Heavy Quark Production:
Prediction of Uncertainties and Uncertainty of Predictions

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Outline

Assessment of theoretical uncertainties in QCD predictions

A generic heavy quark production process

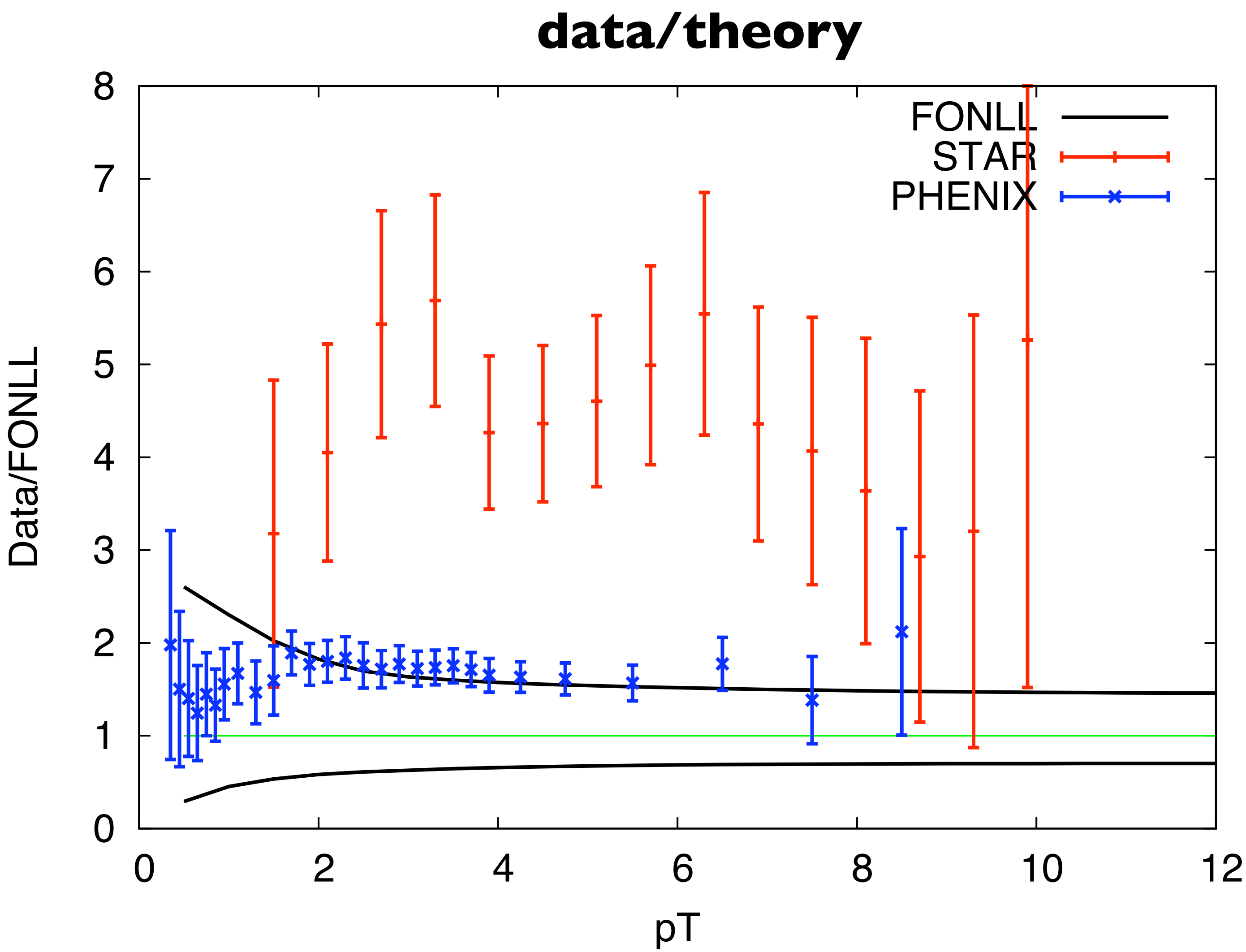
$$pp \xrightarrow{pQCD} Q \xrightarrow{NP\,fragm.} H_Q \xrightarrow{decay} e$$

A generic final state observable

Compare at this level, if possible.
A quark is not a physical object

This part is QCD.
How accurately can we predict it?
What ingredients do we need?

Charm and bottom production @ RHIC



Non-photonic electrons from charm and bottom

What does the theoretical uncertainty band really mean?

How do we assess its reliability?

A modern phenomenological prediction

Two components:

1. The ‘**number**’
2. Its **uncertainty**

(Yes, the theorists finally caught up with the experimentalists.
From time to time, in our best days, we even quote asymmetrical errors.......)

The uncertainty will have (at least) two sub-components:

- intrinsic limitations of the calculation (i.e. truncation of perturbative series)
- imperfect knowledge of numerical inputs to the calculation itself

Theoretical uncertainty components

1. Renormalisation/factorisation scales

Independent scale variations
$0.5 < \mu_{R,F}/m < 2$ && $0.5 < \mu_R/\mu_F < 2$

2. Heavy quark mass

$1.3 < m_{charm} < 1.7$ GeV
$4.5 < m_{bottom} < 5$ GeV

3. Parton distribution functions / α_s

Modern sets provide 'uncertainties'
Are they reliable?

And, if it's a differential cross section we are looking at,

4. Non-perturbative fragmentation

Fixed by e+e- data.
Negligible unc. when properly extracted/used

What can we calculate? What tools are available?

One can of course always use PYTHIA.
For better accuracy, a number of codes based on the full
NLO QCD calculation are available:

Total cross sections

Implementation of analytical NDE NLO calculation

(see also Ramona's talk)

1-particle inclusive distributions

FONLL (NLO+NLL resummation, NP matching)

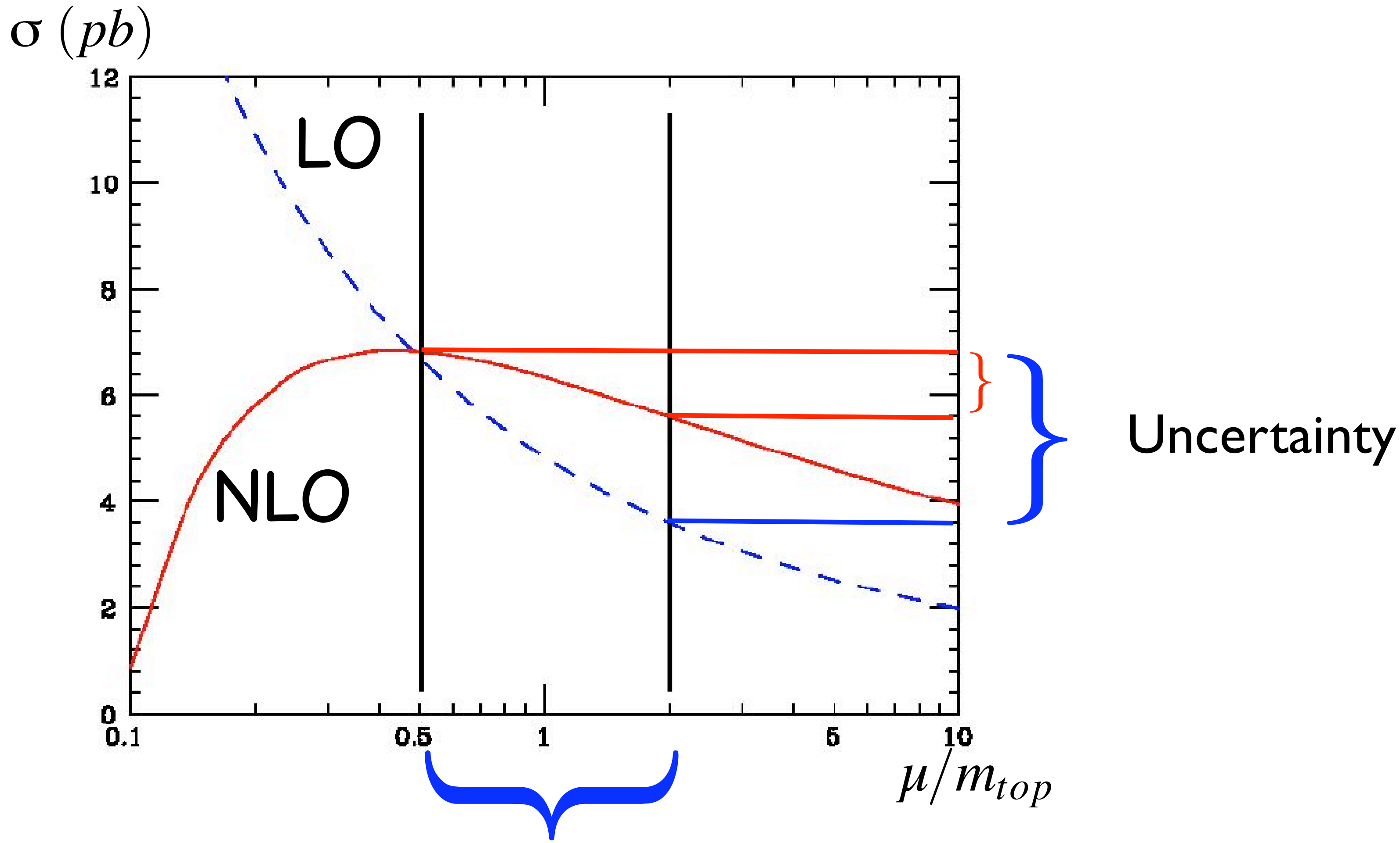
2-particle correlations (i.e. fully exclusive codes)

MNR
MC@NLO
POWHEG

Not covered today

The rule of thumb on uncertainties

“Typical” behaviour of a cross-section w.r.t. scale variations

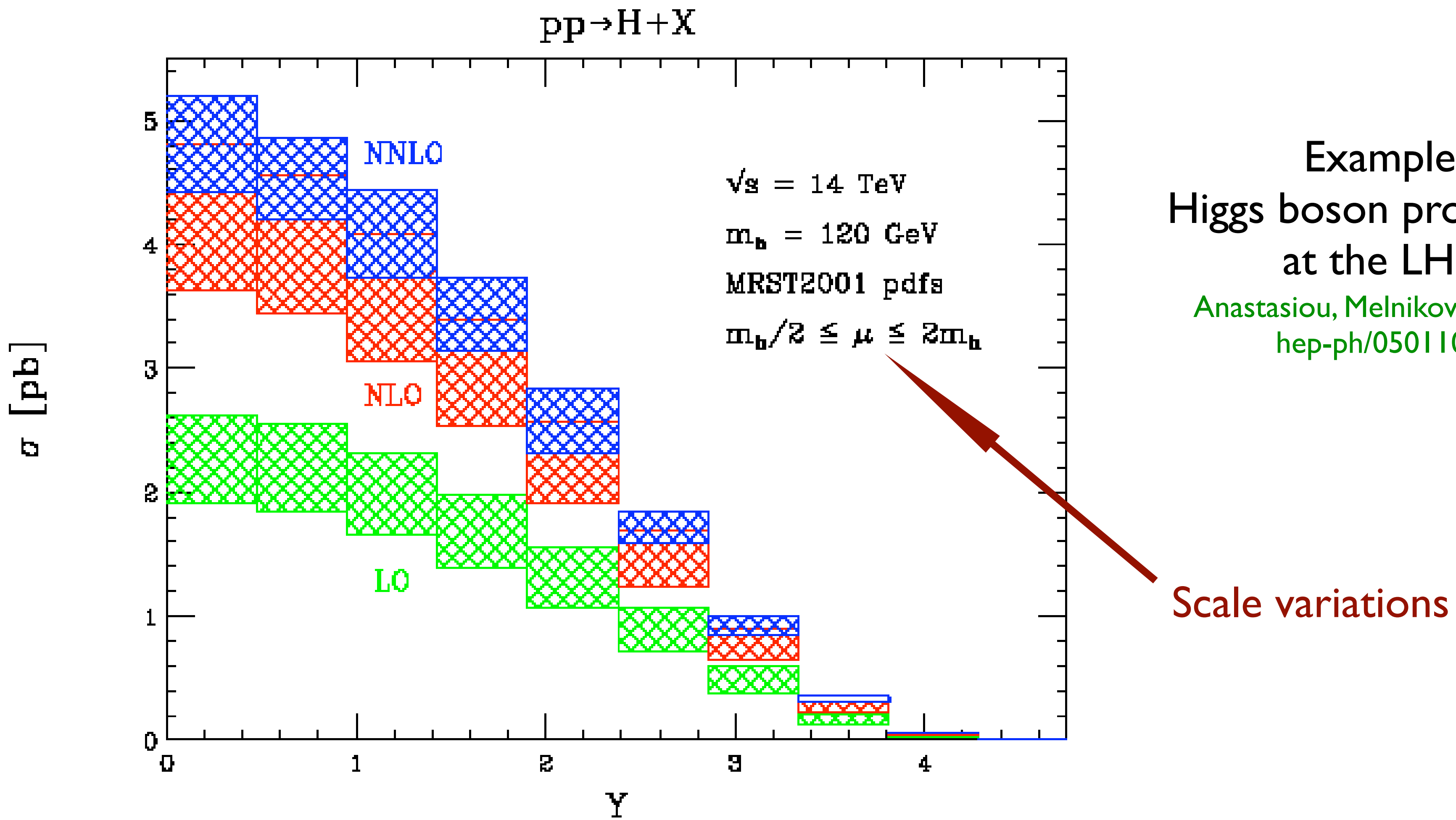


- A **LO** calculation gives you a **rough estimate** of the cross section

- A **NLO** calculation gives you a **good estimate** of the cross section and a **rough estimate** of the uncertainty

The rule of thumb on uncertainties

- A **NNLO** calculation gives you a **good estimate** of the uncertainty



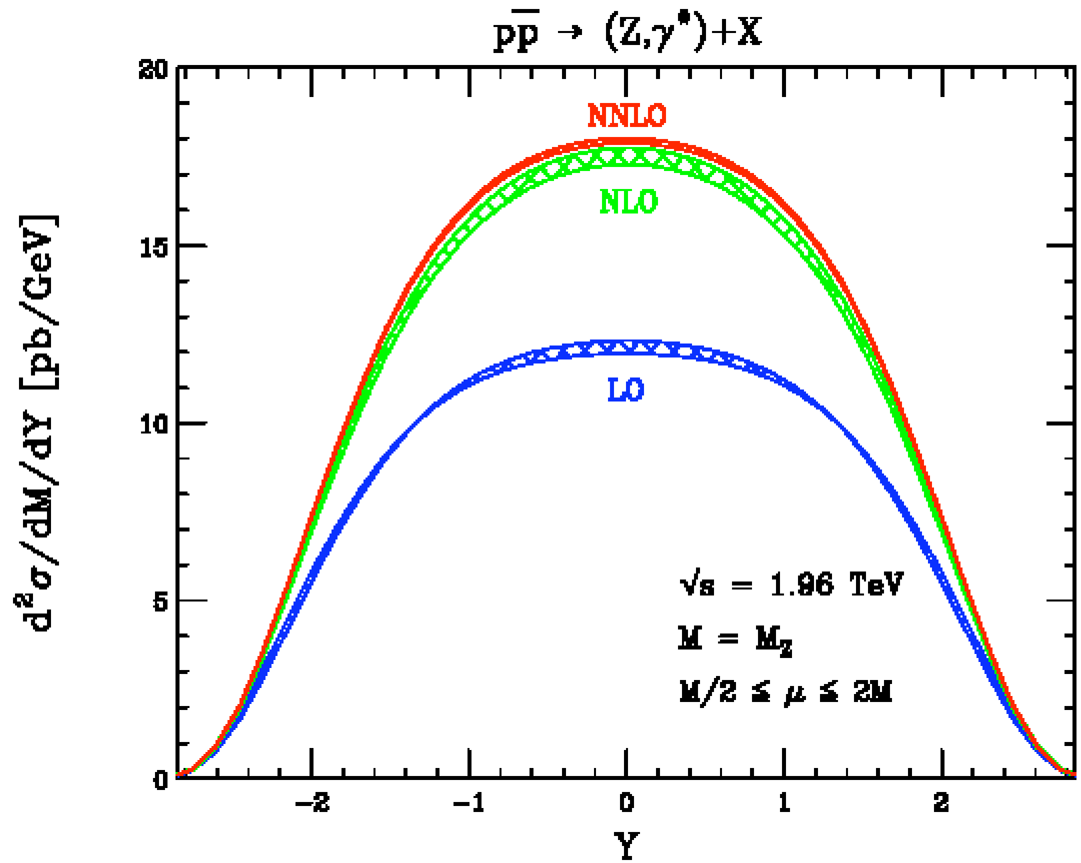
Example:
Higgs boson production at the LHC
Anastasiou, Melnikov. Petriello, hep-ph/05011030

NB. This example shows that the center of the NLO band has nothing to do with the most accurate theoretical prediction.

Theoretical uncertainty bands are not gaussian errors!

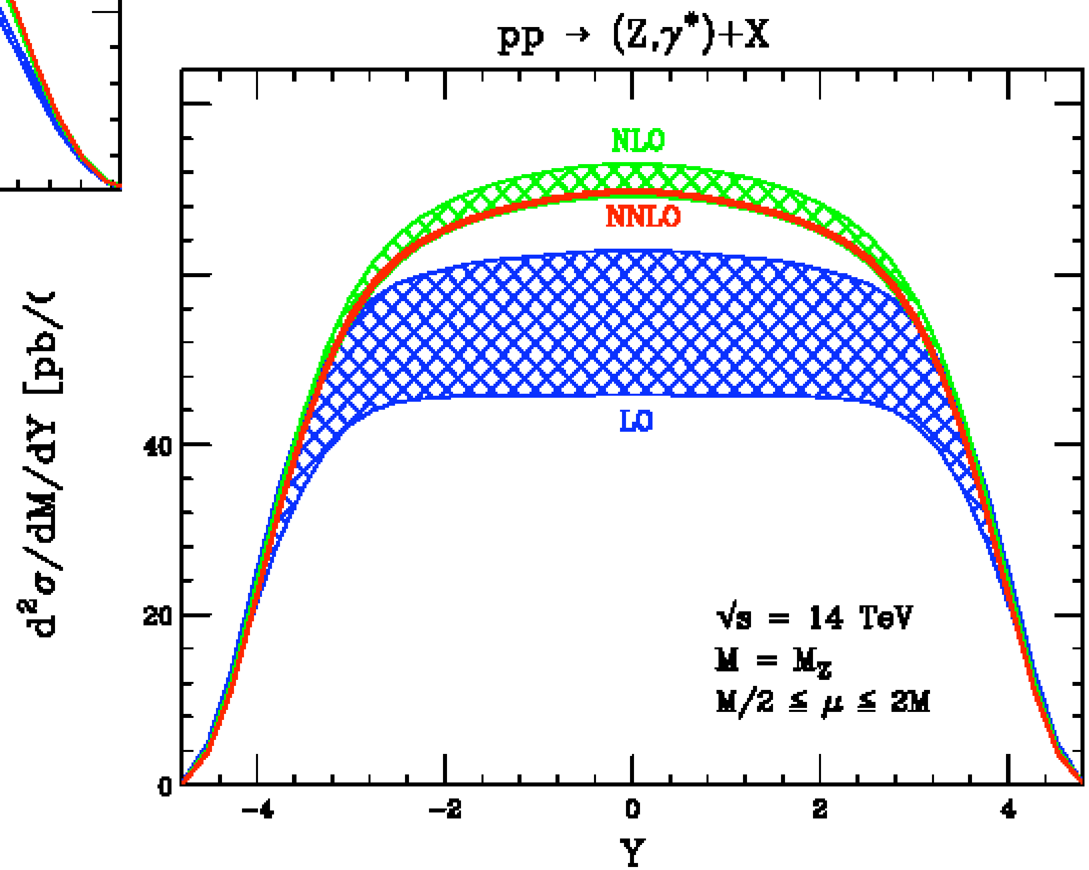
One more example

Anastasiou, Dixon, Melnikov. Petriello, hep-ph/0312266



Z production at the Tevatron

If you think you've found a standard rule, *"NNLO is on the upper limit of the NLO uncertainty band"*, think again



Z production at the LHC:
NNLO now on the lower side of the NLO uncertainty band

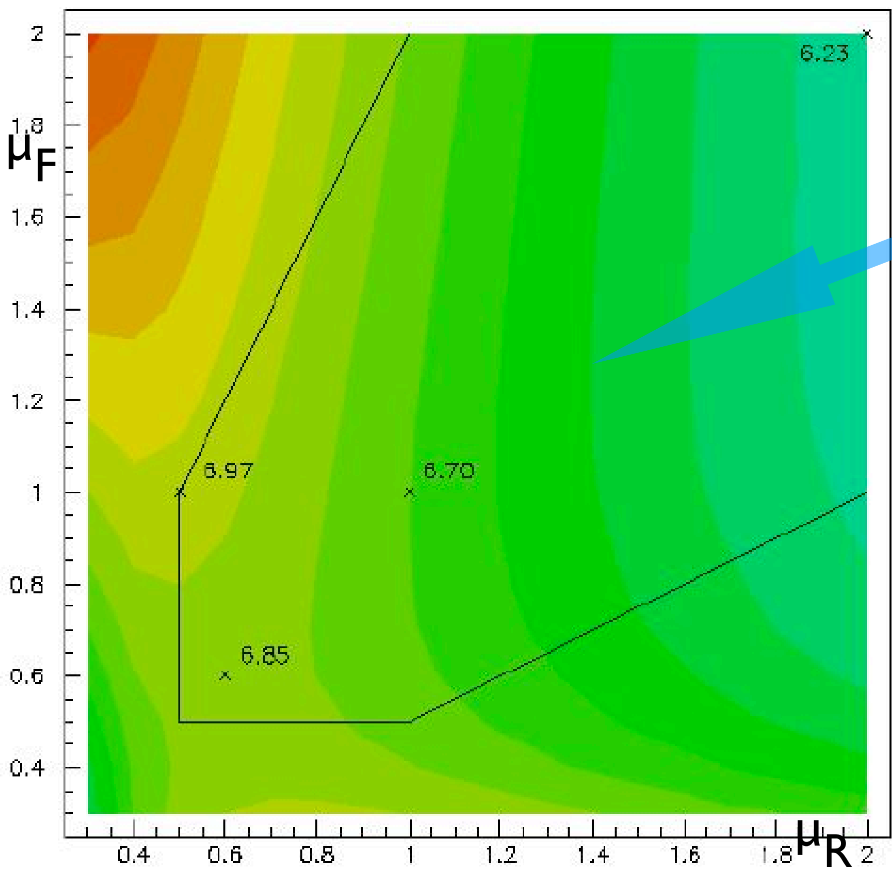
A theoretical *uncertainy band* is meant to be just that: you don't know where the higher order will be

Uncertainties estimate: top @ Tevatron

Standard procedure: vary renormalization and factorization scales.
But, better do so **independently**

σ: 6.82 > 6.70 > 6.23 pb $0.5 < \mu_{R,F}/m < 2$

σ: 6.97 > 6.70 > 6.23 pb $0.5 < \mu_{R,F}/m < 2$ && $0.5 < \mu_R/\mu_F < 2$

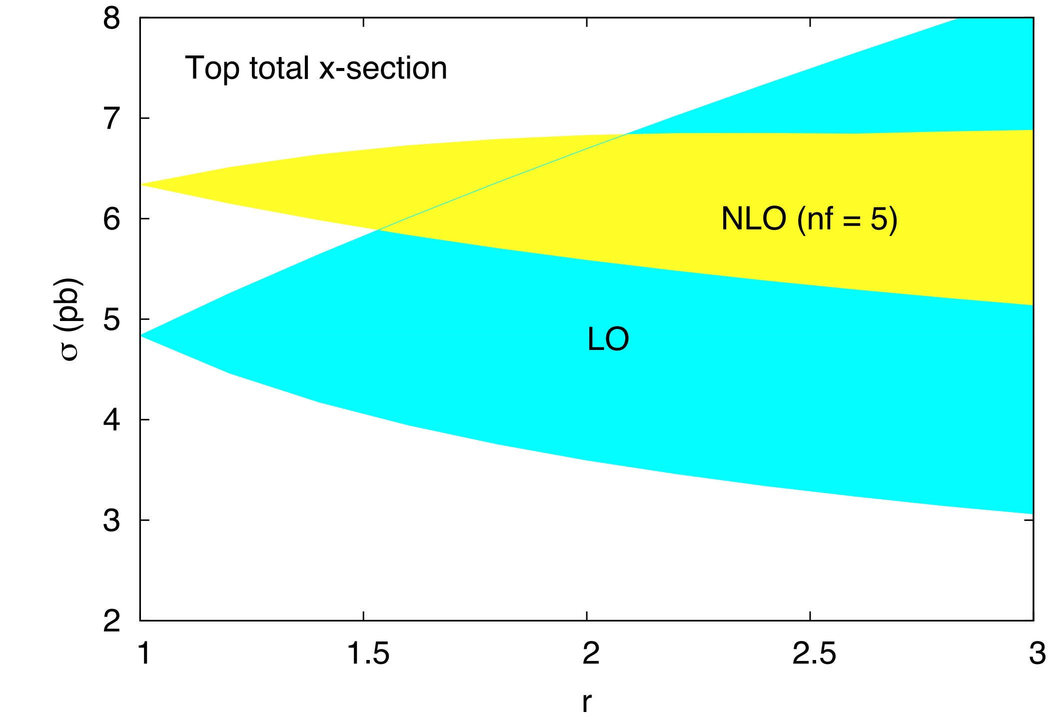


"Fiducial" region

Order **±5%** uncertainty along the diagonal, a little more when considering independent scale variations

NB. The PDF uncertainty (±10-15%) is the dominant one here

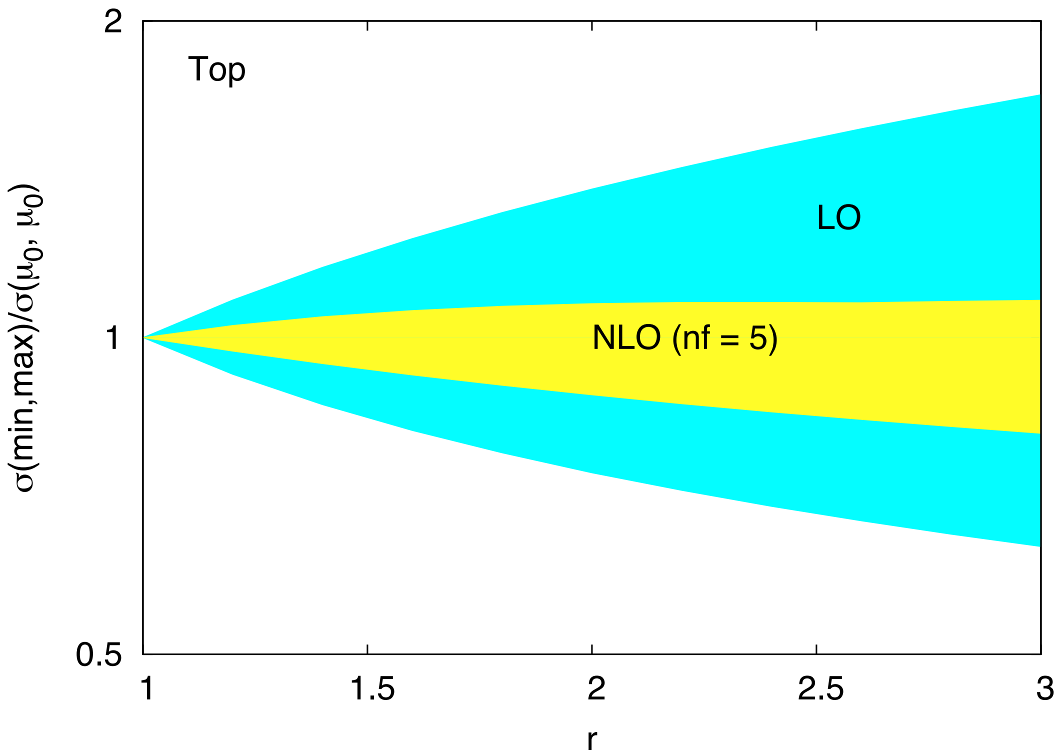
Top total cross section



Uncertainty as a function of r, calculated as envelope of

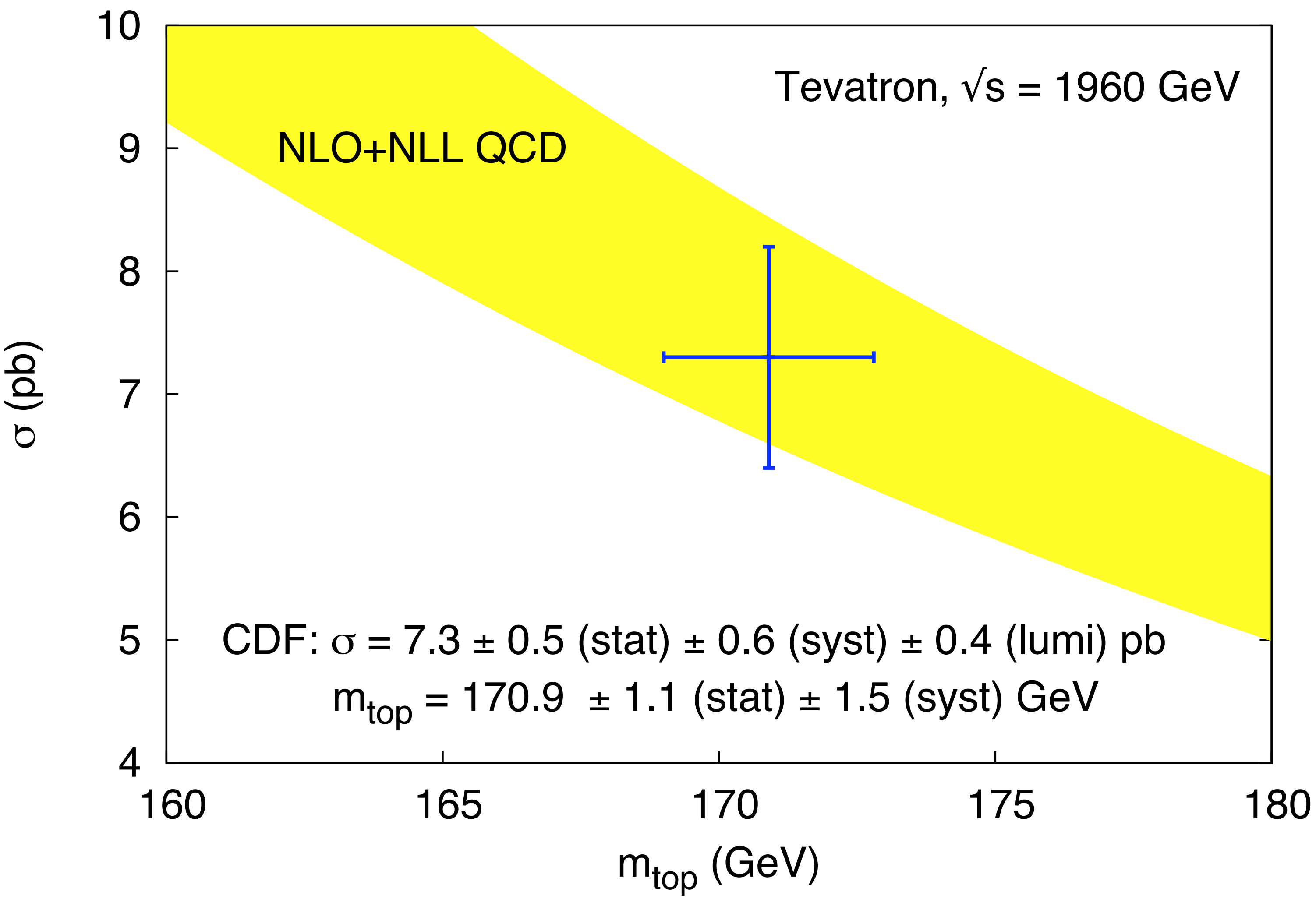
$$\frac{\mu_0}{r} \leq \mu_{R,F} \leq r\mu_0 \quad \&\& \quad \frac{1}{r} \leq \frac{\mu_R}{\mu_F} \leq r$$

[r=2 is the standard choice. Why? Arbitrary to a large extent]



Ratio of min,max to central value

Top total cross section



Good agreement with QCD predictions

NB: cross section data and theory almost good enough to extract mass from comparison

Not yet competitive with direct measurement, but getting there
Bonus: this would be a NLO pole mass (i.e. better defined than LO PYTHIA mass)

Uncertainties estimate: bottom @ Tevatron Run II

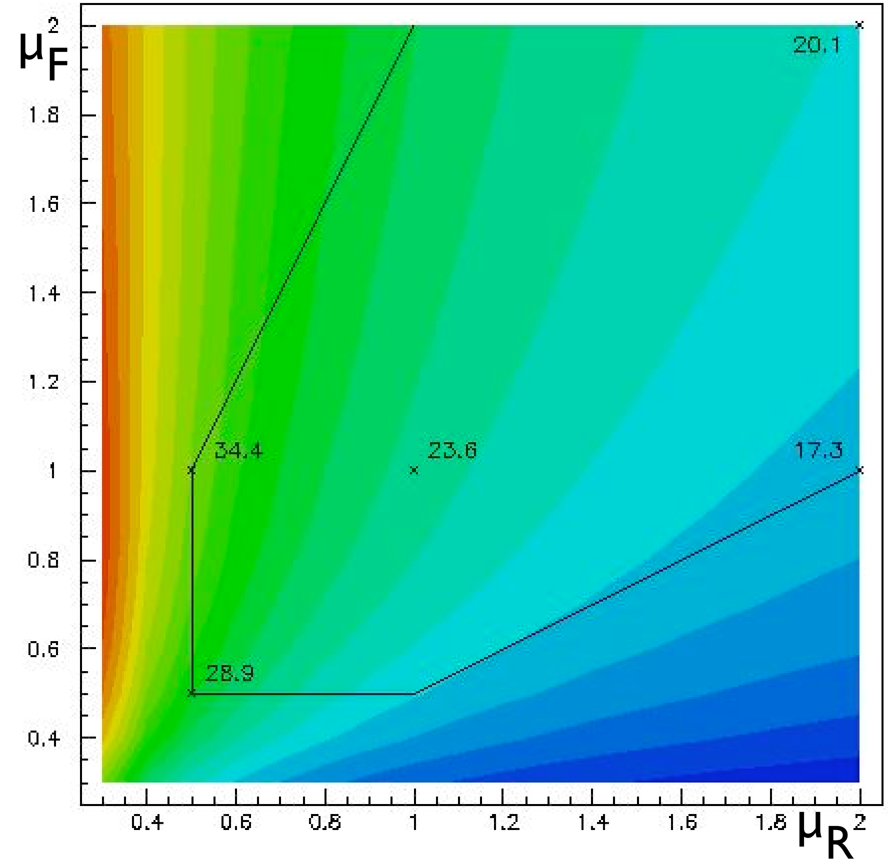
Scales uncertainty:

$\sigma(|y|<1)$: 28.9 > 23.6 > 20.1 μb

$0.5 < \mu_{R,F}/\mu_0 < 2$

$\sigma(|y|<1)$: 34.4 > 23.6 > 17.3 μb

$0.5 < \mu_{R,F}/\mu_0 < 2$ && $0.5 < \mu_R/\mu_F < 2$



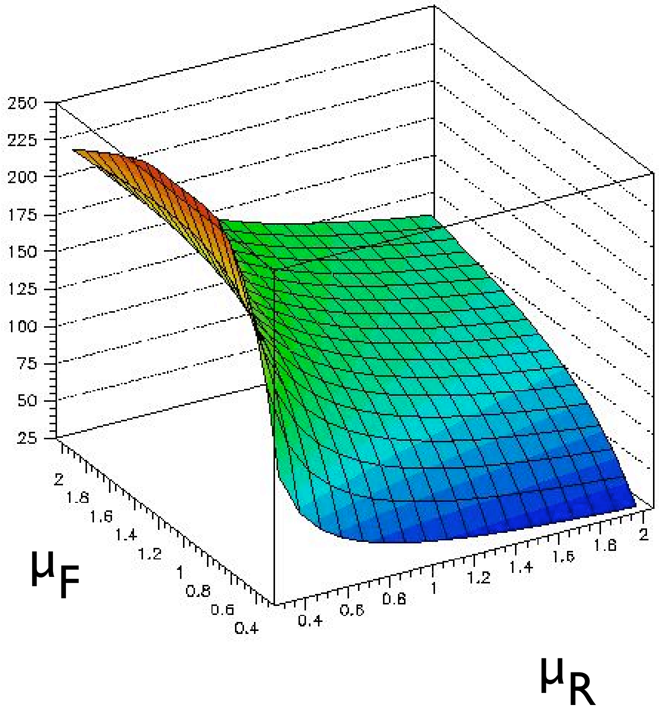
The scales uncertainty increases from **±18%** to **±35%**
when going off-diagonal

→ a first example of the importance of properly exploring the uncertainty sources

Uncertainties estimate: bottom @ LHC

$\sigma(|y|<1)$: 122 > 120 > 115 μb
$0.5 < \mu_{R,F}/\mu_0 < 2$

Only a **±4%** uncertainty when varying the scales together.......

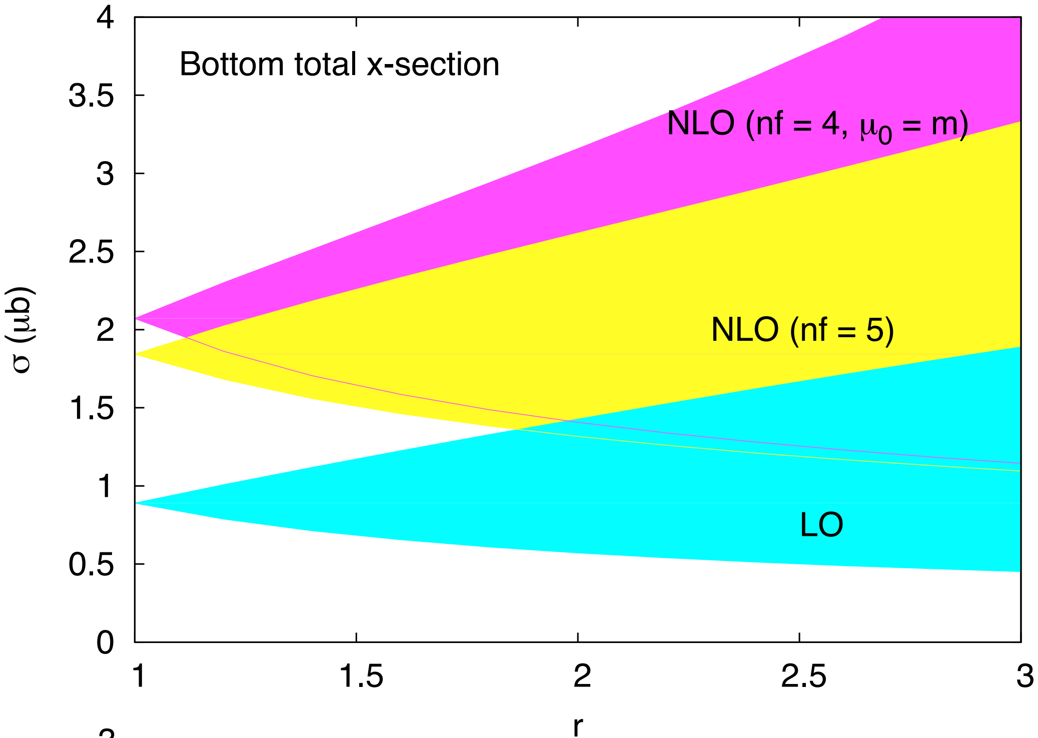


$\sigma(|y|<1)$: 178 > 120 > 75 μb
$0.5 < \mu_{R,F}/\mu_0 < 2$ && $0.5 < \mu_R/\mu_F < 2$

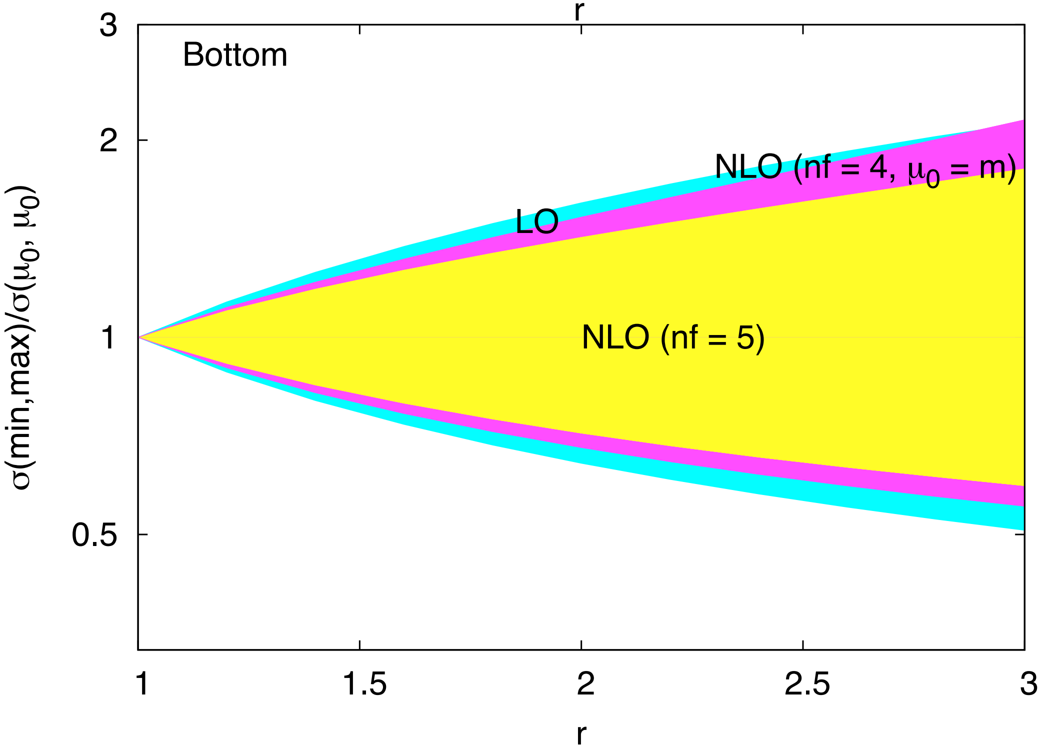
....which becomes a **±40%** one when going off-diagonal!

Note difference with Tevatron case.
The behaviour of the scales uncertainty cannot be reliably extrapolated

Uncertainties estimate: bottom @ RHIC

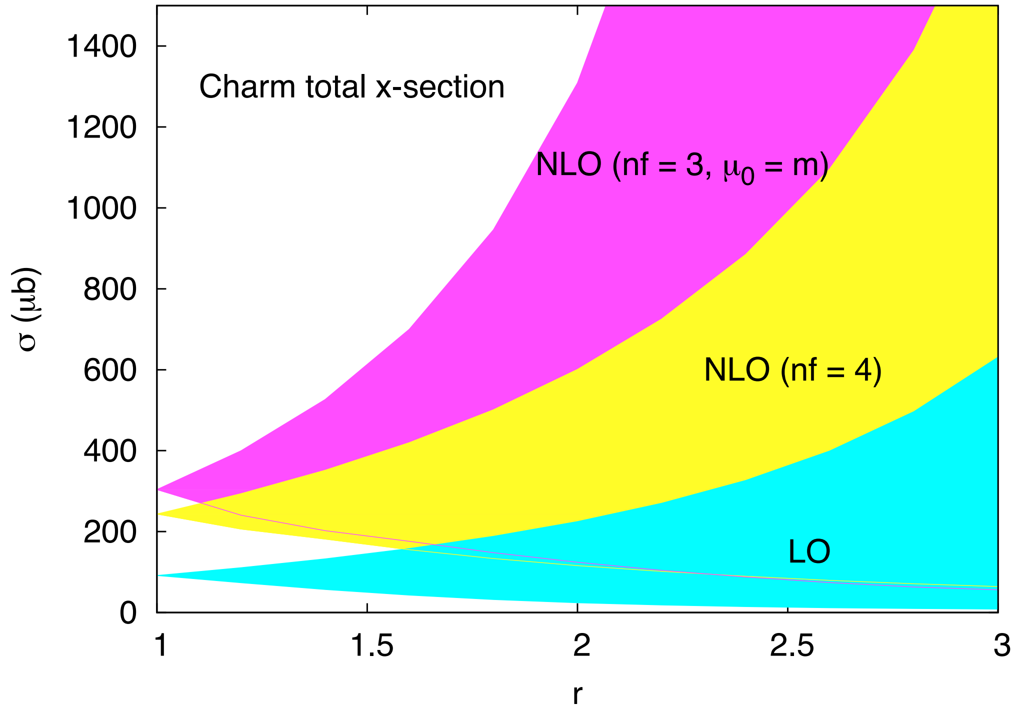


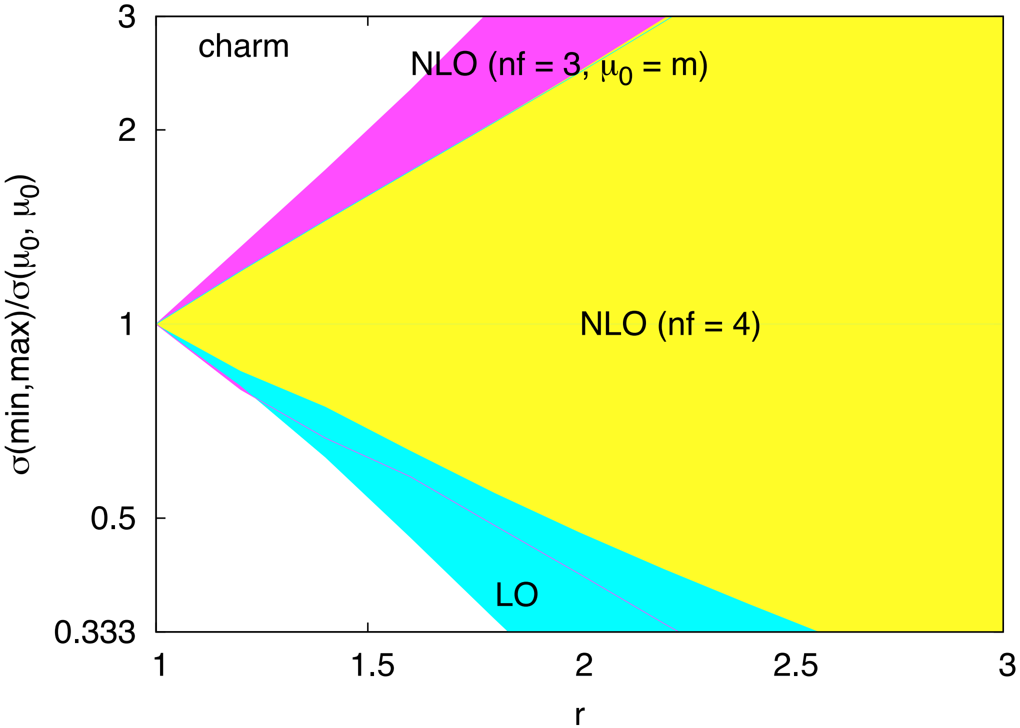
Convergence not that good.
NLO marginally better than LO



A different scheme (4 rather than 5 active flavours, and fixed central scales) starts showing non fully negligible differences

Uncertainties estimate: charm @ RHIC





Uncertainties fairly huge

nf = 3 and fixed central scale schemes 'predict' even larger uncertainties

$$\sigma = 243^{+382}_{-153}\ \mu b$$ nf = 4 running cent. sc.

$$\sigma = 304^{+789}_{-210}\ \mu b$$ nf = 4 fixed cent. sc.

$$\sigma = 304^{+1022}_{-212}\ \mu b$$ nf = 3 fixed cent. sc.

$$\sigma = 236^{+440}_{-150}\ \mu b$$ nf = 3 running cent. sc.

[NB. Central values reasonably stable]

Let's get differential

Total cross sections are rarely really measured.

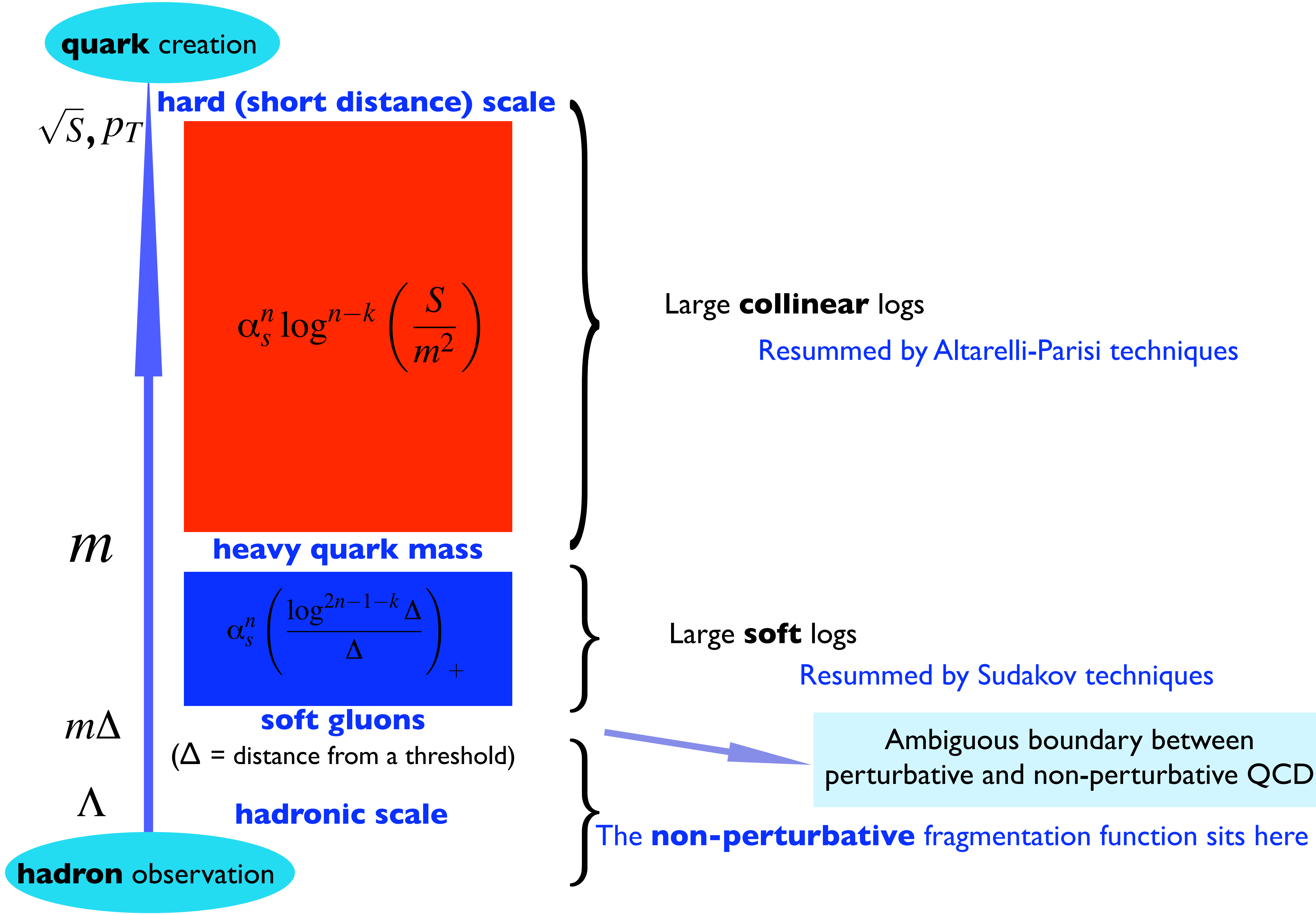
Usually they are obtained by deconvoluting and/or extrapolating the real measurement
This introduces a potential bias from theoretical prejudice that we'd like to avoid

Alternative: **differential** cross section

However, predictions for differential distributions are **harder**:

- Any multi-scale quantity in QCD will display possibly **large logarithms** in the perturbative expansion. These logs will tend to spoil the convergence of the series. Hence, **resummations** will be needed
- Eventually, resummations will not be enough, and genuinely **non-perturbative** contributions will need to be added. They should be included in a correct and minimal way, so as not to spoil the predictivity of pQCD

The many scales in heavy quark production



Phenomenological implementation

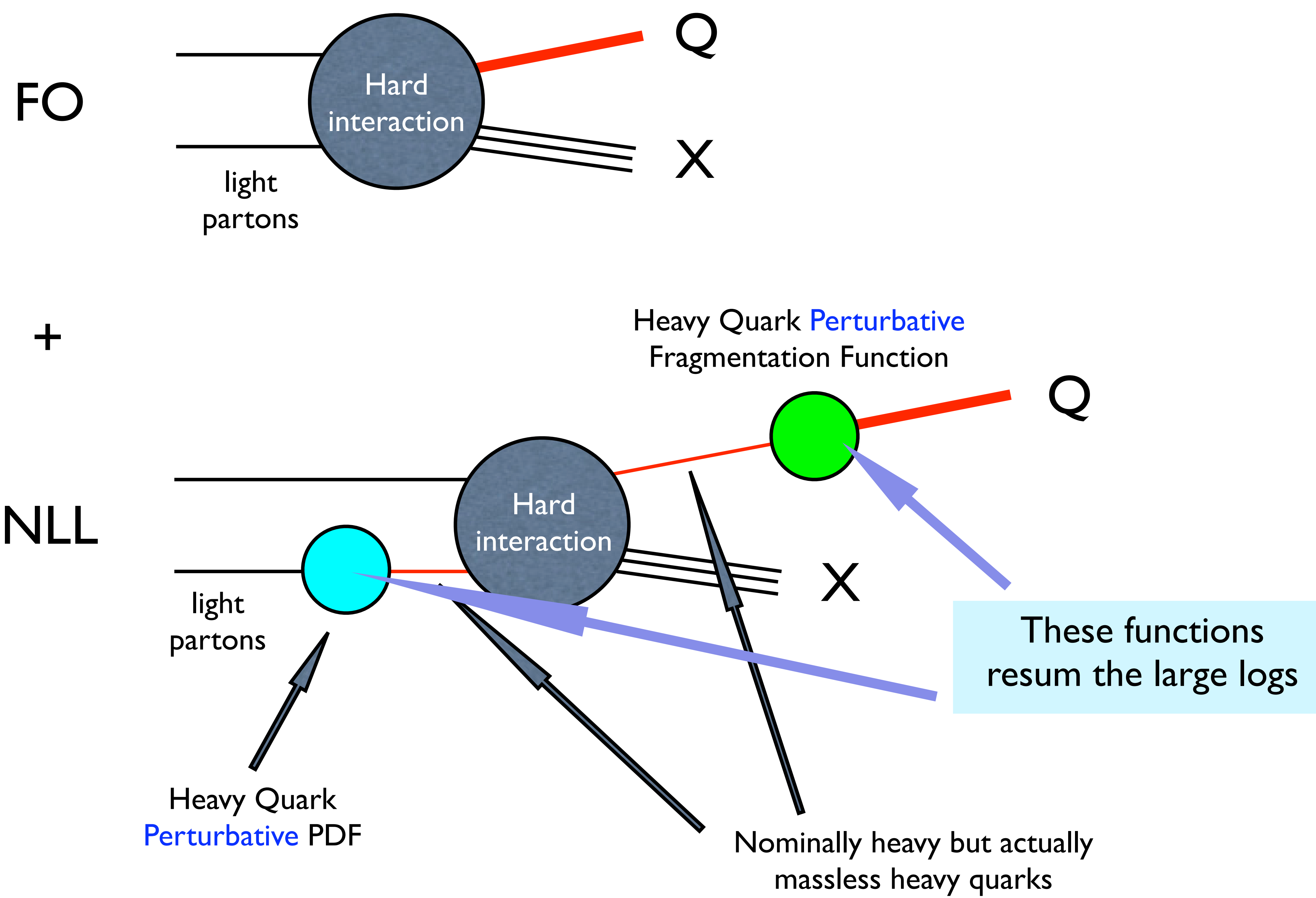
$$\frac{d\sigma_H}{dp_T} = \frac{d\sigma_Q}{dp_T} \otimes D^{np}$$

measured cross section

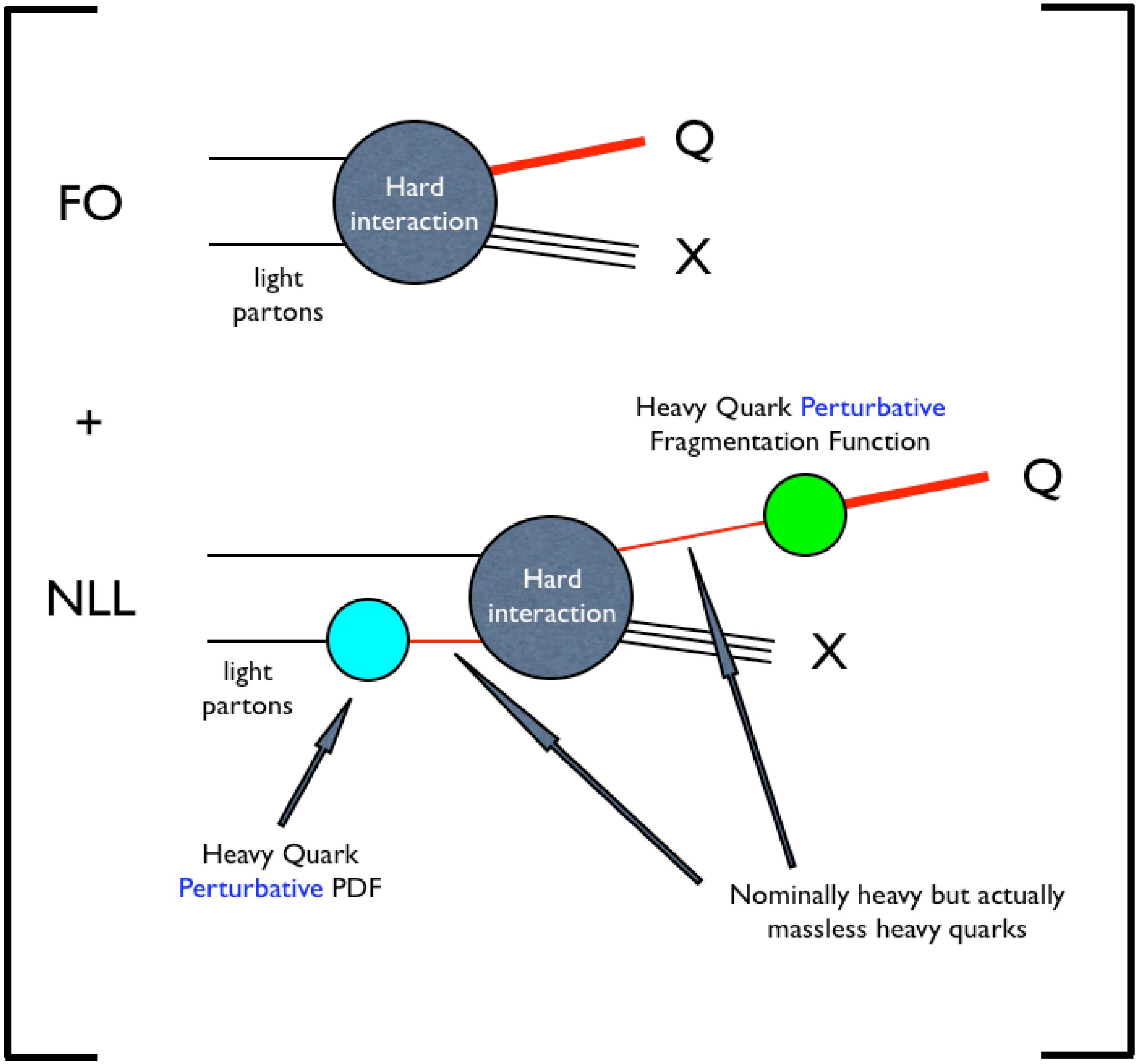
NLO (+NLL) calculation

non-perturbative fragmentation
(usually extracted from e+e- data)

FONLL: How does it work?



FONLL: inclusion of NP fragmentation

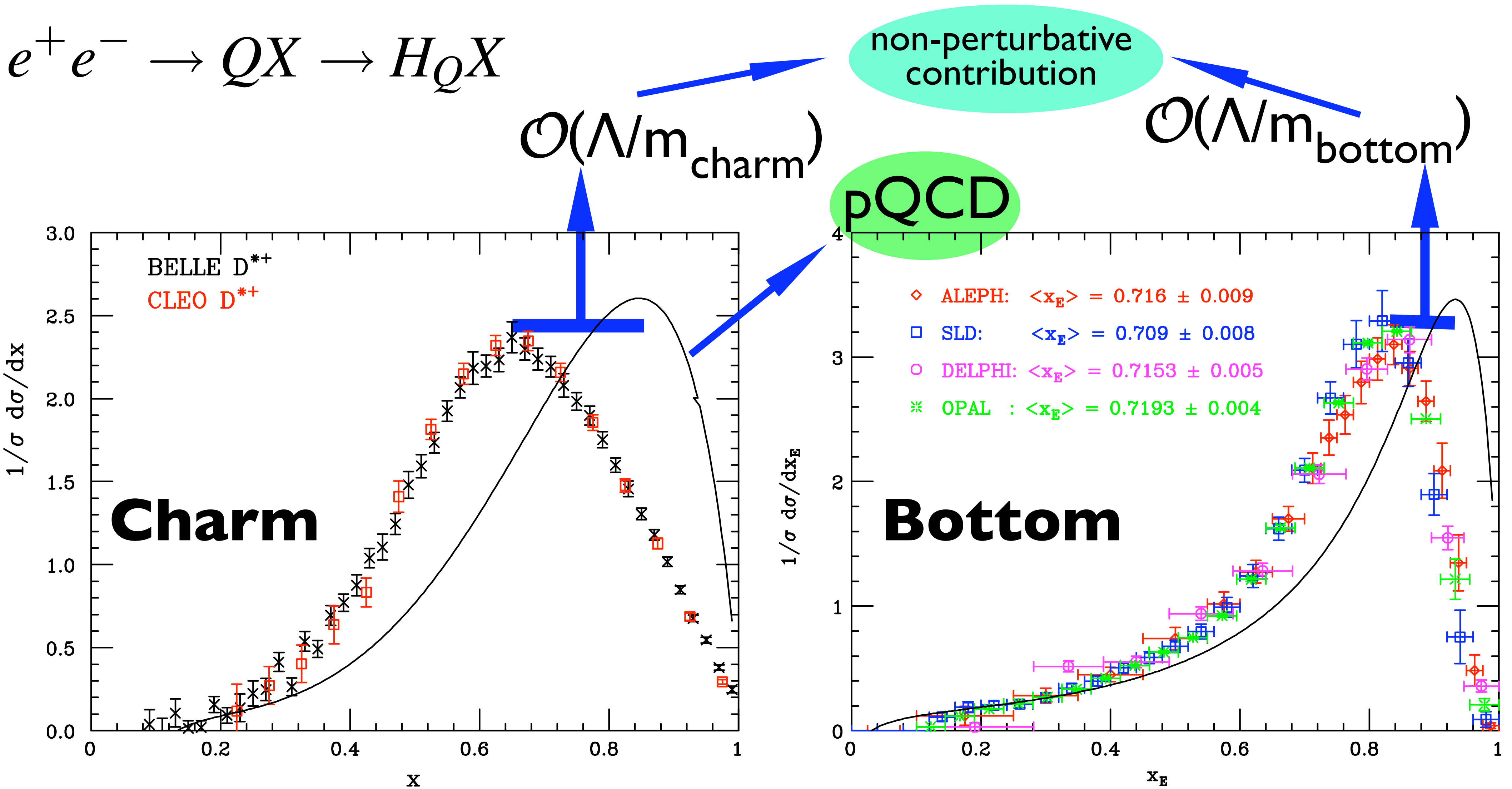


$$\otimes \quad D_{Q\to H}$$

Fitted to e+e- data
in the **same scheme**

Non-perturbative fragmentation

$$e^+e^- \to QX \to H_Q X$$



- non-perturbative contribution limited in size and compatible with expectations
- high-accuracy expt. data allow it to be precisely determined

Non-perturbative fragmentation

$\langle x^{N-1} \rangle$ moments can give a more quantitative picture:

N	2
c @ 10.58 GeV	0.7359
c @ 91.2 GeV (NS)	0.5858
c @ 91.2 GeV (full)	0.5954
b @ 91.2 GeV	0.7634
BELLE $D^{*+} \to D^0$ (ISR corr.)	0.6418 ± 0.0042
ALEPH D^{*+} (ISR corr.)	0.4920 ± 0.0152
ALEPH B	0.7163 ± 0.0085
CLEO D^{*+}	$0.877^{+0.009}_{-0.010}$
BELLE $D^{*+} \to D^0$	$0.872^{+0.005}_{-0.006}$
ALEPH D^{*+}	$0.840^{+0.022}_{-0.031}$
Tab. 2 and eq. (4.2)	0.868
ALEPH B	$0.938^{+0.009}_{-0.014}$
SLD B	$0.931^{+0.016}_{-0.030}$

N=2 moments (i.e. 〈x〉)

pQCD (NLL)

data
(very precise!)

$$D^{np} = \frac{\text{data}}{\text{pQCD}}$$

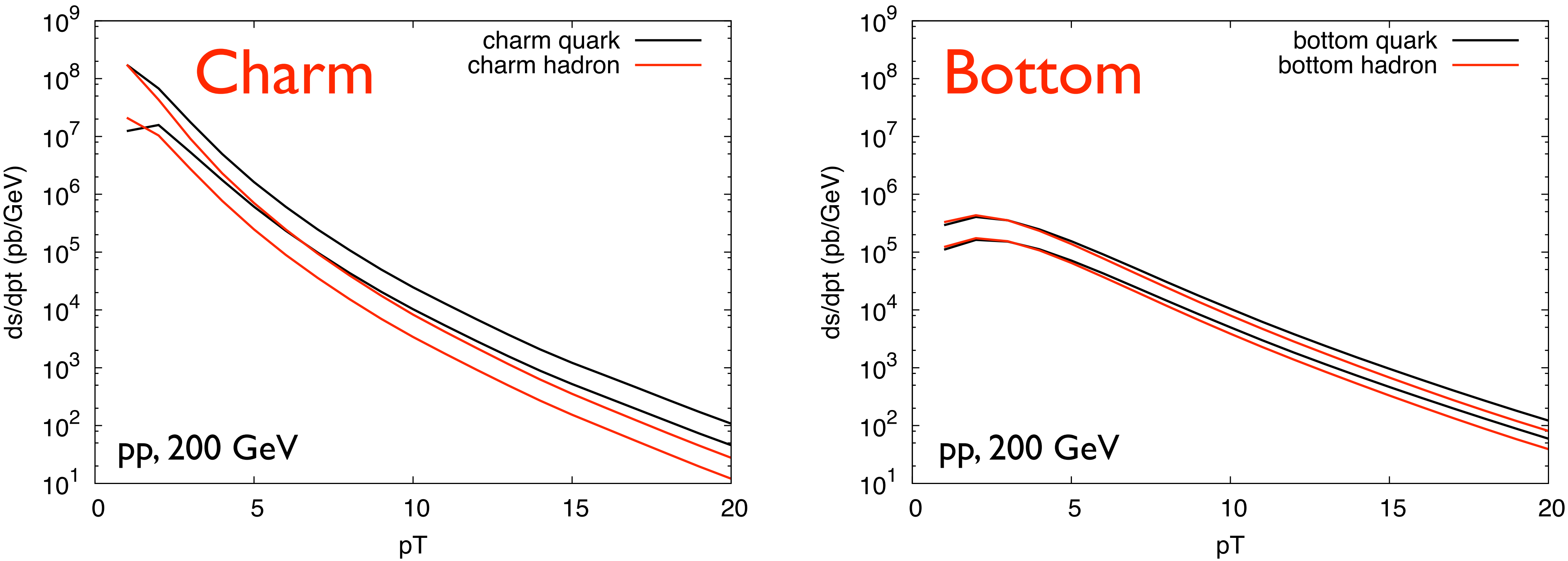
charm ~ 1 - 0.16
bottom ~ 1 - 0.06

Compatible with $D_N^{np} = 1 - \frac{(N-1)\Lambda}{m} + \cdots$ and $\Lambda \simeq 0.25$ GeV

Heavy quark cross sections

Heavy quarks are special:
their **total number** (and that of **heavy hadrons)**
is a **genuine prediction of pQCD**

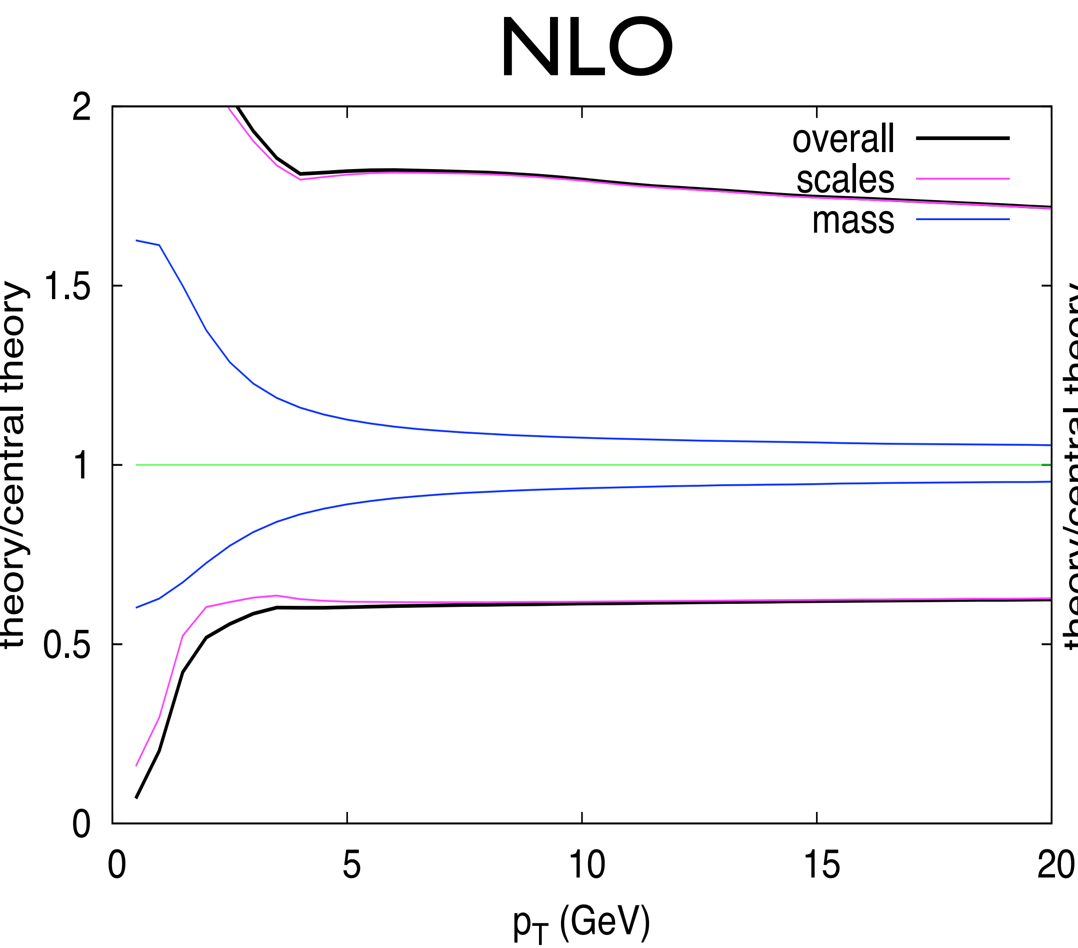
Not so for **differential** distributions: hadrons and quarks differ

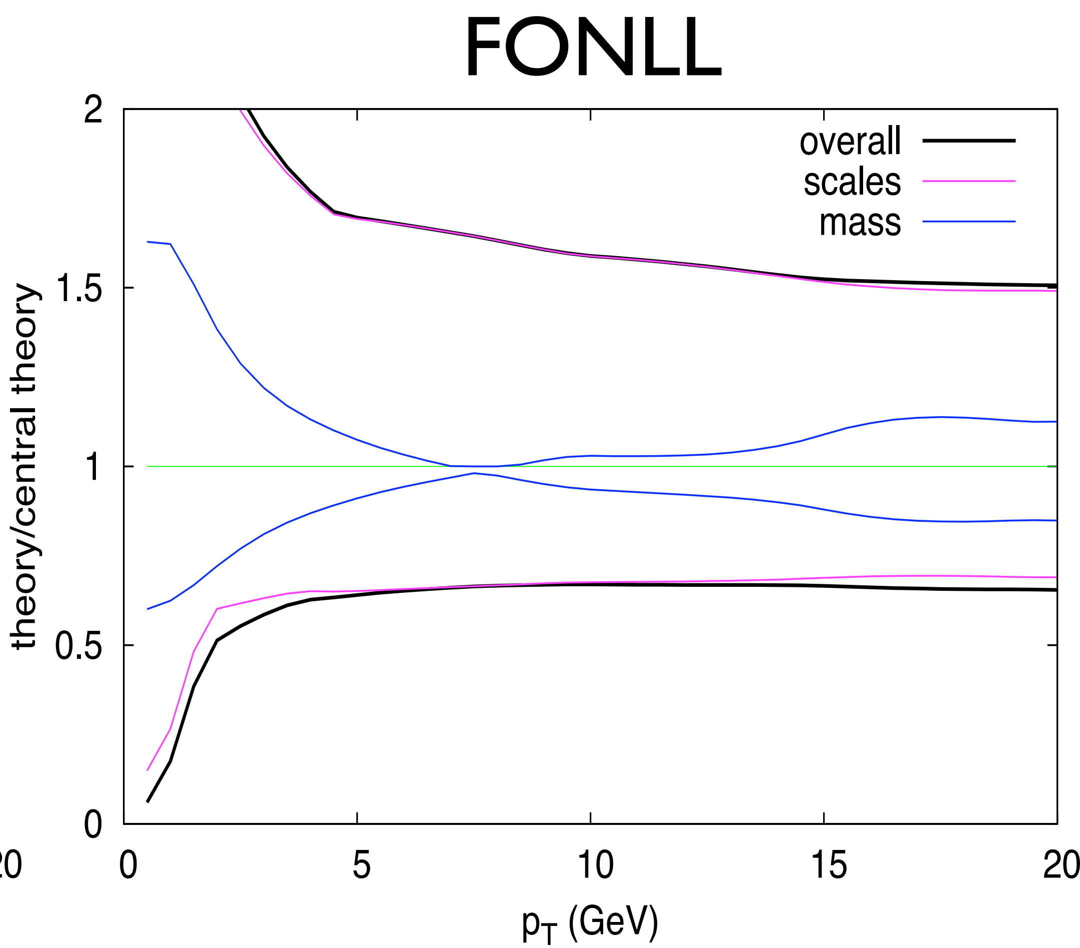


However, the non-perturbative correction is expected
(and observed) to be **parametrically small,** $\mathcal{O}(\Lambda/m)$
(Still, at large p_T the effect can be large)

Uncertainties estimate: charm @ RHIC

(max,min)/central theory as a function of p_T



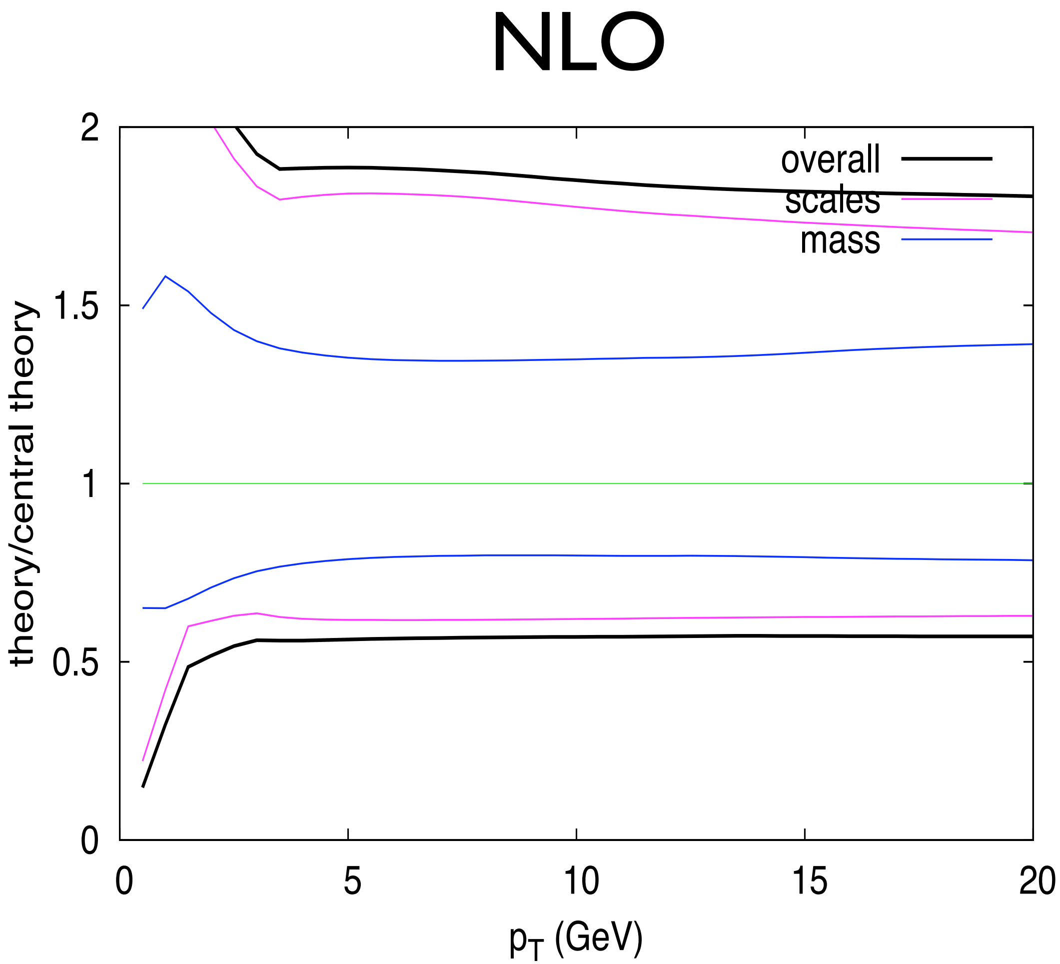


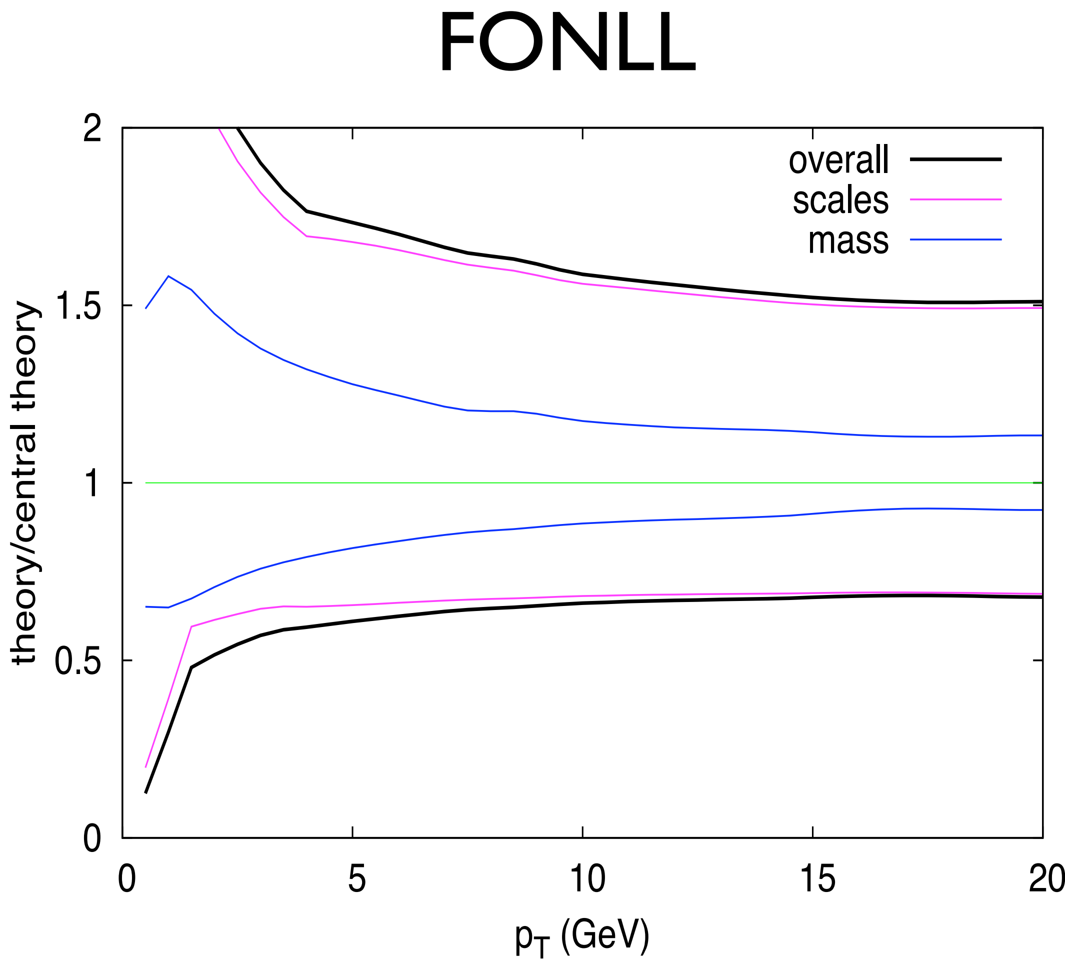
Uncertainty becomes reasonable at large p_T (>5 GeV)

FONLL a little better than NLO

Uncertainties estimate: charm @ RHIC

(max,min)/central theory as a function of p_T





Charmed **hadrons** distributions.
Note reduction of mass uncertainty in FONLL
(proper matching of non-perturbative fragmentation)

More uncertainties: non-perturbative fragmentation

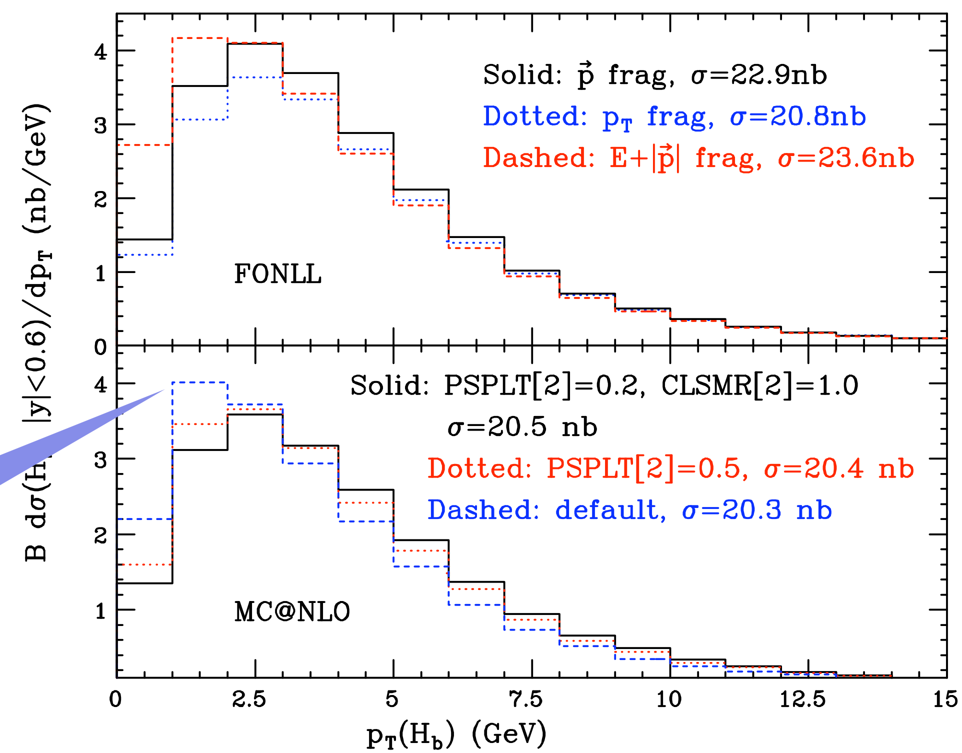
The non-perturbative FF is usually employed in hadronic collisions by writing

$$E_H \frac{d^3\sigma_H(p_H)}{dp_H^3} = E_Q \frac{d^3\sigma_Q(p_Q)}{dp_Q^3} \otimes D_{Q\to H}^{np}$$

Bear in mind that when the transverse momentum is small two things happen:

1. The "independent fragmentation" picture fails, as factorization-breaking higher twists grow large. So, whatever the result of the convolution above, there will be further uncertainties looming over it

2. Scaling a massive particle's 4-momentum is an ambiguous operation. One can scale the transverse momentum at constant rapidity, the 3-momentum at constant angle in a given frame, etc.

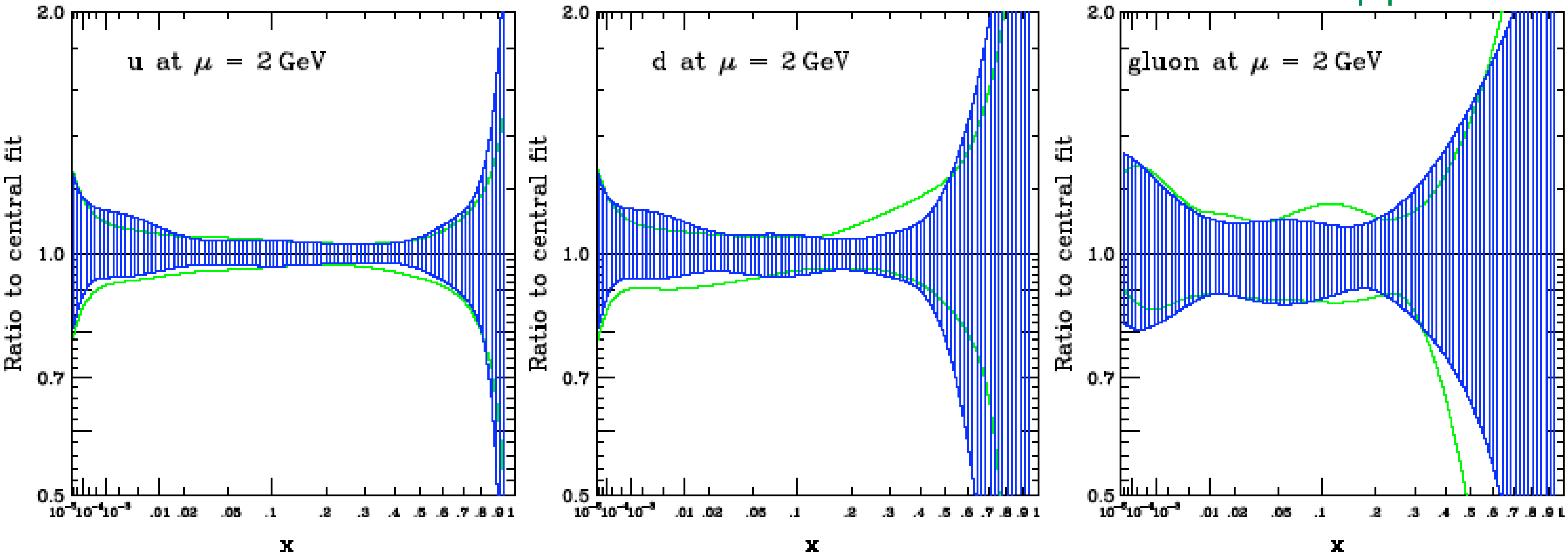


Different fragmentation choices

More uncertainties: PDFs

Modern PDF sets have smaller uncertainties, and should have them under control

hep-ph/0611254



Uncertainty estimate of CTEQ 6.5

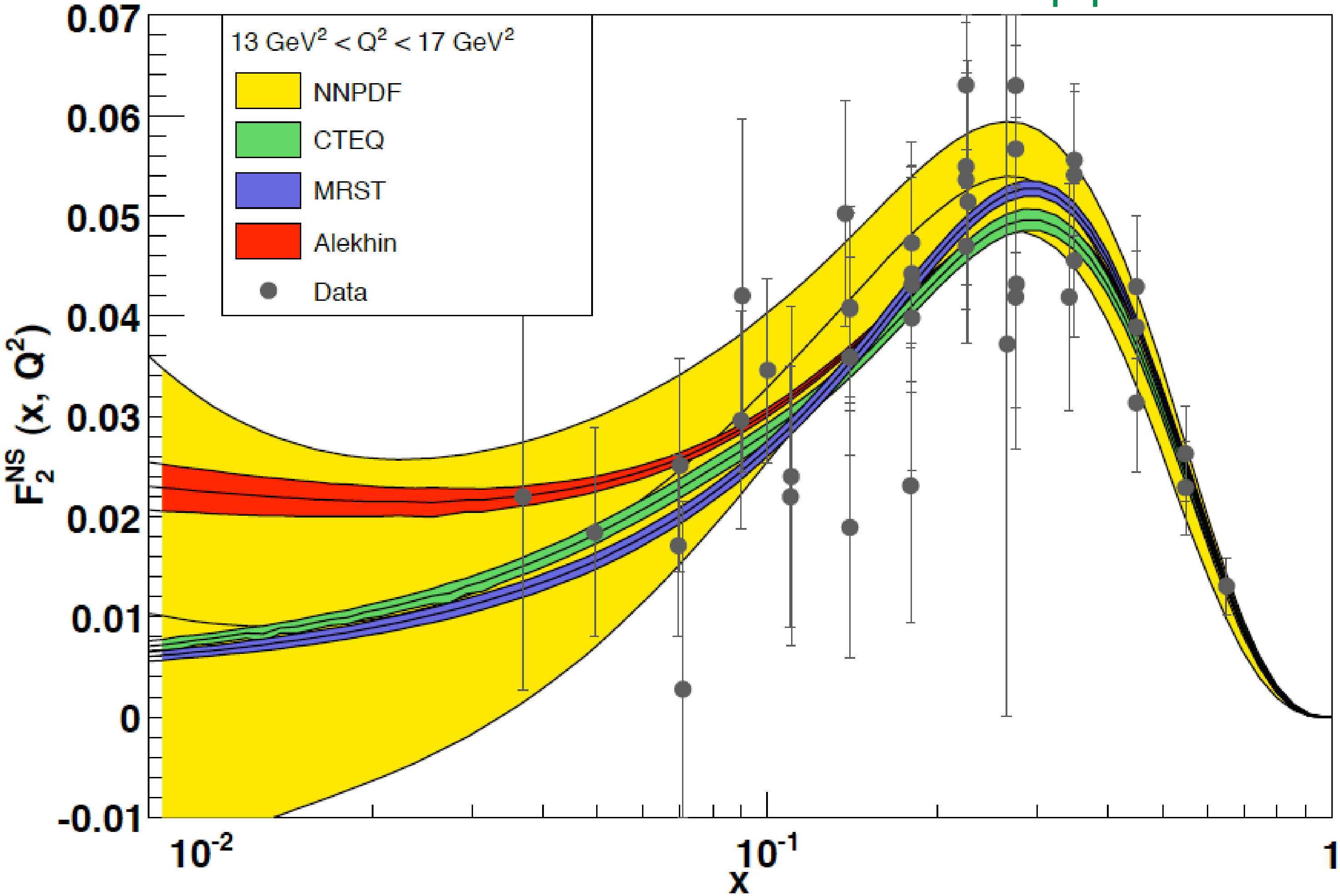
Order 10-20% uncertainty in region of interest ($x \sim 10^{-2}$), and therefore usually smaller than, or at most comparable to, perturbative uncertainties

Is this estimate reliable?

More uncertainties: PDFs

The recent extraction of a new PDF set using neural network methods (and therefore without an a priori choice of a functional form) shows that ‘standard’ uncertainties might be underestimated

hep-ph/0701127



This is non-singlet only. What will happen with the gluon?

Summary of uncertainties @ RHIC

Higher orders: dominant uncertainty

For charm, ± factor of three at low p_T , 50% at large p_T (large ~ 20 GeV)

For bottom, 50% at low p_T , 30% at large p_T

Mass: Only sizable at low p_T. Dwarfed by perturbative uncertainty

Non-perturbative fragmentation:

10-20% at low p_T , smaller at large p_T

Never dominant if properly implemented

PDF's:

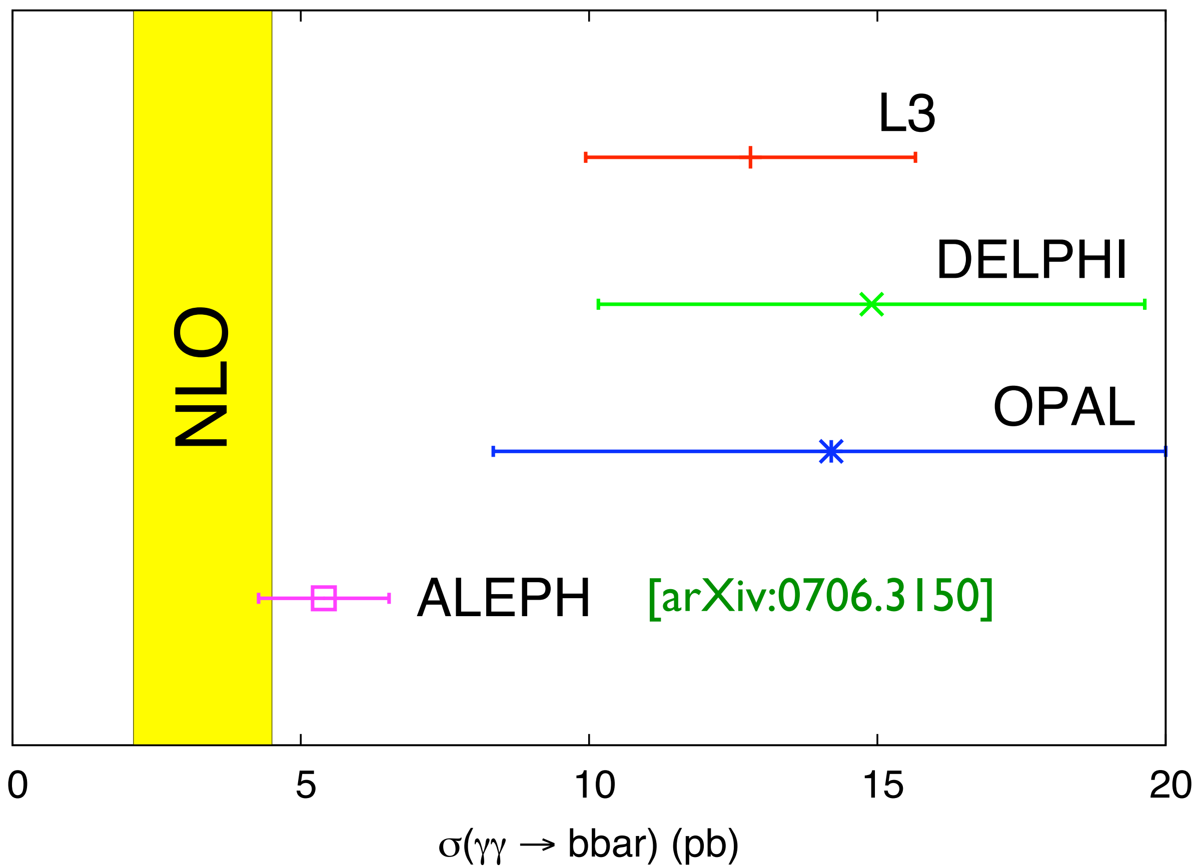
Likely of the order of 10-20%.

If you don’t believe any of this,
just compare the predictions to the experimental data

A bottom total cross section measurement

(Beware: you never know where your extrapolation tool might have been)

$$\gamma\gamma \to b\bar{b}$$

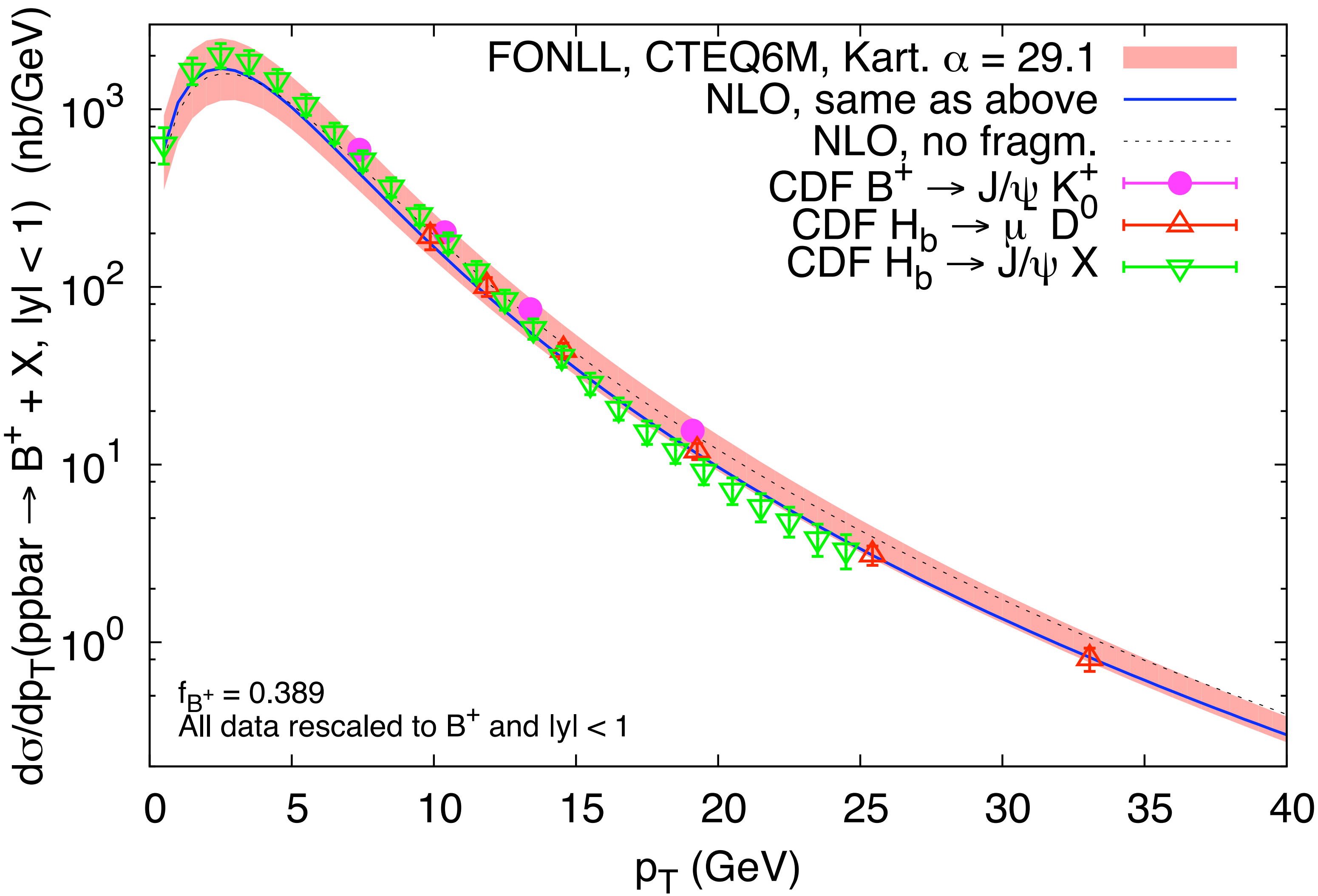


Old analyses, all based on B decay into muons, seemed to consistently indicate an excess, albeit with large uncertainties

A recent ALEPH measurement, which uses instead lifetime tagging, is in good agreement with the NLO prediction

[For details see e.g. Alex Finch's talk at PHOTON 2007]

Bottom differential cross sections @ Tevatron

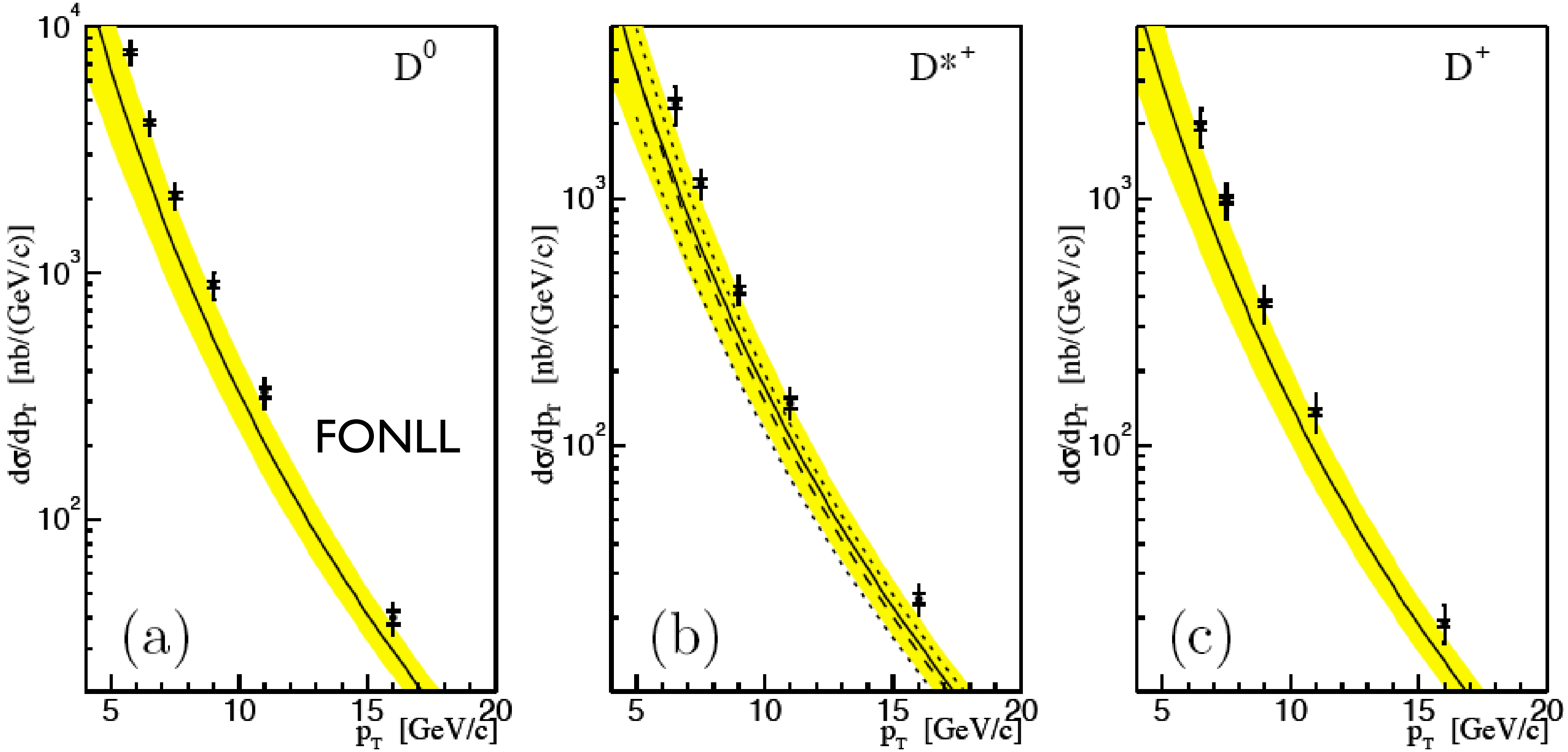


Good agreement, with minimal non-perturbative correction

NLO is sufficient for correct total rate prediction

Charm production @ Tevatron Run 2

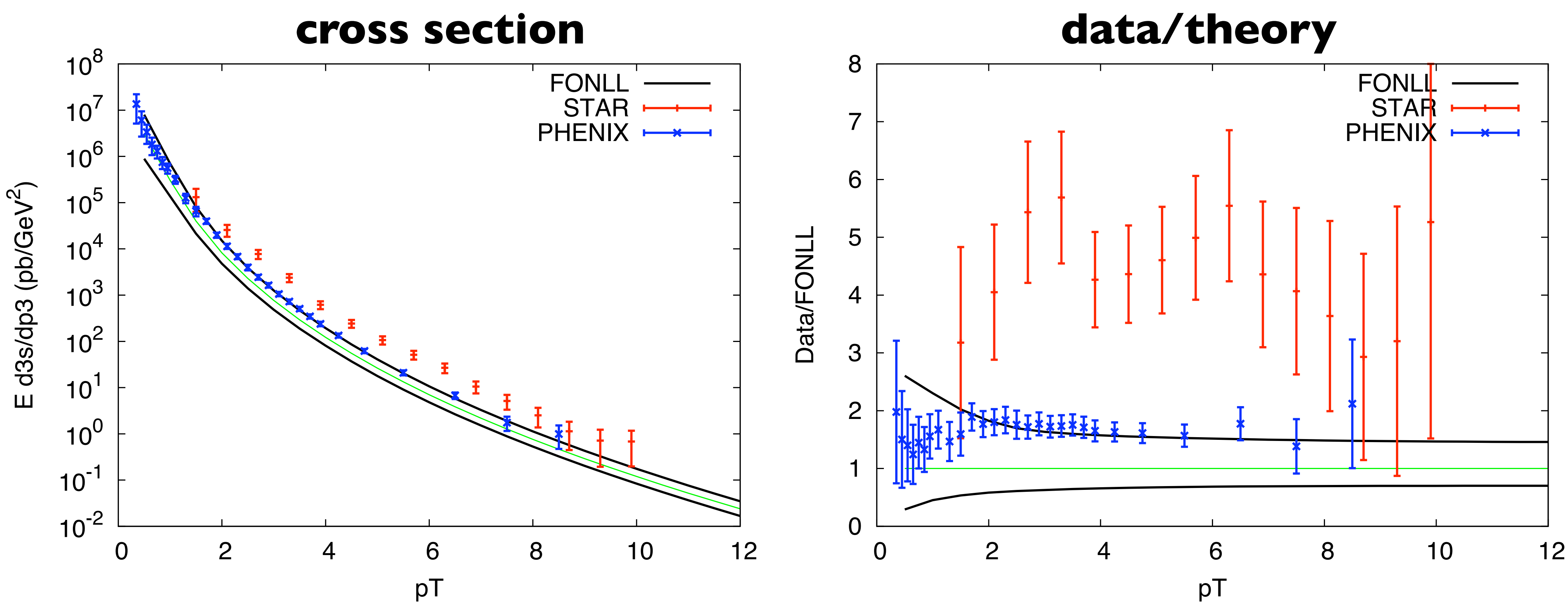
CDF Run II   c → D data   [PRL 91:241804,2003]



The non-perturbative charm fragmentation needed to describe the c → D hadronization has been extracted from moments of ALEPH data at LEP.

Charm and bottom production @ RHIC

Non-photonic electrons from charm and bottom



Phenix data in good agreement.

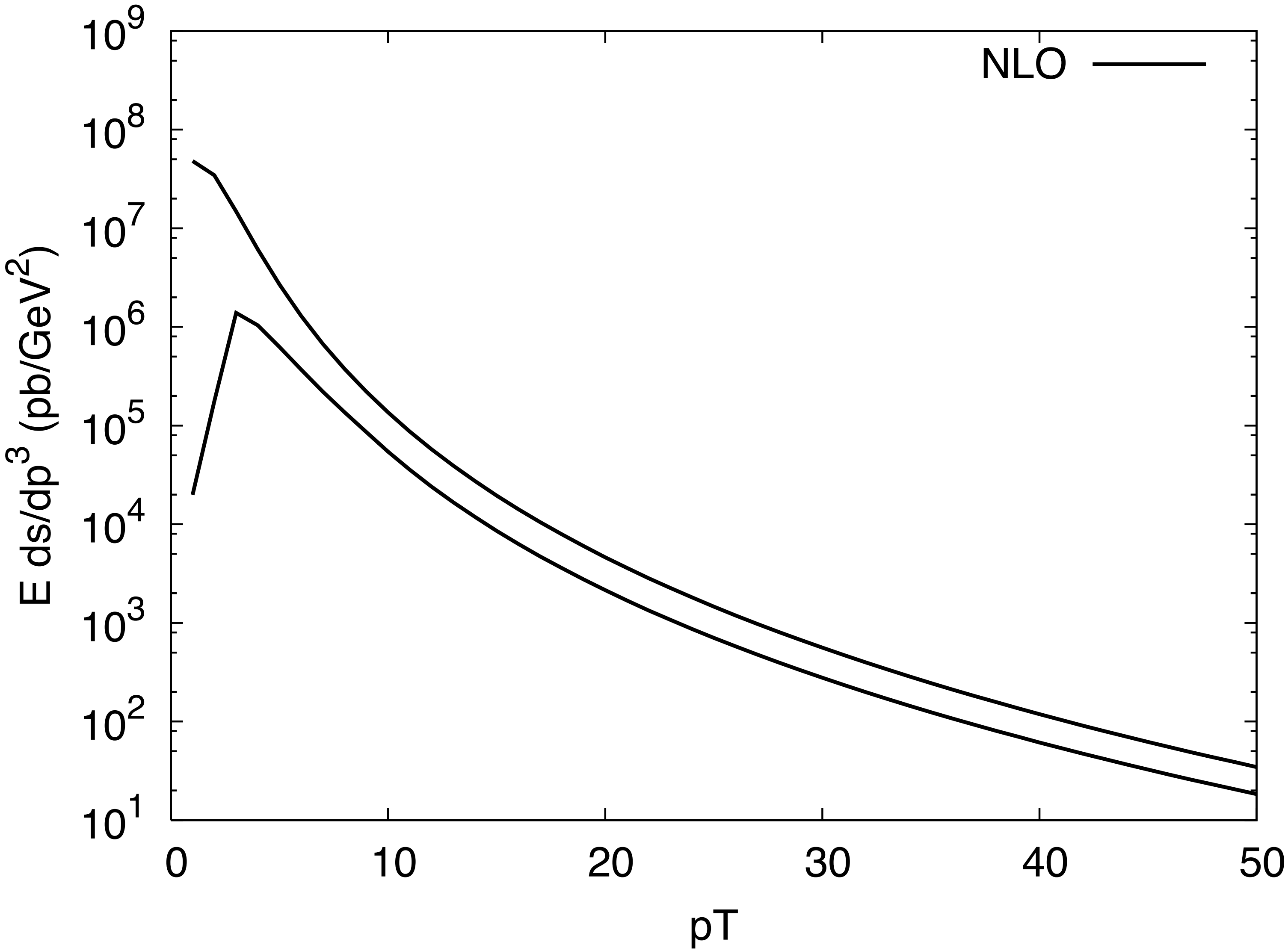
STAR data a little larger, and larger than most theory v. charm data comparisons

Conclusions

- Total charm cross sections suffer from large perturbative uncertainties, essentially related to the low(ish) scale set by the charm mass. pQCD can barely try to give a feeling for the cross section value, a solid prediction of the uncertainty is at present probably beyond reach
- At large transverse momentum the situation is a lot better. The uncertainties are around 50% or below, and should be under control. Comparisons with HERA and Tevatron data seem to support a successful description.
- One open issue is what precise meaning to give to a theoretical uncertainty band: it cannot readily be characterized in terms of 'sigmas'. Perhaps a Bayesian analysis? Next workshop....

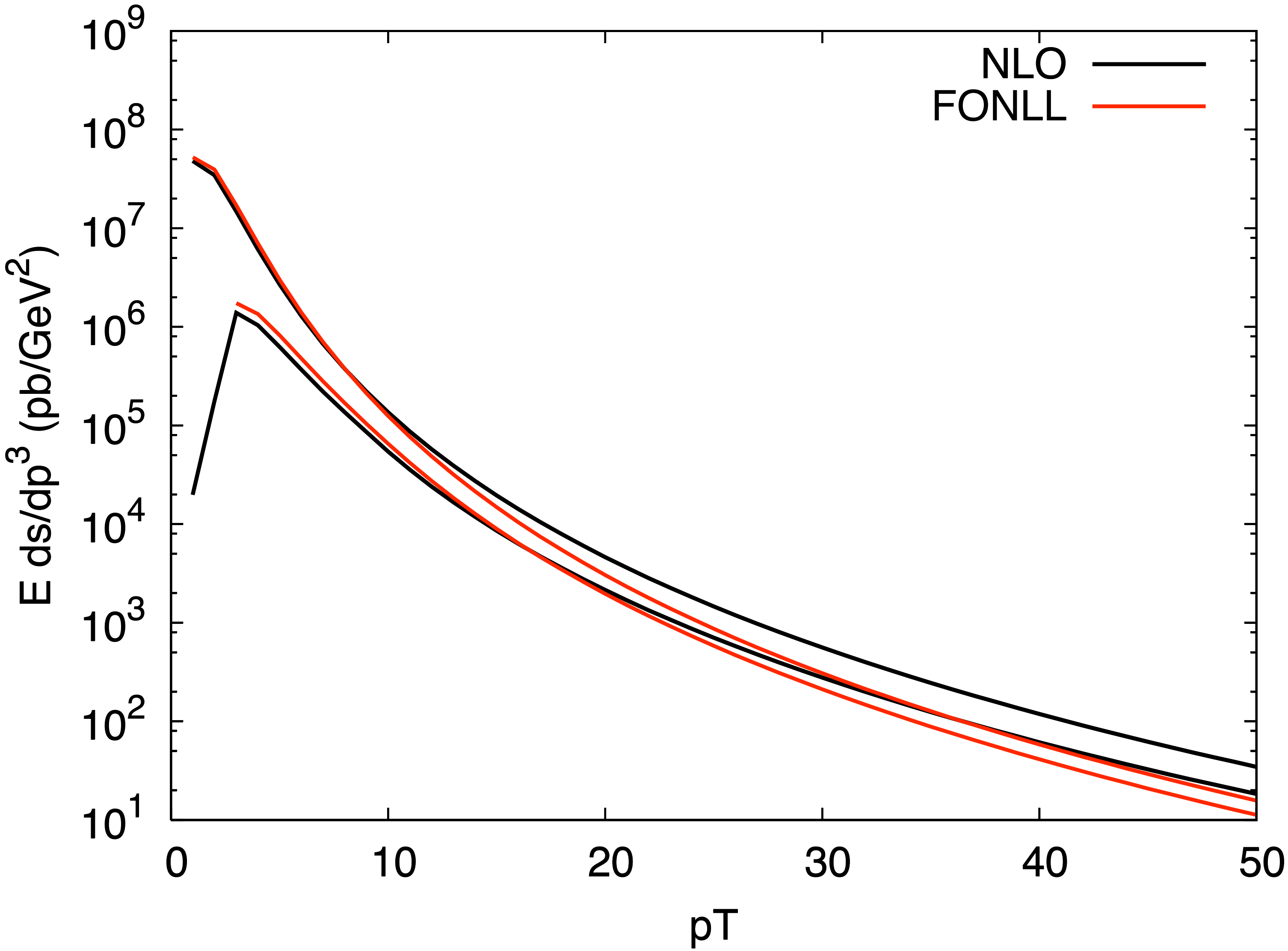
Backup slides

Charm @ LHC



Huge uncertainty at low p_T

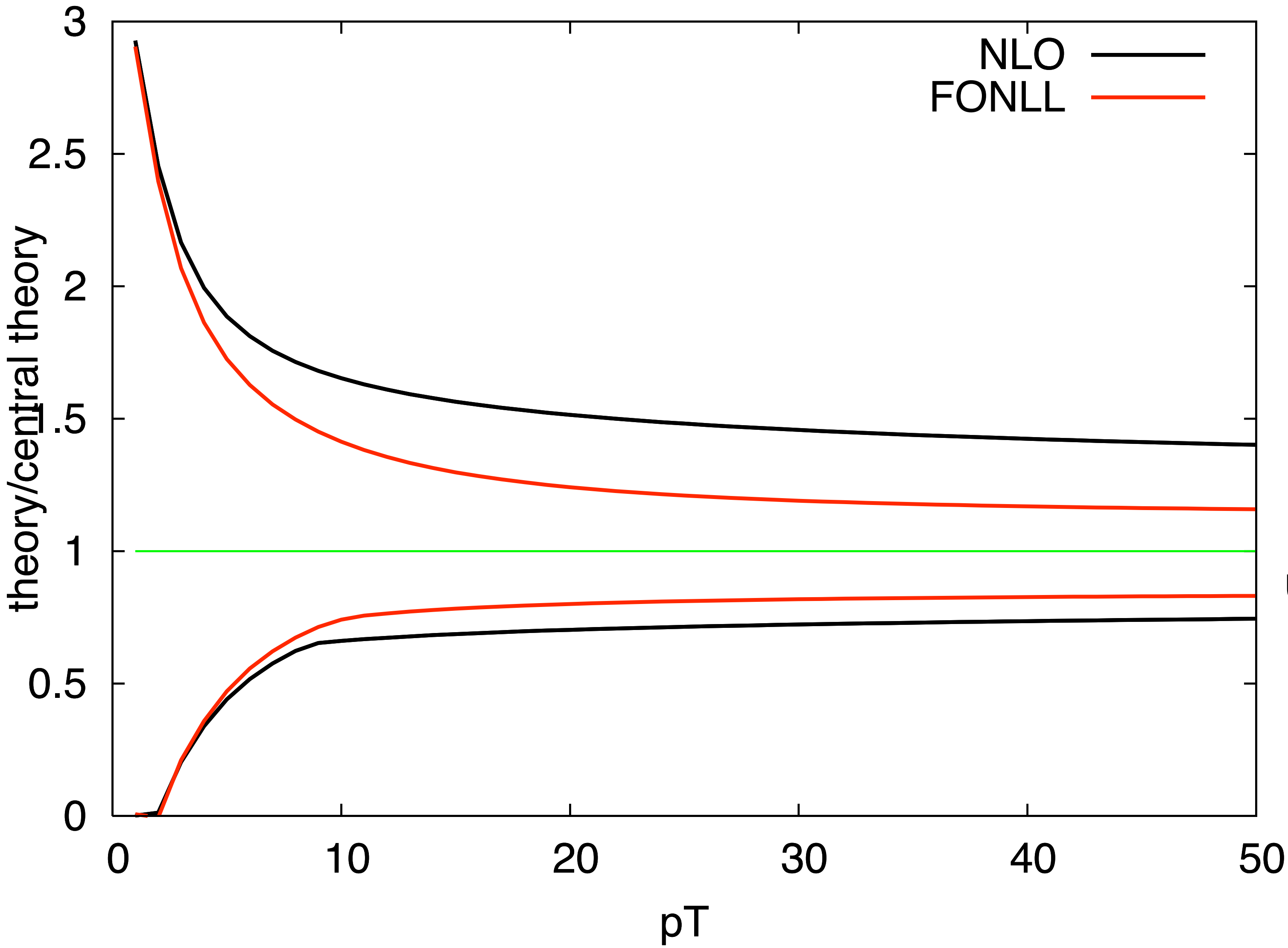
Charm @ LHC



Huge uncertainty at low p_T

FONLL softer and more reliable at large p_T

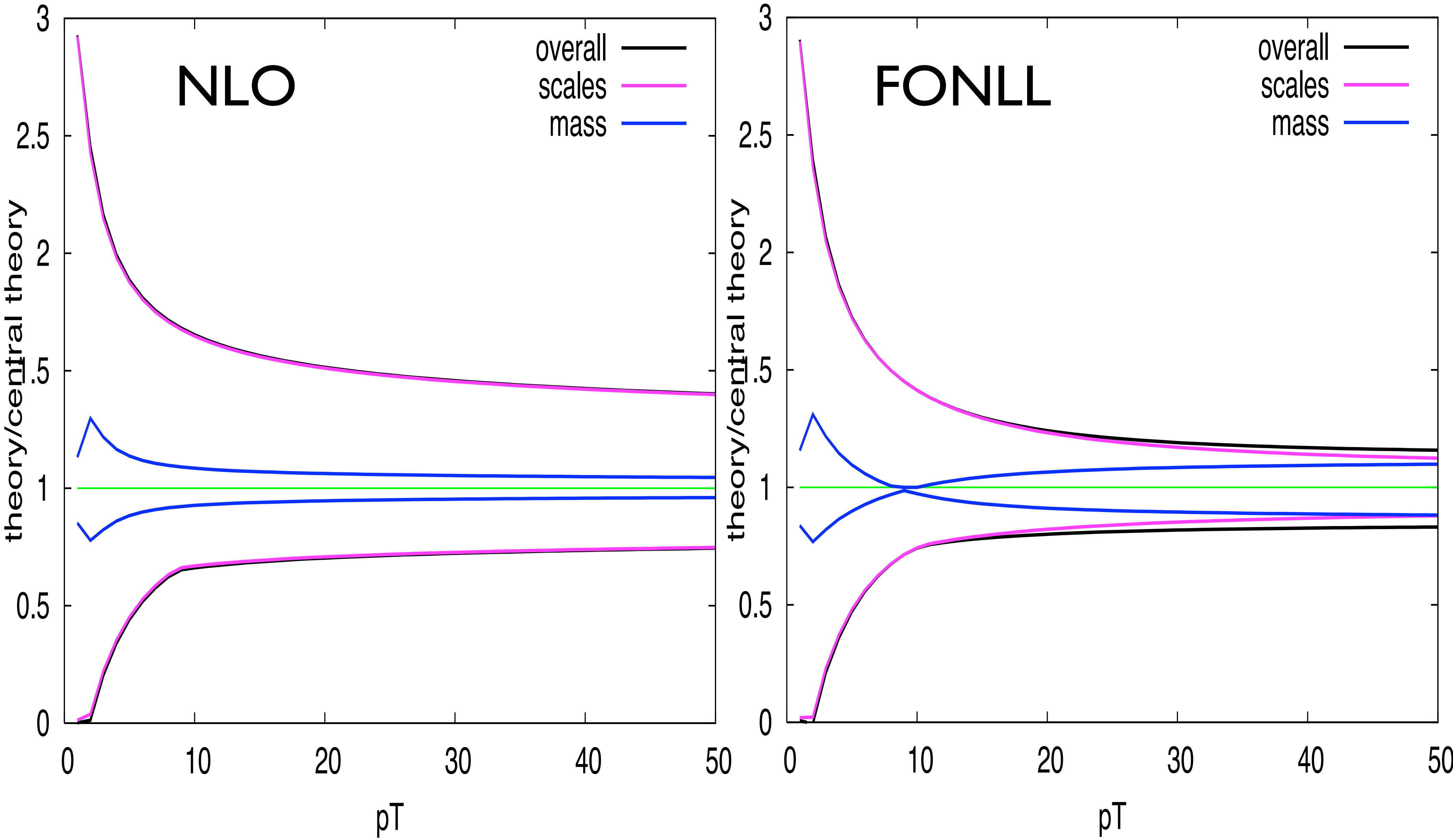
Charm @ LHC



10-20% uncertainty

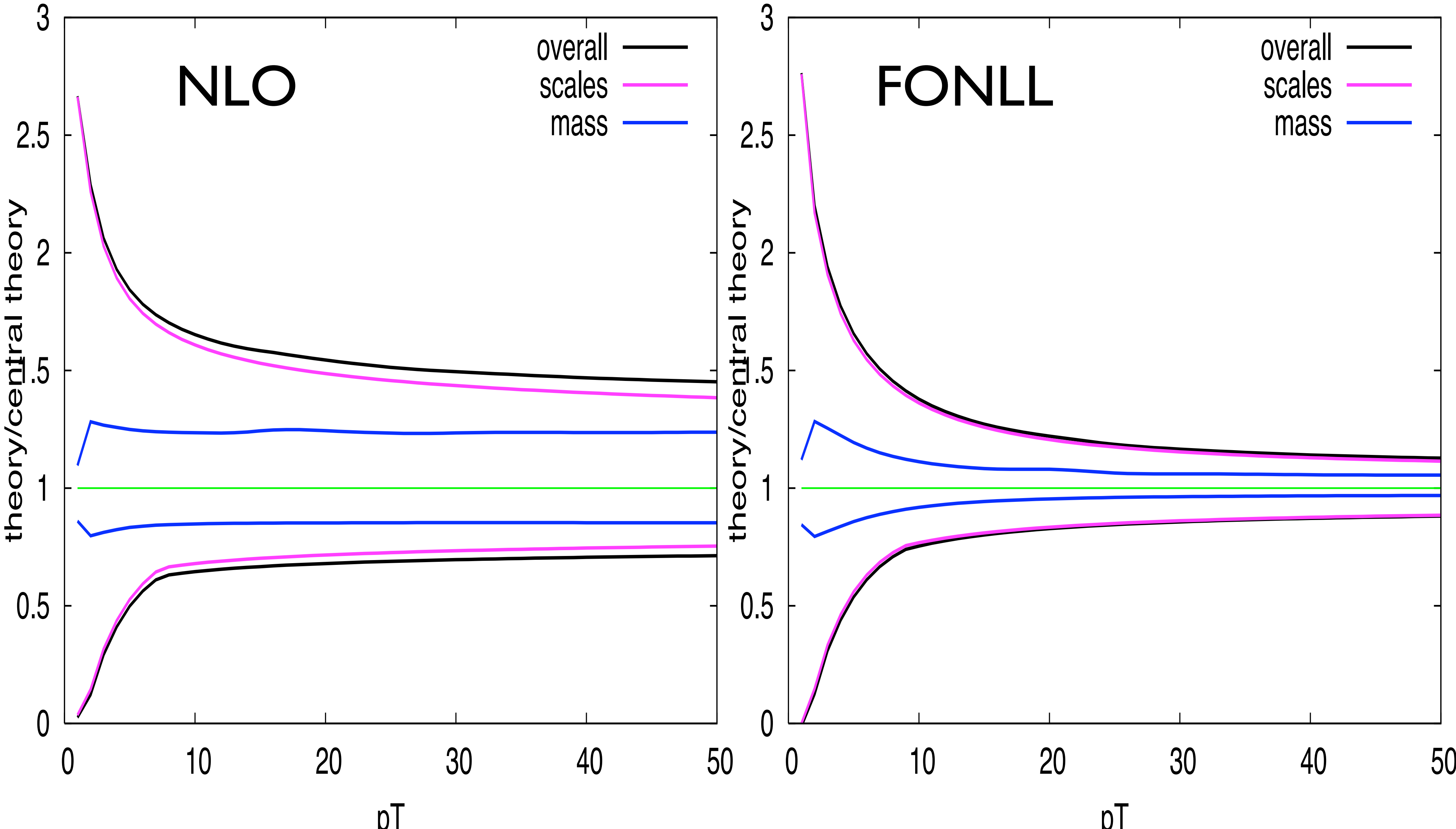
Sizable reduction of uncertainty at large p_T

Charm @ LHC: structure of uncertainties



Uncertainty dominated by factorisation/renormalisation scales (i.e. higher orders)

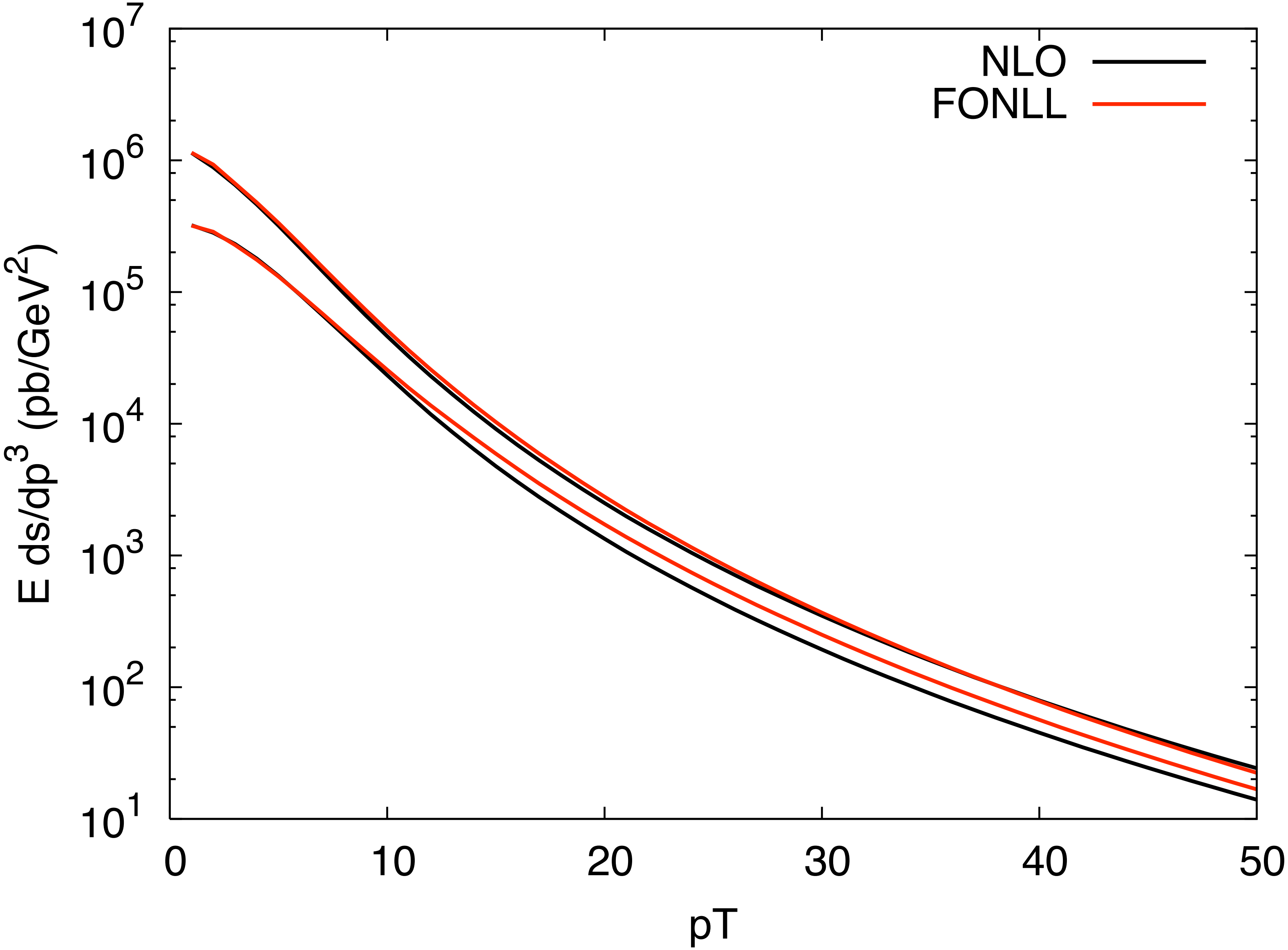
Charmed hadrons @ LHC: non-perturbative effects



Proper inclusion of NP fragmentation **reduces** mass effects at large p_T in FONLL

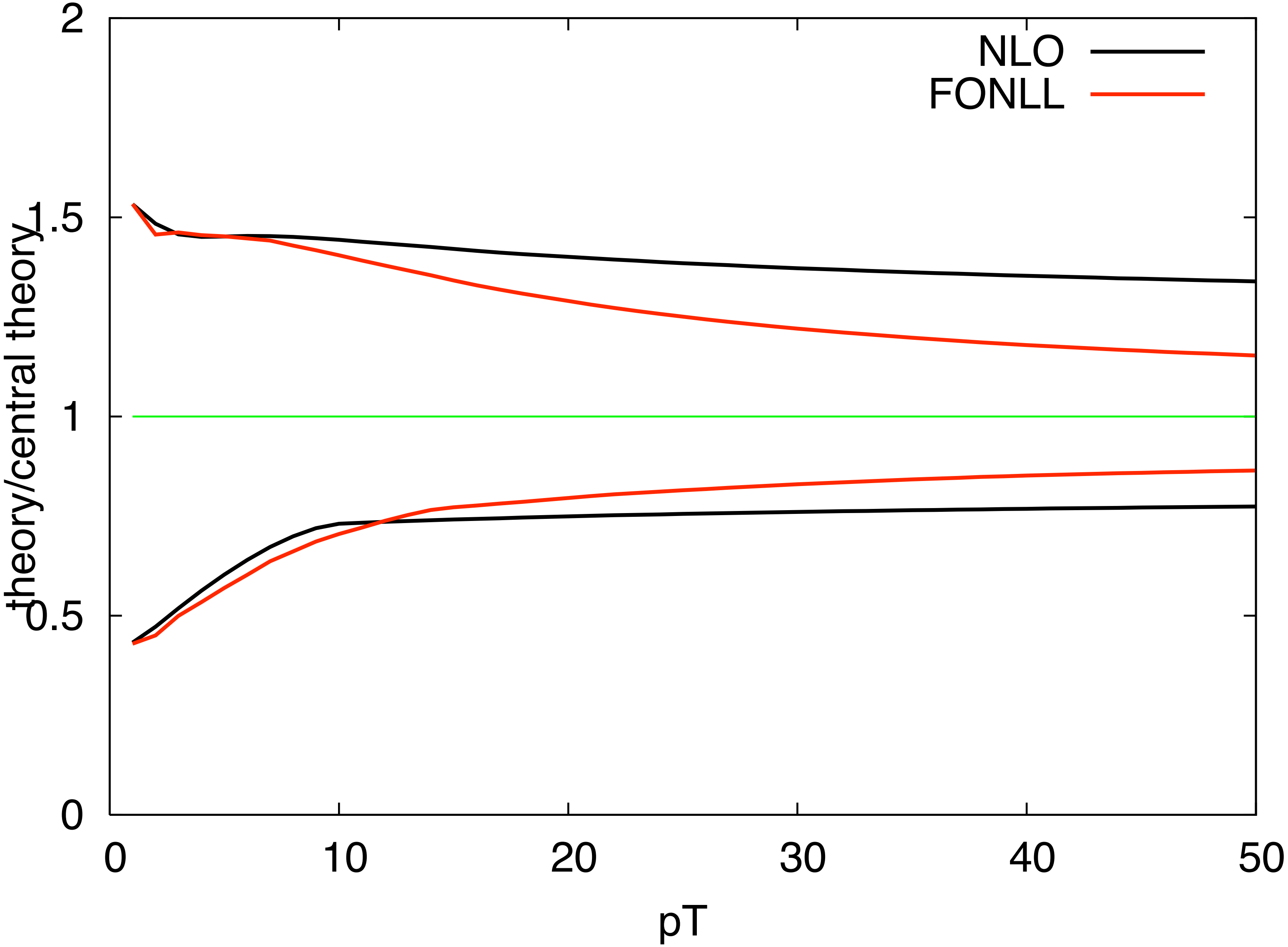
→ specific example of 'good matching'

Bottom @ LHC



NLO and FONLL more similar for bottom (or, if you prefer, NLO more reliable)

Bottom @ LHC



10-20% uncertainty