Theory uncertainties in the extraction of α_S from the $Z\, p_T$ spectrum

QCD@LHC 2024 - 07/10/24
Freiburg, Germany

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arXiv:24xx.yyyyy

with T. Cridge and F. Tackmann

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Plan of the talk

- Theory uncertainty with Theory Nuisance Parameters (TNPs)
- Theory uncertainties in the extraction of α_S from the $Z\,p_T$ spectrum
  - Perturbative uncertainties
  - Nonperturbative uncertainties
- Conclusions

But why?

A precise determination of the strong-coupling constant from the recoil of Z bosons with the ATLAS experiment at $\sqrt{s}$ = 8 TeV

A precise measurement of the Z-boson double-differential transverse momentum and rapidity distributions in the full phase space of the decay leptons with the ATLAS experiment at $\sqrt{s}$ = 8 TeV

[arXiv:2309.12986, 2309.09318]

super precise ATLAS measurement of $Z\,p_T$ spectrum

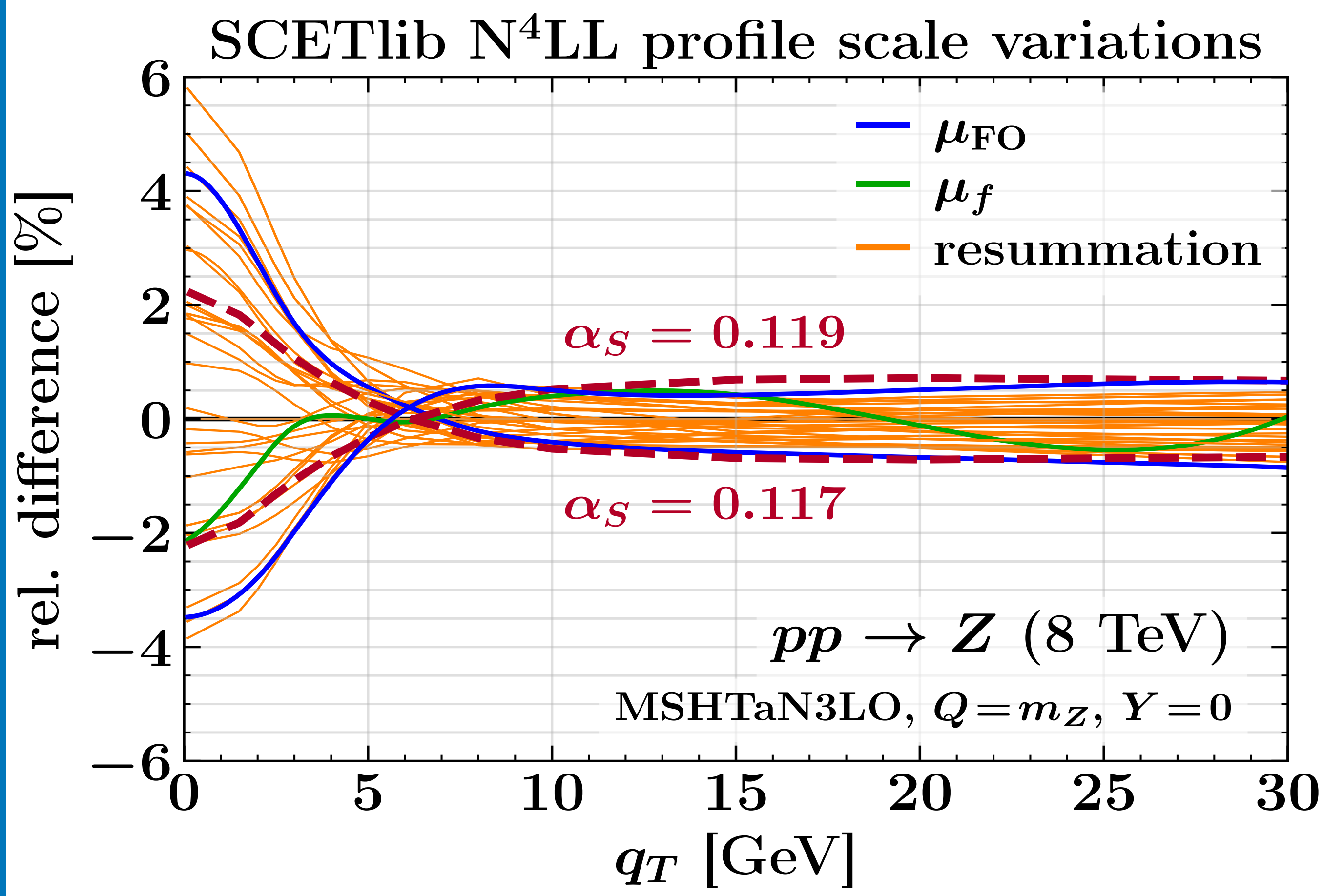
no fiducial cuts, cross-section from $Z \to ll$ full phase space

$$\alpha_S(m_Z) = 0.1183 \pm 0.0009$$

In units of 10^{-3}

Experimental uncertainty	± 0.44	
PDF uncertainty	± 0.51	
Scale variation uncertainties	± 0.42	
Matching to fixed order	0	-0.08
Non-perturbative model	$+0.12$	-0.20
Flavour model	$+0.40$	-0.29
QED ISR	± 0.14	
N^4LL approximation	± 0.04	
Total	$+0.91$	-0.88

Naive approach: scale variations

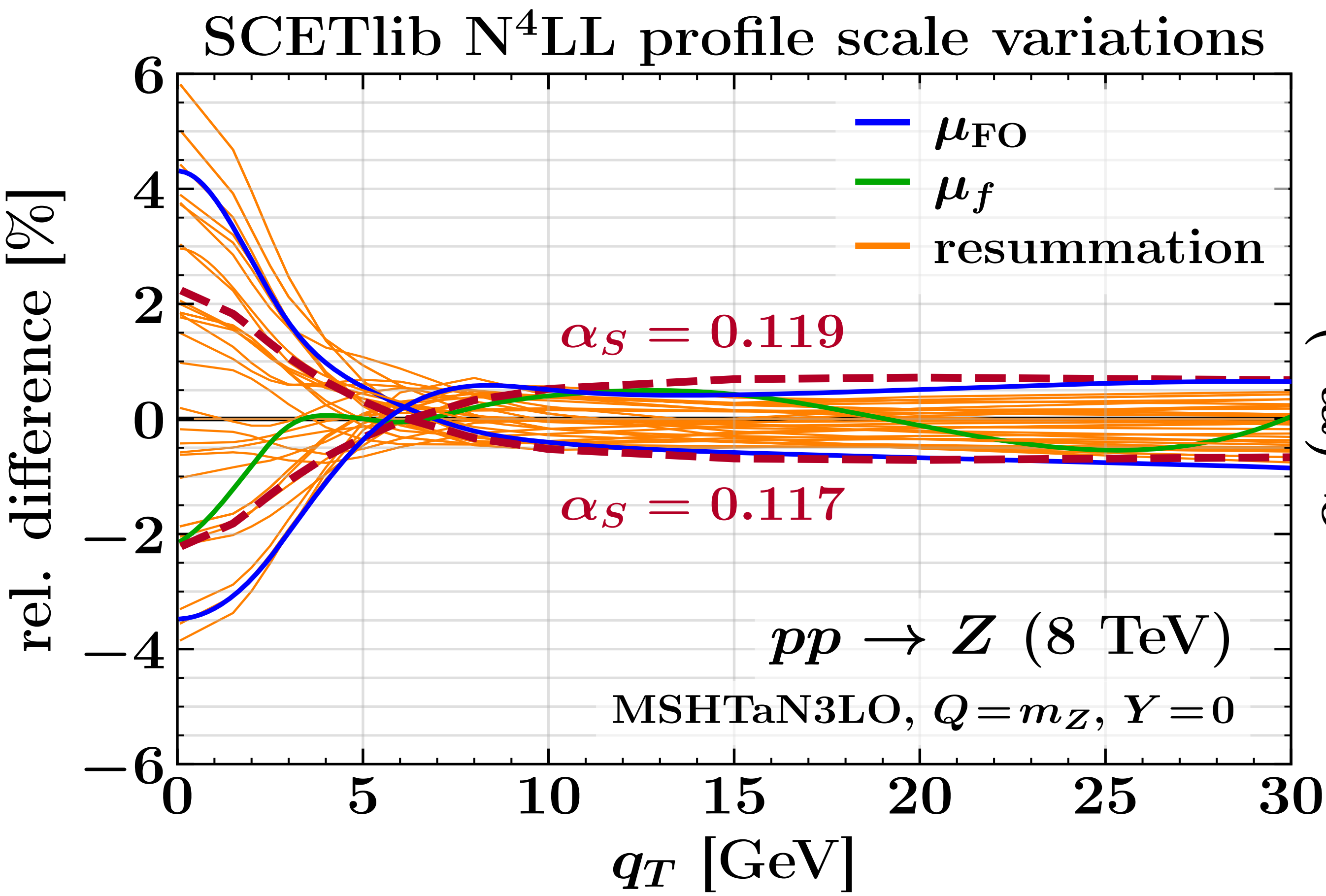


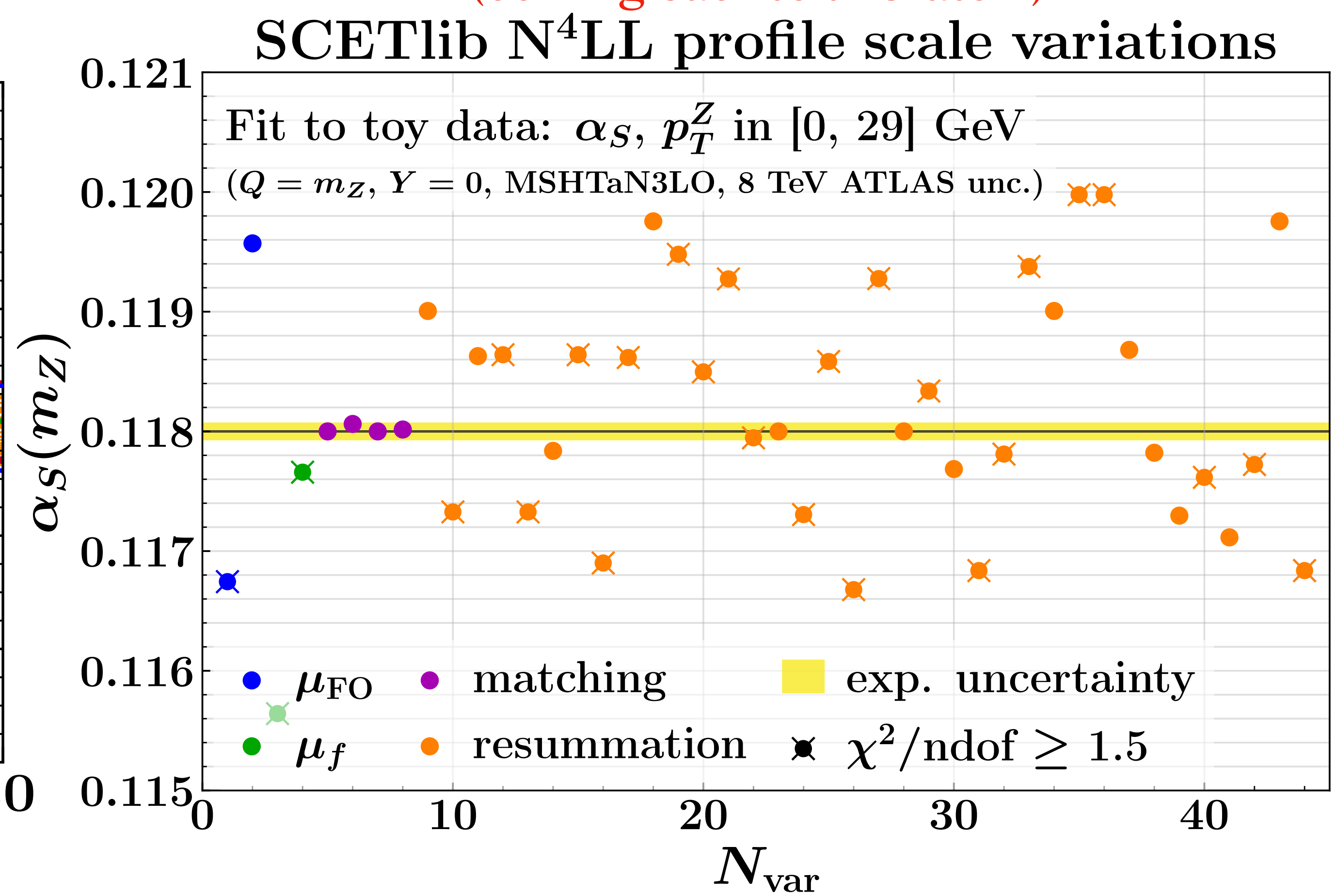
- α_S sensitivity in the q_T spectrum is a shape effect ⟶ theory correlations are crucial

* uncertainties in units of 10^{-3}

Naive approach: scale variations and scanning

Only fitting α_S, Asimov fit
(coming back to this later..)





- α_S sensitivity in the q_T spectrum is a shape effect $\longrightarrow$ theory correlations are crucial
- Each variation is a 100 % (anti)correlated correlation model, strongly impacts the result:

Sum in quadrature: $\Delta_{\rm total} = \sqrt{\Delta^2_{\rm FO} + \Delta^2_{\rm resum} + \Delta^2_{\rm match}} \sim 2.6$ [neglecting μ_f]

Envelope: $\Delta_{\rm total} \sim 2.1$

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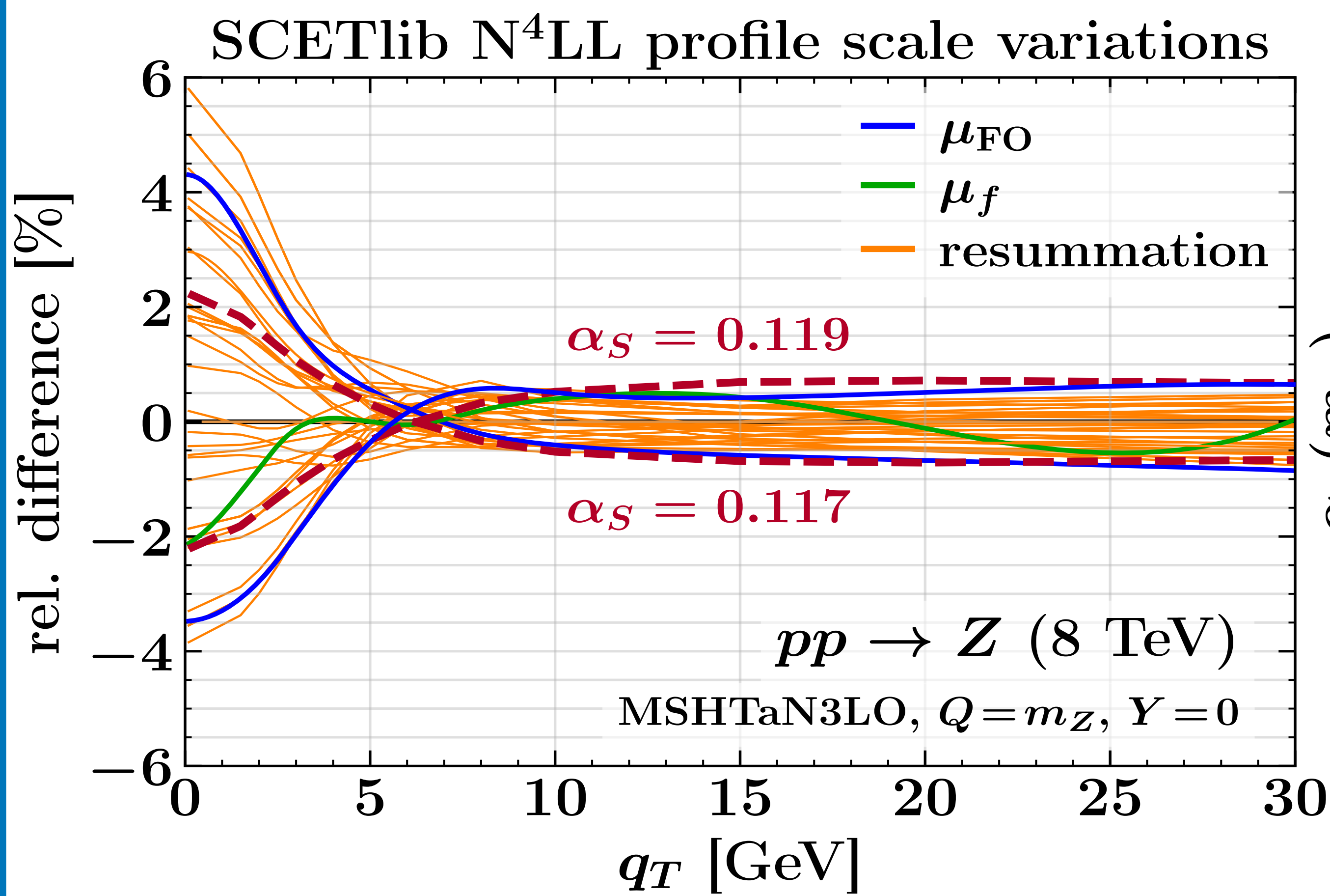

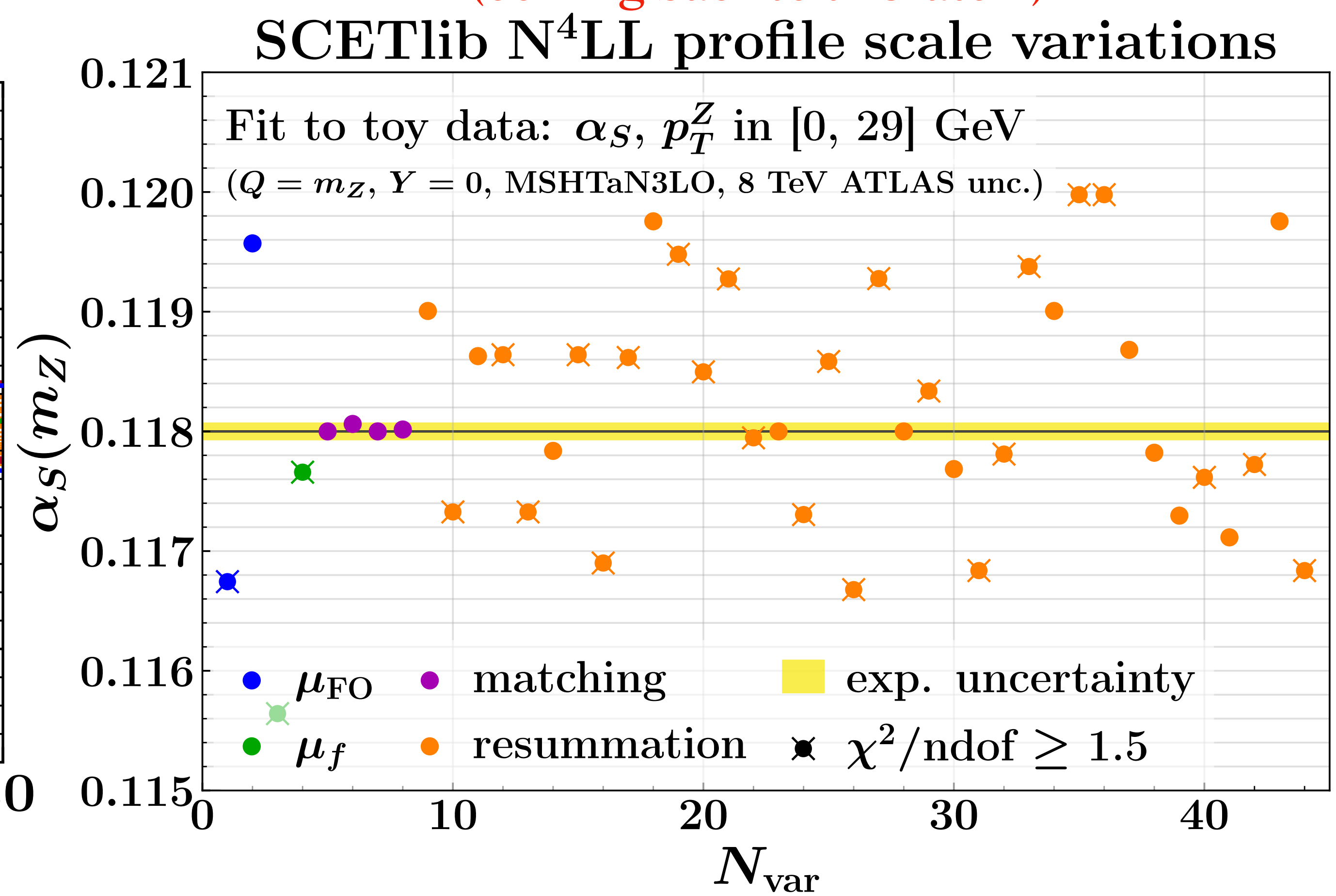

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Envelope: $\Delta_{\rm total} \sim 2.1$

scale variations are not sufficient! can we do better?

* uncertainties in units of 10^{-3}

Theory Nuisance Parameters (TNPs)

Consider a series expansion in a small parameter α:

$$f(\alpha) = \underbrace{f_0 + \alpha f_1 + \alpha^2 f_2}_{\text{NNLO}} + \alpha^3 f_3 + \alpha^4 f_4 + \mathcal{O}(\alpha^5)$$

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$$f(\alpha) = f_0 + \alpha f_1 + \alpha^2 f_2 + \alpha^3 f_3 + \alpha^4 f_4 + \mathcal{O}(\alpha^5)$$

2. Parametrized and include the leading source of uncertainty:

$$f^{\text{pred}}(\alpha) = f_0 + \alpha f_1 + \alpha^2 f_2 + \alpha^3 f_3\left(\theta_3\right) + \mathcal{O}\left(\alpha_S^4\right) \longrightarrow \text{named N}^{2+1}\text{LO}$$

using theory nuisance parameters θ_n ;

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using theory nuisance parameters θ_n ;

- the expansion converges, so the next order [f_4] is not yet relevant;
- once f_3 is known (or strongly constrained), include the next order;
- θ_n have physical value, true parameters

Theory Nuisance Parameters (TNPs)

3 How to ***define*** these θ_n?

- simplest case: $f_3(\theta_3) \equiv \theta_3$
- better: account for the internal structure of f_3
  (given the process: partonic channels, color, ...)

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Consider the p_T spectrum, leading power p_T dependence is know to all orders:

$$p_T \frac{d\sigma}{dp_T} = \left[H \times B_a \otimes B_b \otimes S \right] (\alpha_S, L \equiv \ln p_T/m_Z) + \mathcal{O}\left(\frac{p_T^2}{m_Z^2}\right)$$

$F = \{H, B, S\}$ solution to RGE equations

$$F(\alpha_S, L) = F(\alpha_S) \exp \int_0^L dL' \{ \Gamma[\alpha_S(L')] L' + \gamma_F [\alpha_S(L')] \}$$

$F(\alpha_S)$: boundary conditions

$\Gamma[\alpha_S(L')]$ and $\gamma_F[\alpha_S(L')]$: anomalous dimensions

TNPs in the p_T spectrum

Have three independent scalar perturbative series, for N^{2+1}LL:

$$F(\alpha_S) = 1 + \sum_{n=1} \left(\frac{\alpha_S}{4\pi}\right)^n F_n \longrightarrow F(\alpha_S) = 1 + \frac{\alpha_S}{4\pi} F_1 + \left(\frac{\alpha_S}{4\pi}\right)^2 F_2(\theta_2^F)$$

$$\gamma(\alpha_S) = \sum_{n=0} \left(\frac{\alpha_S}{4\pi}\right)^{n+1} \gamma_n$$

$$\gamma_F(\alpha_S) = \frac{\alpha_S}{4\pi}\gamma_{F0} + \left(\frac{\alpha_S}{4\pi}\right)^2 \gamma_{F1} + \left(\frac{\alpha_S}{4\pi}\right)^3 \gamma_{F,2}(\theta_3^\gamma)$$

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- Pulling out known color factor:

$$F_n(\theta_n) = 4C_r(4C_A)^{n-1}(n-1)!\,\theta_n^F \qquad C_r \text{ leading color factor}$$

$$\gamma_n(\theta_n) = 2C_r(4C_A)^n\,\theta_n^\gamma \qquad C_A^{n-1} \text{ leading } n\text{−loop color factor}$$

TNPs in the p_T spectrum

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factorizing out $\left(\frac{\alpha_S}{4\pi}\right)^n$	1	+4.9	−24.0	−4065.5	−123979.0	C_{gg}

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factorizing out $C_r C_A^{n-1}$	1	+0.4	−0.2	−2.4	−5.9	
factorizing out $(n-1)!$	1	+0.4	−0.2	−1.2	−1.0	

$\longrightarrow$ $\theta_n \sim \mathcal{O}(1)$

TNPs in the p_T spectrum

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factorizing out $\left(\frac{\alpha_S}{4\pi}\right)^n$	1	+4.9	−24.0	−4065.5	−123979.0	C_{gg}
	1	−8.5	−48.6	−1386.7	−42014.9	$C^V_{q\bar{q}}$
factorizing out 4^n	1	+1.2	−1.5	−63.5	−484.3	
	1	−2.1	−3.0	−21.7	−164.1	
factorizing out $C_r C_A^{n-1}$	1	+0.4	−0.2	−2.4	−5.9	
	1	−1.6	−0.8	−1.8	−4.6	
factorizing out $(n-1)!$	1	+0.4	−0.2	−1.2	−1.0	
	1	−1.6	−0.8	−0.9	−0.8	

⟶ $\theta_n = 0 \pm \mathcal{O}(1)$

TNPs in the p_T spectrum

4 How to ***vary*** θ_n?

$$\gamma_n(\theta_n) = 2C_r(4C_A)^n\,\theta_n^{\gamma}$$

$$\text{AD:}\quad \gamma(\alpha_S) = \frac{\alpha_S}{4\pi}\gamma_1 + \left(\frac{\alpha_S}{4\pi}\right)^2\gamma_2 + \left(\frac{\alpha_S}{4\pi}\right)^3\gamma_3 + \left(\frac{\alpha_S}{4\pi}\right)^4\gamma_4 + \left(\frac{\alpha_S}{4\pi}\right)^5\gamma_5 + \mathcal{O}\left(\alpha_S^6\right)$$

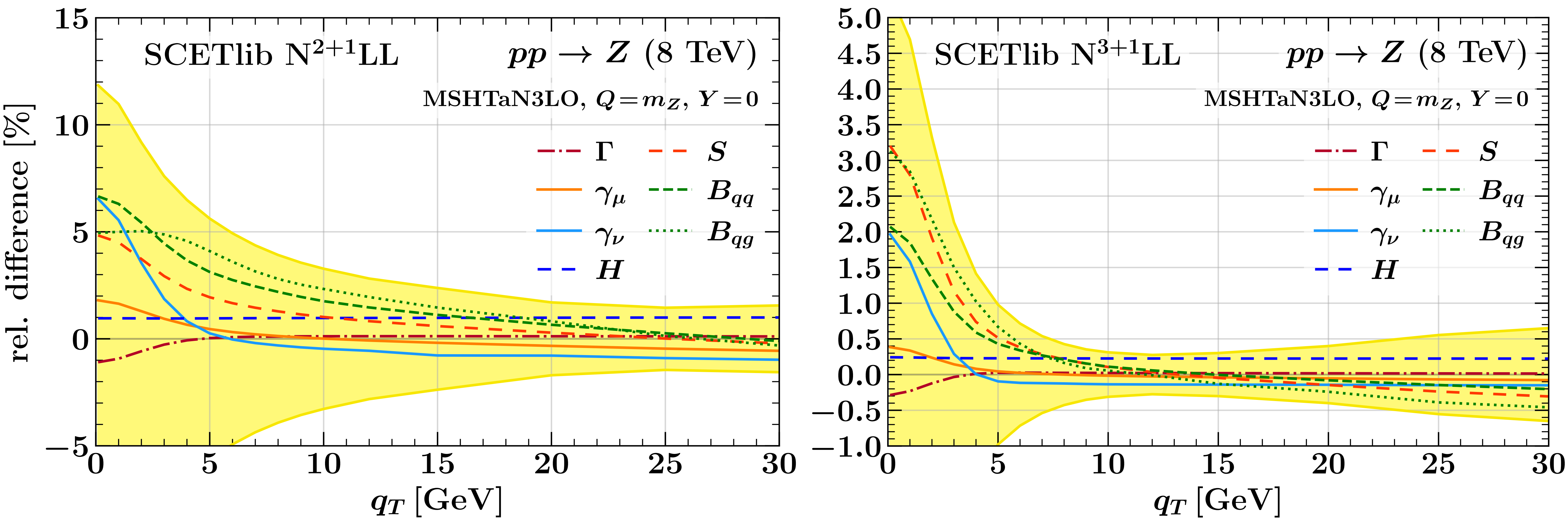
factorizing out $\left(\frac{\alpha_S}{4\pi}\right)^n$	4.0	56.2	474.9	2824.8	42824.1	$-\gamma_m/2$
	5.3	36.8	239.2	141.2	70000.0	Γ_{cusp}
factorizing out $2\cdot 4^n$	2.0	7.0	14.8	22.1	83.6	
	2.7	4.6	7.5	1.1	136.7	
factorizing out $C_rC_A^n$	1.5	1.8	1.2	0.6	0.8	
	2.0	1.5	0.6	0.03	1.3	

- Iterate this game with different functions and do some "statistics": $\longrightarrow$ $\theta_n = 0 \pm 1$

  look at known $n-$loop coefficients from population sample here

Application of TNPs to Z p_T spectrum

Remember $N^{k+1}LL$: $N^{k+1}LL$ resummation structure + highest-order boundary conditions/ anomalous dim. as TNPs



- Varying each θ_i independently: correctly describe correlation across q_T
- Add in quadrature for the total uncertainty
- For the beams B_{qj} : $f_n = (0 \pm 1.5) \times f_n^{\text{true}}$, DGLAP splitting functions not varied

many other interesting plots here

Going towards α_S

Asimov test fitting $\alpha_S(m_Z)$ from $Z\, p_T$

Use TNPs to study the expected uncertainty/sensitivity on α_S on toy data (**Asimov test**)

Our theory inputs:

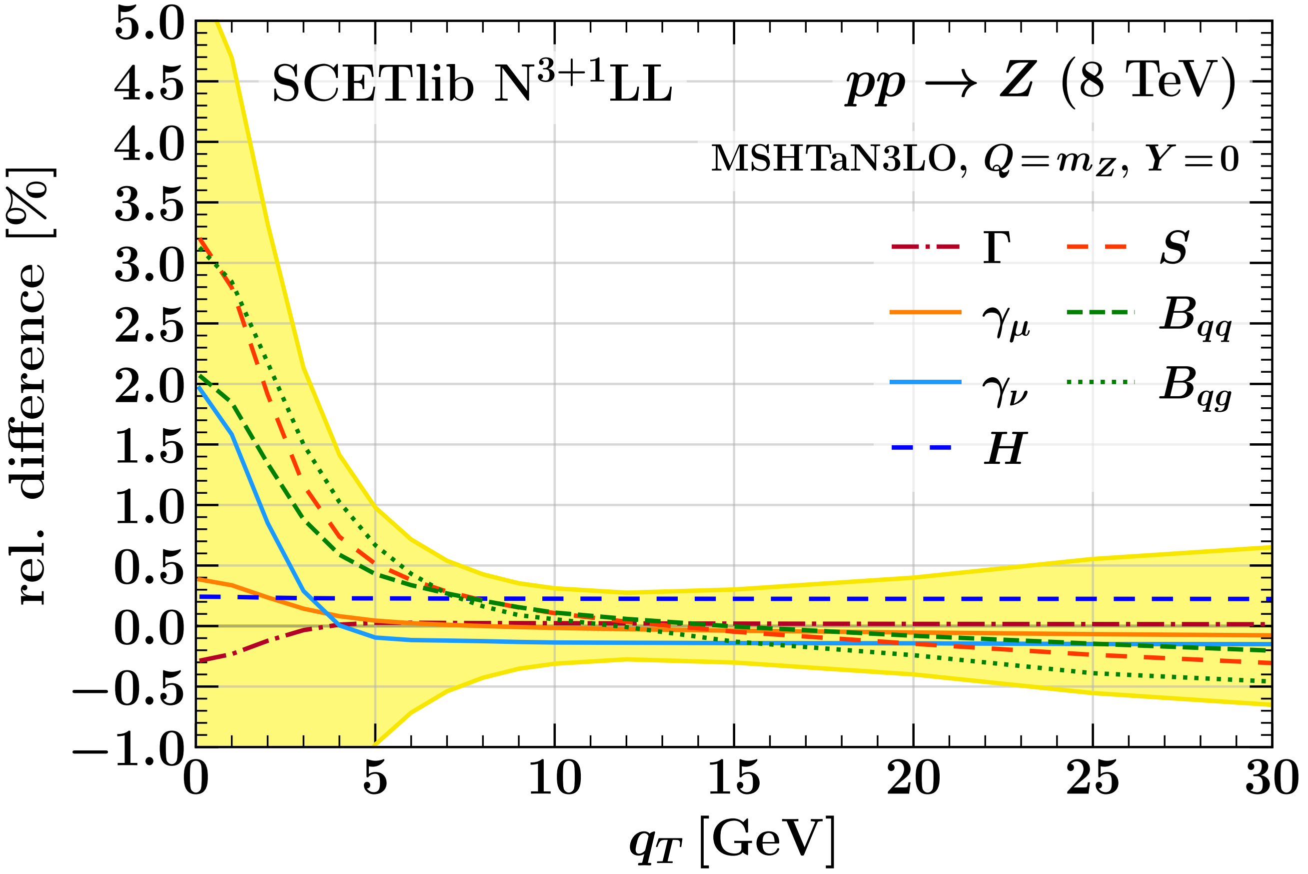
- SCETlib only $\mathrm{N^{3+1}LL}$ resummed contribution
  [default central scales and variations, no mass corrections and nonsingular power corrections*]

Our toy data:

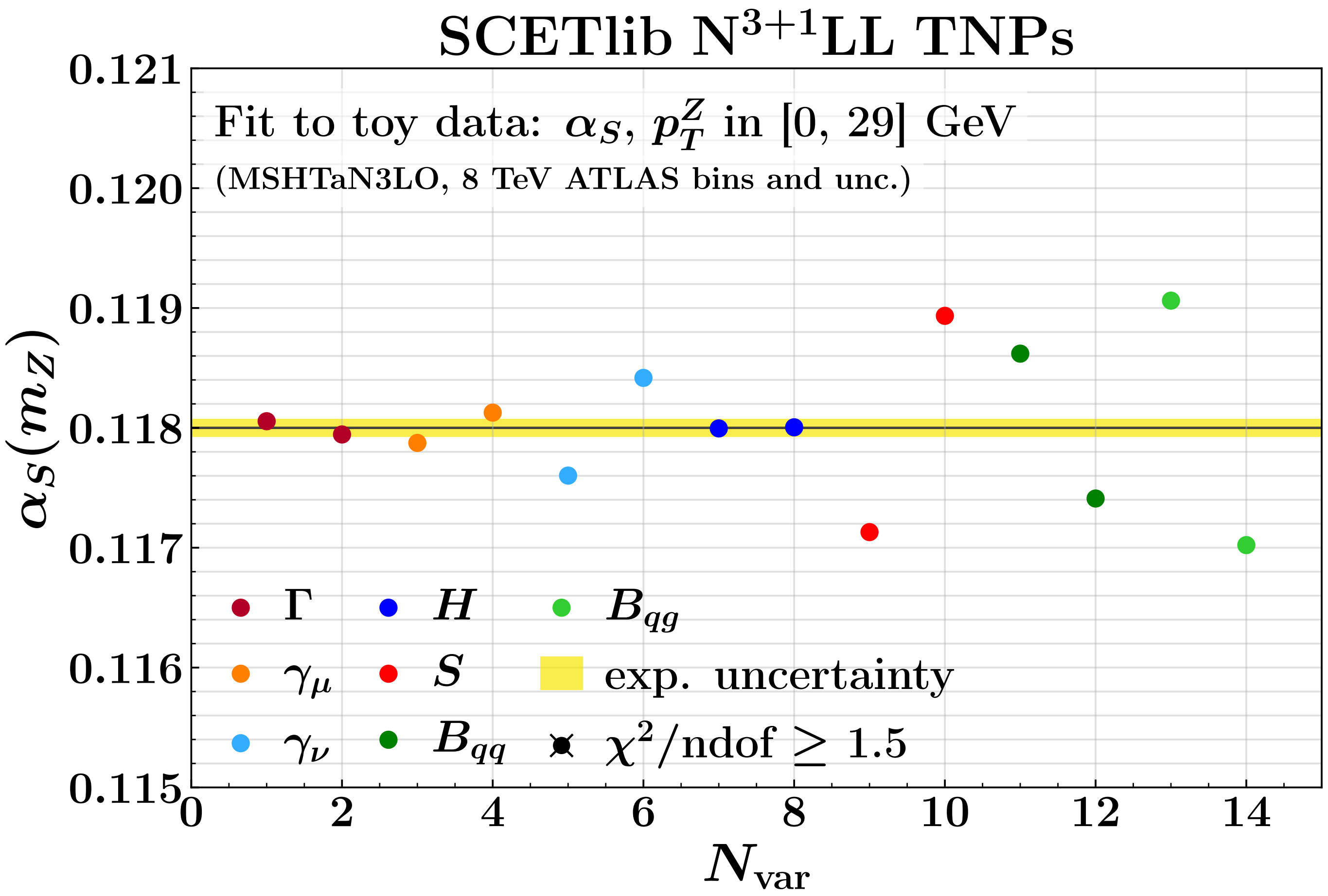
- Data defined as central theory prediction $[\alpha_S = 0.118]$
  [fixed nonp. params, MSHT20aN3LO PDF set]
- 72 data points in ATLAS binning,
  9 q_T bins in [0,29] GeV for each 8 Y bin in [0.0,3.6]
  [integrated in q_T, Y and Q]
- Using ATLAS exp. uncertainties and complete correlations for all 72 bins
- Using Minuit as minimizer for the fit

[*nonsingular p.c. don't affect our conclusions, obviously necessary when fitting against real data]

Scanning TNPs



Only fitting α_S



Repeat fit for each TNP variation, using TNPs at $N^{3+1}LL$;
still does not let the fit decide between moving α_S or theory

TNPs correctly account for their correlations being an independent source of uncertainty ⟶ sum in quadrature: $\Delta_{\text{total}} = 1.6$

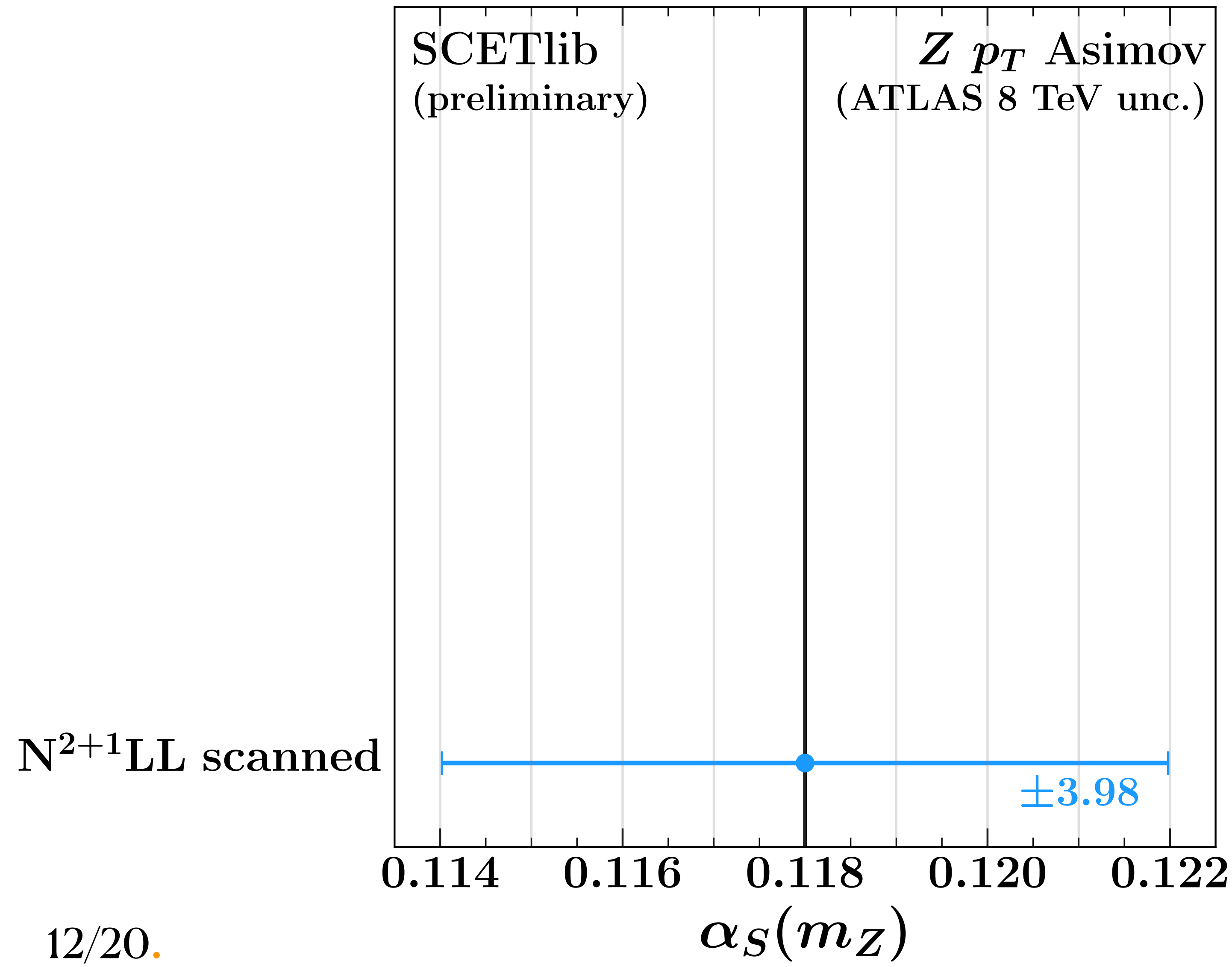
* uncertainties in units of 10^{-3}

Perturbative uncertainty in Asimov fit

Scanning: vary one TNP at a time and re-fit α_S

Profiling: fitting α_S *together* with all TNPs (allow the fit to decide what to do)

- Fit $N^{2+1}LL$ against $N^{2+1}LL$ data



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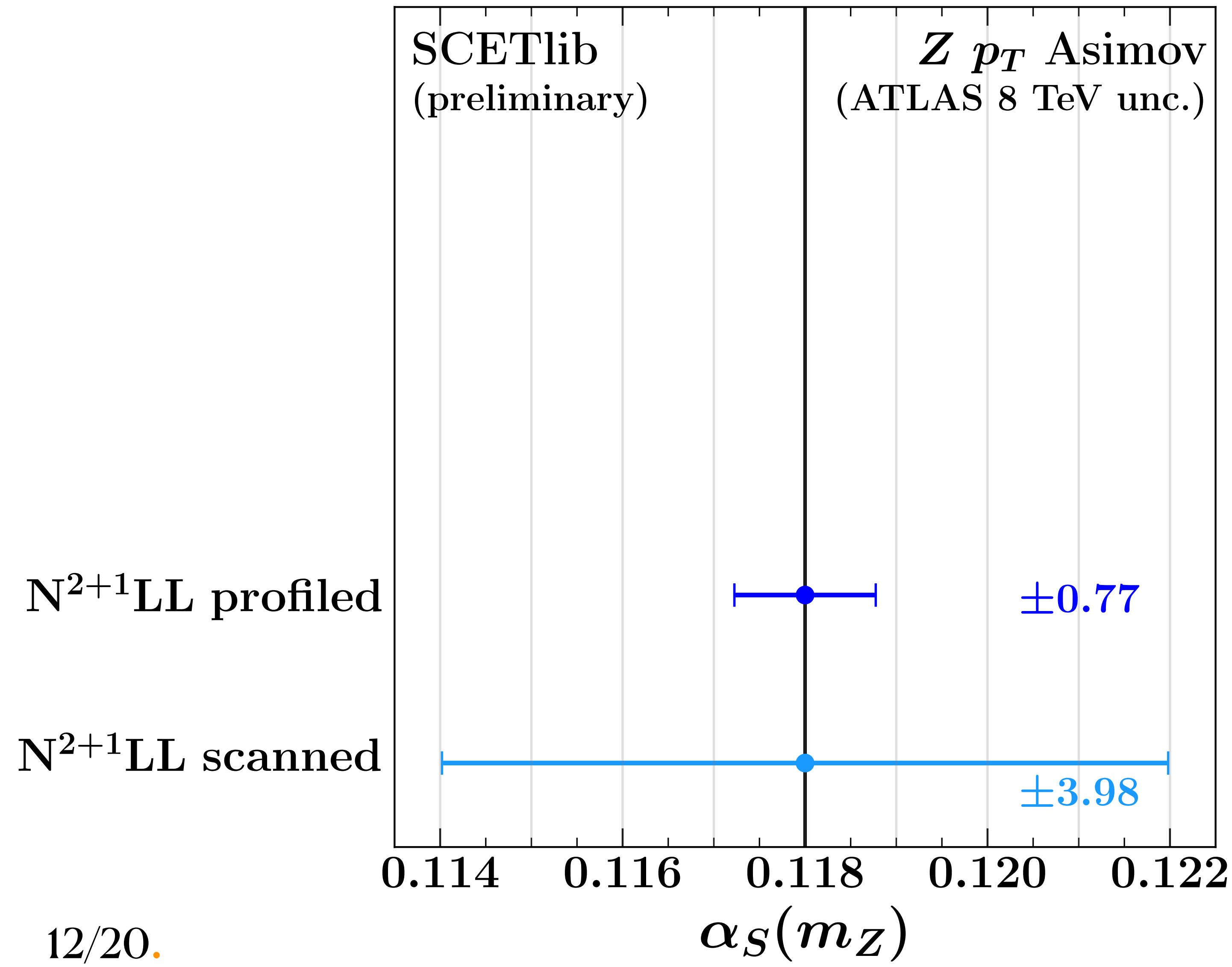

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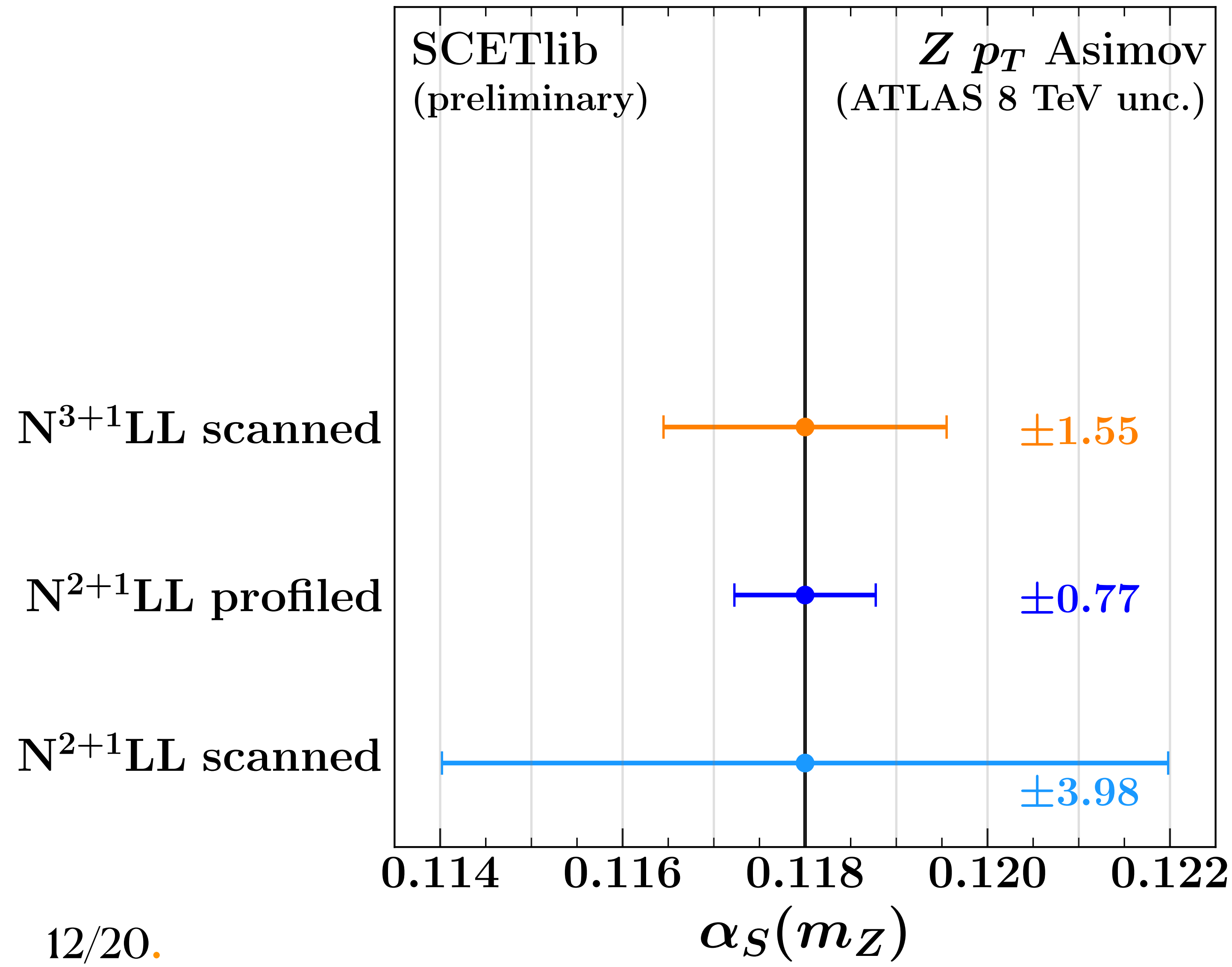
- Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



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Perturbative uncertainty in Asimov fit

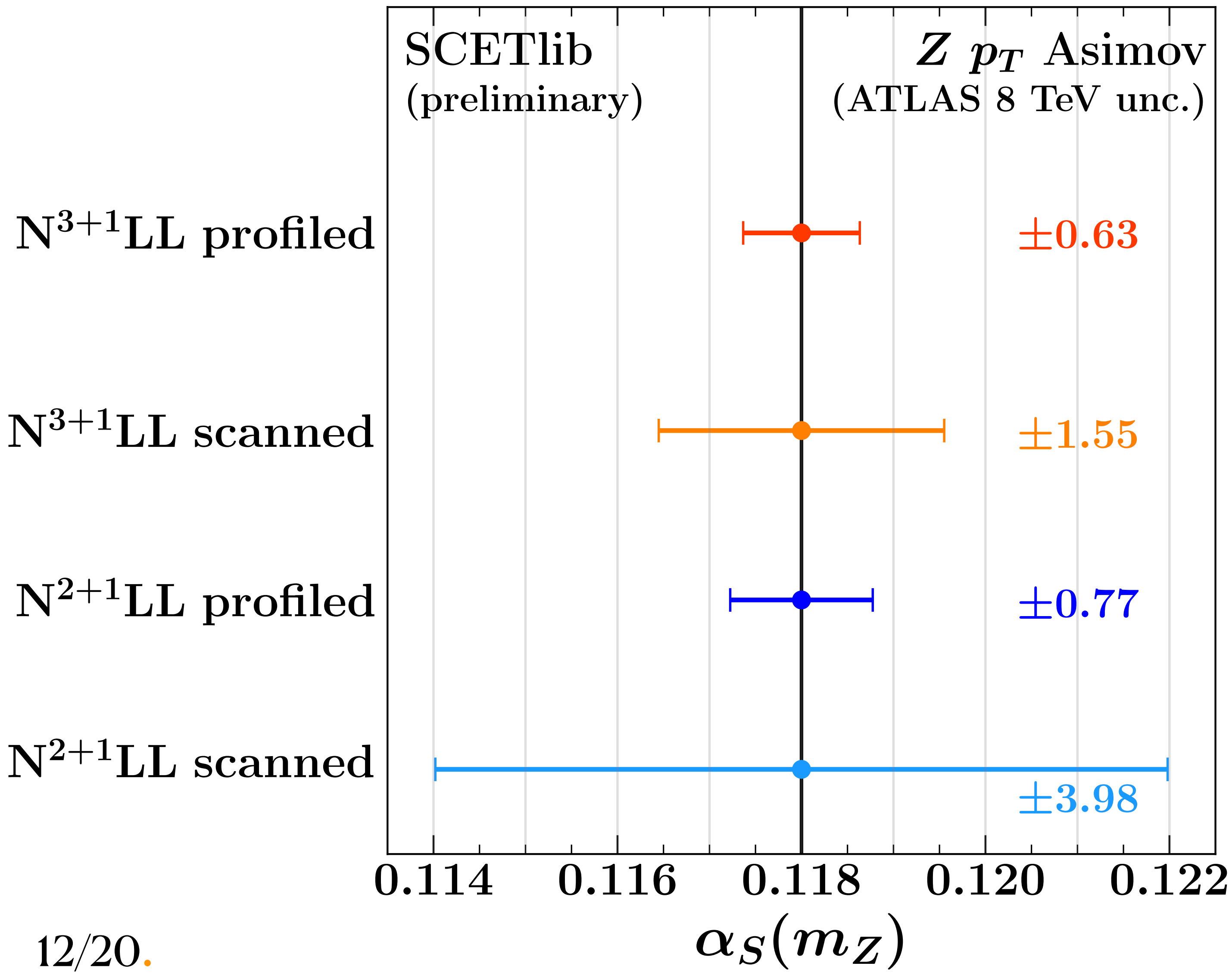
Scanning: vary one TNP at a time and re-fit α_S

Profiling: fitting α_S *together* with all TNPs (allow the fit to decide what to do)

- Fit $N^{2+1}LL$ against $N^{2+1}LL$ data
- Fit $N^{3+1}LL$ against $N^{3+1}LL$ data

profiling constraints the TNPs allowing data to reduce the theory uncertainty!

still need to look at the TNPs pull plot to understand the post-fit uncertainty



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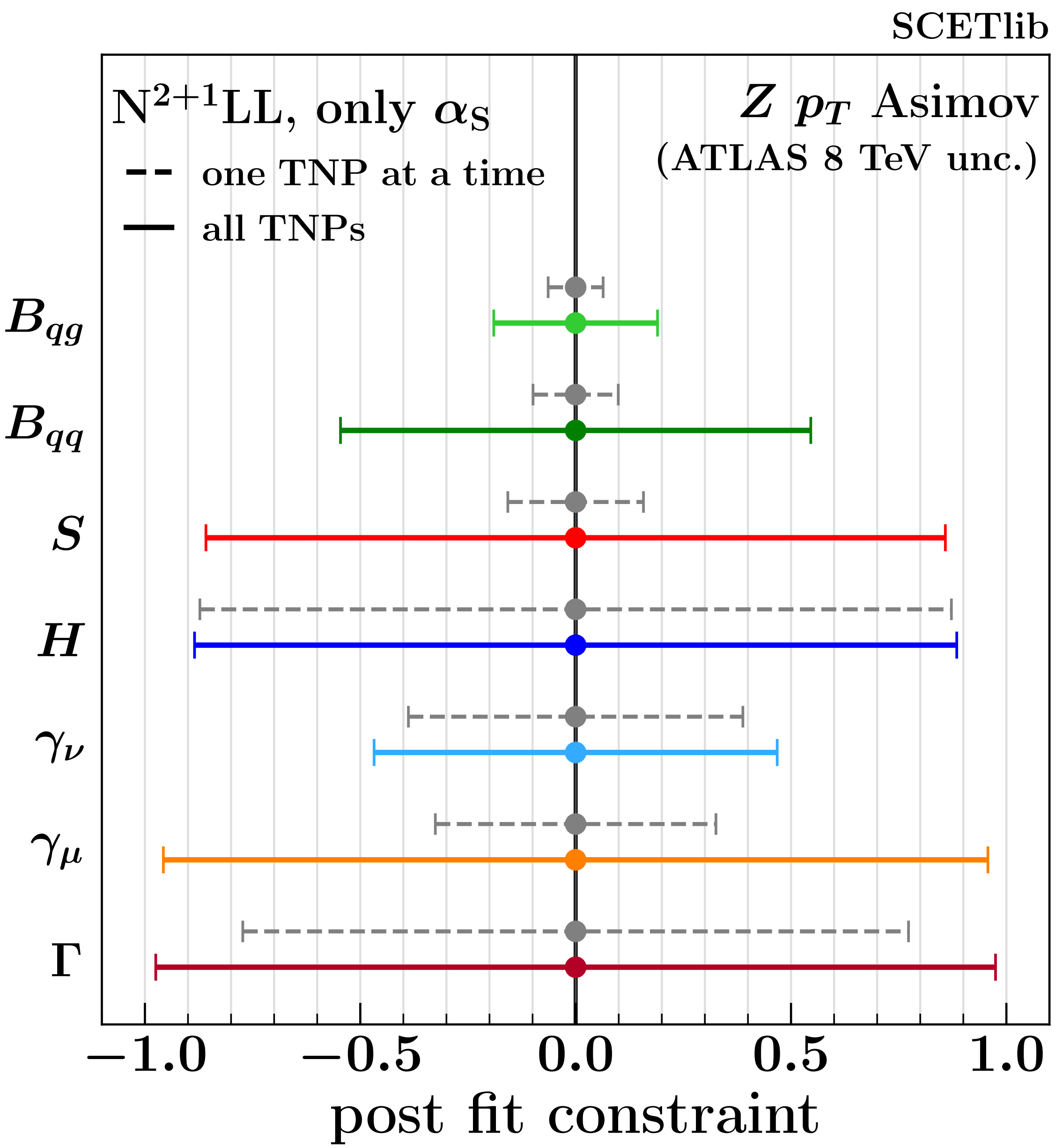
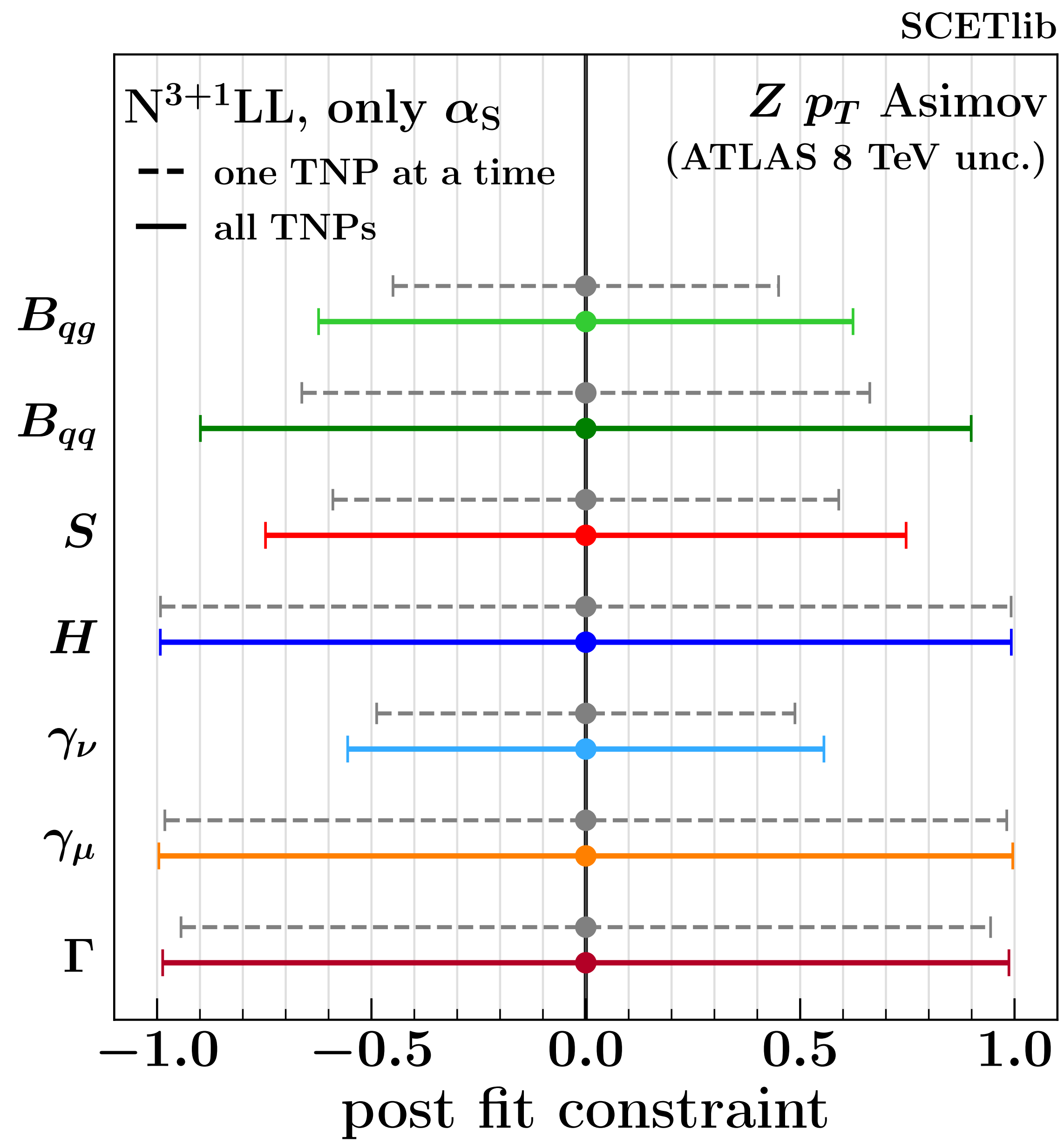
Constraints on TNPs





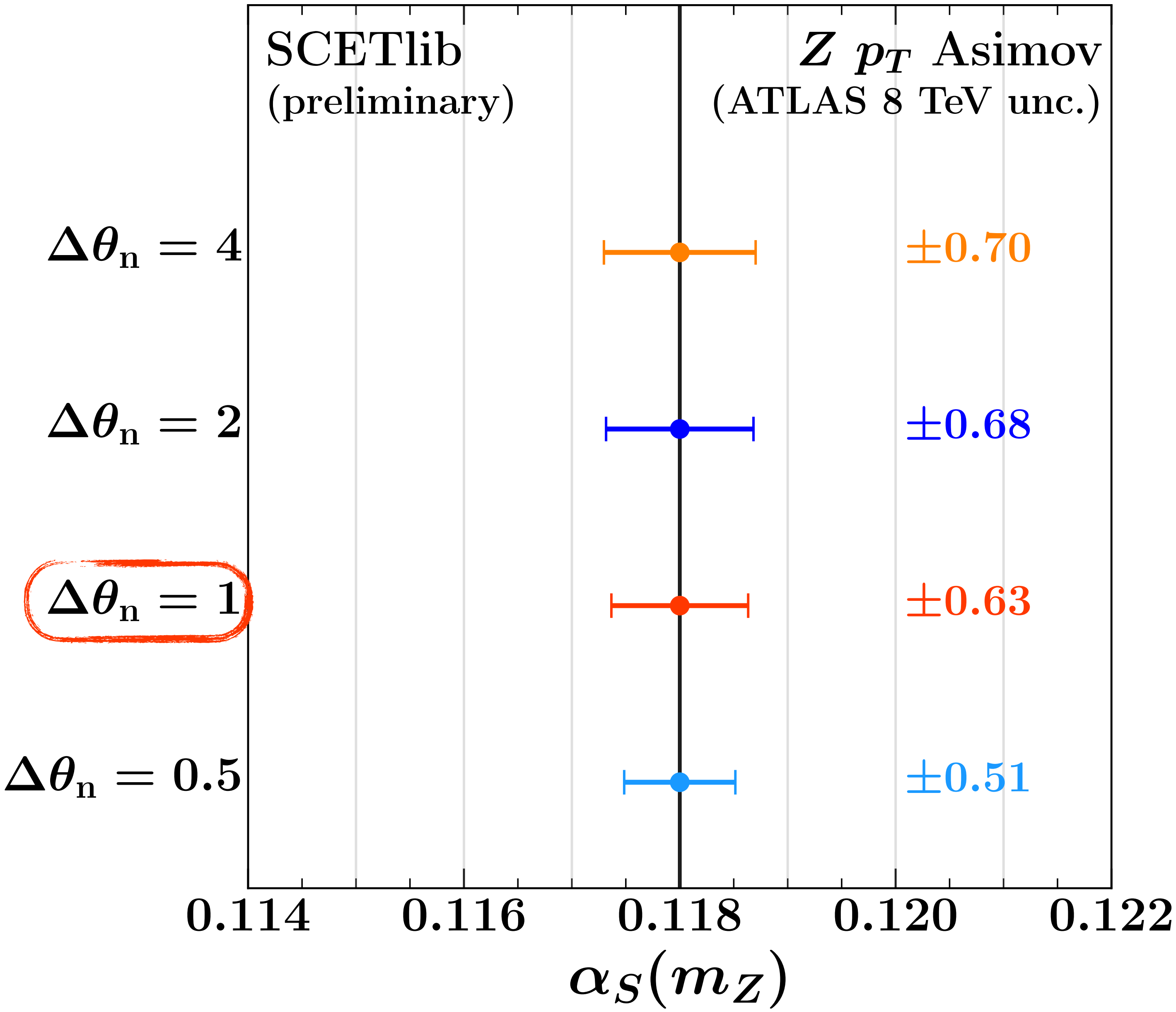
- $N^{2+1}LL$: TNPs much more constrained than at $N^{3+1}LL$
- If TNPs get strongly constrained, the next order becomes relevant for the uncertainty correlations!

Different constraints on TNPs

What happens by changing the prior theory constraint?

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 0.5, 1, 2, 4$

Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



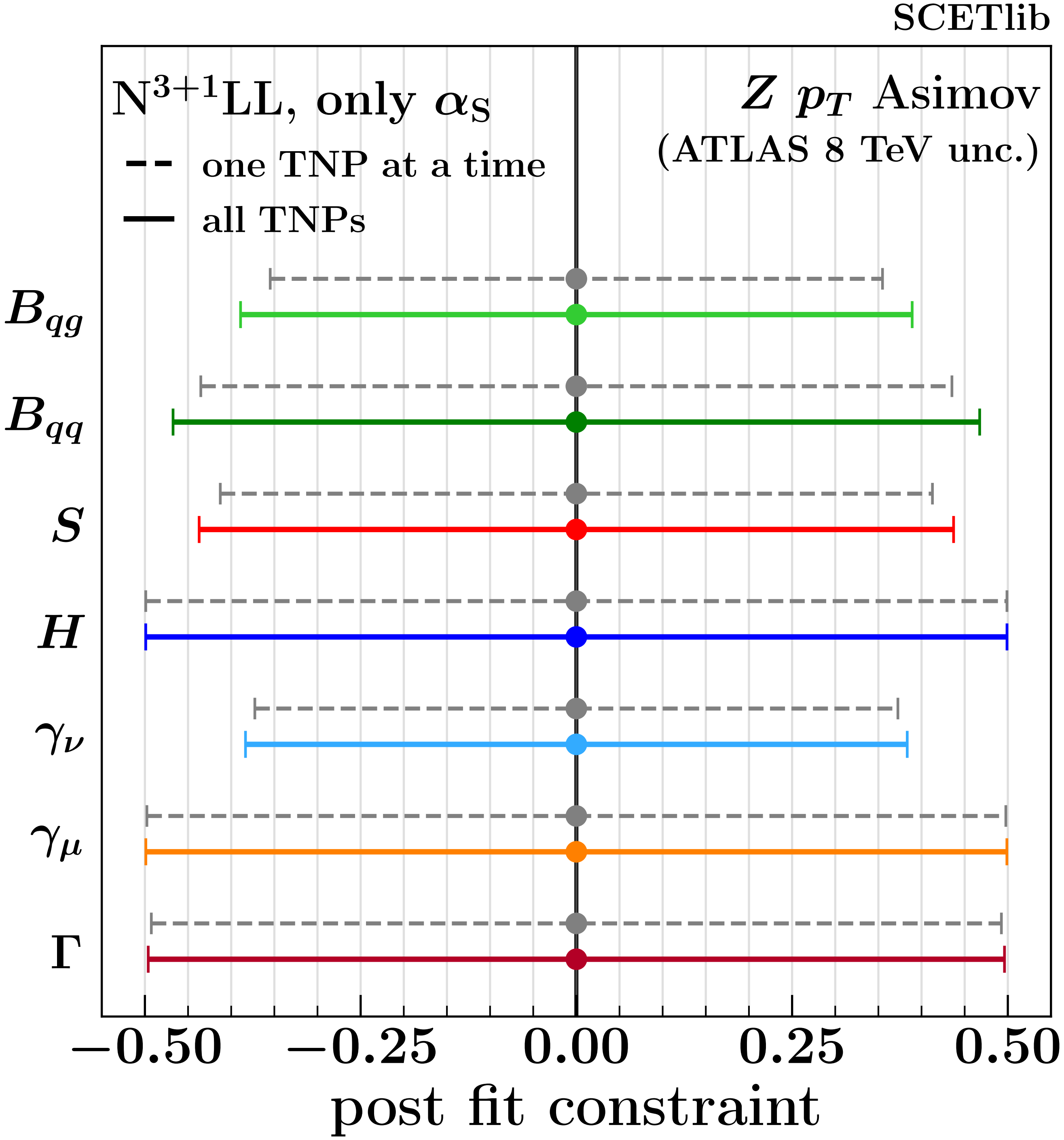
- The effect strongly depends on the power of the experimental constraint
- Only slight increase in the uncertainties when relaxing the TNPs constraint
- Again, need to look at the TNPs pull plot to understand the post-fit uncertainty

* uncertainties in units of 10^{-3}

Different constraints on TNPs

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 0.5$

Fit N^{3+1}LL against N^{3+1}LL data

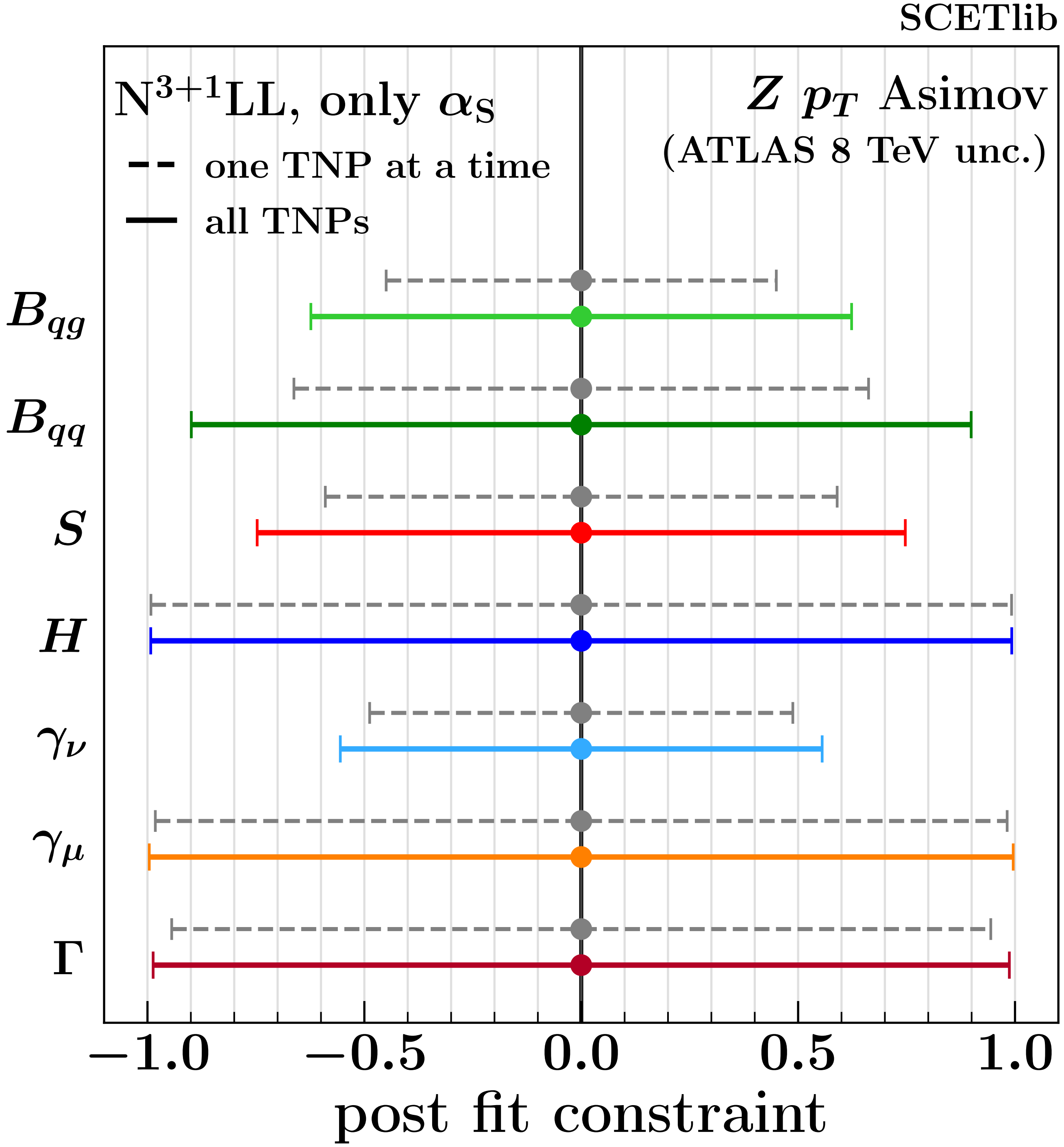


[don't be fooled by the different range!]

1. $\Delta\theta_n = 0.5$ not really constrained by exp., but very tight theory constraint for TNPs [exp. uncert. $\gtrsim$ theory uncert.]

Different constraints on TNPs

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 1$



[don't be fooled by the different range!]

Fit N^{3+1}LL against N^{3+1}LL data

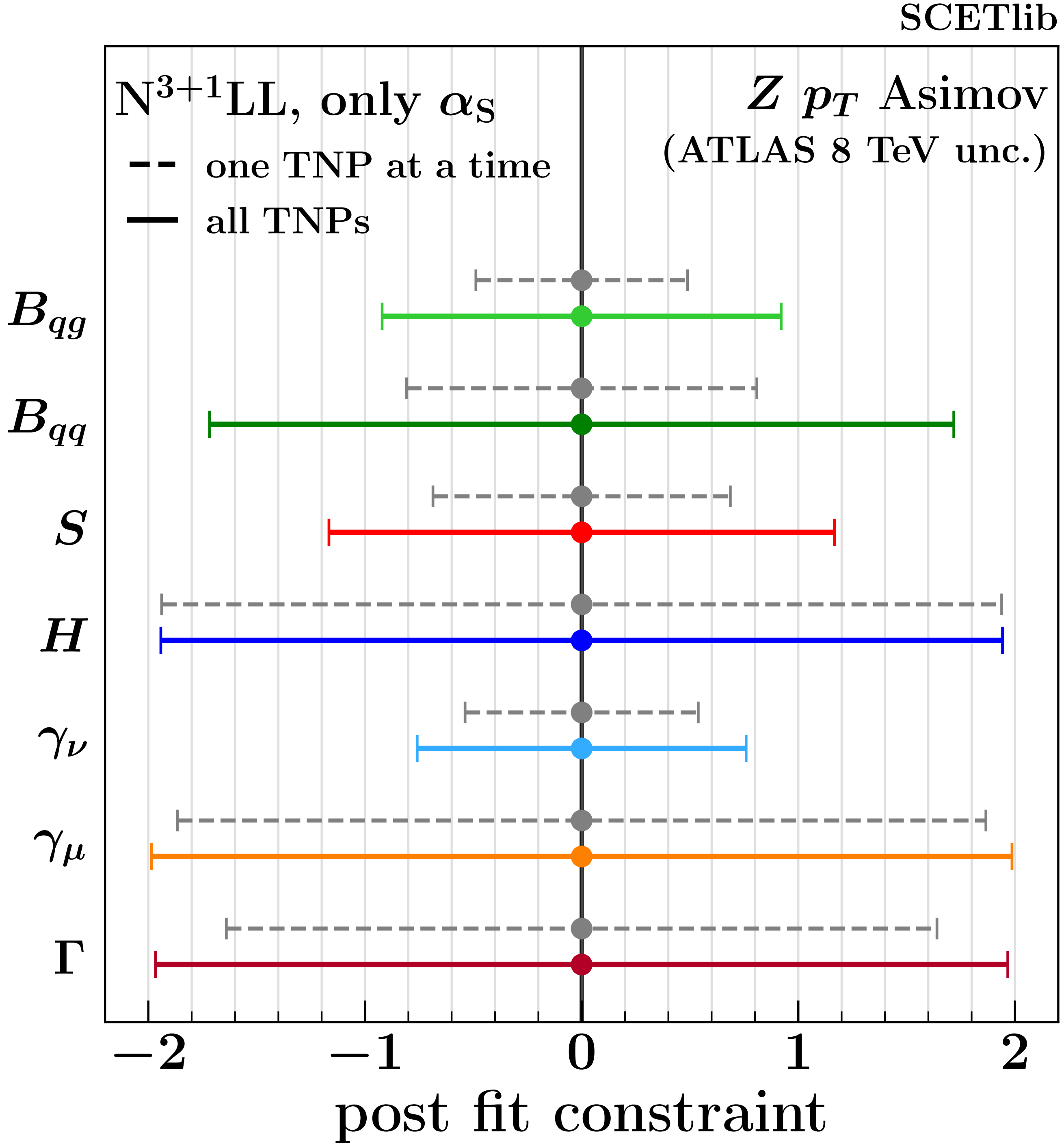
1. $\Delta\theta_n = 0.5$ not really constrained by exp., but very tight theory constraint for TNPs
   [exp. uncert. $\gtrsim$ theory uncert.]

2. $\Delta\theta_n = 1$ start seeing the exp. constraint

Different constraints on TNPs

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 2$

Fit N^{3+1}LL against N^{3+1}LL data



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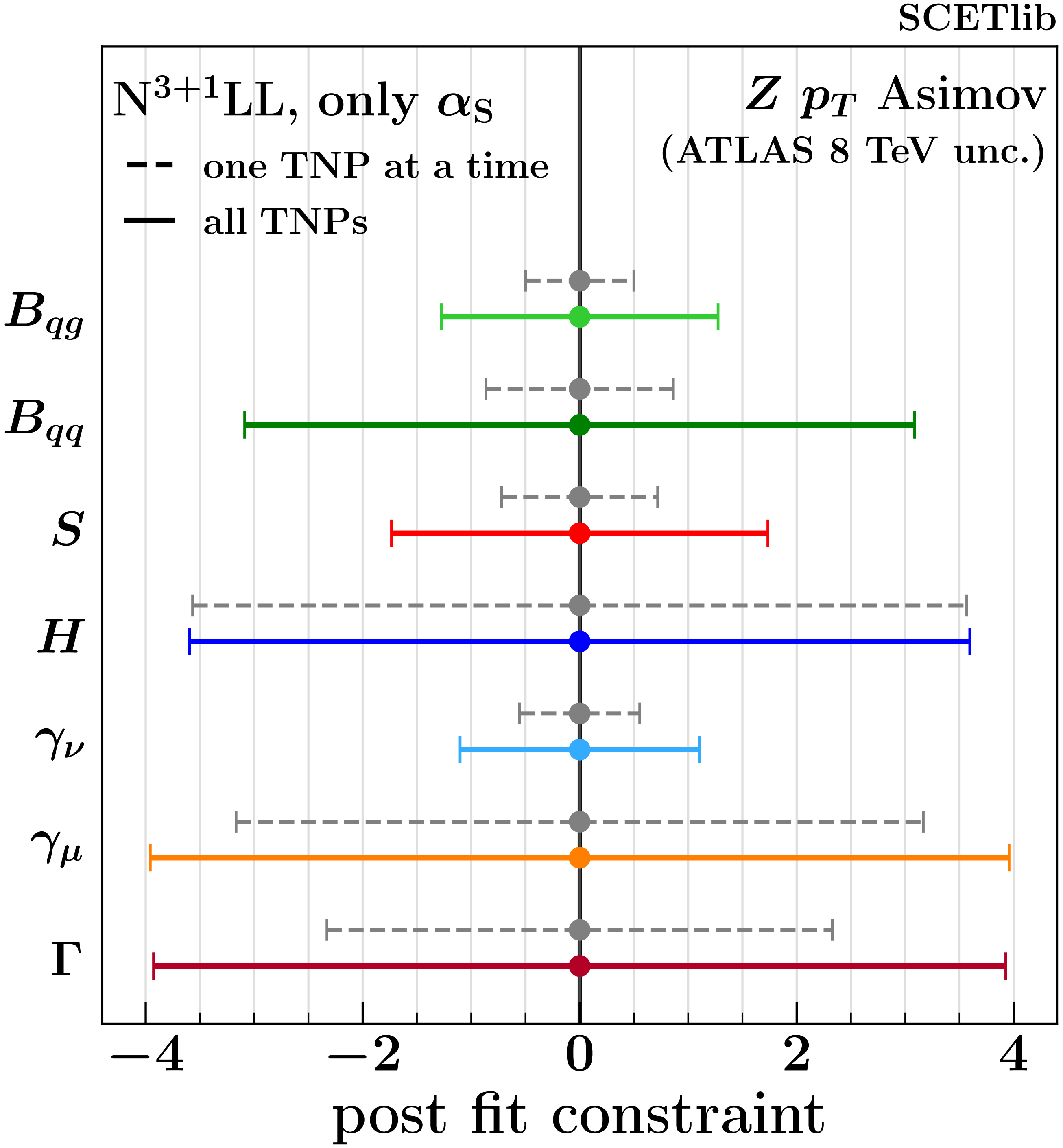
1. $\Delta\theta_n = 0.5$ not really constrained by exp., but very tight theory constraint for TNPs [exp. uncert. $\gtrsim$ theory uncert.]
2. $\Delta\theta_n = 1$ start seeing the exp. constraint
3. $\Delta\theta_n = 2$ it's basically a factor 2 w.r.t $\Delta\theta_n = 1$

Different constraints on TNPs

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 4$

Fit N^{3+1}LL against N^{3+1}LL data



[don't be fooled by the different range!]

1. $\Delta\theta_n = 0.5$ not really constrained by exp., but very tight theory constraint for TNPs [exp. uncert. $\gtrsim$ theory uncert.]
2. $\Delta\theta_n = 1$ start seeing the exp. constraint
3. $\Delta\theta_n = 2$ it's basically a factor 2 w.r.t $\Delta\theta_n = 1$
4. with $\Delta\theta_n = 4$ data can constrain TNPs more

Nonperturbative uncertainty in Asimov fit

1 Collins-Soper (CS) kernel [~ rapidity anomalous dimensions]:

$$\tilde{\gamma}_\nu(b_T) = \tilde{\gamma}_\nu^{\text{pert}}\left(b_6^*(b_T)\right) + \tilde{\gamma}_\nu^{\text{nonp}}(b_T) \qquad \tilde{\gamma}_\nu^{\text{nonp}}(b_T) = -\lambda_\infty f_\nu\left(\frac{\lambda_2}{\lambda_\infty}b_T^2 + \frac{\lambda_4}{\lambda_\infty}b_T^4\right)$$

2 Transverse Momentum Distributions (TMDs)[~ intrinsic k_T of the partons inside the protons]:

$$\tilde{f}(b_T) = \tilde{f}_{\text{pert}}(b_T)\, \tilde{f}_{\text{nonp}}(b_T) \qquad \ln\left(\tilde{f}_{\text{nonp}}(b_T)\right) = -\Lambda_\infty b_T\, f\left(\frac{\Lambda_2}{\Lambda_\infty}b_T + \frac{\Lambda_4}{\Lambda_\infty}b_T^3\right)$$

λ_2, λ_4 and Λ_2, Λ_4 quadratic/quartic small b_T coefficients

$\lambda_\infty, \Lambda_\infty$ determine $b_T \to \infty$ behavior

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From Collins and Rogers '14, $f_\nu(x)$ and $f(x)$ behavior

$$f_\nu(x \to 0) \sim x^2, \qquad f_\nu(x \to \infty) \sim const$$
$$\log\left(f(x \to 0)\right) \sim x^2, \qquad \log\left(f(x \to \infty)\right) \sim x$$

Nonperturbative uncertainty in Asimov fit

What is used in our fits:

$$f_\nu\left(\frac{\lambda_2}{\lambda_\infty}b_T^2+\frac{\lambda_4}{\lambda_\infty}b_T^4\right)=\tanh\left(\frac{\lambda_2}{\lambda_\infty}b_T^2+\frac{\lambda_4}{\lambda_\infty}b_T^4\right)$$

$$f\left(\frac{\Lambda_2}{\Lambda_\infty}b_T+\frac{\Lambda_4}{\Lambda_\infty}b_T^3\right)=2\tanh\left(\frac{\Lambda_2}{\Lambda_\infty}b_T+\frac{\Lambda_4}{\Lambda_\infty}b_T^3\right)$$

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Also using inputs from lattice QCD for the CS kernel [some details here]:

- exploit lattice QCD calculations of the CS kernel to obtain good constraints on λ_∞, λ_2 and λ_4

representative values:

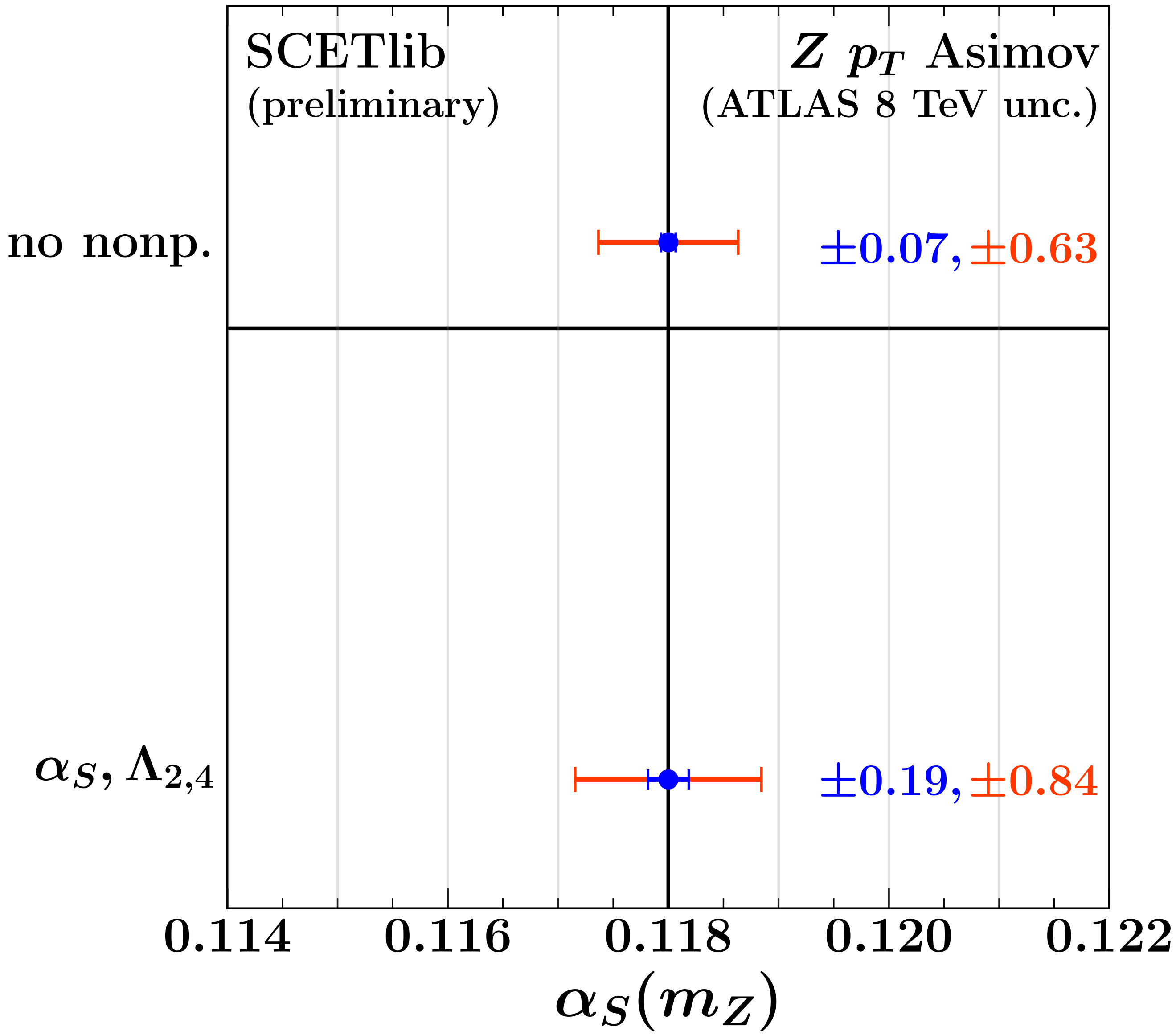
$$\lambda_\infty = 1.7 \pm 0.5$$
$$\lambda_2 = 0.09 \pm 0.03$$
$$\lambda_4 = 0.007 \pm 0.007$$

+ full covariance matrix from lattice fit

Nonperturbative uncertainty in Asimov fit

fit unc. only: fitting *only* α_S and nonp.
$N^{3+1}LL$ profiled: including TNPs

Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



- Fit only α_S, Λ_2 and Λ_4 (fixed $\tilde{\gamma}_\nu^{\rm nonp}$)

* uncertainties in units of 10^{-3}

Nonperturbative uncertainty in Asimov fit

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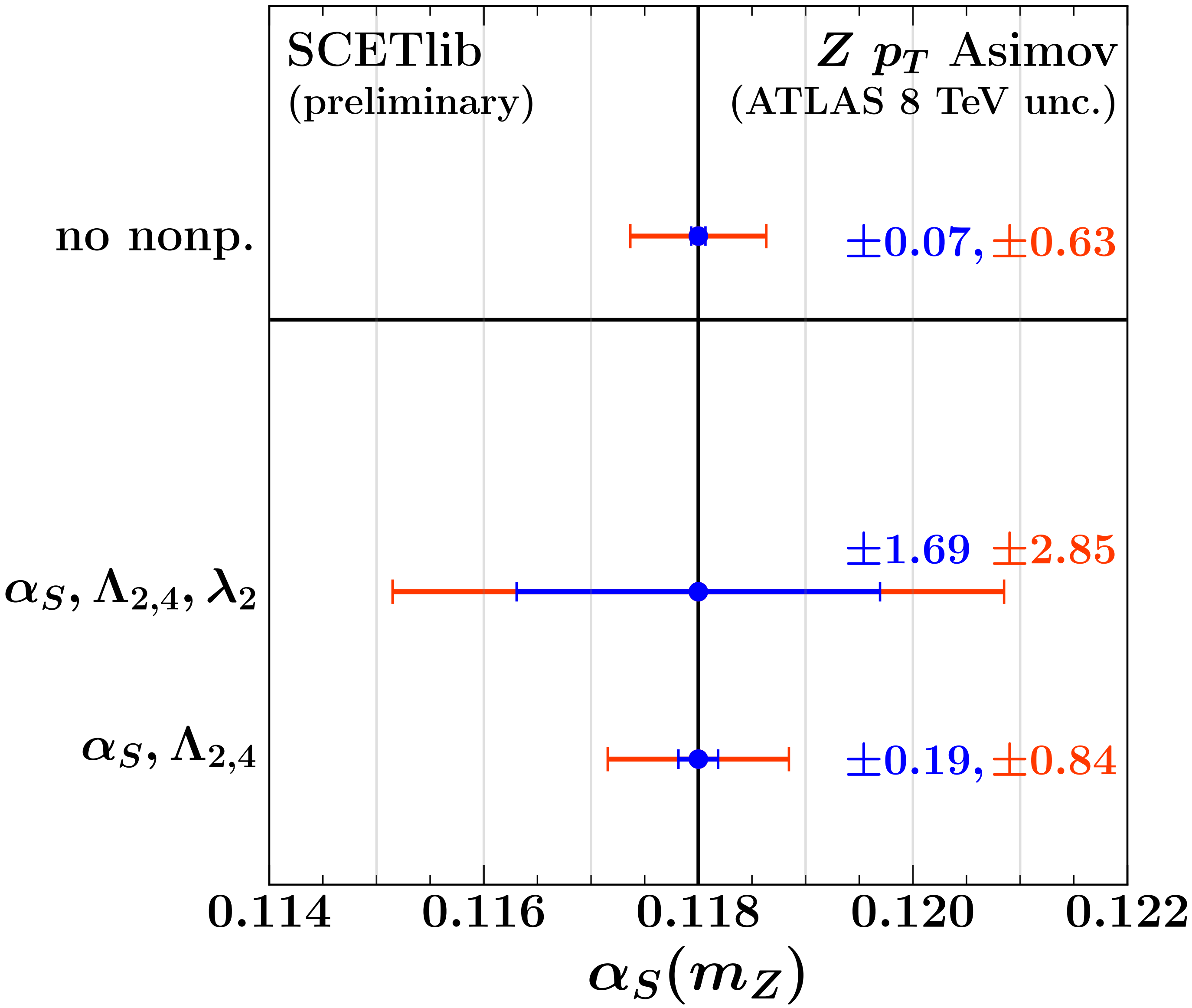

- Fit only α_S, Λ_2 and Λ_4 (fixed $\tilde{\gamma}_\nu^{\mathrm{nonp}}$)
- Not using lattice constraints
  parameters fitted: λ_2, Λ_2, Λ_4

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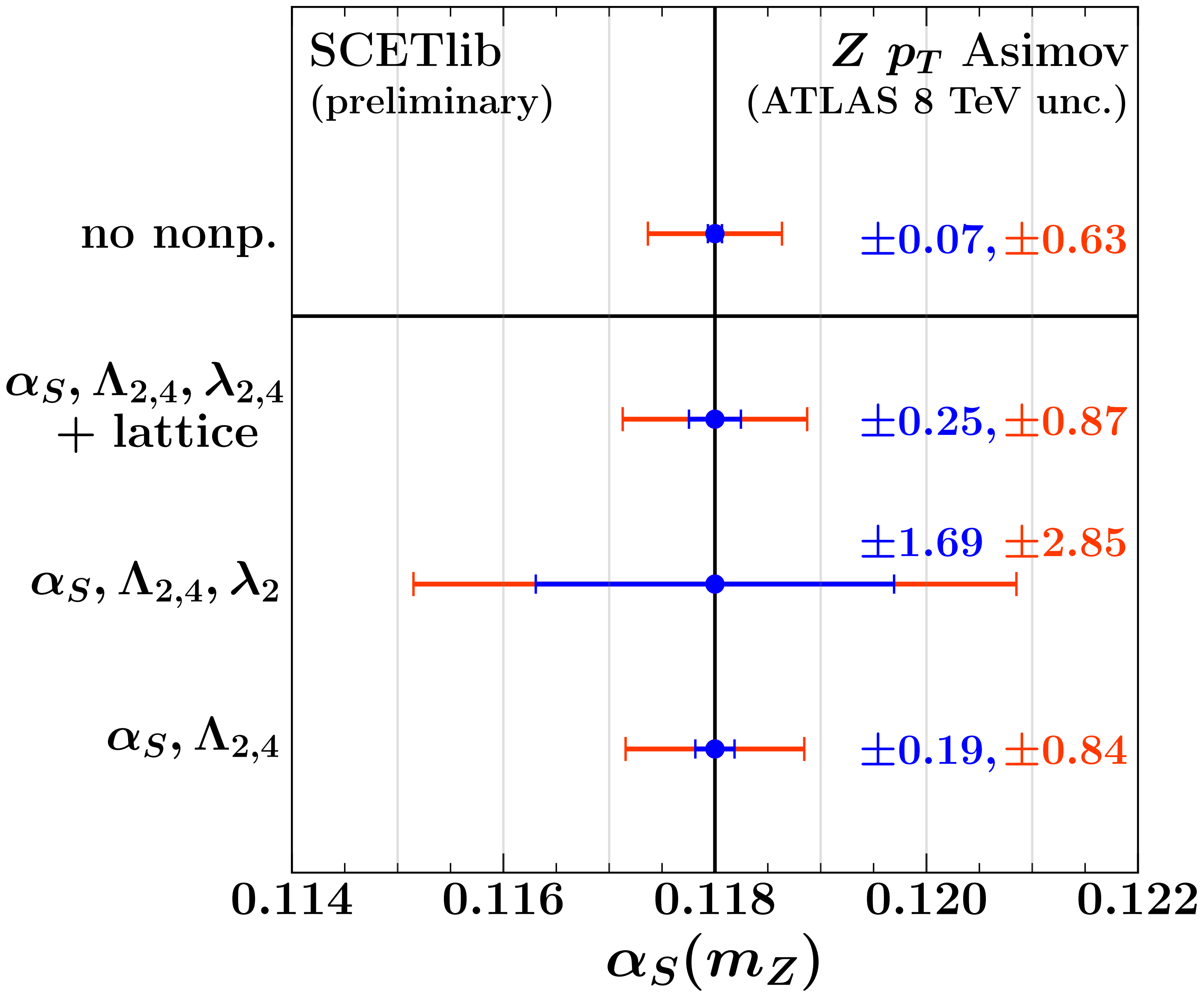
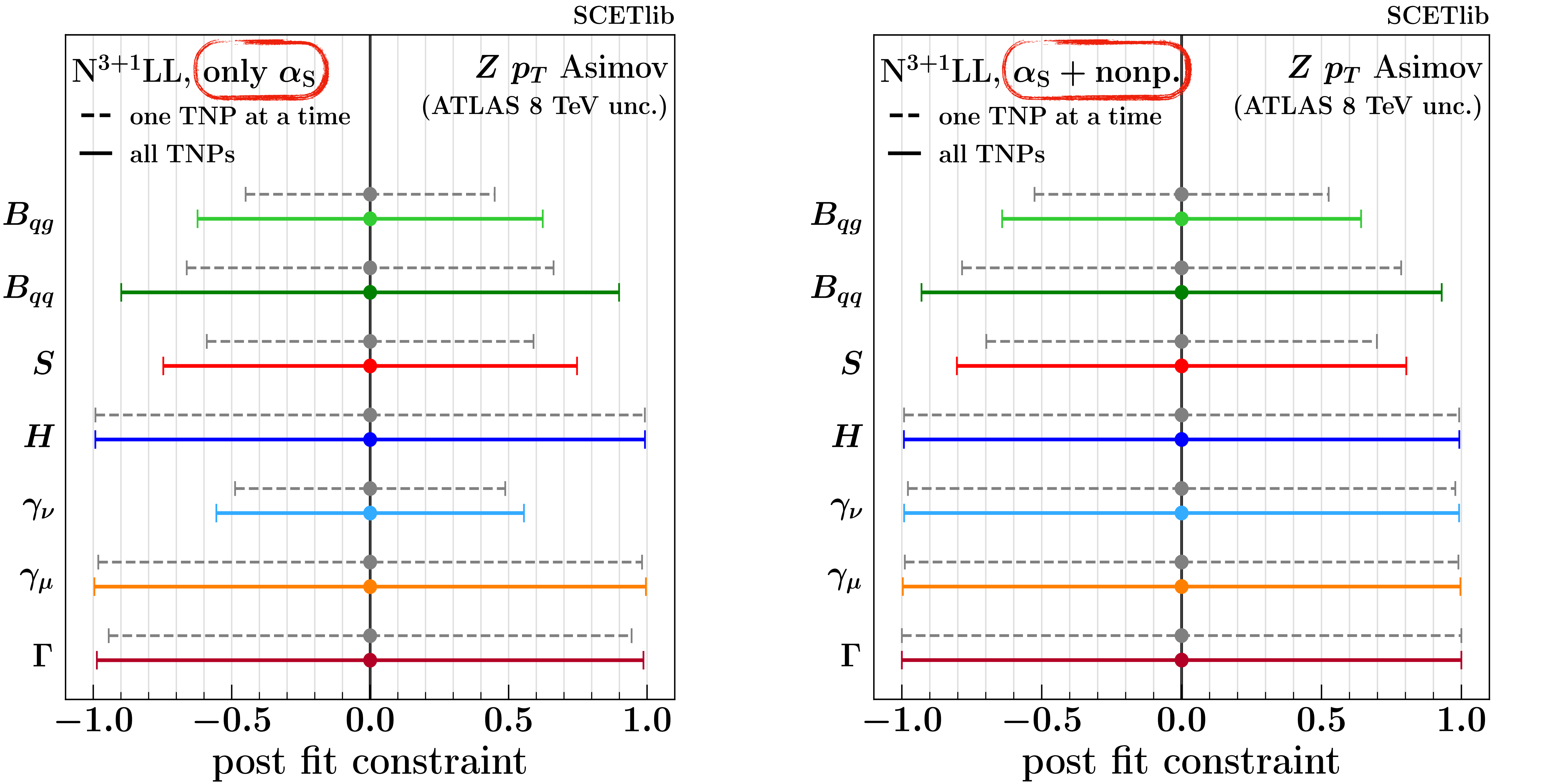


- Fit only α_S, Λ_2 and Λ_4 (fixed $\tilde{\gamma}_\nu^{\text{nonp}}$)
- Not using lattice constraints parameters fitted: λ_2, Λ_2, Λ_4
- Using lattice constraints parameters fitted: λ_2, λ_4, Λ_2, Λ_4

* uncertainties in units of 10^{-3}

Nonperturbative uncertainty in Asimov fit

- parameters fitted λ_2, λ_4, Λ_2, Λ_4 + lattice QCD constraints



Data now also constraint nonperturbative parameters, therefore less constraint on TNPs

plots with different $\Delta\theta_n$ for TNPs here

Conclusions

Need for theoretical predictions including correlations for interpretation of LHC precision measurements:

1. Theory Nuisance Parameters perfect candidate
   - include correct correlations across the p_T spectrum
   - can be constrained by data reducing theory uncertainty
   - work as advertised for Asimov tests
2. Nonperturbative model
   - importance of fitting CS kernel
   - can be improved with lattice constraints

Conclusions

Need for theoretical predictions including correlations for interpretation of LHC precision measurements:

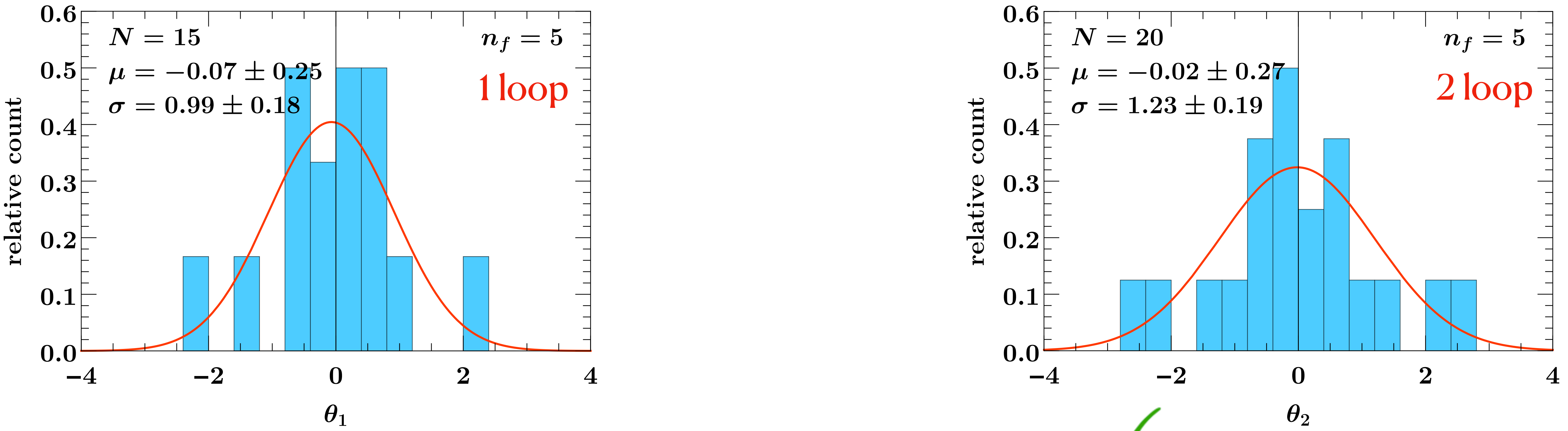
1. Theory Nuisance Parameters perfect candidate
   - include correct correlations across the p_T spectrum
   - can be constrained by data reducing theory uncertainty
   - work as advertised for Asimov tests
2. Nonperturbative model
   - importance of fitting CS kernel
   - can be improved with lattice constraints
3. Under investigation:
   - PDFs: scanning and/or profiling
   - Quark mass effects
   - Fits against real data

THANK YOU!

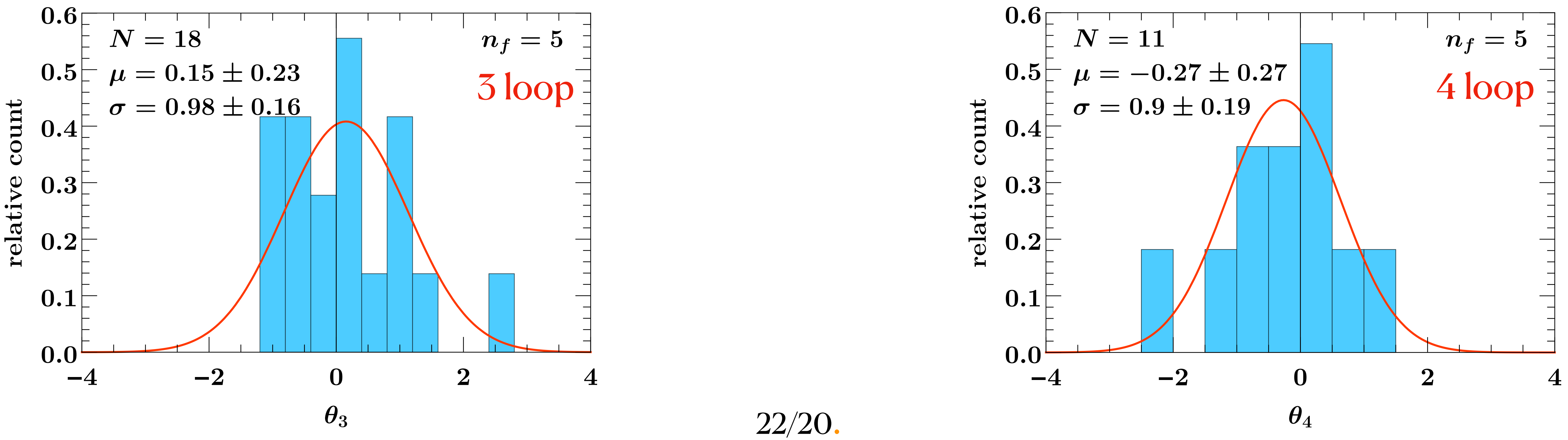
Backup slides

TNPs for Boundary Conditions

$$F_n(\theta_n) = 4C_r(4C_A)^{n-1}(n-1)!\,\theta_n^F$$

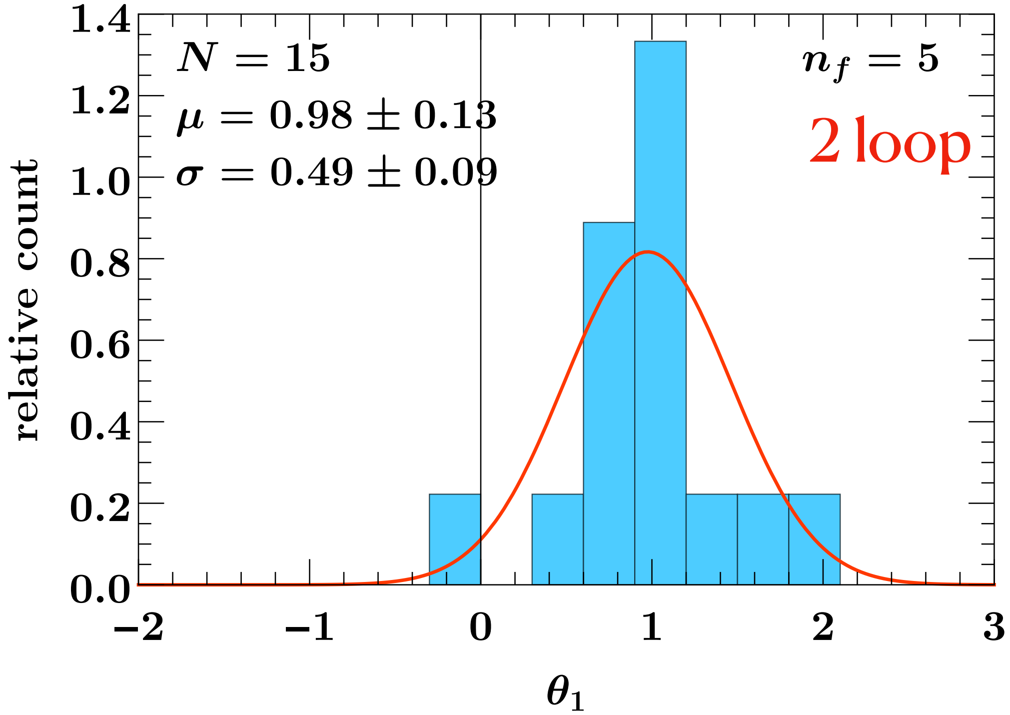


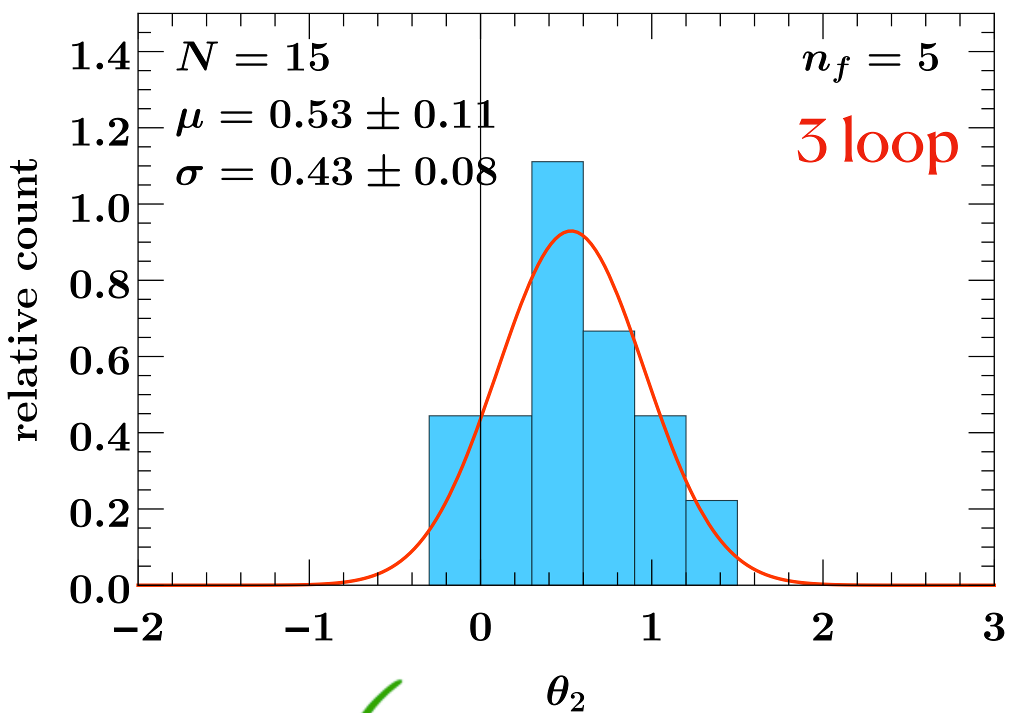
Fit to a Gaussian with $\theta = 0$ and $\Delta\theta_n = 1$ ✓



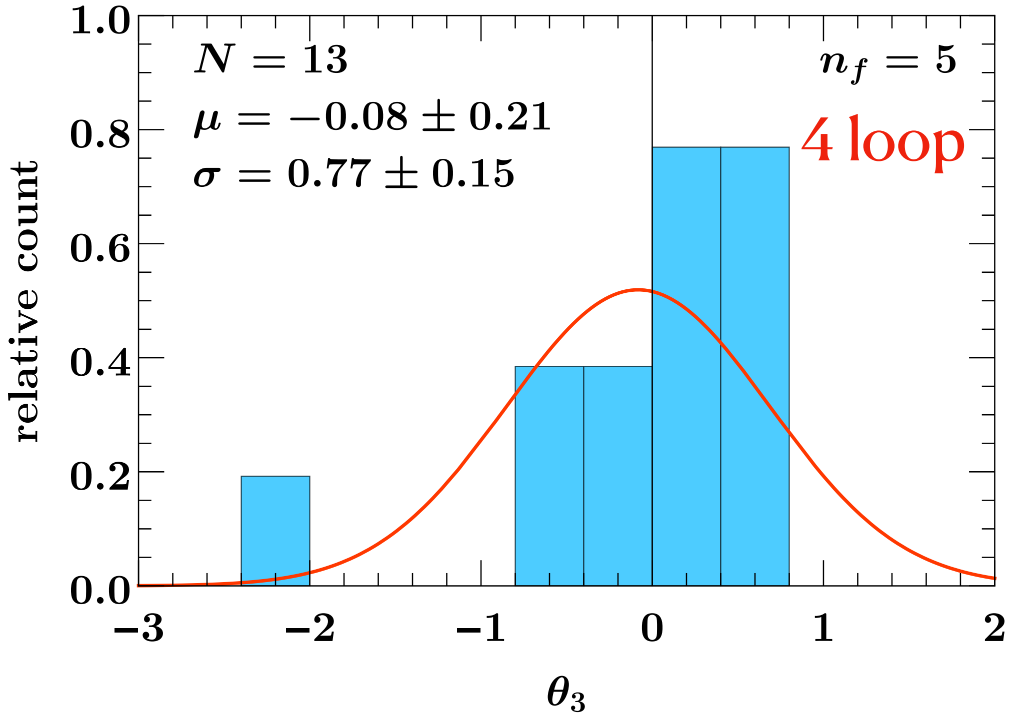
TNPs for Anomalous Dimensions

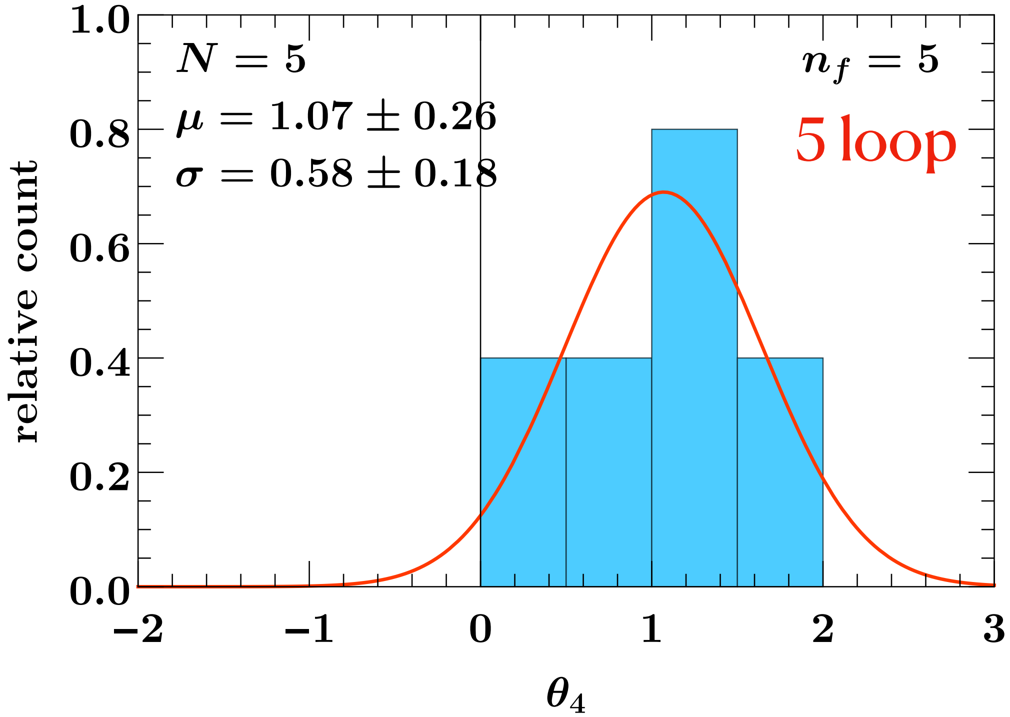
$$\gamma_n(\theta_n) = 2C_r(4C_A)^n\,\theta_n^\gamma$$





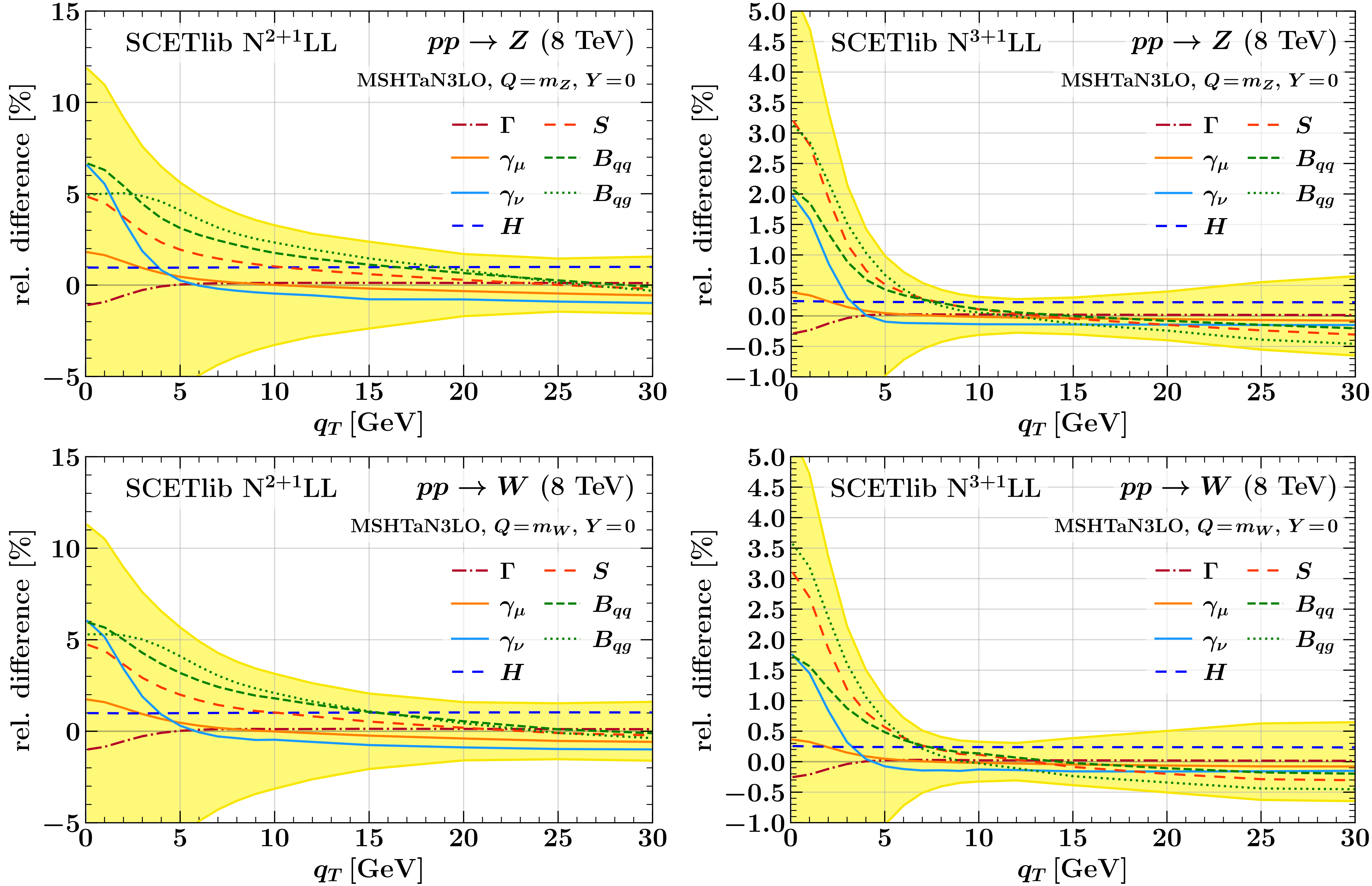
Fit to a Gaussian with $\theta \neq 0$ and $\Delta\theta_n = 0.5$ ✓





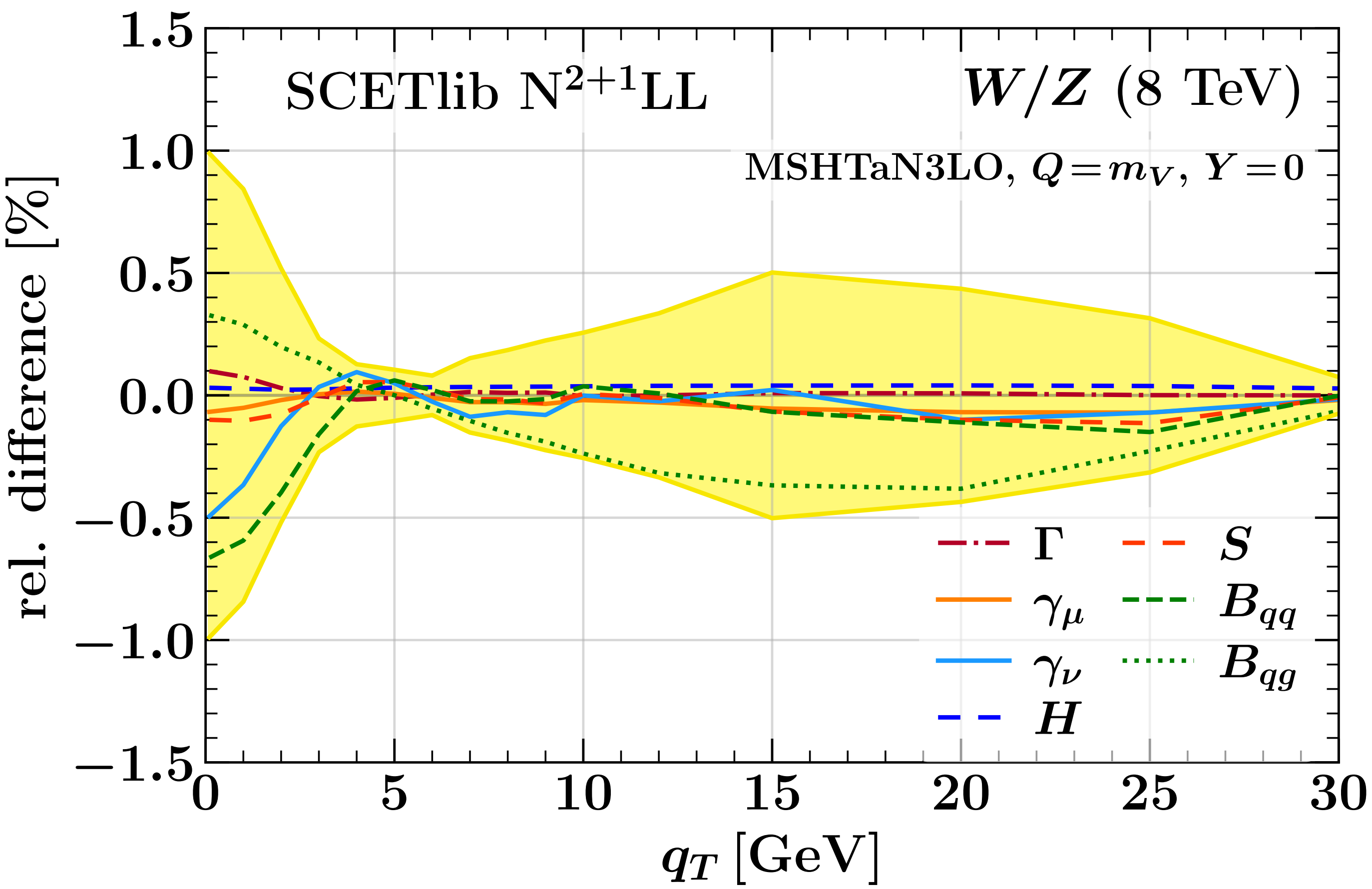
go back slide

Application to Drell-Yan p_T spectrum

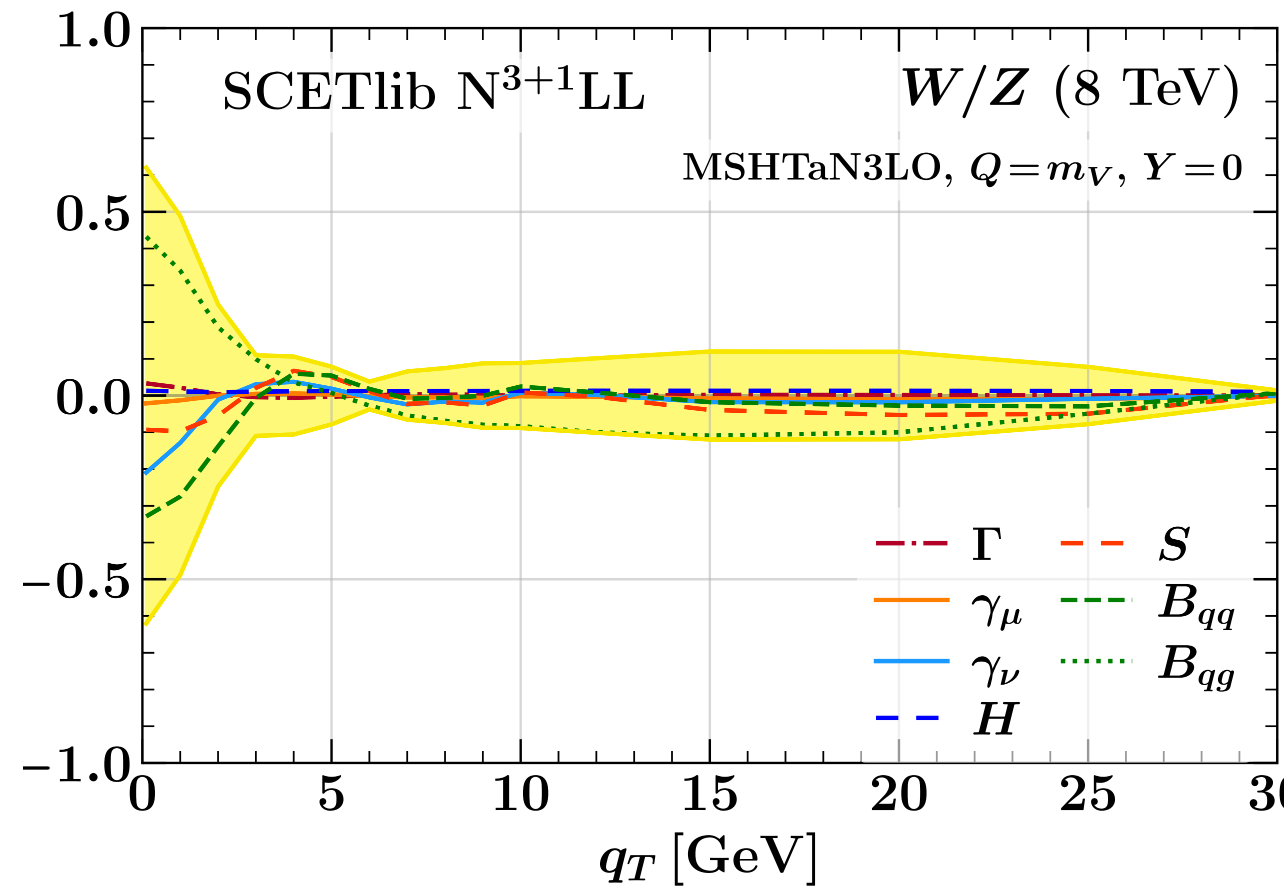


Application to Drell-Yan p_T spectrum

relative impact for W/Z



relative impact for W/Z

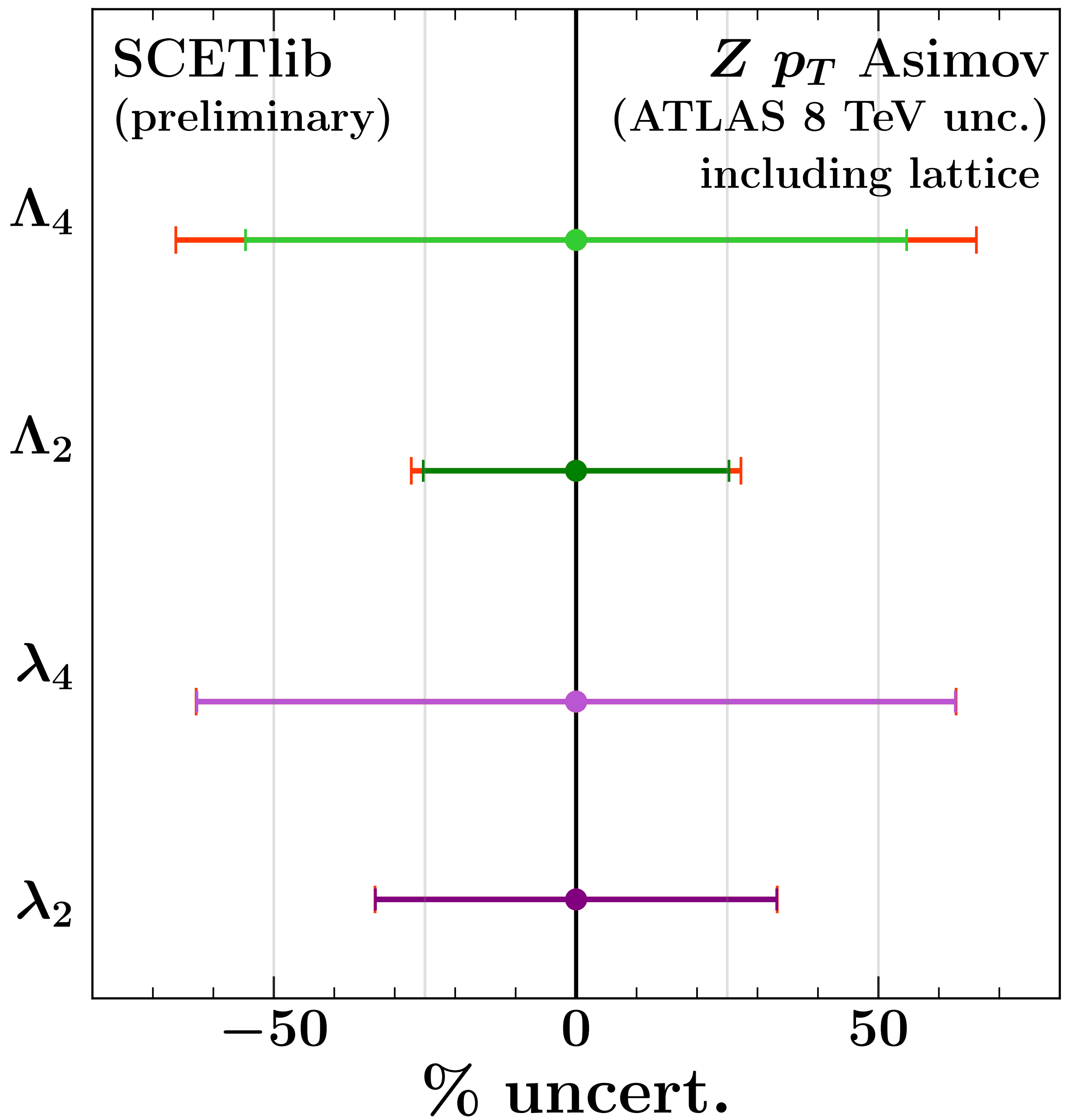


Correlation in p_T between W and Z captured ✓

go back slide

Constraints on nonp. parameters

- parameters fitted λ_2, λ_4, Λ_2, Λ_4 + lattice QCD constraints

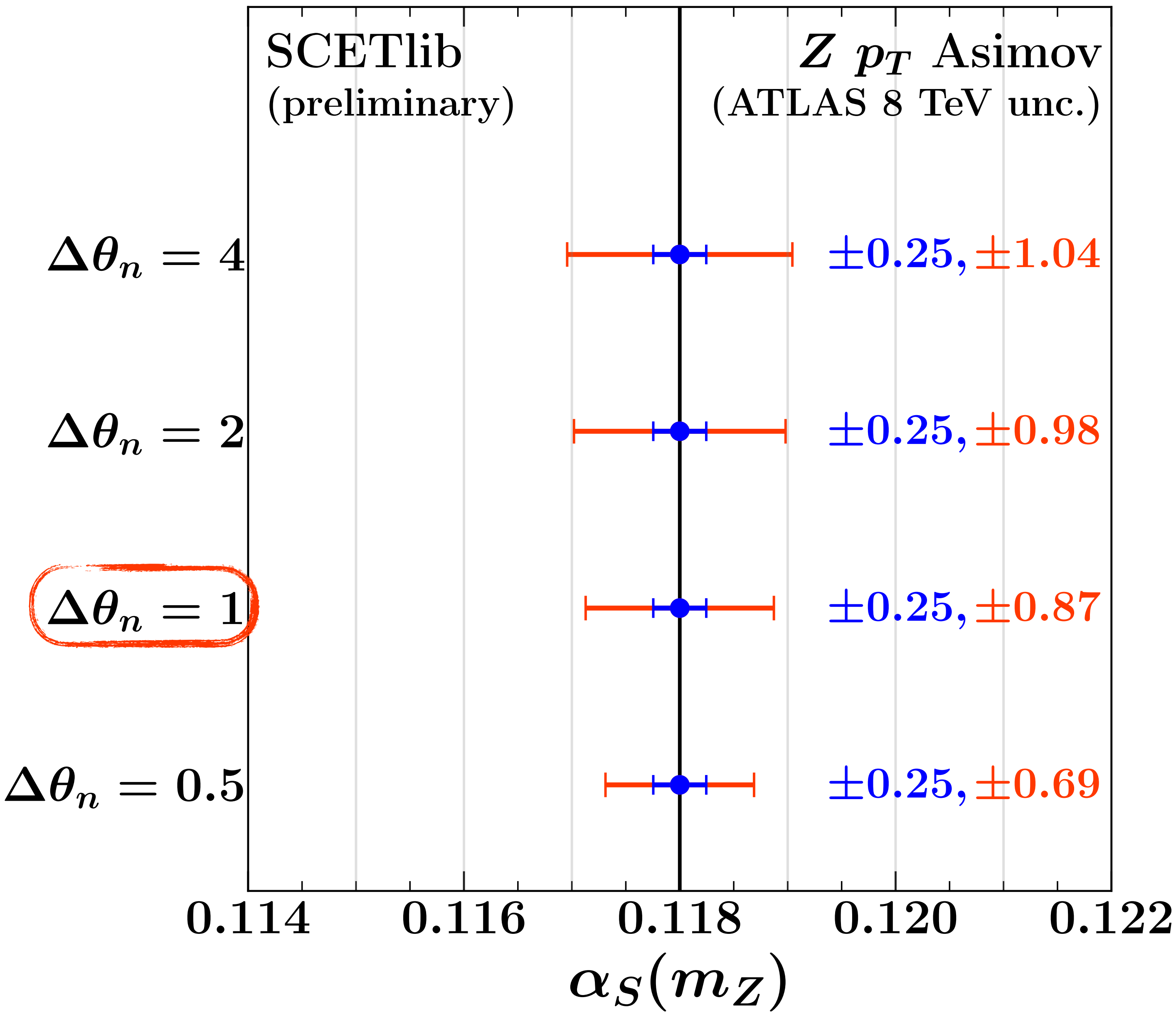


Different constraints on TNPs including nonp.

What happens by changing the constraint?

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 0.5, 1, 2, 4$

Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



fit unc. only: fitting *only* α_S and nonp.

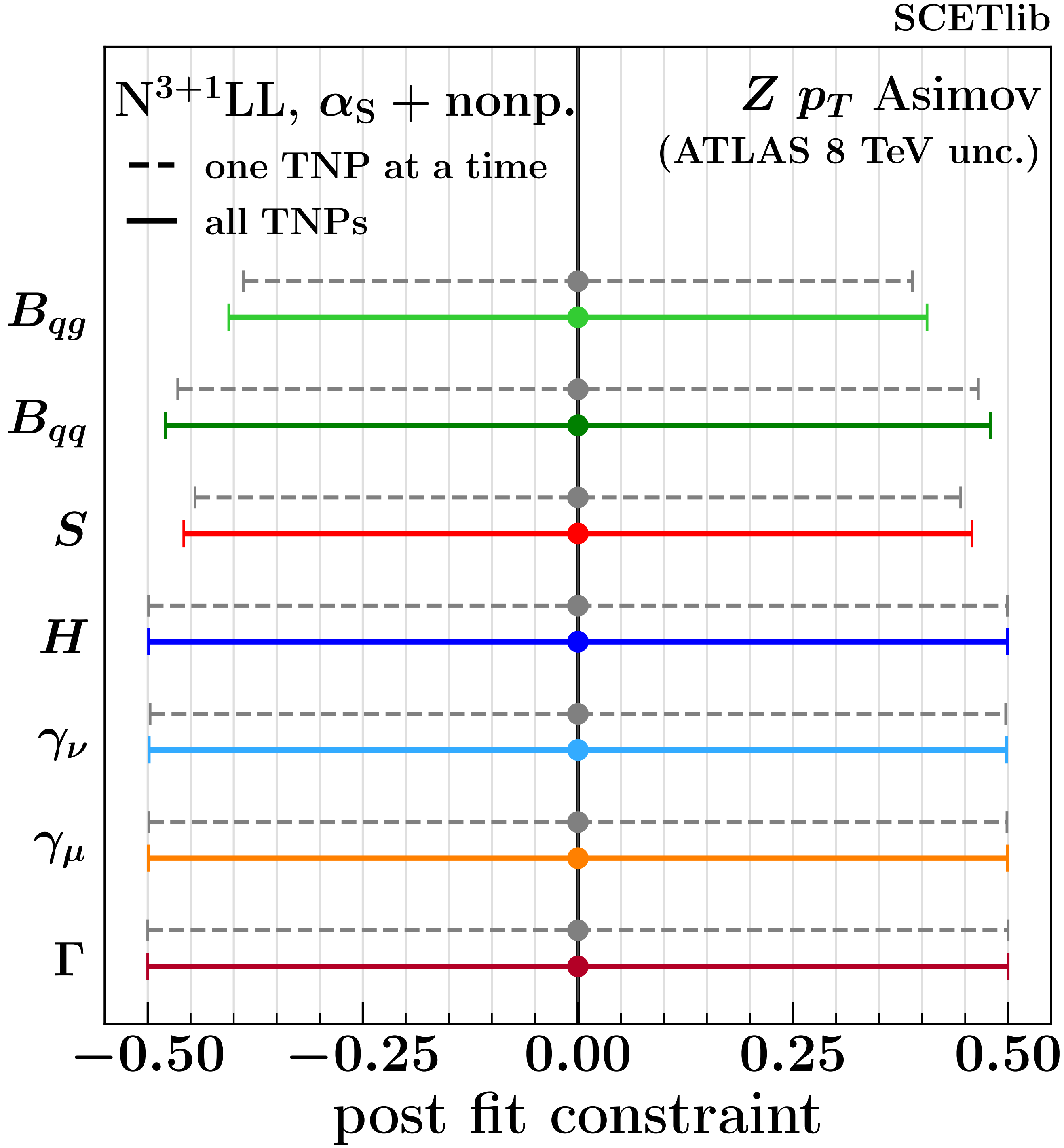
$N^{3+1}LL$ profiled: including TNPs

* uncertainties in units of 10^{-3}

Different constraints on TNPs including nonp.

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 0.5$

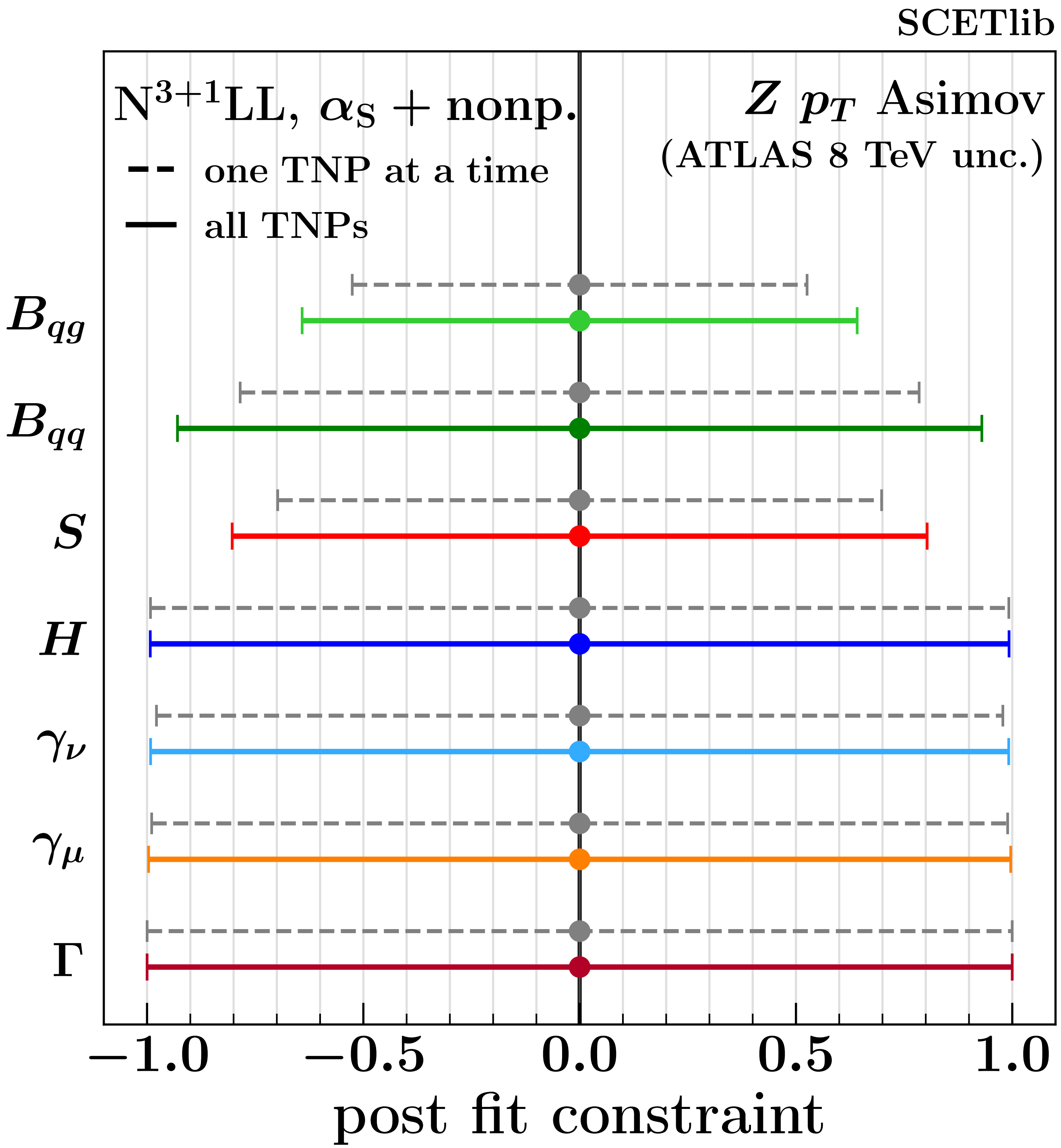
Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



Different constraints on TNPs including nonp.

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 1$

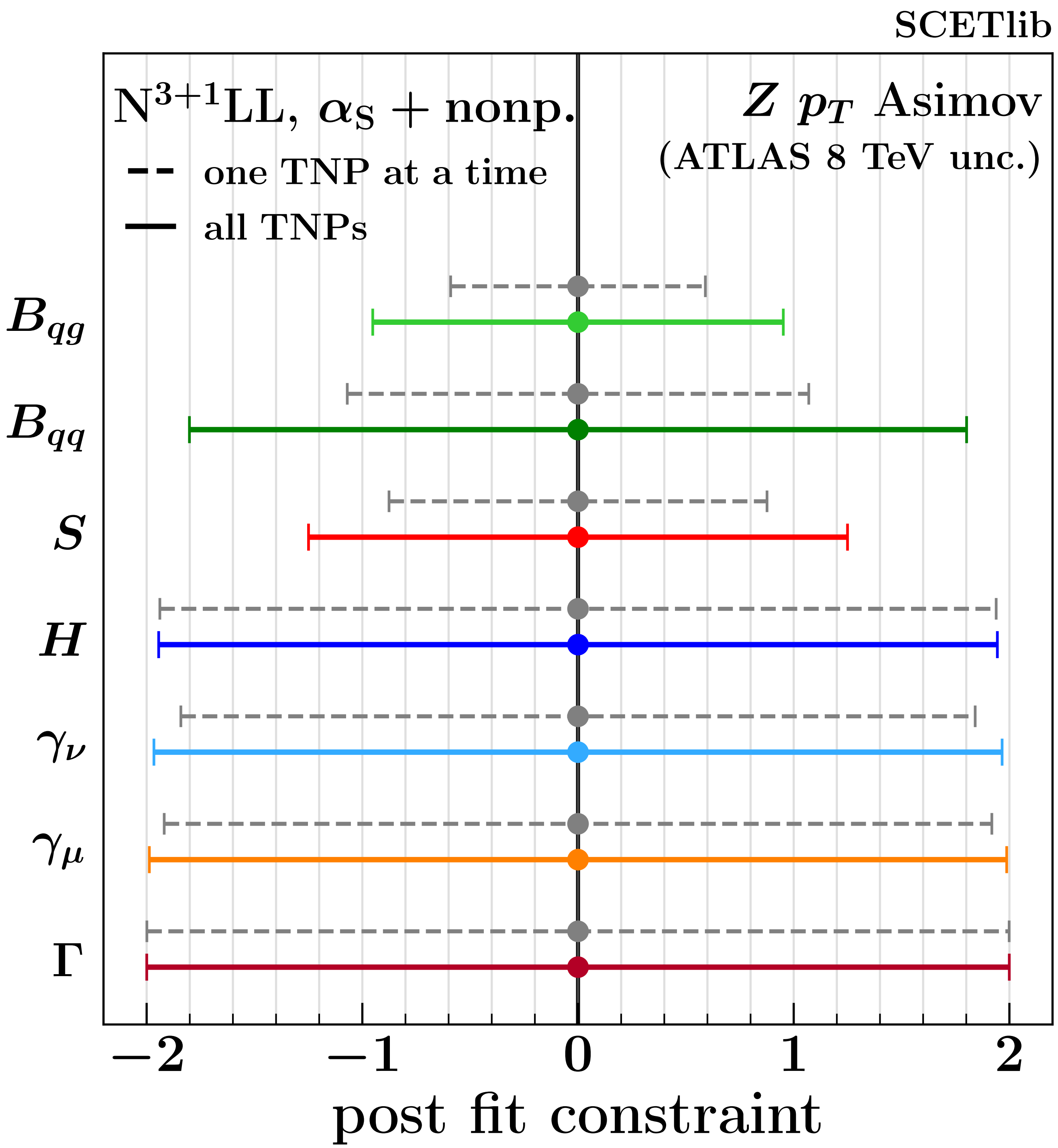
Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



Different constraints on TNPs including nonp.

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 2$

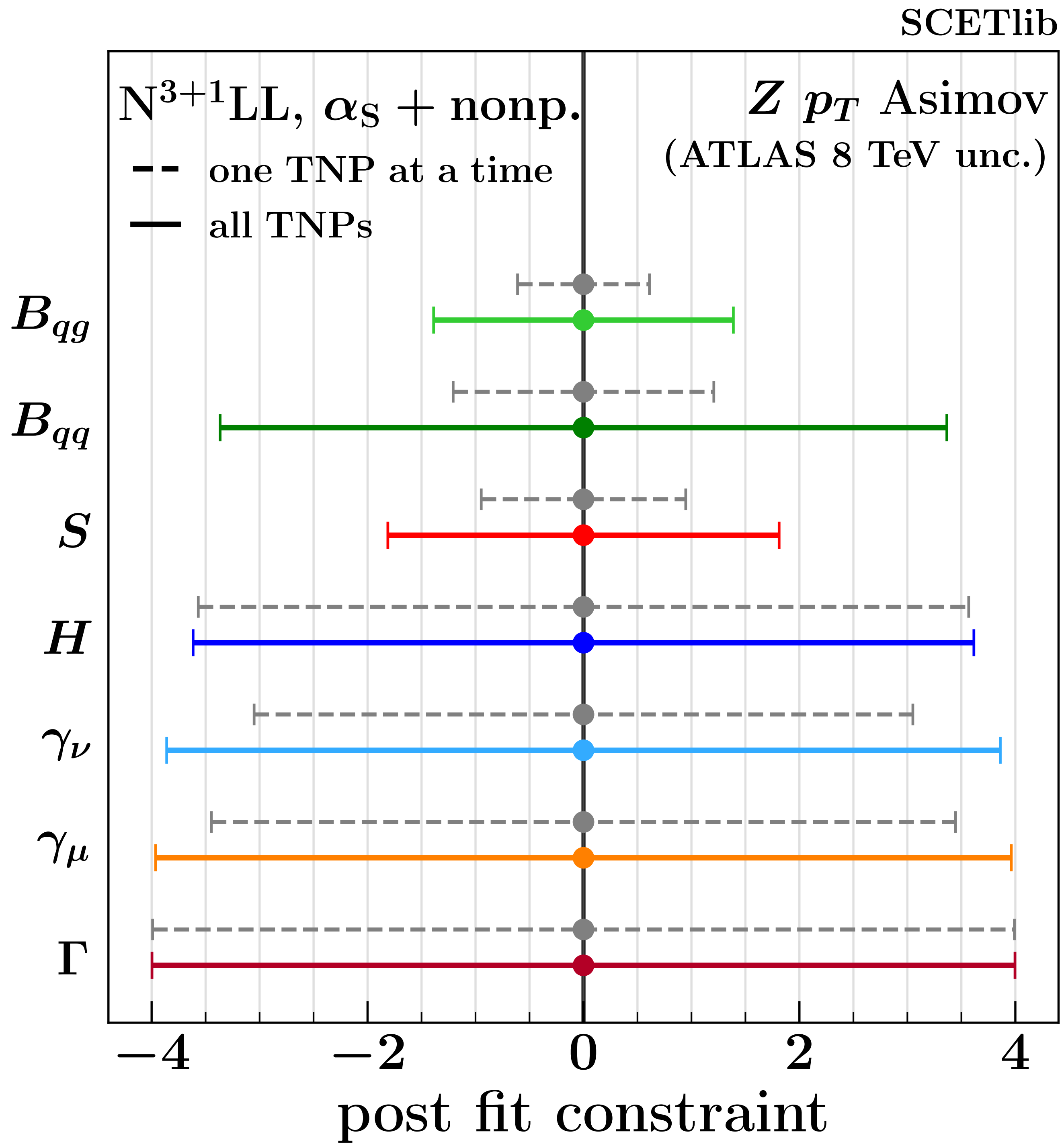
Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



Different constraints on TNPs including nonp.

Using now $\theta_n = 0 \pm \Delta\theta_n$ with $\Delta\theta_n = 4$

Fit $N^{3+1}LL$ against $N^{3+1}LL$ data



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Acknowledgments

This project has received funding from the European Research Council (ERC)
under the European Union's Horizon 2020
research and innovation programme
(Grant agreement No. 101002090 COLORFREE)

European Research Council

Established by the European Commission