

# SCALE VARIATION AND PDF UNCERTAINTIES

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SCALES 2017

CAMBRIDGE, MARCH 31, 2017

## THE PROBLEM:

# THEORETICAL UNCERTAINTIES ON PDFs:

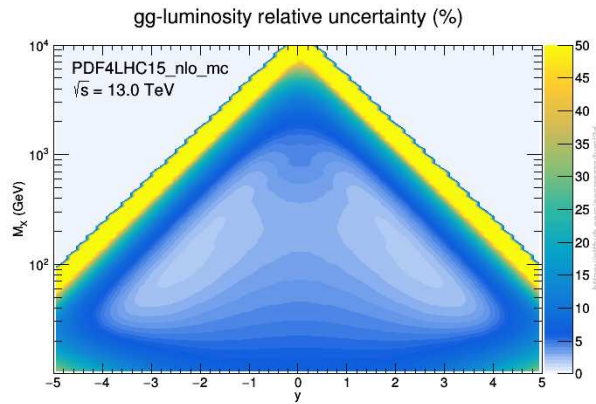
- PDFs ARE DETERMINED BY COMPARING TO DATA THEORY AT SOME FINITE ORDER
- AFFECTED BY THEORETICAL UNCERTAINTY JUST LIKE HARD CROSS-SECTIONS
- NOT INCLUDED IN CURRENT “PDF UNCERTAINTY”  
(ACCOUNTS ONLY DATA & METHODOLOGY)
- TERMINOLOGY:
  - “PDF UNCERTAINTY”  $\Leftrightarrow$  PROPAGATED FROM DATA I.E. DATA+METHODOLOGY
  - “THEORY UNCERTAINTY”  $\Leftrightarrow$  DUE TO MHO IN QCD EVOLUTION AND MATRIX ELEMENTS IN FIT
- NOTE PDF UNCERTAINTY TESTED TO BE FAITHFUL THROUGH CLOSURE TEST

## THEORY UNCERTAINTIES: QUESTIONS

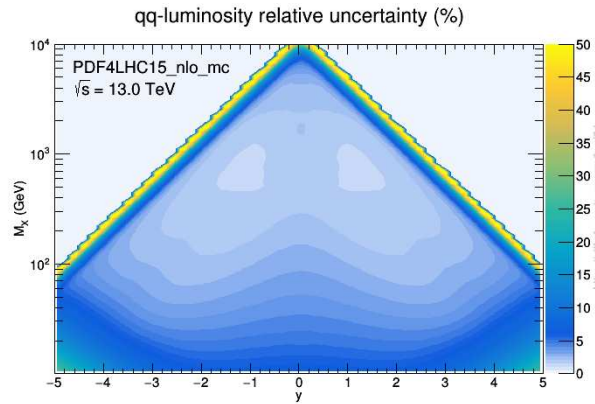
- HOW LARGE ARE THEY IN COMPARISON TO PDF UNCERTAINTIES
- HOW DO THEY RELATE TO THE UNDERLYING MHO
- CAN WE ESTIMATE THEM

# PDF UNCERTAINTIES: THE STATE OF THE ART (PDF4LHC15, NLO)

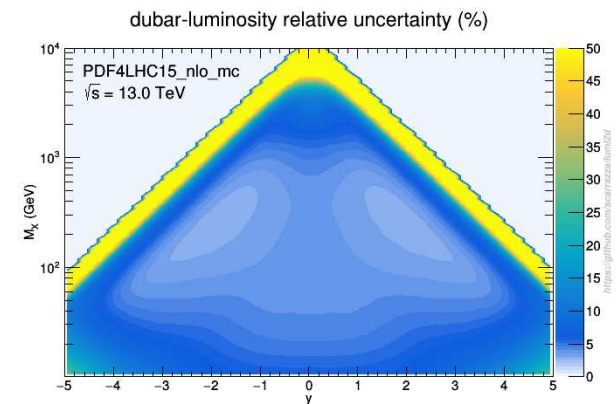
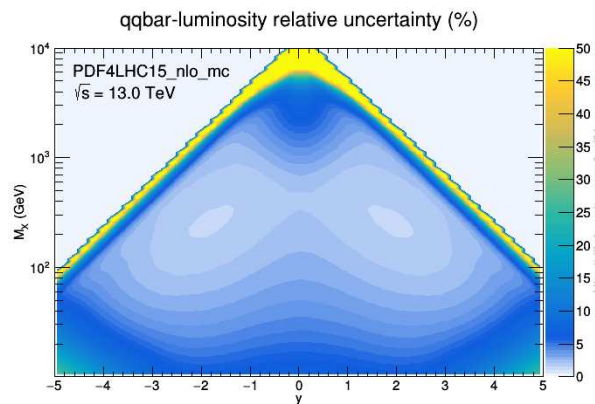
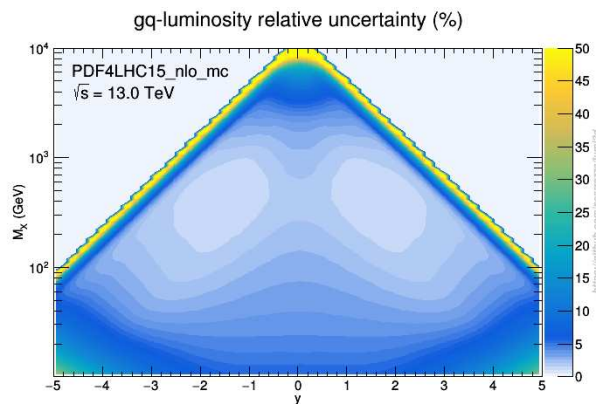
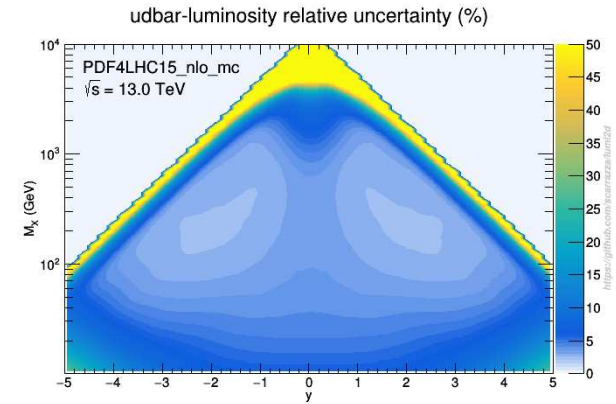
GLUON



SINGLET



FLAVORS



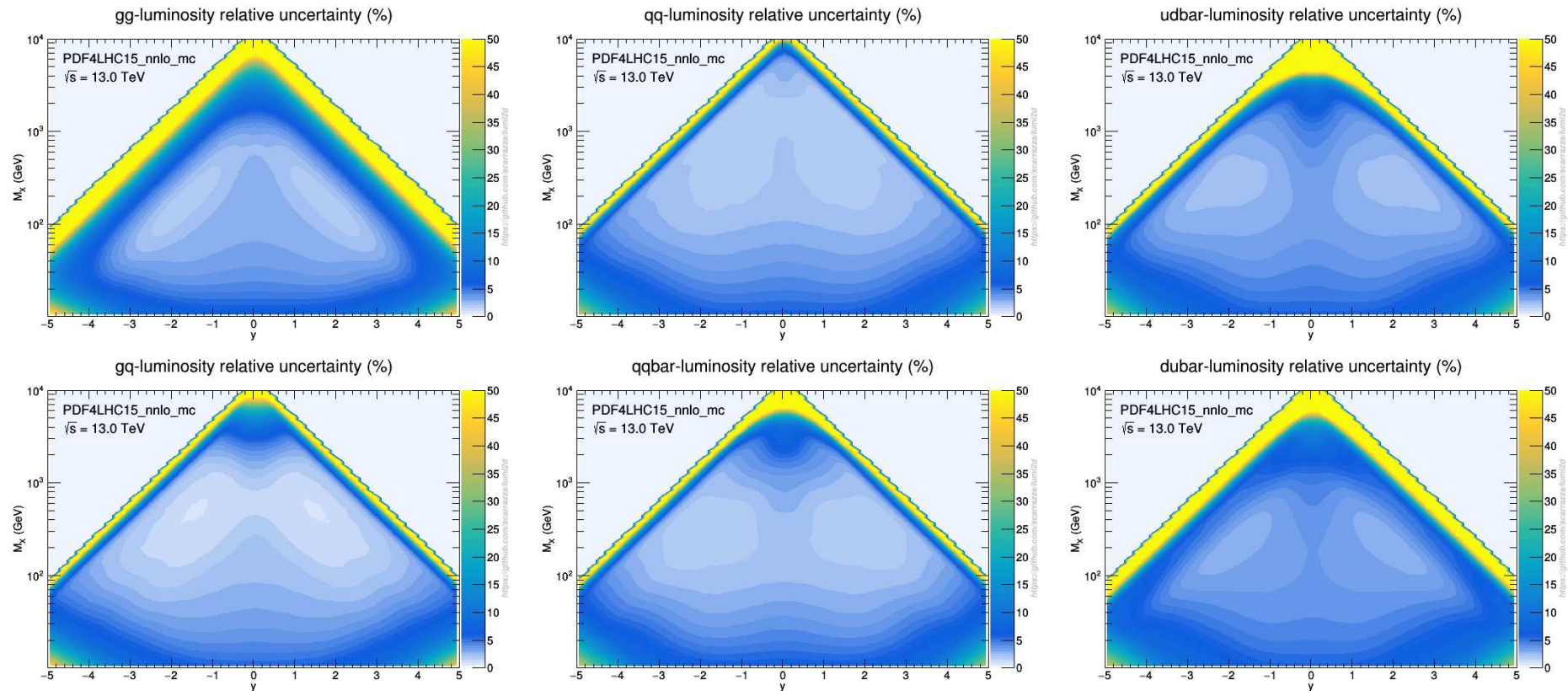
- GLUON BETTER KNOWN AT SMALL  $x$ , VALENCE QUARKS AT LARGE  $x$ , SEA QUARKS IN BETWEEN
- SWEET SPOT: VALENCE Q - G; UNCERTAINTIES DOWN TO 1%
- UP BETTER KNOWN THAN DOWN; FLAVOR SINGLET BETTER THAN INDIVIDUAL FLAVORS

# PDF UNCERTAINTIES: THE STATE OF THE ART (PDF4LHC15, NNLO)

GLUON

SINGLET

FLAVORS

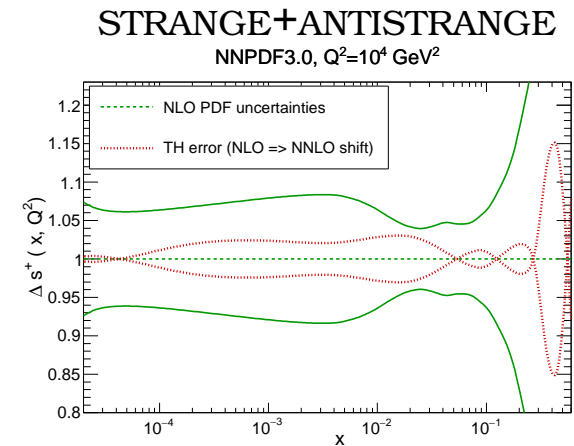
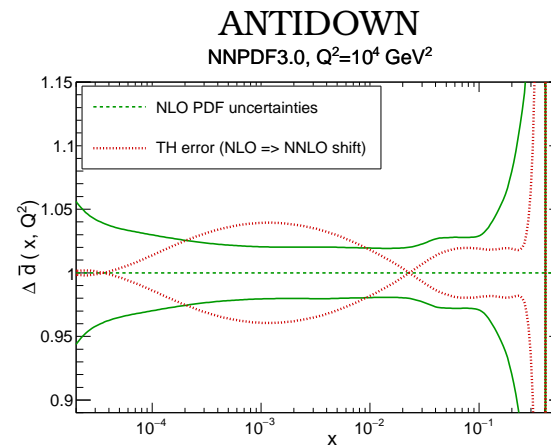
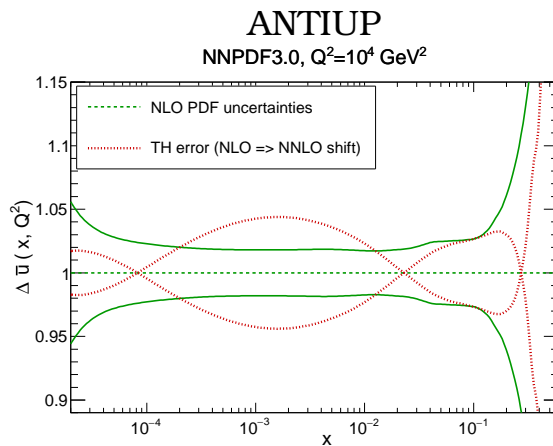
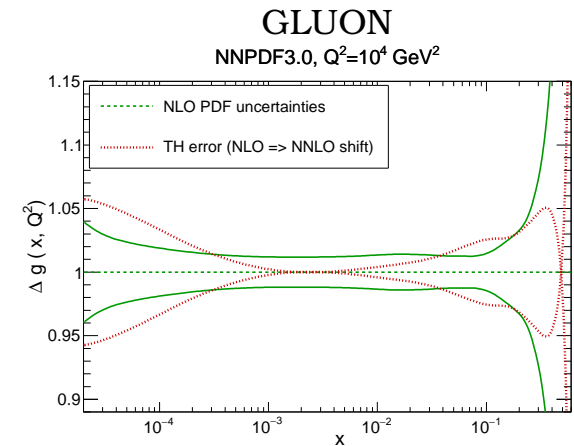
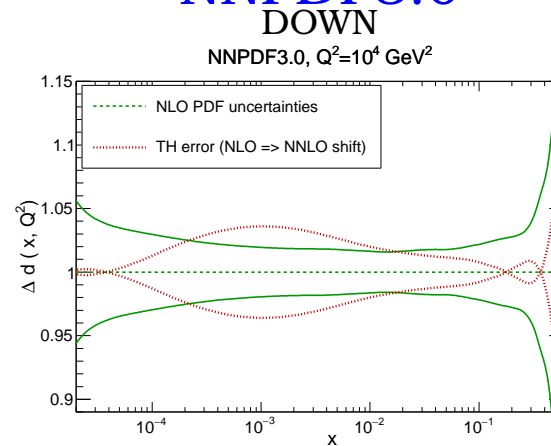
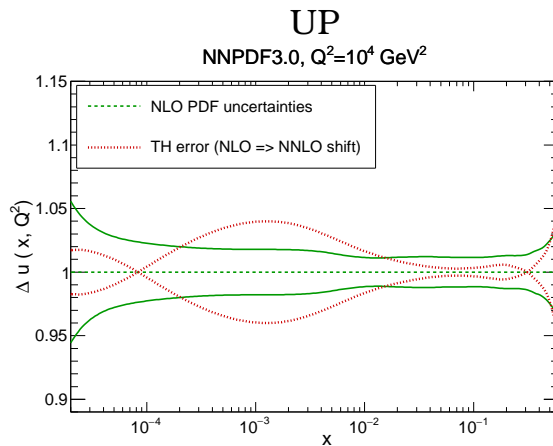


- GLUON BETTER KNOWN AT SMALL  $x$ , VALENCE QUARKS AT LARGE  $x$ , SEA QUARKS IN BETWEEN
- SWEET SPOT: VALENCE Q - G; UNCERTAINTIES DOWN TO 1%
- UP BETTER KNOWN THAN DOWN; FLAVOR SINGLET BETTER THAN INDIVIDUAL FLAVORS
- NO QUALITATIVE DIFFERENCE BETWEEN NLO AND NNLO
- AT 1% LEVEL, CAN WE NEGLECT THEORY UNCERTAINTIES?

# PDF UNCERTAINTIES vs. NLO THEORY UNCERTAINTIES

- AT NLO, THE THEORY UNCERTAINTY IS JUST THE NNLO-NLO SHIFT
- HOW DOES IT COMPARE TO THE PDF UNCERTAINTY?

## NNPDF3.0

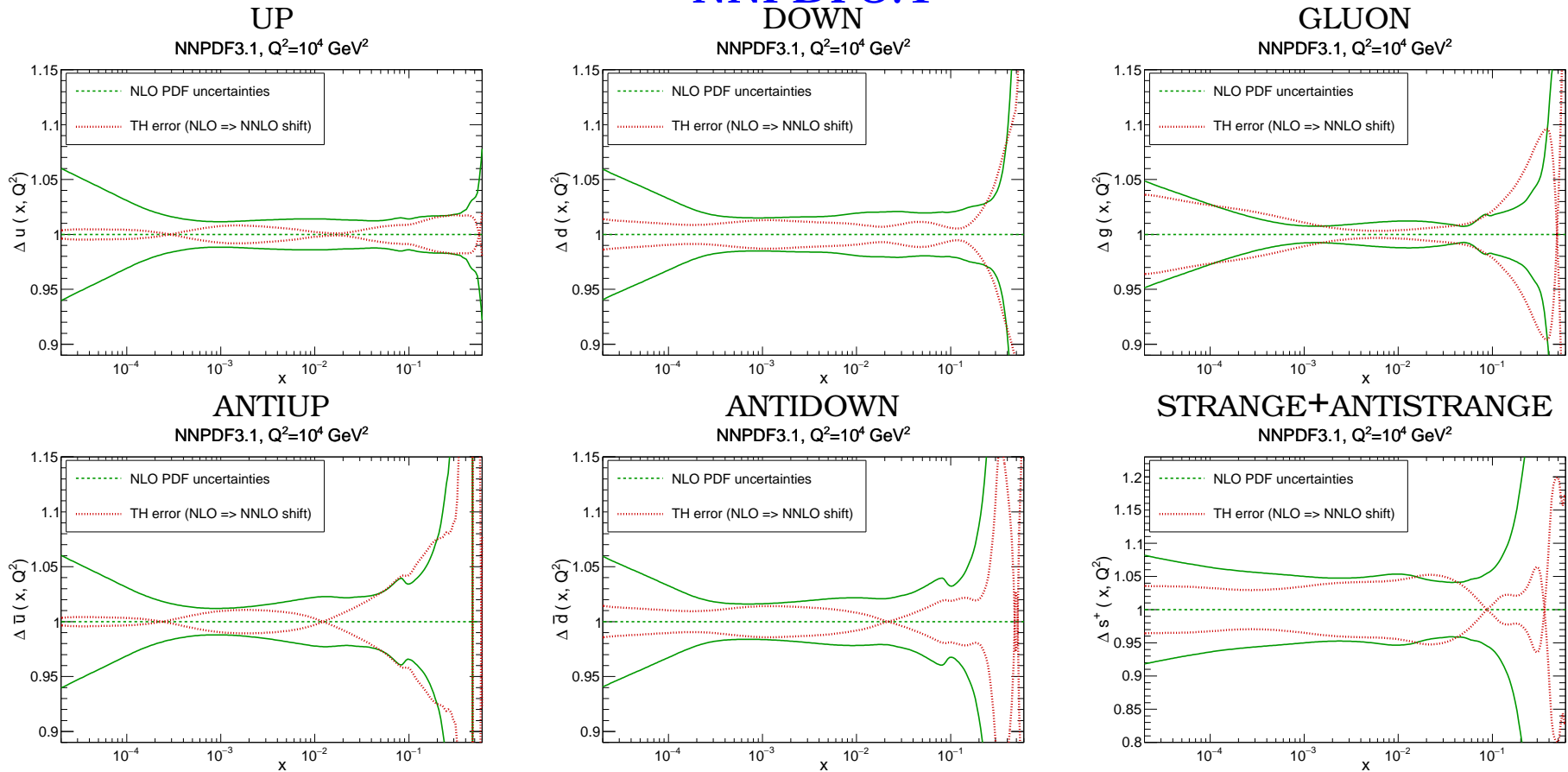


IN CURRENT NLO SETS **MISSING THEORY UNCERTAINTY COMPARABLE TO**  
PDF UNCERTAINTY

# PDF UNCERTAINTIES vs. NLO THEORY UNCERTAINTIES

- AT NLO, THE **THEORY UNCERTAINTY** IS JUST THE **NNLO-NLO SHIFT**
- HOW DOES IT COMPARE TO THE **PDF UNCERTAINTY**?

## NNPDF3.1



NEW NLO SETS: **MISSING THEORY SMALLER BUT STILL COMPARABLE** TO PDF UNCERTAINTY

CAN WE ESTIMATE WHAT HAPPENS AT NNLO?



# CACCIARI-HOUDEAU FOR PDFs

(slides from 2011)

## IDEA

- ASSUME COEFFICIENT OF PERTURBATIVE EXPANSION BOUNDED FROM ABOVE AND WITH SOME (UNIFORM?) DISTRIBUTION
- ESTIMATE SIZE OF NEXT ORDER BASED ON KNOWN COEFFICIENTS

series in  $\alpha_s$  starting at  $\alpha_s^0$ ; uncertainty on  $k$ -th order:

$$\Delta_k = \begin{cases} \alpha_s^{k+1} \max\{|c_l|, \dots, |c_k|\} \frac{n_c+1}{n_c} p & \text{if } p \leq \frac{n_c}{n_c+1} \\ \alpha_s^{k+1} \max\{|c_l|, \dots, |c_k|\} [(n_c+1)(1-p)]^{-1/n_c} & \text{if } p > \frac{n_c}{n_c+1} \end{cases}$$

$n_c = k + 1$  number of known coefficients;  $P \Rightarrow$  c.l. (one  $\sigma \leftrightarrow P = 0.68$ )

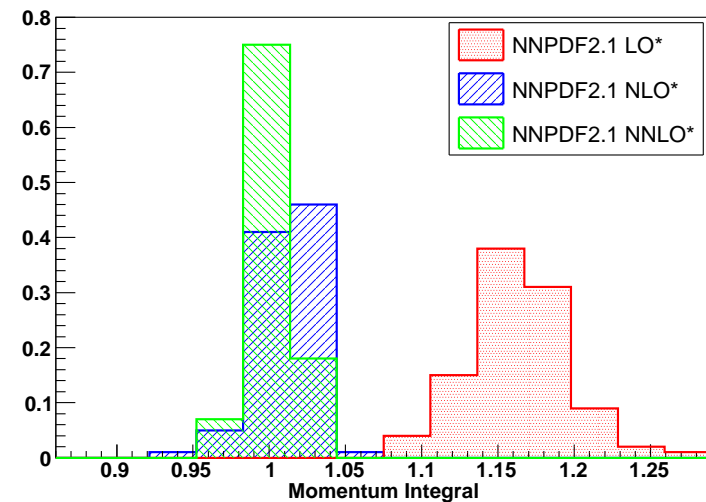
# HOW WELL DOES IT WORK?

WHEN WE KNOW THE ANSWER

## THE MOMENTUM SUM RULE

- PERFORM LO, NLO, NNLO PDF FITS WITHOUT MOMENTUM CONSTRAINT
- DETERMINE  $[M] = \int_0^1 dx \Sigma(x) + g(x)$   
(AT ANY SCALE)
- VIEW LO, NLO, NNLO RESULTS AS SERIES IN  $\alpha_s$

- LO  $[M] = 1.161 \pm 0.032^{\text{exp}}$
- NLO  $[M] = 1.011 \pm 0.018^{\text{exp}}; \Delta^{\text{th,CH}} = 0.019$
- NNLO  $[M] = 1.002 \pm 0.014^{\text{exp}}; \Delta^{\text{th,CH}} = 0.002$



WORKS QUITE WELL, ACCURACY IMPROVES WITH ORDER!



# THE CACCIARI-HOUDEAU METHOD

## APPLICATION TO PDFs

- CONSIDER PDFs FOR GIVEN  $x, Q^2$  AS A SERIES IN  $\alpha_s$
- AT NLO USE FORMULA WITH  $k = 1$  ETC. (HENCEFORTH,  $\alpha_s = 0.119$ )

# THEORETICAL UNCERTAINTIES

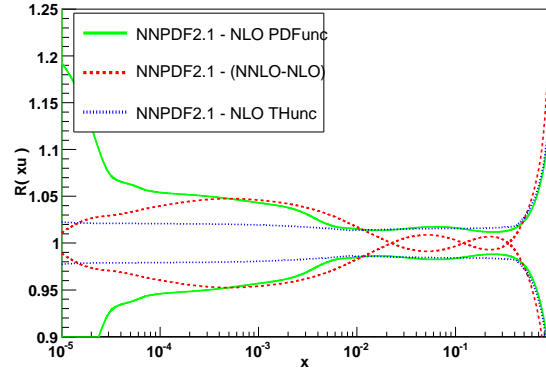
NLO PDF UNC. VS NLO-NNLO SHIFT VS NLO CACCIARI-HOUDEAU (NNPDF2.1)

UP

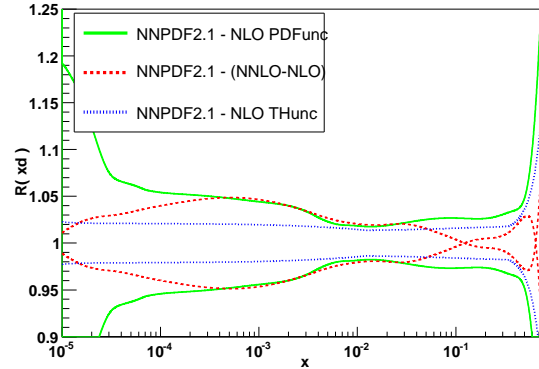
DOWN

STRANGE

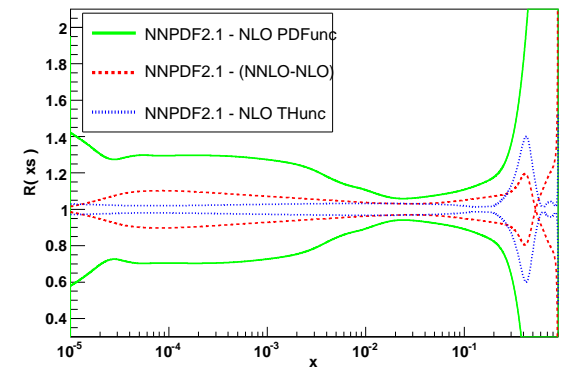
Relative Errors,  $Q^2 = 10^4 \text{ GeV}^2$



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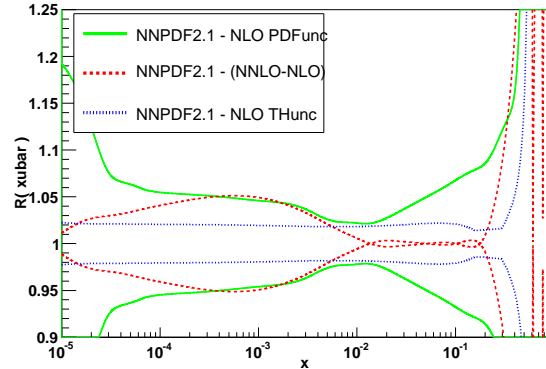


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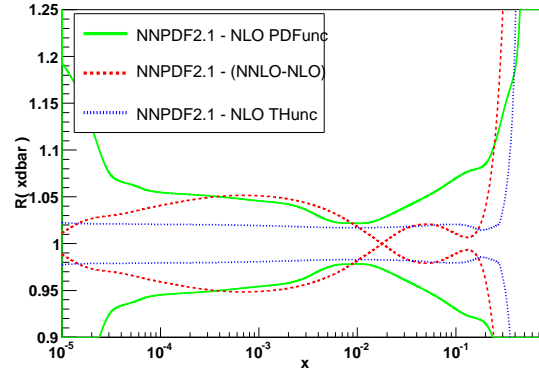
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ANTISTRANGE

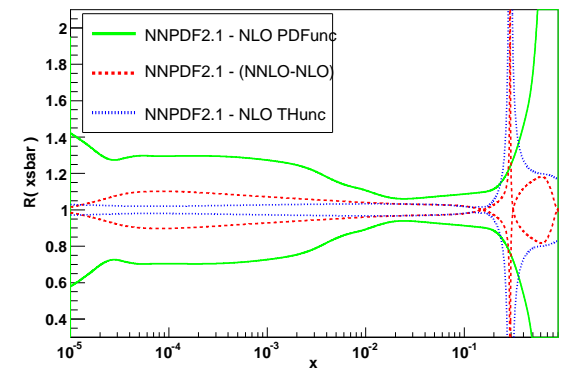
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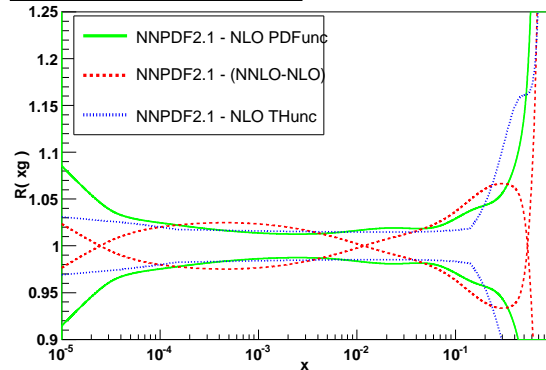


GLUON

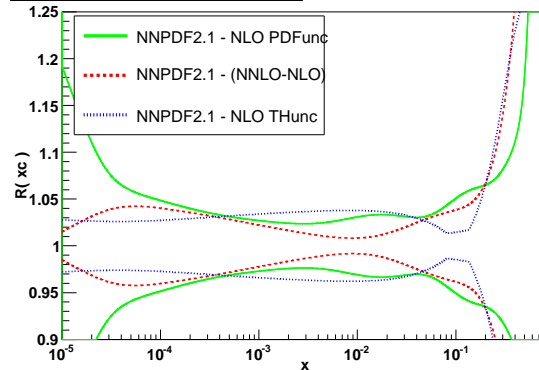
CHARM

BOTTOM

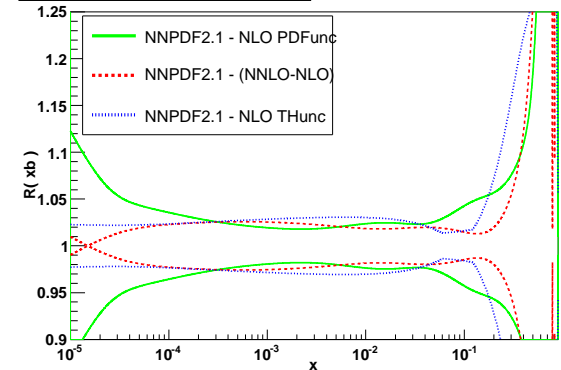
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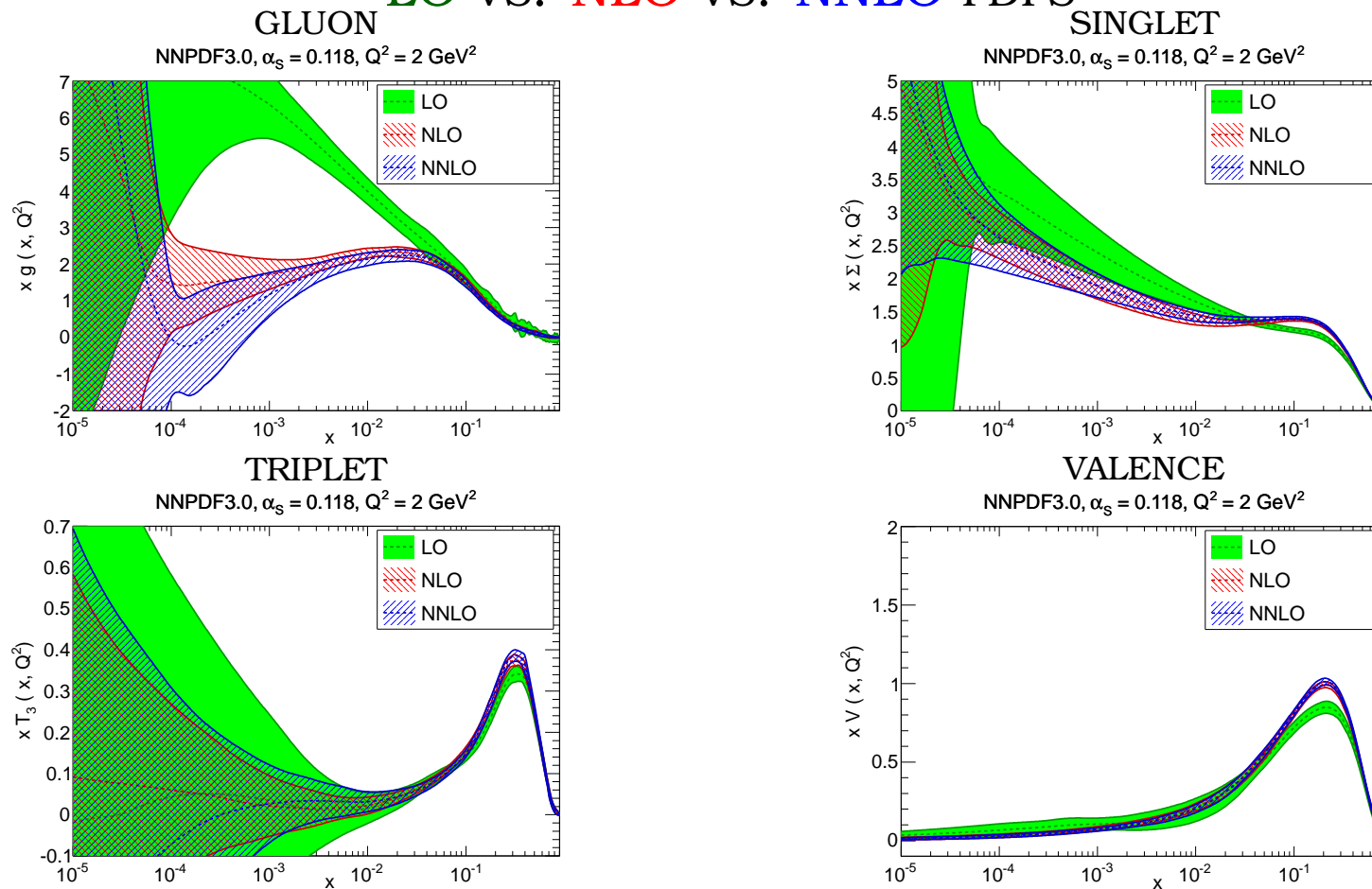


# THE PERTURBATIVE EXPANSION FOR PDFs

## OBJECTIONS:

- CAN WE REALLY TAKE PDFs AS SERIES IN  $\alpha_s$ ?
- IS IT MEANINGFUL TO EXTRAPOLATE BASED ON ONE SINGLE ORDER?
- LO PDFs ARE SPECIAL: POSITIVITY, GLUON,  $\alpha_s$

## LO VS. NLO VS. NNLO PDFs



## CACCIARI HOUDEAU FOR PDFS

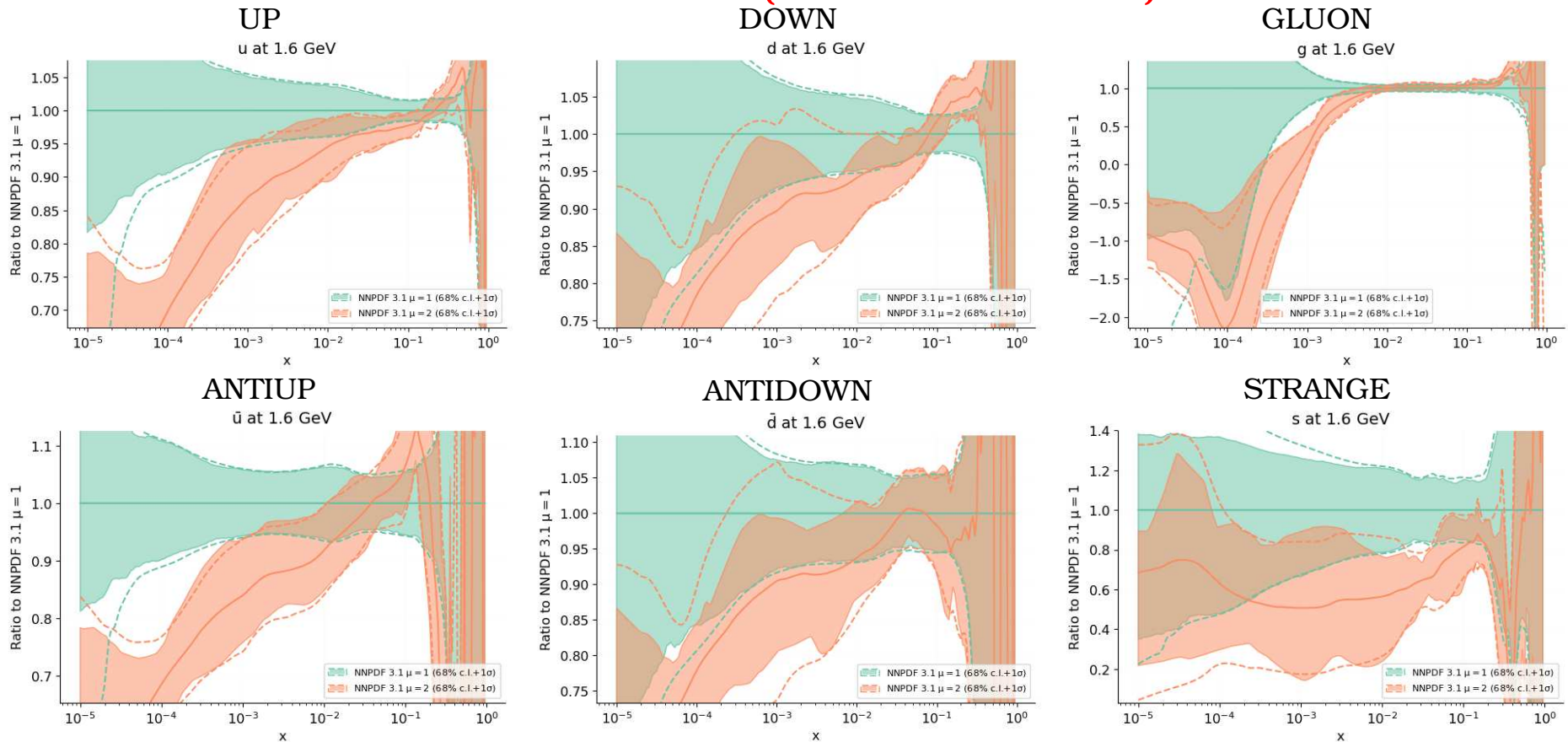
### PROs AND CONs

- CORRECTLY INCLUDES UNCERTAINTY DUE TO IMPERFECT FIT QUALITY LEADING TO SUBOPTIMAL CONVERGENCE
- POTENTIALLY UNSTABLE AT LOW PERTURBATIVE ORDERS DUE TO SPECIAL NATURE OF LO FITS

# SCALE VARIATION IN PDF FITS

- REPEAT PDF DETERMINATION WITH DIFFERENT CHOICES OF RENORMALIZATION AND FACTORIZATION SCALE
- HOW SHOULD THE SCALE VARIATION CORRELATE BETWEEN DATAPOINTS?

## NNPDF3.1: CENTRAL VS $2\times \mu_R$ & $\mu_F$ PRELIMINARY (ONLY 57 REPLICAS)



- AT MEDIUM & LARGE  $x$ , APPEARS TO BE IN BROAD AGREEMENT WITH ACTUAL NLO-NNLO SHIFT
- LARGE DEVIATION AT SMALL  $x$  (SCALE VARIATION MISSES DOUBLE SCALING?)

# NEW IDEA

## PDF THEORY ERROR AS A FIT UNCERTAINTY

(Del Debbio, Ubiali, unpublished)

- PDFS ARE DETERMINED BY **MAXIMIZING THE LIKELIHOOD**

$$P = N \exp - \left( \frac{d - t}{2\sigma_{exp}^2} \right)$$

$d, t$  ARE REALLY VECTORS AND  $1/\sigma^2$  THE INVERSE COVARIANCE MATRIX

- CAN VIEW THIS AS THE **PROBABILITY OF THE THEORY**  $t$  BEIN CORRECT GIVEN DATA  $d$ , WHICH BY **BAYES** IS

$$P(t|d) \propto P(d|t)P(t)$$

- IF THEORY WAS KNOWN EXACTLY, THEN  $P(t) = \delta(t - t^{\text{exact}})$
- IN ACTUAL FACT **ONLY SOME PERTURBATIVE RESULT**  $t_p$  IS **EXACTLY KNOWN** SO  $t^{\text{exact}} = t_p + \Delta_p$ , WHERE  $\Delta_p$  INCLUDES MHO
- ASSUMING  $\Delta$  TO BE GAUSSIANLY DISTRIBUTED, WITH UNCERTAINTY  $\sigma_{th}$  AND INTEGRATING OUT

$$P = N \exp \left[ \frac{d - t_p}{2(\sigma_{exp}^2 + \sigma_{th}^2)} \right]$$

- **THEORETICAL UNCERTAINTY** ADDED IN QUADRATURE, **PROPAGATES INTO PDF UNCERTAINTY** UPON MINIMZATION
- **CAN COMPUTE PDF UNCERTAINTY GIVEN MHO**

## SUMMARY

- AT 1% LEVEL **MUST INCLUDE THEORY UNCERTAINTIES** ON PDFs
- NLO-NNLO **SHIFT COMPARABLE TO NLO PDF UNCERTAINTIES**
- CACCIARI-HOUDEAU & SCALE VARIATION **PROMISING BUT PROBLEMATIC**
- THEORY UNCERTAINTIES **CAN BE INCLUDED IN OVERALL PDF UNCERTAINTY**  
THROUGH BAYESIAN ARGUMENT



NO EFFECT THAT REQUIRES MORE THAN 10% ACCURACY IN  
MEASUREMENT IS WORTH INVESTIGATING

Walther Nernst

~~NO EFFECT THAT REQUIRES MORE THAN 10% ACCURACY IN  
MEASUREMENT IS WORTH INVESTIGATING~~

Walther Nernst

ACCURACY OF OBSERVATION IS THE EQUIVALENT OF  
ACCURACY OF THINKING

Wallace Stevens

**EXTRAS**

# THEORETICAL UNCERTAINTIES

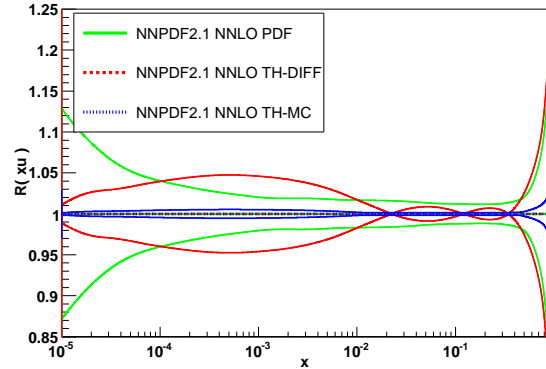
NNLO PDF UNC. VS NLO-NNLO SHIFT VS NNLO CACCIARI-HOUDEAU (NNPDF2.1)

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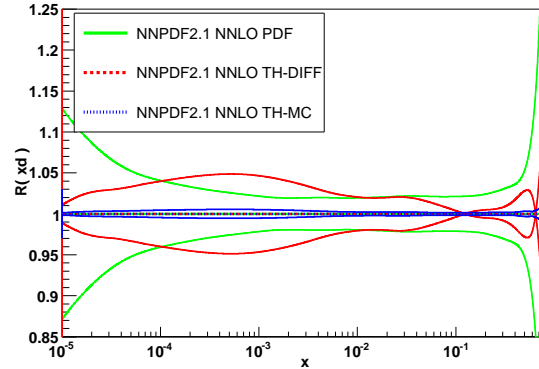
DOWN

STRANGE

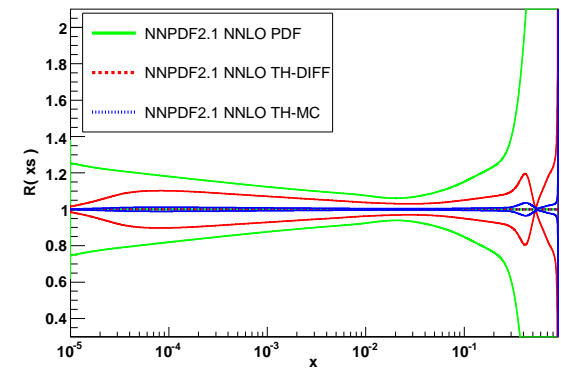
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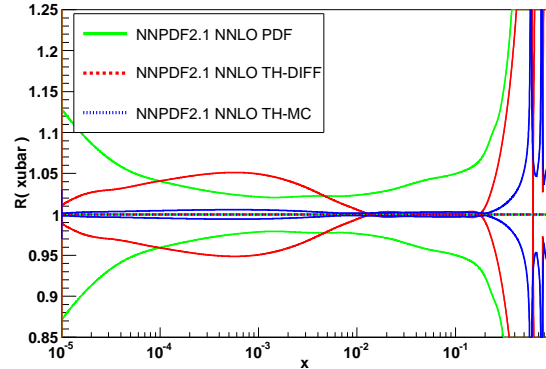


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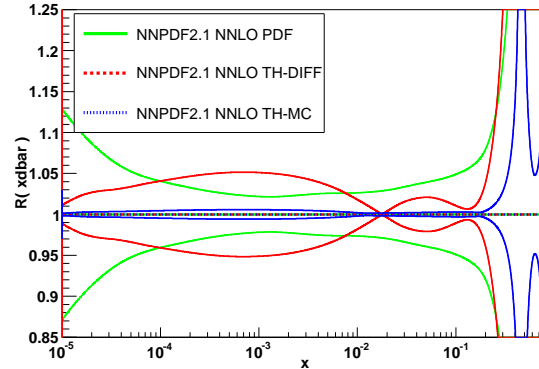
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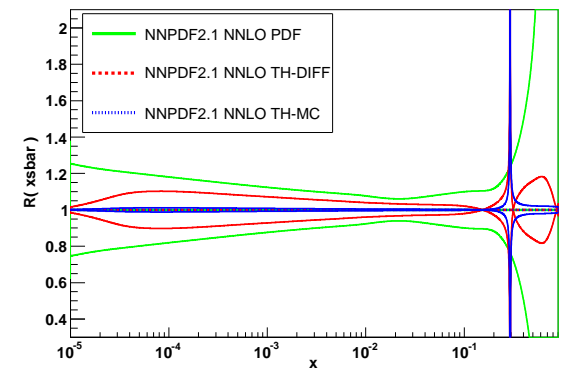
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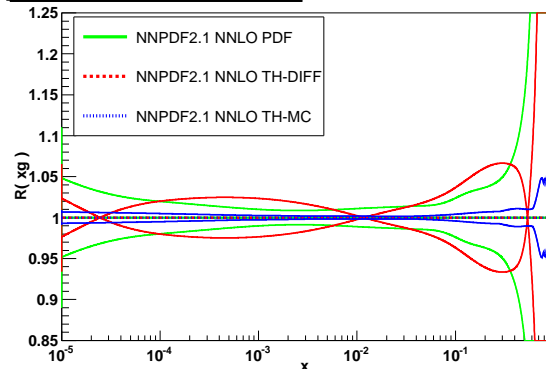


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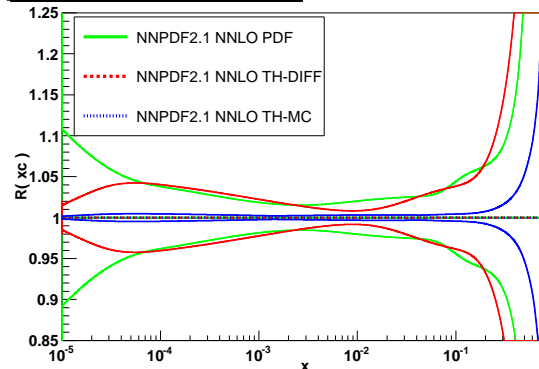
CHARM

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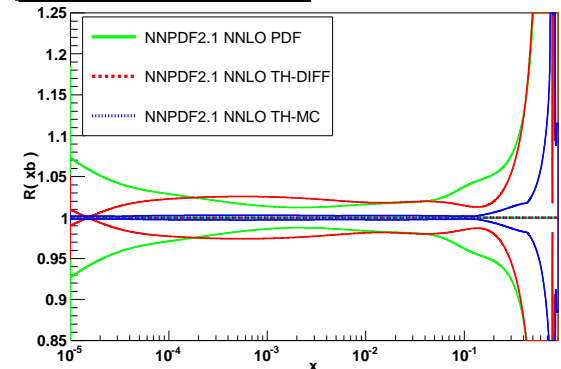
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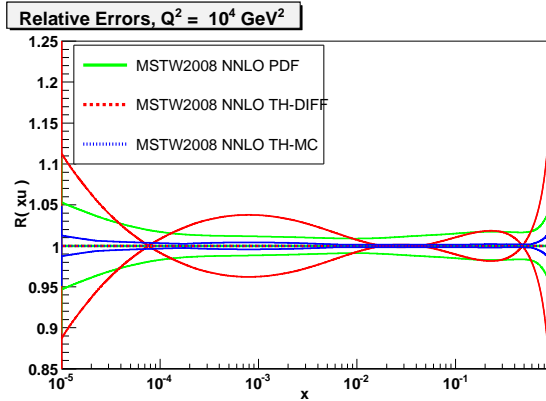
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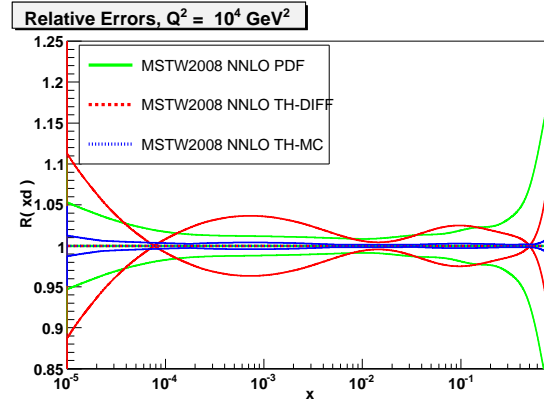
# THEORETICAL UNCERTAINTIES

NNLO PDF UNC. VS NLO-NNLO SHIFT VS NNLO CACCIARI-HOUDEAU (MSTW08)

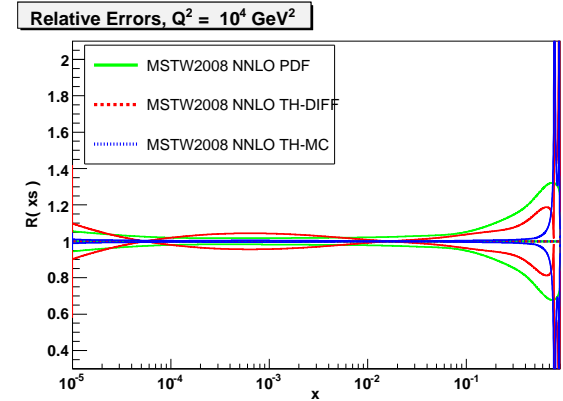
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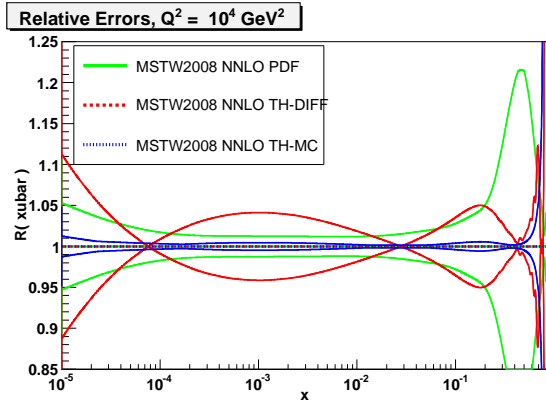
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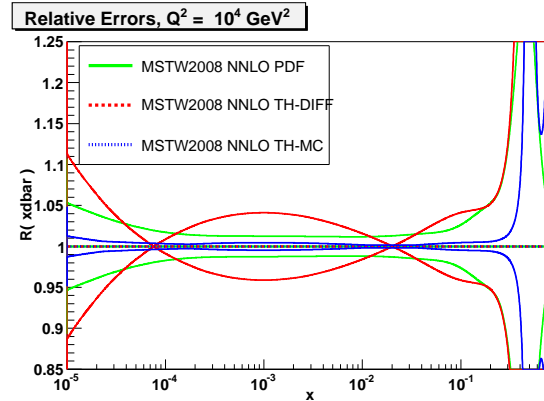
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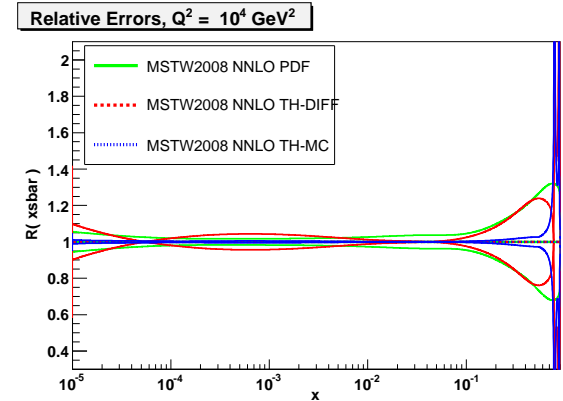
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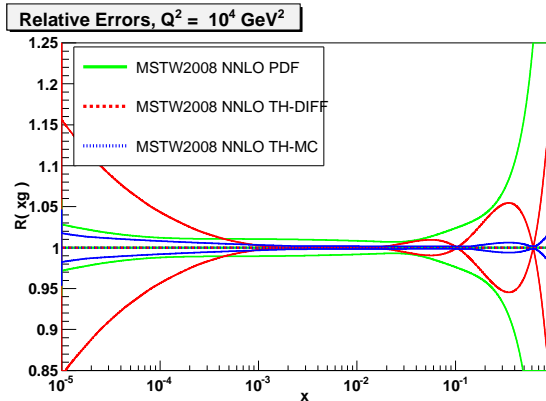
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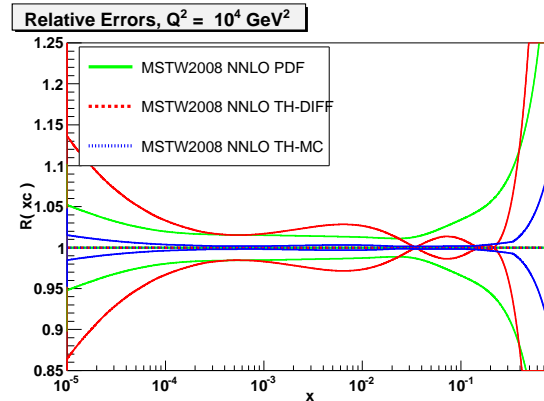
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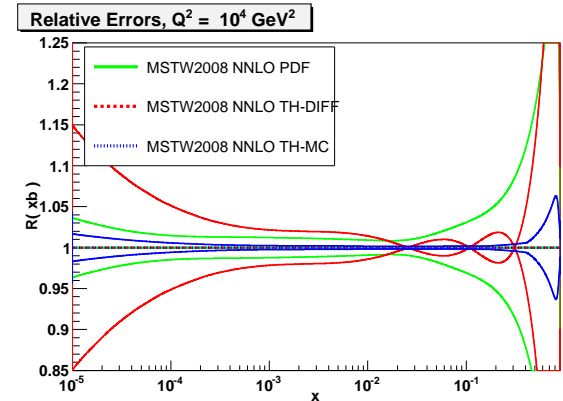
GLUON



CHARM



BOTTOM

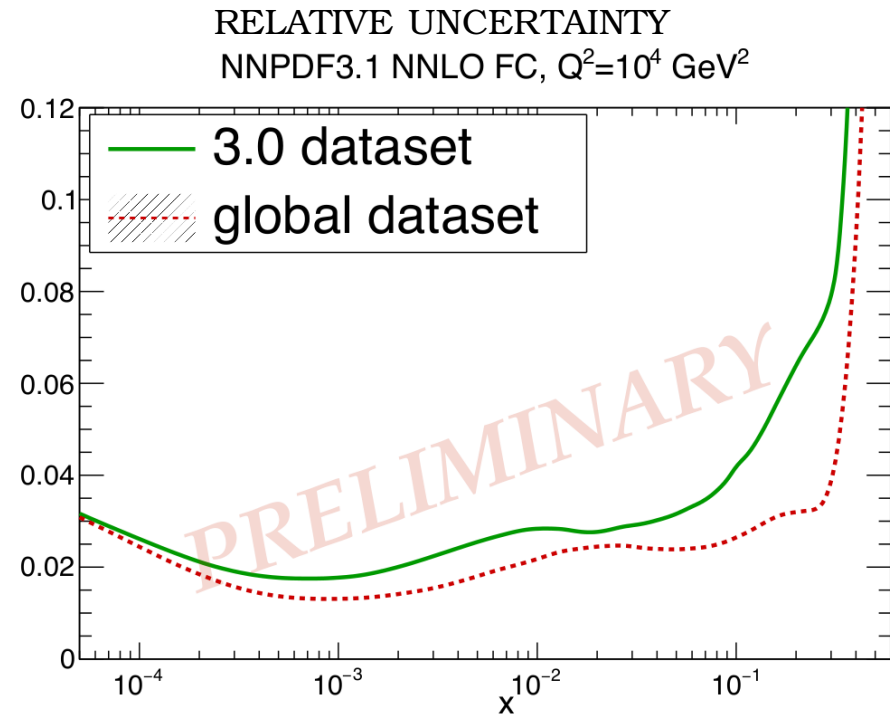
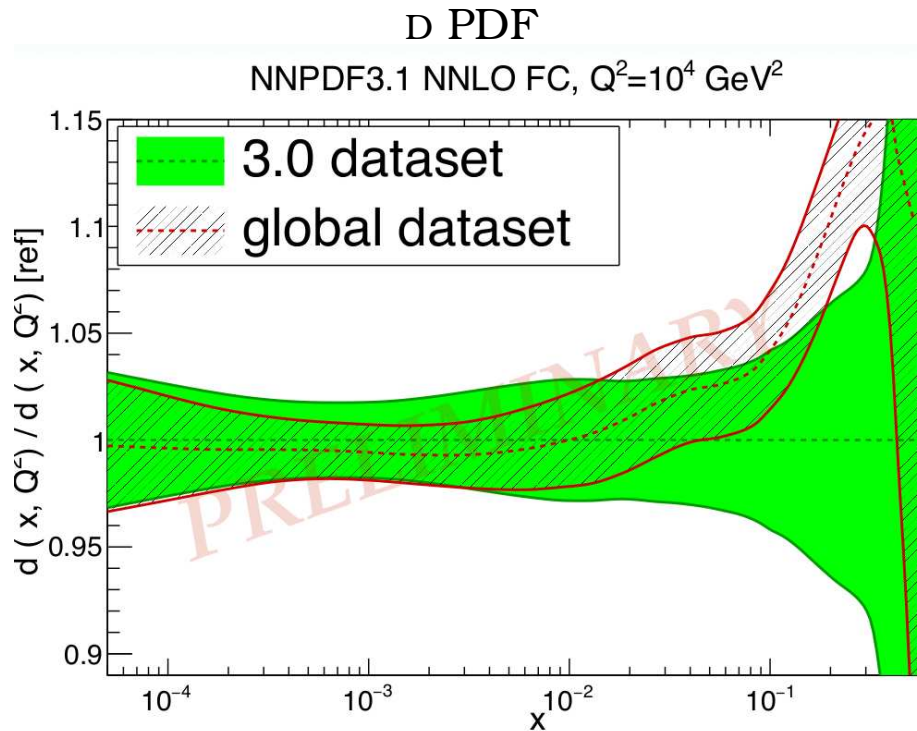


# A SOLUTION: NEXT GENERATION PDFs

## AN EXAMPLE: NNPDF3.1 NNPDF3.0 DATASET SUPPLEMENTED BY

- Tevatron legacy  $Z$  rapidity,  $W$  asymmetry & jet data
- ATLAS  $W$ ,  $Z$  rapidity, and total xsect (incl. 13TeV), high and low mass DY, jets
- CMS  $W$  asymmetry,  $W + c$  total & ratio, double-differential DY and jets
- LHCb  $W$  and  $Z$  rapidity distributions
- ATLAS and CMS  $Z$   $p_T$  distributions
- ATLAS and CMS top total cross-section & differential rapidity distribution

### NNPDF3.1 (PRELIM.)



- SURELY HIGHER PRECISION
- HOPEFULLY BETTER ACCURACY

# CLOSURE TESTS:

## THE BASIC IDEA

- ASSUME PDFS KNOWN: GENERATE FAKE EXPERIMENTAL DATA
- CAN DECIDE DATA UNCERTAINTY (ZERO, OR AS IN REAL DATA, OR . . .)
- FIT PDFS TO FAKE DATA
- CHECK WHETHER FIT REPRODUCES UNDERLYING “TRUTH”:
  - CHECK WHETHER TRUE VALUE GAUSSIANLY DISTRIBUTED ABOUT FIT
  - CHECK WHETHER UNCERTAINTIES FAITHFUL
  - CHECK STABILITY(INDEP. OF METHODOLOGICAL DETAILS)



# LEVEL-0 CLOSURE TESTS

- ASSUME VANISHING EXPERIMENTAL UNCERTAINTY
- MUST BE ABLE TO GET  $\chi^2 = 0$
- UNCERTAINTY AT DATA POINTS TENDS TO ZERO (NOT NECESSARILY ON PDF!)

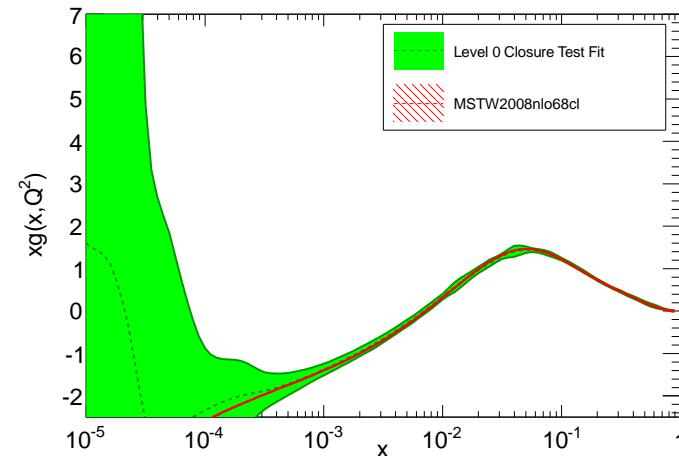
DEFINE  $\phi \equiv \sqrt{\langle \chi_{rep}^2 \rangle - \chi^2}$ ,

EQUALS FIT UNCERTAINTY/DATA UNCERTAINTY; CHECK  $\phi \rightarrow 0$

- BEST FIT ON TOP OF “TRUTH” IN DATA REGION

## THE GLUON

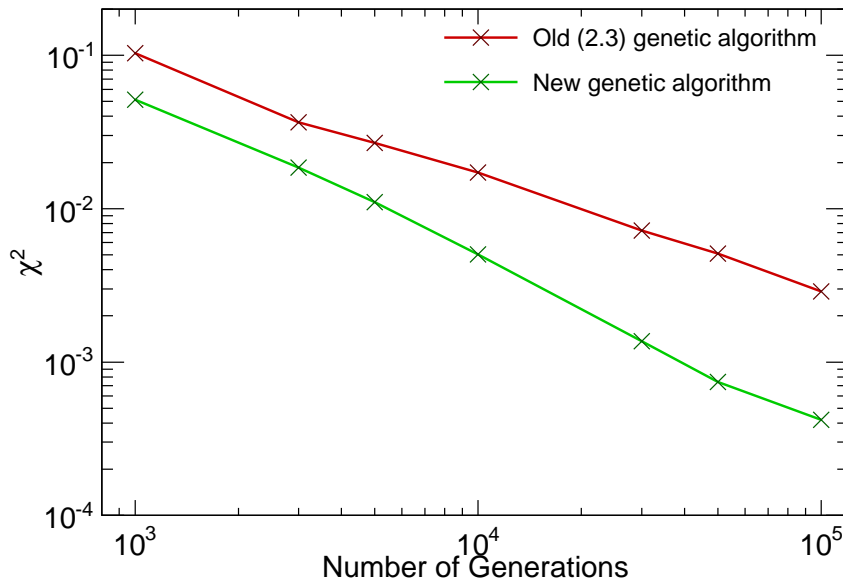
Level 0 closure test vs. MSTW



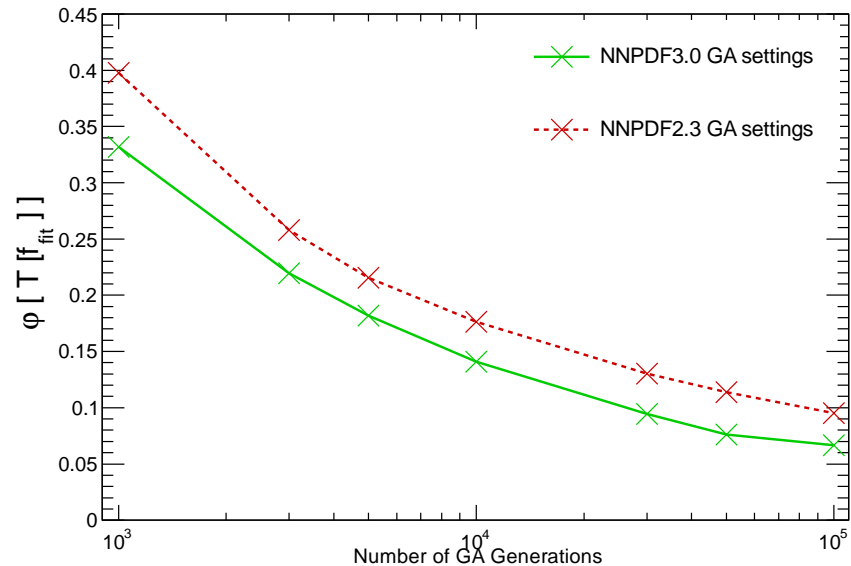
FRACTIONAL UNCERTAINTY VS TRAINING LENGTH

## $\chi^2$ VS TRAINING LENGTH

Effectiveness of Genetic Algorithm in Level 0 Closure Tests



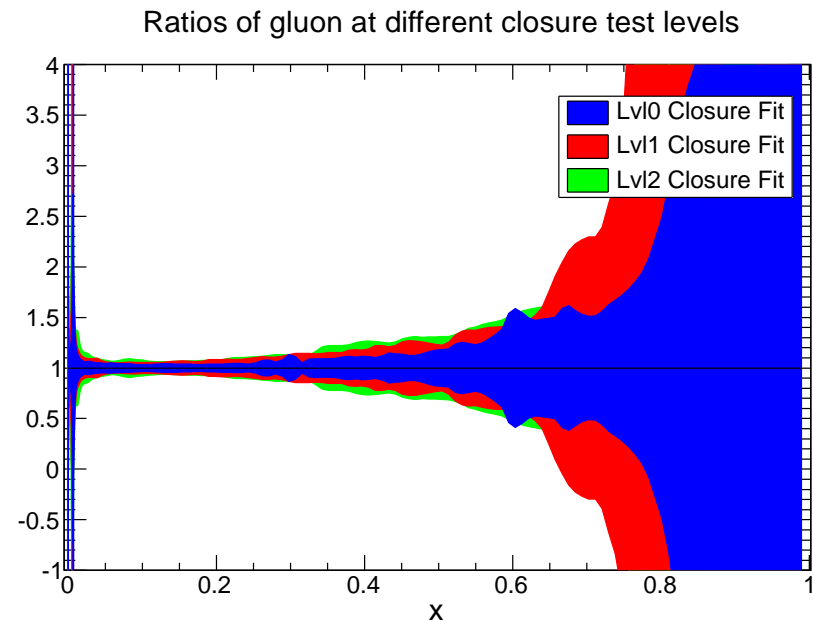
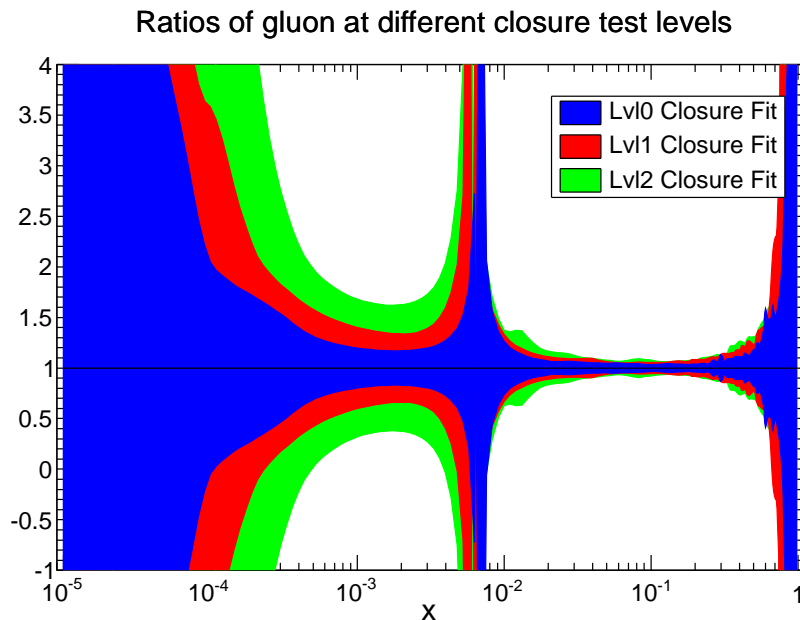
Effectiveness of Genetic Algorithms in Level 0 Closure Tests



# LEVEL-0, LEVEL-1 AND LEVEL-2

- **LEVEL 0**: FAKE DATA GENERATED WITH NO UNCERTAINTY  
→ INTERPOLATION AND EXTRAPOLATION UNCERTAINTY
- **LEVEL 1-2**: FAKE DATA GENERATED WITH SAME UNCERTAINTY AS REAL DATA (INCLUDING CORRELATIONS)
- **LEVEL 1**: NO PSEUDODATA REPLICAS:  
⇒ REPLICAS FITTED TO SAME DATA OVER AND OVER AGAIN  
→ FUNCTIONAL UNCERTAINTY DUE TO INFINITY OF EQUIVALENT MINIMA
- **LEVEL 2**: STANDARD NNPDF METHODOLOGY  
⇒ REPLICAS FITTED TO PSEUDODATA REPLICAS  
→ DATA UNCERTAINTY
- THREE SOURCES OF UNCERTAINTY COMPARABLE IN DATA REGION

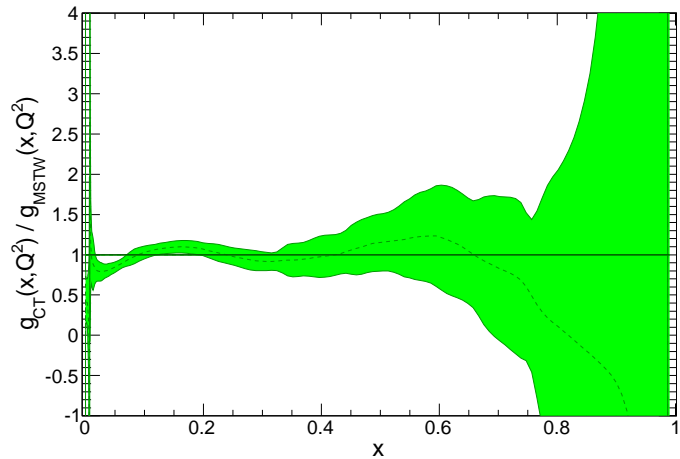
## THE GLUON: LEVEL 0, LEVEL 1 AND LEVEL 2



# LEVEL-2: CENTRAL VALUES AND UNCERTAINTIES

THE GLUON: FITTED/"TRUE"

Ratio of Closure Test g to MSTW2008

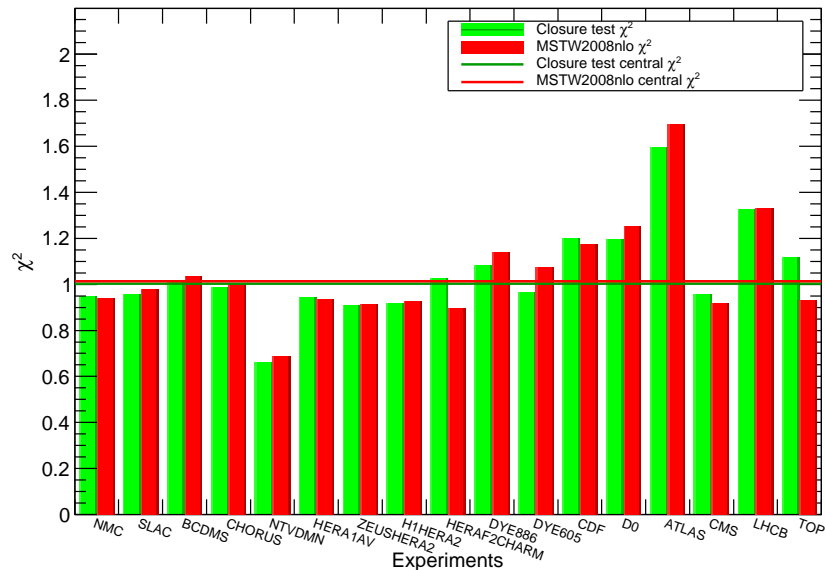


- **CENTRAL VALUES:**  
COMPARE FITTED VS. "TRUE"  $\chi^2$   
BOTH FOR INDIVIDUAL EXPERIMENTS  
& TOTAL DATASET  
FOR TOTAL  $\Delta\chi^2 = 0.001 \pm 0.003$

- **UNCERTAINTIES:** DISTRIBUTION OF DEVIATIONS BETWEEN FITTED AND "TRUE" PDFs  
SAMPLED AT 20 POINTS BETWEEN  $10^{-5}$  AND 1  
FIND 0.699% FOR ONE-SIGMA,  
0.948% FOR TWO-SIGMA C.L.

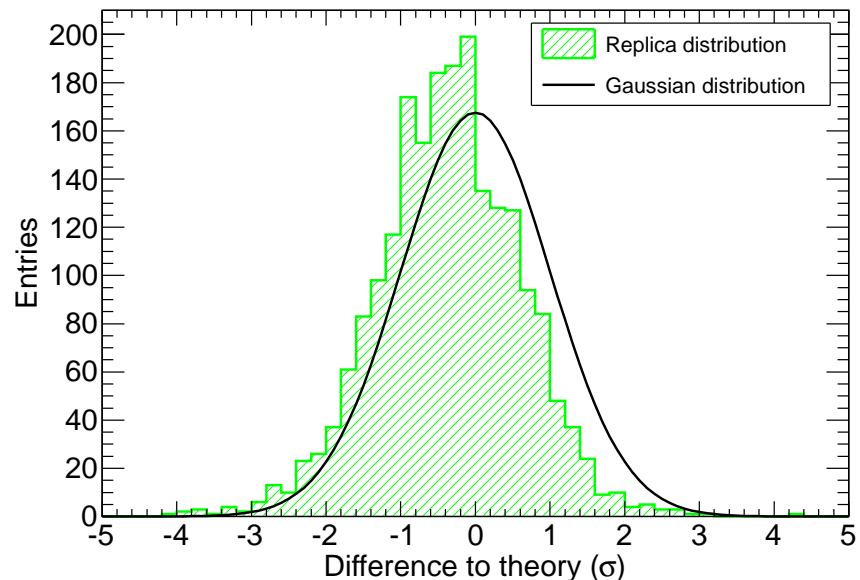
## LEVEL-2 FITTED $\chi^2$ VS "TRUE"

Distribution of  $\chi^2$  for experiments



## NORM. DISTRIBUTION OF DEVIATIONS

Distribution of single replica fits in level 2 uncertainties



# LEVEL-2 STABILITY TESTS

- CHANGE UNDERLYING PDF SET (CT10, NNPDF2.3)
- INCREASE MAXIMUM GA TRAINING LENGTH TO 80K  
TESTS EFFICIENCY OF CROSS-VALIDATION
- INCREASE NN ARCHITECTURE TO 2-20-15-1  
NUMBER OF FREE PARAMETRES INCREASE BY MORE THAN 10×
- CHANGE PDF PARAMETRIZATION BASIS  
OLD: ISOTRIplet,  $\bar{u} - \bar{d}$ ,  $s + \bar{s}$ ,  $s - \bar{s}$ ;  
NEW: ISOTRIplet, SU(3)-OCTET, BOTH TOTAL ( $q + \bar{q}$ ) & VALENCE ( $q - \bar{q}$ )

## STATISTICAL EQUIVALENCE!

DISTANCES BETWEEN REF. AND NEW FIT:

difference in unites of standard deviation of the mean

30K GENS VS 80K GENS

2.3 BASIS VS 3.0 BASIS

300 VS 37 PARMS

