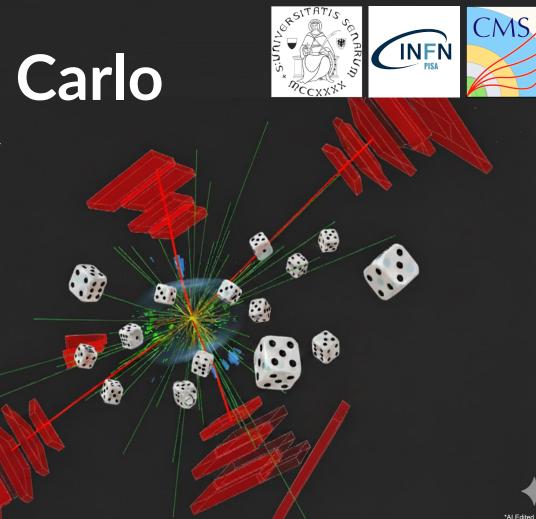
**Data - Monte Carlo** Compatibility Check

Sayan Dhani

University of Siena 24 / 10 / 25





# Why Data-Monte Carlo Compatibility Matters — The Reality Check



- Physics Goal: Before any discovery or precision measurement, we must verify that our detector and simulations agree on what the world looks like.
- **Benchmark Channel:** The  $Z \to \mu^+\mu^-$  process clean, well-understood, and sensitive to detector and modelling differences.
- The Question: Do our Monte Carlo templates truly represent what CMS recorded?
- The Approach:
  - Start with simple shape tests (KS test)
  - Move to likelihood fits to extract scaling parameters
  - Iterative KS tests with new scaling parameters
  - Introduce shape morphing to test systematic effects
- End Goal: Build a statistically consistent bridge between simulation and reality.

# Data and Samples (Event Selection : Tag & Probe Method)



Data	DoubleMuon primary dataset in NANOAOD format from RunH of 2016		
Signal	Simulated dataset ZToMuMu_M-50To120_TuneCP5_13TeV-powheg-pythia8		
Background-1	Simulated dataset TTTo2L2Nu_TuneCP5_13TeV-powheg-pythia8		
Background-2	Simulated dataset WJetsToLNu_TuneCP5_13TeV-madgraphMLM-pythia8		
Background-3	Simulated dataset ZZTo2L2Nu_TuneCP5_13TeV_powheg_pythia8		
Background-4	Simulated dataset ZZTo4L_M-1toInf_TuneCP5_13TeV_powheg_pythia8		

# Tag & Probe Method: Event Selection:

- Event Trigger : HLT\_IsoMu22\_eta2p1
- MET p<sub>T</sub> > 40 GeV
- nMuon >= 2

#### **Electron Veto:**

- Good electron :  $[p_T^e > 10 \text{ GeV}, \eta^e < 2.5, no \mu \text{ within } \Delta R = 0.4]$
- If good electron, reject the event

#### Tag Selection:

- $p_T^{\mu} \ge 24 \; GeV$
- $\eta^{\mu} < 2.1$
- $iso^{\mu} < 0.3$
- $[tight\ id]^{\mu} = 1$

#### Jet Veto:

- Good Jet:  $[p_T^{Jet} > 30 \text{ GeV}, \eta^{Jet} < 4.7, no \ \mu \text{ within } \Delta R = 0.4]$
- If >3 good Jets, reject the event

#### **Probe Selection:**

- Probe\_chrg \* Tag\_chrg < 0
- $\eta^{\mu} < 2.1$
- $M_{\{\mu^{Tag}\mu^{Probe}\}} < 2000 \text{ GeV}$

#### b-Jet Veto:

- Good b-Jet:  $[p_T^{Jet} > 30 \text{ GeV}, \eta^{Jet} < 4.7, no \ \mu \text{ within } \Delta R = 0.4, btag \ge 0.33]$
- If good b-jet, reject the event.

Trigger & Event Selection

Tag Selection Probe Selection

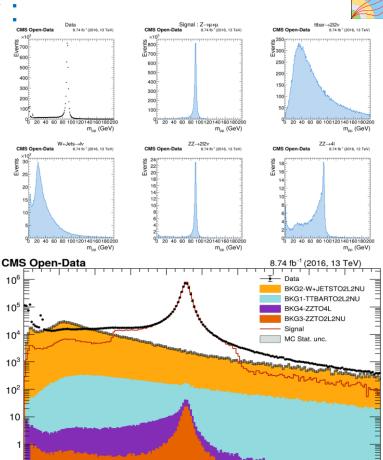
Election Veto

Jet & b-Jet Veto Store the observables in histograms

# MC Normalization to Data Luminosity

- MC samples are arbitrary number of events generated → randomize mixture of random numbers
- Real Process Info. (Randomness in reality) corresponds to a known
   Integrated Luminosity >> encoded in Data << MC (randomness
   implemented to mimic reality) should be look similar to Data if we know the
   process</li>
- So, each MC event is assigned a **weight** = how many real events it represents?
- Otherwise, our understanding, = + +
- General formula :  $w_{event} = w_{norm} \cdot (genWeight) \cdot w_{PU} \cdot w_{SF}^{\mu\mu} \cdot w_{prefire}$
- Where,  $w_{norm} = \frac{L_{data}[fb^{-1}] \cdot \sigma[fb] \cdot \epsilon \cdot k}{\sum w}$
- Ensures total MC yield matches expected yield for 8.74 fb<sup>-1</sup> (2016, 13 TeV)

Process	Cross-section $(pb)$	Events
Data		5025648
Signal : $Z \rightarrow \mu^+ + \mu^-$	2008.4	5412870.60
Bkg-1 : $t\bar{t}  o 2\mu + 2\nu$	88.29	7928.12
Bkg-2 : W + Jets $\rightarrow \mu + \nu$	61529.7	173500.67
Bkg-3 : ZZ $ ightarrow 2\mu + 2\nu$	0.564	155.67
Bkg-4 : ZZ $ ightarrow 4\mu$	1.256	304.84



100

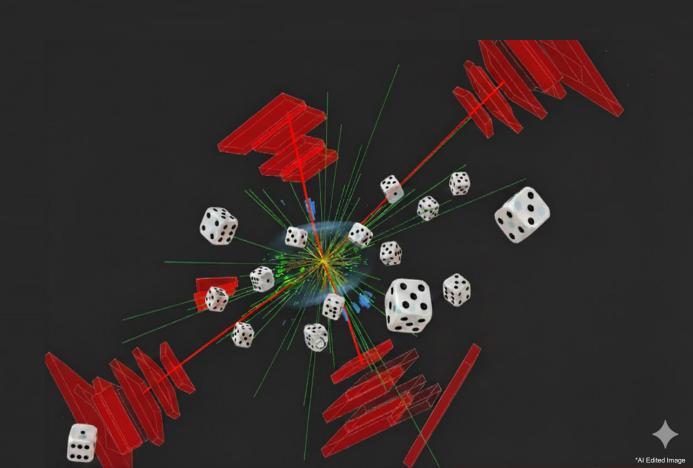
140

Events / bin

180

m<sub>μμ</sub> [GeV]

# **KS Test**



# Data-MC Comparison: Kolmogorov-Smirnov (K-S) Test



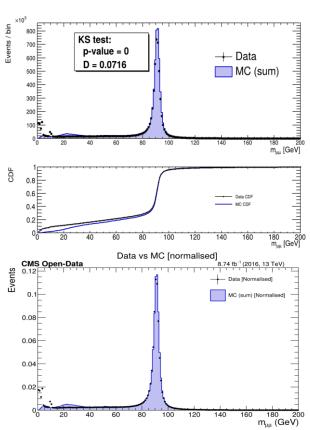
A non-parametric statistical test used to compare two probability distributions ⇒ Draws conclusion whether those two PDFs are drawn from the same underlying distribution or not.

#### How it Works :

- The test is based on empirical cumulative distribution functions (ECDFs).
- For each PDF, the ECDF is given by :  $F_n(x) = \frac{Number\ of\ data\ points \le x}{Total\ number\ of\ points:\ n}$
- KS Test Statistics :  $D = \sup_{x} [F_n(x) F_m(x)] = \sup_{x} [F_{Data}(x) F_{MC}(x)]$  i.e, the largest vertical distance b/w 2 CDFs
- P-value ≥ 0.05 → Good Agreement but P-value ≪ 0.05 → Significant Mismatch

#### Why it matters :

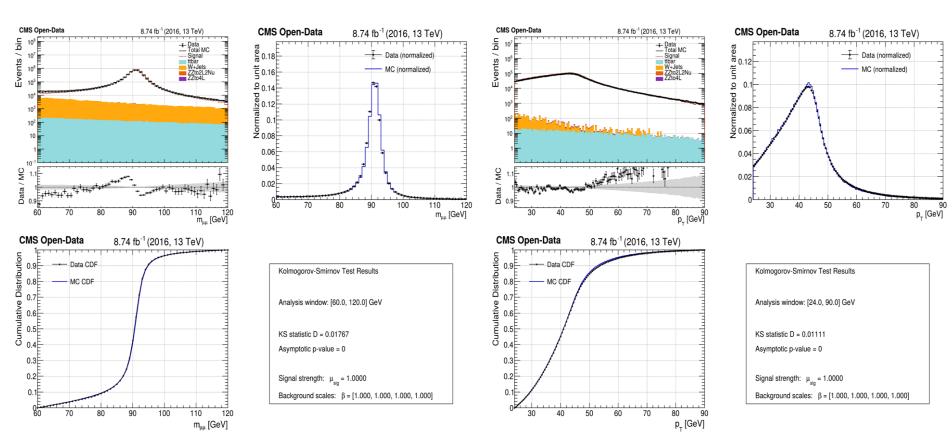
- O Non-parametric, so no assumption about the form of distribution
- Sensitive to difference in both location (mean shift) and shape (skew)
- O Used check Data-Monte Carlo agreement for generators and detector simulation validation
- O Comparison between different unfolding methods.



Result : Data and MC differ notably around the Z-peak region  $\rightarrow$  indicates modeling or detector bias  $\rightarrow$  motivates fit-based approach.

# Kolmogorov–Smirnov (K-S) Test of different Observables



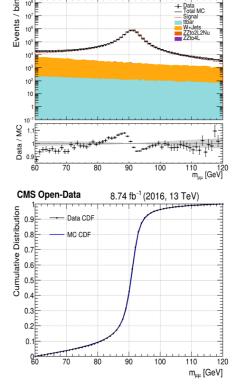


# Kolmogorov–Smirnov (K-S) Test : Scope of Improvement ??

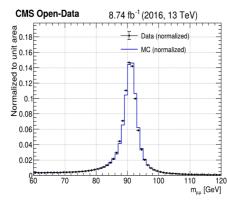


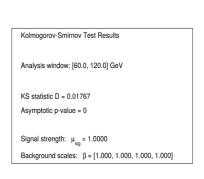
- Made a 12% shift of bin-contents of to the consecutive left bins → Shape Improves!!
- Also the  $\mu_{sig}$  and  $\beta's$  are **ASSUMED to 1**

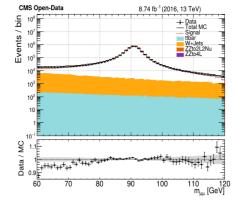
8.74 fb<sup>-1</sup> (2016, 13 TeV)

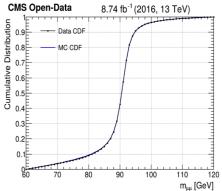


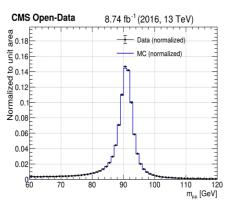
CMS Open-Data

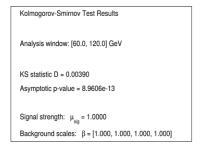




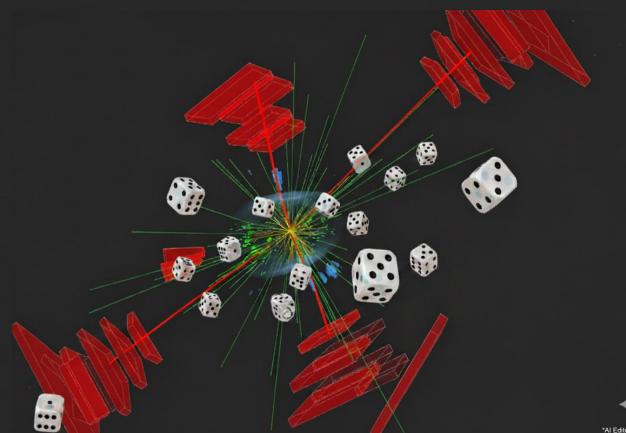








# **Template Fit**





# Template Fit Framework — Estimating Signal Strength



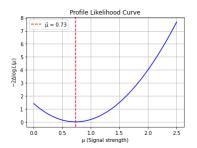
- We have binned hist. Data and MC templated for process (Signal & Backgrounds)
- For each bin (say in i<sup>th</sup> bin of  $m_{\mu\mu}$  histogram), the expected event is  $v_i(m_{\mu\mu}) = \mu_s \cdot s_i(m_{\mu\mu}) + \sum_{k \in bka_s} \beta_k \cdot b_{k,i}(m_{\mu\mu})$ 
  - Where  $s_i, b_{k,i}$  are signal and background shape templates respectively (MC yields per bin, possibly deformed by shape nuisances  $\phi$ )
  - $\circ$   $\mu_s$  is the signal strength scaling (parameter if interest)
  - $\circ$   $\beta_k$  is the background scaling factors (can be treated as nuisance)
- Likelihood:
  - For observed count  $n_i$ ,  $P(n_i | v_i) = \frac{e^{-v_i} v_i^{n_i}}{n_i!}$
  - $L_{nrimarv}(\mu_s, \beta, \phi) = \prod_{i=1}^{N_{bins}} Pois(n_i | \nu_i(\mu_s, \beta, \phi))$
  - $L_{auxiliary}(\eta) = \prod_k \pi_k(\beta_k) \cdot \prod_i \pi_i(\phi_i) \cdot (MC stat \ constraints)$

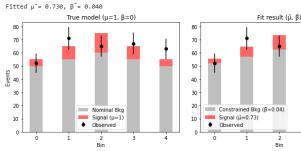
$$\pi(\beta_k) = \begin{cases} N(1, \sigma_k) \text{ (Gaussian Constriant)} \\ LogNormal(1, \sigma_k) \text{ (Positive, multiplicative constraint)} \end{cases}$$

$$\text{With } \sigma_k = 0.10 \rightarrow 10\% \text{ prior uncertainty}$$

- Full likelihood :  $L(\mu_s, \beta, \phi) = L_{primary} \cdot L_{aux}$ .
- Profiling :
  - $\circ$  To estimate  $\mu_s$ , profile all nuisances :

$$\widehat{\widehat{\eta}}(\mu_s) = \arg\max_{n} L(\mu_s, \eta), \ \widehat{\mu_s}, \widehat{\eta} = \arg\max_{n} \mu_s n$$

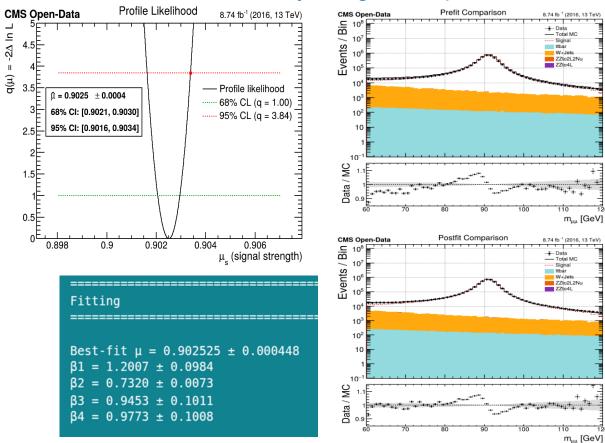




## Constraints on Backgrounds to Nominal with Uncertainty, Singal is kept Free

CMS

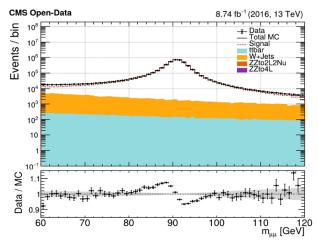
- We trust our background predictions reasonably well; constrained with Gaussian priors (σ = 10%)
- Only the main component = Signal float freely
- Parameters  $egin{cases} \mu_{s} \ [free\ to\ float\ ] \ eta_{k} \ [constrained\ by\ \pi(eta_{k})\ ] \end{cases}$

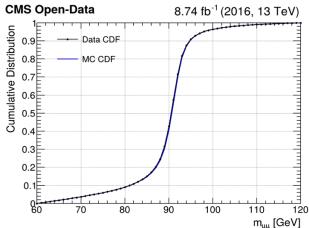


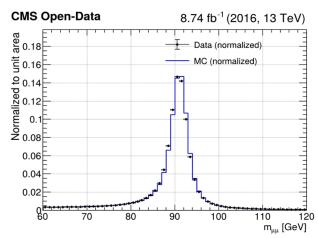
Allowing  $\mu_s$  to float improves the overall shape agreement, but residual mismatch near Z-mass remains — hinting at small shape bias

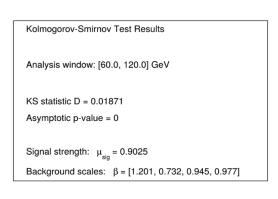
## Post-fit Validation: KS Test











- KS test after fit:
- D = 0.0187, p = 0  $\rightarrow$  Data and MC still not statistically compatible
- Agreement improved but not perfect → likely due to mass-scale or shape modeling differences

## Shape Adjustment — 12 % Left Shift of Signal Template



#### [Testing possible mass-scale bias around Z peak]

**Goal:** Investigate whether a small **mass-scale bias** in simulation can explain the Data–MC shape mismatch.

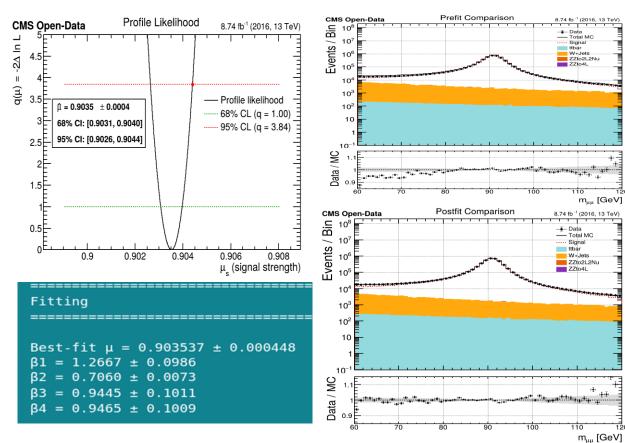
#### Approach:

- Shift the signal template by 12 % toward lower mass
- Keep backgrounds Gaussian-constrained (σ = 10 %)
- Allow μ<sub>s</sub> (signal strength) to float freely

#### Interpretation:

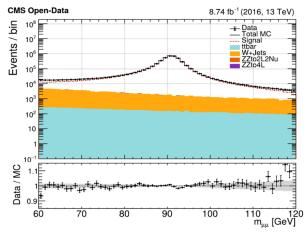
- · Fit quality improved compared to nominal
- KS test shows better Data–MC compatibility

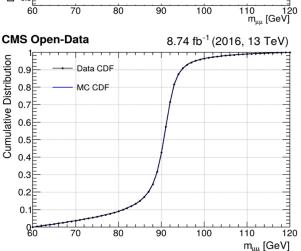
**Result:** Applying a 12 % left shift aligns the Z peak and improves both fit and Data–MC consistency.

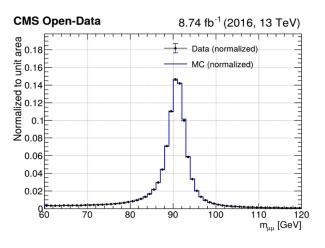


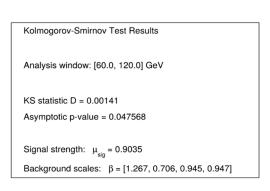
# Post-fit Validation — Improved Data–MC Agreement











- The **KS p-value rises from** ≈ 0 → 0.05, confirming better shape consistency.
- Indicates a small mass-scale mismatch between Data and MC — corrected by shifting signal.

After shape adjustment, Data and MC are statistically consistent within 5 % level.

## **Unconstrained Background Fit**

Goal: Test whether freeing background normalizations can improve the overall fit and Data-MC agreement.

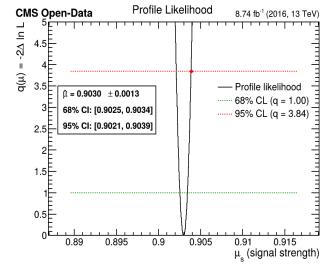
#### Setup:

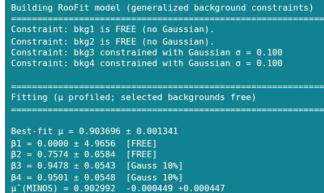
- Backgrounds  $\beta_{1,2,3,4}$  allowed to float (some unconstrained, some with 10% prior)
- Signal strength  $\mu_s$  free to float

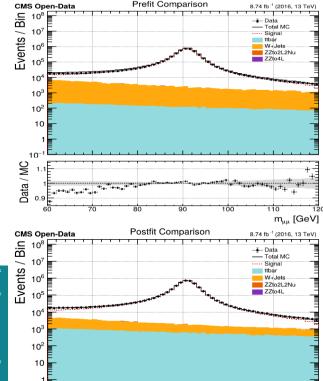
#### Interpretation:

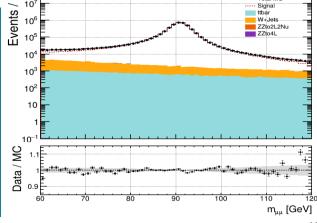
- Fit still converges near  $\mu_s \approx 0.90$
- Uncertainty increases as expected
- Backgrounds adjust within reasonable physical range
- Expect further KS improvement

**Result:** Letting background yields float freely improves shape flexibility and slightly enhances post-fit agreement, without biasing µ<sub>s</sub>.



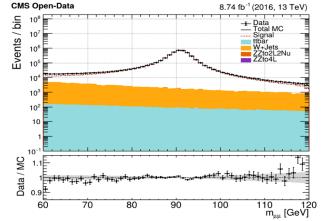


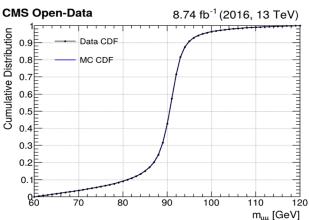


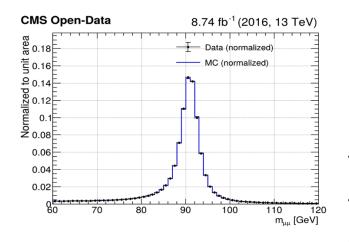


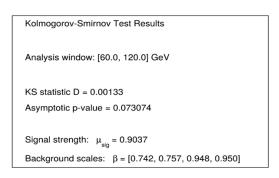
# Post-fit Validation — Improved Data–MC Agreement







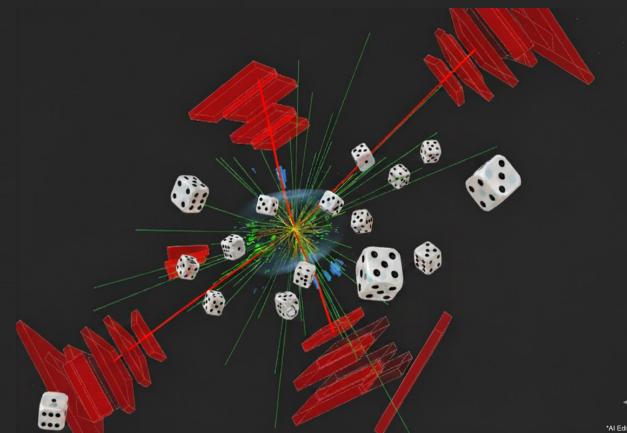




- Data–MC shape compatibility further improved (p-value from  $0.048 \rightarrow 0.073$ ).
- Confirms that allowing background flexibility helps fine-tune modeling differences.
- $\mu_s$  remains stable  $\rightarrow$  fit is statistically reliable.

With unconstrained backgrounds, Data and MC are statistically consistent and stable around  $\mu_s\approx 0.90.$ 

# **Systematics Estimation**





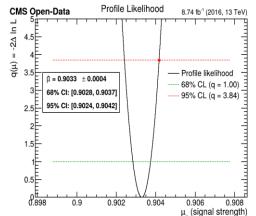
# Shape Systematics (Morphing)

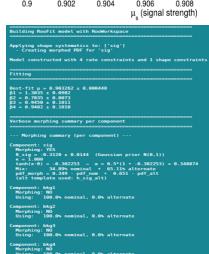
CMS

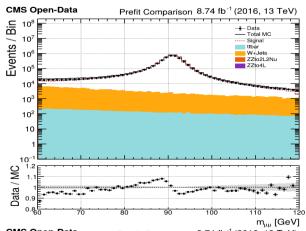
- Goal: Quantify residual shape uncertainty in the signal using morphing between the nominal and shifted templates.
- Concept: The morphed shape is built as a linear combination of nominal and shifted templates:

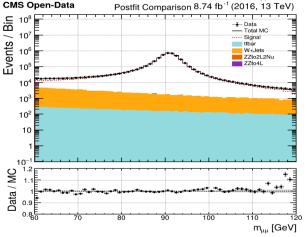
  - $\alpha = \frac{1}{2} [1 + \tanh(k\theta)]$  controls the deformation strength.
- It captures possible detector or modeling biases that shift or skew the signal shape.

Result: Applying a 12 % left shift aligns the Z peak and improves both fit and Data–MC consistency.



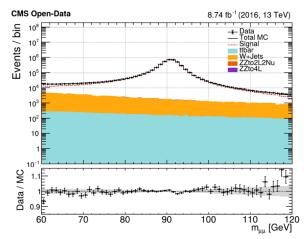


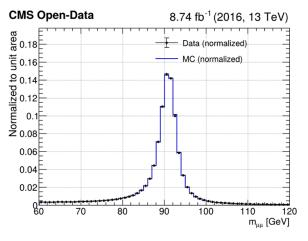


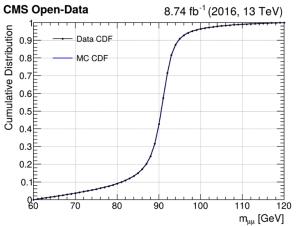


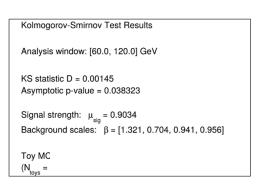
# Post-fit Validation — KS Test with Shape Morphing











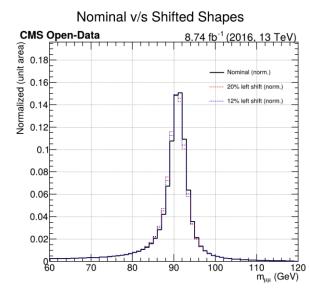
No morphing : D = 0.0187, p = 0No morphing but shift applied: D = 0.00141, p = 0.046With morphing: D = 0.00145, p = 0.038

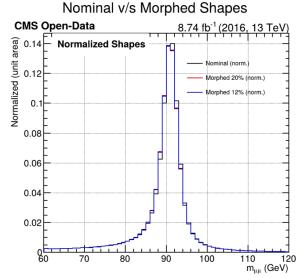
Slight improvement  $\rightarrow$  residual shape mismatch absorbed.

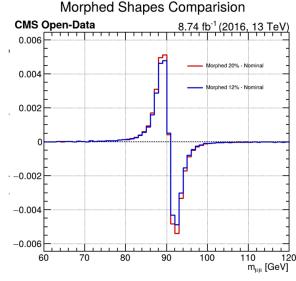
Morphing captures small residual shape systematics, leading to marginally better Data–MC consistency without altering  $\mu_{\text{s}}.$ 

# Visualizing Morphing









Nominal vs shifted templates show the Z-peak movement.

Morphed shapes interpolate smoothly between them.

Difference plots confirm that morphing introduces only minimal distortion, very less.

**Morphing provides a smooth, data-driven way to incorporate shape uncertainties** into the fit. It bridges between the nominal and shifted signal templates, allowing the fit to marginalize over realistic shape variations.

# Final Signal-Strength Estimate



- The key message:  $\mu_s \approx 0.903 \pm 0.001$  is consistent across all configurations.
- The Data–MC compatibility steadily improves, demonstrating that our modeling corrections genuinely fix the shape discrepancy.

Fit Configuration	μ̂s ± Δμ	KS D	KS p-value	Comment / Observation
Constrained Backgrounds (baseline)	0.9025 ± 0.0004	0.0716	≈ 0.00	Poor shape match, MC Z-peak slightly off
12 % Shifted Signal	0.9035 ± 0.0004	0.00141	0.048	Better alignment around Z-peak
Unconstrained Backgrounds (robustness)	0.9037 ± 0.0013	0.00133	0.073	Background flexibility improves fit
Morphing (shape systematics included)	0.9033 ± 0.0004	0.00145	0.038	Residual mismatch absorbed by morphing

# Discussion & Takeaways



#### To wrap up:

- $Z \rightarrow \mu\mu$  serve as a good benchmark for validation of detector calibration and MC modelling
- The **KS test** offers a shape-level diagnostic, complementing likelihood-based fits.
- Step-wise modeling : from constraints → shift → morphing :: systematically improves Data-MC agreement.
- The final  $\mu_s$  result is robust to statistical and systematic choices.
- And this same workflow extends naturally to more complex analyses, from precision measurements to newphysics searches.
- In essence: we've shown that careful statistical modelling including both rate and shape systematics can turn a simple benchmark process into a powerful validation tool for high-energy-physics analyses.
- Combining shape tests and likelihood fits provides a complete, data-driven validation of Monte Carlo models — an essential step for precision and discovery analyses.

#### My extra learnings:

- I learned to use brilcalc and golden JSON and normtag files to calculate the luminosity
- Learned about the RooFit, and RooStat etc fitting modules
- Leaned about the usage of Open-Data

# Comments, Questions?

# Thank you!!

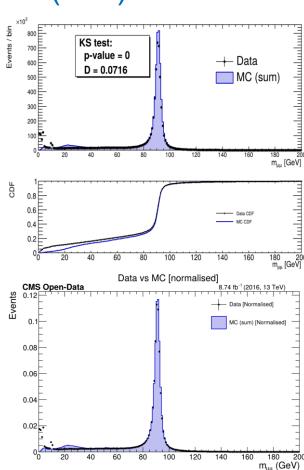
# Back-up

# Data-MC Comparison: Kolmogorov-Smirnov (K-S) Test



A non-parametric statistical test used to compare two probability distributions ⇒ Draws conclusion whether those two PDFs are drawn from the same underlying distribution or not.

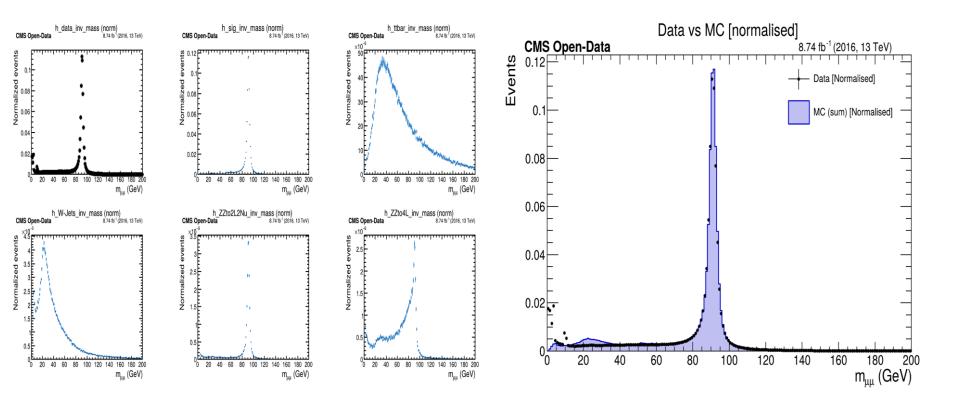
- The test is based on empirical cumulative distribution functions (ECDFs).
- For each PDF, the ECDF is given by :  $F_n(x) = \frac{Number\ of\ data\ points \le x}{Total\ number\ of\ points : n}$
- KS Test Statistics :  $D = \sup_{x} [F_n(x) F_m(x)] = \sup_{x} [F_{Data}(x) F_{MC}(x)]$  i.e, the largest vertical distance b/w 2 CDFs
- Effective sample size :  $N_{eff} = \frac{nm}{n+m}$ , but our `Data` is unweighted but the `MC` is weighted ( not integer sample size). So,  $\mathbf{n}_{\mathrm{MC}} = \frac{\left(\sum_{j} w_{j}\right)^{2}}{\sum_{i} w_{i}^{2}}$ , then  $n = n_{Data}$  and  $m = n_{MC}$
- P-value [ asymptotically ; large n ] :  $p \approx Q_{KS}(\lambda) = 2 \sum_{k=1}^{\infty} (-1)^{k-1} e^{-2k^2 \lambda^2}$  where  $\lambda = \sqrt{N_{eff}} D$
- So, if p=value is very low (→ 0), then samples drawn from different distributions OR, if p-value ≥ **0.05** (!!!), then samples are consistent to each other.
- Non-parametric, so no assumption about the form of distribution
- Sensitive to difference in both location (mean shift) and shape (skew)
- Used check Data-Monte Carlo agreement for generators and detector simulation validation
- Comparison between different unfolding methods.



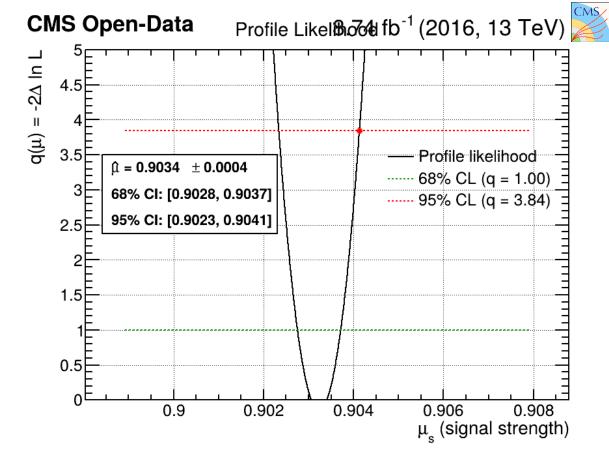


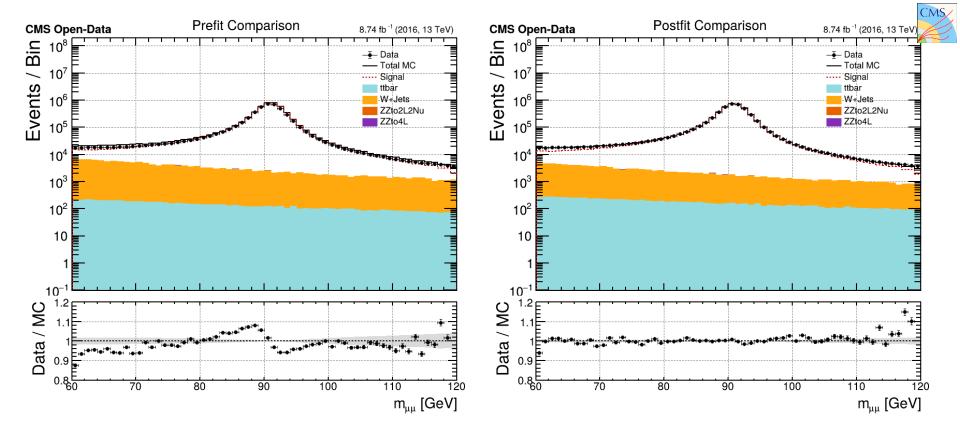
Shape Systematics 12% left shift





```
Preparing histograms in window [60.0, 120.0] GeV
                     5412870.60
                    7928.12
173500.67
Background 1:
Background 2:
Background 3:
                        304.84
Background 4:
Total MC:
                    5594759.90
                     5025648.00
Data:
Building RooFit model with RooWorkspace
Applying shape systematics to: ['sig']
  - Creating morphed PDF for 'sig'
Model constructed with 4 rate constraints and 1 shape constraints
Fitting
Best-fit u = 0.903411 ± 0.000448
\beta 1 = 1.3215 \pm 0.0977
\beta 2 = 0.7044 \pm 0.0073
\beta 3 = 0.9410 \pm 0.1012
84 = 0.9556 \pm 0.1007
Verbose morphing summary per component
   Morphing summary (per component) ---
 Component: siq
  Morphing: YES
 0_sig = -3.0852 ± 0.1308 (Gaussian prior N(0,1))
 tanh(\kappa \cdot \theta) = -0.995828 \rightarrow \alpha = 0.5*(1 + -0.995828) = 0.002086
            0.21% nominal + 99.79% alternate
 pdf morph = 0.002 · pdf nom + 0.998 · pdf alt
  (alt template used: h sig alt)
Component: bkg1
 Using: 100.0% nominal, 0.0% alternate
 Using: 100.0% nominal, 0.0% alternate
Component: bkg3
 Using: 100.0% nominal, 0.0% alternate
Component: bkg4
 Using: 100.0% nominal, 0.0% alternate
 Yields (scale parameters):
 μ (signal strength) = 0.903411 \pm 0.000448 β1 = 1.3215 \pm 0.0977 (10% Gaussian prior)
 β2 = 0.7044 ± 0.0073 (10% Gaussian prior)
  β3 = 0.9410 ± 0.1012 (10% Gaussian prior)
  β4 = 0.9556 ± 0.1007 (10% Gaussian prior)
Shape nuisance parameters:
 \theta sig = -3.0852 ± 0.1308
Computing profile likelihood
68% CI: [0.902757, 0.903718]
95% CI: [0.902342, 0.904132]
[postfit] bins with data>0 and MC==0: 140
 first few: [(61, 17463.0, 0.0), (62, 17634.0, 0.0), (63, 17934.0, 0.0), (64, 18029.0, 0.0), (65, 18099.0, 0.0)
```



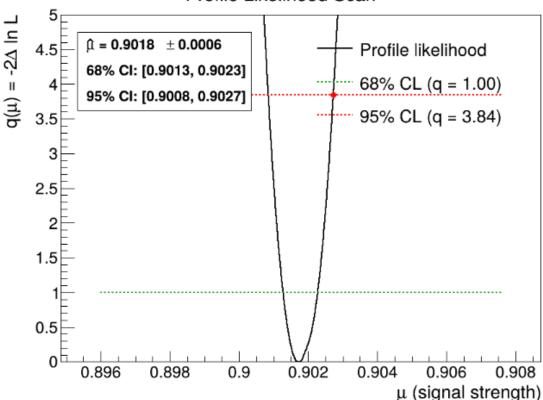


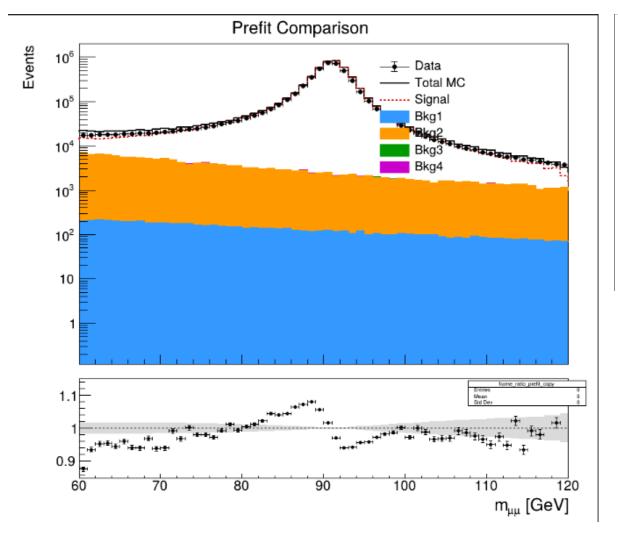


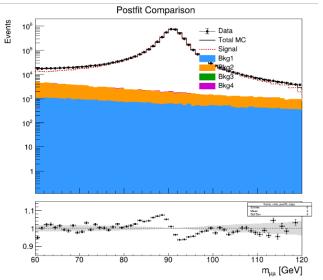
beta\_k without any shift

```
Preparing histograms in window [60.0, 120.0] GeV
Signal:
                    5412870.60
Background 1:
                       7928.12
Background 2:
                     173500.67
Background 3:
                        155.67
Background 4:
                        304.84
Total MC:
                    5594759.90
                    5025648.00
Data:
Building RooFit model (generalized background constraints)
Constraint: bkgl is FREE (no Gaussian).
Constraint: bkg2 is FREE (no Gaussian).
Constraint: bkg3 is FREE (no Gaussian).
Constraint: bkg4 is FREE (no Gaussian).
Fitting (µ profiled; selected backgrounds free)
Best-fit \mu = 0.901779 \pm 0.000579
\beta 1 = 5.0000 \pm 0.0592
                      [FREE]
82 = 0.5723 \pm 0.0083
                       [FREE]
\beta 3 = 3.5535 \pm 2.9430
                       [FREE]
\beta 4 = 5.0000 \pm 0.2167 [FREE]
Computing profile likelihood
68% CI: [0.901273, 0.902276]
95% CI: [0.900845, 0.902726]
Done! Four plots created:
  1. Profile likelihood scan
  2. RooFit postfit
  3. Prefit comparison with ratio
  4. Postfit comparison with ratio
```

#### Profile Likelihood Scan







Info in <TCanvas::Print>: png file cKS\_postfit.png has been created

