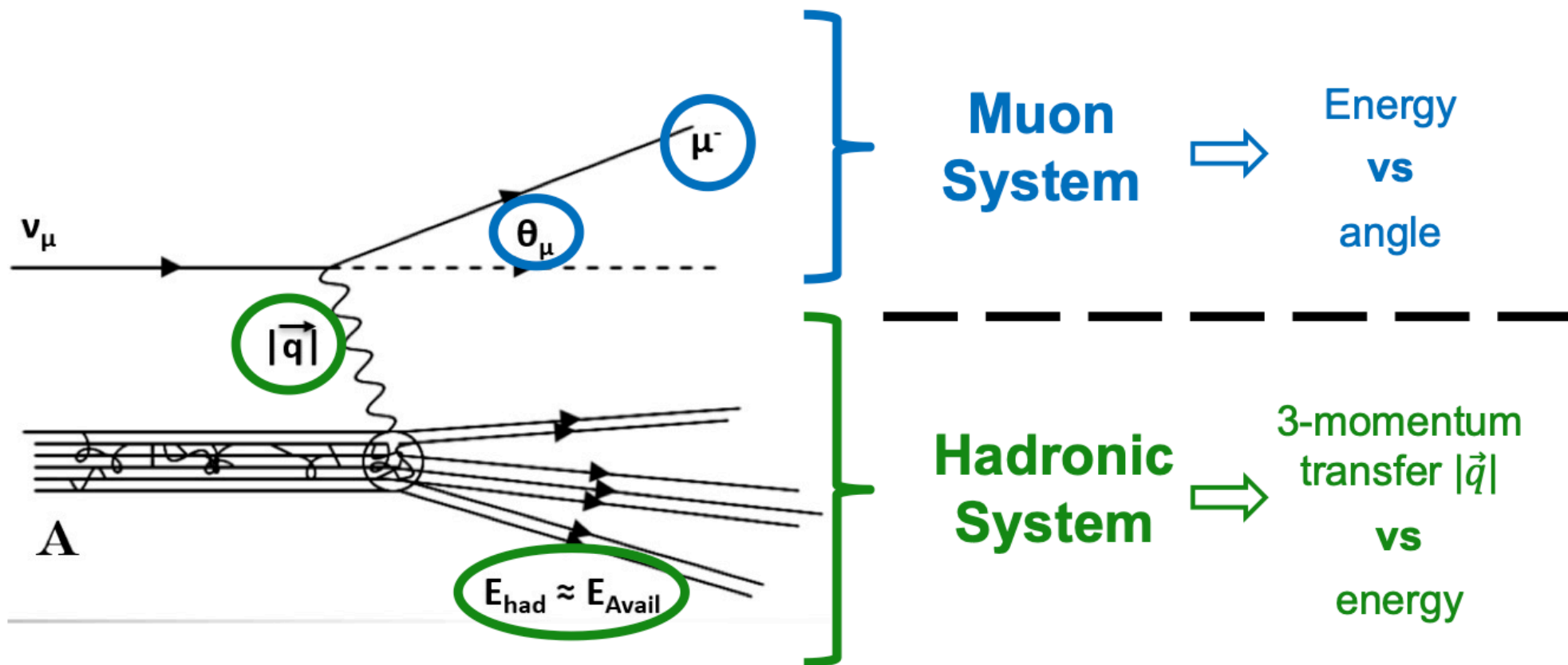
FD



+



NOvA ND Variables



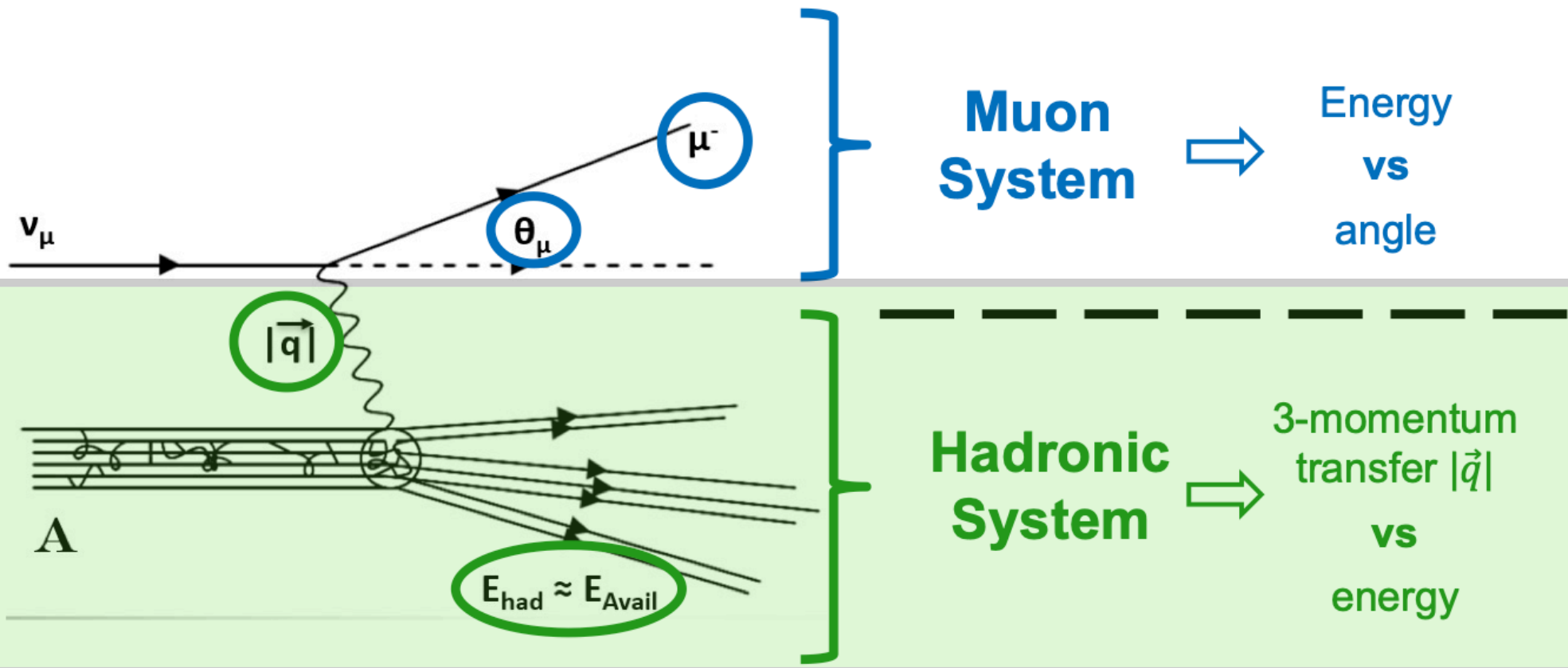
NOvA ND Variables

▸ $Reco E_{had}^{vis}$

- hadronic visible energy
- energy observed by detector imparted into the hadronic system.
- proxy for true energy transfer, q_0 .

▸ $Reco |\vec{q}|$

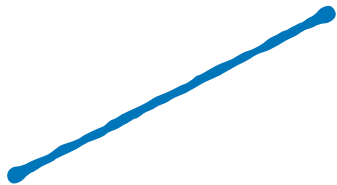
- reconstructed three-momentum transfer
- scales with interaction type.
- proxy for true momentum transfer, $\vec{q}_3$.



NOvA ND Topologies

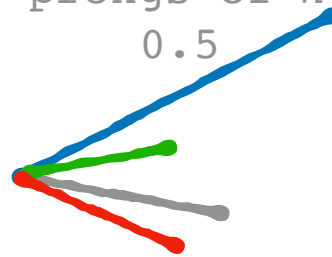
Muon

- μ CVN > 0.5
- length $> 5m$



Muon + Pion + other

- $2 \geq 3D$ prongs
- μ CVN score > 0.5
- length $> 5m$
- 1 3D prong π score > 0.7
- "other" prongs of π score < 0.5



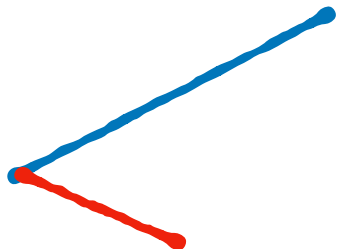
Remaining

- Everything else



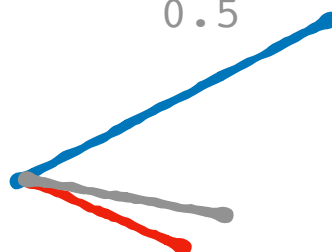
Muon + Proton

- Exactly 2 prongs
- μ CVN > 0.5
- μ length $> 5m$
- 1 3D prong proton score ≥ 0.5



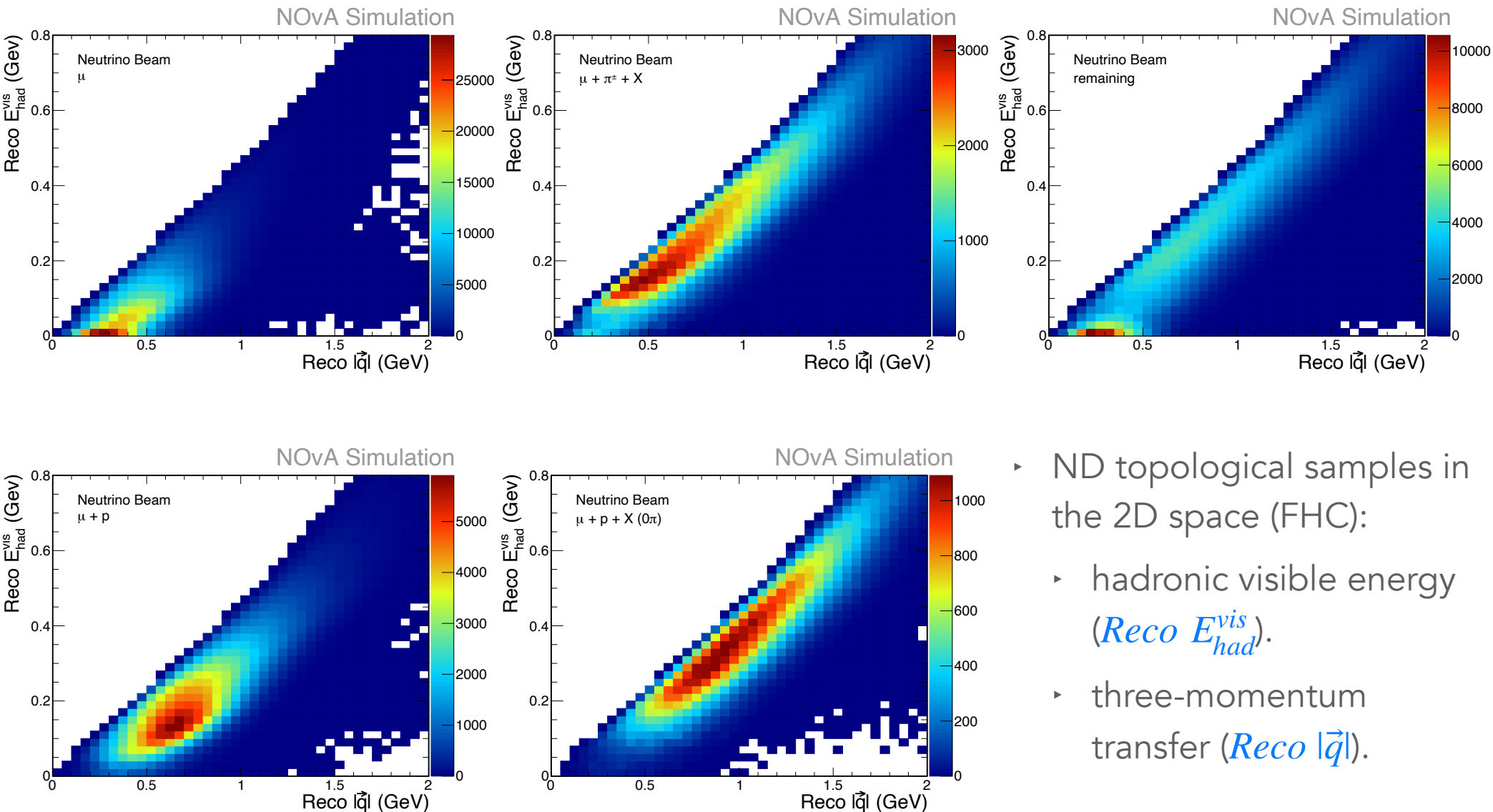
Muon + (Proton) + other

- $2 (3) \geq 3D$ prongs
- 1 prong μ CVN score > 0.5
- μ length $> 5m$
- 1 3D prong proton score ≥ 0.5
- "other" prongs of π score < 0.5



NOvA's ND Topological Samples

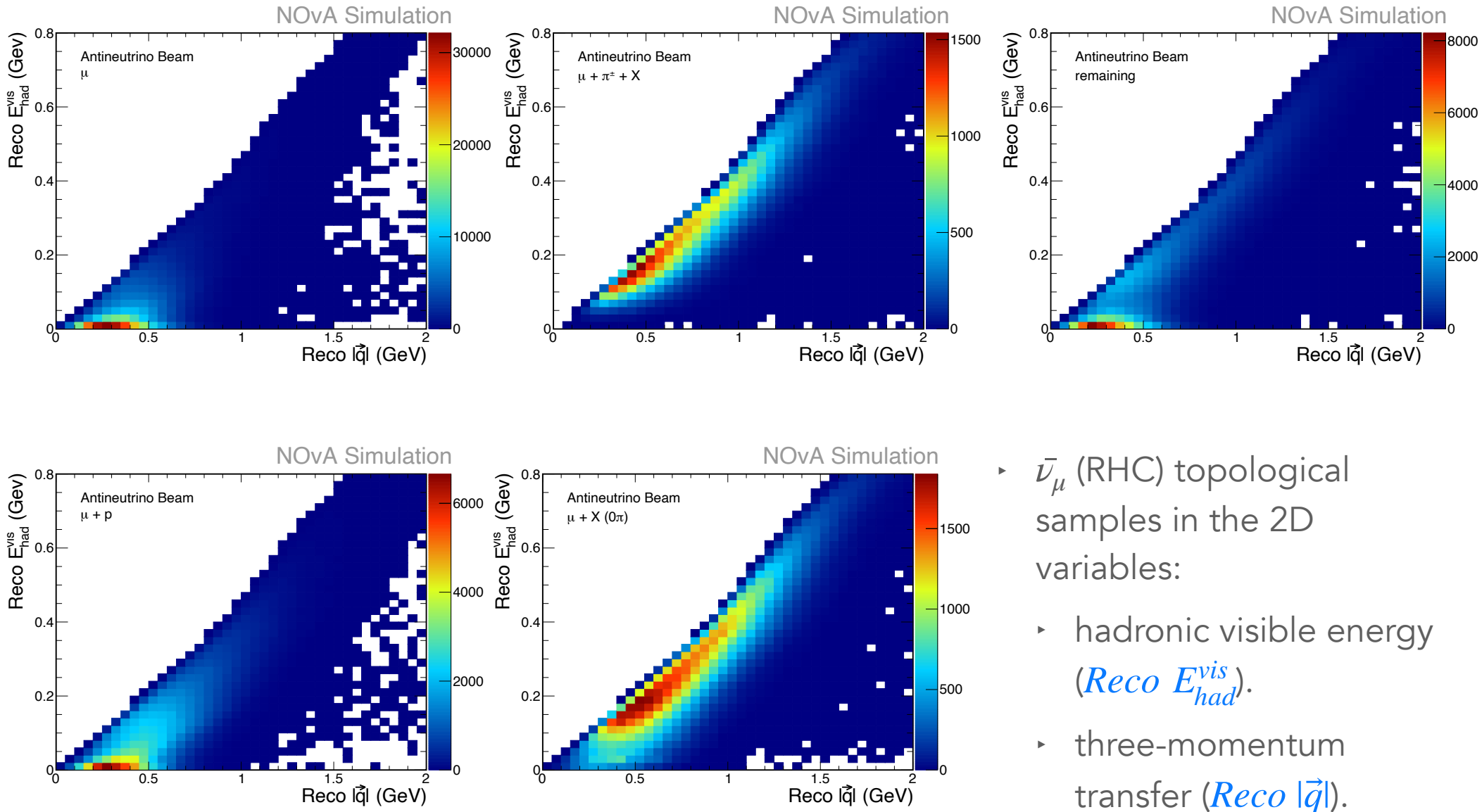
ν mode



- ▶ ND topological samples in the 2D space (FHC):
 - ▶ hadronic visible energy ($Reco E_{had}^{vis}$).
 - ▶ three-momentum transfer ($Reco |\vec{q}|$).

NOvA's ND Topological Samples

$\bar{\nu}$ mode

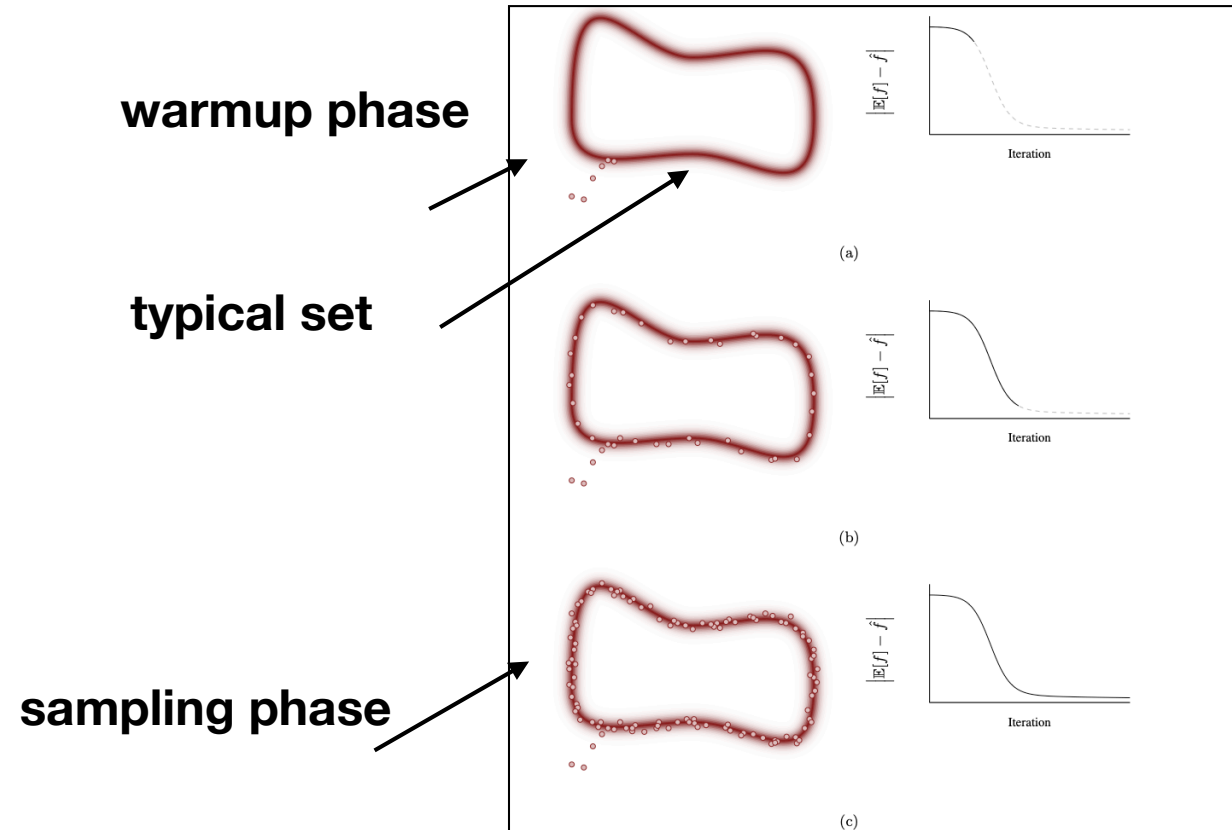


- ▶ $\bar{\nu}_\mu$ (RHC) topological samples in the 2D variables:
 - ▶ hadronic visible energy ($Reco E_{had}^{vis}$).
 - ▶ three-momentum transfer ($Reco |\vec{q}|$).

Markov Chain Monte Carlo (MCMC)

<https://arxiv.org/abs/1701.02434>

- Bayesian parameter estimation tool.
- Goal is to efficiently locate maximum of posterior parameter space.
 - **typical set**: region of high probability.
 - done with Hamilton's equations.
- MCMC fitting is divided into two phases **warmup** and **sample**:
 - warmup — locate the typical set.
 - sampling — maximize statistics from the typical set.
- The warmup phase is uninformative, but crucial.



Bayes Theorem

$$P(\vec{\theta} | \vec{\mathcal{X}}) \propto P(\vec{\mathcal{X}} | \vec{\theta}) \times P(\vec{\theta})$$

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

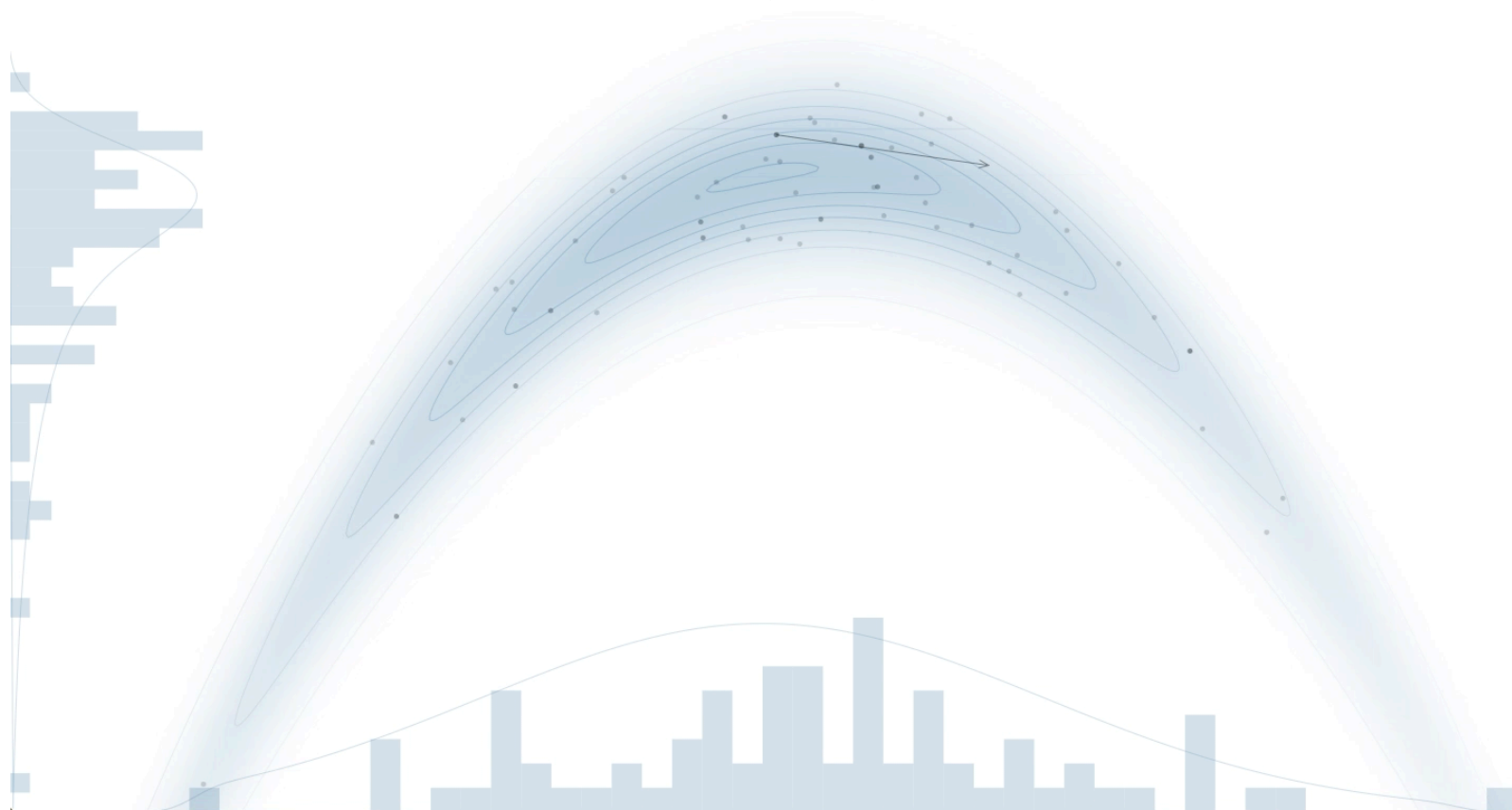
$$\text{posterior} \propto e^{-\frac{\chi^2}{2}} \times \mathcal{N}(0, \approx 1)^*$$

*Gaussian-like

Hamiltonian Monte Carlo

Hamiltonian Monte Carlo

Open Controls

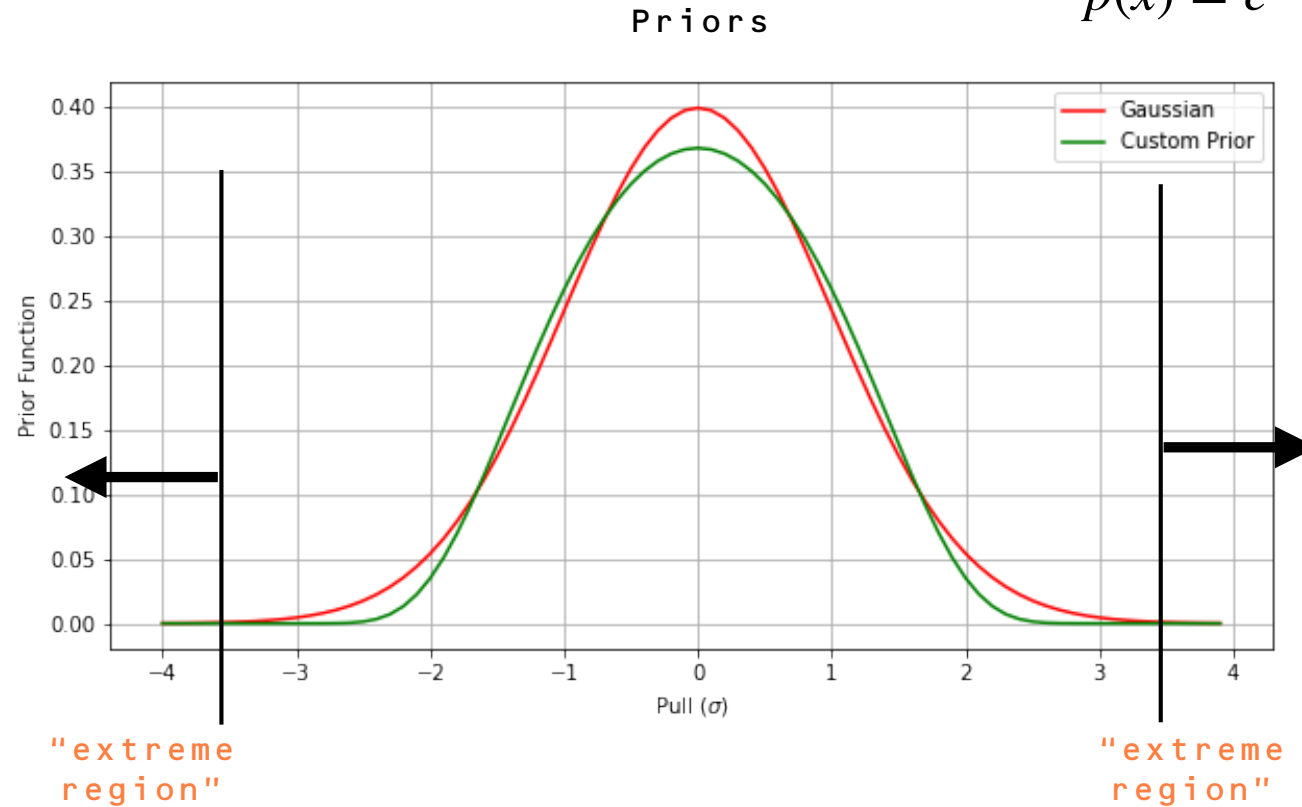


<https://chi-feng.github.io/mcmc-demo/app.html>

Bayesian Prior Choice

Custom Prior:

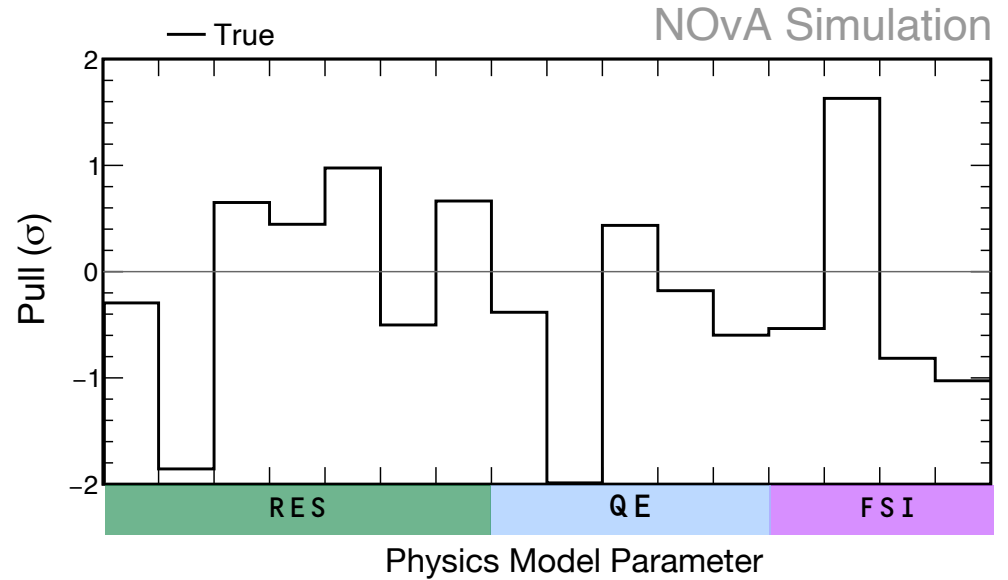
$$p(x) = e^{-e^{0.3025x^2}}$$



- We use a Gaussian-like "**custom prior**" for fitting NOvA's physics model uncertainties.
- NOvA's uncertainty model cannot predict pulls $> \pm 3\sigma$.

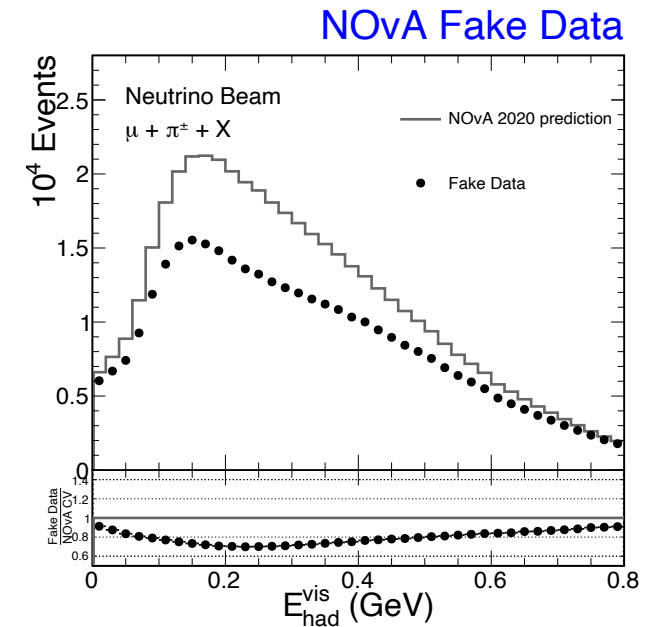
Fake Data

- Demonstrate MCMC machinery:
 - fit subset of NOvA uncertainties in the ND topologies with ND fake data.
- Assign random values from a uniform distribution $[-3,+3]$ to physics parameters — **true values**.
- MCMC explores posterior to locate typical set (and find the true values).



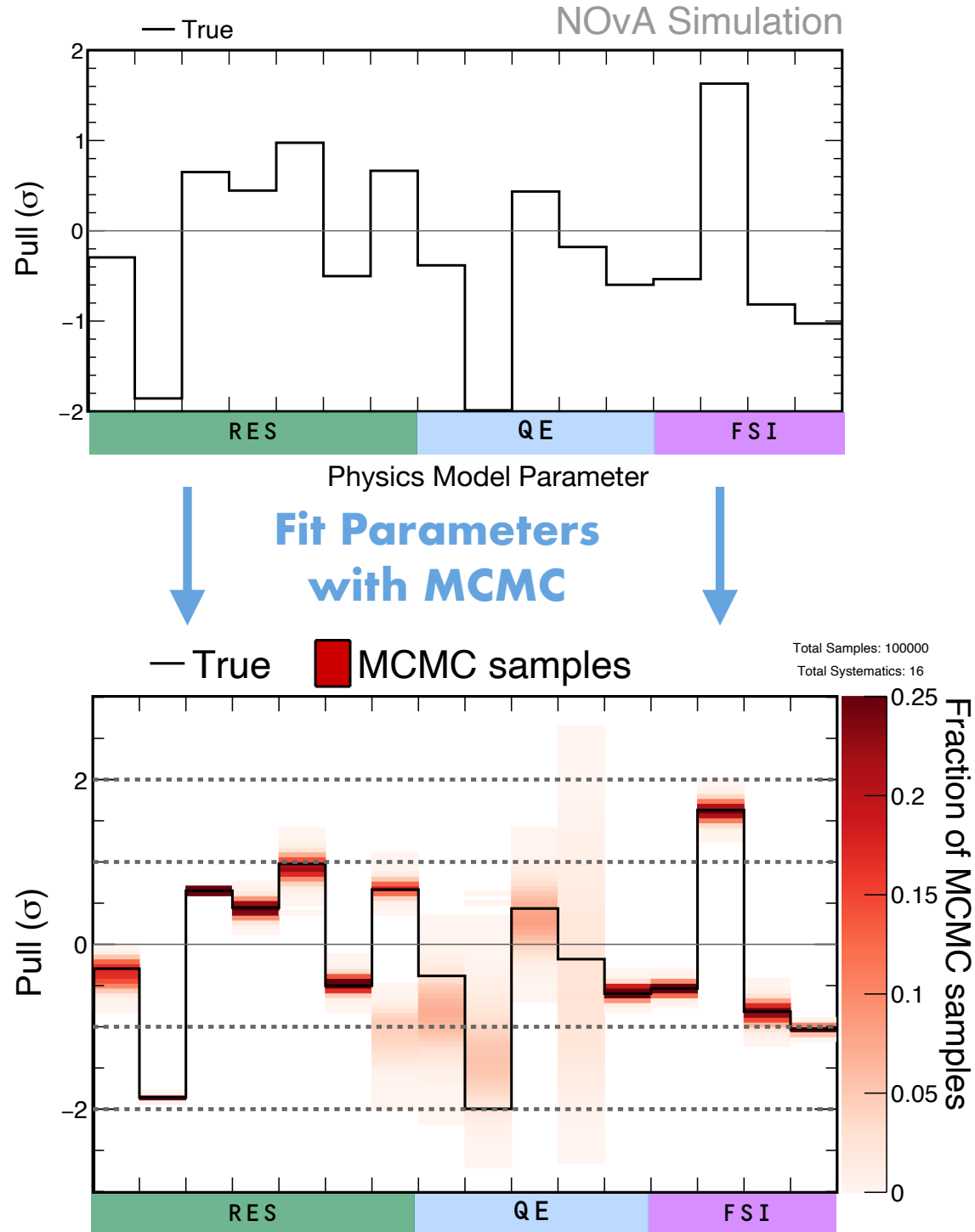
Systematic Name	Physics Model
Low Q^2 Suppression	RES
M_A Resonance	RES
M_V Resonance	RES
Adler Angle $\theta_{\Delta \rightarrow N+\pi}$	RES
1η	RES
RES Decay B.R.	RES
RPA Shape Enhancement	QE
RPA Shape Suppression	QE

Systematic Name	Physics Model
hN Mean Free Path	FSI
hN “Fate Fraction” Eigen Vector 1, 2, 3	FSI
Z-Expansion Axial Form Factor Eigen Vector 1, 2, 3, 4	QE
Z-Expansion Normalization	QE



Fake Data Fit

- Plot MCMC **samples** for each systematic uncertainty (bottom).
- MCMC **samples**:
 - densely overlap **RES** and **FSI** **true pull values**.
 - are broad for **QE** parameters — not as well constrained by fake data.
- We will use this summary plot again...

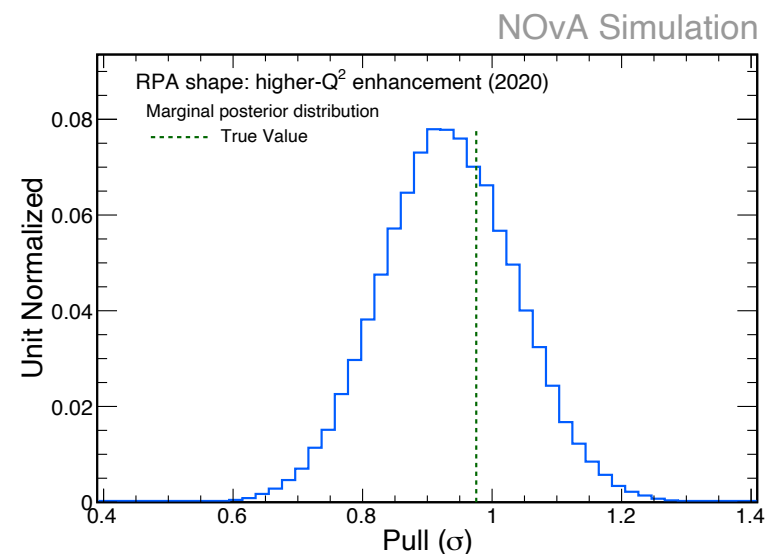
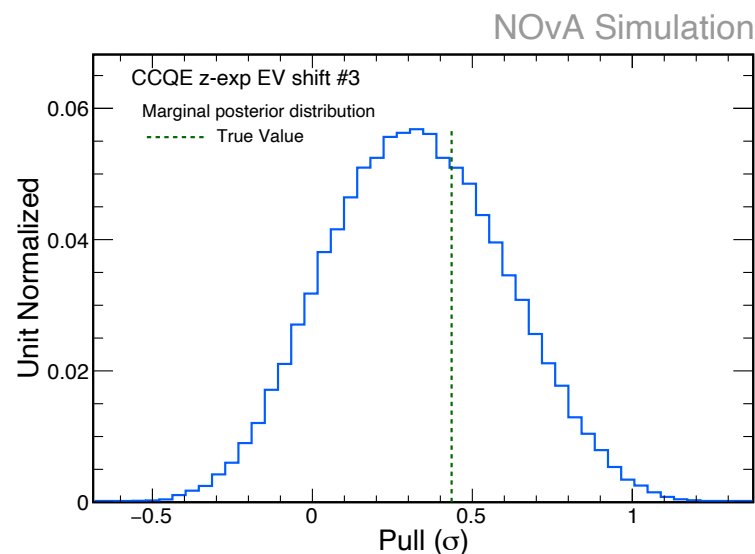
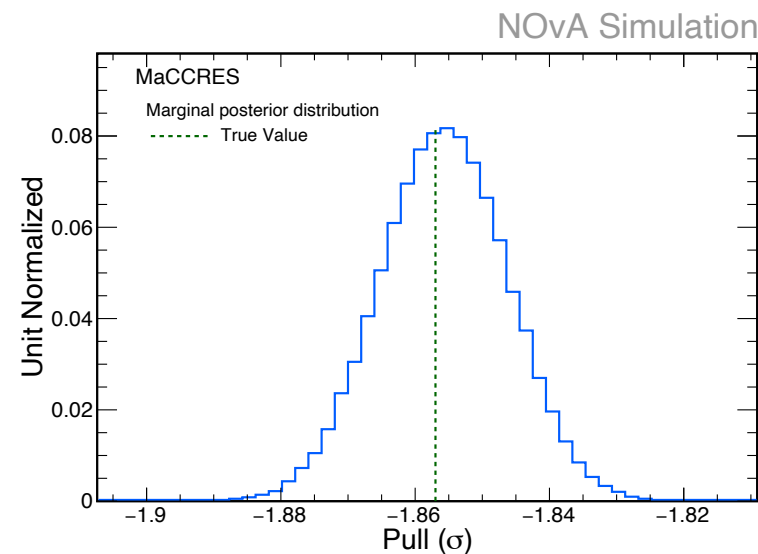
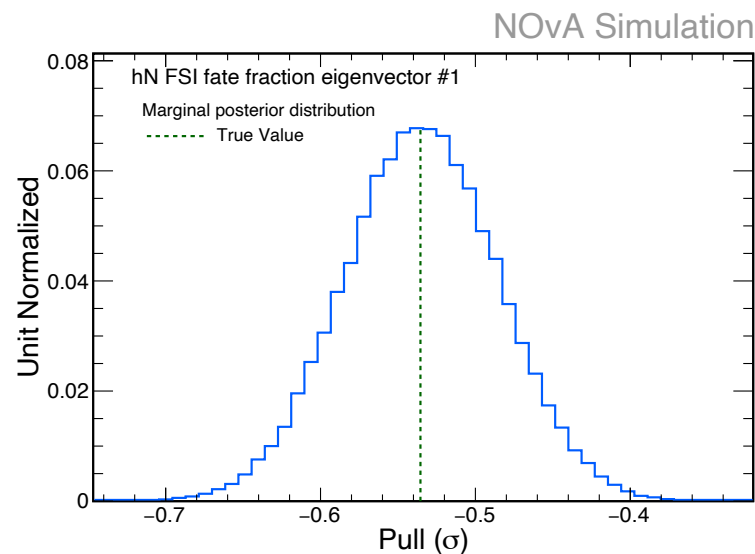


Takeaway: Why MCMC?

- Bayesian inference offers advantage of **marginalization** of nuisance parameters, $\vec{\delta}$.
- 1D marginal distributions** integrate out extraneous parameters for desired one, θ_i .
 - comes “free” (no need to profile over parameters).
- Easy means of quantifying fit uncertainties — width of marginal.

Marginalization

$$\mathcal{P}(\vec{\theta}|\vec{x}) = \int \mathcal{P}(\vec{\theta}, \vec{\delta}|\vec{x}) d\vec{\delta}$$

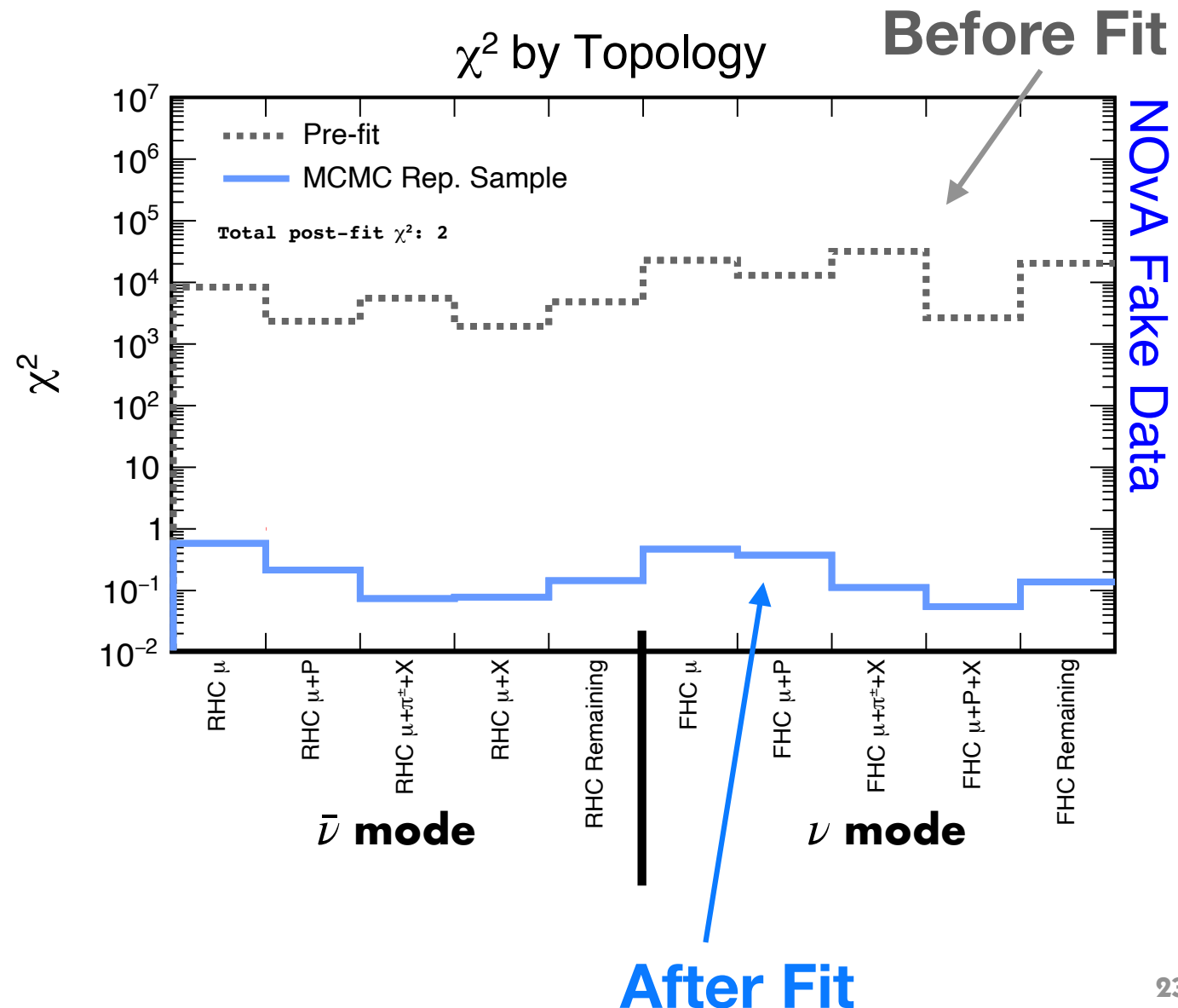


Evaluating MCMC Fit

- Evaluate fit with χ^2 metric:

$$\chi^2 = \sum_{i \in \text{bins}} -2 \left(-\lambda_i + x_i + x_i \log \left(\frac{\lambda_i}{x_i} \right) \right),$$

- Pre-fit — fake data vs. nominal simulation.
- Post fit — fake data vs. fitted simulation.
 - MCMC “**Representative Sample**”, maximum likelihood MCMC sample.
- “**Rep. Sample**” $\chi^2 \approx 0$ for each topology:
- We have verified:
 - MCMC can fit NOvA uncertainties.



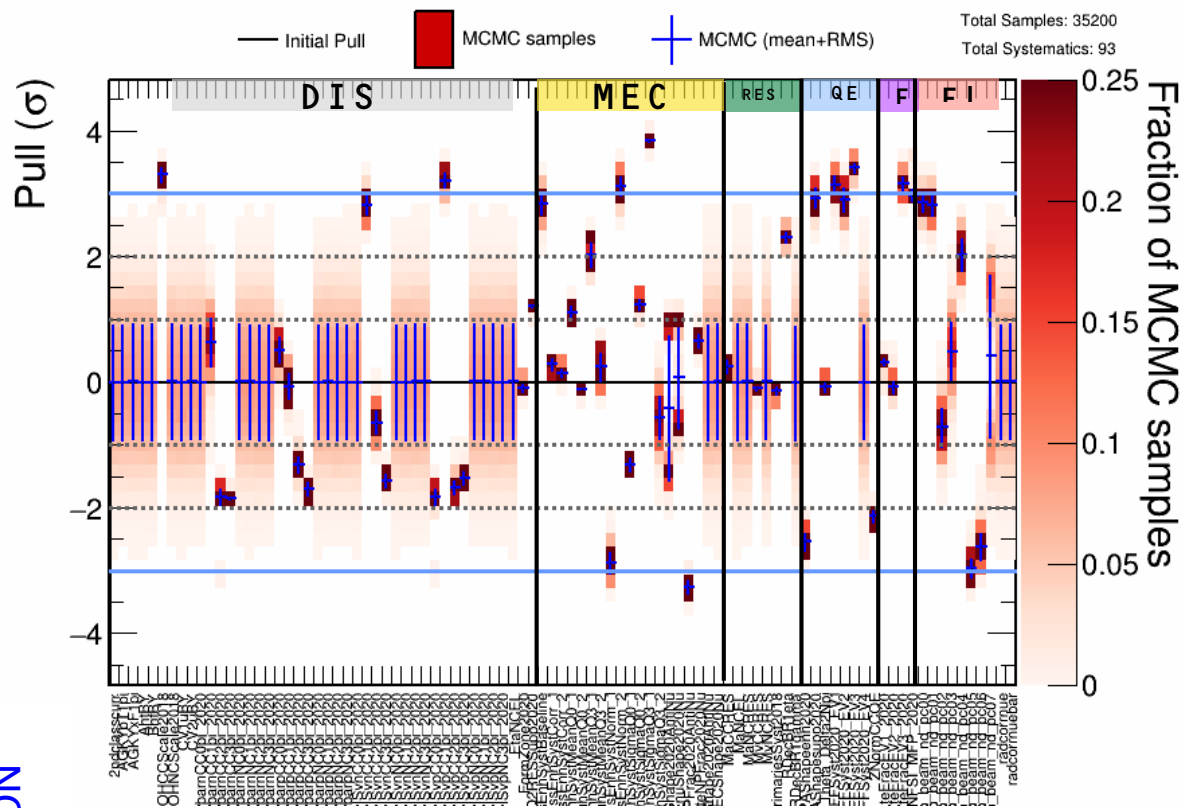
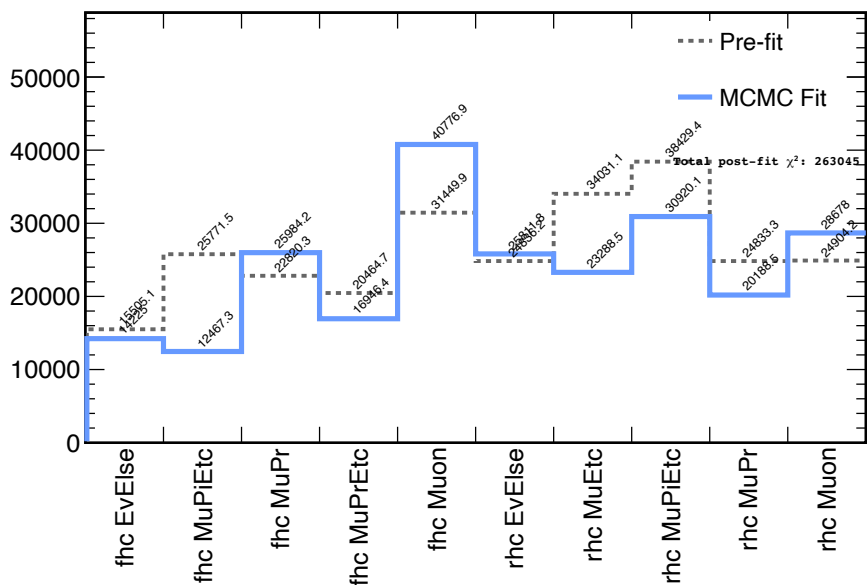
Moving to ND data fit

fake → real data...

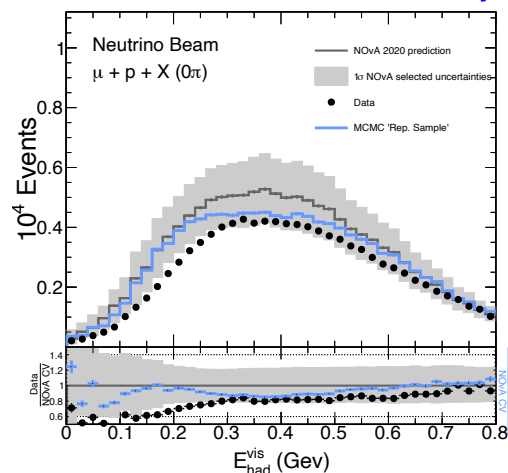
Poor agreement in ND data fit

- ▶ Fitting all NOvA ND uncertainties is intractable.
 - ▶ Too **few samples** produced.
 - ▶ ND data **cannot constrain** several uncertainties — the prior is returned.
- ▶ χ^2 in some topologies has gotten worse.
- ▶ Agreement only marginally improved.

χ^2 by Topology



NOvA Preliminary



Takeaway: What's wrong with GENIE?

- GENIE over-predicts $\mu+P+X$ events consistently.

Improving the ND fit

- There are two keys obstacles of MCMC fitting:

quality

- agreement of fit.
 - the data-Rep. Sample (i.e. fitted) agreement needs to be improved.
 - how can we improve the agreement?

quantity

- number of samples.
 - fits are slow.
 - need more MCMC samples to draw conclusions.
 - how can we make MCMC faster?

Fit to data

- Implemented improvements to address the **quality** and **quantity**:
 - uniform priors.
 - covariance matrix.
 - minimal differentiation.
 - ranking systematics by χ^2 .
 - new RES/DIS uncertainties.
 - variable binning.
 - phase space cut.

Fit to data

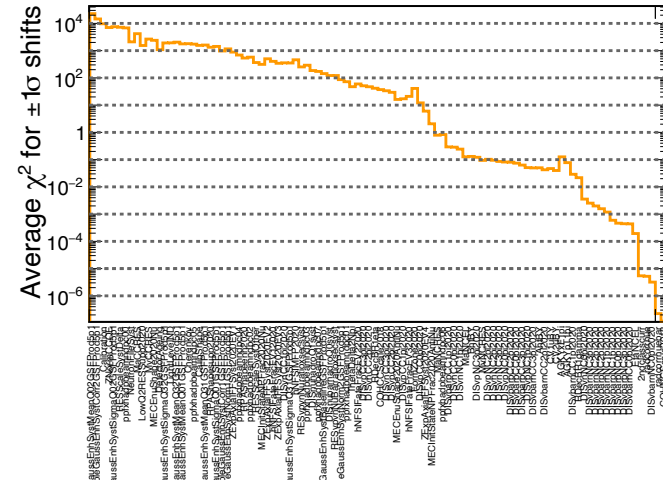
- Implemented improvements to address the **quality** and **quantity**:
 - uniform priors. ✗
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Available in back-up

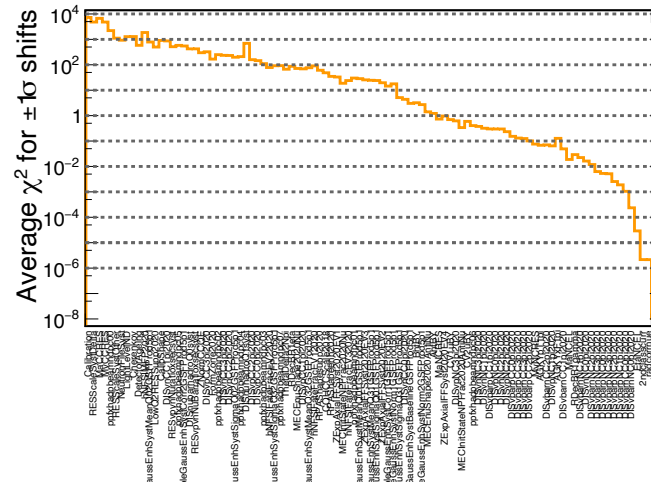
Ranking systematics by χ^2

quantity

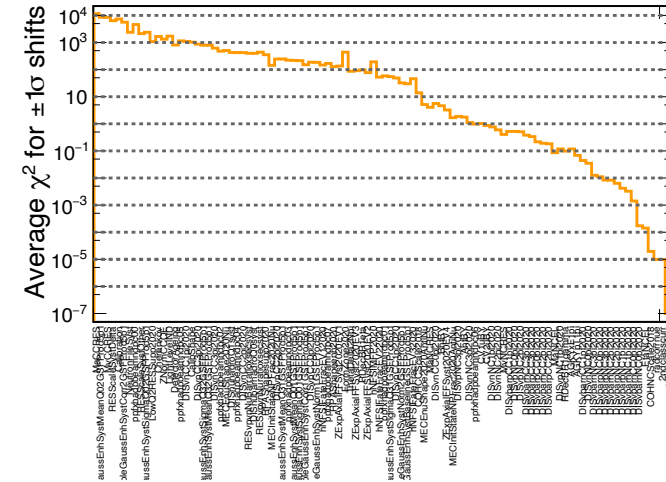
FHC ND μ Topology



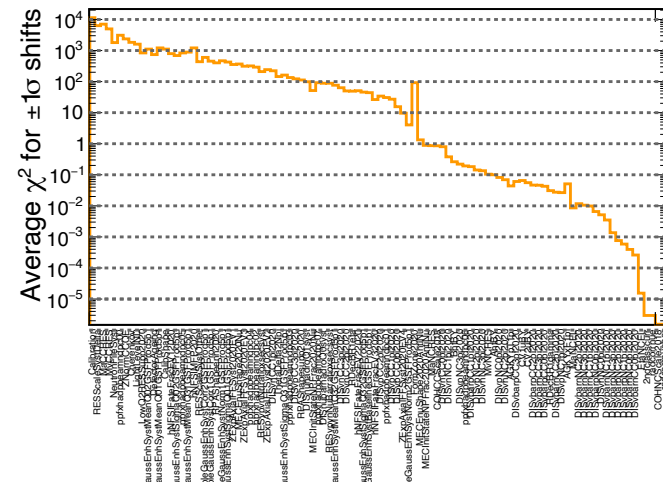
FHC ND $\mu+\pi^++X$ Topology



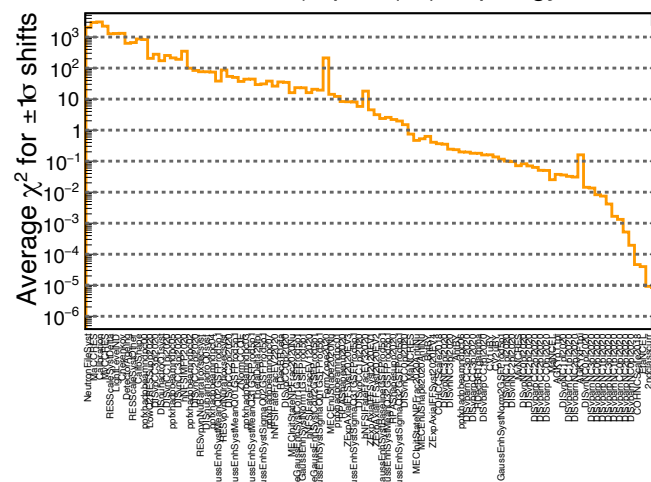
FHC ND Remaining Topology



FHC ND $\mu + p$ Topology



FHC ND $\mu+p+X$ (0π) Topology

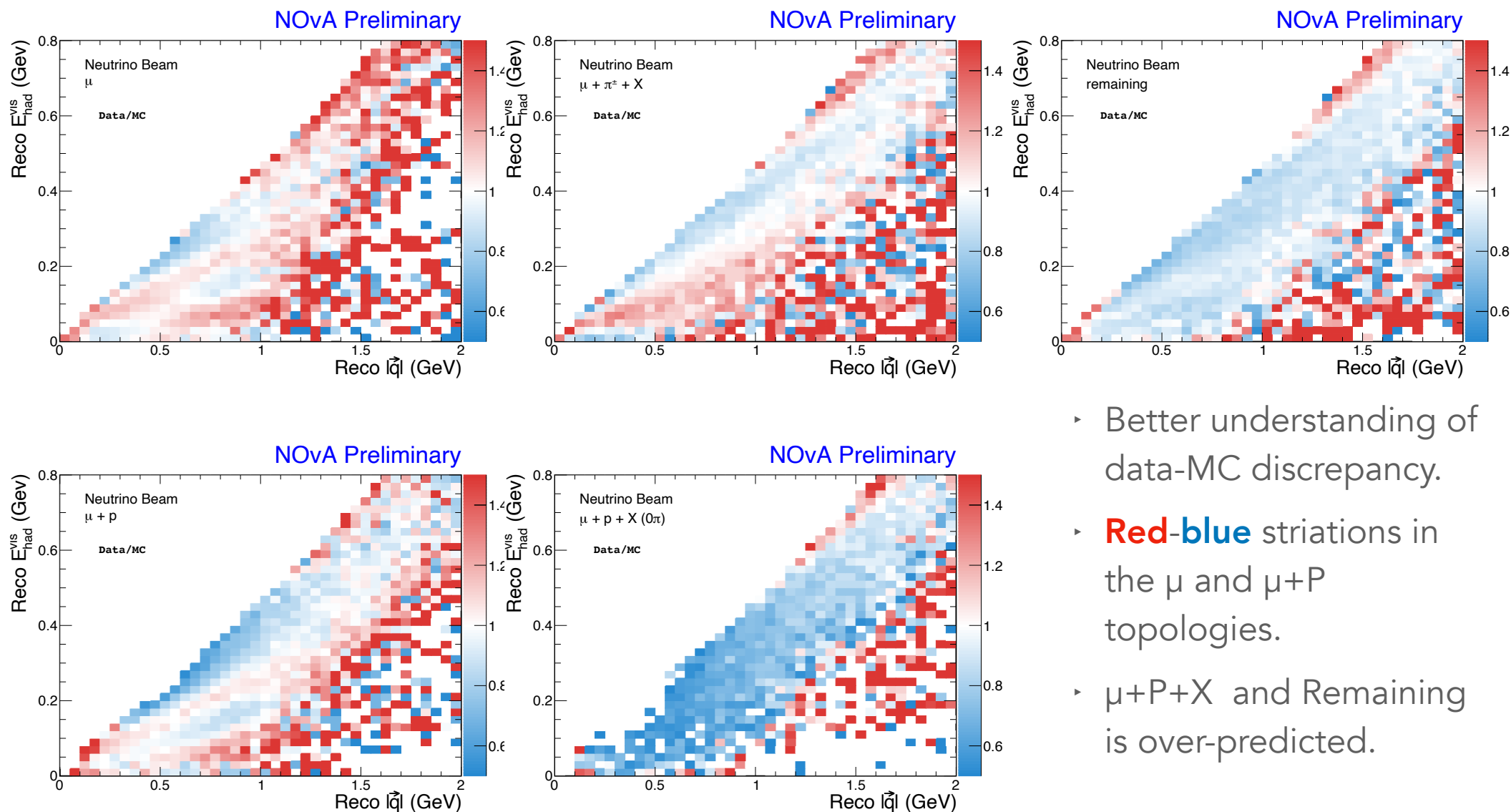


- ▶ Which systematics change the prediction the most?
- ▶ Calculate χ^2 for:
 - ▶ 1σ shifted MC vs. Nominal MC
 - ▶ for each systematic uncertainty
 - ▶ in each topology.
- ▶ Log scale.
- ▶ Fit only important systematics
~10-20 for each topology.

Fit to data

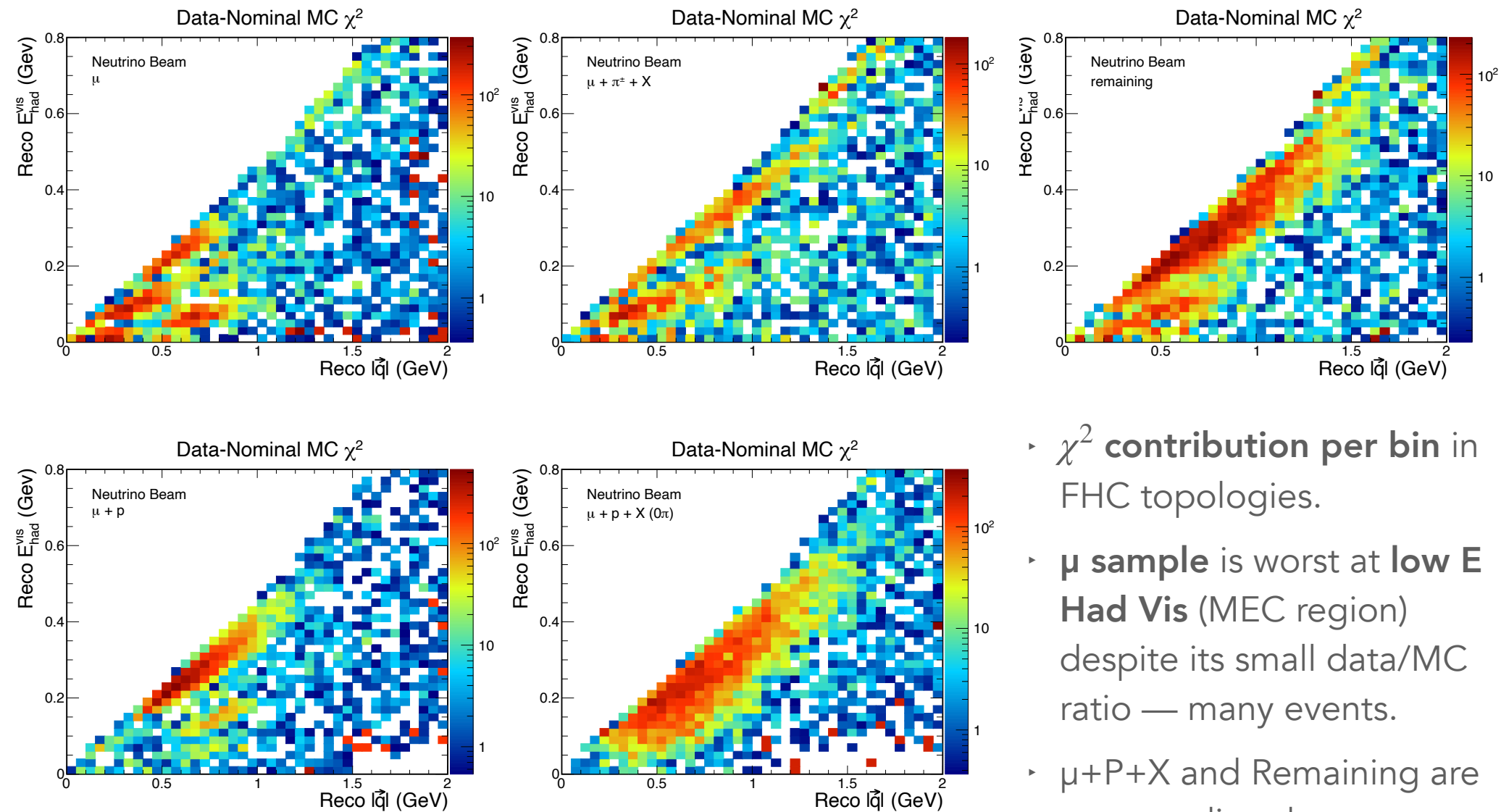
- Implemented improvements to address the **quality** and **quantity**:
 - uniform priors. ✗
 - covariance matrix. ✗
 - minimal differentiation. ✓
 - ranking systematics by χ^2 . ✓
 - new RES/DIS uncertainties.
 - variable binning.
 - phase space cut.

Breaking down the prediction quality



- Better understanding of data-MC discrepancy.
- **Red-blue** striations in the μ and $\mu+P$ topologies.
- $\mu+P+X$ and Remaining is over-predicted.

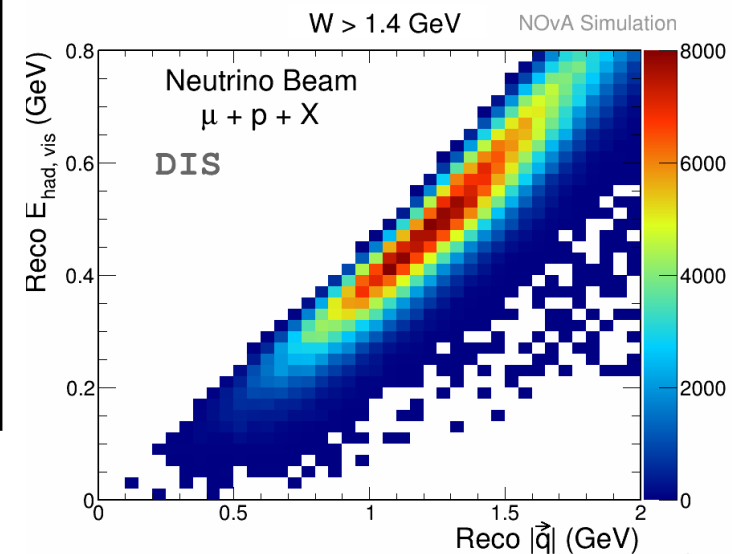
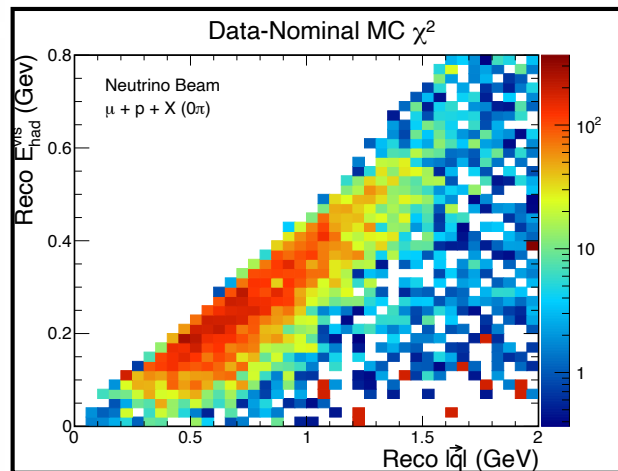
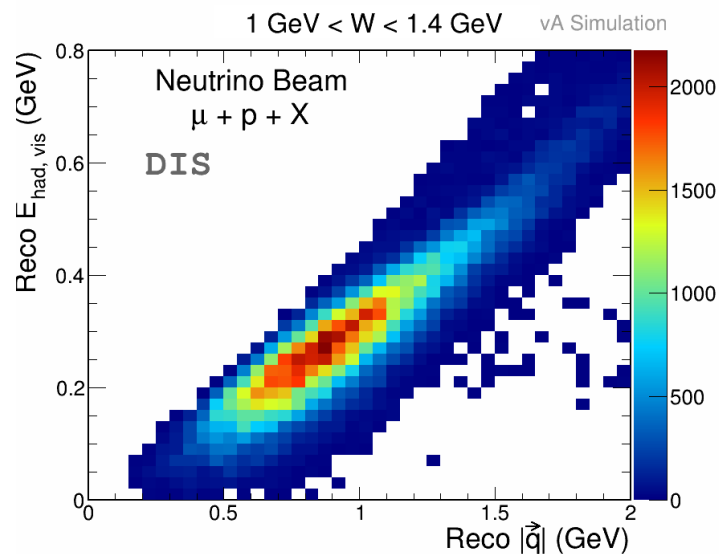
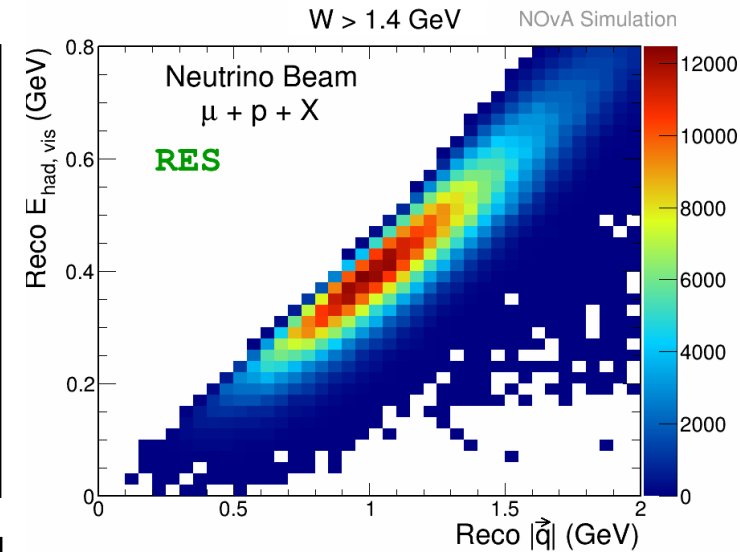
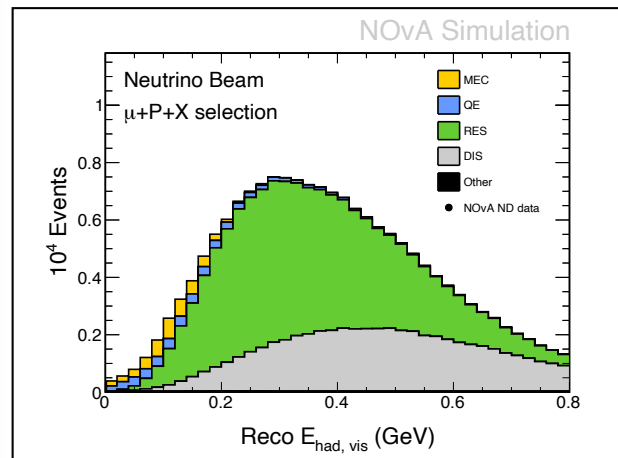
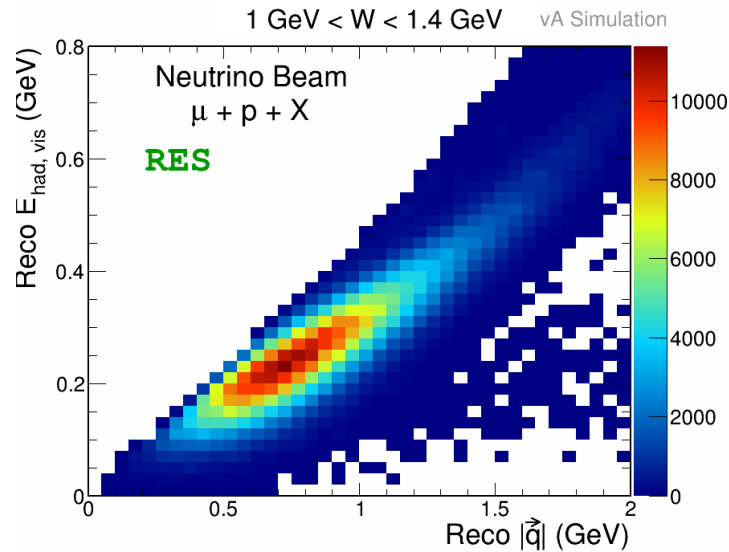
Breaking down the prediction



- χ^2 contribution per bin in FHC topologies.
- μ sample is worst at **low $E_{\text{Had Vis}}$** (MEC region) despite its small data/MC ratio — many events.
- $\mu + p + X$ and Remaining are over-predicted.

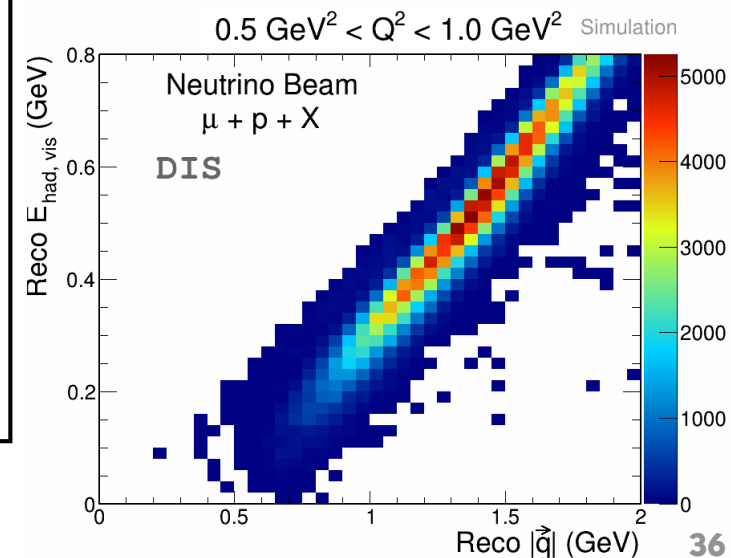
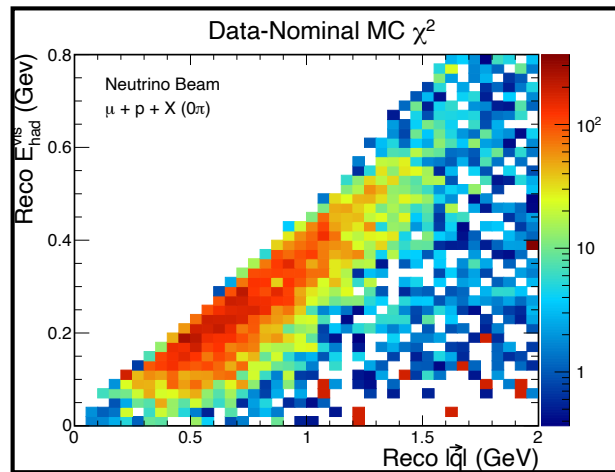
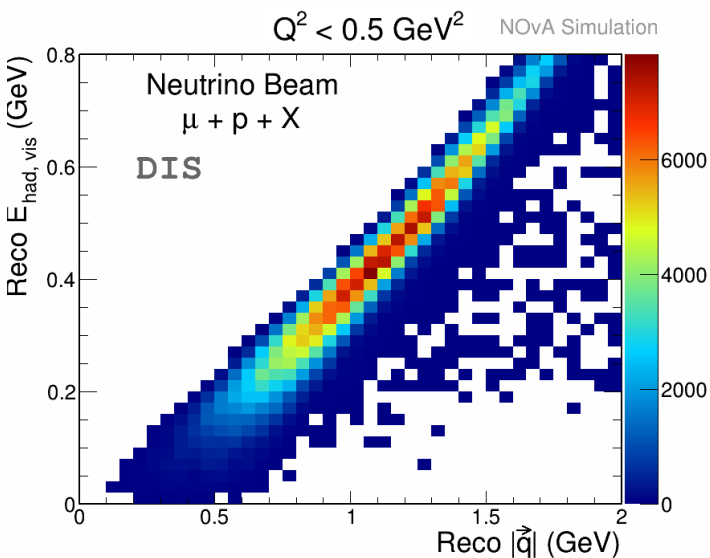
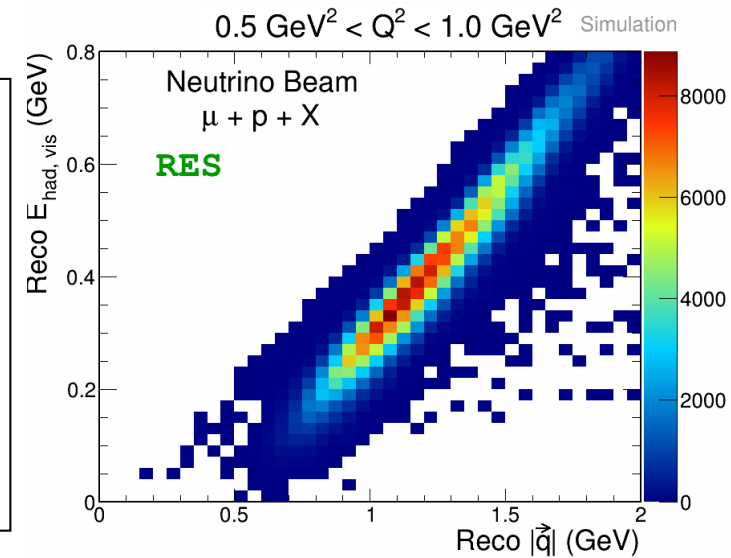
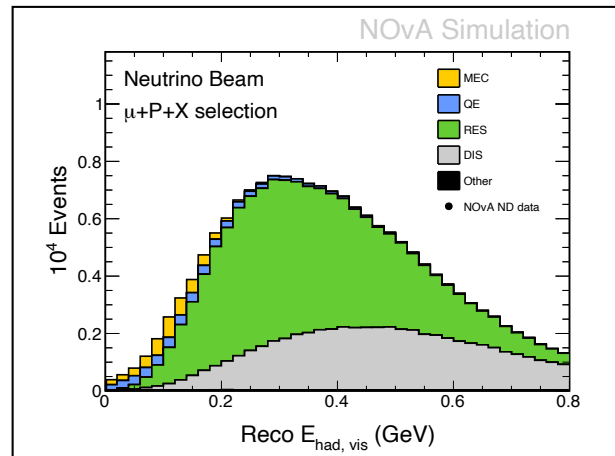
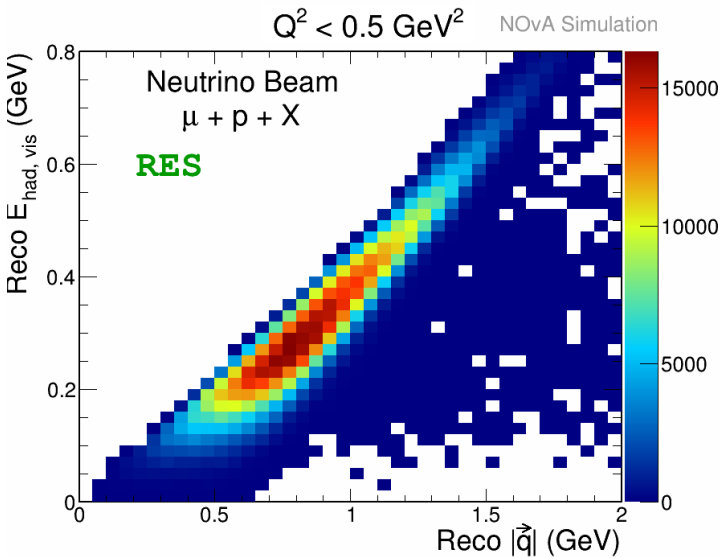
Breaking down the prediction

- $\mu + P + X$ sample, in slices of true W , by interaction type.



Breaking down the prediction

- $\mu + P + X$ sample, in slices of true Q^2 , by interaction type.



Takeaway: What's wrong with GENIE?

- GENIE over-predicts μ +P+X events consistently.
- GENIE over-predicts RES and DIS events at low- Q^2 in all topologies.

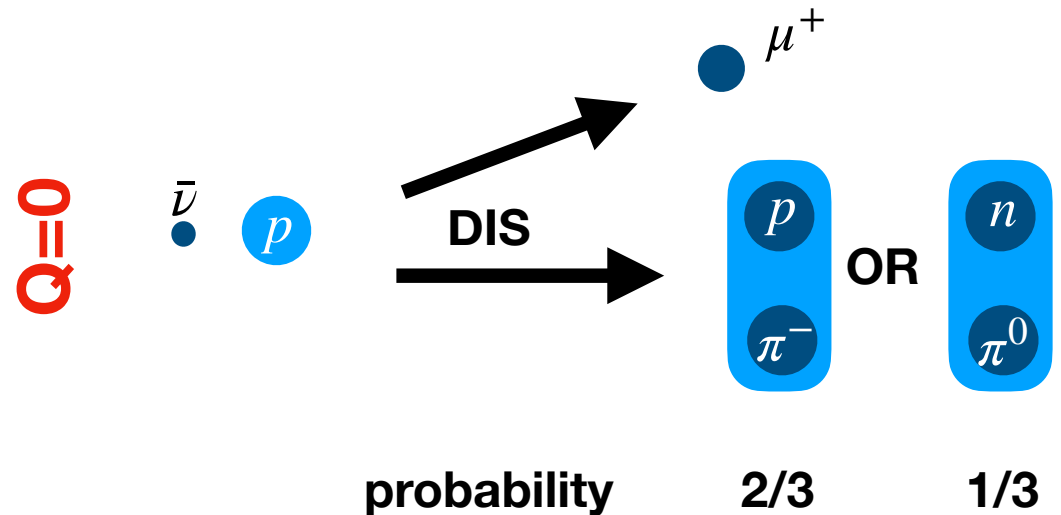
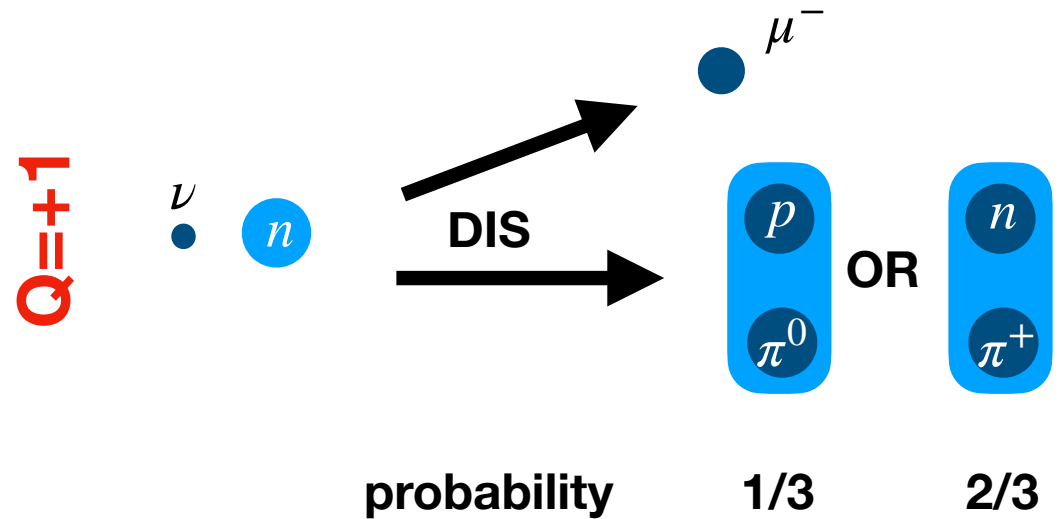
Fit to data

- Implemented improvements to address the **quality** and **quantity**:
 - uniform priors. ✗
 - covariance matrix. ✗
 - minimal differentiation. ✓
 - ranking systematics by χ^2 . ✓
 - new RES/DIS uncertainties.
 - DIS hadron final states.
 - $\text{RES} \frac{\sigma(\nu p)}{\sigma(\nu n)}$.
 - RES scale.
 - variable binning.
 - phase space cut.

A new DIS systematic

quality

- In GENIE, a ν CC DIS, with final state $Q=+1,0$, and multiplicity=2 **has fixed probabilities**:
 - proton = 1/3.
 - neutron = 2/3.
- Associated with isospin amplitudes.
- Allow flexibility in the final states $\rightarrow$ topology.



A new DIS systematic

quality

DIS events

topological impact....

ν

$$\nu + n \rightarrow \mu^- + p + \pi^0$$



more MuPrEtc

$+2\sigma$

no events

-1σ

$$\nu + n \rightarrow \mu^- + n + \pi^+$$



no events

more MuPiEtc

$\bar{\nu}$

$$\bar{\nu} + p \rightarrow \mu^+ + n + \pi^0$$



no events

$+1\sigma$

more MuEtc

-2σ

$$\bar{\nu} + p \rightarrow \mu^+ + p + \pi^-$$



more MuPiEtc

no events

Fit to data

- Implemented improvements to address the **quality** and **quantity**:
 - uniform priors. ❌
 - covariance matrix. ❌
 - minimal differentiation. ✅
 - ranking systematics by χ^2 . ✅
 - new RES/DIS uncertainties.
 - DIS hadron final states. ✅
 - $\text{RES} \frac{\sigma(\nu p)}{\sigma(\nu n)}$.
 - RES scale.
 - variable binning.
 - phase space cut.

Takeaway: What's wrong with GENIE?

- GENIE over-predicts $\mu+P+X$ events consistently.
- GENIE over-predicts RES and DIS events at low- Q^2 in all topologies.
- GENIE does not have enough flexibility to determine hadronic final state particles from the DIS (and probably SIS) regime.

Fit to data

▸ Implemented improvements to address the **quality** and **quantity**:

- uniform priors. ❌
- covariance matrix. ❌
- minimal differentiation. ✅
- ranking systematics by χ^2 . ✅
- new RES/DIS uncertainties. ✅
 - DIS hadron final states. ✅
 - $\text{RES} \frac{\sigma(\nu p)}{\sigma(\nu n)}$. ✅
 - RES scale. ✅
- variable binning.
- phase space cut.

**RES vp / vn available in
back-up.**

Adjust relative x-secs

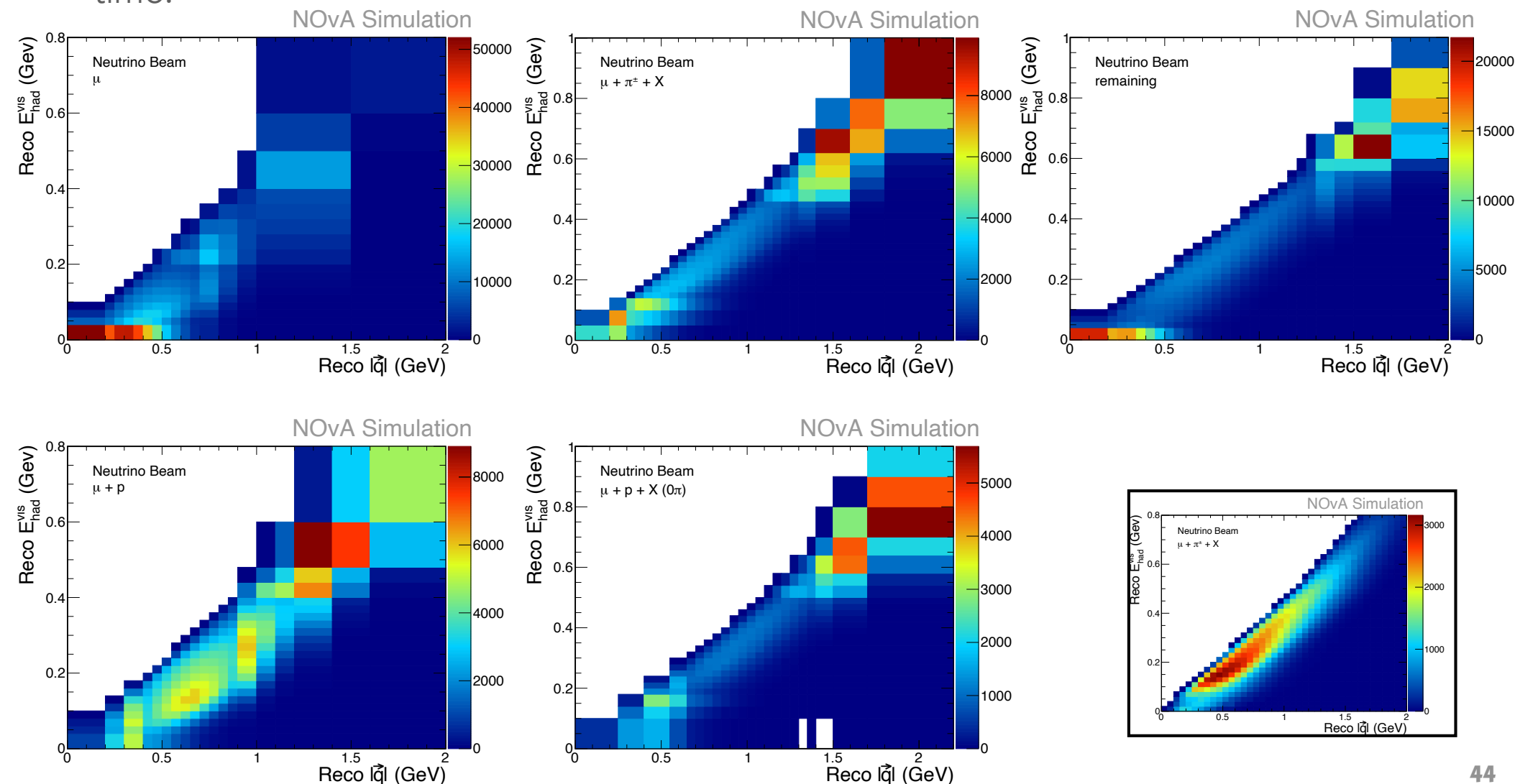
**RES scale available in
back-up.**

**20% scale to Δ and other
resonances.**

Variable binning

quality + quantity

- Large bins at low-event regions of phase space.
- These changes will “improve” the χ^2 with fewer bins — should see speedup in CPU time.



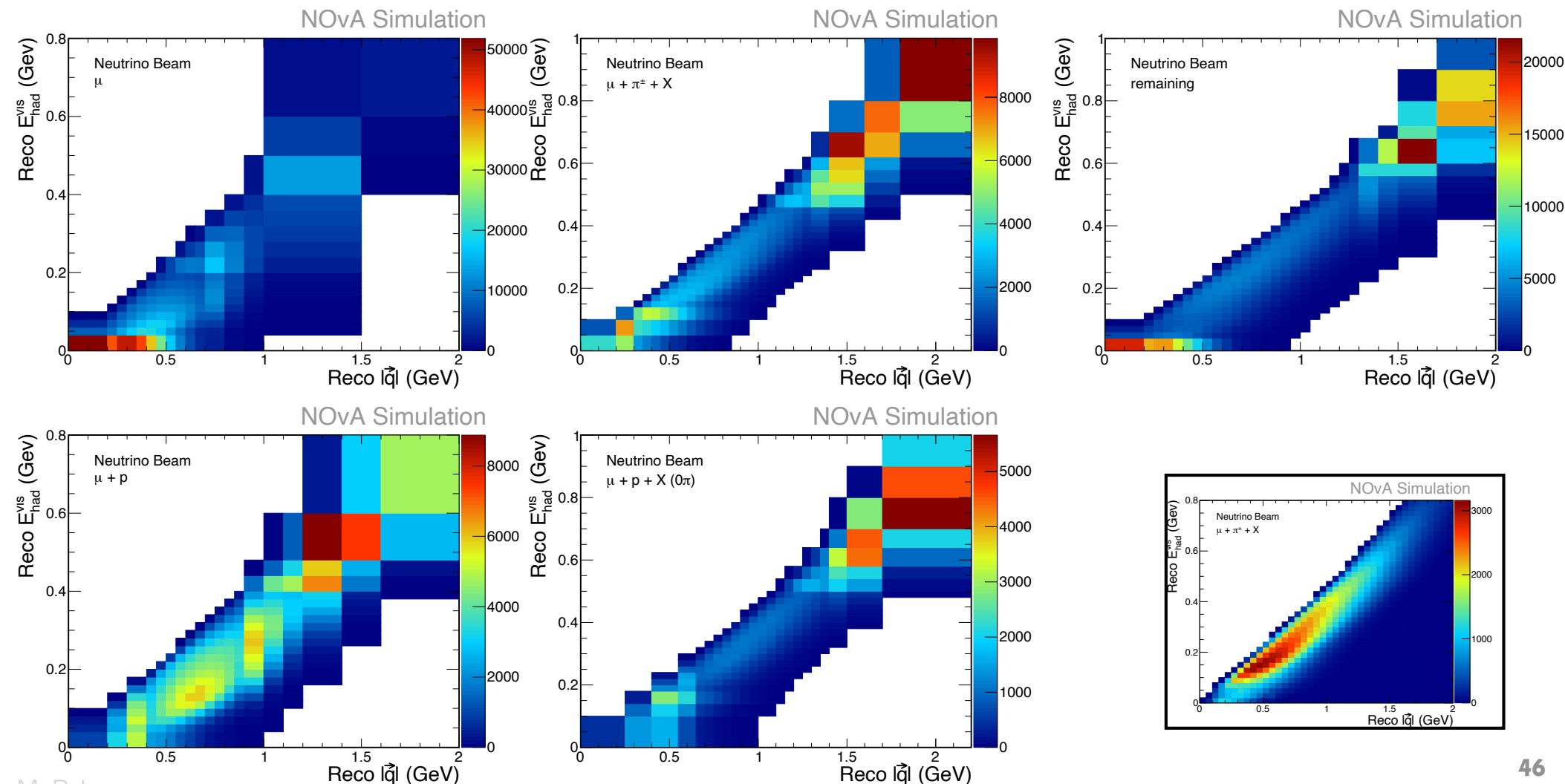
Fit to data

- Implemented improvements to address the **quality** and **quantity**:
 - uniform priors. ❌
 - covariance matrix. ❌
 - minimal differentiation. ✅
 - ranking systematics by χ^2 . ✅
 - new RES/DIS uncertainties. ✅
 - DIS hadron final states. ✅
 - RES $\frac{\sigma(\nu p)}{\sigma(\nu n)}$. ✅
 - RES scale. ✅
 - variable binning. ✅
 - phase space cut.

Phase space cut

quality + quantity

- Remove events at low E Had Vis, high Reco lql.
- These changes will “improve” the χ^2 by removing the low statistics region of the predictions.



Fit to data

- Implemented improvements to address the **quality** and **quantity**:
 - uniform priors. ❌
 - covariance matrix. ❌
 - minimal differentiation. ✅
 - ranking systematics by χ^2 . ✅
 - new RES/DIS uncertainties. ✅
 - DIS hadron final states. ✅
 - RES $\frac{\sigma(\nu p)}{\sigma(\nu n)}$. ✅
 - RES scale. ✅
 - variable binning. ✅
 - phase space cut. ✅

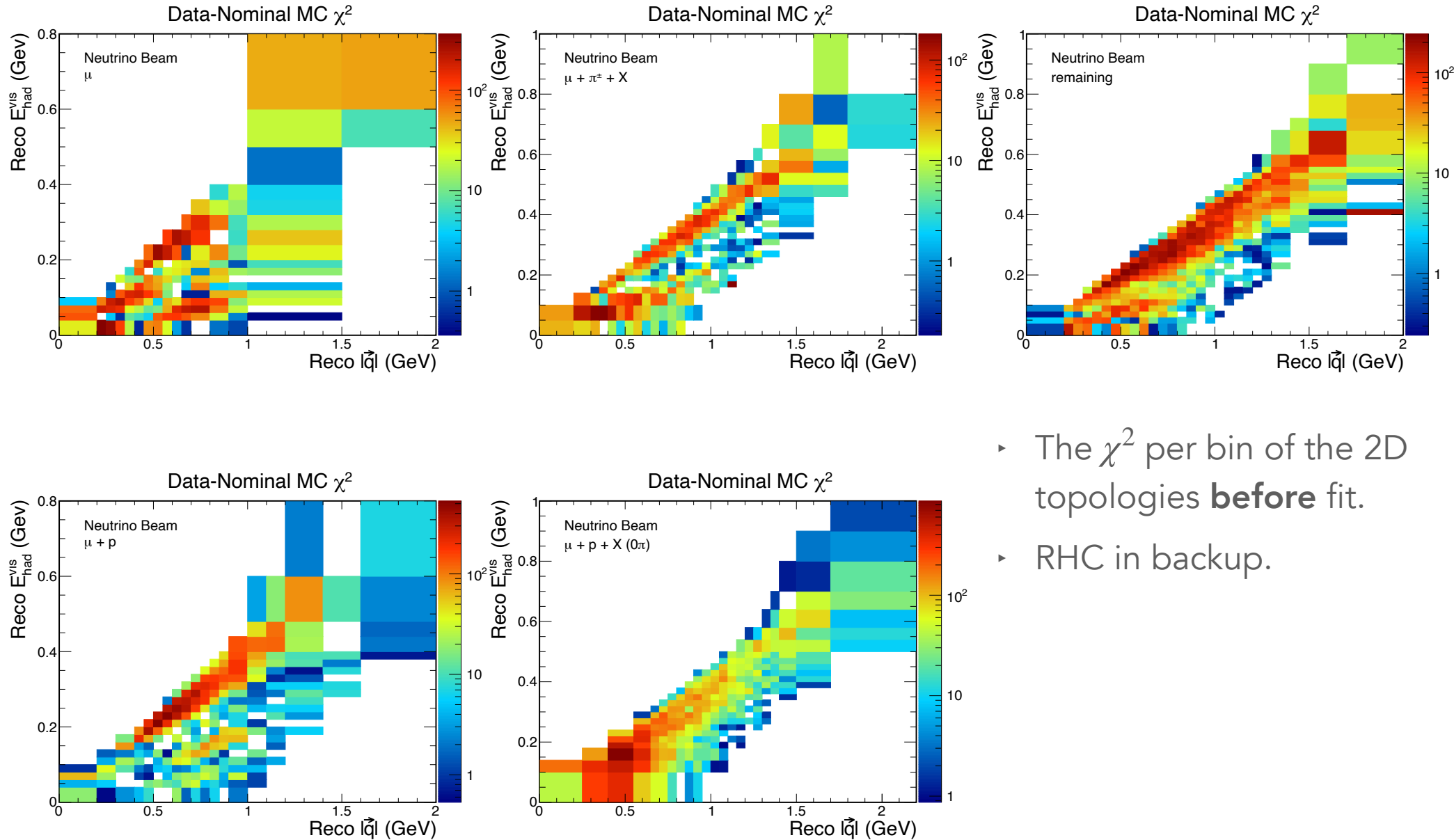
Fit to data

▸ Implemented improvements to address the **quality** and **quantity**:

- uniform priors. ❌
- covariance matrix. ❌
- minimal differentiation. ✅
- ranking systematics by χ^2 . ✅
- new RES/DIS uncertainties. ✅
 - DIS hadron final states. ✅
 - $\text{RES} \frac{\sigma(\nu p)}{\sigma(\nu n)}$. ✅
 - RES scale. ✅
- variable binning. ✅
- phase space cut. ✅

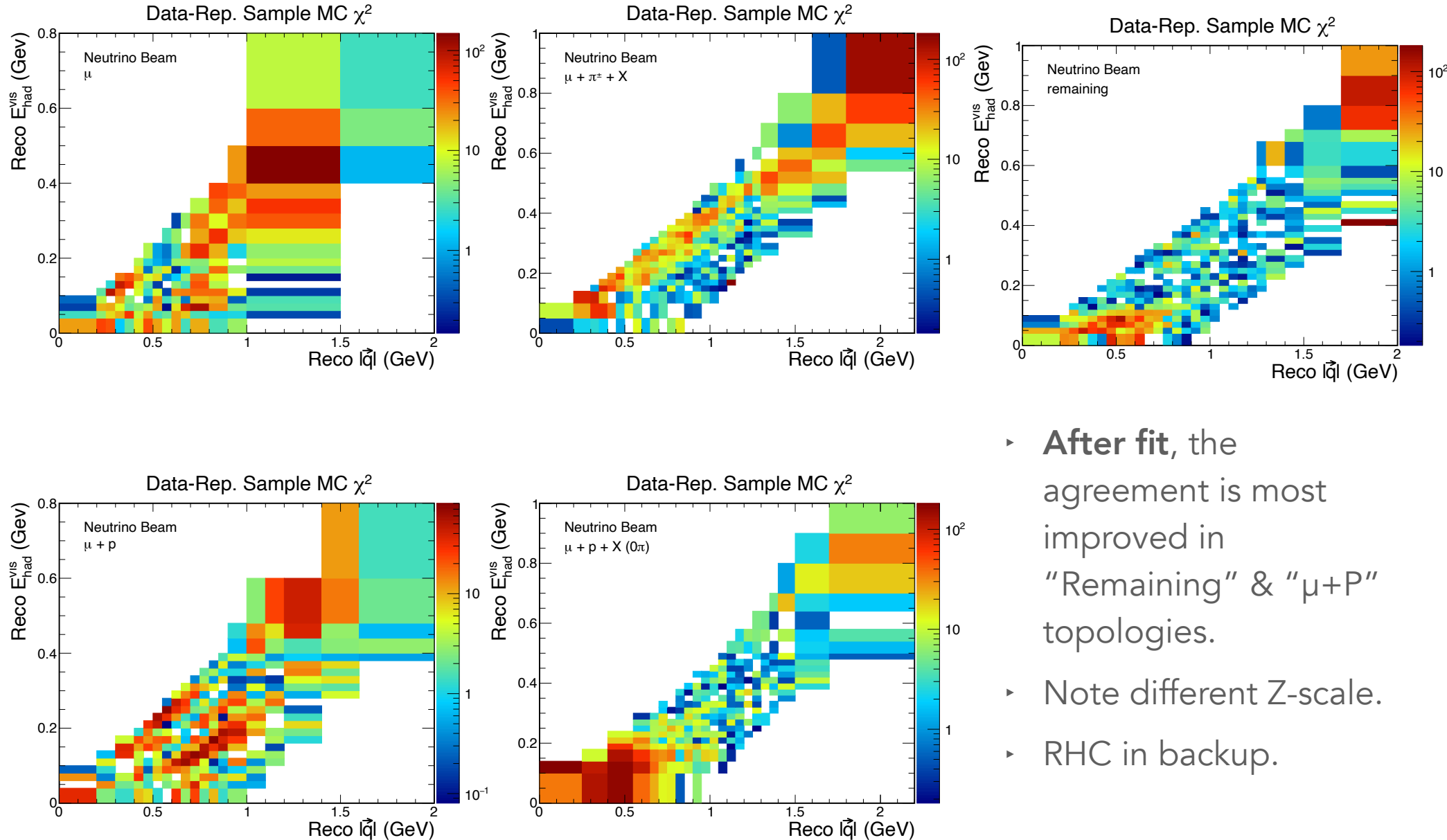
Generate ND predictions with
these developments →
Ready to fit ND data.

Data-Nominal MC χ^2 — FHC



- The χ^2 per bin of the 2D topologies **before** fit.
- RHC in backup.

Data-Rep Sample MC χ^2 — FHC



- **After fit**, the agreement is most improved in "Remaining" & " $\mu + p$ " topologies.
- Note different Z-scale.
- RHC in backup.

Data-Rep Sample MC χ^2

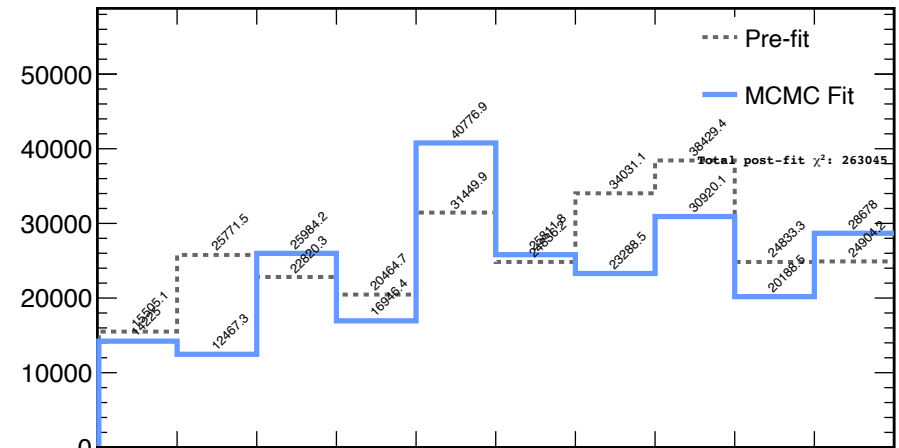
- χ^2 per topology improved.
- But is this level of agreement "good enough"?
- Need to do full **ND + FD fake data fit** to assess the ND fit quality....
- this is the next to-do item.

**Before
Developments**

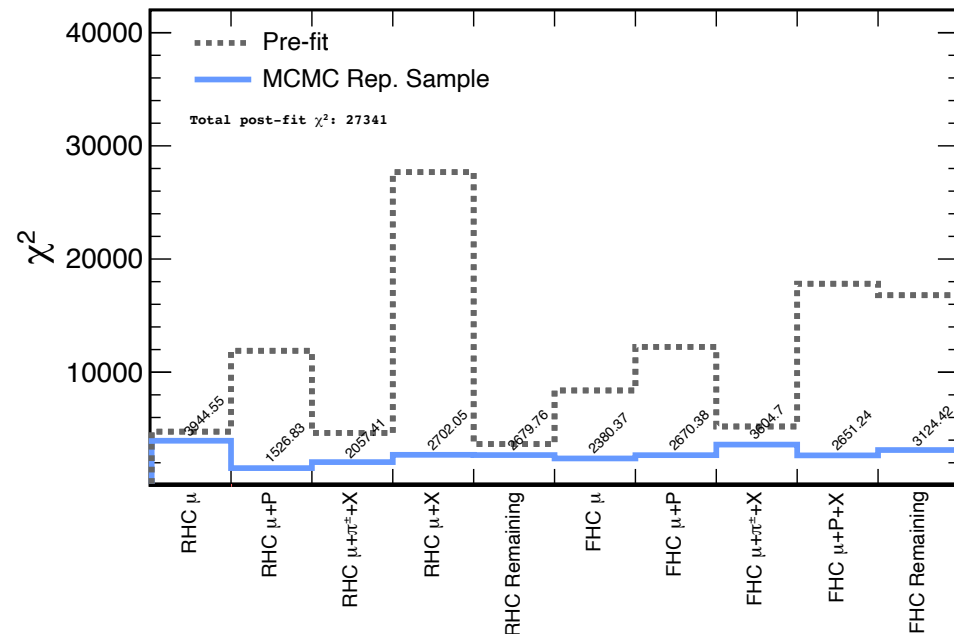


**After
Developments**

χ^2 by Topology



χ^2 by Topology



Some important takeaways

▸ Why a joint fit?

- Maximize the information (i.e. statistical power) of the ND dataset.
- Provides novel means of interrogating NOvA data — akin to ongoing NOvA-T2K joint fit.
- More transparent about NOvA's MC deficiencies.

▸ Why MCMC?

- Complements Frequentist analyses well.
- Marginalizing over uncertainties comes “free” — no computational cost (no FC).

▸ What's wrong with GENIE?

- NOvA's tune of GENIE:
 - over-predicts SIS/DIS + RES interactions at low- Q^2 .
 - over-predicts lowest hadronic visible energy events (QE + MEC).

Summary

- MCMC is a Bayesian parameter estimation tool.
- Verified MCMC can be applied to estimate NOvA's physics model uncertainties (and ultimately oscillation parameters).
- Initial MCMC fits to data proved intractable.
 - Numerous improvements made to MCMC and ND predictions:
 - to reduce CPU demand (**quantity**) and
 - to improve agreement (**quality**).
- Can efficiently run ND fits to data.
- Now, critical junction: **"Does this ND post-fit discrepancy matter for an ND + FD fit?"**
- Creating machinery for ND + FD fake data fits.

Thank you!

Backup

NOvA Simulation

- NOvA uses neutrino generator GENIE 3.0.6 with a custom combination of physics models.
 - the Valencia 2p2h model — added **NOvA tune**.
 - hN Final State Interaction (FSI) model — added **NOvA tune**.

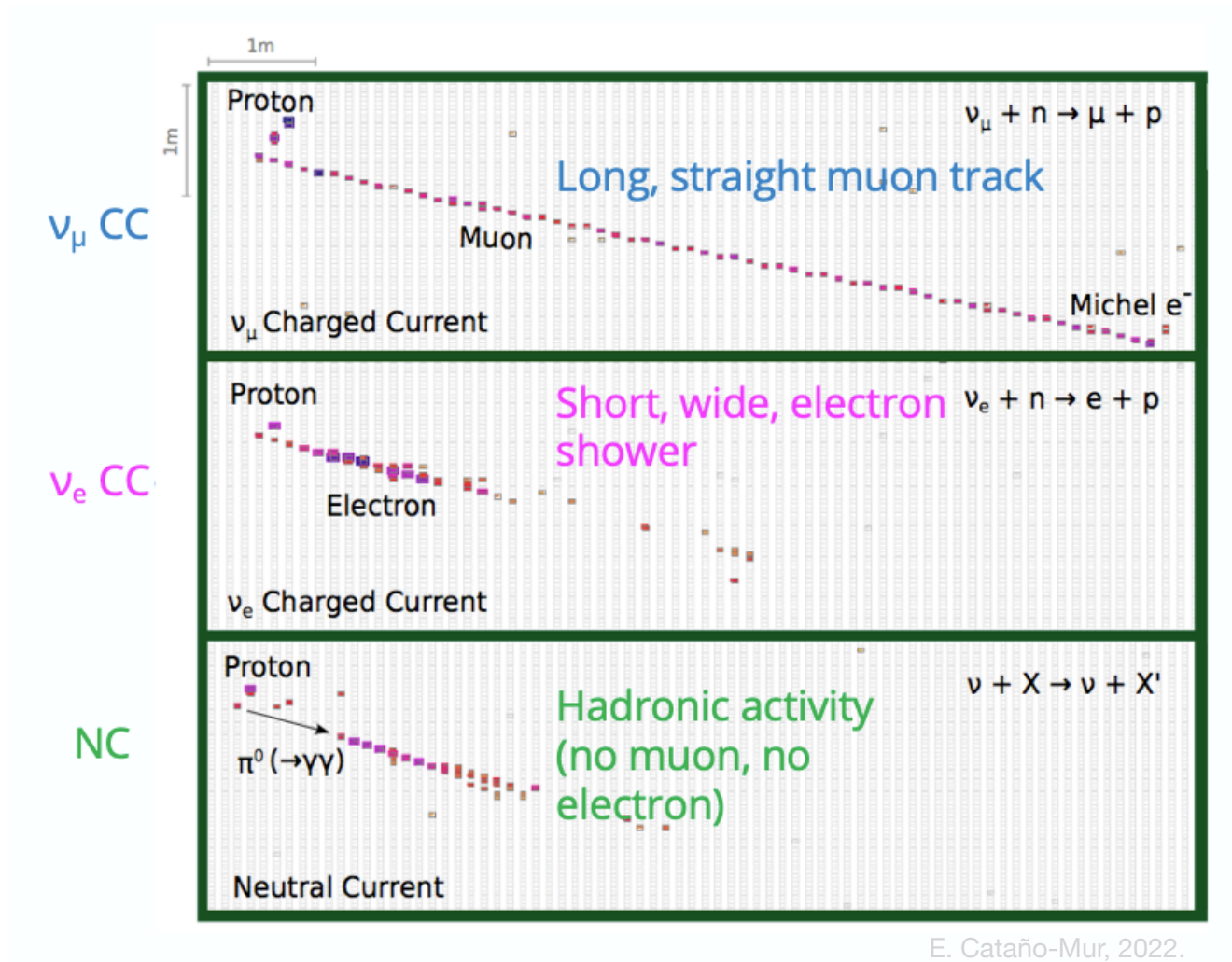
Process	Model	Reference
Quasielastic	Valencia 1p1h	J. Nieves, J. E. Amaro, M. Valverde, Phys. Rev. C 70 (2004) 055503
Form Factor	Z-expansion	A. Meyer, M. Betancourt, R. Gran, R. Hill, Phys. Rev. D 93 (2016)
Multi-nucleon	Valencia 2p2h	R. Gran, J. Nieves, F. Sanchez, M. Vicente Vacas, Phys. Rev. D 88 (2013)
Resonance	Berger-Sehgal	Ch. Berger, L. M. Sehgal, Phys. Rev. D 76 (2007)
DIS	Bodek-Yang	A. Bodek and U. K. Yang, NUINT02, Irvine, CA (2003)
Final State Int.	hN semi-classical cascade	S. Dytman, Acta Physica Polonica B 40 (2009)

* We call our tune N1810j_0211a, and it is built by starting with G1810b_0211a and substituting the Z-expansion form factor for the dipole one. This combination was not available in the 3.0.6 release, but it may be available in future versions.

Fig: Teppei Katori, "Meson Exchange Current (MEC) Models in Neutrino Interaction Generators" AIP Conf.Proc. 1663 (2015) 030001

A. Himmel, Neutrino 2020

NOvA Experiment

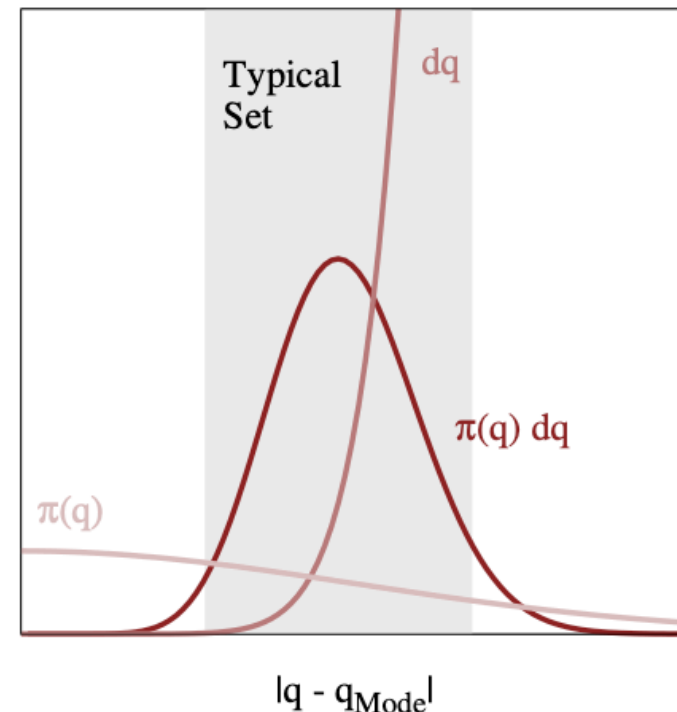


E. Cataño-Mur, 2022.

Markov Chain Monte Carlo (MCMC)

<https://arxiv.org/abs/1701.02434>

- The objective of MCMC is to locate the maximum of the posterior parameter space.
 - Most of the volume is low probability, $\pi(q)$.
 - volume element grows with dimension, dq .
- **typical set:** product of $\pi(q) dq$ is maximal.
 - $\mathbb{E}(f) = \int f(q) \pi(q) dq$



Markov Chain Monte Carlo (MCMC)

- Want to reach typical set as efficiently as possible.
- Hamiltonian Monte Carlo algorithm **samples** posterior $\propto$ probability.
 - Sampling is analogous to a particle in a gravitational field:
 - particle follows gradient of “gravitational” potential.
 - region(s) where particle traverses more frequently $\rightarrow$ more probable.
- **Sample repeatedly** for increased statistics.

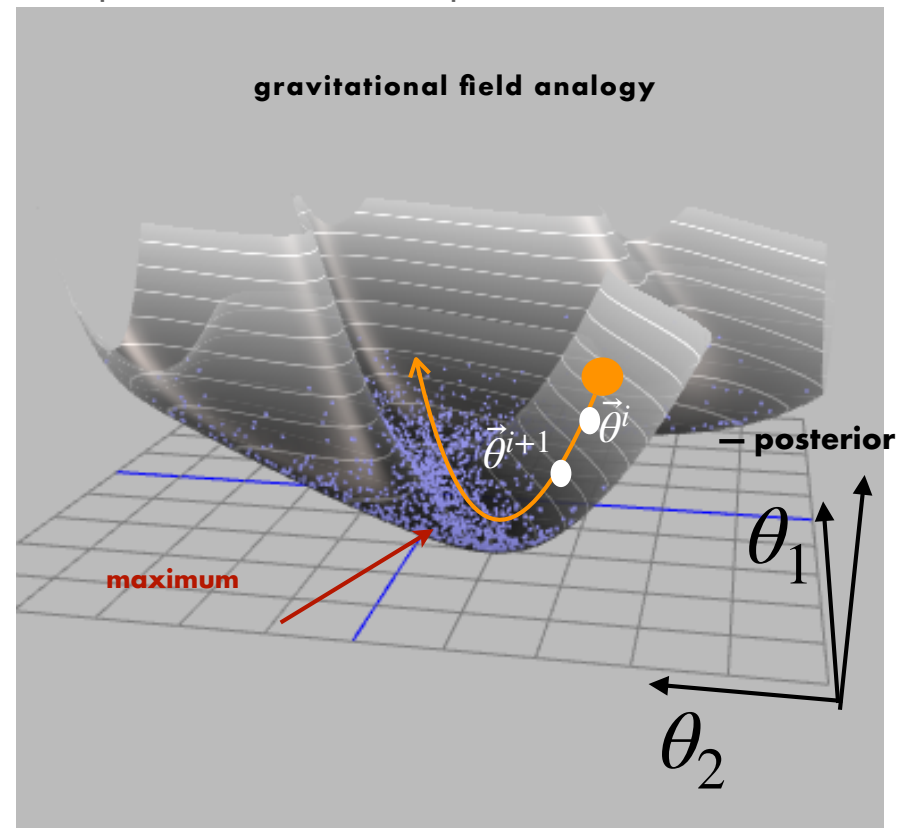
Bayes Theorem

$$P(\vec{\theta}|\vec{\mathcal{X}}) \propto P(\vec{\mathcal{X}}|\vec{\theta}) \times P(\vec{\theta})$$

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

$$\text{posterior} \propto e^{-\frac{\chi^2}{2}} \times \mathcal{N}(0, \approx 1)^*$$

*Gaussian-like



2D posterior example

Markov Chain Monte Carlo (MCMC)

- Consider a 2-dimensional posterior, $\{\theta_1, \theta_2\}$, as a **topological** space, with peaks and valleys.
 - 1. Introduce a conjugate variable, $\{p_1, p_2\}$, analogous to momentum.
 - 2. Describe single point in space as: $pdf(\vec{\theta}, \vec{p}) \equiv H(\vec{\theta}, \vec{p}) = KE(\vec{\theta}, \vec{p}) + V(\vec{\theta})$.
 - 3. Utilize Hamilton's Eqns and kinematic motion to "travel" the posterior $\frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{\theta}} = \frac{\partial V}{\partial \vec{\theta}}$.
- Markov Chain uses gradient of the parameter space to moves towards increasing probability.
 - The chain ends once it turns back on itself (No U-Turn Sampling, NUTS).
- One complete chain is a **sample** — repeat to maximize statistics.
- Samples that end at specific pull value $\rightarrow$ more probable value.

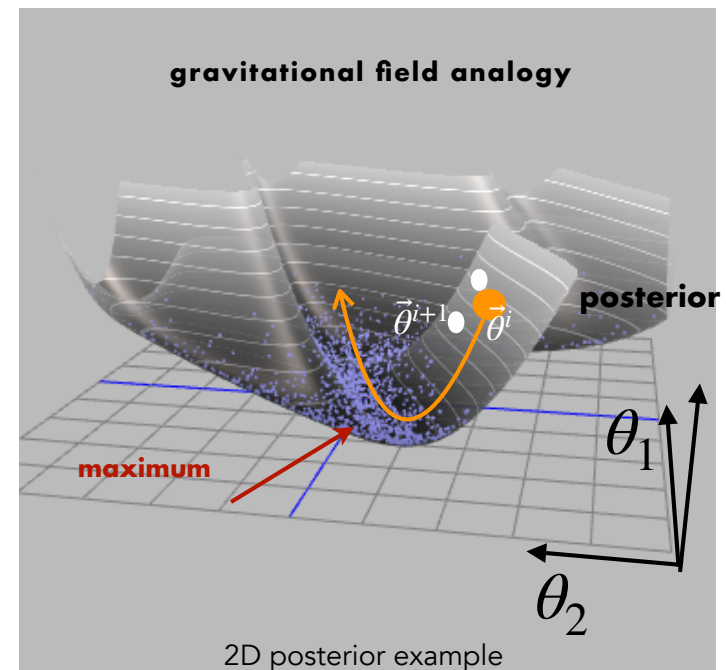
Bayes Theorem

$$P(\vec{\theta} | \vec{\mathcal{X}}) \propto P(\vec{\mathcal{X}} | \vec{\theta}) \times P(\vec{\theta})$$

$$\text{posterior} \propto \text{likelihood} \times \text{prior}$$

$$\text{posterior} \propto e^{-\frac{\chi^2}{2}} \times \mathcal{N}(0, \approx 1)^*$$

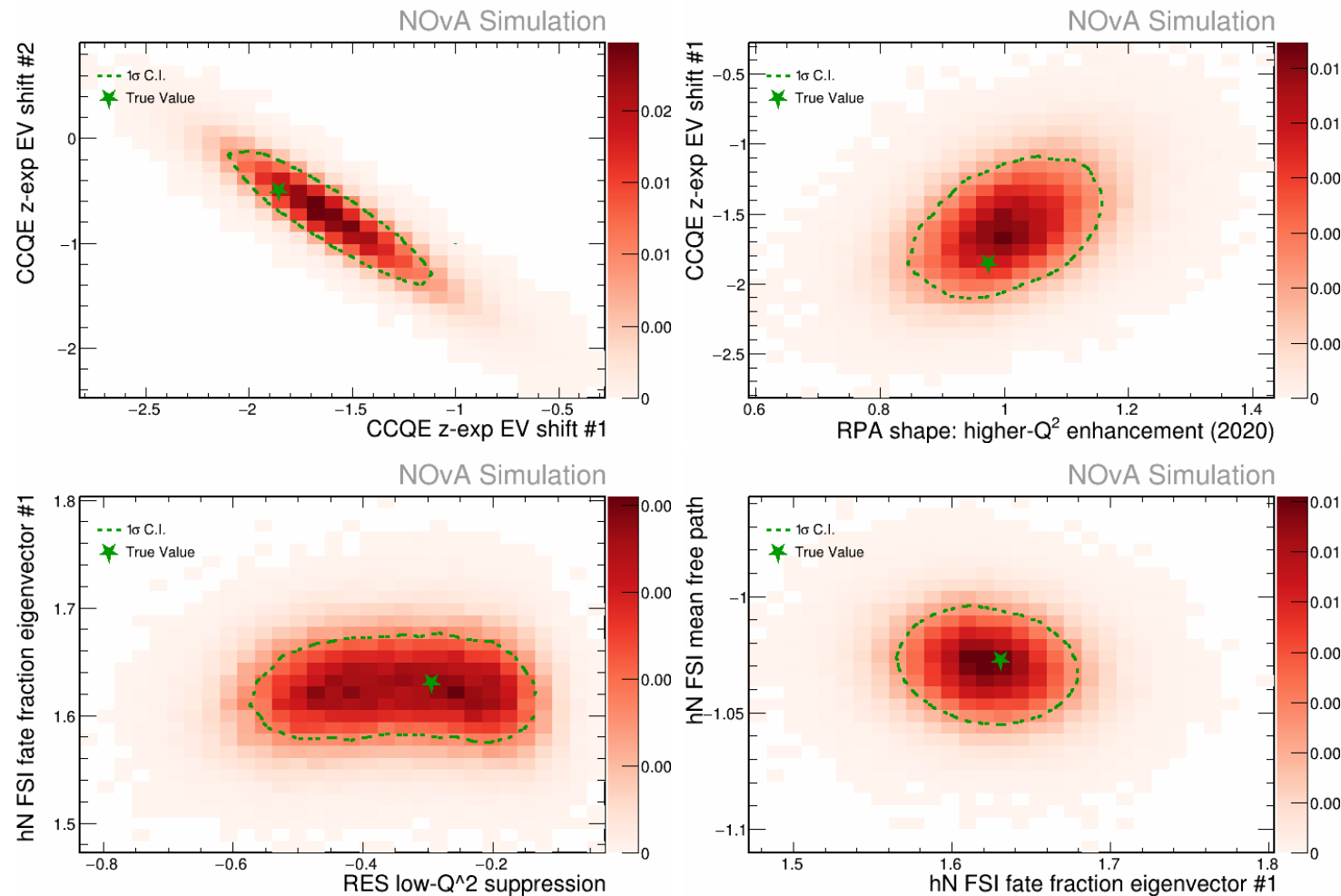
*Gaussian-like



Takeaway: Why MCMC?

Marginalization $\mathcal{P}(\vec{\theta}|\vec{x}) = \int \mathcal{P}(\vec{\theta}, \vec{\delta}|\vec{x}) d\vec{\delta}$

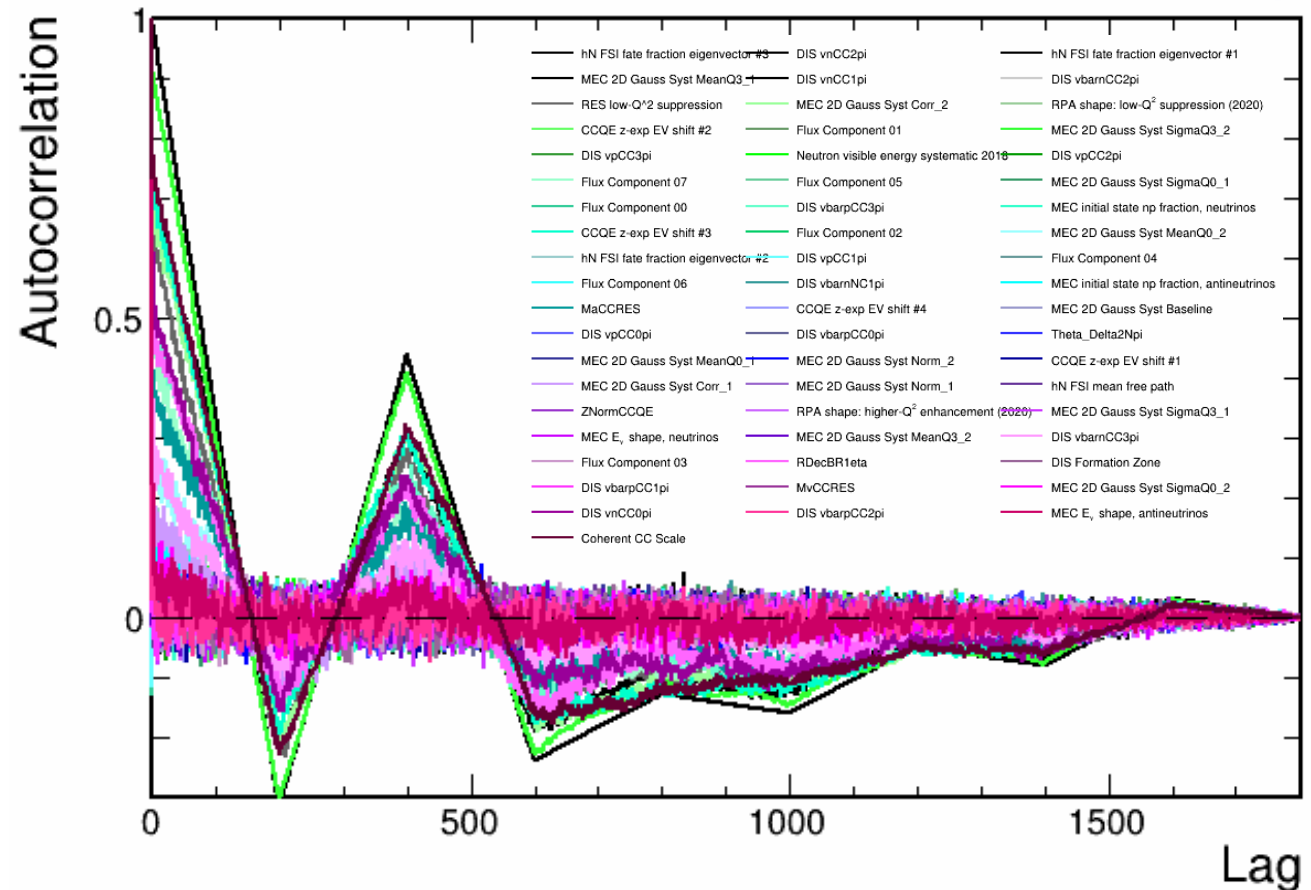
- Bayesian inference offers advantage of **marginalization** of nuisance parameters, $\vec{\delta}$.
- 2D marginal distributions** — easy access to correlations of parameters.



Diagnose MCMC samples

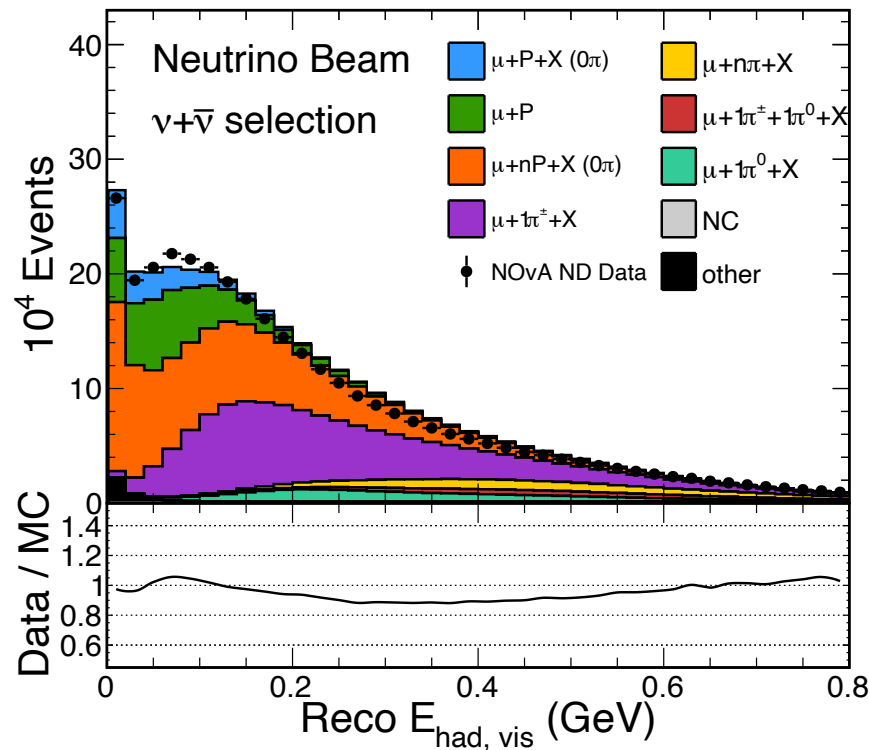
- Evaluate the efficiency of sampling with **auto-correlations**.
- Each step in posterior should be uncorrelated from prior step.
 - Most parameters move to 0 quickly.
 - Several have large correlations.
 - larger step-size or more samples needed.

NOvA Preliminary



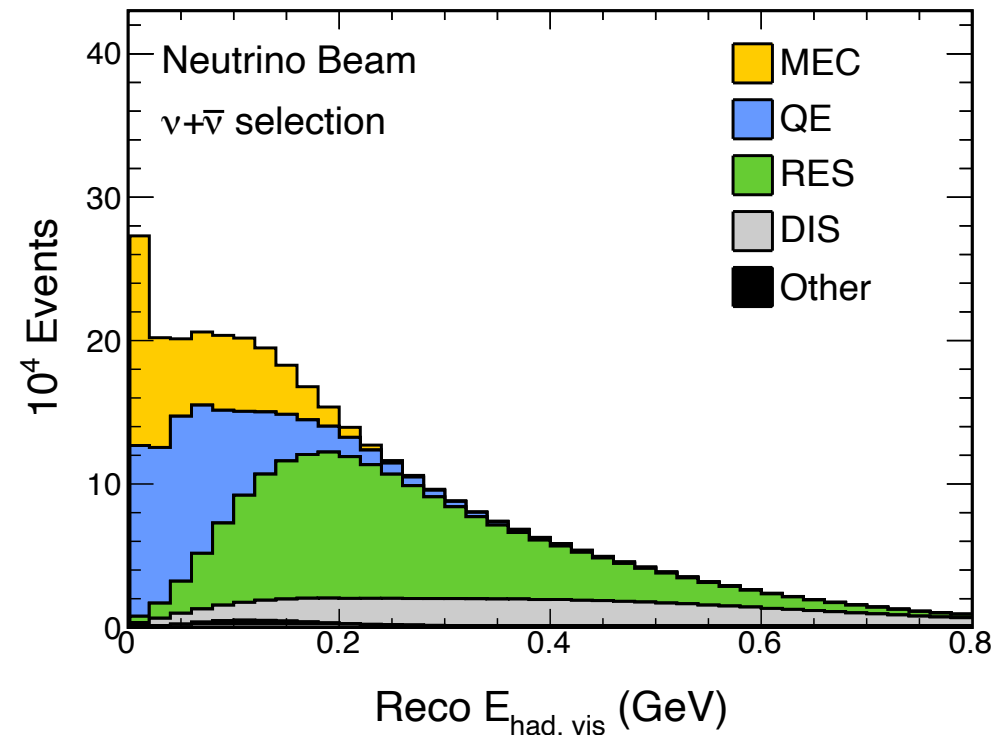
NOvA's ND Topological Samples

NOvA Preliminary



ν mode — Hadronic Visible Energy

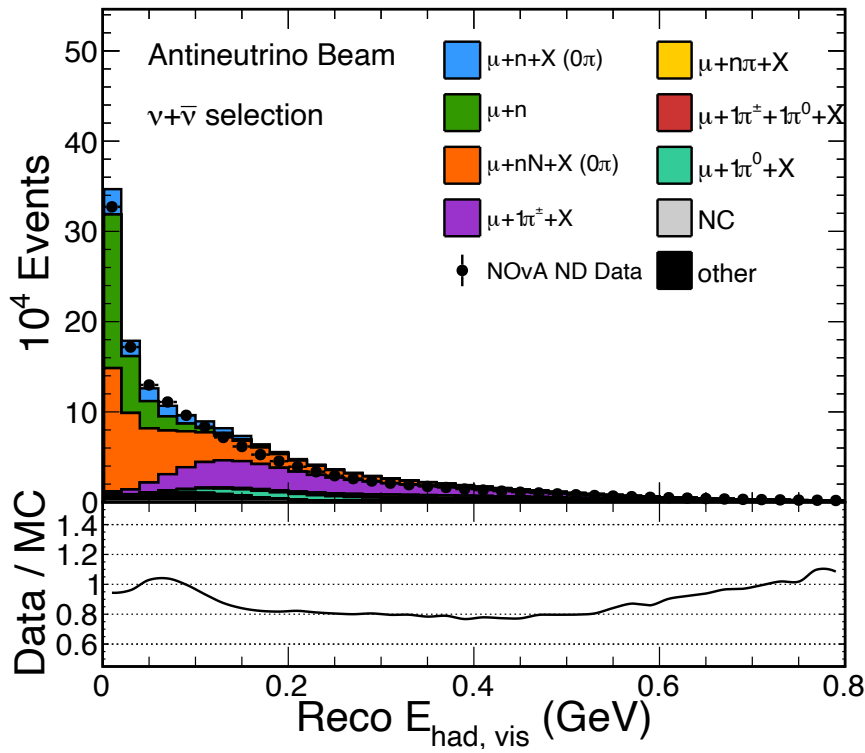
NOvA Simulation



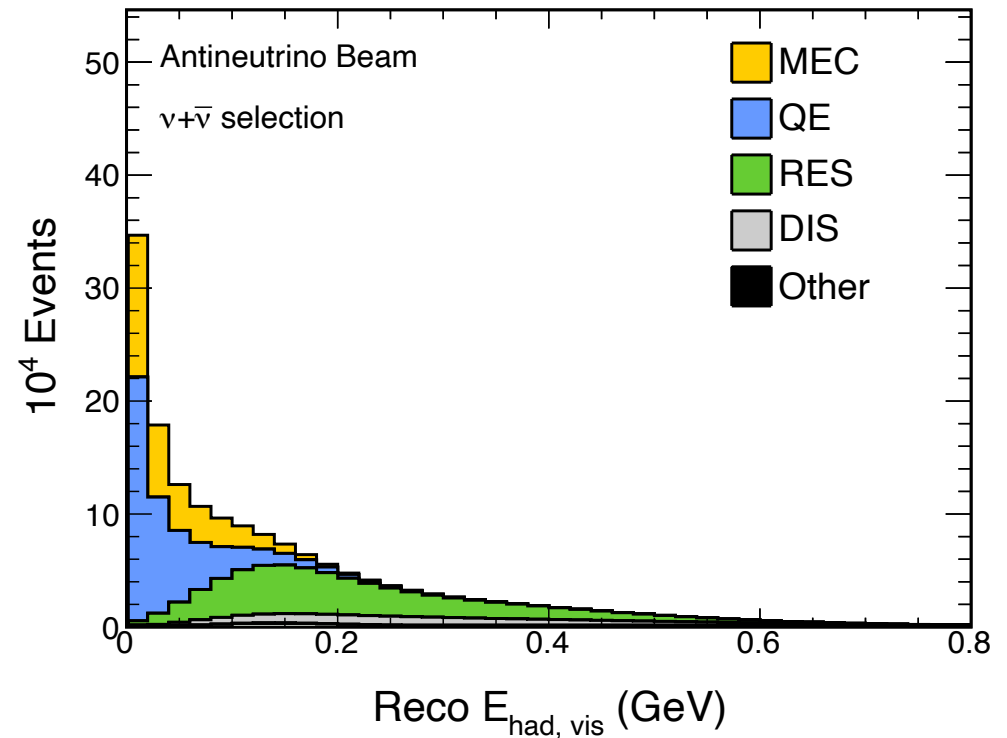
NOvA's ND Topological Samples

$\bar{\nu}$ mode — Hadronic Visible Energy

NOvA Preliminary



NOvA Simulation

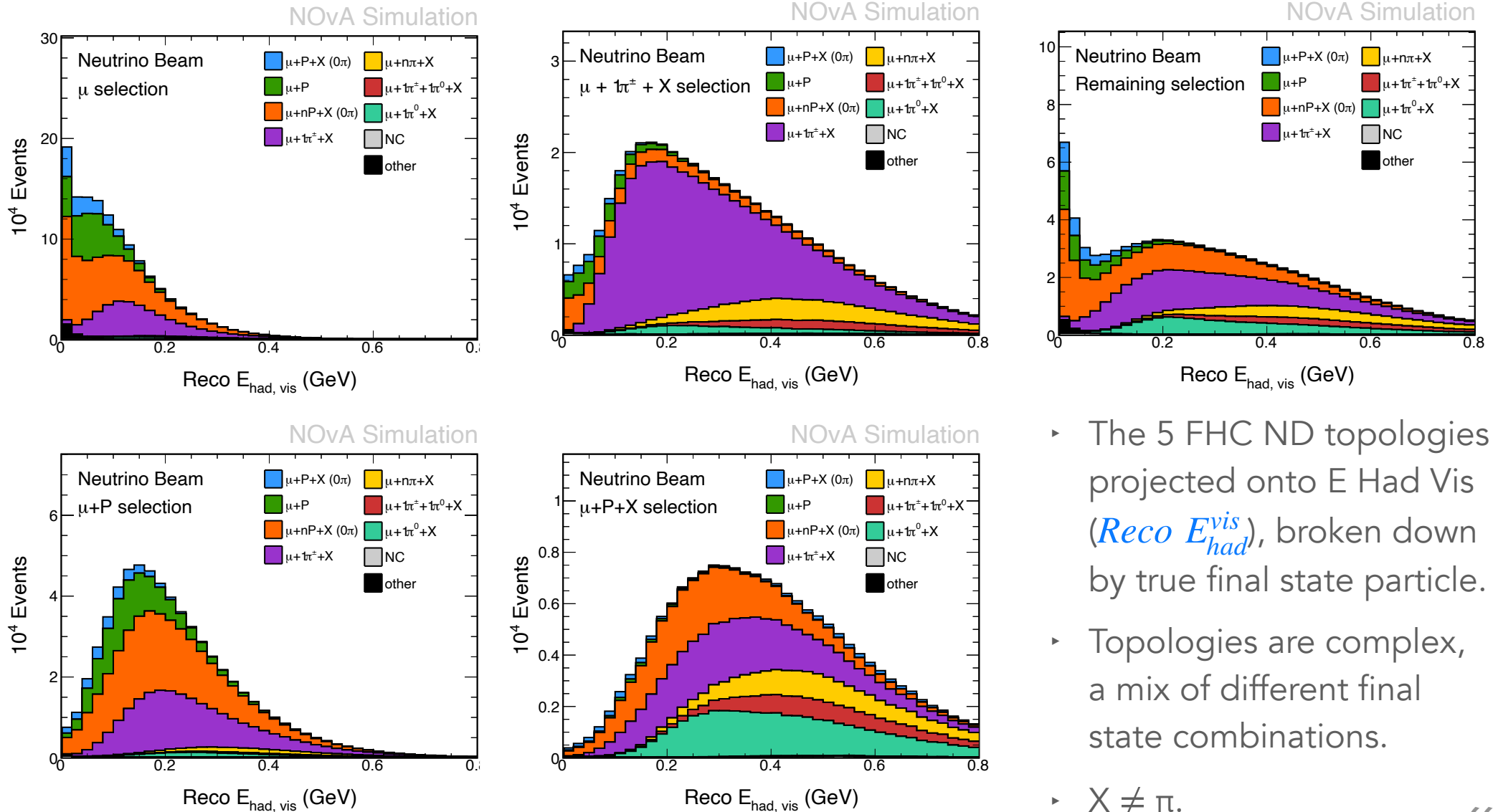


NOvA ND Topologies

- **Mu:** μ
 - * 1 3D prong with μ cvn score $> .5$ or longer than 500 cm.
- **MuPr:** $\mu + p$
 - * Exactly 2 3D prongs required
 - * 1 3D prong with μ cvn score $> .5$ or longer than 500 cm.
 - * 1 3D prong with p-score ≥ 0.5
- **MuPi:** $\mu + \pi^\pm + X$
 - * 2 or more 3D prongs required
 - * 1 3D prong with μ cvn score $> .5$ or longer than 500 cm.
 - * 1 3D prong with π -score ≥ 0.7
- **MuPrEtc:** $\mu + p + X(0\pi)$ (only FHC)
 - * 3 or more 3D prongs required
 - * 1 3D prong with μ cvn score $> .5$ or longer than 500 cm.
 - * 1 3D prong with p-score ≥ 0.5
 - * Exclude most pions by only accepting other prongs with π score < 0.5
- **MuEtc:** $\mu + X(0\pi)$ (only RHC)
 - * 2 or more 3D prongs required
 - * 1 3D prong with μ cvn score $> .5$ or longer than 500 cm.
 - * Exclude most pions by only accepting other prongs with π score < 0.5
- **EvElse:** Everything not in previous categories

NOvA's ND Topological Samples

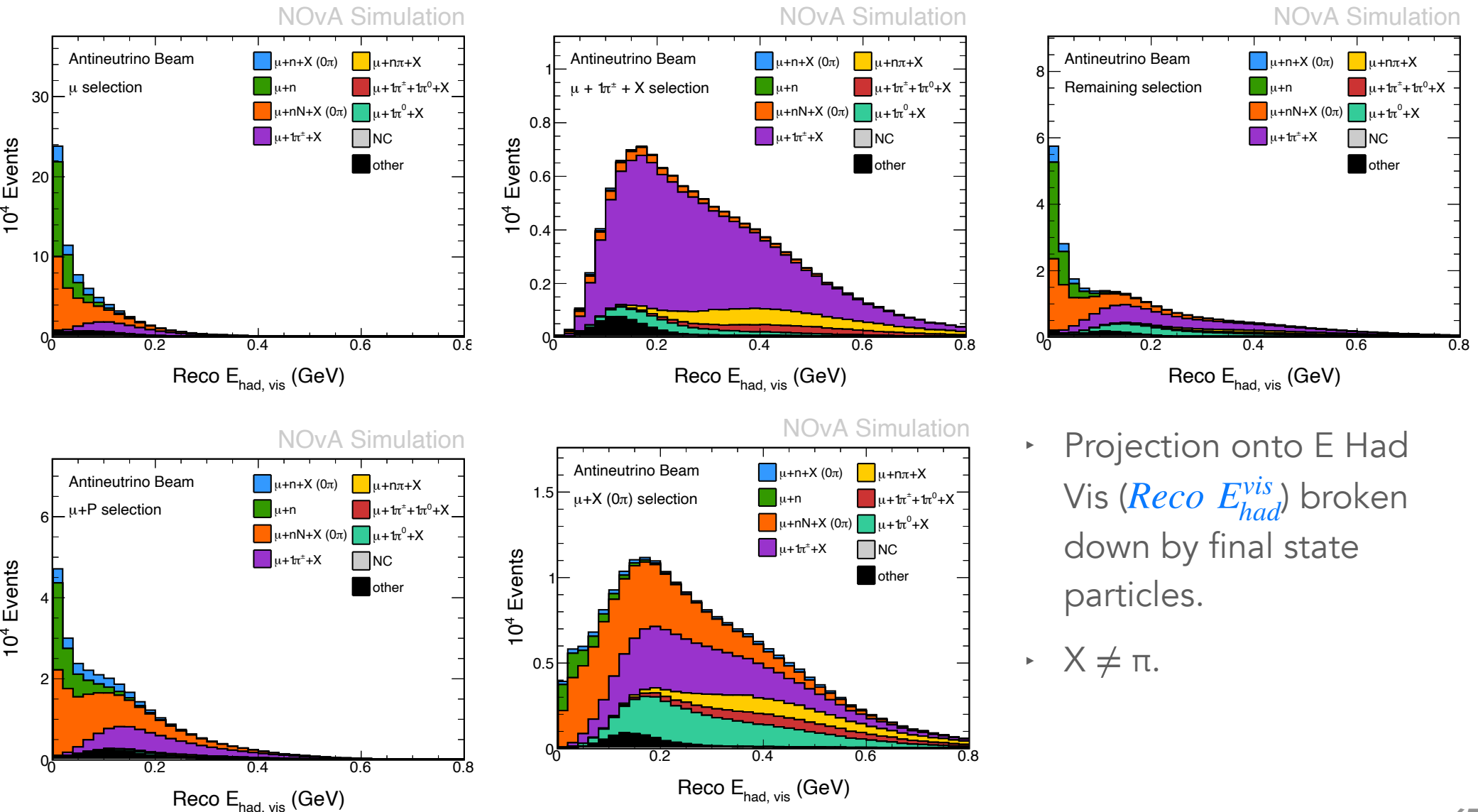
ν mode — Hadronic Visible Energy



- ▶ The 5 FHC ND topologies projected onto $E_{\text{Had Vis}}$ ($\text{Reco } E_{\text{had}}^{\text{vis}}$), broken down by true final state particle.
- ▶ Topologies are complex, a mix of different final state combinations.
- ▶ $X \neq \pi$.

NOvA's ND Topological Samples

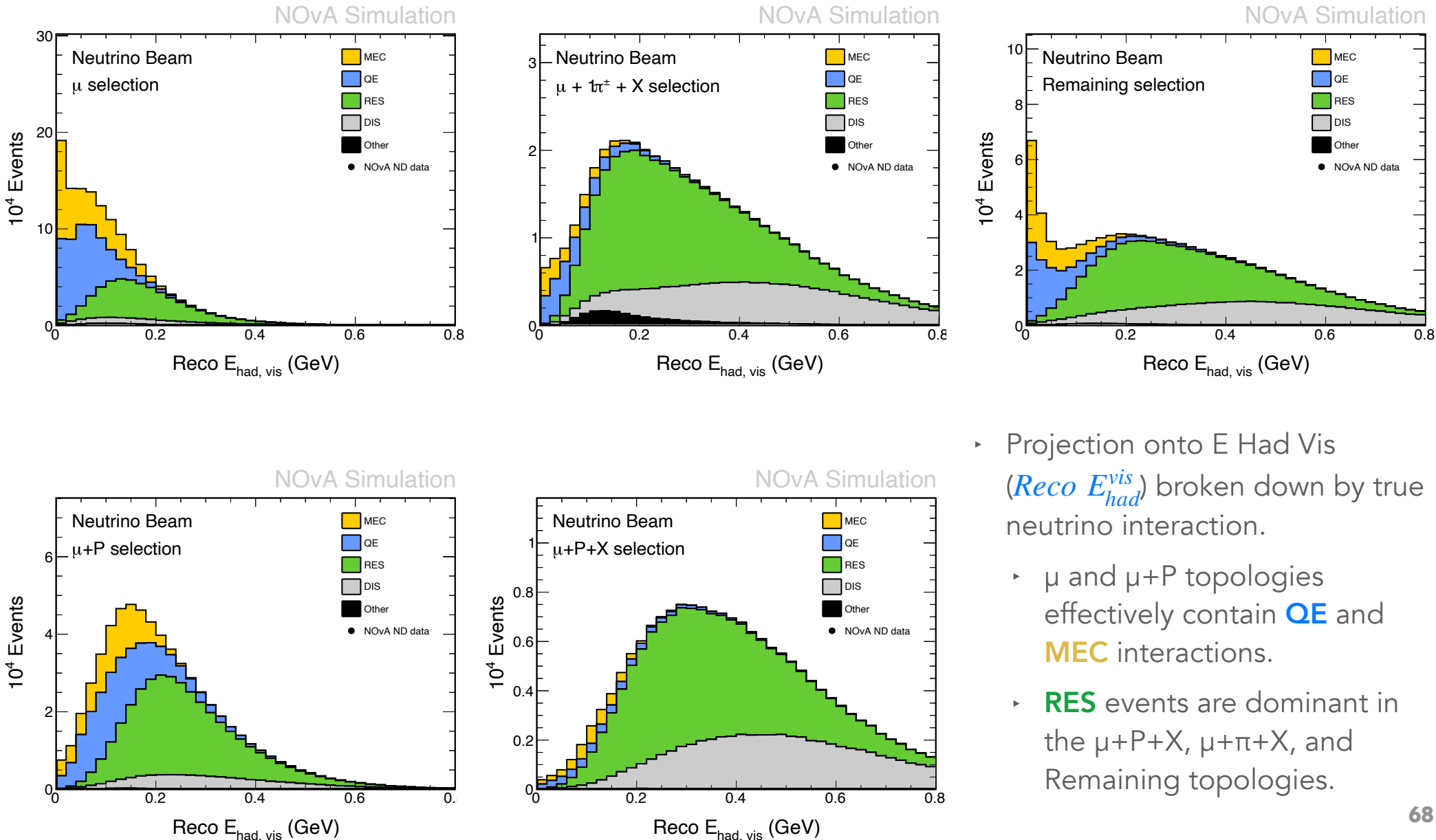
$\bar{\nu}$ mode — Hadronic Visible Energy



- Projection onto E_{Had} Vis ($Reco E_{had}^{vis}$) broken down by final state particles.
- $X \neq \pi$.

NOvA's ND Topological Samples

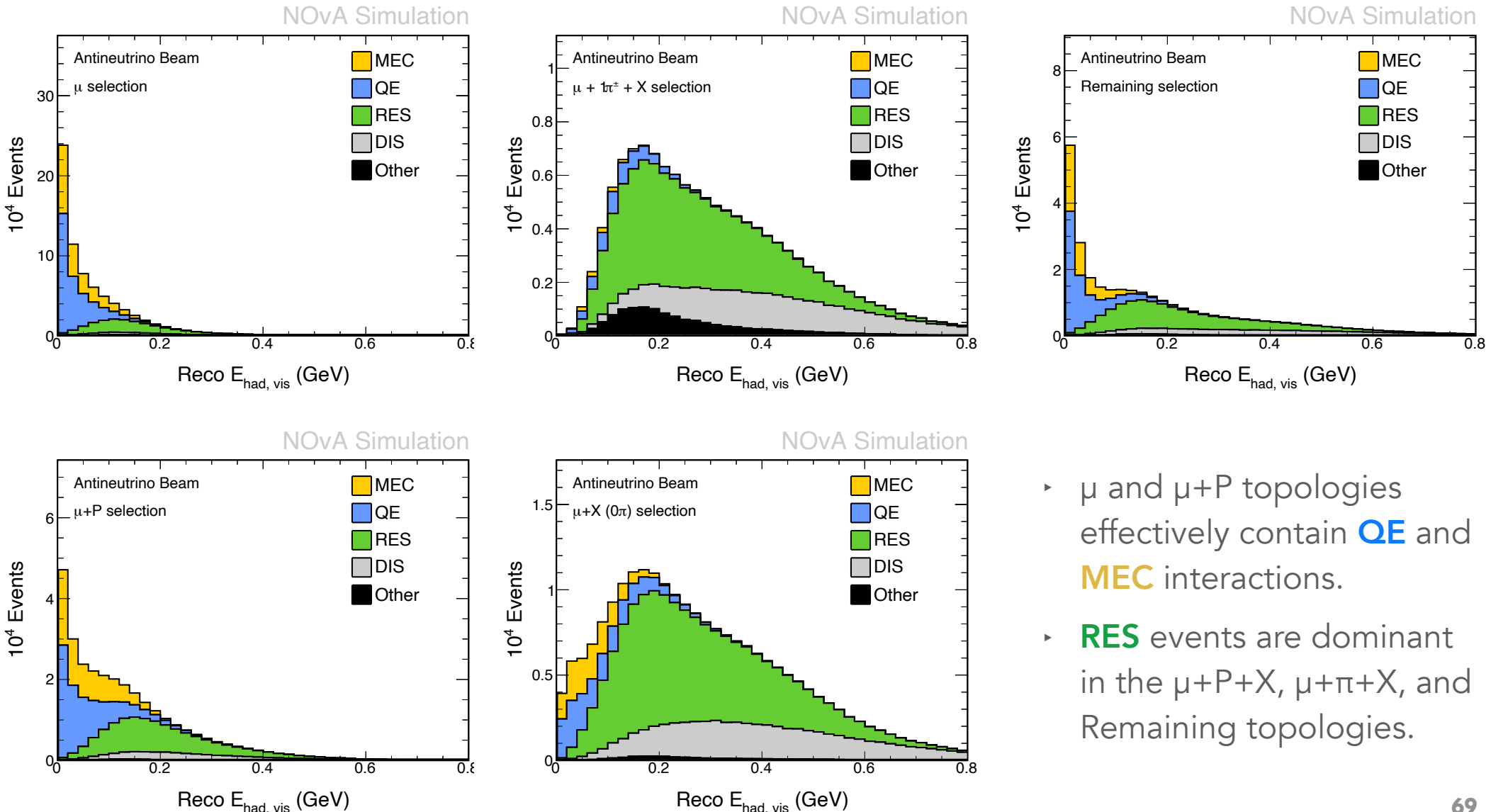
ν mode



- Projection onto $E_{\text{Had Vis}}$ ($\text{Reco } E_{\text{had}}^{\text{vis}}$) broken down by true neutrino interaction.
 - μ and $\mu+P$ topologies effectively contain **QE** and **MEC** interactions.
 - RES** events are dominant in the $\mu+P+X$, $\mu+\pi+X$, and Remaining topologies.

NOvA's ND Topological Samples

$\bar{\nu}$ mode — Hadronic Visible Energy

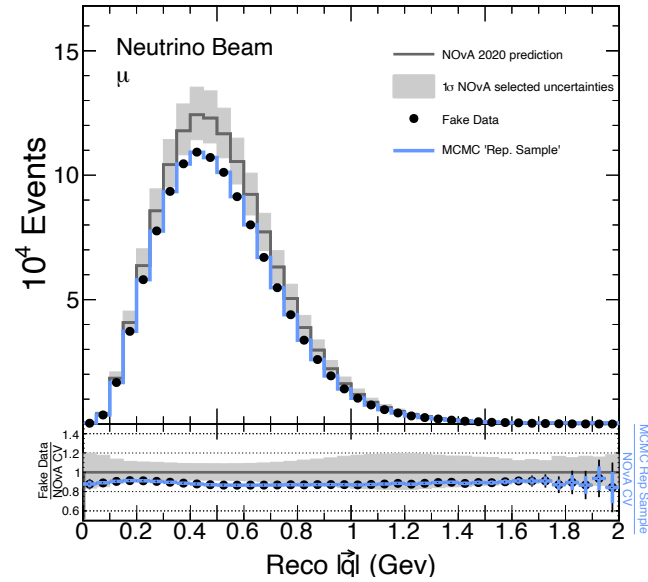


- ▶ μ and $\mu+P$ topologies effectively contain **QE** and **MEC** interactions.
- ▶ **RES** events are dominant in the $\mu+P+X$, $\mu+\pi+X$, and Remaining topologies.

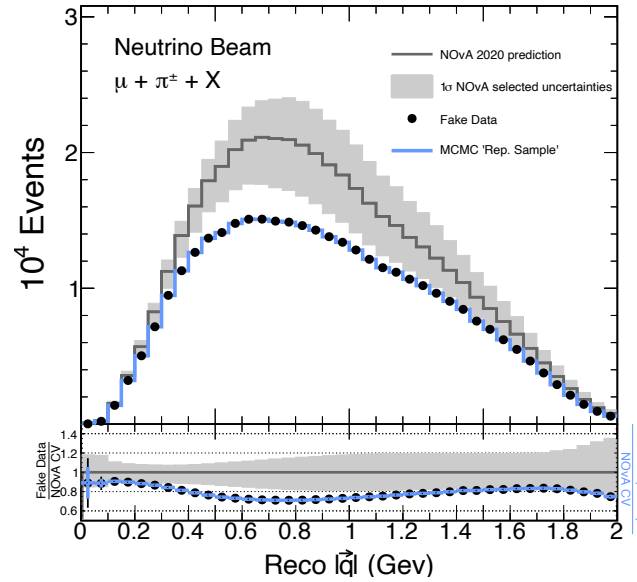
Results of Fake Data Fit

ν mode — Reconstructed $|\vec{q}|$

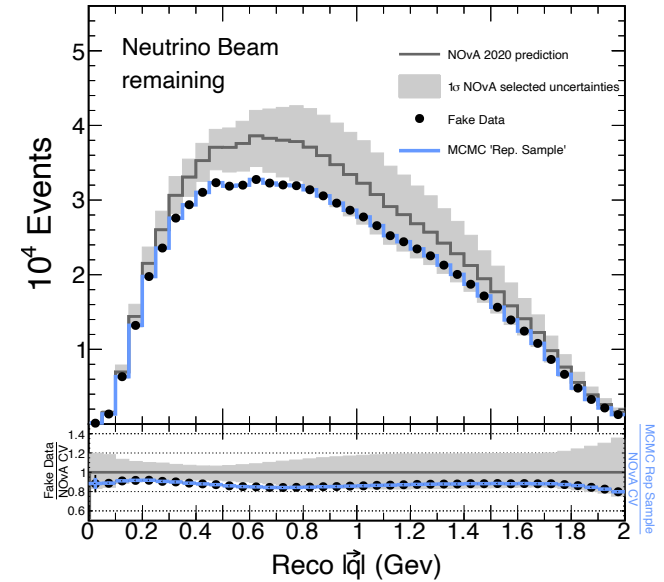
NOvA Fake Data



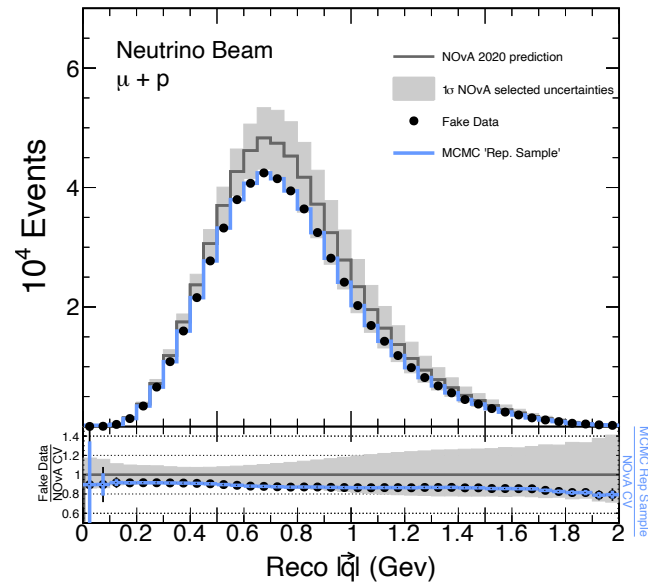
NOvA Fake Data



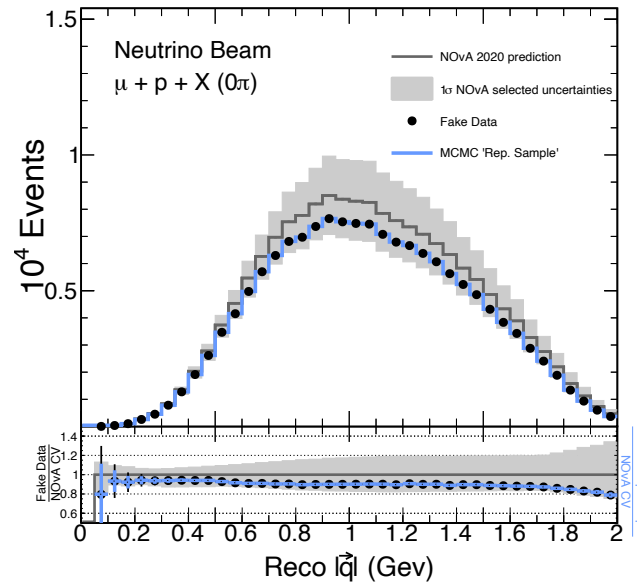
NOvA Fake Data



NOvA Fake Data

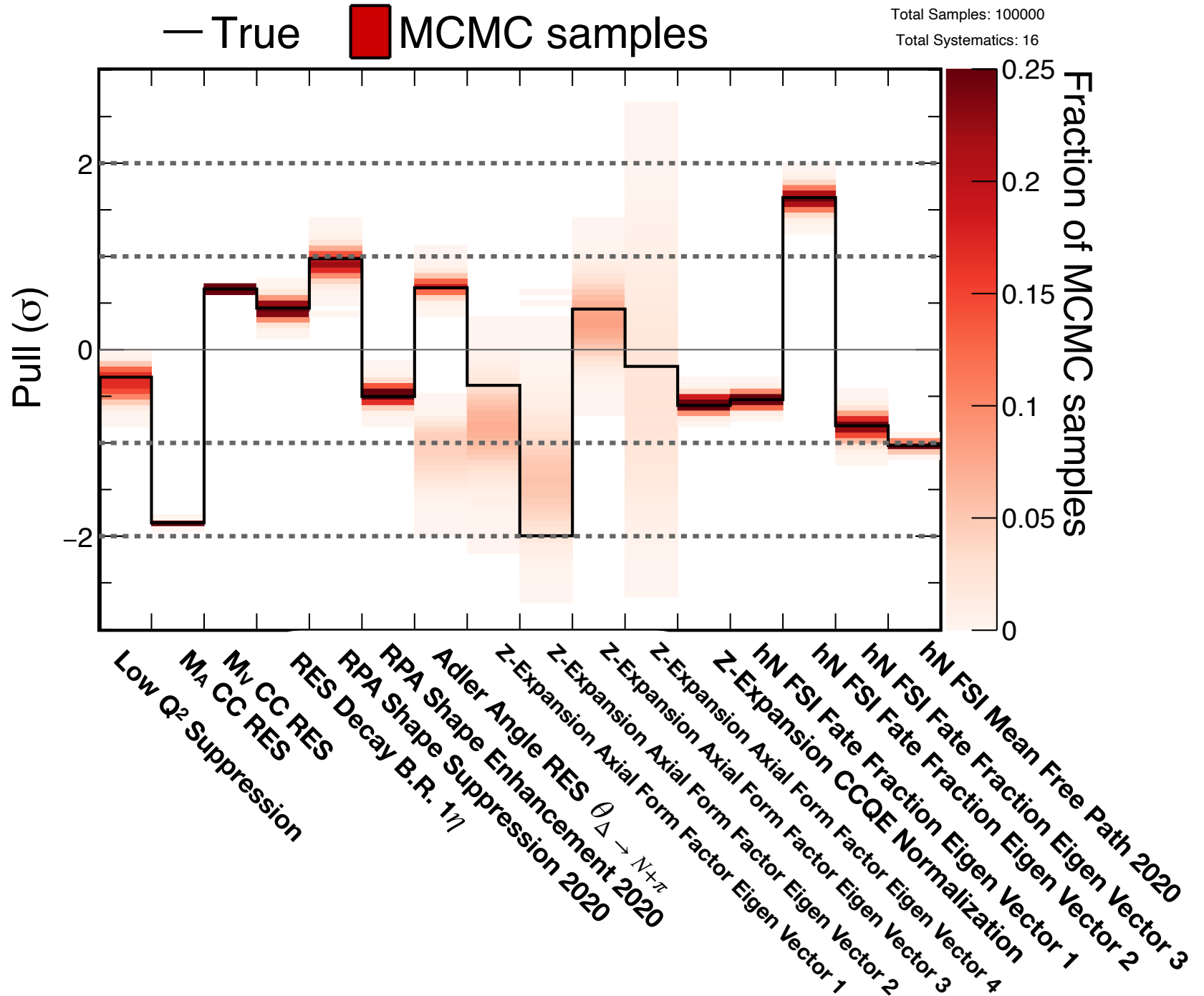


NOvA Fake Data



- ▶ The “Representative Sample” of the ν topologies in reconstructed three-momentum transfer, $Reco |\vec{q}|$.
- ▶ “Rep. Sample” perfectly agrees with the fake data.
- ▶ The grey band represents the 1 σ error of the 16 parameters used in the fit.

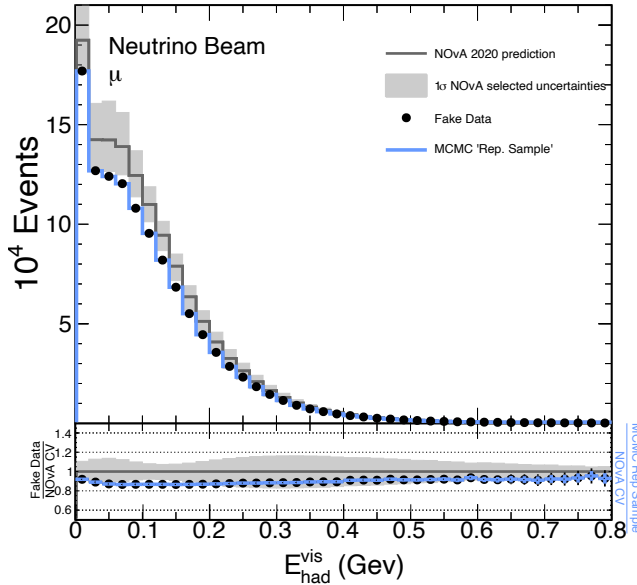
Fake Data Fit



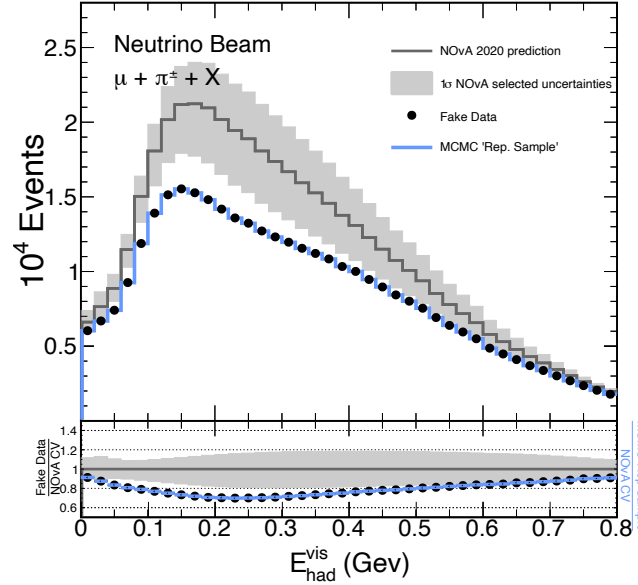
Results of Fake Data Fit

ν mode — Hadronic Visible Energy

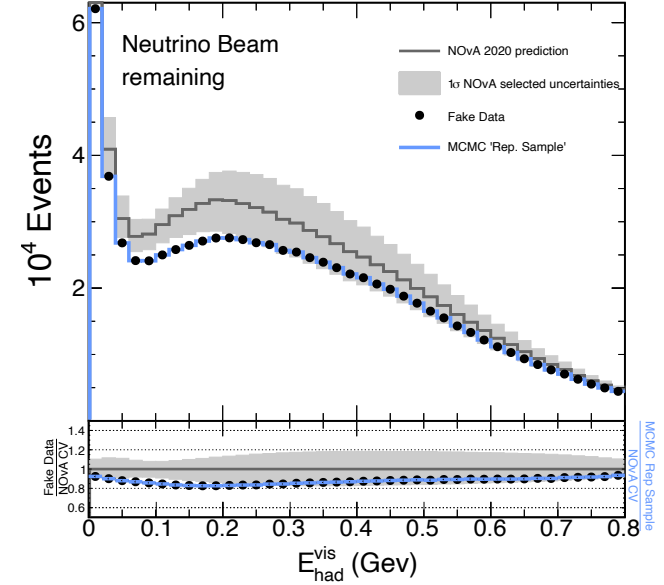
NOvA Fake Data



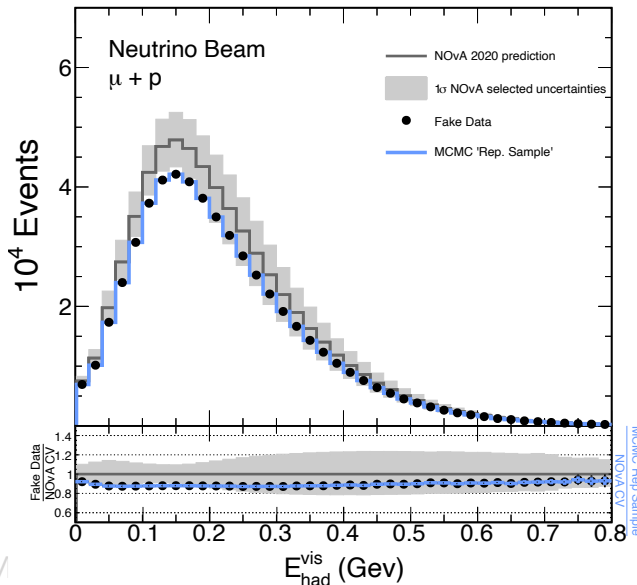
NOvA Fake Data



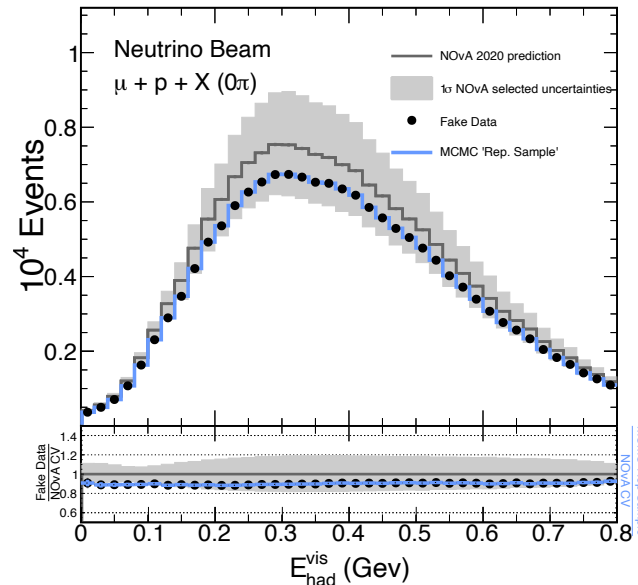
NOvA Fake Data



NOvA Fake Data

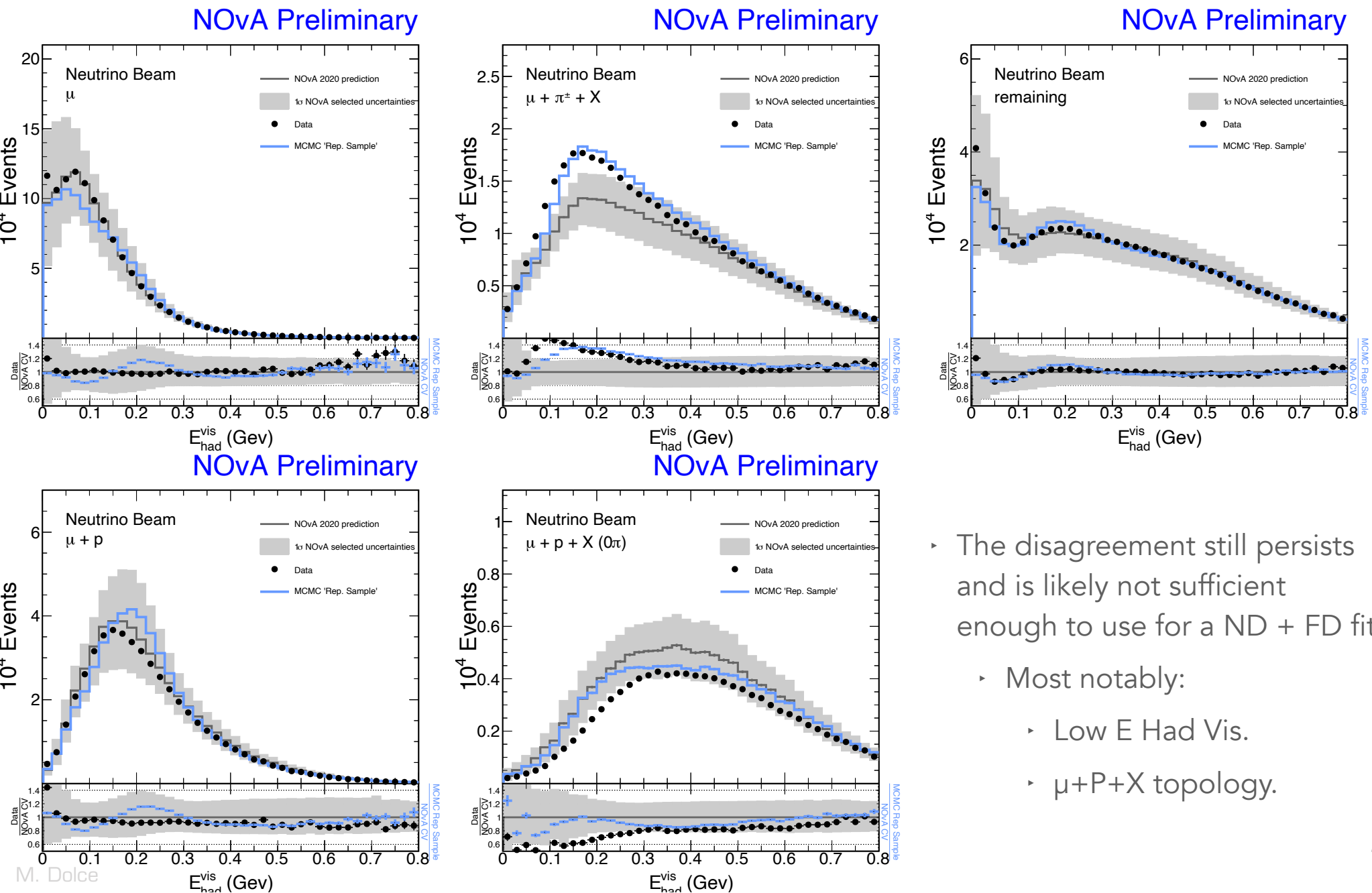


NOvA Fake Data



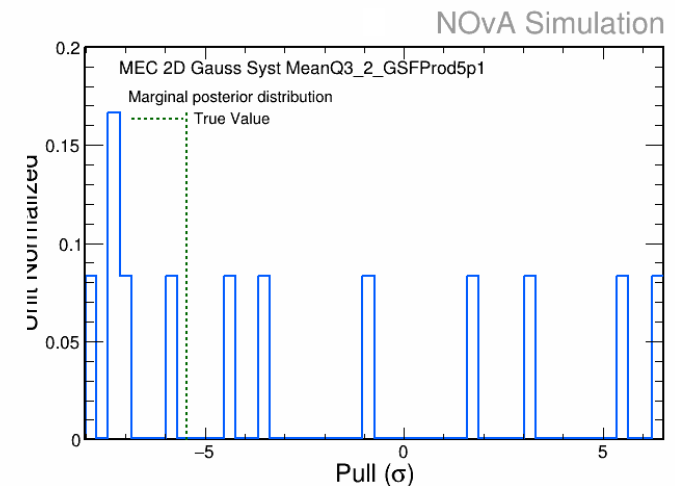
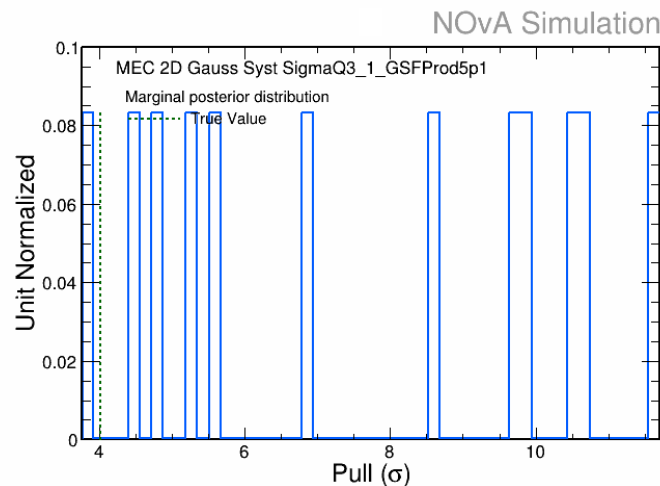
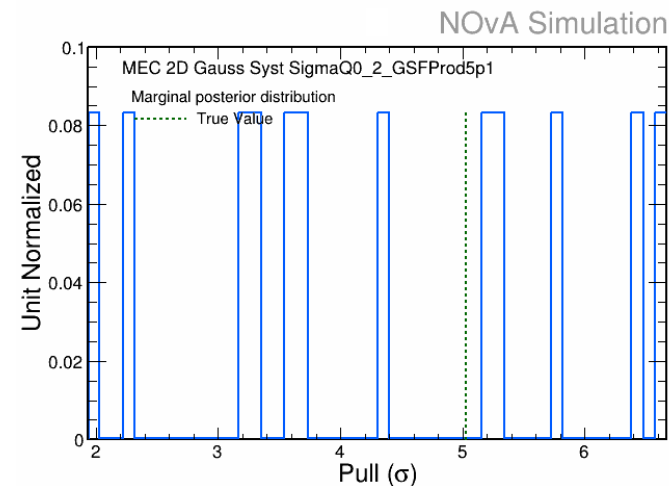
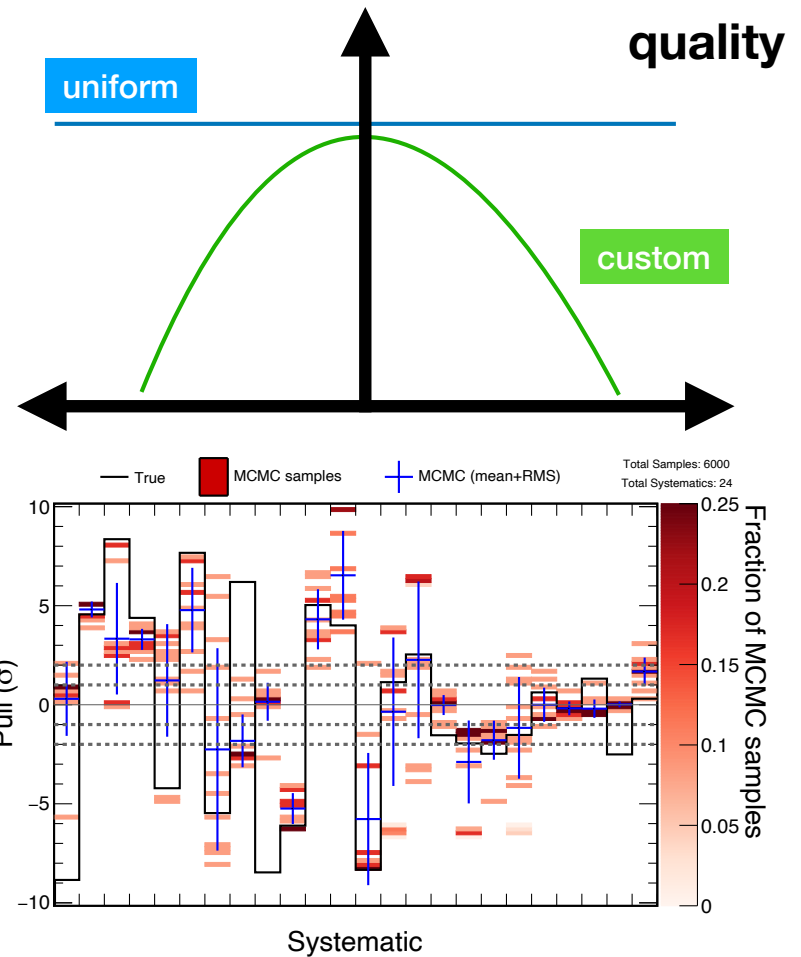
- ▶ The “Representative Sample” of the ν topologies in hadronic visible energy, E_{had}^{vis} .
- ▶ “Rep. Sample” perfectly agrees with the fake data.
- ▶ The grey band represents the 1σ error of the 16 parameters used in the fit.

Poor agreement in ND data fit



Uniform Priors

- Implemented option to specify the prior for a given systematic.
- Added uniform prior as an option.
- Tested with a fake data fit to:
 - MEC Double Gaussian parameters — Uniform priors.
 - CCQE parameters — “Custom” priors.
- This further slowed our fitting, unsurprisingly.
 - Unrestricted pull values requires much more sampling.
 - Option has been aborted. **✗**

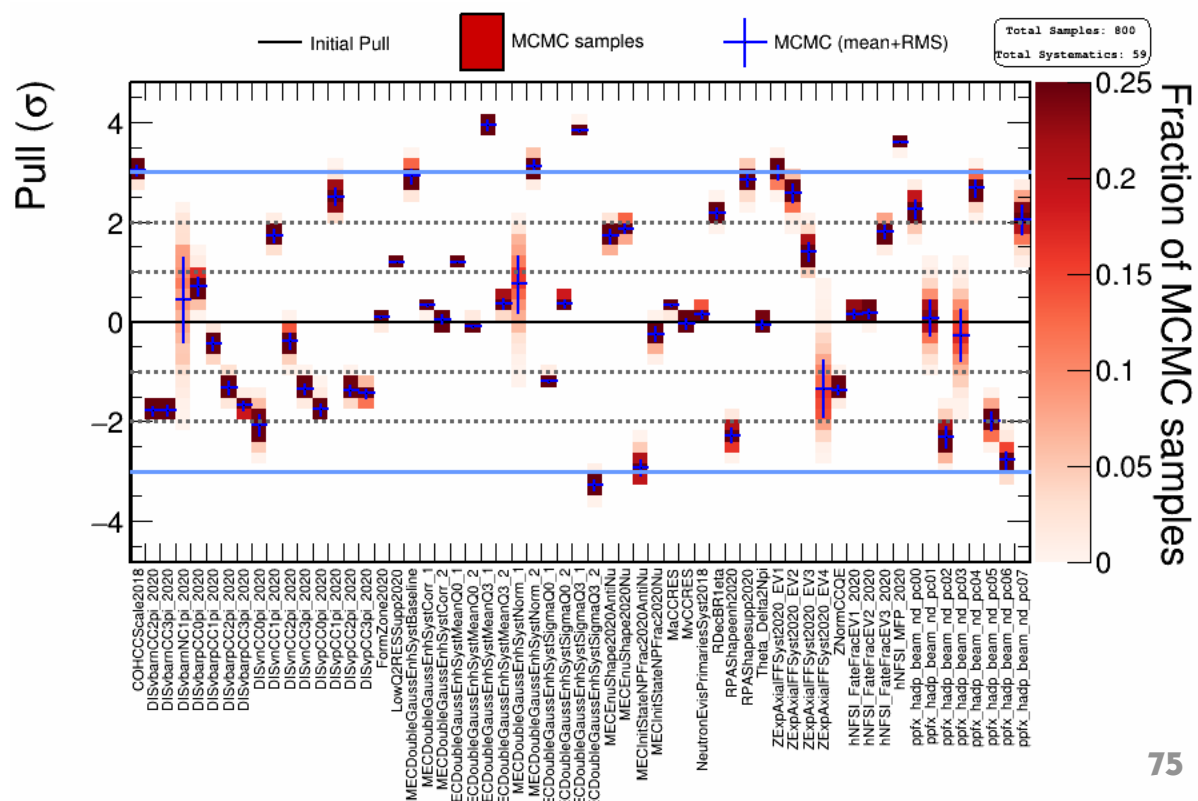
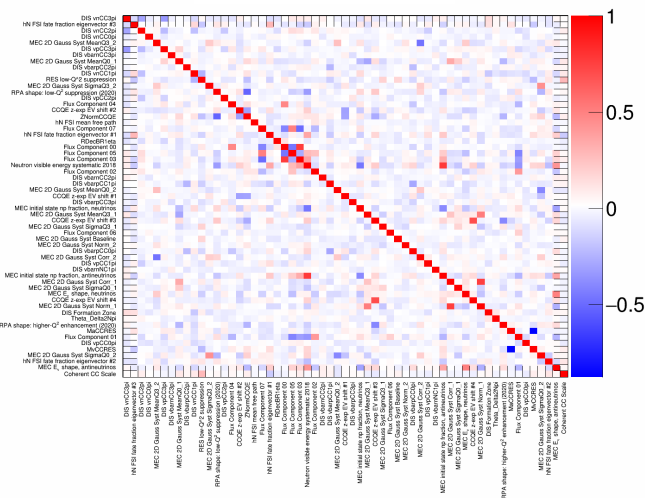


Covariance matrix input

quantity

- Feed in covariance matrix of parameters to **replace warmup phase**.
 - MCMC effectively does this with its warmup phase.
 - Can save CPU time by providing the matrix of correlations (obtained from a previous fit).
- Likely slower because a **dense** mass matrix is required.
- Did not yield optimal results.
 - The matrix can be read by Stan, but the fitting is even slower...
 - an open question, unresolved. **✗**

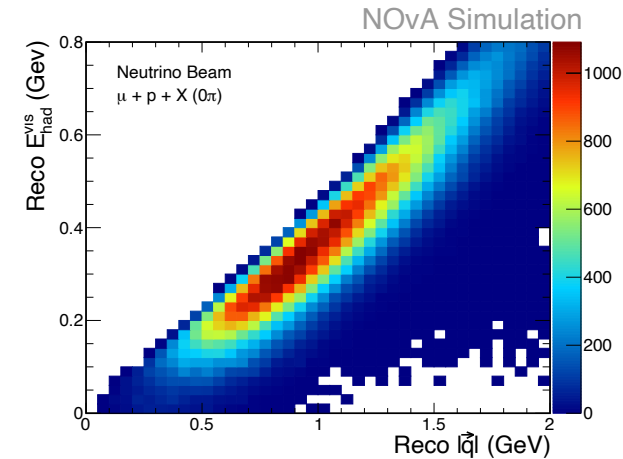
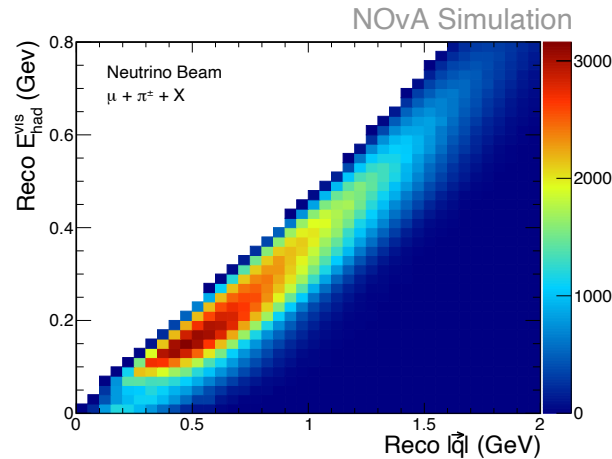
Correlation Matrix



Technical Improvements

quantity

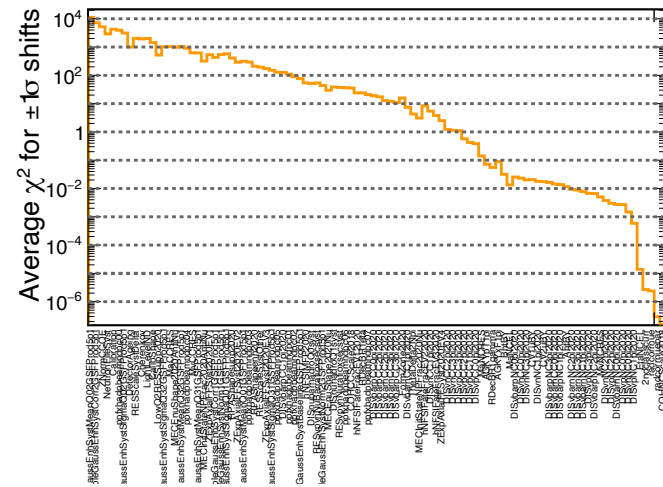
- Stan calculates Hamilton's equations for bins that are empty — wasteful.
 - In all samples there are many empty bins.
- MCMC now skips the calculations for empty bins.
 - ~ 30-40% faster.
 - But still not at the level where we want.



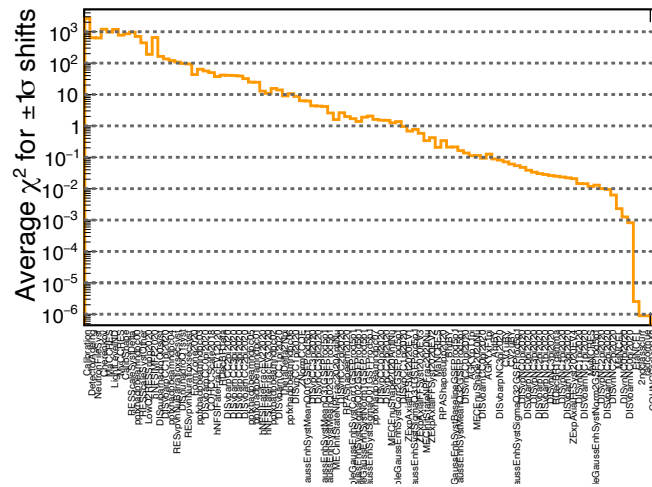
- 160 bins of a 2-D topological distribution (40 bins in $E_{had,vis}$, 40 bins in $|\vec{q}| Reco$).
- 10 topologies of neutrino interactions (5 FHC, 5 RHC).
- ≈ 100 of NOvA's systematic parameters to fit with MCMC.
- 5 “knots” in a cubic “spline” of a NOvASoft's PredInterp object, which attempts to interpolate in between these knots.

Ranking the physics model uncertainties

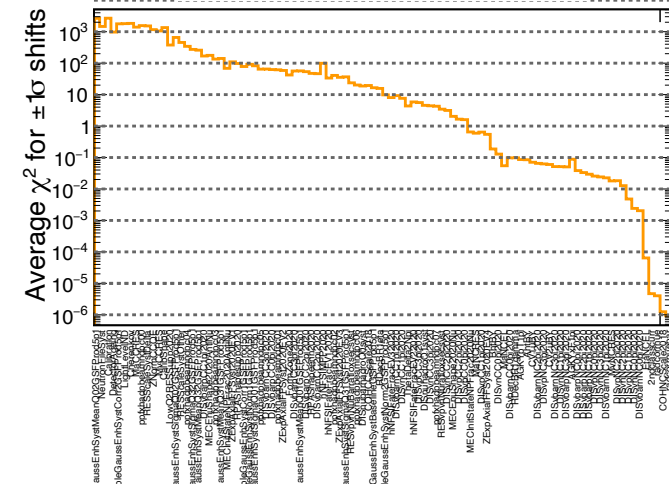
RHC ND μ Topology



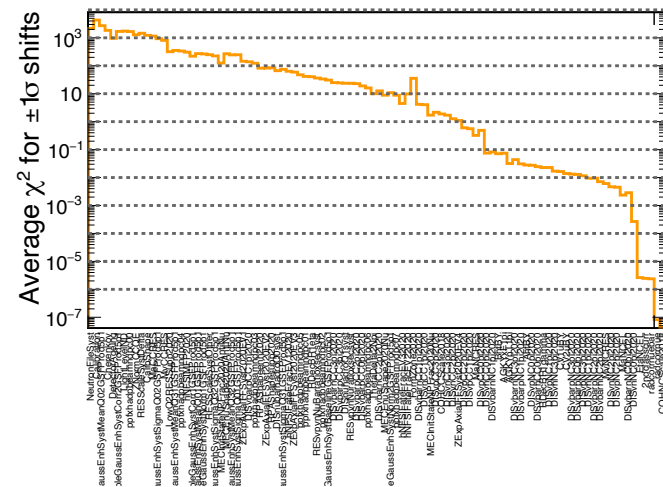
RHC ND $\mu + \pi^+ + X$ Topology



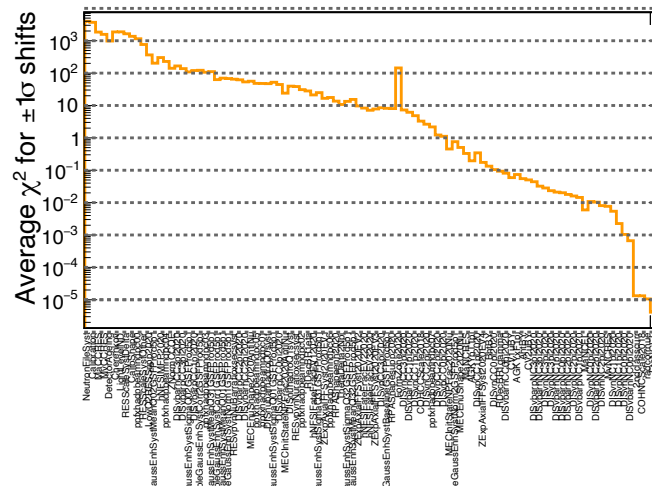
RHC ND Remaining Topology



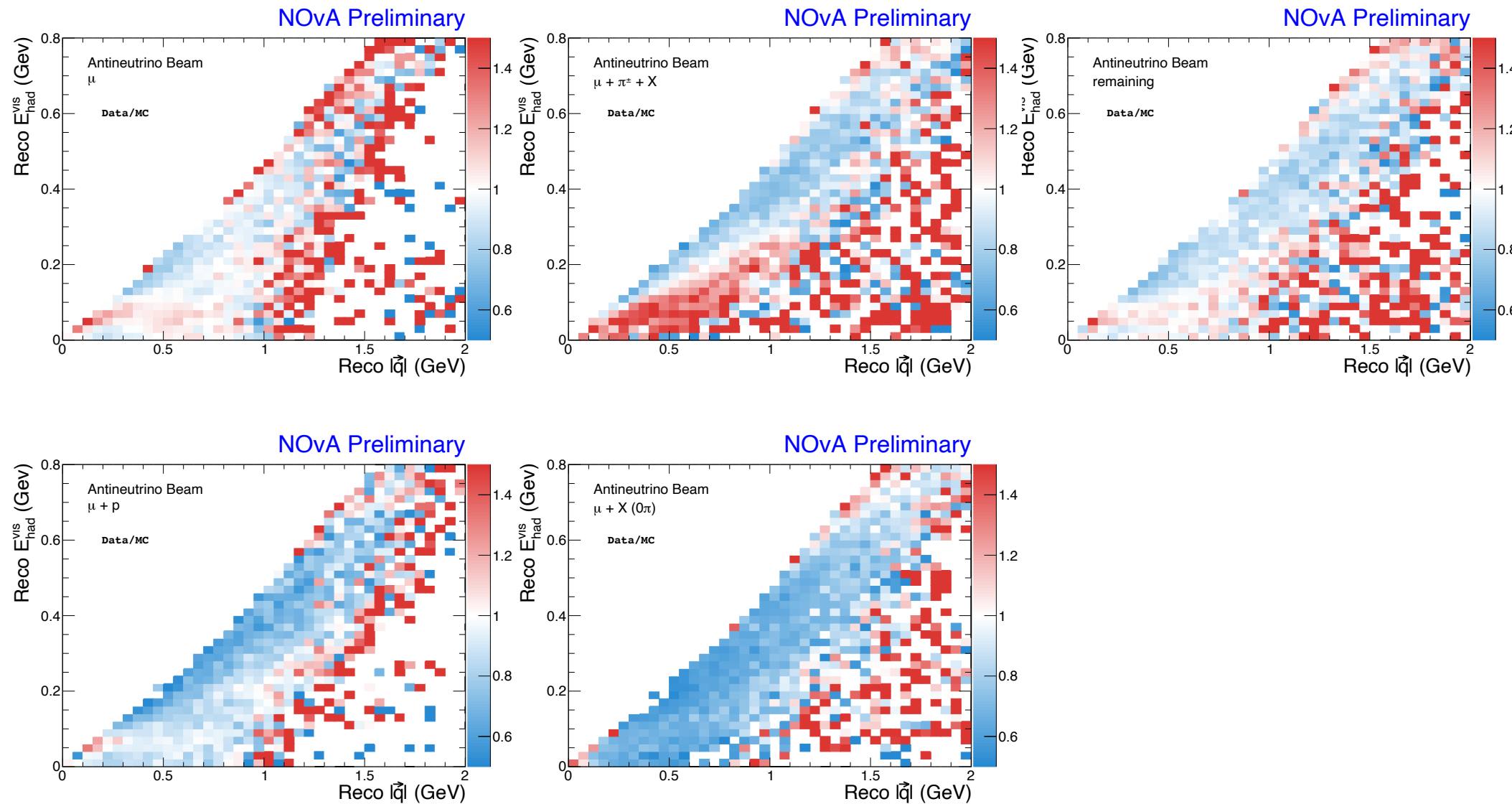
RHC ND $\mu + p$ Topology



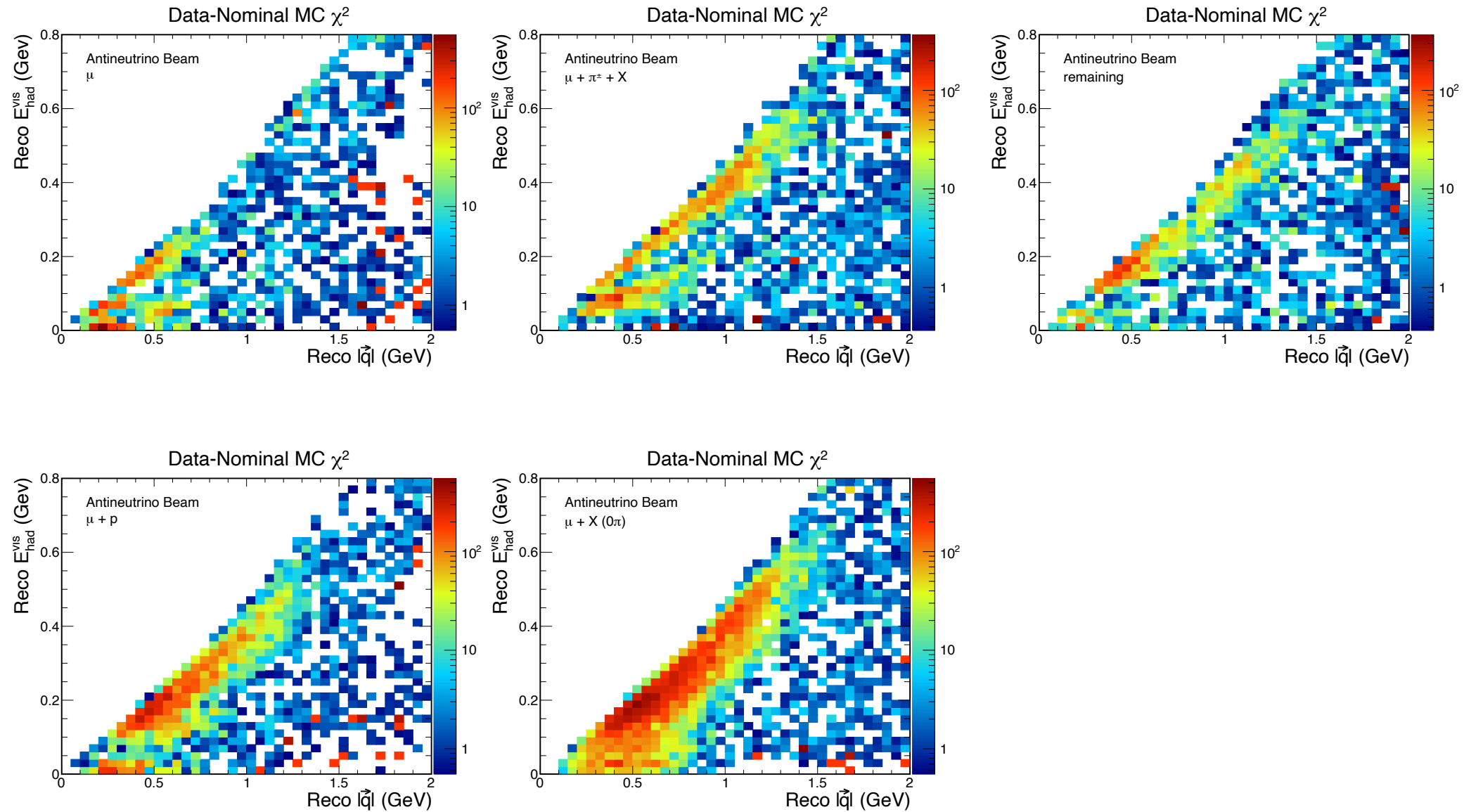
RHC ND $\mu + X$ (0π) Topology



Breaking down the topologies

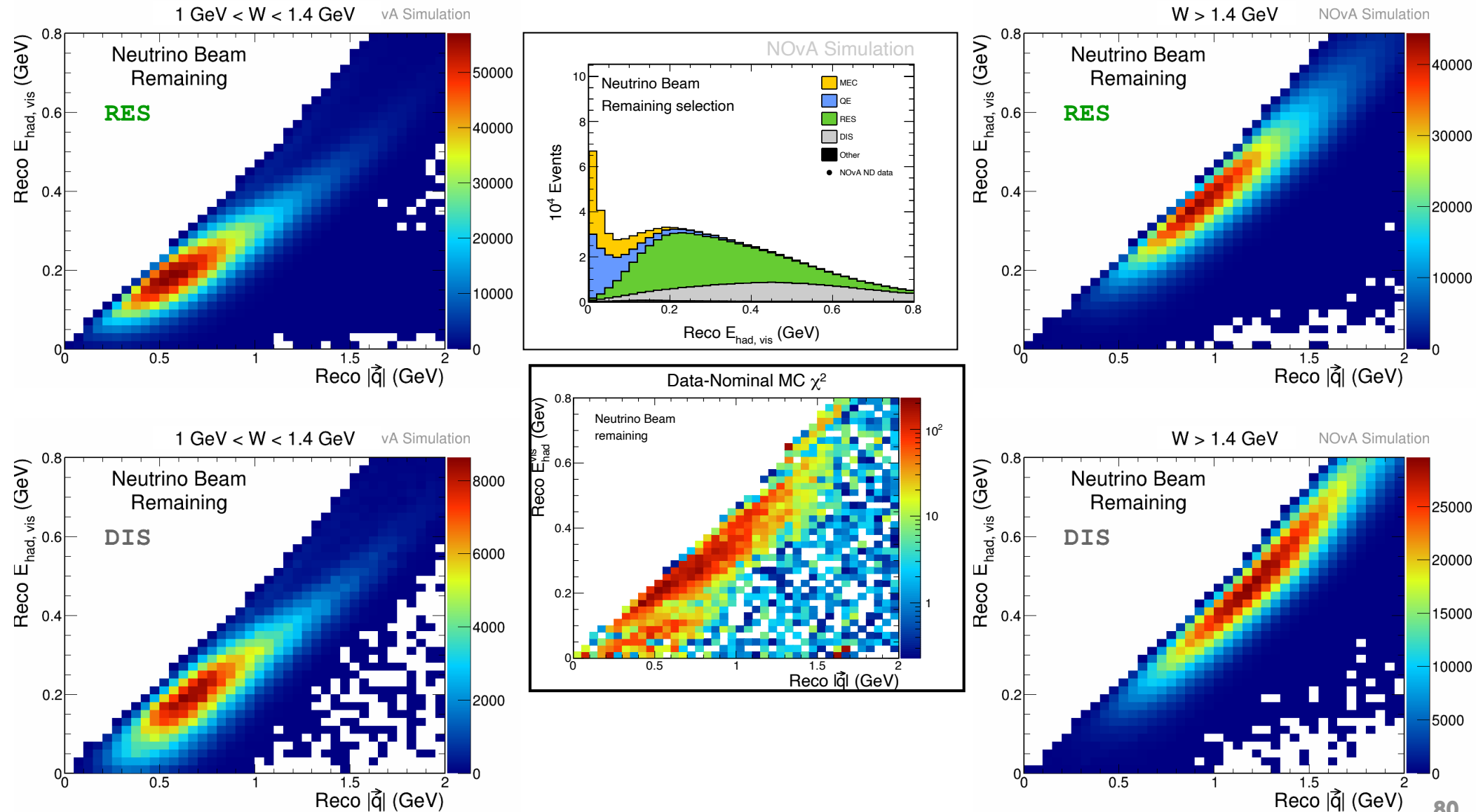


Breaking down the topologies



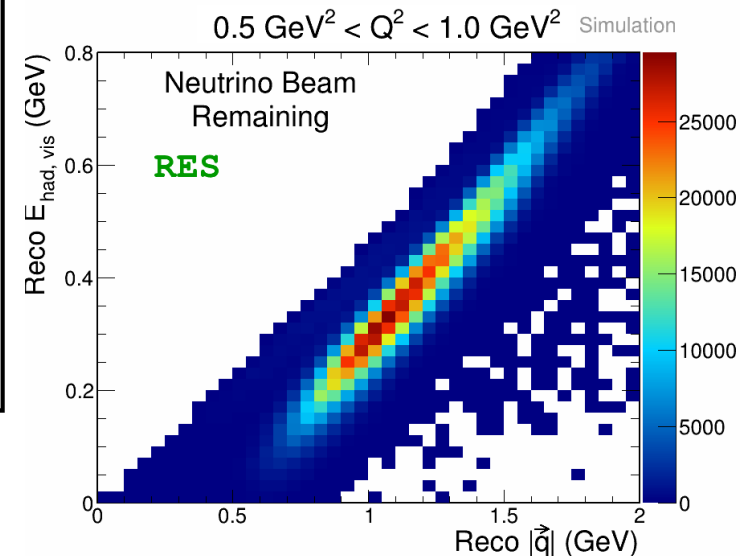
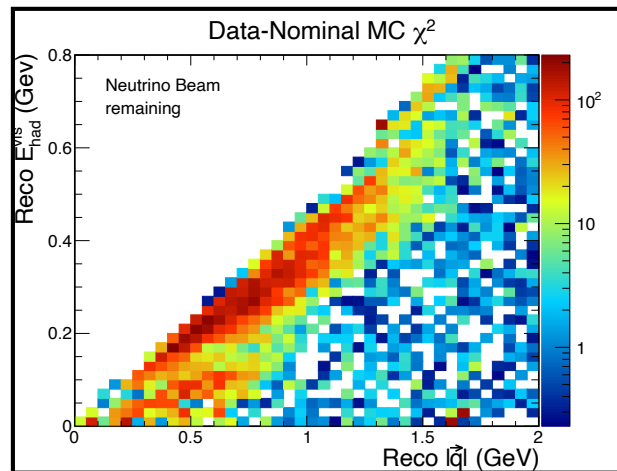
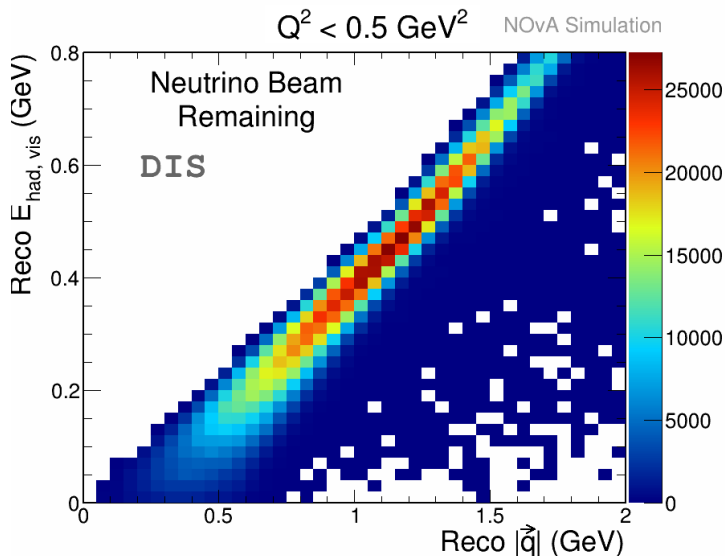
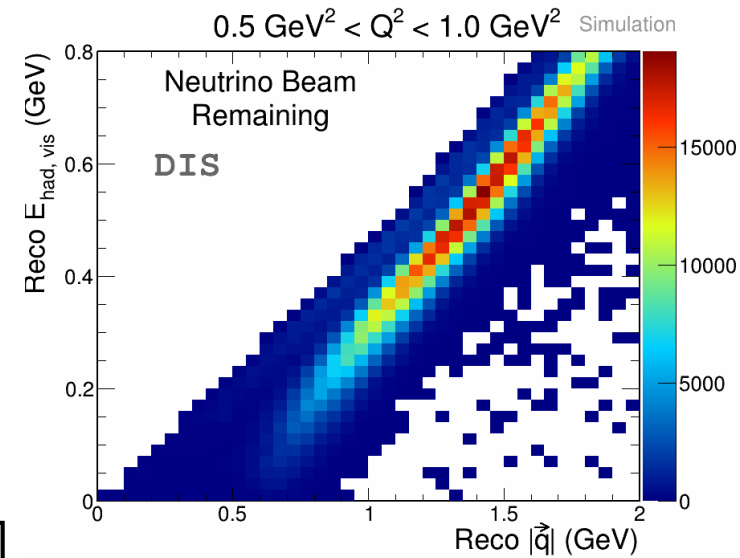
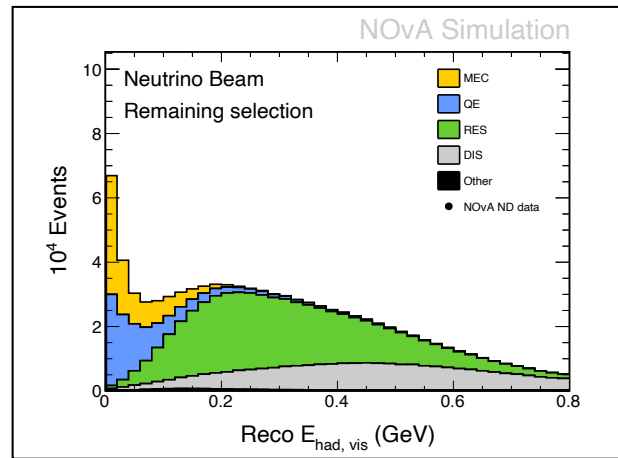
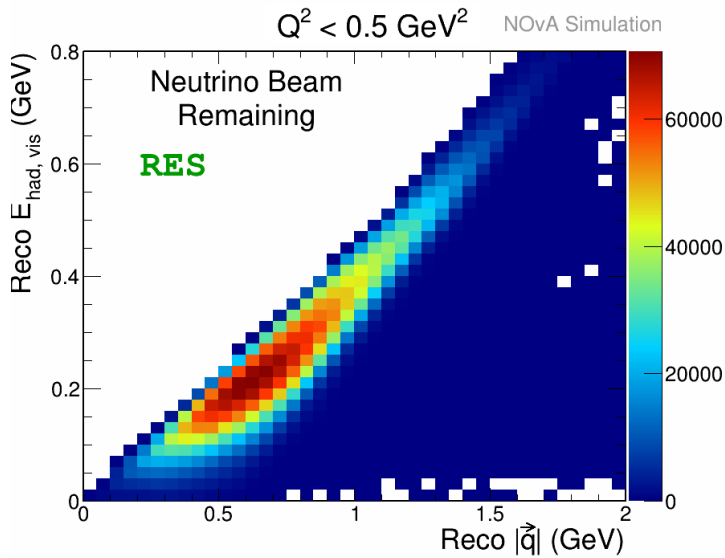
Breaking down the topologies

- (~0.75 GeV, ~0.4 GeV) is the problematic region.



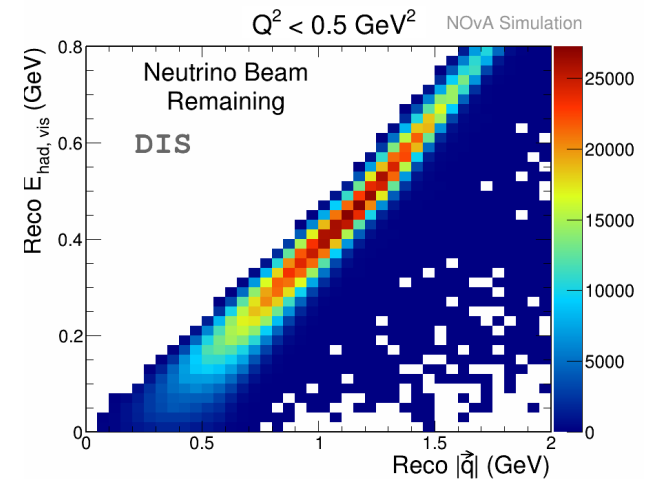
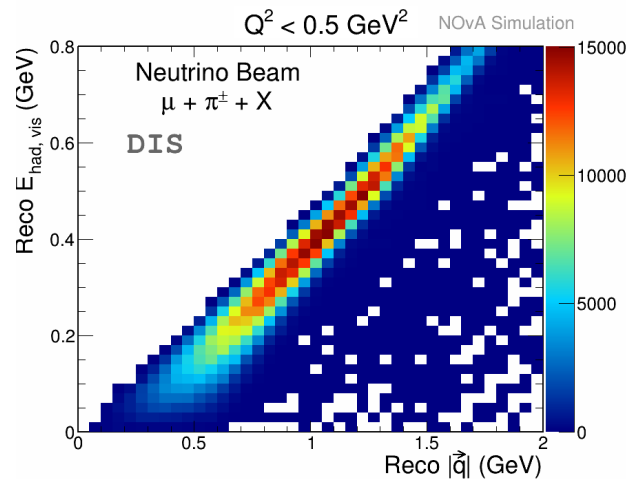
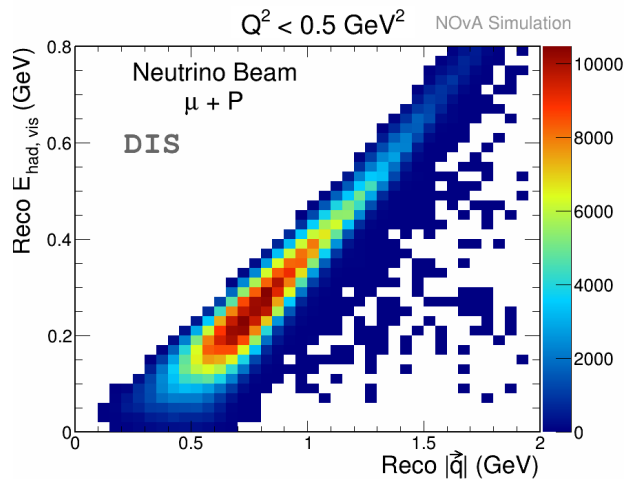
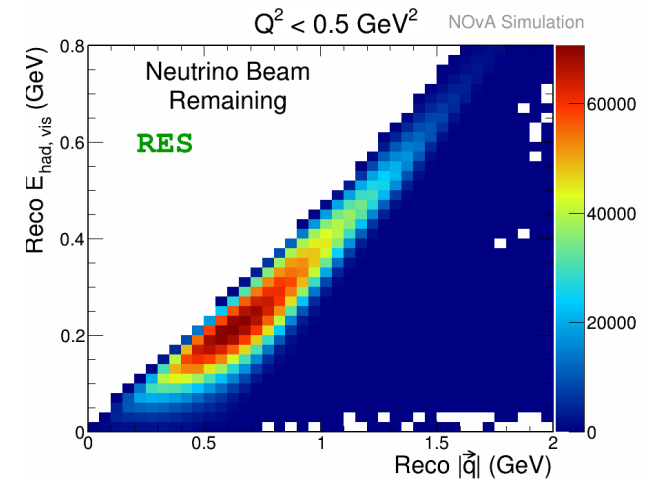
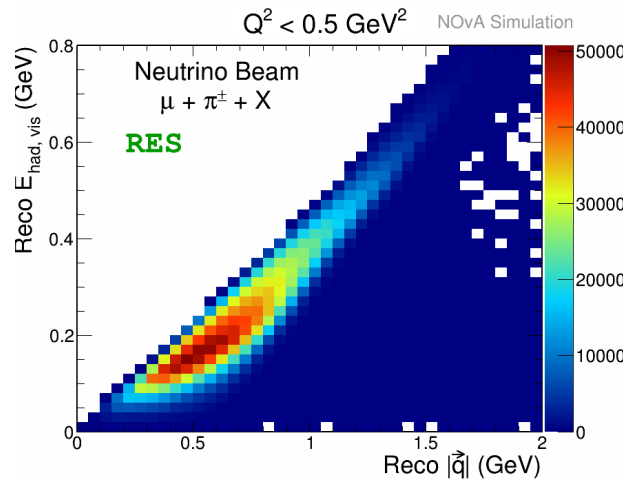
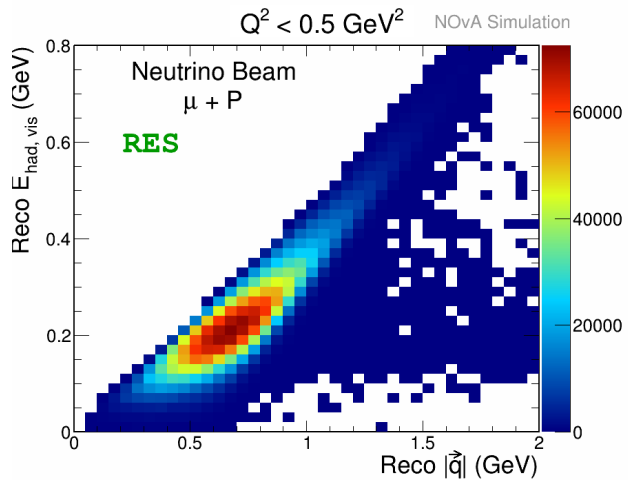
Breaking down the topologies

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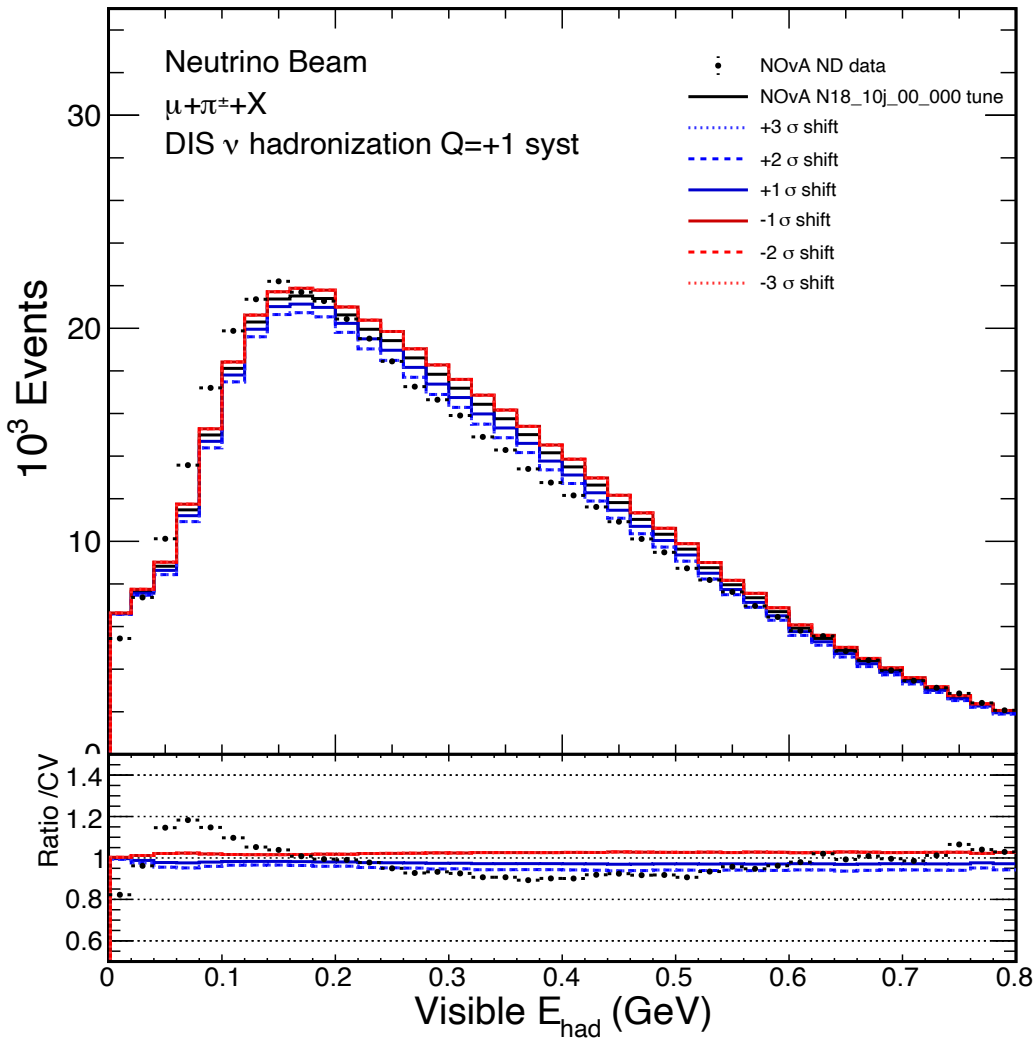
Breaking down the topologies

- (~ 0.75 GeV, ~ 0.4 GeV) is the problematic region.

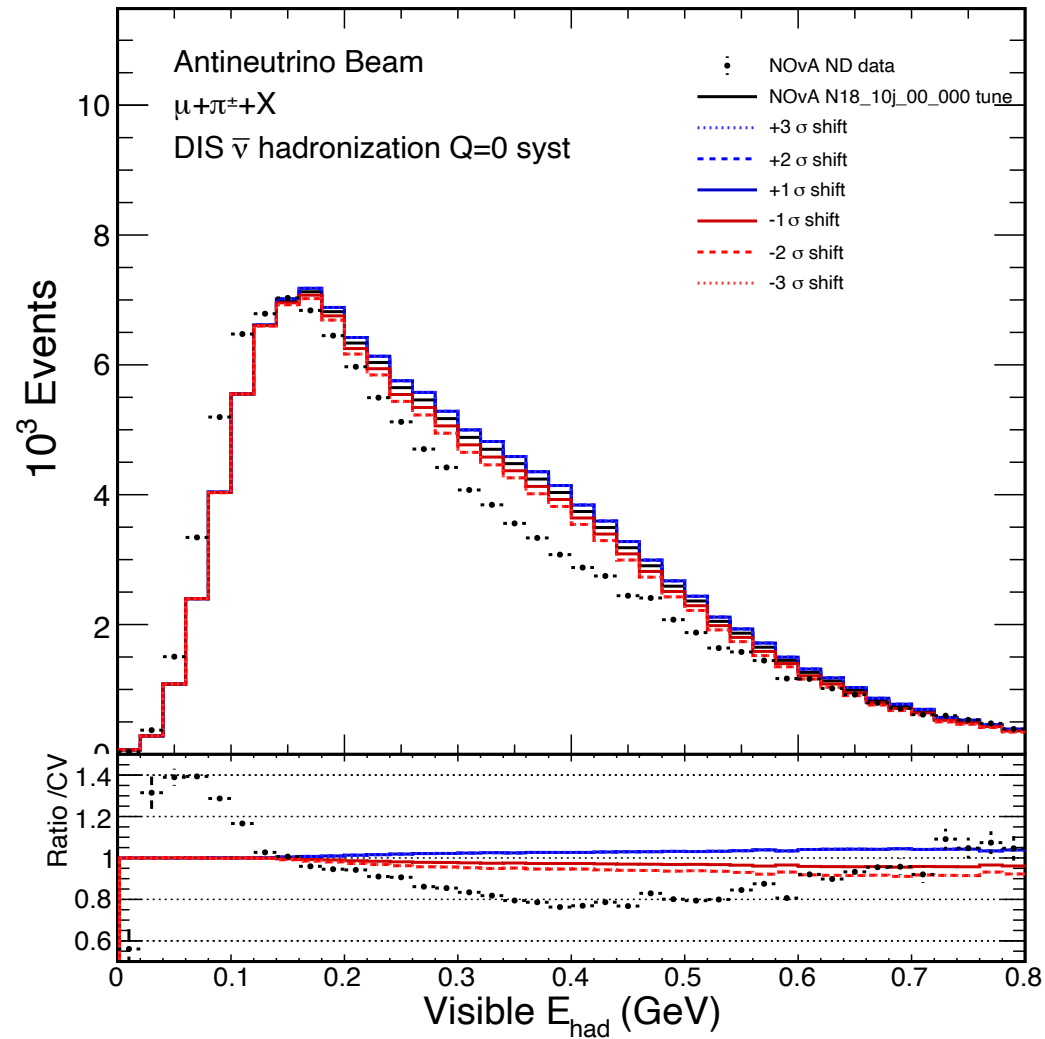


DIS hadron final states ^{quality}

NOvA preliminary



NOvA preliminary



A new RES systematic quality

Δ decays....

+3 σ shift....

$$\nu + p \rightarrow \mu^- + \Delta^{++}$$

$$\Delta^{++} \rightarrow p + \pi^+$$



more events in MuPiEtc
(and possibly MuPr)

- Adjust the relative $\nu p / \nu n$ RES cross section.

$$\nu + n \rightarrow \mu^- + \Delta^+$$

$$\Delta^+ \rightarrow \pi^+ + n$$

$$\Delta^+ \rightarrow \pi^0 + p$$



less events in MuPiEtc



less events in MuPrEtc
and less MuPr

- Added flexibility in the final states $\rightarrow$ topology.

$$\bar{\nu} + p \rightarrow \mu^+ + \Delta^0$$

$$\Delta^0 \rightarrow \pi^0 + n$$

$$\Delta^0 \rightarrow \pi^- + p$$



less events in MuPrEtc



more events in MuPiEtc

$$\bar{\nu} + n \rightarrow \mu^+ + \Delta^-$$

$$\Delta^- \rightarrow n + \pi^-$$

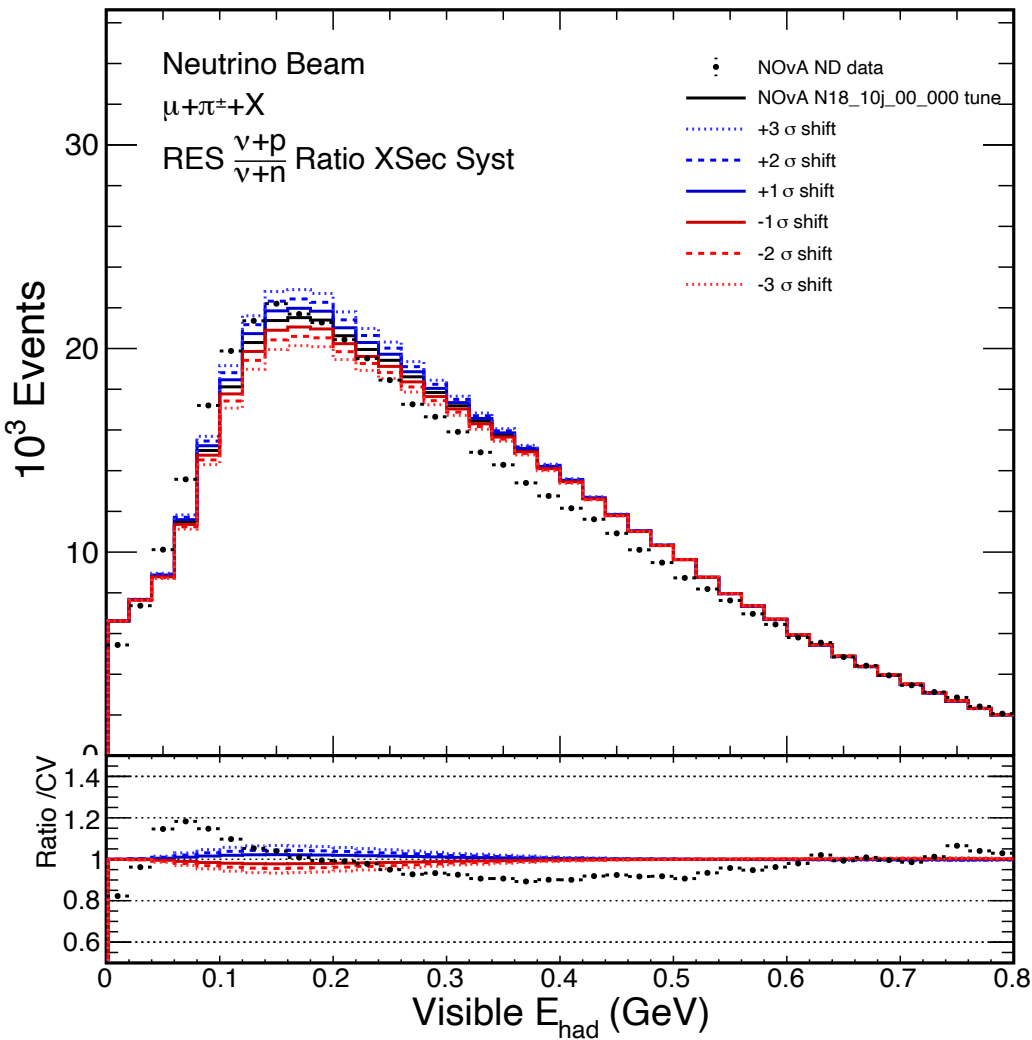


less events in MuPrEtc

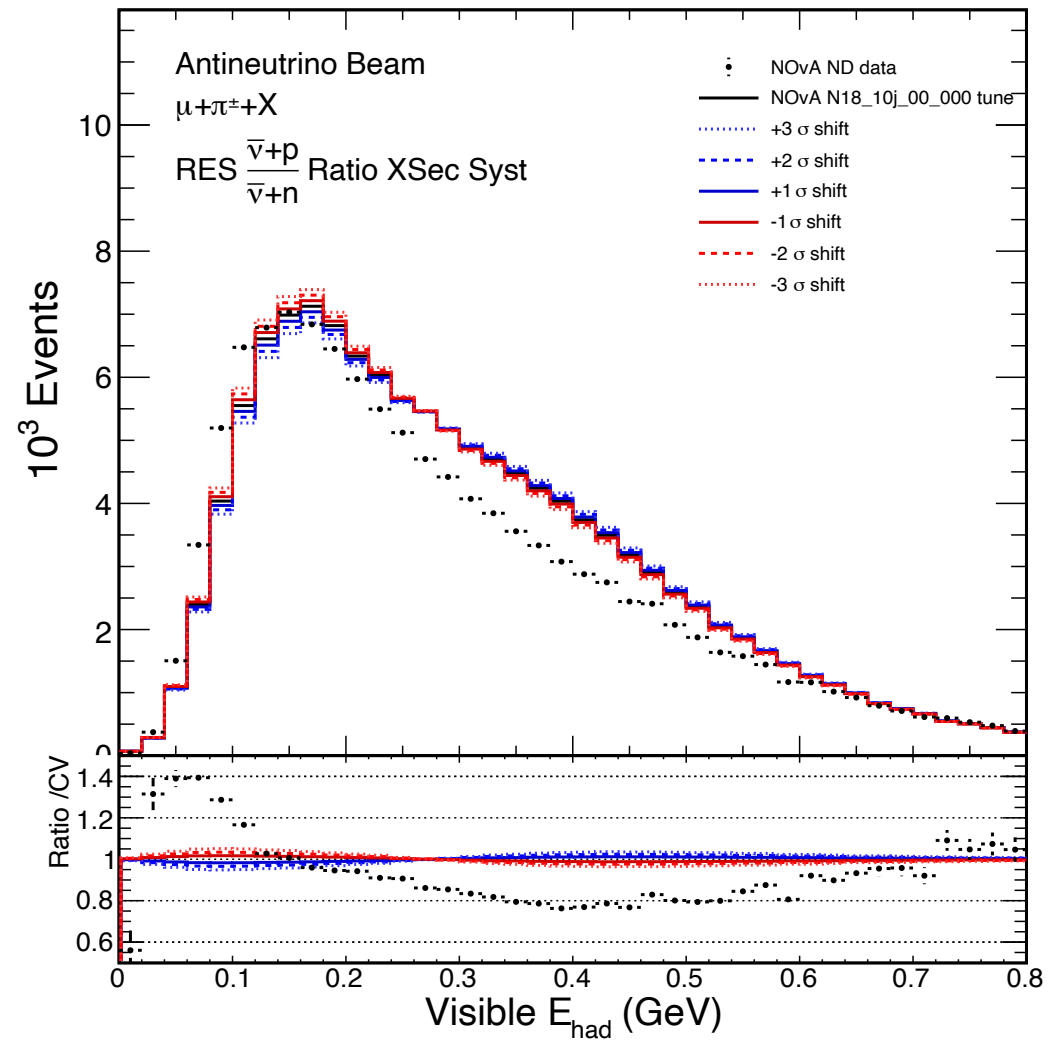
RES $\nu p / \nu n$ scaling

quality

NOvA preliminary



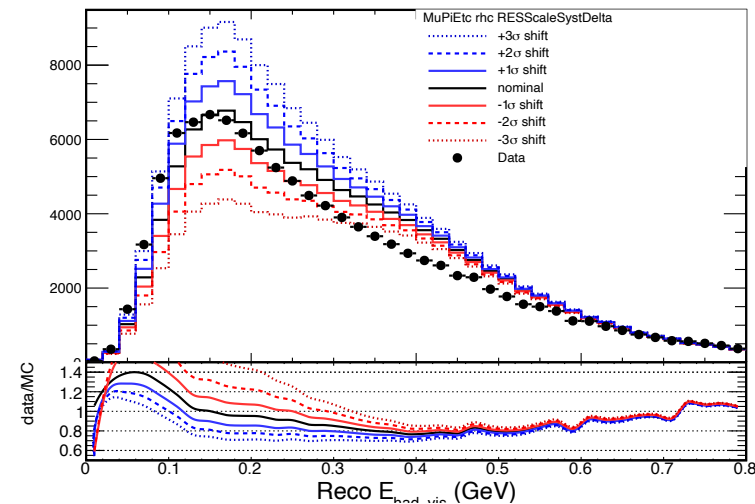
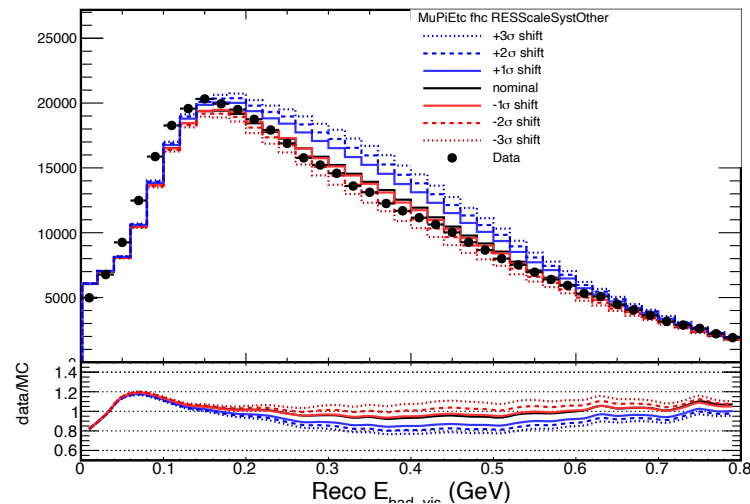
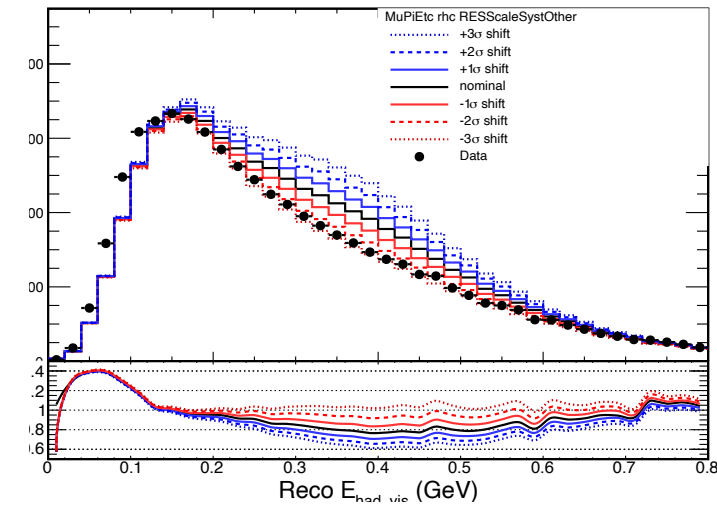
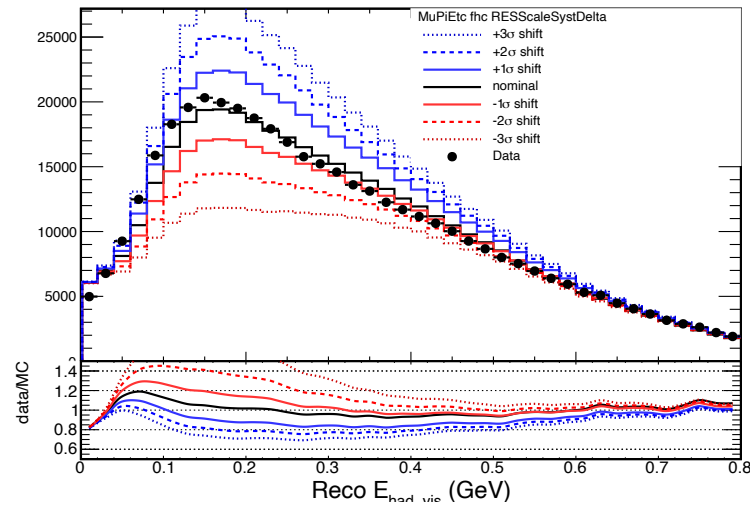
NOvA preliminary



RES Scale

quality

- Added a 20% uncertainty at 1σ on the Δ resonance and higher resonances ($W > 1.4$ GeV).
- This is the largest uncertainty we have introduced.



Complete list of systematics

CalibShape
Calibration
Cherenkov
DetectorAgeing
Light_Level_ND

Detector

NeutronEvisPrimariesSyst2018

Neutron

DIS_nu_hadro_Q1_syst
DIS_nubar_hadro_Q0_syst
DISvbarnCC3pi_2020
DISvbarpCC1pi_2020
DISvbarpCC3pi_2020
DISvnCC1pi_2020
DISvnCC2pi_2020
DISvnCC3pi_2020
DISvpCC0pi_2020
DISvpCC2pi_2020
DISvpCC3pi_2020
FormZone2020

DIS

LowQ2RESSupp2020
Theta_Delta2Npi
MaCCRES
MvCCRES
RESDeltaScaleSyst
RESOtherScaleSyst
RES_vpvN_NuBar_ratio_xsec_syst
RES_vpvN_Nu_ratio_xsec_syst

RES

RPAShapeenh2020
RPAShapessupp2020
ZExpAxialFFSyst2020_EV1
ZExpAxialFFSyst2020_EV2
ZExpAxialFFSyst2020_EV3
ZNormCCQE

QE

hNFSI_FateFracEV1_2020
hNFSI_MFP_2020

FSI

- We have removed the MEC DG MeanQ0_2, MEC DG Norm_2, and MEC DG Corr_2 systematic — despite their large χ^2 contribution — they are on the edge of phase space.

MECDoubleGaussEnhSystBaseline_GSFProd5p1
MECDoubleGaussEnhSystCorr_1_GSFProd5p1
MECDoubleGaussEnhSystMeanQ0_1_GSFProd5p1
MECDoubleGaussEnhSystMeanQ3_1_GSFProd5p1
MECDoubleGaussEnhSystMeanQ3_2_GSFProd5p1
MECDoubleGaussEnhSystNorm_1_GSFProd5p1
MECDoubleGaussEnhSystSigmaQ0_1_GSFProd5p1
MECDoubleGaussEnhSystSigmaQ0_2_GSFProd5p1
MECDoubleGaussEnhSystSigmaQ3_1_GSFProd5p1
MECDoubleGaussEnhSystSigmaQ3_2_GSFProd5p1
MECEnuShape2020AntiNu
MECEnuShape2020Nu
MECInitStateNPfrac2020AntiNu -
MECInitStateNPfrac2020Nu -

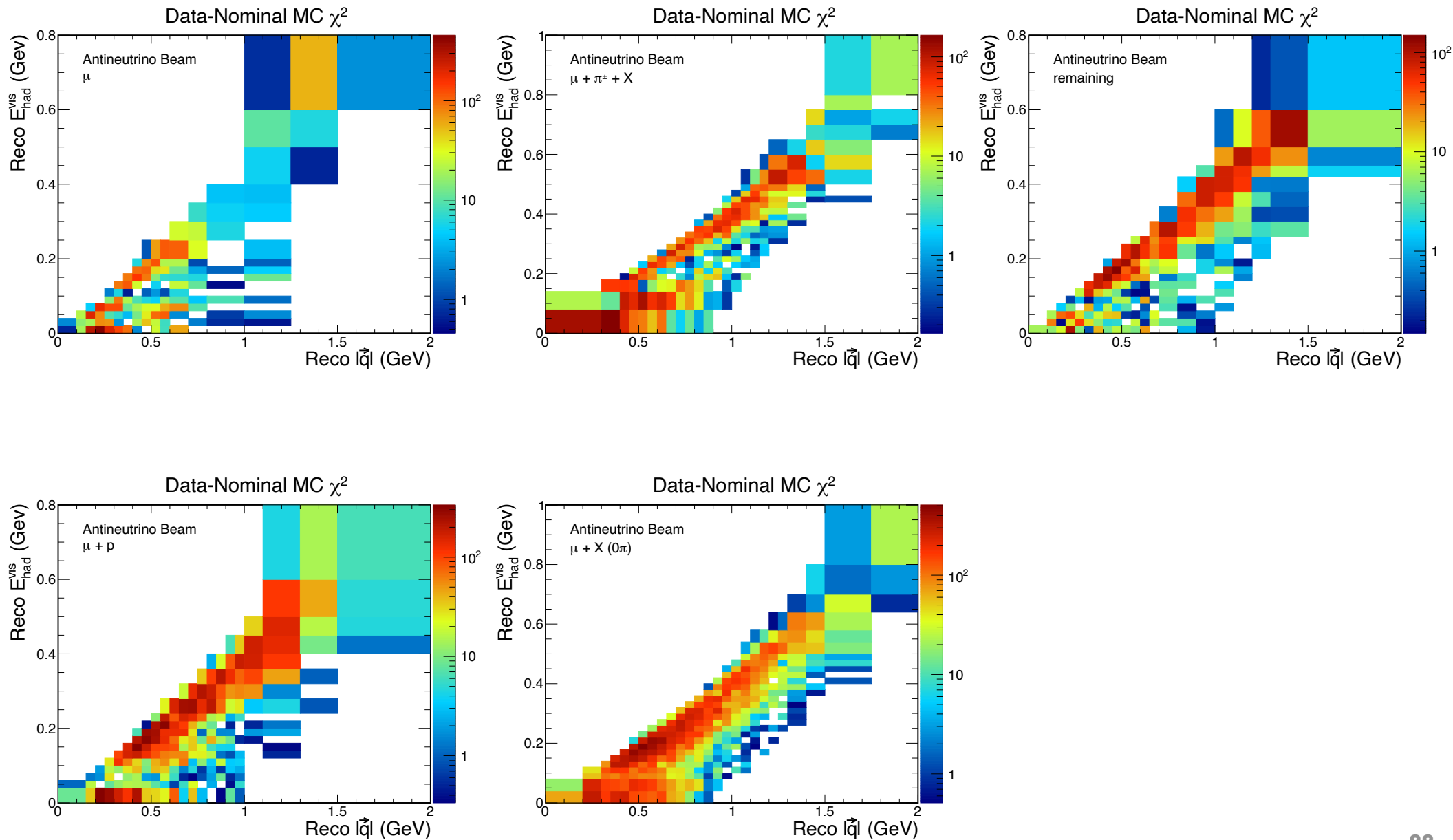
MEC

ppfx_hadp_beam_nd_pc00
ppfx_hadp_beam_nd_pc01
ppfx_hadp_beam_nd_pc02
ppfx_hadp_beam_nd_pc03
ppfx_hadp_beam_nd_pc04
ppfx_hadp_beam_nd_pc05
ppfx_hadp_beam_nd_pc07

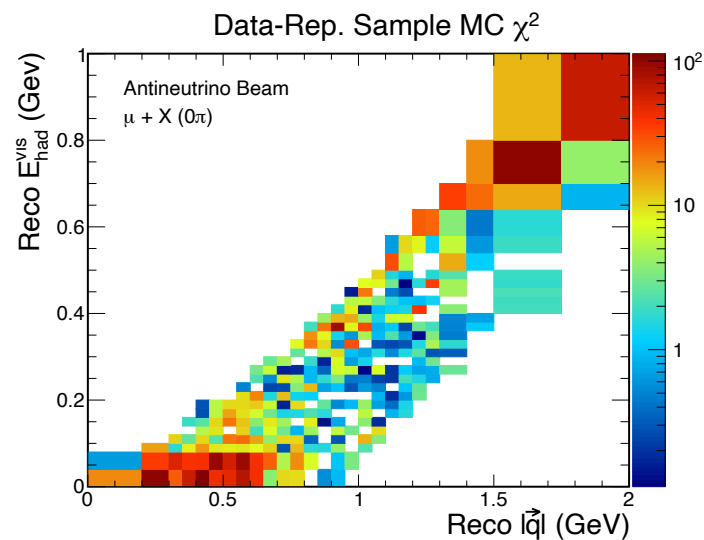
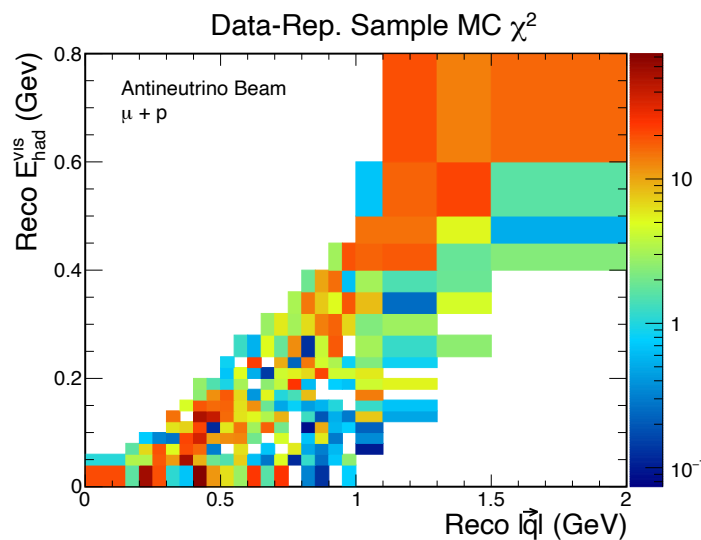
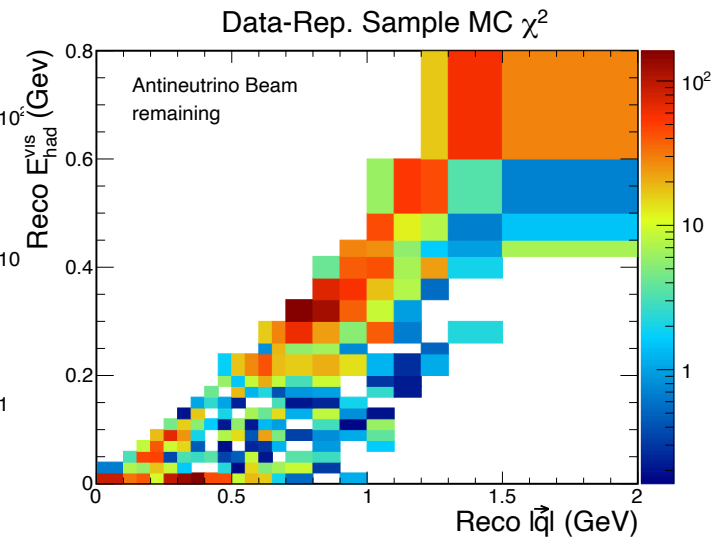
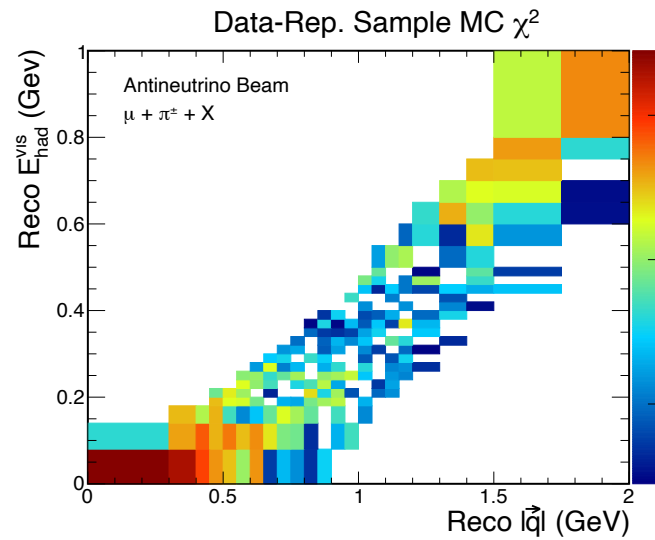
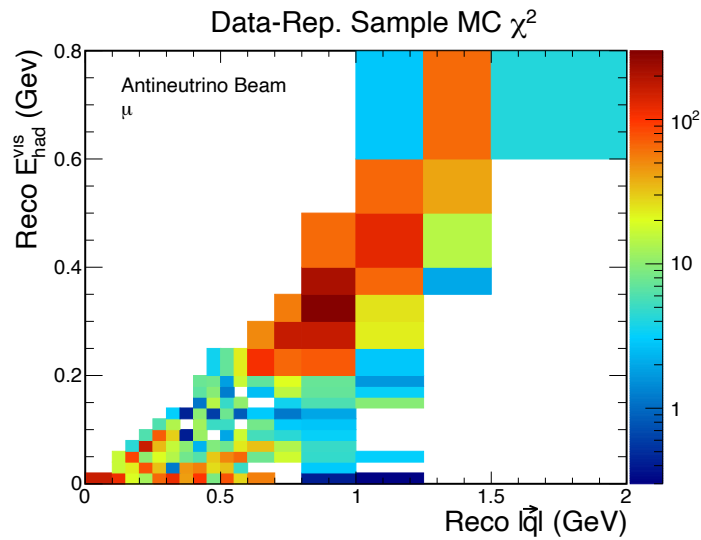
Flux

- The systematics used in our fits, with a $\chi^2 > 100$.

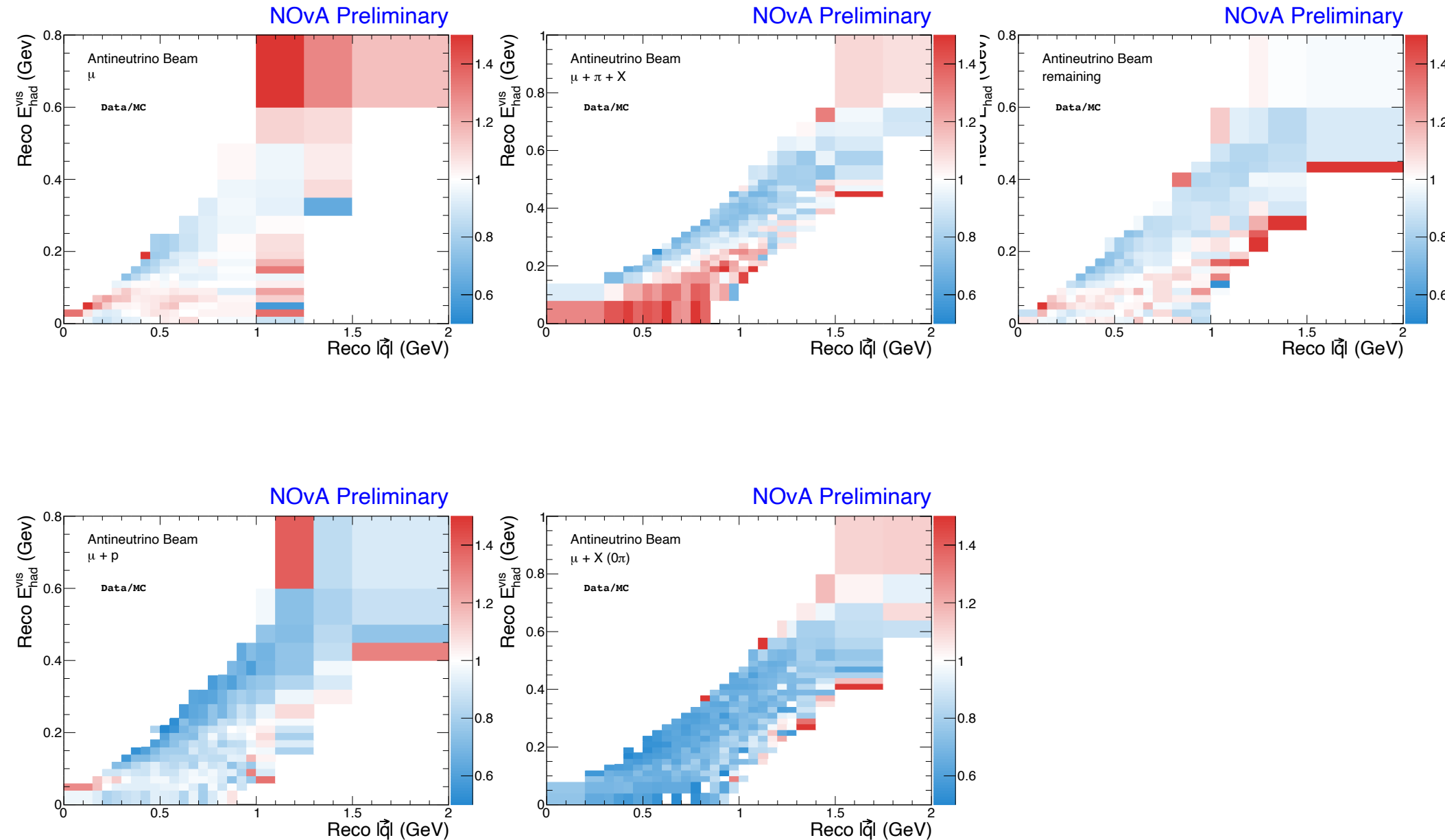
Data-Nominal MC χ^2 — RHC



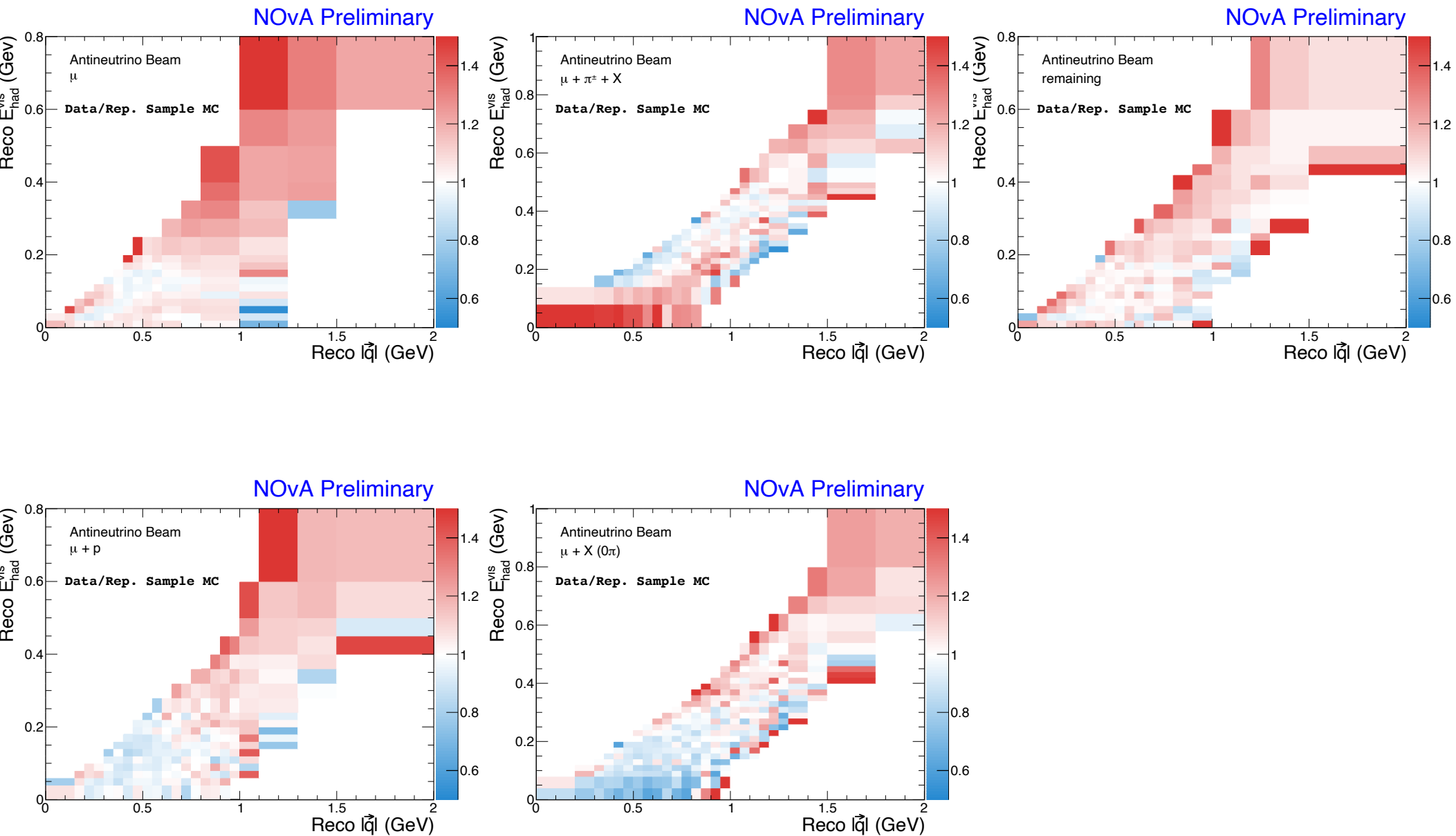
Data-Rep Sample MC χ^2 — RHC



Data-Nominal MC Ratio — RHC

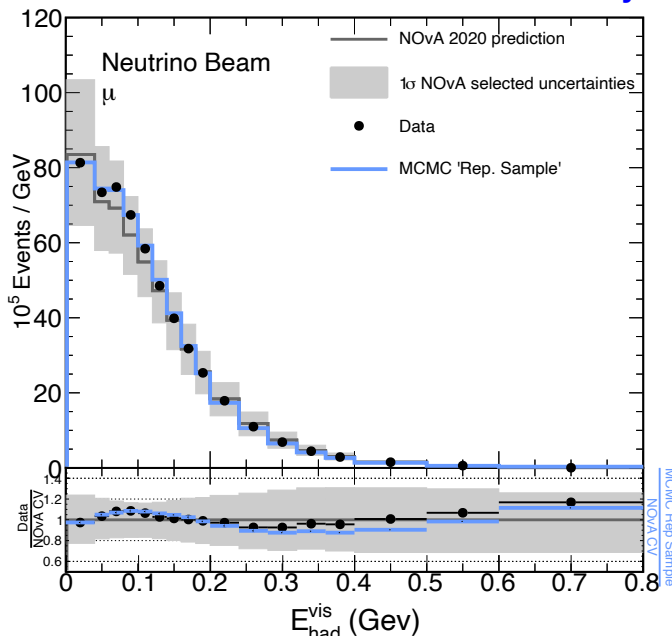


Data-Rep Sample MC Ratio — RHC

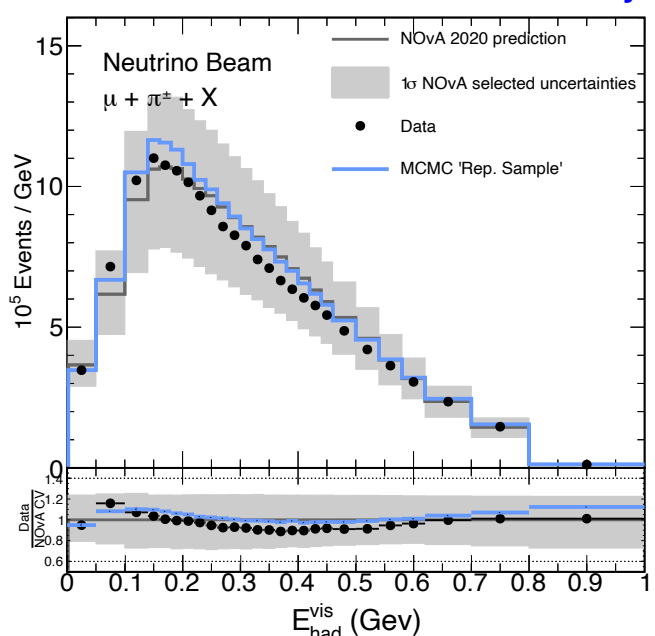


1D Projections — FHC

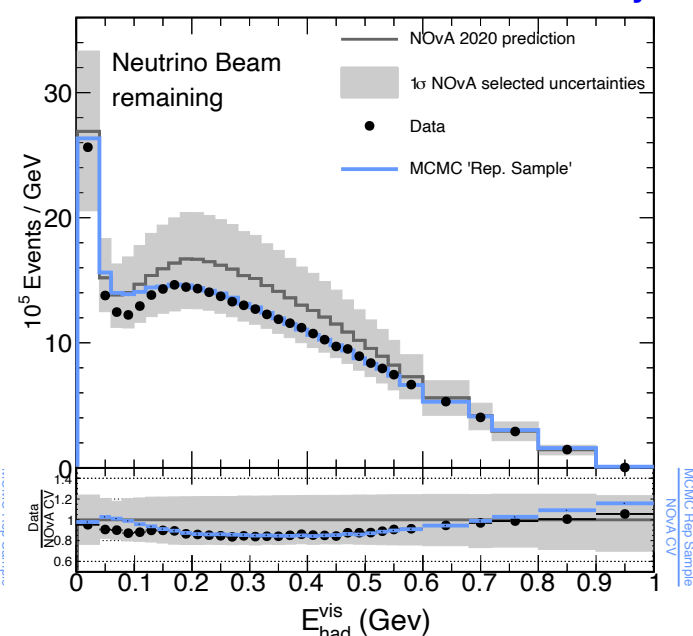
NOvA Preliminary



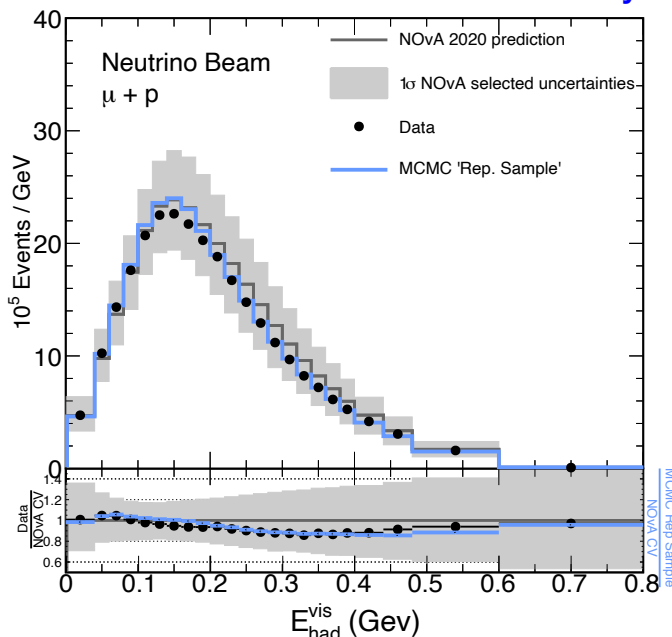
NOvA Preliminary



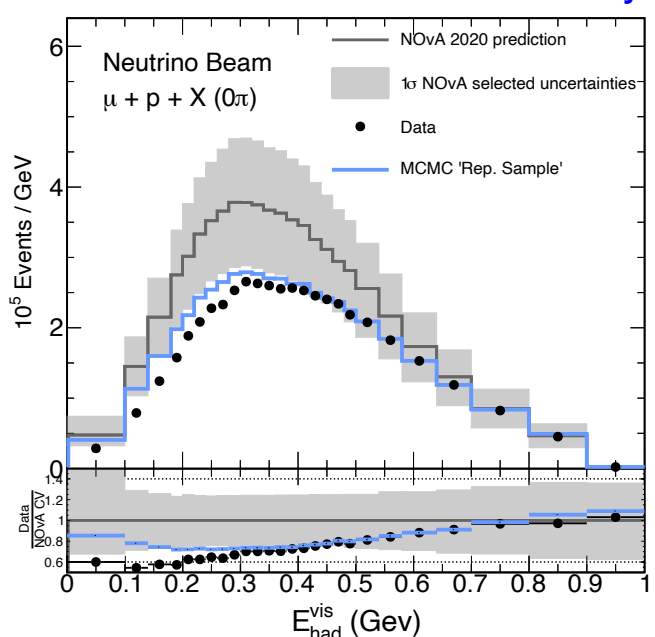
NOvA Preliminary



NOvA Preliminary



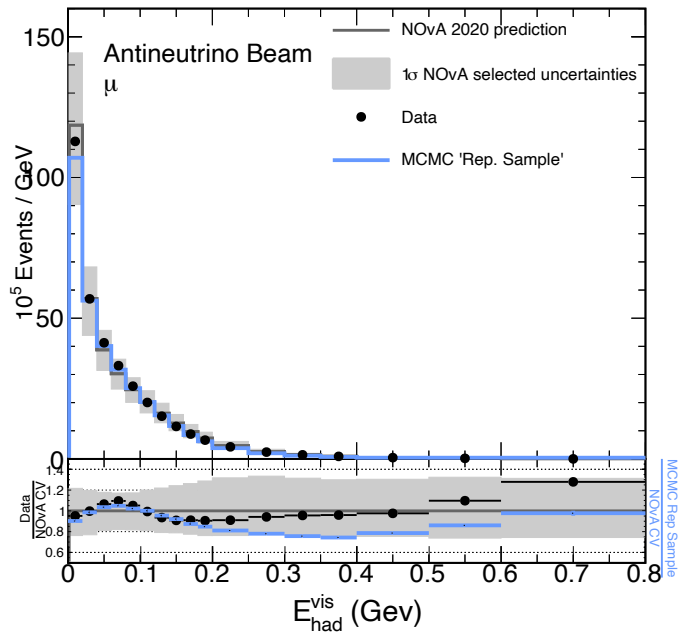
NOvA Preliminary



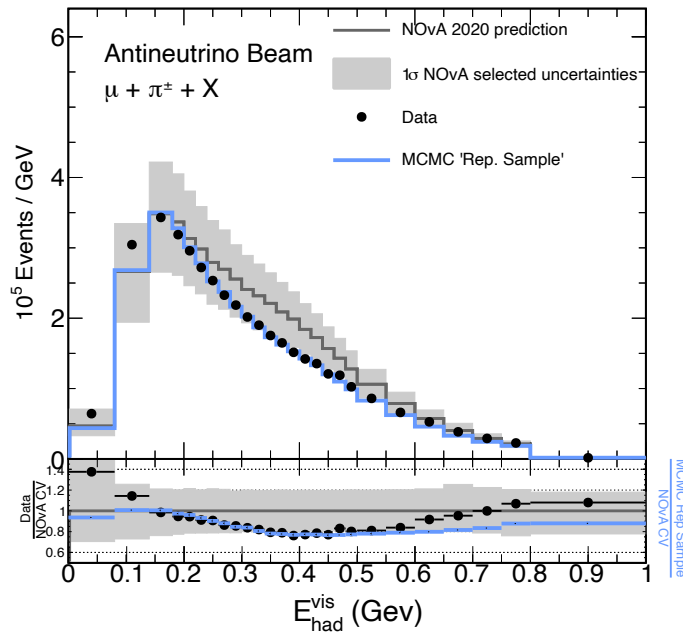
- The agreement in 1D projections look good, even in low E_{HadVis} bins.

1D Projections — RHC

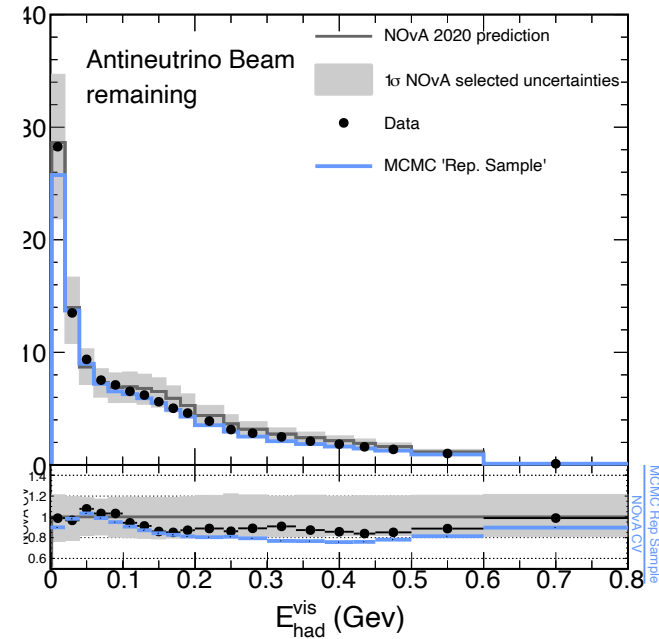
NOvA Preliminary



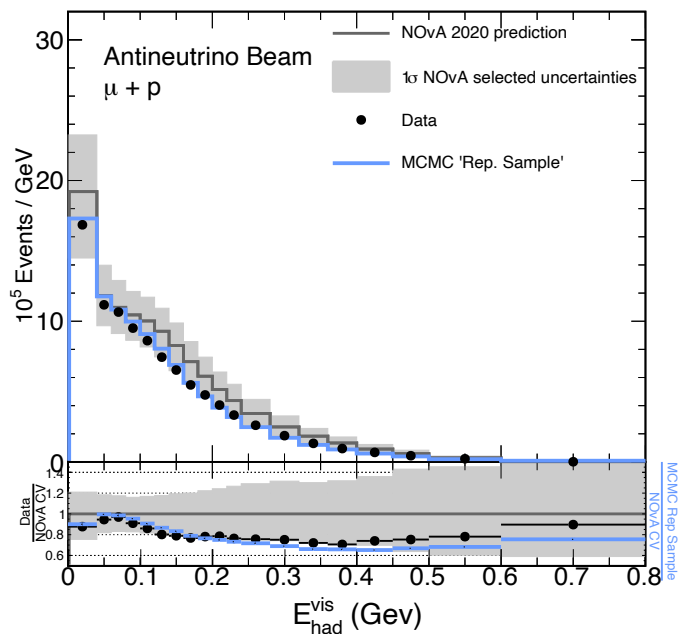
NOvA Preliminary



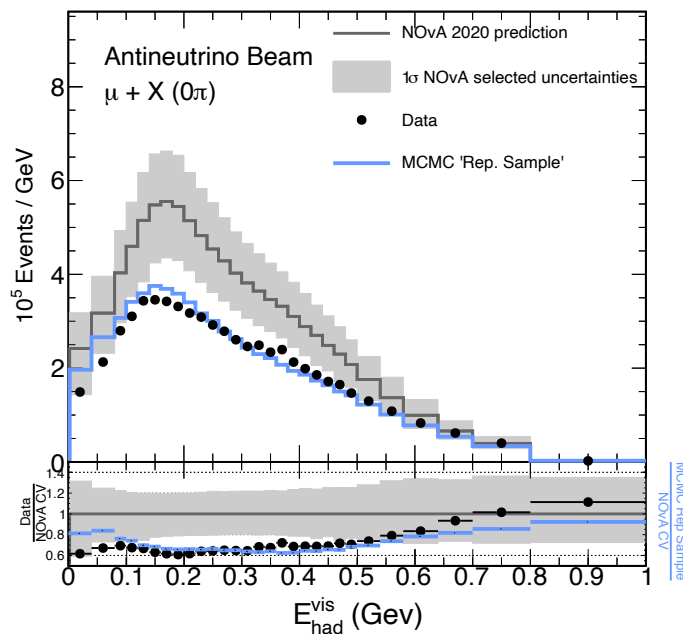
NOvA Preliminary



NOvA Preliminary



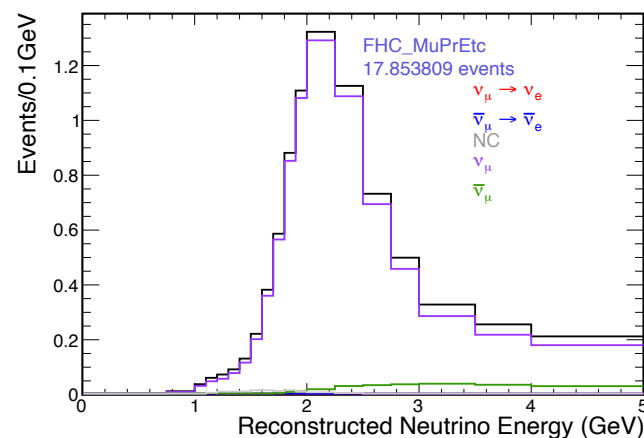
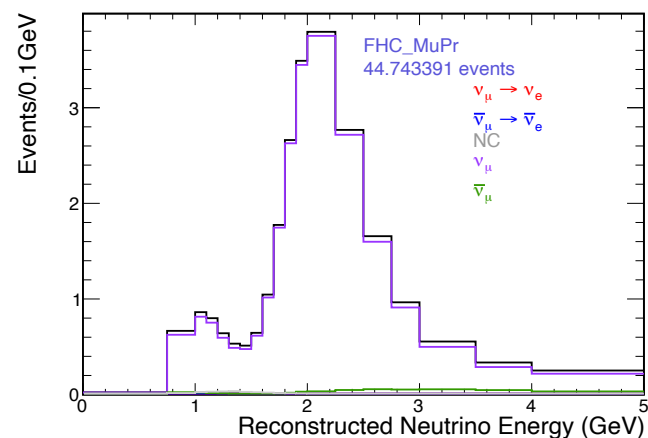
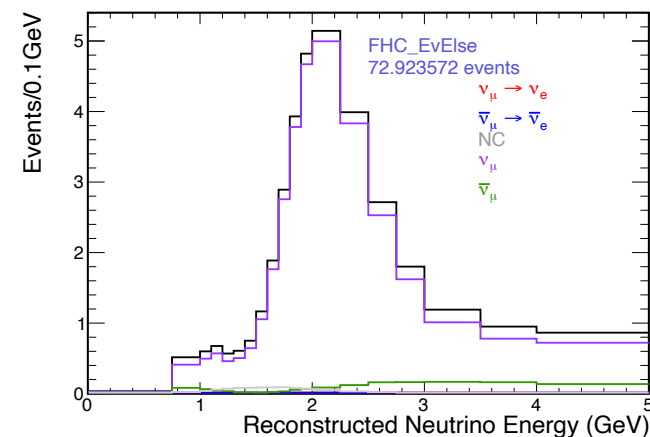
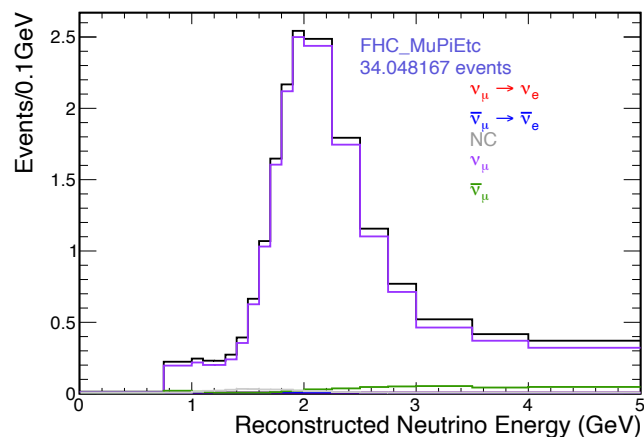
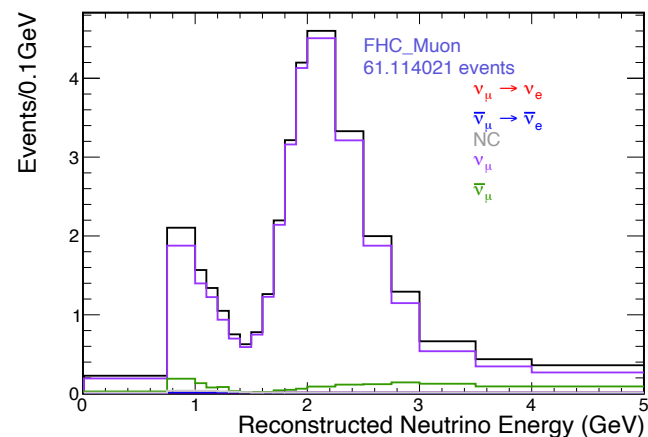
NOvA Preliminary



- The agreement in 1D projections look good, even in low E_{HadVis} bins.

Moving to the Far Detector

NOvA Simulation

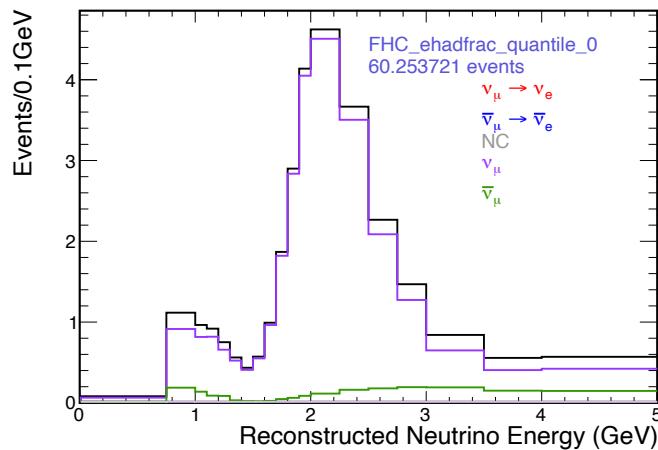


- Machinery for ND + FD fake data fits under development. 🛠️
- Use topological samples for FD predictions?

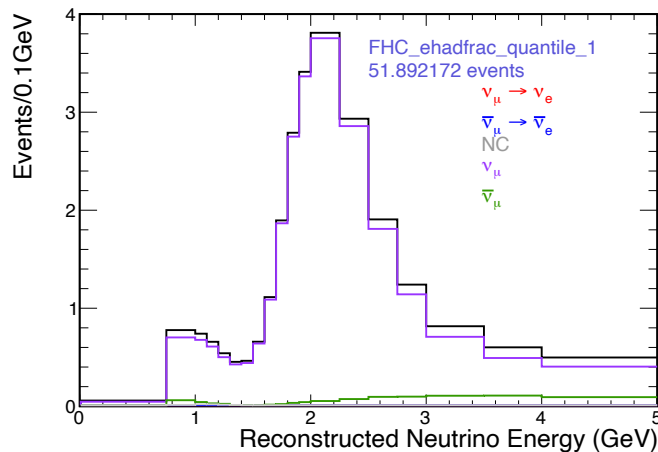
Moving to the Far Detector

- NOvA traditionally divides FD data & MC into **quantiles** of hadronic energy resolution.
 - cosmic background grouped into last quartile (worst resolution).
- Or use traditional quantiles?

6%
hadronic
energy
resolution

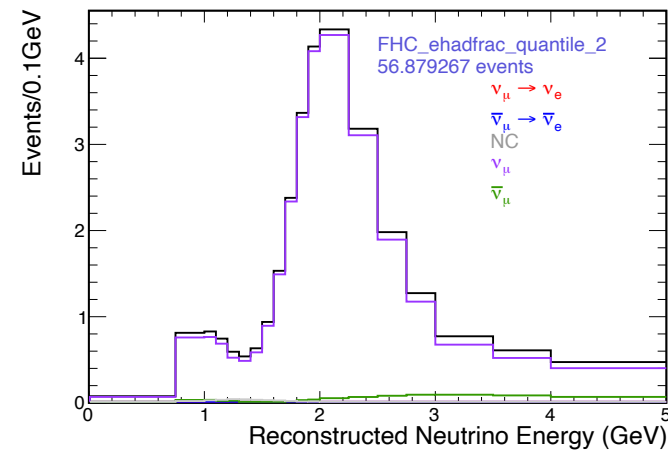


8%



NOvA Simulation

10%



12%

