Scale choices and uncertainties for inclusive/exclusive and *complex* processes

…some points for discussion

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Snowmass 2013: Energy Frontier Workshop on QCD Physics
…some of the work in collaboration with Steve Ellis

Consider scale dependence at NLO

- Write cross section indicating explicit scale-dependent terms
- First term (lowest order) in (3) leads to monotonically decreasing behavior as scale increases (the LO piece)
- Second term is negative for $\mu < p_T$, positive for $\mu > p_T$
- Third term is negative for factorization scale $M < p_T$
- Fourth term has same dependence as lowest order term
- Thus, lines one and four give contributions which decrease monotonically with increasing scale while lines two and three start out negative, reach zero when the scales are equal to p_T, and are positive for larger scales
- At NLO, result is a roughly parabolic behavior (if you're lucky)
- Note that each of these terms depends on the kinematics of the cross section under investigation

Consider a large transverse momentum process such as the single jet inclusive cross section involving only massless partons. Furthermore, in order to simplify the notation, suppose that the transverse momentum is sufficiently large that only the quark distributions need be considered. In the following, a sum over quark flavors is implied. Schematically, one can write the lowest order cross section as

$$E\frac{d^3\sigma}{dp^3} \equiv \sigma = a^2(\mu)\,\hat{\sigma}_B \otimes q(M) \otimes q(M) \qquad (1)$$

where $a(\mu) = \alpha_s(\mu)/2\pi$ and the lowest order parton-parton scattering cross section is denoted by $\hat{\sigma}_B$. The renormalization and factorization scales are denoted by μ *and* M, respectively. In addition, various overall factors have been absorbed into the definition of $\hat{\sigma}_B$. The symbol $\otimes$ denotes a convolution defined as

$$f \otimes g = \int_x^1 \frac{dy}{y}\, f\!\left(\frac{x}{y}\right) g(y). \qquad (2)$$

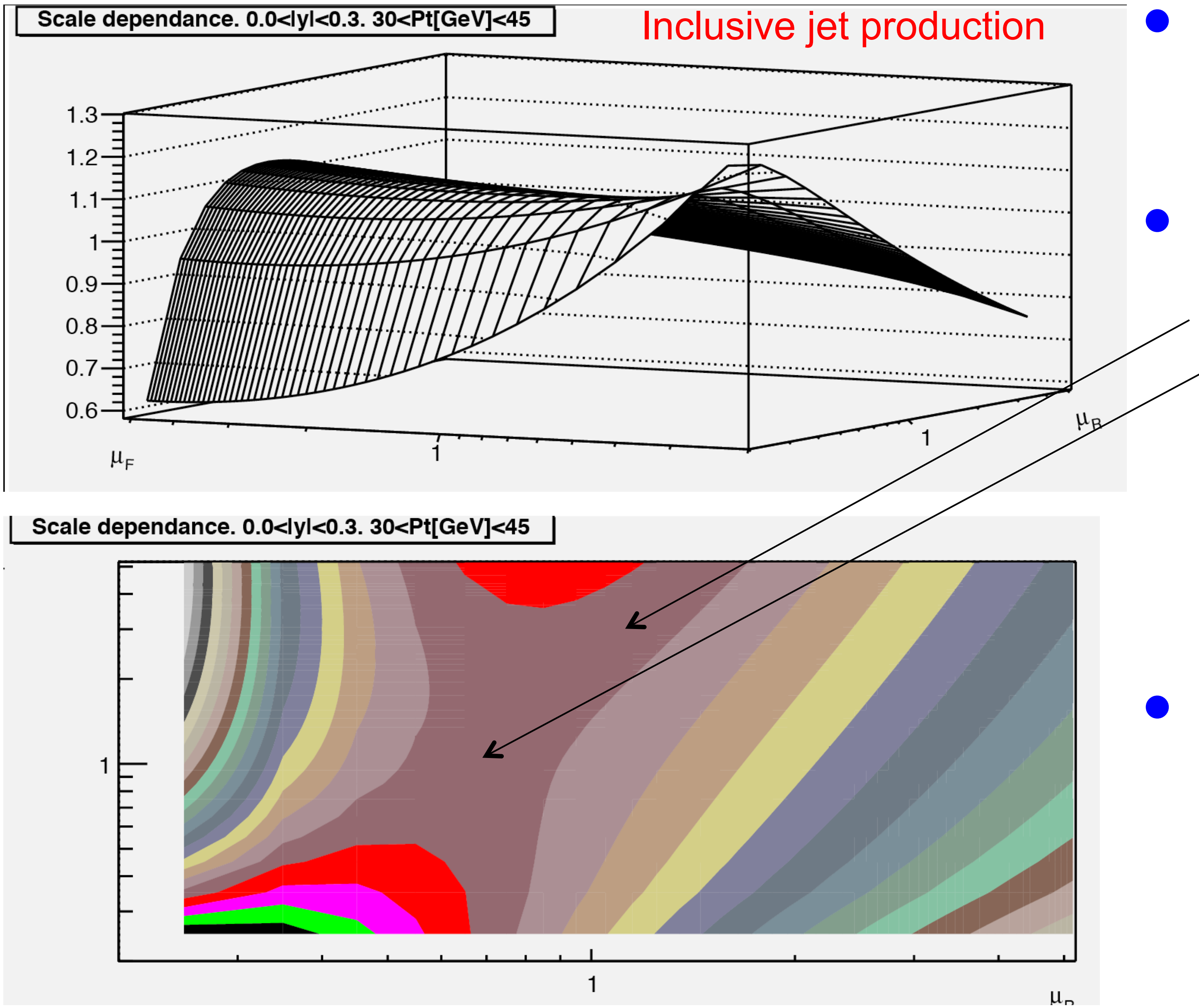
When one calculates the $\mathcal{O}(\alpha_s^3)$ contributions to the inclusive cross section, the result can be written as

$$\begin{aligned}
(1)\quad \sigma &= a^2(\mu)\,\hat{\sigma}_B \otimes q(M) \otimes q(M) \\
(2)\quad &+ 2a^3(\mu)\, b \ln(\mu/p_T)\hat{\sigma}_B \otimes q(M) \otimes q(M) \\
(3)\quad &+ 2a^3(\mu)\, \ln(p_T/M) P_{qq} \otimes \hat{\sigma}_B \otimes q(M) \otimes q(M) \\
(4)\quad &+ a^3(\mu)\, K \otimes q(M) \otimes q(M). \qquad (3)
\end{aligned}$$

In writing Eq. (3), specific logarithms associated with the running coupling and the scale dependence of the parton distributions have been explicitly displayed; the remaining higher order corrections have been collected in the function K in the last line of Eq. (3). The μ

Jeff Owens in CTEQ.1 paper

Look in 2-D, with logarithmic scales

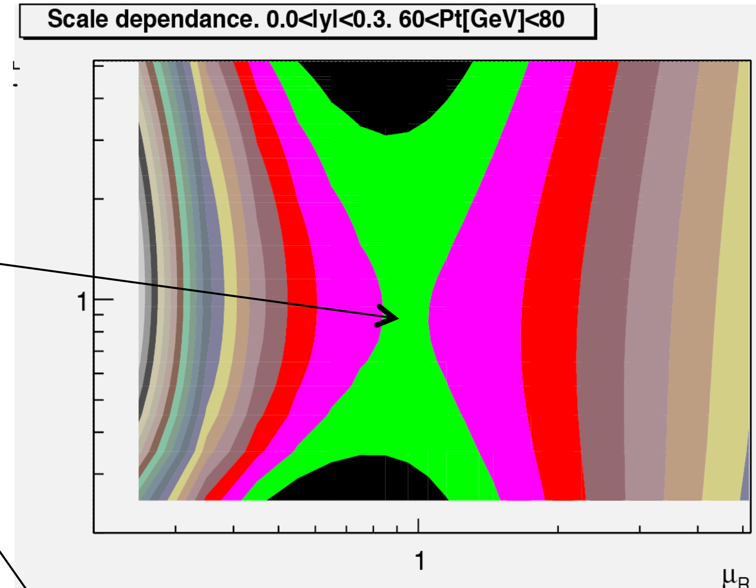


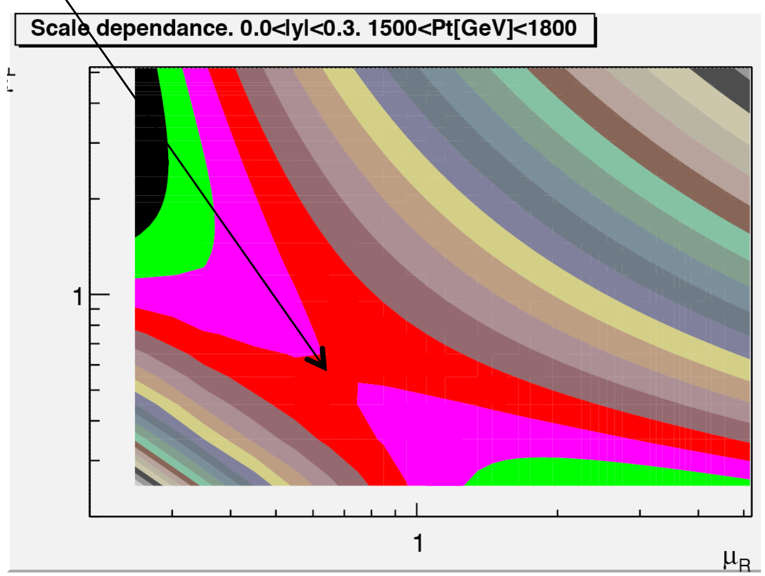
- …since perturbative QCD is logarithmic
- Note that there's a saddle region, and a saddle point, where locally there is no slope for the cross section with respect to the two scales
- This is kind of the 'golden point' and typically around the expected scale (p_T^{jet} in this case)

Scale choices

- Take inclusive jet production at the LHC
- Canonical scale choice at the LHC is $\mu_r=\mu_f=1.0*p_T$
  - CDF used $0.5p_T$
  - CTEQ6.6 used this scale for determination of PDFs
  - new CT PDFs use p_T
- Close to saddle point for low p_T
- But saddle point moves down for higher p_T (and the saddle region rotates)
- Our typical scale choices don't work for all LHC kinematics; more extreme movements for some of measured cross sections
- Rather than look for some magic formula, we should try to understand what is going on the kinematic/scale point-of-view both to establish a central scale, and to calculate the range of uncertainty

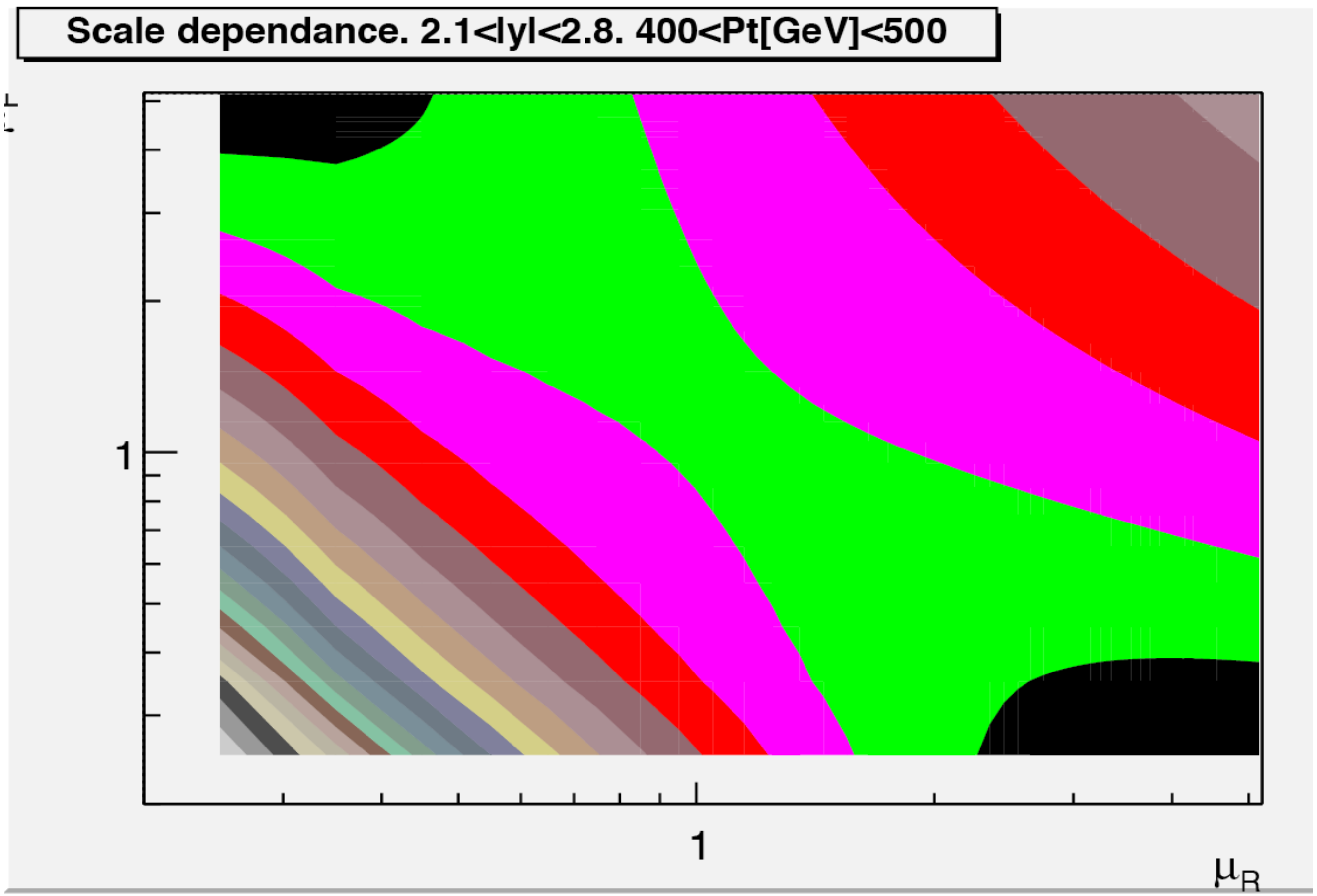
R=0.4
antikT





Scale dependence depends on rapidity

- The saddle point tends to move upwards in scale as the rapidity increases
- Is the physics changing; no, just the kinematics



Scale dependence also depends on jet size

R=0.4
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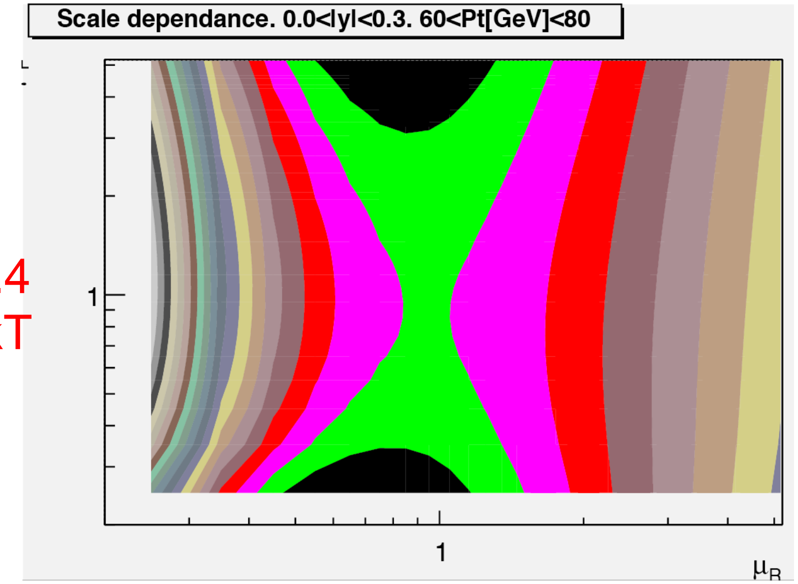
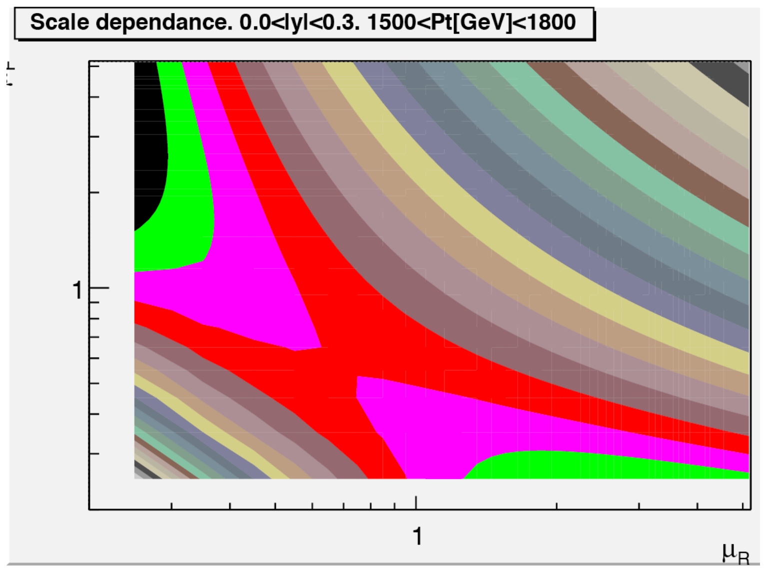
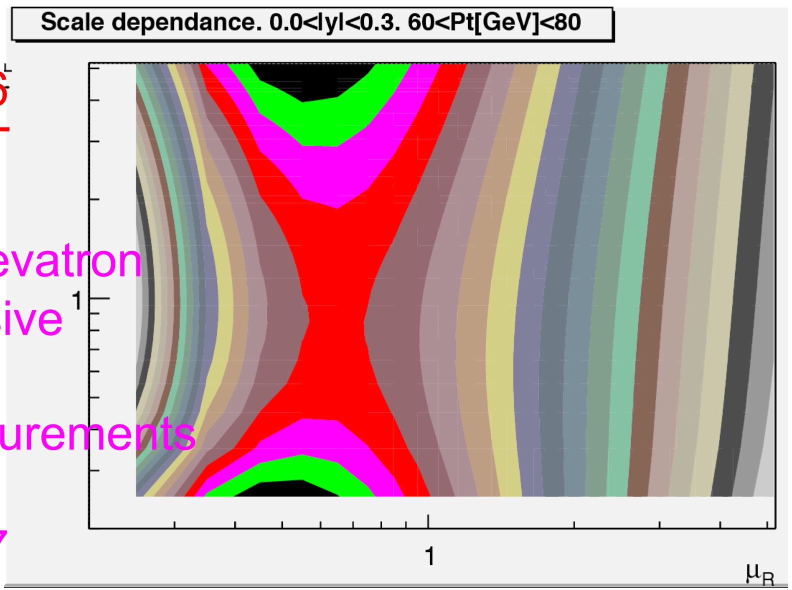
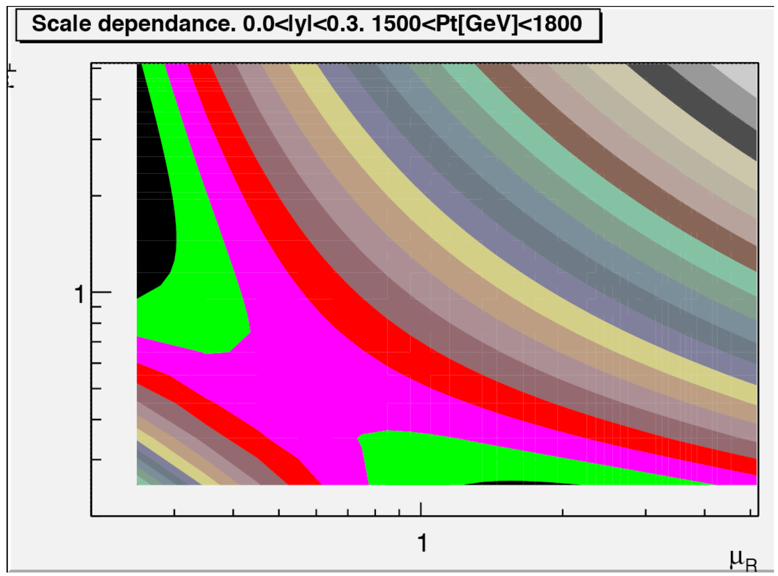




R=0.6
antikT

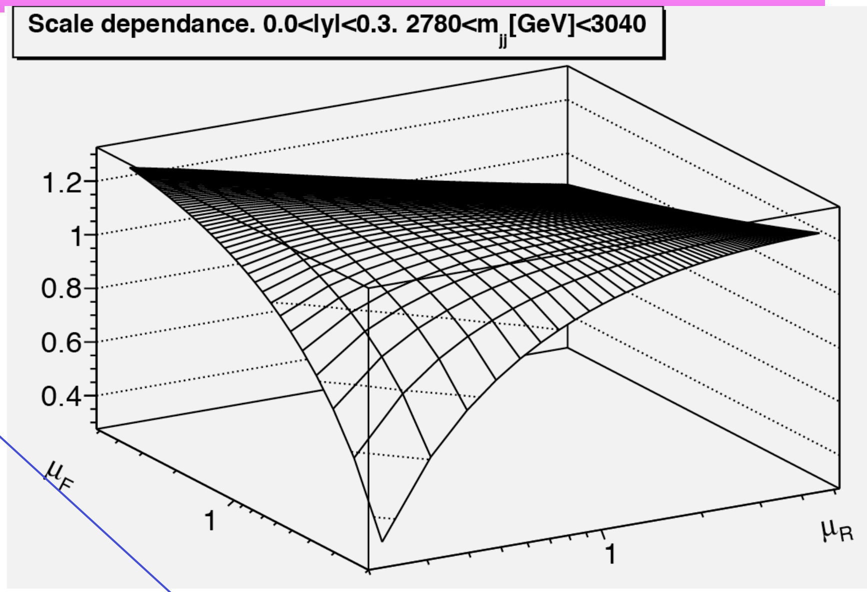
NB:Tevatron inclusive jet measurements with R=0.7

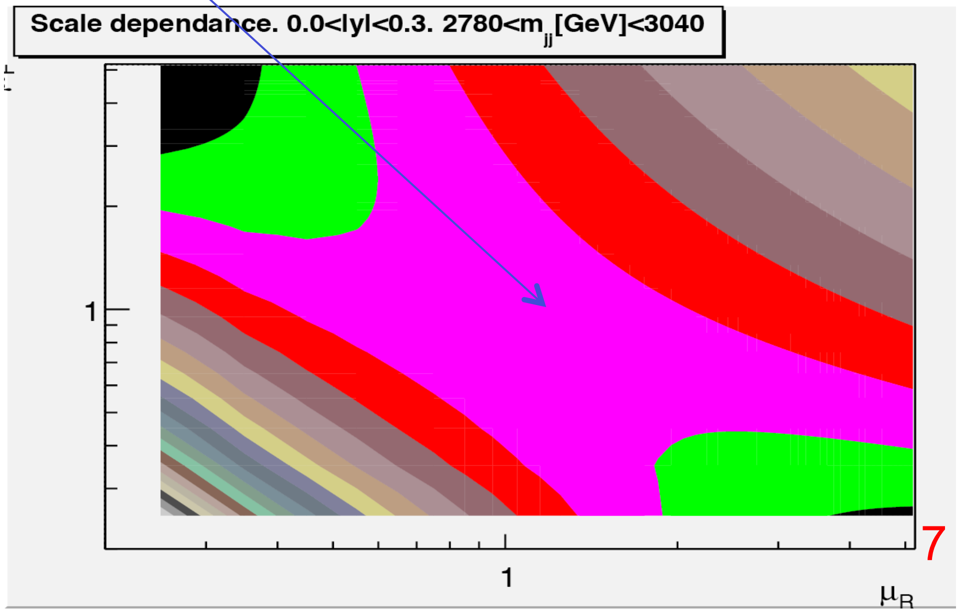




Now look at the dijet mass cross section

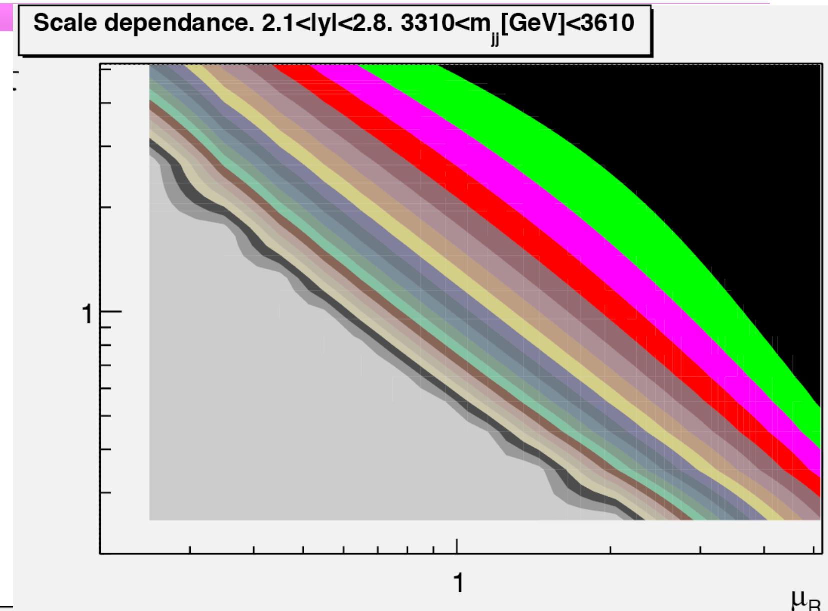
- In most cases, get a nice saddle region around p_T^{jet}

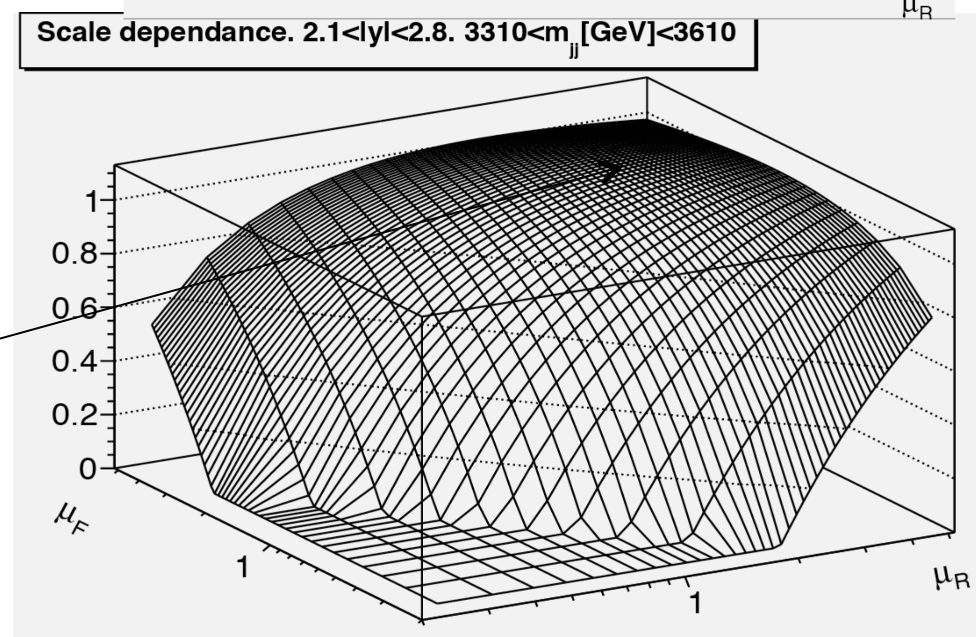




…but not for forward rapidities

- Is perturbation theory not valid here?
- It's ok as long as *reasonable scales* are chosen
- It's a continuation of the effect that we've been looking at
- To be on the plateau requires scales of the order of 3-4*p_T
- Our 'motivated' scale, though, is p_T
  - in this case, I would argue that kinematics forces us to change
  - in most cases, we tend to ignore the kinematic effects; this is so severe we have to take them into account





Saddle points and scale uncertainties

- Cross sections depend on the renormalization scale μ_R and factorization scale μ_F
- Consider default values for these two scales, $\mu_{o,F}$ and $\mu_{o,R}$ and expand around these values
- Can write the NLO cross section near the reference scales as

$$\sigma(\mu_F,\mu_R) \approx \sigma(\mu_{0,F},\mu_{0,R})\left[1 + b_R \ln\left(\frac{\mu_R}{\mu_{0,R}}\right) + b_F \ln\left(\frac{\mu_F}{\mu_{0,F}}\right) + c_R \ln^2\left(\frac{\mu_R}{\mu_{0,R}}\right) + c_F \ln^2\left(\frac{\mu_F}{\mu_{0,F}}\right) + c_{RF} \ln\left(\frac{\mu_R}{\mu_{0,R}}\right)\ln\left(\frac{\mu_F}{\mu_{0,F}}\right)\right]$$

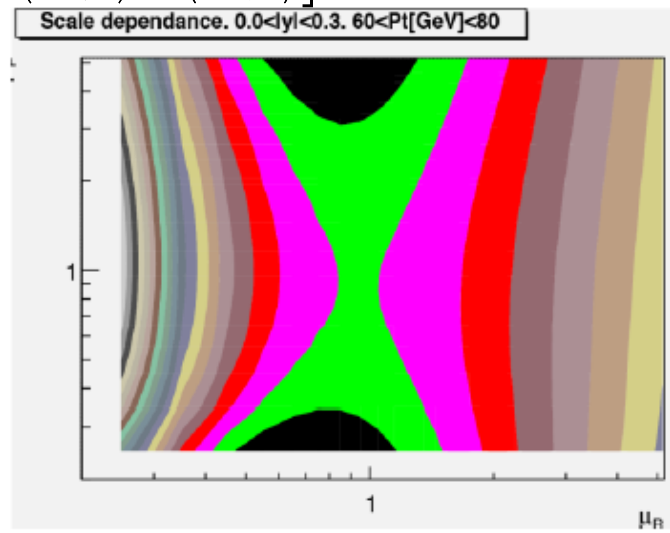
- …where the explicit logarithmic dependences have been factorized out; the b and c variables will depend on the kinematics
- In general, there will be a saddle point, where the local slope as a function of μ_R,μ_F is zero, i.e. the *b's* vanish
- Around the saddle point, can write the scale dependence as

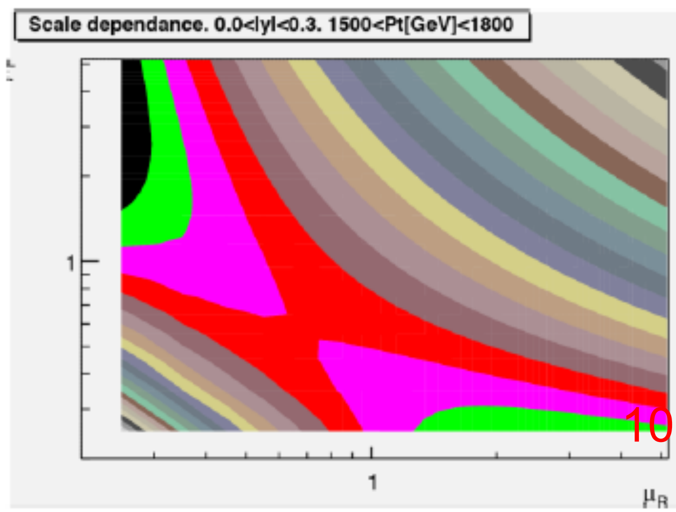
$$\sigma(\mu_F,\mu_R) \approx \sigma(\mu_{S,F},\mu_{S,R})\left[1 + c_R \ln^2\left(\frac{\mu_R}{\mu_{S,R}}\right) + c_F \ln^2\left(\frac{\mu_F}{\mu_{S,F}}\right) + c_{RF} \ln\left(\frac{\mu_R}{\mu_{S,R}}\right)\ln\left(\frac{\mu_F}{\mu_{S,F}}\right)\right]$$

Consider inclusive jet cross section at NLO

$$\sigma(\mu_F,\mu_R) \approx \sigma(\mu_{S,F},\mu_{S,R})\left[1 + c_R \ln^2\left(\frac{\mu_R}{\mu_{S,R}}\right) + c_F \ln^2\left(\frac{\mu_F}{\mu_{S,F}}\right) + c_{RF} \ln\left(\frac{\mu_R}{\mu_{S,R}}\right)\ln\left(\frac{\mu_F}{\mu_{S,F}}\right)\right]$$

- For $c_F>0, c_R<0$ and $c_F, |c_R| >> |c_{RF}|$, the saddle point axes are aligned with the plot axes, as shown at the top right
- At higher p_T values, $c_{RF}<0$ and $c_F, |c_R| << |c_{RF}|$, the saddle position rotates by about 45°, as we've already seen
- Should we follow the saddle point to determine the central scale? Should we make sure that any scale uncertainty includes the saddle point?





One scheme

- F. Olness and D. Soper, arXiv: 0907.5052
- Define x_1 and x_2

$$x_1 = \log_2\left(\frac{\mu_{\rm uv}}{P_T/2}\right)$$

$$x_2 = \log_2\left(\frac{\mu_{\rm col}}{P_T/2}\right)$$

- Make a circle of radius |x|=2 around a central scale (could be saddle point, or could be some canonical scale) and evaluate the scale uncertainty

$$\left[\frac{d\sigma(x_1,x_2)}{dP_T}\right]_{\rm NLO} \approx \left[\frac{d\sigma(0,0)}{dP_T}\right]_{\rm NLO} [1 + P(\vec{x})]$$

where

$$P(\vec{x}) = \sum_J x_J A_J + \sum_{J,K} x_J M_{JK} x_K$$

A_J and M_{JK} carry information on the scale dependence beyond NLO

$$\mathcal{E}^2_{\rm scale} = \frac{1}{2\pi}\int_0^{2\pi} d\theta\ P(|\vec{x}|\cos\theta, |\vec{x}|\sin\theta)^2$$

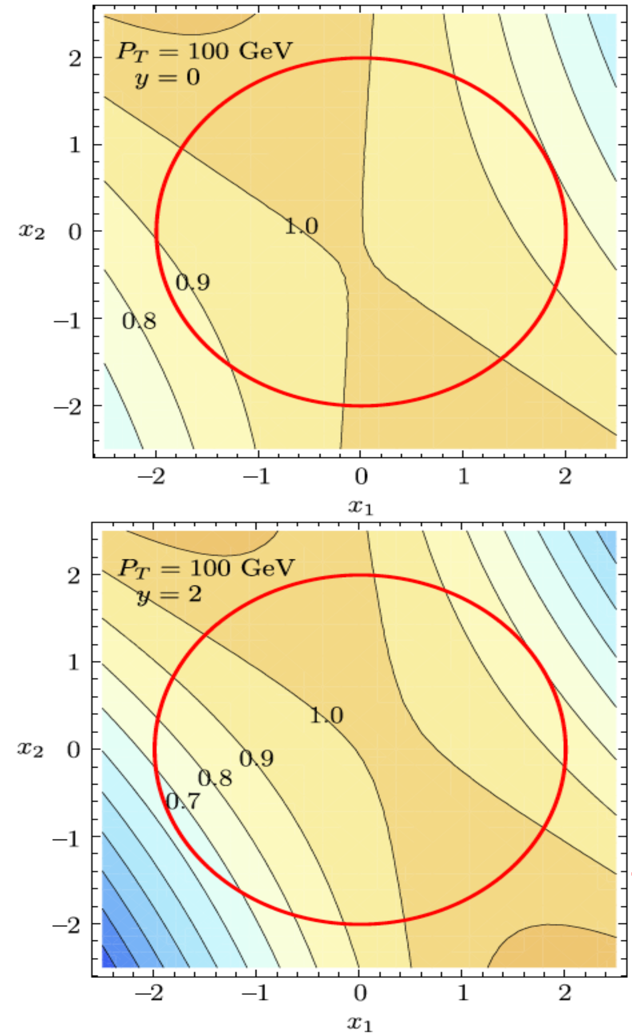


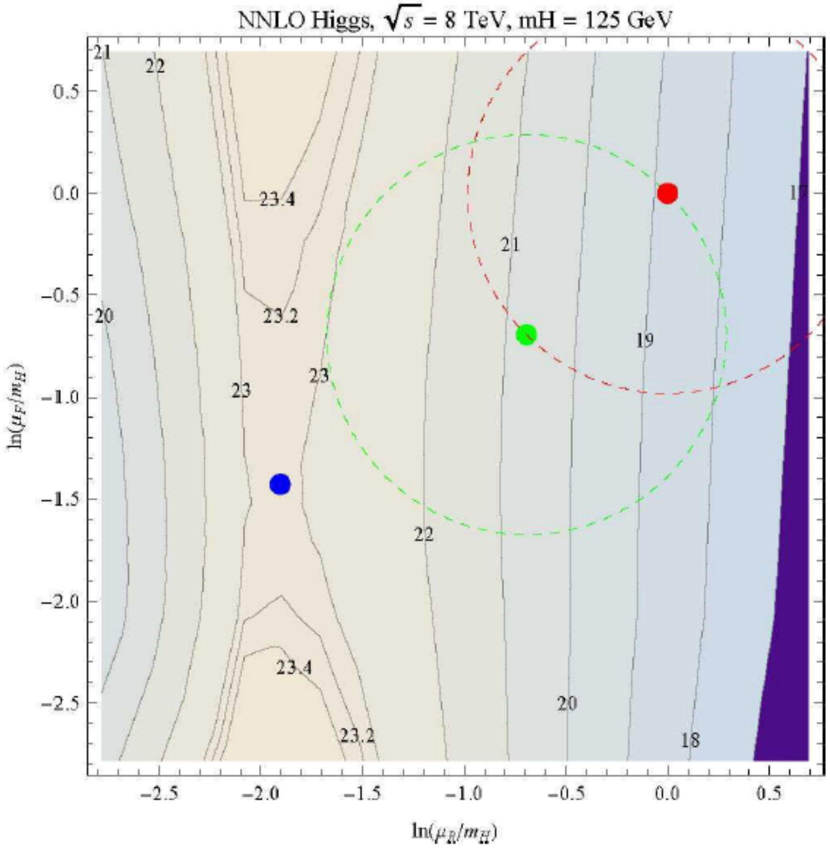
Figure 2: Contour plot of the jet cross section in the $\{x_1, x_2\}$ plane for the Tevatron ($\sqrt{s} = 1960$ GeV) with $P_T = 100$ GeV and a) central rapidity $y = 0$ and b) forward rapidity $y = 2$. We plot the ratio of the cross section compared to the central value at $\{x_1, x_2\} = \{0, 0\}$. Contour lines are drawn at intervals of 0.10. The (red) circle is at radius $|x| = 2$.

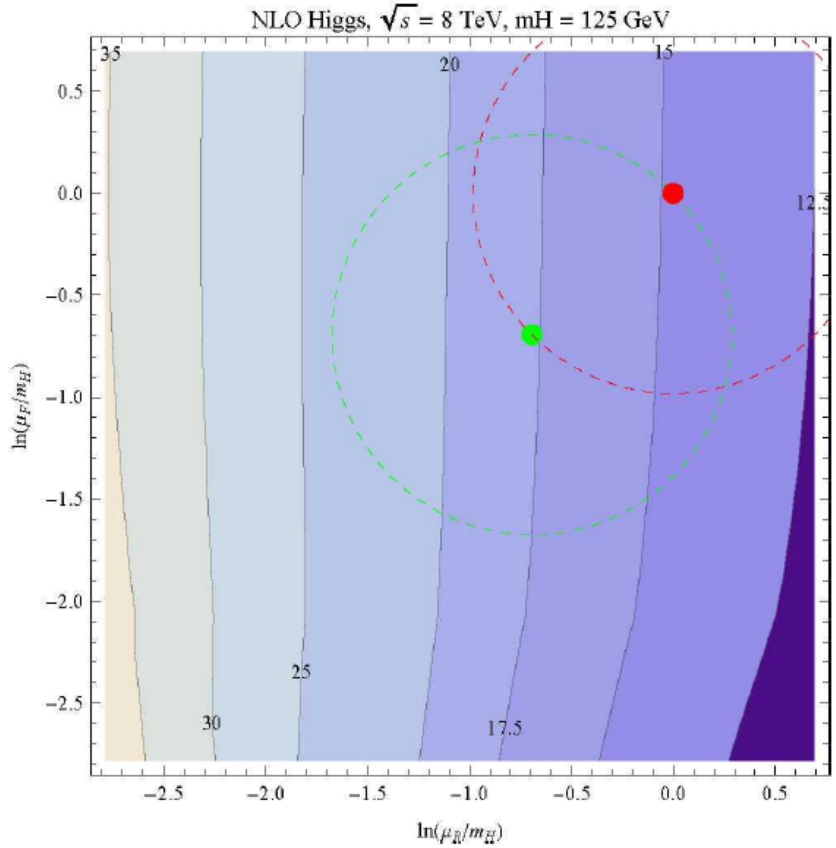
I don't know if any measurement has explicitly used this, but it would be useful to see.

2-D plots for ggF for Higgs

- The NNLO scale dependence looks similar to that for low p_T inclusive jet production, steep at low values of μ_R, shallow in μ_F
- Note that there is no saddle point at NLO in the range of scales plotted; it looks similar to LO for inclusive jet production

ihixs

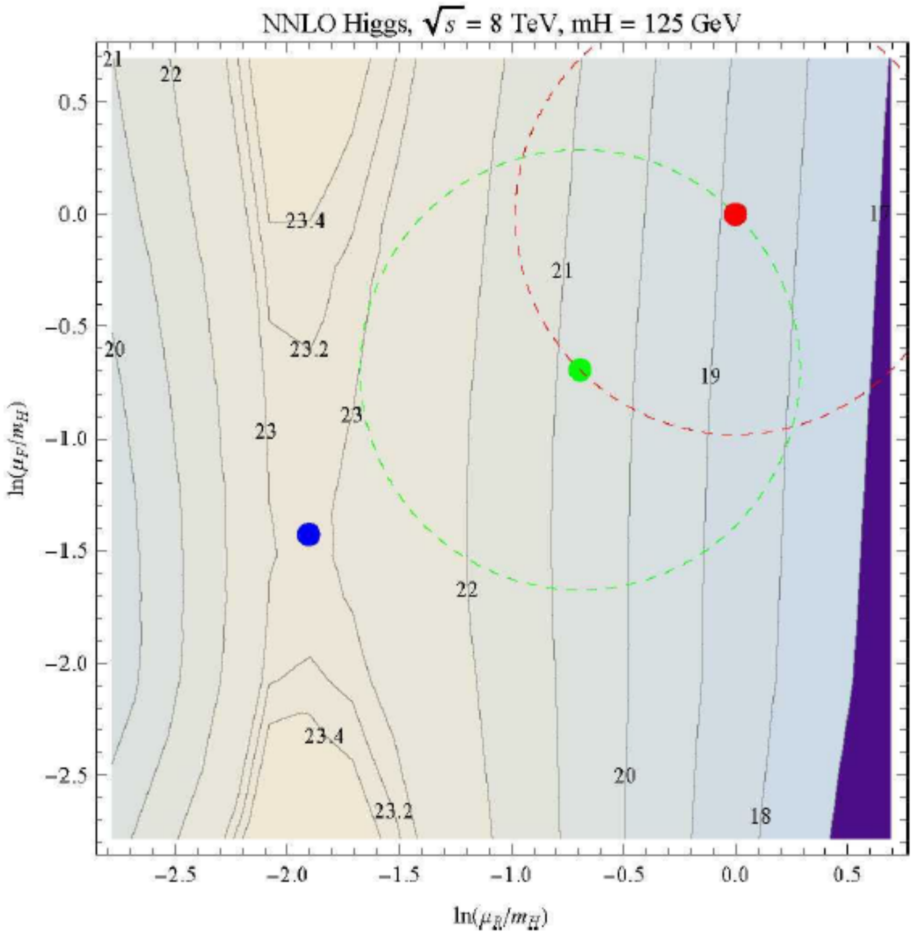




Achilleas Lazopoulos and Stephan Buehler, with Steve Ellis

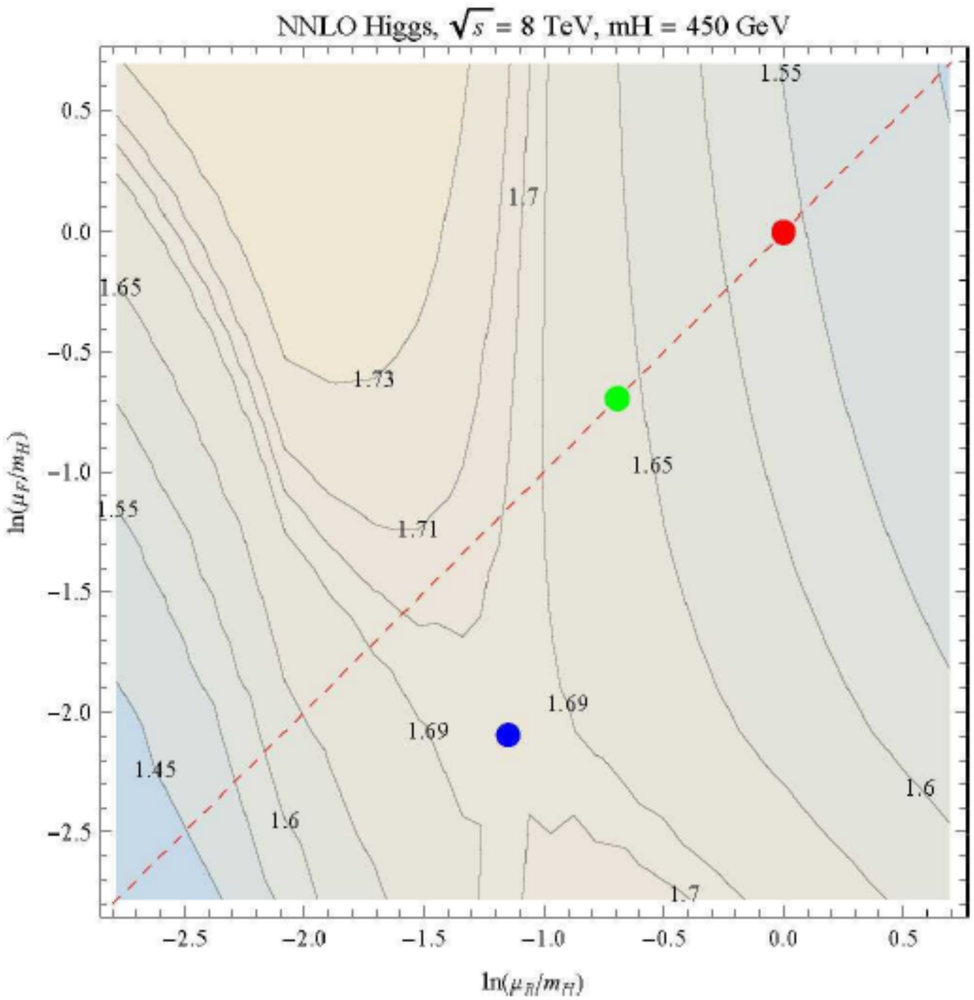
ggF at NNLO

- Note that the location of the saddle point is at ~(0.15m_H, 0.24m_H), i.e. outside of the range of uncertainties typically taken into account when using a scale of either m_H or 0.5 m_H
- Saddle point ~23.1pb compared to 20.7pb for m_H/2
- Maybe the saddle point is not magic, but it may be disturbing that it is not included in the uncertainty calculation
- …especially since we're now worrying/are excited about the ggF data cross section perhaps being larger than the 'SM' prediction



ggF at NNLO

- Now consider a 450 GeV Higgs produced by ggF
- There's some rotation of the saddle region as you would expect from the jet analysis
- Saddle point also moves to smaller μ_F



What about complex processes?

- …where there are multiple scales
- Most of the recent conquests of the Les Houches NLO wishlist deal with such complex final states
- …such as V+4(5) jets
- What is the appropriate scale to use?
- See also Kalanand Mishra's talk this afternoon

Process ($V \in \{Z, W, \gamma\}$)	Comments
Calculations completed since Les Houches 2005	
1. $pp \to VV$jet	WWjet completed by Dittmaier/Kallweit/Uwer [4, 5]; Campbell/Ellis/Zanderighi [6]. ZZjet completed by Binoth/Gleisberg/Karg/Kauer/Sanguinetti [7]
2. $pp \to$ Higgs+2jets	NLO QCD to the gg channel completed by Campbell/Ellis/Zanderighi [8]; NLO QCD+EW to the VBF channel completed by Ciccolini/Denner/Dittmaier [9, 10]
3. $pp \to VVV$	ZZZ completed by Lazopoulos/Melnikov/Petriello [11] and WWZ by Hankele/Zeppenfeld [12] (see also Binoth/Ossola/Papadopoulos/Pittau [13])
4. $pp \to t\bar{t}b\bar{b}$	relevant for $t\bar{t}H$ computed by Bredenstein/Denner/Dittmaier/Pozzorini [14, 15] and Bevilacqua/Czakon/Papadopoulos/Pittau/Worek [16]
5. $pp \to V$+3jets	calculated by the Blackhat/Sherpa [17] and Rocket [18] collaborations
Calculations remaining from Les Houches 2005	
6. $pp \to t\bar{t}$+2jets	relevant for $t\bar{t}H$ computed by Bevilacqua/Czakon/Papadopoulos/Worek [19]
7. $pp \to VV\,b\bar{b}$,	relevant for VBF $\to H \to VV$, $t\bar{t}H$
8. $pp \to VV$+2jets	relevant for VBF $\to H \to VV$ VBF contributions calculated by (Bozzi/)Jäger/Oleari/Zeppenfeld [20–22]
NLO calculations added to list in 2007	
9. $pp \to b\bar{b}b\bar{b}$	$q\bar{q}$ channel calculated by Golem collaboration [23]
NLO calculations added to list in 2009	
10. $pp \to V$+4 jets	top pair production, various new physics signatures
11. $pp \to Wb\bar{b}j$	top, new physics signatures
12. $pp \to t\bar{t}t\bar{t}$	various new physics signatures
Calculations beyond NLO added in 2007	
13. $gg \to W^*W^*\ \mathcal{O}(\alpha^2\alpha_s^3)$	backgrounds to Higgs
14. NNLO $pp \to t\bar{t}$	normalization of a benchmark process
15. NNLO to VBF and Z/γ+jet	Higgs couplings and SM benchmark
Calculations including electroweak effects	
16. NNLO QCD+NLO EW for W/Z	precision calculation of a SM benchmark

W+4 jets at 7 TeV

- Blackhat+Sherpa collaboration suggests using (large) scale of $H_T/2$, with variations a factor of 2 around that
- Result is generally in agreement with the data, with reasonably small scale uncertainty, and small+stable LO->NLO corrections

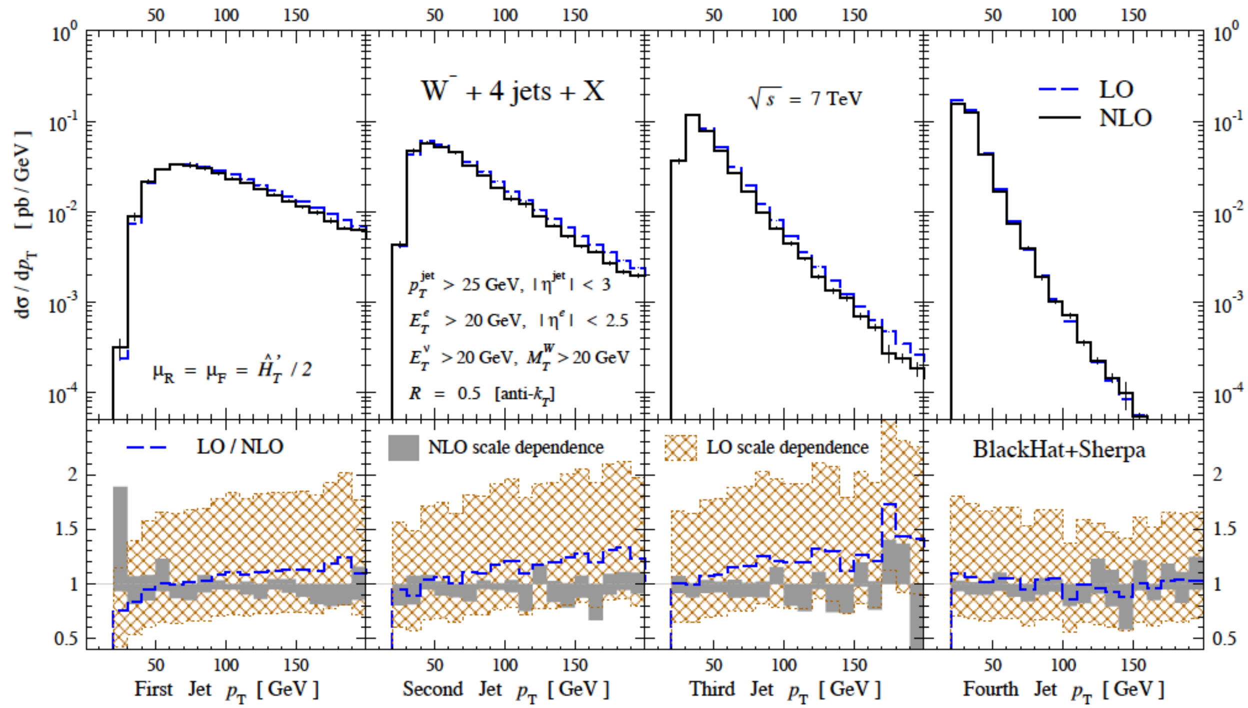
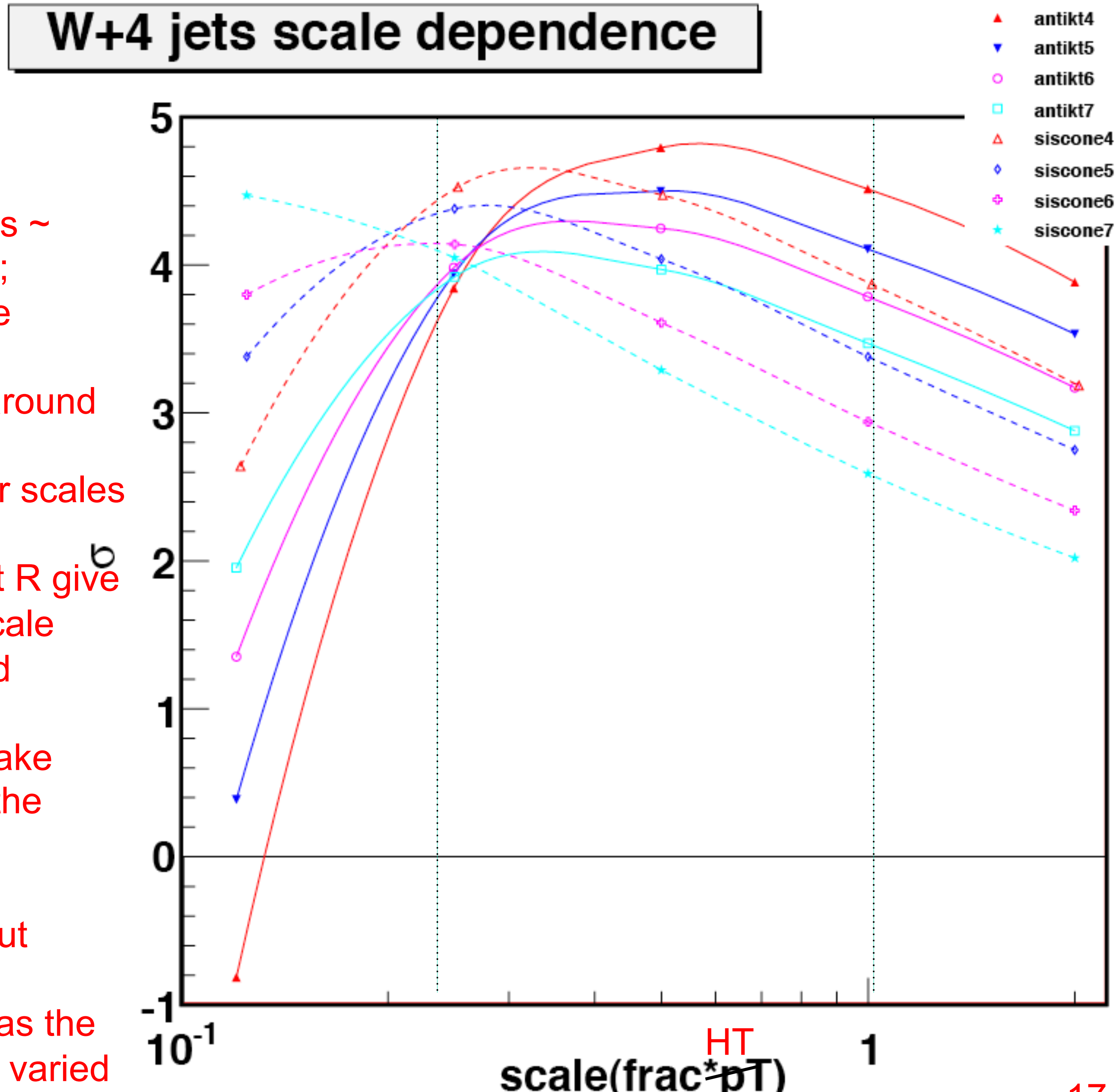


FIG. 2: A comparison of the p_T distributions of the leading four jets in $W^- + 4$-jet production at the LHC at $\sqrt{s} = 7$ TeV. In the upper panels the NLO distribution is the solid (black) histogram and the LO predictions are shown as dashed (blue) lines. The thin vertical line in the center of each bin (where visible) gives its numerical integration error. The lower panels show the distribution normalized to the central NLO prediction. The scale-dependence bands are shaded (gray) for NLO and cross-hatched (brown) for LO.



- A scale of HT/2 is ~ the peak for antikt4; so all deviations are negative
- Siscone peaks around HT/3
- Moves to smaller scales for larger R
- @HT/4, all antikt R give same result; that scale seems to be around HT/5 for siscone
- it is difficult to make conclusions about the uncertainty of any particular W + n jet cross section without understanding the scale dependence as the jet size/algorithm is varied

Scales: CKKW and NLO

- Applying a CKKW-like scale at LO also leads to better agreement for shapes of kinematic distributions
- Now we have CKKW@NLO and MINLO(->Keith Hamilton talk)
- Connection between large scales (H_T) and small scales (MINLO/CKKW) with appropriate Sudakov suppression?

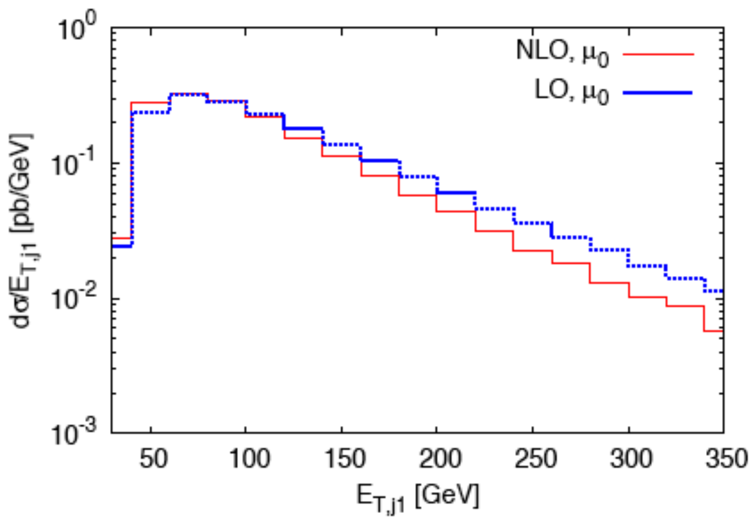


FIG. 3: The transverse momentum distribution of the leading jet for $W^+ + 3$ jet inclusive production cross section at the LHC. All cuts and parameters are described in the text. The leading color adjustment procedure is applied.

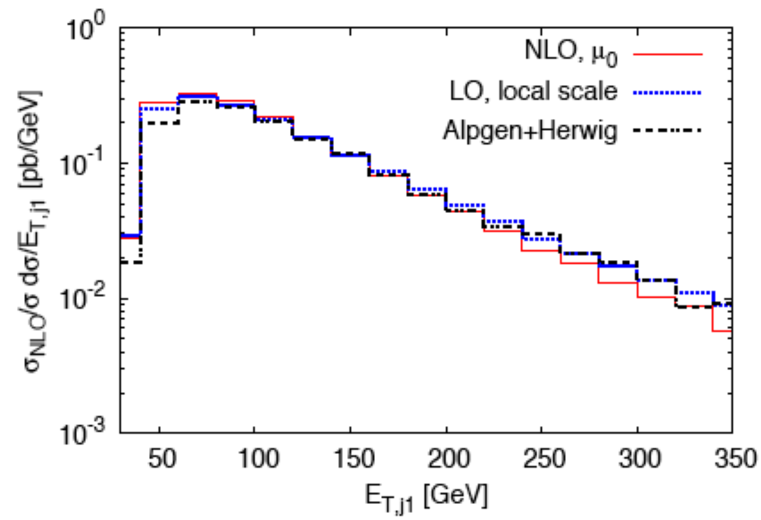


FIG. 4: The transverse momentum distribution of the leading jet for $W^+ + 3$ jet inclusive production cross section at the LHC. All cuts and parameters are described in the text. The leading color adjustment procedure is applied. All LO distributions are rescaled by constant factor, to ensure that the LO and NLO normalizations coincide.

See review of W + 3 jets in Les Houches 2009 NLM proceedings

0910.3671 Melnikov, Zanderighi

- So far we have been talking about inclusive cross sections
- What about exclusive cross sections where jet vetoes, or severe kinematic cuts have been applied?
- One of the biggest topics of discussion at Les Houches 2011
- …as it will continue to be at Les Houches 2013

Start with Stewart-Tackmann

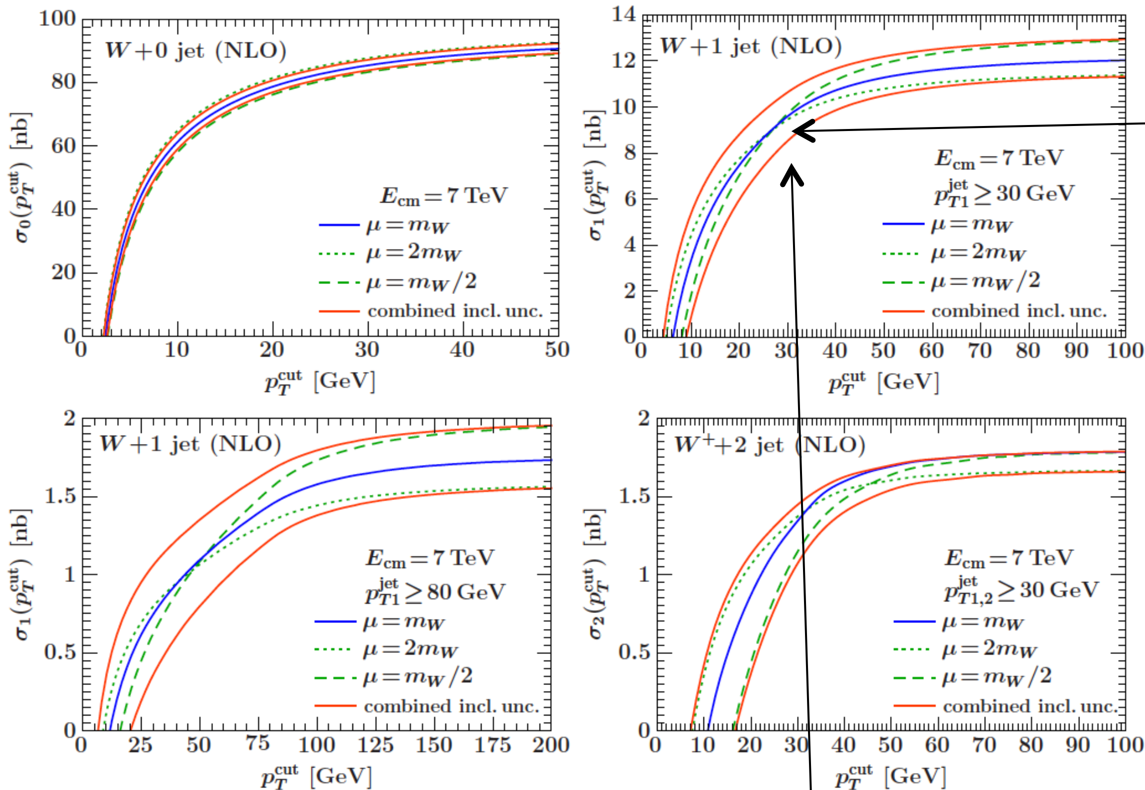


FIG. 3: Fixed-order perturbative uncertainties for the exclusive $pp \to W + 0, 1, 2$ jet cross sections at NLO for the LHC with $E_{cm} = 7$ TeV. Central values are shown by blue solid curves, naive scale variation in the exclusive jet bin by the green dashed and dotted curves, and the result of combining independent inclusive uncertainties to get the jet-bin uncertainty by the outer red solid curves.

clearly, scale uncertainty for exclusive cross sections don't vanish, so naïve scale uncertainty estimate is probably too low

Stewart-Tackmann: n-jet exclusive σ is difference between two inclusive cross sections

$$\sigma_N = \sigma_{\geq N} - \sigma_{\geq N+1}$$

The two series are independent of each other; for example W+>=2 jets has large double logs of p_T^{jet2}/m_W; so have to add scale dependence in quadrature

$$\Delta_N^2 = \Delta_{\geq N}^2 + \Delta_{\geq N+1}^2$$

$$\sigma_{\geq 1}(p_{T1}^{jet} \geq 30\,\text{GeV}) = (8.61\,\text{nb})\left[1 + 3.4\,\alpha_s + \mathcal{O}(\alpha_s^2)\right]$$

$$\sigma_{\geq 2}(p_{T1}^{jet} \geq 30\,\text{GeV}, p_{T2}^{jet} \geq 30\,\text{GeV}) = (8.61\,\text{nb})\left[2.5\,\alpha_s + \mathcal{O}(\alpha_s^2)\right].$$

The result is a significant (but perhaps more realistic) increase in the scale uncertainty.

…continued

- One solution is to use inclusive distributions
  - or to show both inclusive and exclusive
- For a ratio of two exclusive cross sections (like W+1 jet/Z+1 jet), the S-T approach now increases the uncertainty 'beyond reason', as there are now 4 cross sections, all of which need to be treated as uncorrelated
- Given that the central prediction, using a scale such as $H_T/2$ for the case of W/Z+jets, is in good agreement with the data, are the scale uncertainties really so large?

Z+jet

Impact on exclusive jet multiplicity

Njet	S&T	naive
0p	+- 1%	+ 2% - 2%
1p	+- 6%	+ 1% - 2%
2p	+- 7%	+ 1% - 12%
3p	+-12%	+ 0% - 21%
4p	+-23%	+ 0% - 26%

Njet(Pt>150)	S&T	naive
1p	+-32%	+10% - 20%
2p	+-13%	+13% - 39%
3p	+-18%	+ 8% - 48%
4p	+-38%	+ 2% - 46%

Ratio(N+1/N)	S&T (+uncorrelated)	naive (+correlated)
1/0	+7% - 7%	+ 0% - 2%
2/1	+13% - 12%	+ 1% - 10%
3/2	+20% - 17%	+ 0% - 10%
4/3	+39% - 31%	+ 0% - 6%

Ratio(N+1/N) PT>150GeV	S&T (+uncorrelated)	naive (+correlated)
2/1	+67% - 34%	+ 3% - 25 %
3/2	+36% - 27%	+ 0% - 14%
4/3	+68% - 47%	+ 4% - 5%

Z+4j: Cannot follow the S&T prescription due to lack of Z+5p NLO
Using Z+5p LO instead

- scale uncertainties assumed to be uncorrelated between the multiplicities
- large uncertainties on the jet multiplicities

→ huge uncertainties in the exclusive multiplicity ratio

Ulla Blumenschein

Higgs+jets

- Here it is crucial to use exclusive cross sections because of backgrounds differing with jet multiplicity
  - but because of its importance, a great deal of work has gone into resumming the logs that lead to the increased scale dependence; the result is a decrease of the naïve S-T uncertainty
- My question to Gavin:
  - can we use what has been learned from Higgs+jets resummation techniques to guide us for W/Z+jets?
  - No: Higgs is a special case; gg fusion to Higgs has a large K-factor; with jet-veto that large K-factor partially cancels against Sudakov suppression, resulting in a spurious smaller scale dependence
- But…don't assume that NLO predictions for jet multiplicities are completely uncorrelated, given that much of the underlying physics must be similar
- Another technique: treat the scale uncertainties as completely correlated between different jet multiplicities (for a ratio), but estimate the uncertainty by writing the ratio in ways that are perturbatively equivalent, but whose differences might illuminate the 'real' scale uncertainty

W+jets

- For example, consider W+1 jet and W+2 jets at NLO
- Rewrite as:

$$\sigma_1^{LO} + \sigma_1^{NLO}$$

$$\sigma_2^{LO} + \sigma_2^{NLO}$$

- Then write the series in two ways

a) $Ratio(default) = \dfrac{\sigma_2^{LO} + \sigma_2^{NLO}}{\sigma_1^{LO} + \sigma_1^{NLO}}$

b) $Ratio(alternative) = \dfrac{\sigma_2^{LO}}{\sigma_1^{LO}} + \dfrac{\sigma_2^{NLO}}{\sigma_1^{LO}} - \dfrac{\sigma_1^{NLO} * \sigma_2^{LO}}{\left(\sigma_1^{LO}\right)^2}$

- For Higgs, Gavin took the envelope of all scale variations on a) and the central result from b)
- This may work for inclusive ratios, but not necessarily for exclusive
- It's worth trying

B+S estimates for uncertainty

- Calculate the ratio of Z+jets to γ+jets
- Use the NLO and ME+PS ratios to estimate scale uncertainty
  - divide the absolute value of the difference between the two ratios by the NLO ratio
  - PS effectively serves as an estimator for higher order corrections

Set 1: $H_T^{jet} > 300$ GeV, $|MET| > 250$ GeV;

Set 2: $H_T^{jet} > 500$ GeV, $|MET| > 150$ GeV;

Set 3: $H_T^{jet} > 300$ GeV, $|MET| > 150$ GeV;

Set 4: $H_T^{jet} > 350$ GeV, $|MET| > 200$ GeV;

Set 5: $H_T^{jet} > 500$ GeV, $|MET| > 350$ GeV;

Set 6: $H_T^{jet} > 800$ GeV, $|MET| > 200$ GeV;

Set 7: $H_T^{jet} > 800$ GeV, $|MET| > 500$ GeV.

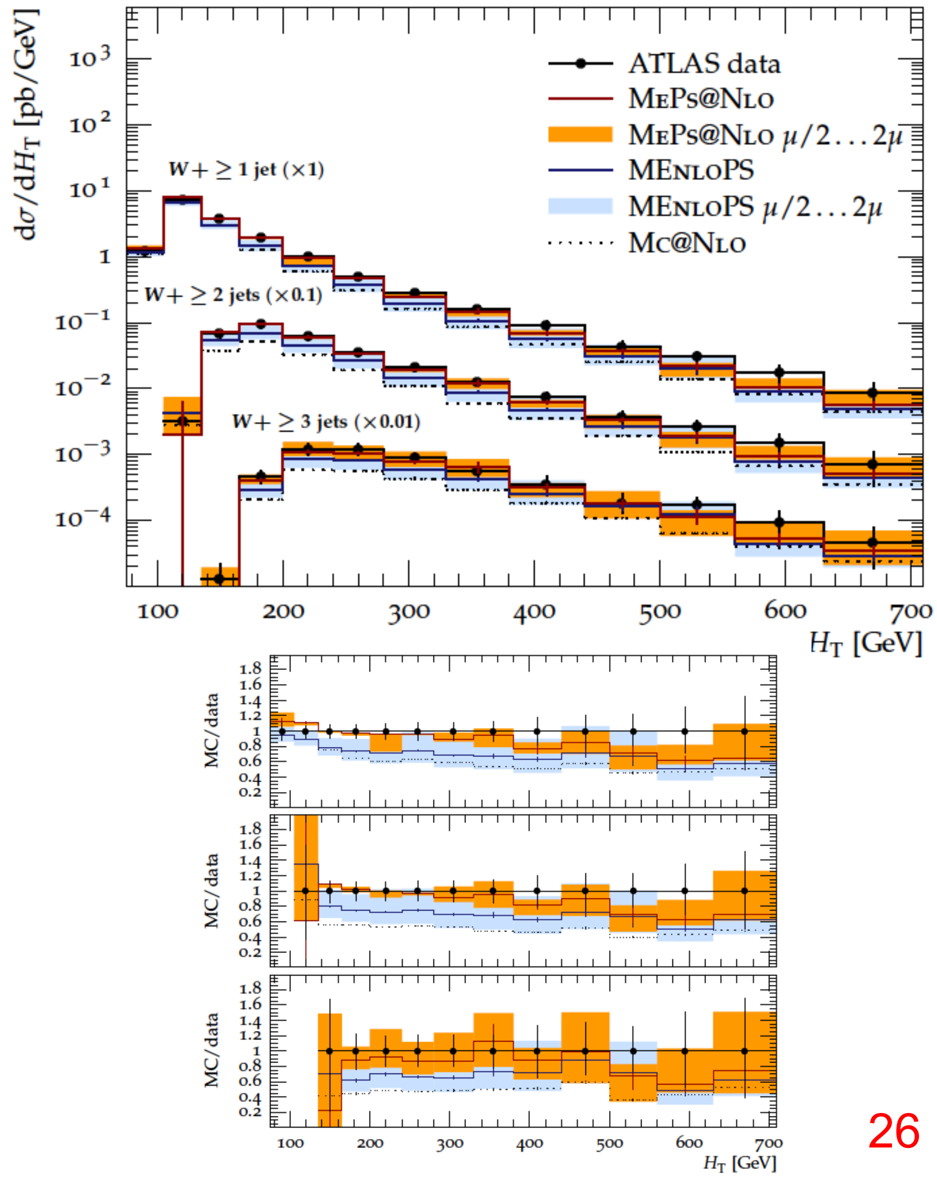
Source \ Set	1	2	3	4	5	6	7
perturbative	0.09	0.03	0.10	0.07	0.05	0.02	0.04
PDF	0.02	0.03	0.02	0.02	0.03	0.04	0.05
photon-cone	0.01	0.01	0.01	0.01	0.01	0.01	0.01
total	0.09	0.04	0.10	0.08	0.06	0.04	0.06

estimates are *reasonably small*

TABLE VI: Estimates of the fractional uncertainty remaining from QCD effects for the Z + 3-jet to γ + 3-jet ratios. The "perturbative" uncertainty comes from comparing the NLO ratio with the ME+PS one, as explained in the text. The "photon-cone" uncertainty is due to the estimated difference in predictions using the standard and Frixione isolation cones.

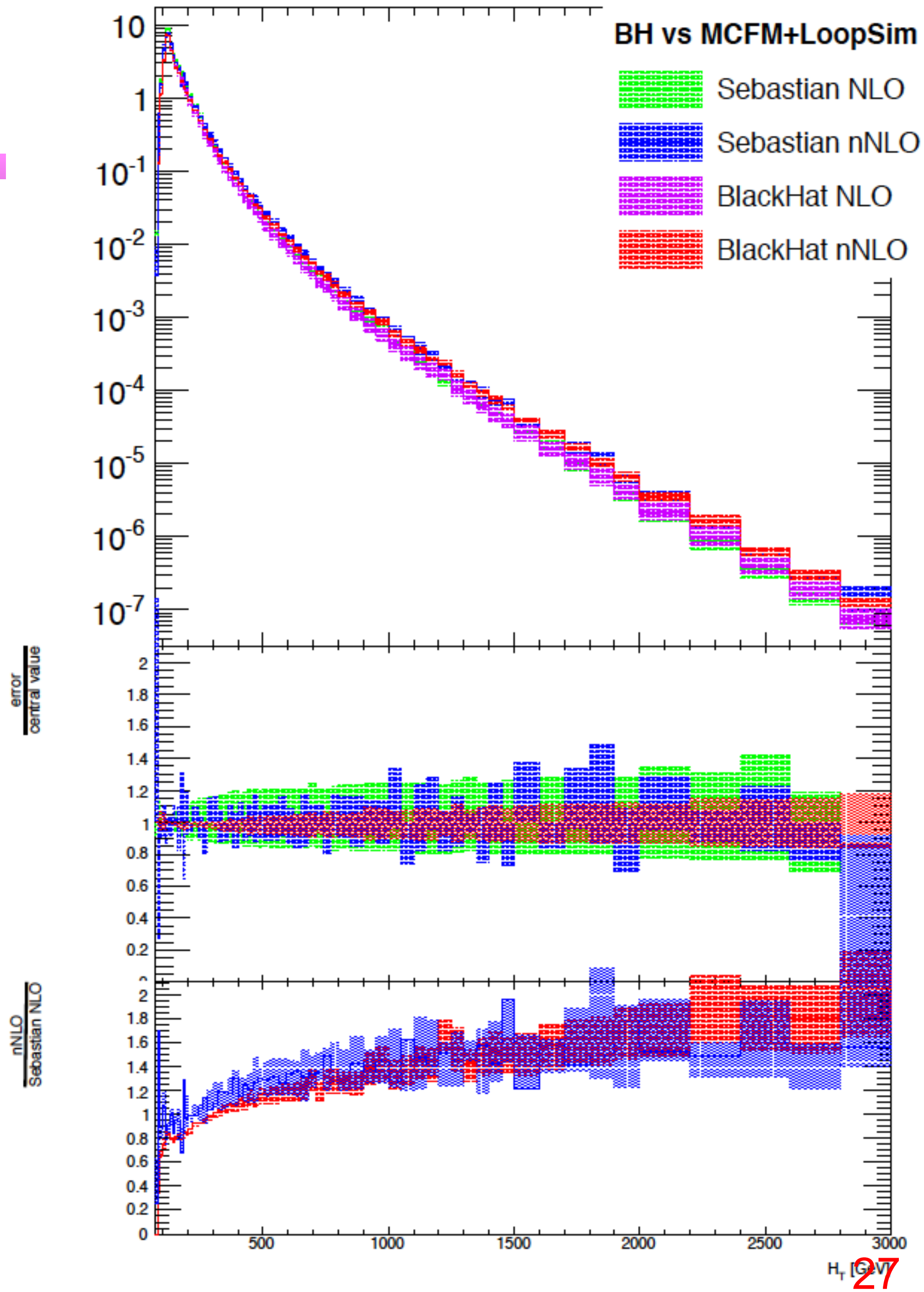
MEPS@NLO (or aMC@NLO)

- I've been running W +0+1+2 jets at NLO with additional jets either by LO or by PS
  - effectively CKKW at NLO
- This may be a better/ different vehicle to estimate scale uncertainties
  - since many of the higher order corrections can be taken in/out in a more sophisticated way than in the previous slide



LoopSim

- Sebastian Sapeta has been running LoopSim for W+>=1 jet to effectively get approximate NNLO (nNLO) predictions for W+>=1 jet
- Compared here to Blackhat +Sherpa exclusive sums approach
- Note that for both, significant scale dependence cancellation by addition of virtual W+2 jet matrix elements
  - this is because of substantial contributions from qq->qqW where W is radiated from quark line
- May be useful for uncertainties for some ratios since it tries to estimate higher order corrections



Summary

- Tremendous progress in the development of tools that allow us to improve the perturbative power of predictions for complex final states at the LHC
- A lot to think about and discuss, both here and in subsequent meetings, including Les Houches, about the best ways of using these tools