QCD Theory and Monte Carlo Tools

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Fermilab-CERN HCPSS18

20-31 August 2018

References

- Useful resources for perturbative QCD — additional background and further reading for more advanced topics — are:

- QCD and Collider Physics
R. K. Ellis, W. J. Stirling and B. R. Webber
Cambridge Monographs on Particle Physics, Nuclear Physics and Cosmology

- The Black Book of Quantum Chromodynamics: A Primer for the LHC Era
JC, J. Huston, F. Krauss
Oxford University Press

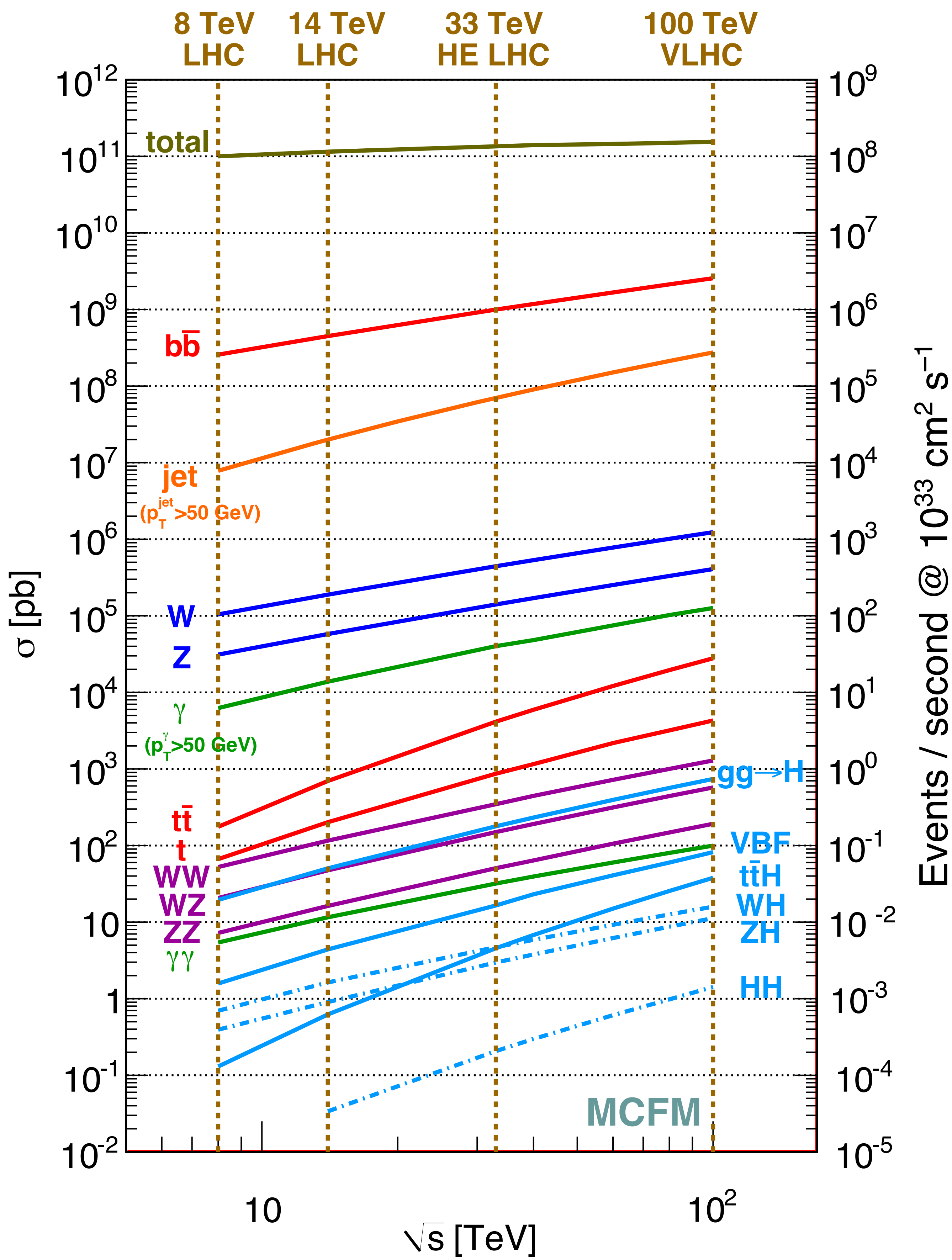
- Resource Letter: Quantum Chromodynamics
A. S. Kronfeld and C. Quigg
arXiv: 1002.5032 [hep-ph], prepared for the American Journal of Physics

Outline

- Introduction to the theory of QCD
  - Lagrangian, color, Feynman rules, strong coupling
- QCD for hadron colliders
  - factorization, parton distribution functions, hard scattering
- Structure of QCD matrix elements
  - infrared singularities, real and virtual radiation
- Beyond leading order
  - techniques for NLO, NNLO and beyond
- Parton shower techniques
  - Sudakov factors, resolvable emissions, hadronization
- Modern event generators
  - merging, matching, hybrid schemes, precision matching

QCD: why we care

- It is no surprise that hadron colliders require an understanding of QCD.
- However, the level of sophistication we require is demonstrated by the inclusive cross-sections for final states that we are typically interested in.
- In order to test the SM (and models of new physics), we require a quantitative understanding of QCD and precise theoretical predictions.
- These lectures will describe the ways in which we reach this goal.



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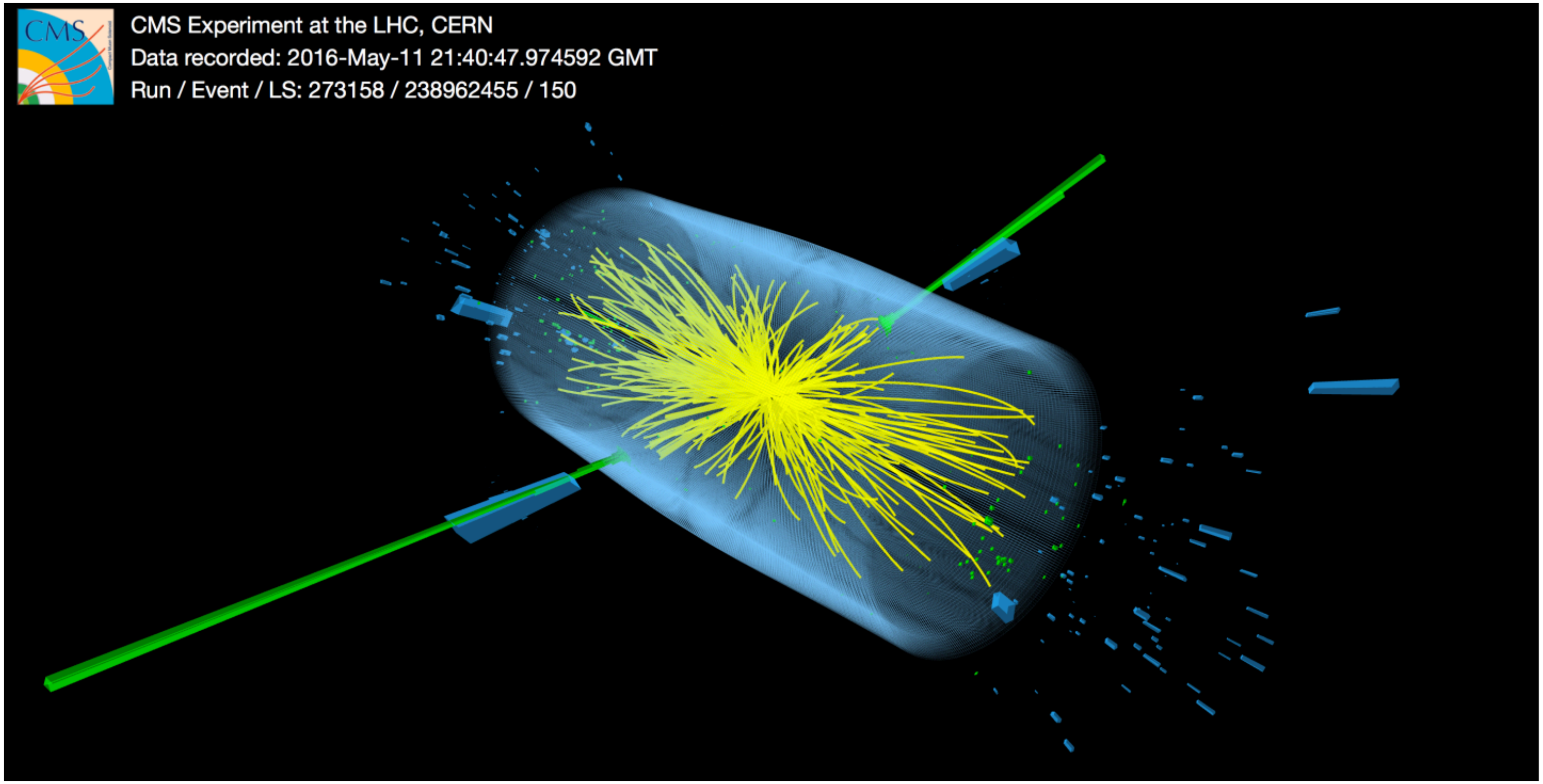
The challenge of QCD

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^{a}_{\mu\nu} F^{\mu\nu}_{a} + \sum_{\text{flavors}} \bar{q}_i \left(i D_\mu \gamma^\mu - m \right)_{ij} q_j$$



QCD and color

- The Lagrangian looks a lot like the one for QED: a field strength term representing the gluon field and a Dirac term for the quarks.
- However, it has one important difference: color.

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^{a}{}_{\mu\nu} F^{\mu\nu}_{a} + \sum_{\text{flavors}} \bar{q}_i \left(i D_\mu \gamma^\mu - m \right)_{ij} q_j$$

- Within the quark model, the additional quantum number of color was initially introduced to accommodate the existence of the Δ^{++} baryon.
  - antisymmetry to satisfy Pauli exclusion principle carried by color
  - quarks and gluons carry color but observed hadrons are colorless
- The color degrees of freedom can also be directly probed in electron-positron collisions, by comparing the production of hadrons and muons.

$$R = \frac{\sigma\left(e^+e^- \to \text{hadrons}\right)}{\sigma\left(e^+e^- \to \mu^+\mu^-\right)} = N_c \sum_f Q_f^2$$

- Q_f^2: quark charge
- N_c: assume N_c colors of quark
- $\sum_f$: sum over active quarks

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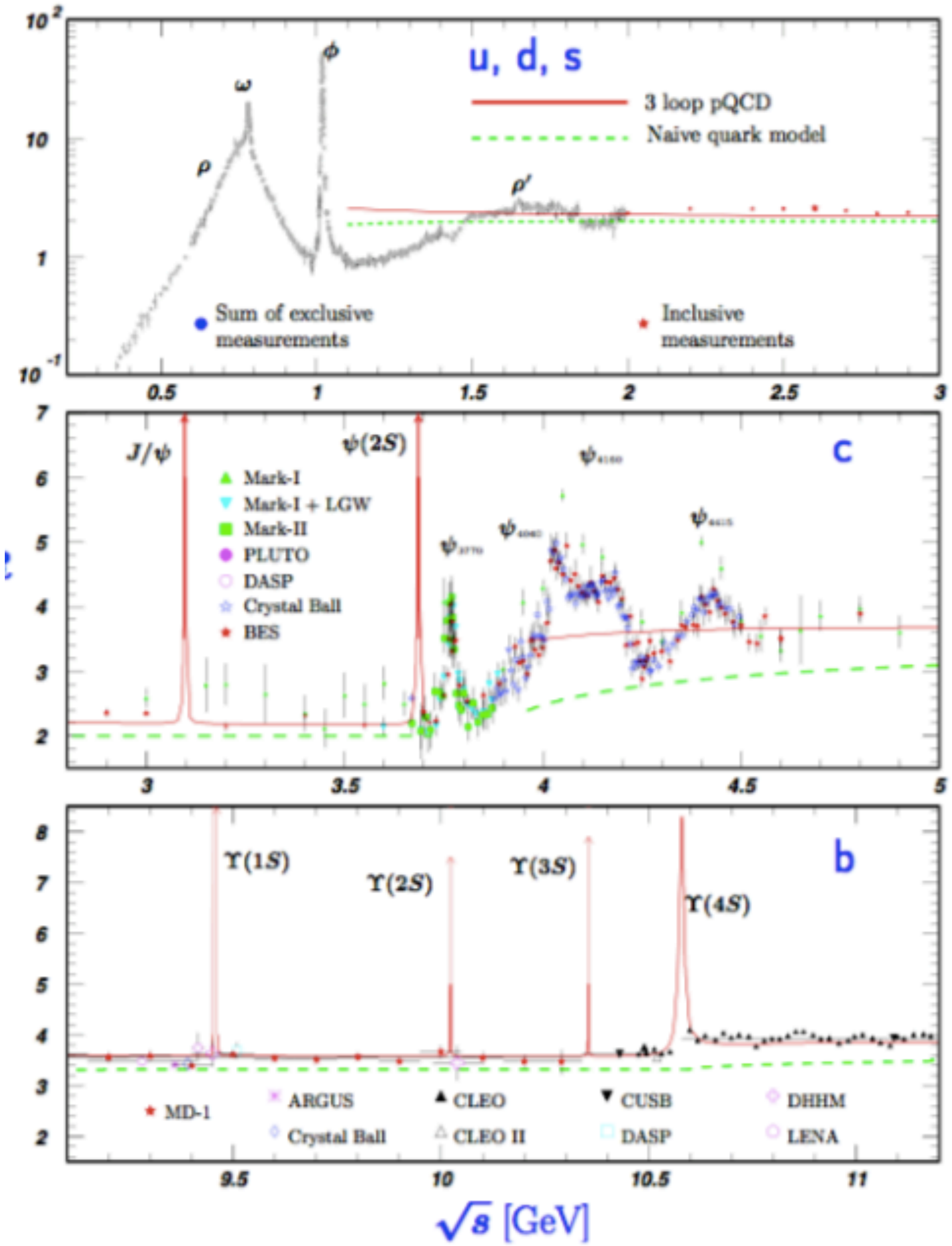
"R-ratio" measurements



$$R_{u,d,s} = 3 \times \left[\left(\frac{2}{3}\right)^2 + \left(-\frac{1}{3}\right)^2 + \left(-\frac{1}{3}\right)^2\right] = 2$$

$$R_{u,d,s,c} = R_{u,d,s} + 3 \times \left(\frac{2}{3}\right)^2 = \frac{10}{3}$$

$$R_{u,d,s,c,b} = R_{u,d,s,c} + 3 \times \left(-\frac{1}{3}\right)^2 = \frac{11}{3}$$

Color in the QCD Lagrangian: quarks

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a{}_{\mu\nu} F^{\mu\nu}_a + \sum_{\text{flavors}} \bar{q}_i \left(i D_\mu \gamma^\mu - m \right)_{ij} q_j$$

- The gauge principle — invariance under local gauge transformations — requires the introduction of the gauge-invariant derivative:

$$(D_\mu)_{ij} = \partial_\mu \delta_{ij} + i g_s \left(t^a A^a_\mu \right)_{ij}$$

- When inserted in the Lagrangian this introduces interactions between quarks of color *i* and *j*, mediated by the gluon field $A^a{}_{ij}$.
- Strength of the interaction depends on the strong coupling (g_s) and a matrix in color space (t^a) that is related to a Gell-Mann matrix (λ^a) by $t^a = \lambda^a/2$.
- These are Hermitian, traceless & satisfy commutation relation:

$$\left[\lambda^a, \lambda^b \right] = 2 i f_{abc} \lambda^c$$

$$\lambda^1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda^2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda^4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \lambda^5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \lambda^6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\lambda^7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \lambda^8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

SU(3)

- The matrices t^a are the generators of the group SU(3) in the fundamental representation: eight 3x3 matrices that satisfy:

$$[t^a, t^b] = i f_{abc} t^c$$

where f_{abc} form a set called the SU(3) structure constants. They're real numbers and are completely antisymmetric in the indices.

$$f_{123} = 1$$
$$f_{147} = f_{165} = f_{246} = f_{257} = f_{345} = f_{376} = \frac{1}{2}$$
$$f_{458} = f_{678} = \frac{\sqrt{3}}{2}.$$

- The matrices also obey a normalization condition:

$$\mathrm{Tr}\left(t^a t^b\right) = T_R\, \delta^{ab} \quad \text{with } T_R = 1/2$$

- By inspection, we can also see that:

$$\sum_a t^a t^a = C_F\, \mathbf{1}$$

$$\text{with } C_F = \frac{4}{3} \equiv \frac{N_c^2 - 1}{2N_c}$$

- The quantity C_F is called a Casimir.

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Color in the QCD Lagrangian: gluons

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a{}_{\mu\nu} F_a^{\mu\nu} + \sum_{\text{flavors}} \bar{q}_i \left(i D_\mu \gamma^\mu - m \right)_{ij} q_j$$

- The field strength tensor in the first term is fundamentally different from the QED case:

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g_s f_{abc} A^b_\mu A^c_\nu$$

- The final term involves the SU(3) structure constants and two gluon fields.
- When inserted into the Lagrangian this leads to self-interactions between gluons, involving three or four fields.

- To handle these gluon interactions we will need a second Casimir:

$$\sum_{c,d} f^{acd} f^{bcd} = C_A \delta^{ab} \quad \text{with } C_A = 3 \equiv N_c$$

(can again check this by inspection)

From the Lagrangian to calculations

- To use this Lagrangian we need to be able to calculate scattering amplitudes and ultimately cross-sections.
- The main toolbox for collider physics is perturbative QCD:
  - expand the Lagrangian about the free (non-interacting) case in powers of the coupling
  - interactions correspond to at least one power of the coupling
  - represent amplitudes as Feynman diagrams, with rules read off from the Lagrangian

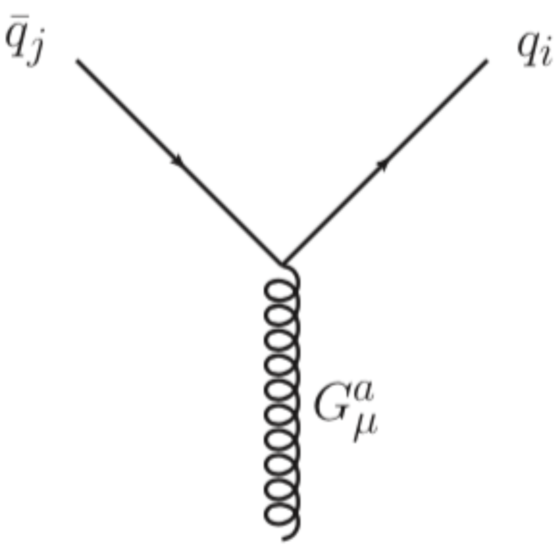
- In the free case ($g_s \to 0$) there are only propagators.
- These are easily read off from two-point interactions in the Lagrangian, that give the inverse propagator, after making the momentum-space replacement (c.f. Fourier expansion): $\partial_\mu \to -ip_\mu$

- E.g. quarks: $\bar{q}_i \left(i\partial_\mu \gamma^\mu - m \right) \delta_{ij} q_j \to \bar{q}_i \left(p_\mu \gamma^\mu - m \right) \delta_{ij} q_j$

$$\frac{(p_\mu \gamma^\mu + m)}{p^2 - m^2} \delta_{ij}$$

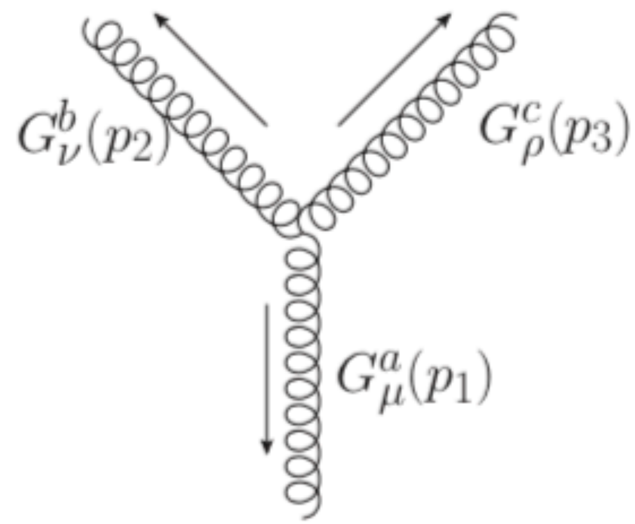
Note: inverse of gluon propagator requires extra gauge-fixing term

QCD interactions



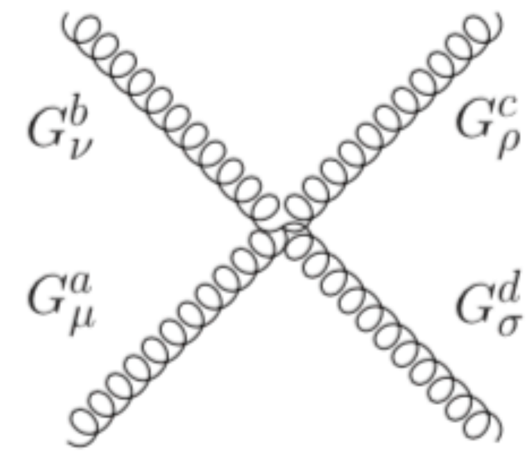
$-ig_s T^a_{ij}\gamma_\mu$

Quark-gluon interaction (gauge-invariant derivative)



$$g_s f^{abc}[(p_1 - p_2)_\rho\, g_{\mu\nu} + (p_2 - p_3)_\mu\, g_{\nu\rho} + (p_3 - p_1)_\nu\, g_{\rho\mu}]$$

Triple-gluon vertex (field-strength tensor, one derivative)



$$ig_s^2[f^{eac}f^{ebd}(g_{\mu\nu}g_{\rho\sigma} - g_{\mu\sigma}g_{\nu\rho}) + f^{ead}f^{ebc}(g_{\mu\nu}g_{\rho\sigma} - g_{\mu\rho}g_{\nu\sigma}) + f^{eab}f^{ecd}(g_{\mu\rho}g_{\nu\sigma} - g_{\mu\sigma}g_{\nu\rho})]$$

Four-gluon vertex (field-strength tensor, no derivatives)

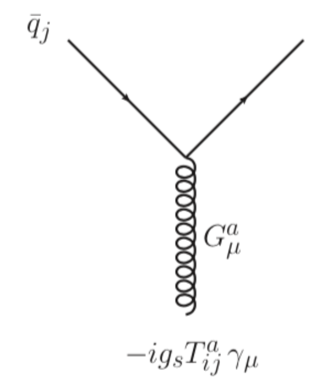
$$(D_\mu)_{ij} = \partial_\mu \delta_{ij} + ig_s\left(t^a A^a_\mu\right)_{ij}$$

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g_s f_{abc} A^b_\mu A^c_\nu$$

Color factors in action

- As an example of how these work, consider additional gluon emission from a hard quark or gluon.
- Looking at just the color matrices (i.e. ignoring kinematics) we can find the effect on gluon emission probabilities from just the Feynman rules so far:

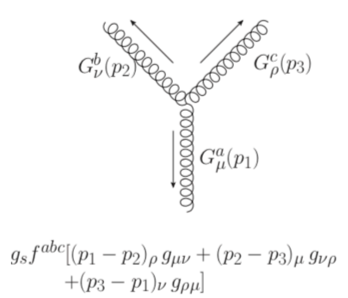
$$P_{\rm emit}(q) \sim \left| \vphantom{\sum} \right.$$



$$\left. \vphantom{\sum} \right|^2 \sim \sum_{a,j} t^a_{ij} \left(t^a_{ij}\right)^* = \sum_{a,j} t^a_{ij}\, t^a_{ji} = C_F$$

(sum over colors) (Hermitian) (Casimir)

$$P_{\rm emit}(g) \sim \left| \vphantom{\sum} \right.$$



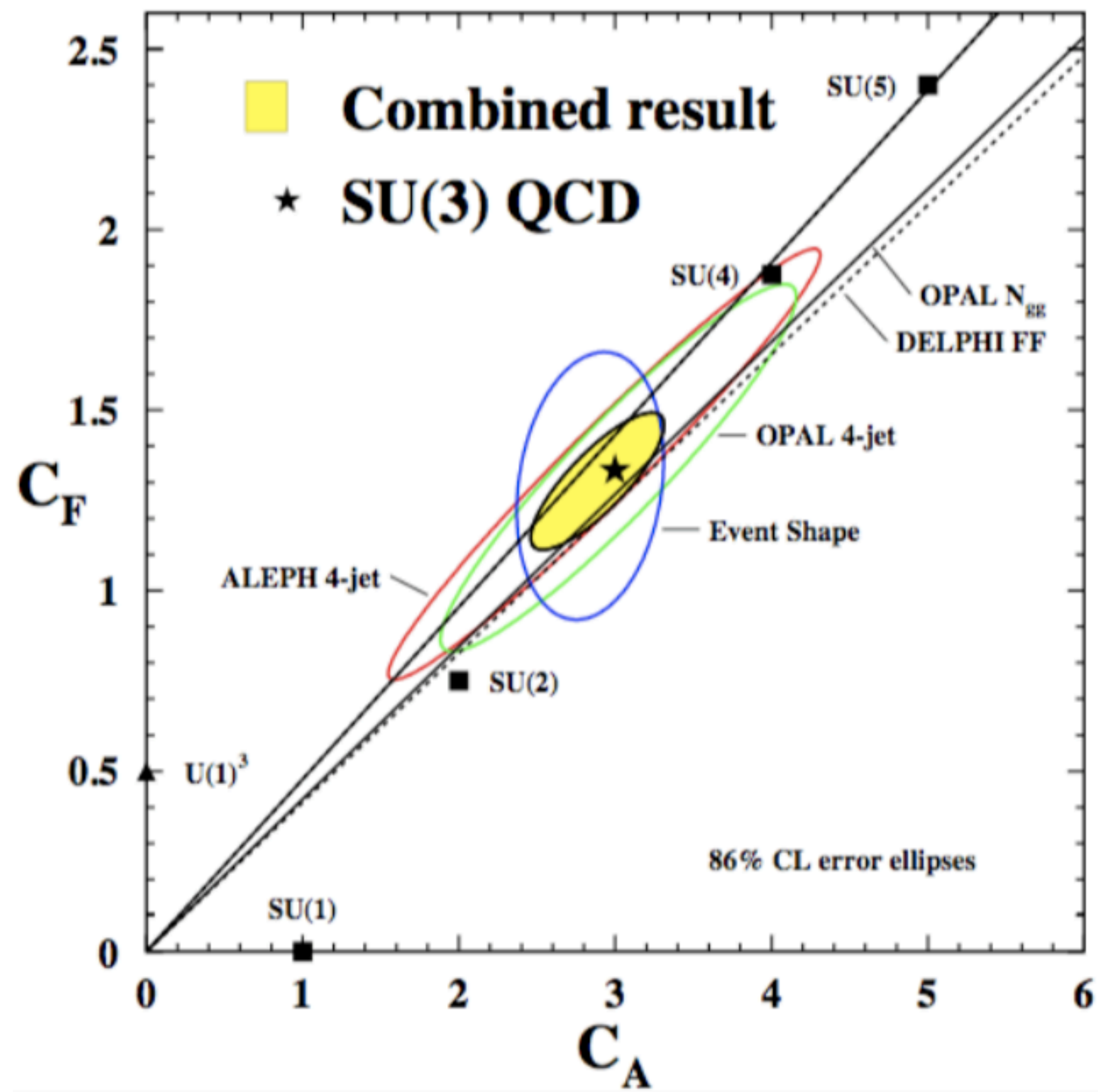
$$\left. \vphantom{\sum} \right|^2 \sim \sum_{b,c} f_{abc}\, f_{abc} = C_A$$

(sum over colors) (Casimir)

- This gives rise to the expectation that gluon jets radiate more copiously than quark jets.

Color factors and cross-sections

- In calculations of cross-sections these sums over color factors are ubiquitous (and can be arduous to handle, for very many colored particles).
- The Casimirs of SU(3), C_A and C_F, are intrinsic to the theory of QCD.
- Their values have been tested, e.g. in measurements of jet event shapes at LEP.
  - A neat demonstration of the manifestation of group theory in physical observables.

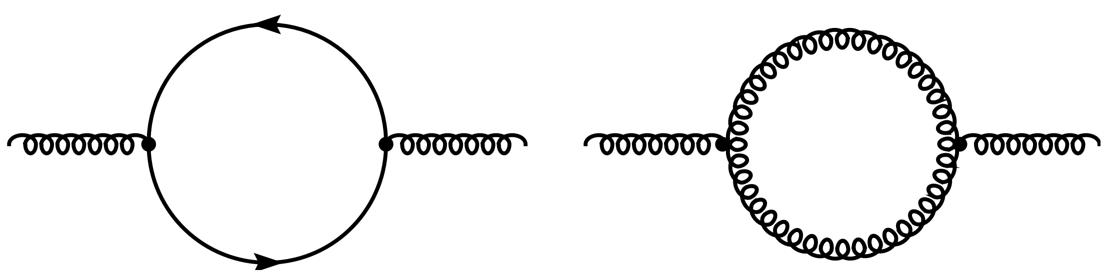


The strong coupling

- The effects of the quantum field theory vacuum — populated by short-lived, virtual quark and gluon pairs — affects the strength of the coupling.
- Trying to measure the coupling of an individual quark by probing with a gluon is only possible at sufficiently high energy.
- At lower energies the probe will instead only resolve a cloud of virtual particles that partially screen the coupling.
- This dependence on the energy scale μ is encoded in the beta function, which governs the running of the strong coupling:

$$\beta(\alpha_s) = \mu \frac{\partial \alpha_s(\mu)}{\partial \mu} = \frac{\partial \alpha_s(\mu)}{\partial(\log \mu)} \qquad \text{with } \alpha_s = \frac{g_s^2}{4\pi}$$

- It can be computed perturbatively by considering exactly these vacuum fluctuation diagrams, e.g. one power of α_s:



Running the strong coupling

- At this order the result is: $\beta(\alpha_s) = -b_0 \alpha_s^2 + \ldots$ $\qquad b_0 = \frac{11 C_A - 2 n_f}{6\pi}$
- With quark loops alone (c.f. QED) the result would be a positive beta-function; in contrast, in QCD the gluon loops make it negative.
- Can now solve for the coupling relative to some other scale *Q*:

$$\frac{\partial \alpha_s(\mu)}{\partial(\log \mu)} = -b_0 \alpha_s(\mu)^2 \quad \Longrightarrow \quad \left[\frac{1}{\alpha_s(\mu)}\right]_{\mu=Q} = b_0 \left[\log \mu\right)\big]_{\mu=Q}$$

$$\Longrightarrow \quad \alpha_s(\mu) = \frac{\alpha_s(Q)}{1 + \alpha_s(Q) b_0 \log(\mu/Q)}$$

- Note that this diverges at the scale Λ≪Q when the denominator vanishes.
- This condition gives an alternate expression for the running:

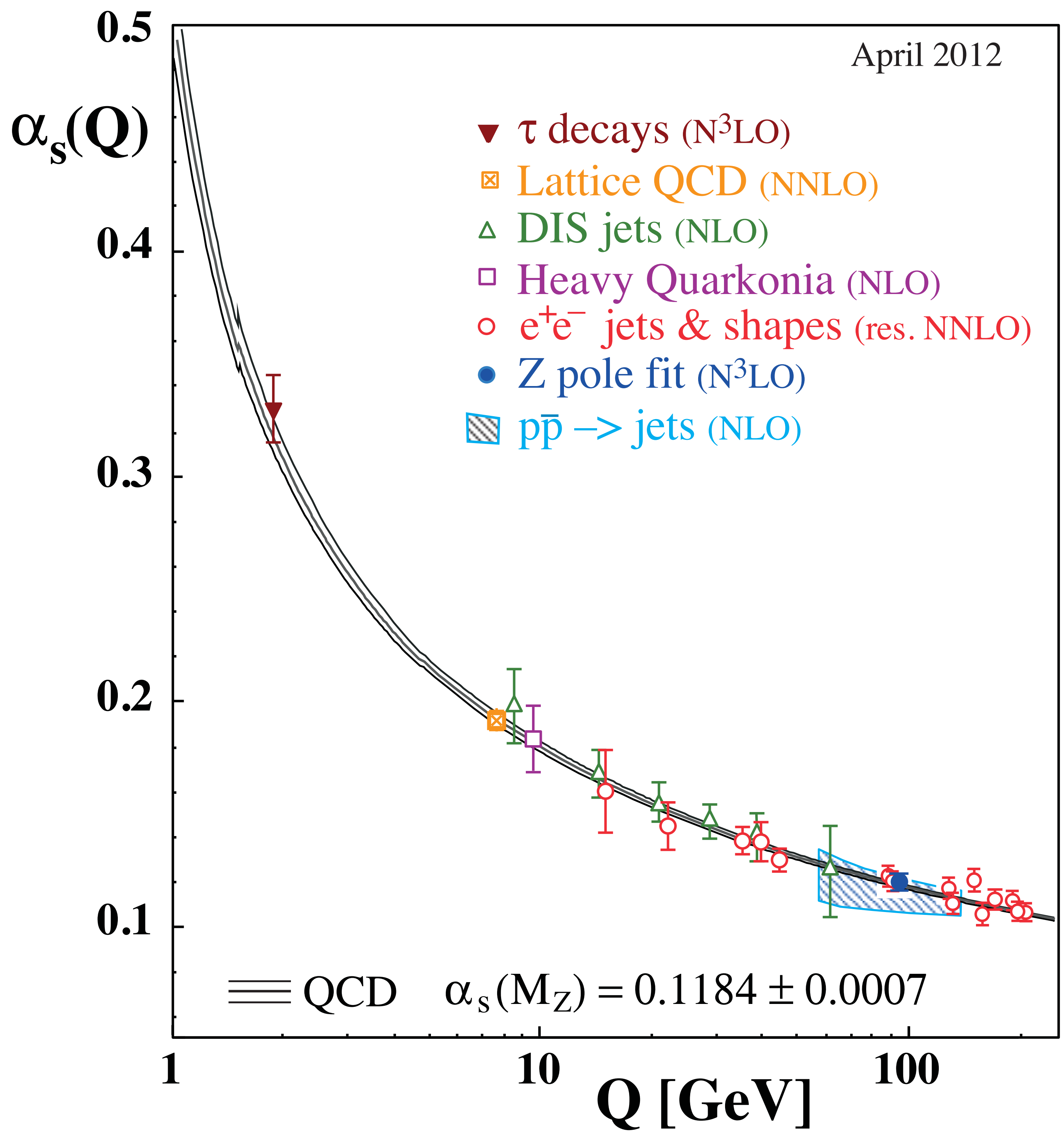
$$\alpha_s(\mu) = \frac{1}{b_0 \log(\mu/\Lambda)}$$

Λ is the QCD scale; it represents the position of the Landau pole in QCD

Consequences and tests

$$\alpha_s(\mu) = \frac{1}{b_0 \log(\mu/\Lambda)}$$

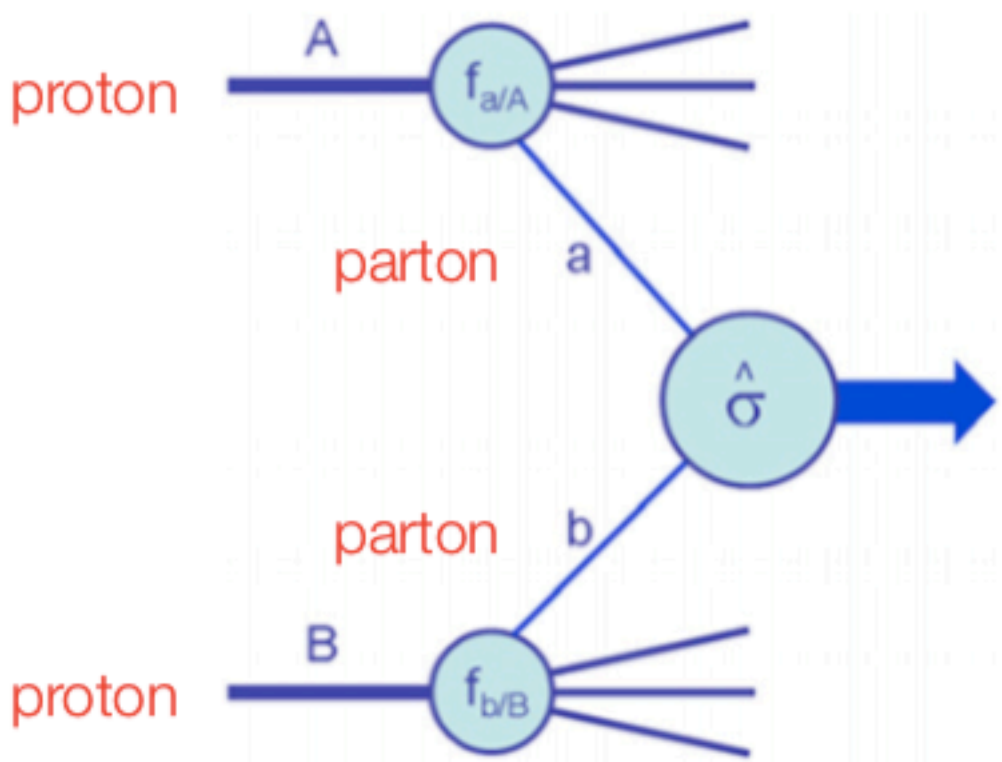
- Strong coupling decreases at high energy: asymptotic freedom.
- Perturbation theory requires sufficiently high energy, unreliable close to Λ.
- Measured value of the strong coupling $\Longleftrightarrow$ values of Λ around 250 MeV.



Protons and partons

- We now have to understand how to apply QCD in the era of hadron colliders.
- To do so, we have to understand how to apply a theory of quarks and gluons to the protons found in the beams.

$$\sigma_{2\to n} = \sum_{a,b} \int_0^1 dx_a dx_b\, f_{a/h_1}(x_a, \mu_F)\, f_{b/h_2}(x_b, \mu_F)\, \hat{\sigma}_{ab\to n}(\mu_F, \mu_R)$$



- The appropriate formalism is called collinear factorization.
- It divides the problem into:
  - soft physics, corresponding to the probability of finding, within a proton, a parton with a given momentum fraction *x*.
  - hard physics, the subsequent scattering between the incident quarks and gluons.
- Strictly only proven in special cases: Drell-Yan and deep inelastic scattering (DIS).

Parton distribution functions (pdfs)

- Depend on the momentum fraction (x_a) and the factorization scale (μ_F), that is implicit in the separation into soft and hard scales: $f_{a/h_1}(x_a, \mu_F)$
- Interpret as a probability ⇒ must integrate over fraction x_a (and x_b)
- In the simplest, non-interacting, picture one might assume the proton consists of just the three valence quarks. With no quark preferred above others one would get:

$$f_{u/p}(x,\,\mu^2) = 2\delta\left(x - \frac{1}{3}\right)$$
$$f_{d/p}(x,\,\mu^2) = \delta\left(x - \frac{1}{3}\right)$$

- By construction, these satisfy the momentum sum rule:

$$\int_0^1 \mathrm{d}x\, x \sum_i f_{i/h}(x,\,\mu^2) = 1 \;\; \forall \mu^2 \text{ and for all hadrons } h$$

- A more sophisticated guess would be to imagine elastic interactions between the quarks, “rubber bands” holding them together
  - only effect would be to smear out the δ-function, smoothing the sharp peak at $x=1/3$.

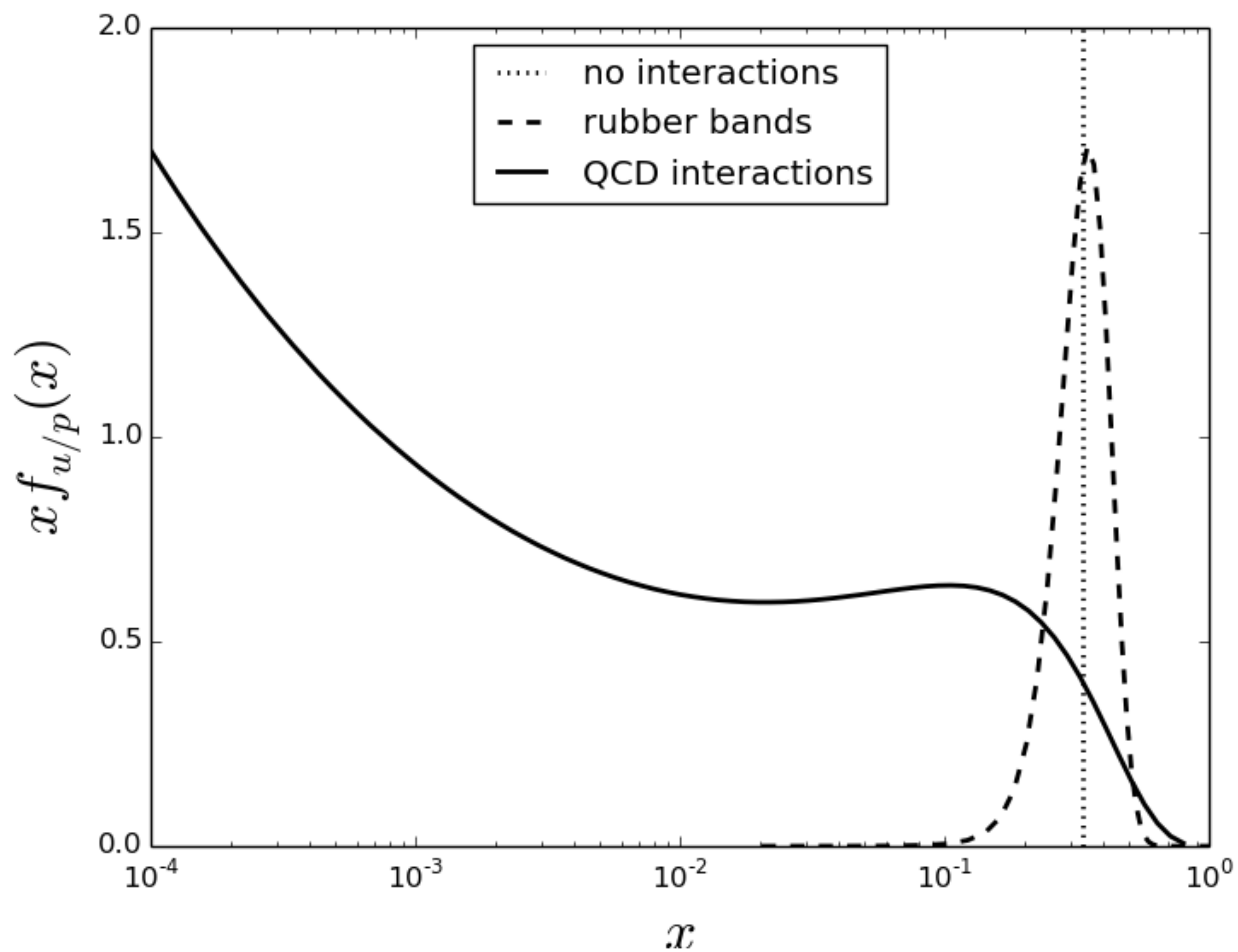
QCD effects in pdfs

- In fact, the valence quarks inside the proton will emit gluons (that can further split into quark-antiquark pairs).
- These emissions will tend to be soft with respect to the original quark, meaning that the additional sea partons will be more likely to be found at small values of *x*.
- In fact, to a fair approximation:

$$f_{\text{sea}/p}(x,\, \mu^2) \propto x^{-\lambda}$$

λ=1 (gluons, sea quarks)

λ=-1/2 (valence quarks)

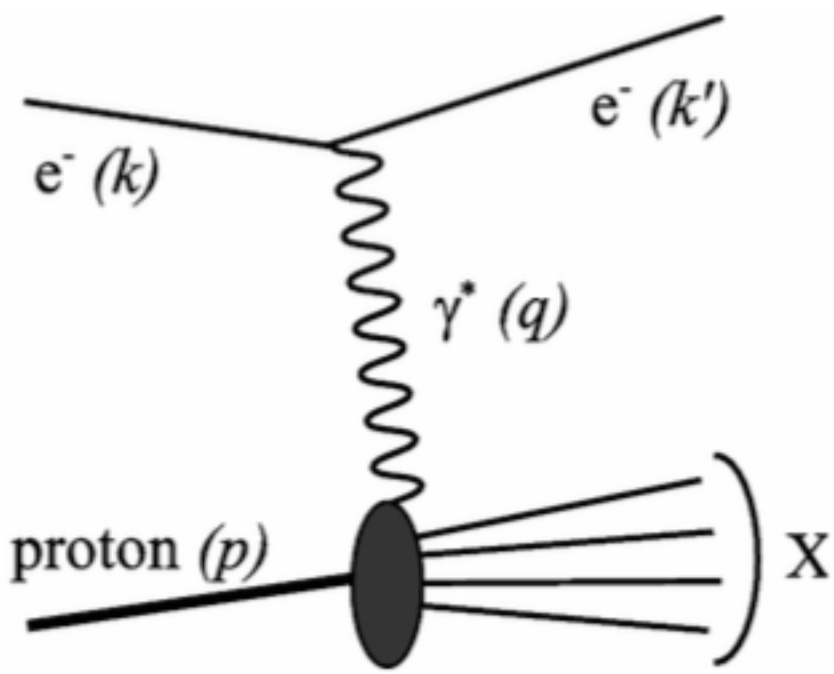


- Effect of QCD interactions:
  - pdfs increase at small *x*
  - valence peak shifts to lower x ≈ 0.1 and broadens (due to emission)

Probing pdfs

- Since they represent truly soft, non-perturbative, physics the pdfs cannot be calculated from first principles.
- However, the factorization procedure is based on the fact that they are universal: independent of the hard scattering and the rest of the collision.
  - therefore they can be extracted from experimental data.
- Deep inelastic scattering in electron-proton collisions, historically at HERA, is an ideal environment for this.
  - pdf enters only in part of the initial state.
  - the rest is well-known QED.
- This process is called "deep" due to the fact that the probing photon is of very high virtuality:

$$Q^2 = -q^2 \gg 1 \text{ GeV}$$



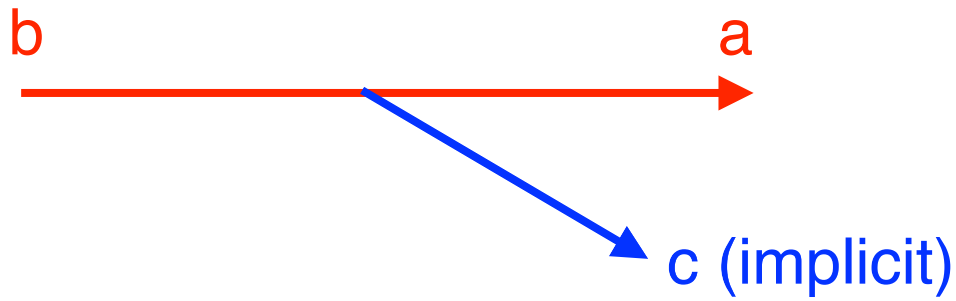
- This is the scale of the pdf that is probed.

Pdf evolution

- Although they are essentially non-perturbative objects, their evolution — the dependence on the probing scale — depends on the emission of quarks and gluons and is calculable in perturbative QCD.
- Just like the strong coupling, the pdfs obey (coupled) evolution equations. At first order these take the form:

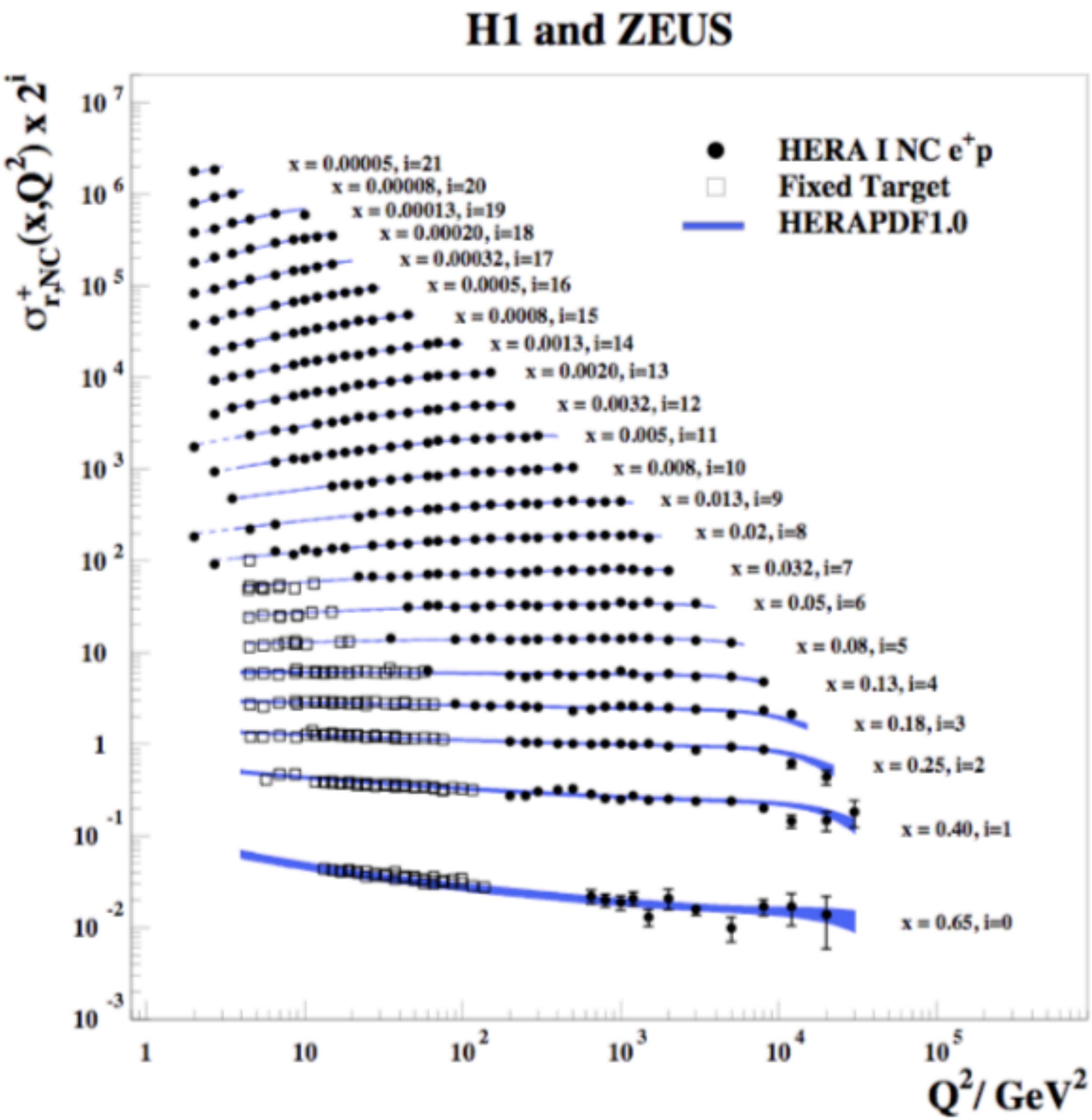
$$\frac{\partial}{\partial \log Q^2} \begin{pmatrix} f_{q/h}(x, Q^2) \\ f_{g/h}(x, Q^2) \end{pmatrix} = \frac{\alpha_s(Q^2)}{2\pi} \int_x^1 \frac{\mathrm{d}z}{z} \begin{pmatrix} \mathcal{P}_{qq}\left(\frac{x}{z}\right) & \mathcal{P}_{qg}\left(\frac{x}{z}\right) \\ \mathcal{P}_{gq}\left(\frac{x}{z}\right) & \mathcal{P}_{gg}\left(\frac{x}{z}\right) \end{pmatrix} \begin{pmatrix} f_{q/h}(z, Q^2) \\ f_{g/h}(z, Q^2) \end{pmatrix}$$

- Called the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equation.
- The kernels of this evolution equation, the quantities P_{ab}, are called splitting functions (more on these later).
- They represent the parton splitting:



QCD-improved parton model

- Taking account of this evolution results in the QCD-improved parton model.
- It gives rise to so-called scaling violation, which is clearly visible in experimental data.
- See for example the combination of HERA data (from experiments H1 and ZEUS) taken over the period 1994-2000.



Pdf fitting: general strategy

- Since the Q^2 evolution of the pdfs is known, the traditional approach is to parametrize them at some reference scale, typically Q_0 = 1-2 GeV.
- Typically starting ansatz is:

$$F(x, Q_0) = x^{A_1}(1-x)^{A_2} P(x; A_3, A_4 \ldots).$$

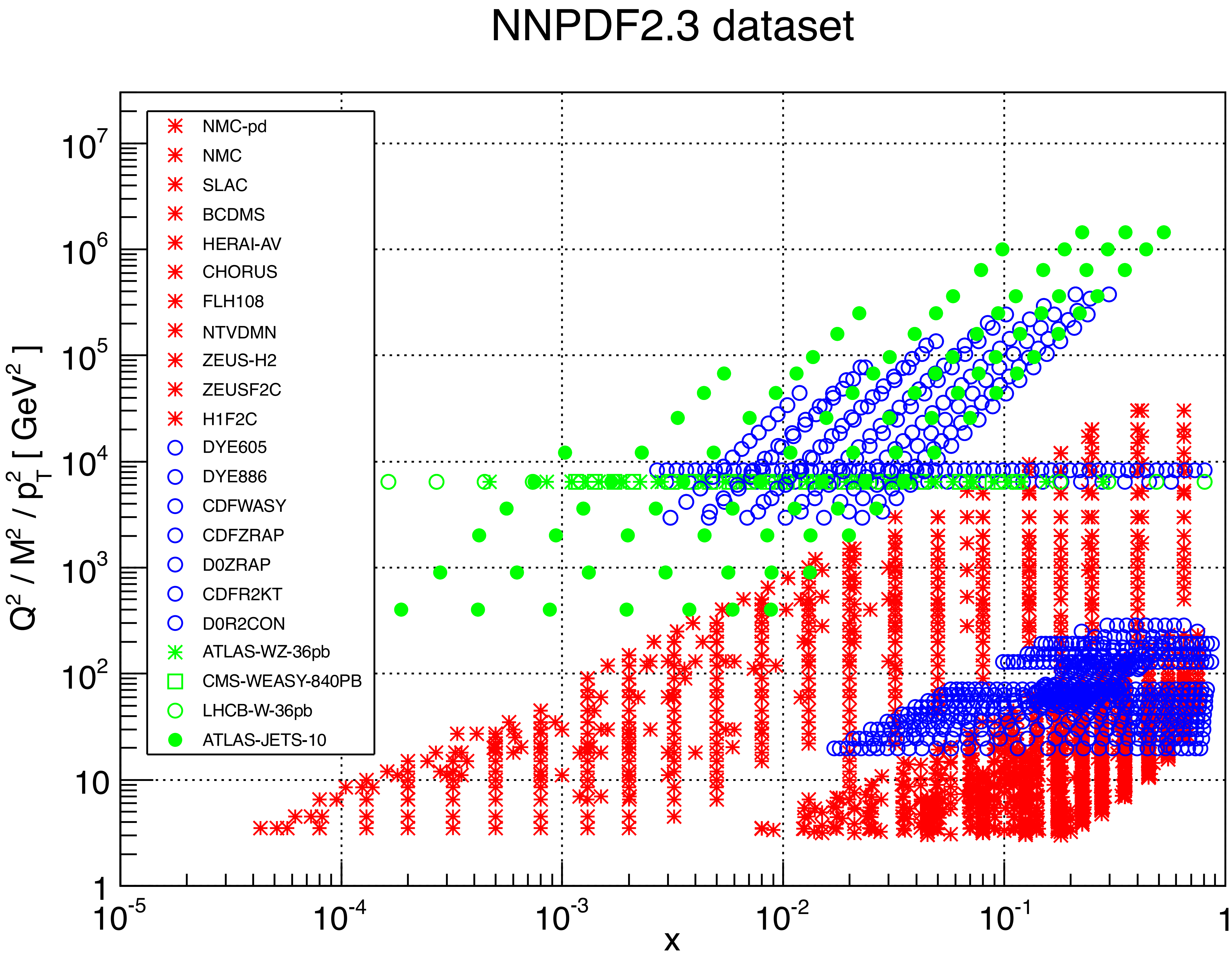
  with a smooth function P and free parameters A_1, A_2, …
- Perform a global fit to available data, using DGLAP equation to evolve the pdfs to the appropriate scale first.
- Lots of room for interpretation:
  - choice of input data sets (especially in cases of conflict)
  - order of perturbation theory (in theory predictions and DGLAP evolution)
  - input parametrization and other theoretical prejudice (e.g. always positive or not).
- Global fitting industry: continuous improvements to the fitting procedure and theoretical input. Main groups are CTEQ, MSTW/MMHT and NNPDF.
- NNPDF has a different approach to starting ansatz, instead using a sample of pdf replicas generated by neural network to try to avoid parametrization bias.

Typical data sets

LHC

fixed-larget, Tevatron

deep inelastic scattering



Pdf requirements

- Simplest case: production of a single particle with mass *M* and rapidity *y*.
- Kinematics:

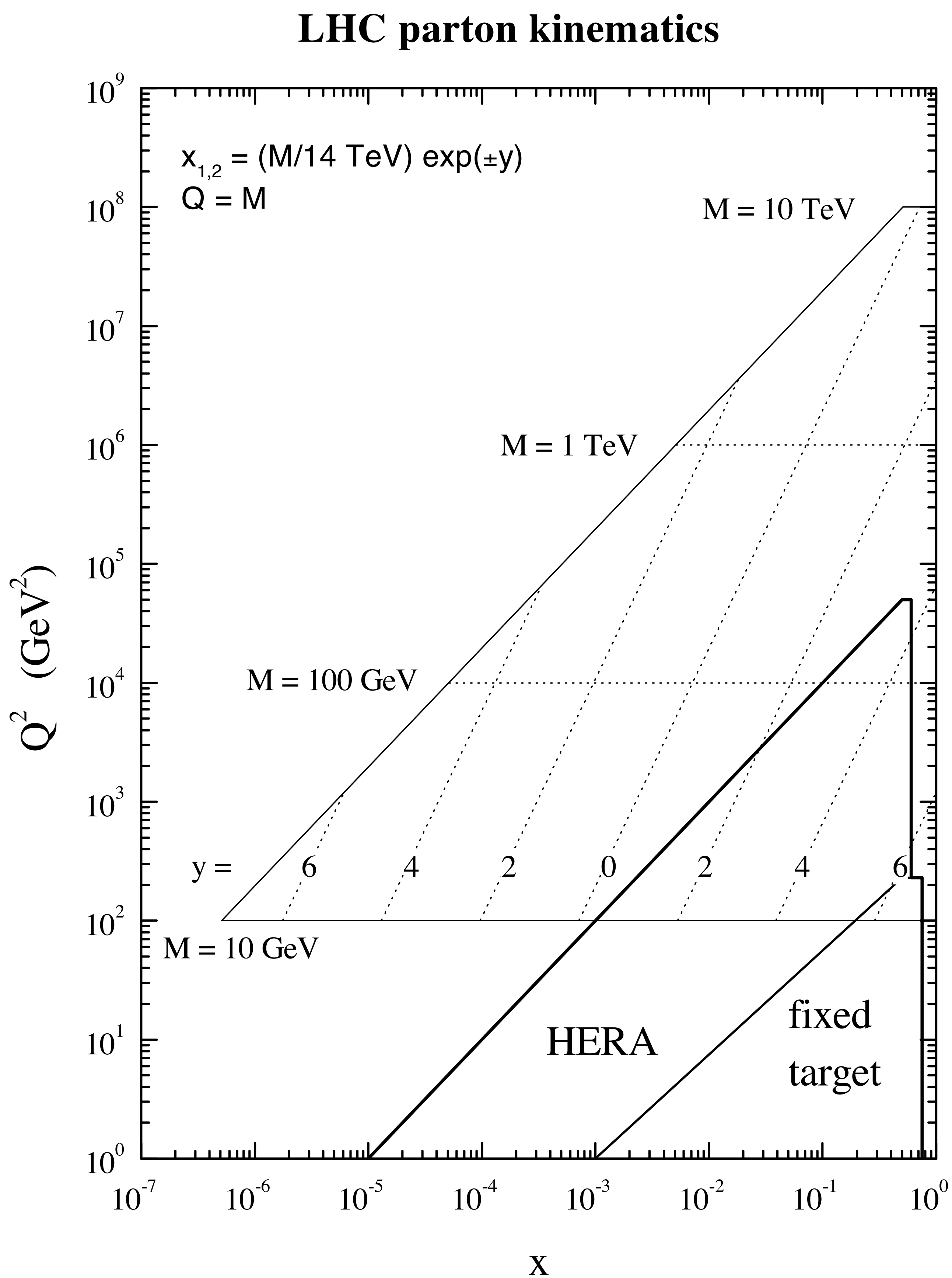
$$p_1 = x_1 \frac{\sqrt{s}}{2} (1,0,0,1)$$

$$p_2 = x_2 \frac{\sqrt{s}}{2} (1,0,0,-1)$$

$$p_f = M (\cosh y, 0, 0, \sinh y)$$

$$\implies x_{1,2} = \frac{M}{\sqrt{s}} e^{\pm y}$$

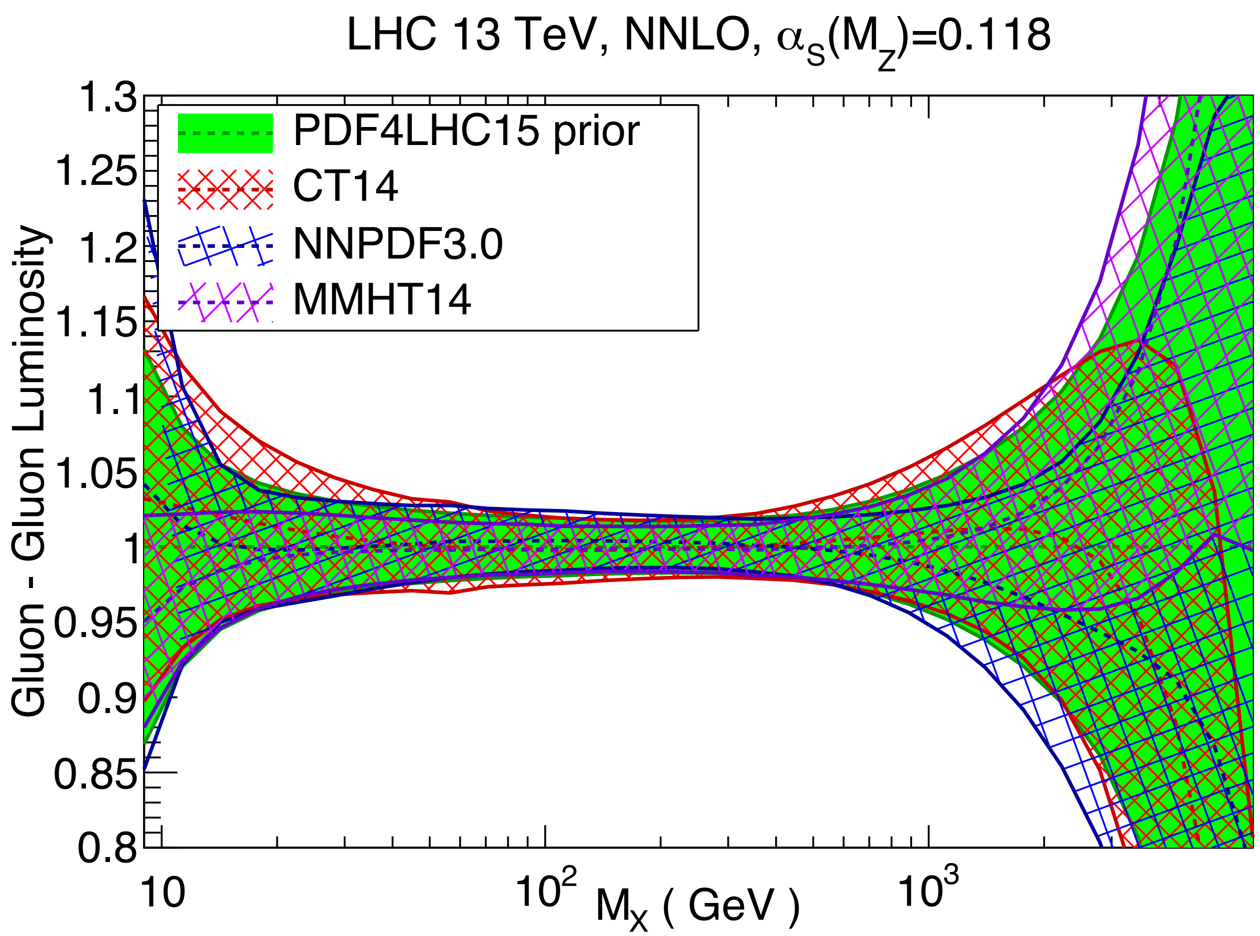
- High-mass or high-rapidity particle production may be outside fit range and suffer from larger pdf uncertainties.



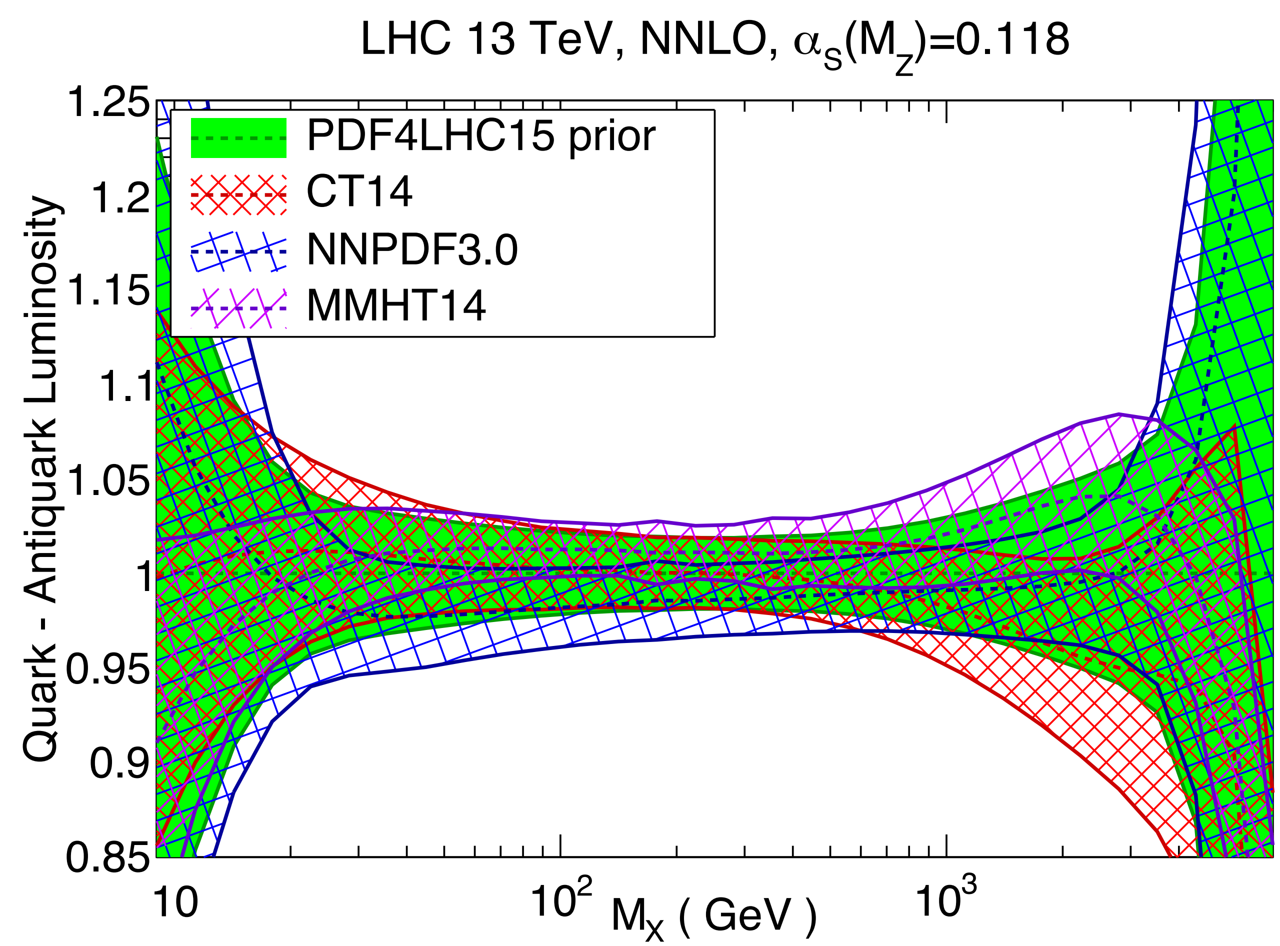
Uncertainties and consistency

- The associated pdf uncertainties typically cover the spread between different fitting groups, at least in the well-constrained region 50 - 500 GeV.
  - uncertainties on cross-sections at the level of 2–4% (important for modern precision!)
- Beyond that, differences begin to emerge and uncertainties are O(10%).
  - prescriptions for combining them to capture the spread exist, e.g. PDF4LHC.

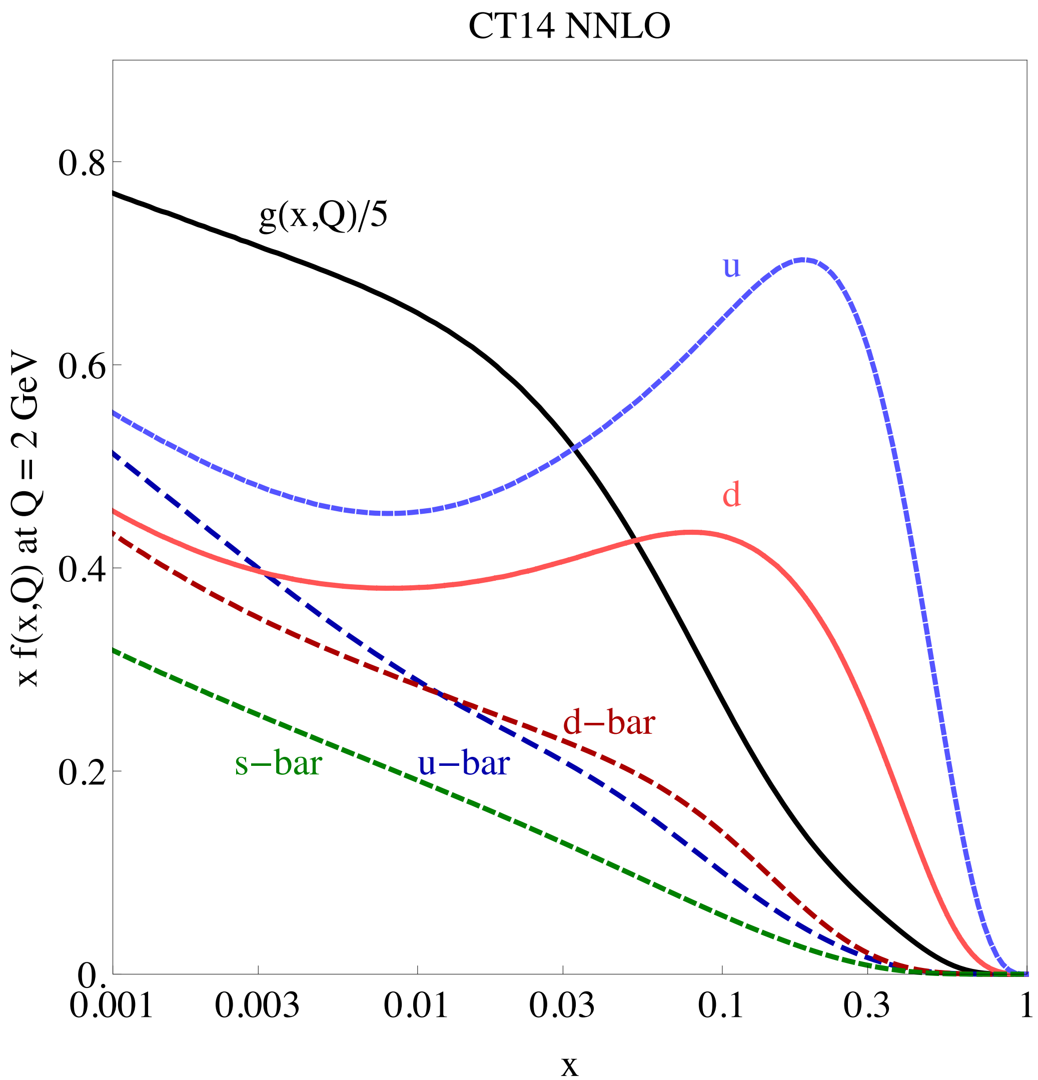
uncertainty for $gg \to X$



uncertainty for $q\bar{q} \to X$

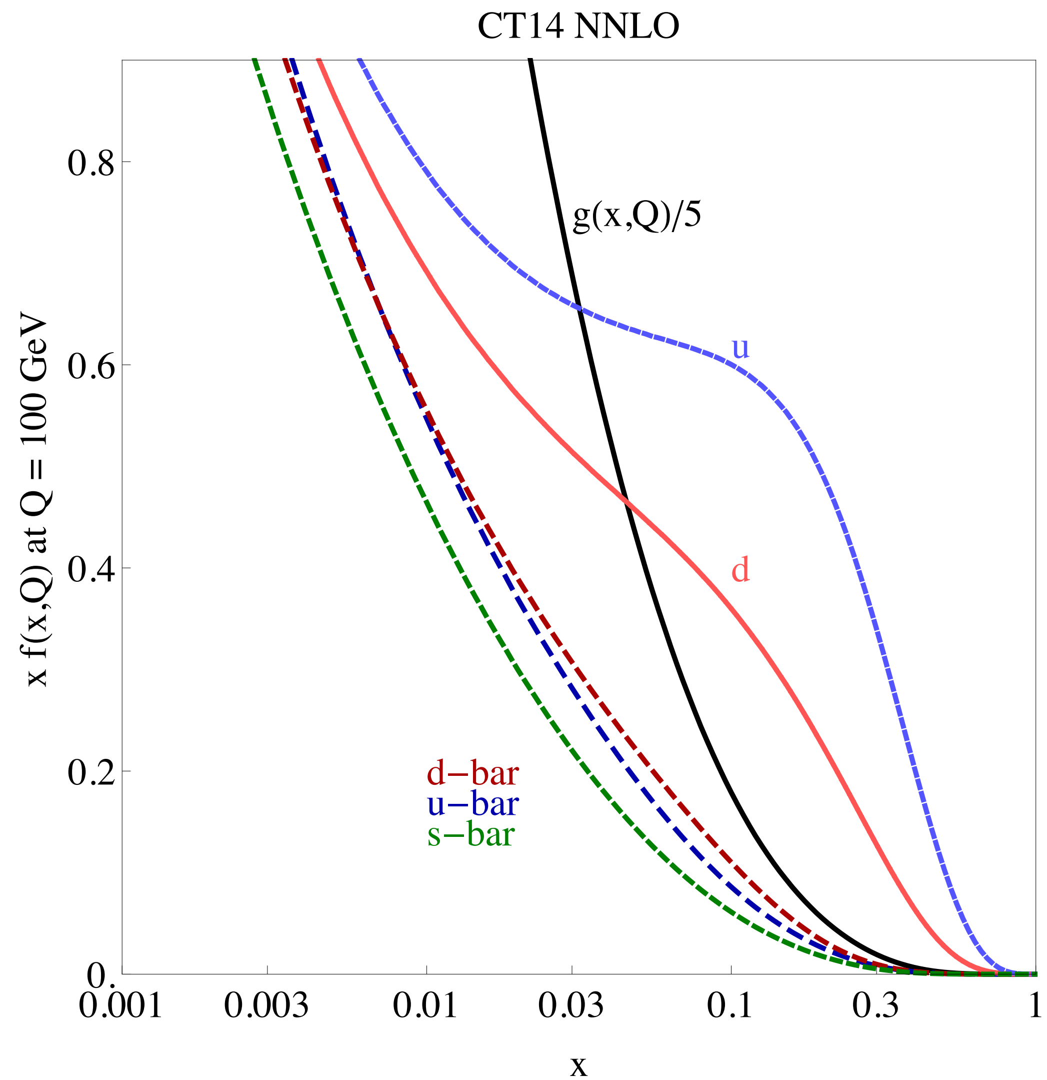


Example pdfs



Q = 2 GeV

- Near starting scale for the evolution.
- u, d still peaked near x=1/3.



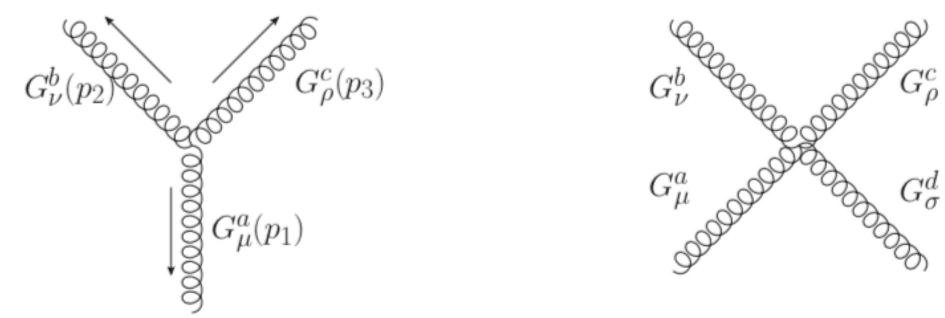
Q = 100 GeV

- Typical LHC kinematics.
- u,d flattened, less important.
- gluon dominant for x < 0.1.

Summary so far

- Have illustrated how the QCD Lagrangian can be translated into Feynman rules, with an emphasis on the special role of color.

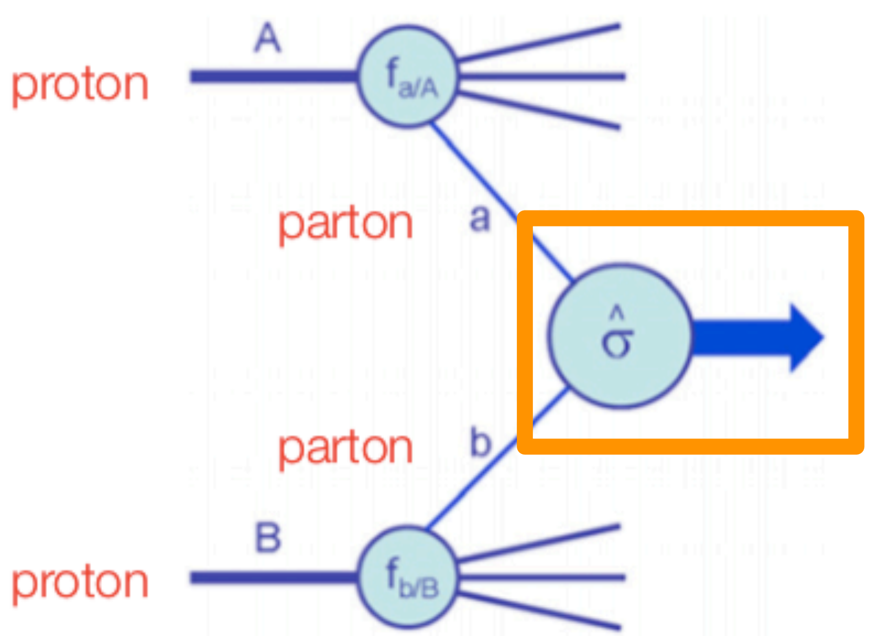
$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F_a^{\mu\nu} + \sum_{\text{flavors}} \bar{q}_i \, (i D_\mu \gamma^\mu - m)_{ij} \, q_j$$



$$g_s f^{abc}[(p_1 - p_2)_\rho \, g_{\mu\nu} + (p_2 - p_3)_\mu \, g_{\nu\rho} + (p_3 - p_1)_\nu \, g_{\rho\mu}]$$

$$i g_s^2 [f^{eac} f^{ebd} (g_{\mu\nu} g_{\rho\sigma} - g_{\mu\sigma} g_{\nu\rho}) + f^{ead} f^{ebc} (g_{\mu\nu} g_{\rho\sigma} - g_{\mu\rho} g_{\nu\sigma}) + f^{eab} f^{ecd} (g_{\mu\rho} g_{\nu\sigma} - g_{\mu\sigma} g_{\nu\rho})]$$

$$\sigma_{2\to n} = \sum_{a,b} \int_0^1 \mathrm{d}x_a \mathrm{d}x_b \, f_{a/h_1}(x_a, \mu_F) \, f_{b/h_2}(x_b, \mu_F) \, \hat{\sigma}_{ab\to n}(\mu_F, \mu_R)$$



- Have discussed the strong coupling and the idea of collinear factorization for hadron collisions and the introduction of pdfs.

- Will now spend some time on the calculation of the **hard scattering process**.

Hard scattering calculations

- First we have to break down the partonic cross-section we identified into a few constituent parts:

$$\hat{\sigma}_{ab\to n}(\mu_F, \mu_R) = \frac{1}{2\hat{s}} \int \mathrm{d}\Phi_n \, |\mathcal{M}_{ab\to n}|^2(\Phi_n; \mu_F, \mu_R)$$

- Incoming partonic flux:

$$\frac{1}{4\sqrt{(p_a \cdot p_b)^2 - p_a^2 p_b^2}} \xrightarrow{m_{a,b}\to 0} \frac{1}{2\hat{s}} = \frac{1}{2x_a x_b s}$$

- Transition amplitude (or matrix element) squared: $|\mathcal{M}_{ab\to n}|^2(\Phi_n; \mu_F, \mu_R)$

- Integrated over the available *n*-parton phase-space element, $\mathrm{d}\Phi_n$.

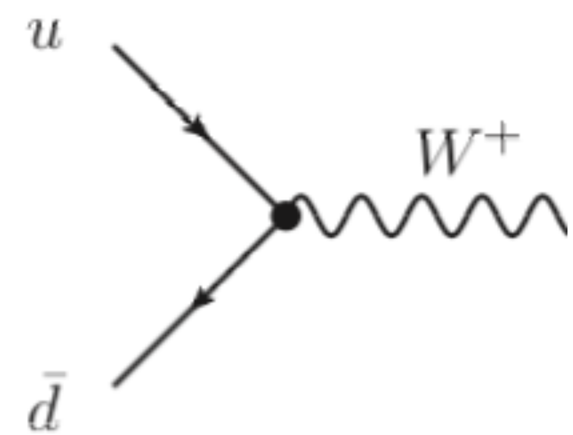
$$\mathrm{d}\Phi_n = \prod_{i=1}^{n} \left[\frac{\mathrm{d}p_i}{(2\pi)^4} (2\pi)\, \delta(p_i^2 - m_i^2) \Theta(p_i^{(0)}) \right] \, (2\pi)^4 \delta^4(p_a + p_b - \sum_{i=1}^{n} p_i)$$

Lorentz-invariant phase-space element for each final state particle

ensure overall four-momentum conservation

W-production

- Consider one of the simplest-possible hadron-collider processes, which is primarily mediated by up-anti-down annihilation.



- Application of the (mostly EW) Feynman rules gives the matrix element:

$$\mathcal{M}_{u\bar{d}\to W^+} = -\frac{iV_{ud}\,g_W\,\delta_{ij}}{\sqrt{2}}\bar{d}_i(p_2)\gamma^\mu\frac{1-\gamma_5}{2}u_j(p_1)\epsilon_\mu^{(W)}$$

CKM element; weak coupling; trivial color factor; quark spinors; Dirac matrices (LH current); polarization vector

- Squaring and summing over spins and colors is an exercise in Dirac algebra:

$$\overline{\sum}|\mathcal{M}_{u\bar{d}\to W^+}|^2 = \frac{3}{9\cdot 4}\,\frac{|V_{ud}|^2 g_W^2}{2}\,\mathrm{Tr}\left[\not{p}_2\gamma^\mu\not{p}_1\gamma^\nu\frac{1-\gamma_5}{2}\right]\left[-g_{\mu\nu}+\frac{Q_\mu Q_\nu}{m_W^2}\right]$$
$$= \frac{|V_{ud}|^2 g_W^2}{12}Q^2 = \frac{|V_{ud}|^2 g_W^2}{12}m_W^2\,,$$

color sum; averaged over initial colors and spins; $Q = p_1+p_2$

Partonic cross-section

- Putting the ingredients together we have:

$$\sigma^{(\mathrm{LO})}_{h_1 h_2 \to W^+} = \int_0^1 \mathrm{d}x_u \mathrm{d}x_{\bar{d}} \sum_{u,\bar{d}} f_{u/h_1}(x_u,\, \mu_F)\, f_{\bar{d}/h_2}(x_{\bar{d}},\, \mu_F)\, \hat{\sigma}^{(\mathrm{LO})}_{u\bar{d} \to W^+}$$

where

$$\hat{\sigma}^{(\mathrm{LO})}_{u\bar{d}\to W^+} = \frac{1}{2\hat{s}} \int \frac{\mathrm{d}^4 p_W}{(2\pi)^4} (2\pi)^4 \delta^4(p_u + p_{\bar{d}} - p_W)(2\pi)\delta(p_W^2 - m_W^2) |\mathcal{M}|^2_{u\bar{d}\to W^+}$$

$$= \frac{\pi \delta(\hat{s} - m_W^2)}{\hat{s}} |\mathcal{M}|^2_{u\bar{d}\to W^+} = \frac{\pi \delta(\hat{s} - m_W^2)}{\hat{s}} \frac{g_W^2 |V_{ud}|^2 m_W^2}{12}$$

- Recalling our earlier kinematics we also have

$$\hat{s} = x_u x_{\bar{d}}\, s \qquad\qquad y_W = \frac{1}{2} \log \frac{x_u}{x_{\bar{d}}}$$

so that we can perform the convenient change of variable: $\mathrm{d}x_u \mathrm{d}x_{\bar{d}} = \frac{\mathrm{d}\hat{s}}{s}\, \mathrm{d}y_W$

Final result

$$\sigma^{(\mathrm{LO})}_{h_1 h_2 \to W^+} = \int_0^1 \mathrm{d}x_u \mathrm{d}x_{\bar d} \sum_{u,\bar d} f_{u/h_1}(x_u, \mu_F)\, f_{\bar d/h_2}(x_{\bar d}, \mu_F)\, \hat\sigma^{(\mathrm{LO})}_{u\bar d \to W^+}$$

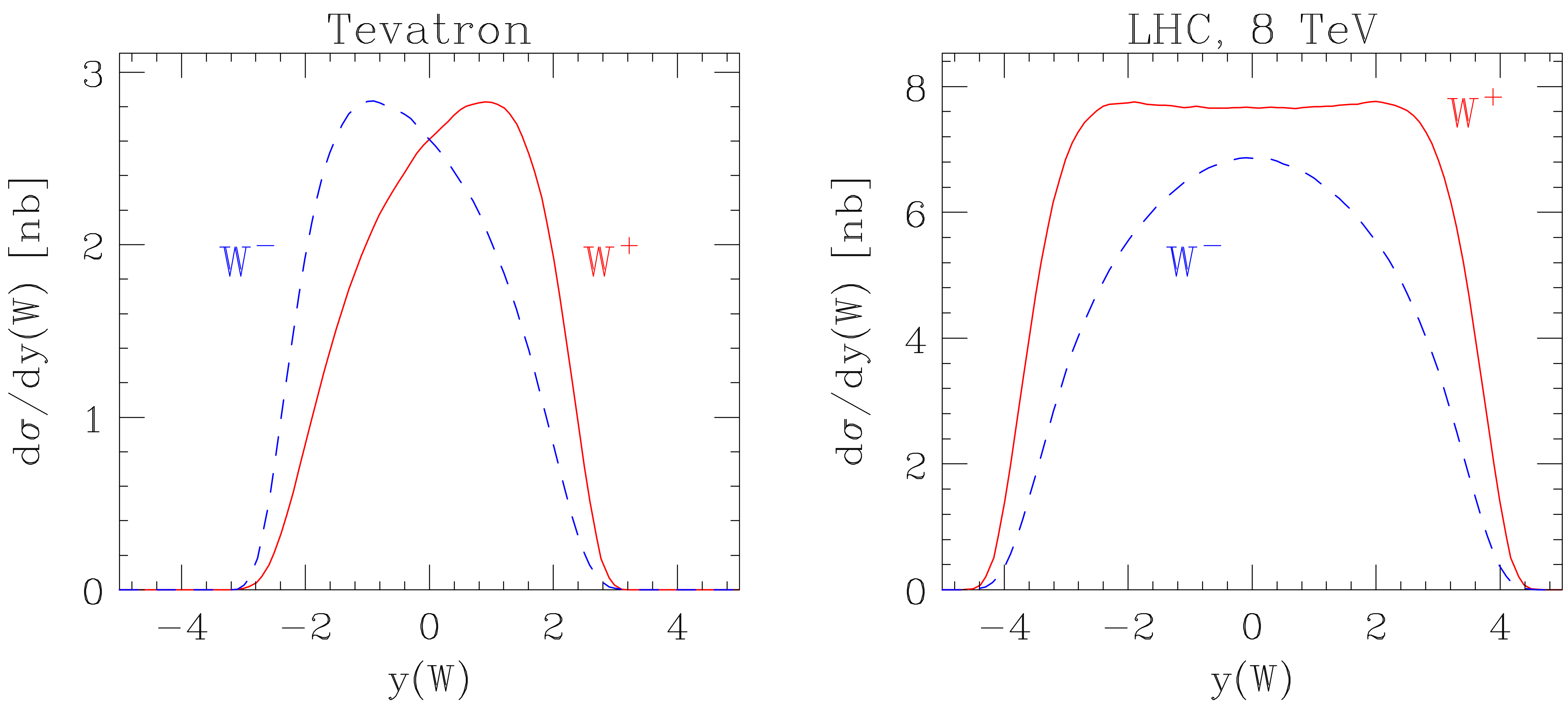
$$= \frac{\pi g_W^2\, |V_{ud}|^2}{12} \int \frac{m_W^2 \mathrm{d}\hat s}{\hat s^2}\, \delta(\hat s - m_W^2)$$

$$\times \int_{-y_{\max}}^{y_{\max}} \mathrm{d}y_W \sum_{u,\bar d} x_u f_{u/h_1}(x_u, \mu_F)\, x_{\bar d} f_{\bar d/h_2}(x_{\bar d}, \mu_F)\Big|_{x_u x_{\bar d} s = m_W^2}$$

$$= \frac{\pi g_W^2\, |V_{ud}|^2}{12 s} \int_{-y_{\max}}^{y_{\max}} \mathrm{d}y_W \sum_{u,\bar d} f_{u/h_1}(x_u, \mu_F)\, f_{\bar d/h_2}(x_{\bar d}, \mu_F)\,,$$

- The maximum rapidity is constrained by x<1 to be: $y_{\max} = \frac{1}{2} \log \frac{s}{m_W^2}$
- This is the lowest order (tree-level) result for the inclusive cross-section.
  - the result for W^- is obtained by interchanging u and anti-d quarks.
- In this form we immediately see that the rapidity distribution of the W-boson is entirely defined by the (quark) pdfs.

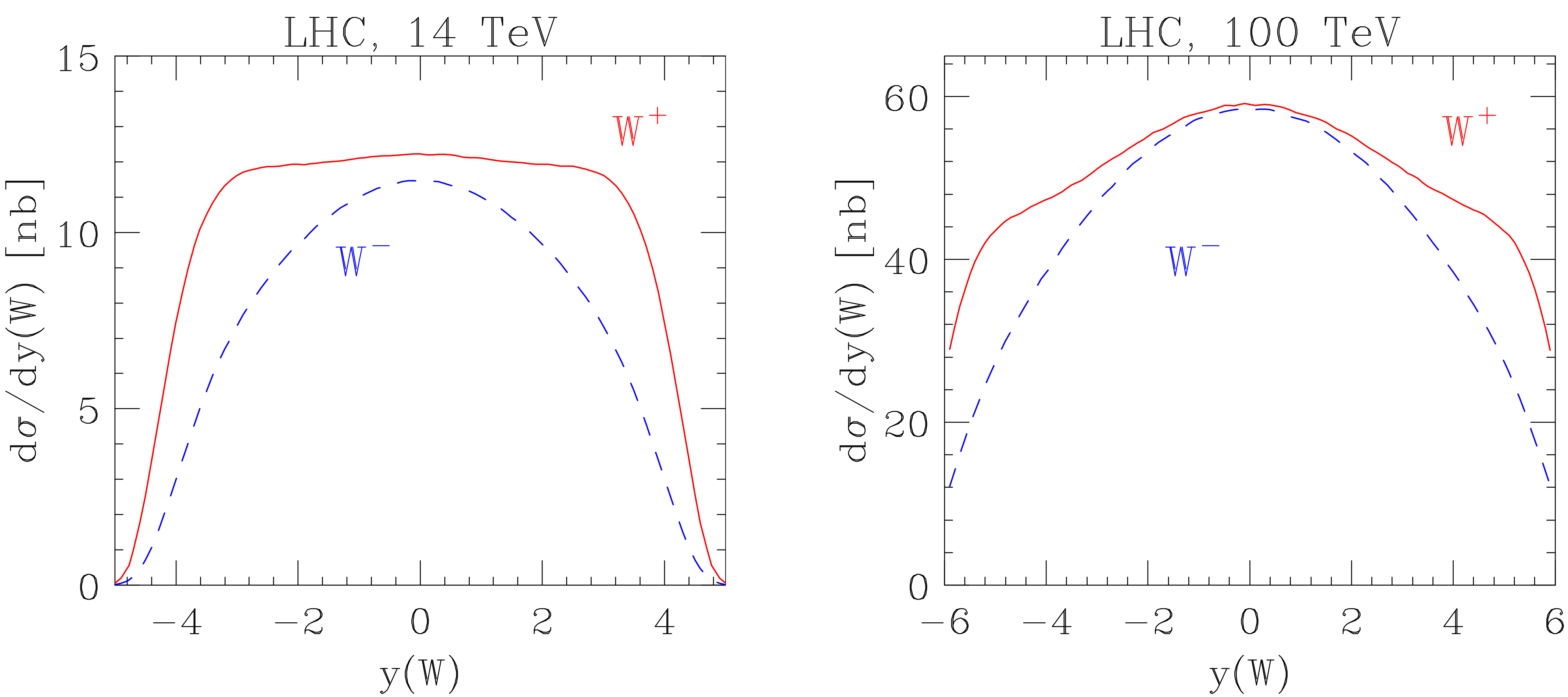
W rapidity distribution: Tevatron vs. LHC



- Tevatron: valence quarks in protons drive production of W^+ to positive rapidity and anti-protons favor W^- at negative rapidity.
  - asymmetry is used to constrain high-*x* valence quark pdfs (although indirectly, through diluted lepton asymmetry)
- LHC: no preferred direction and sea quarks play an important role; impact of valence quarks still evident in wider plateau for W^+.

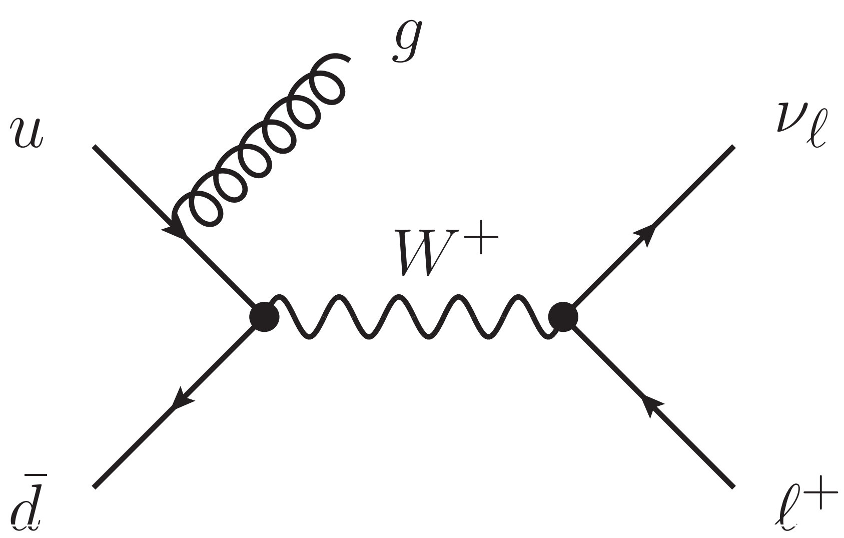
W rapidity at the LHC and beyond

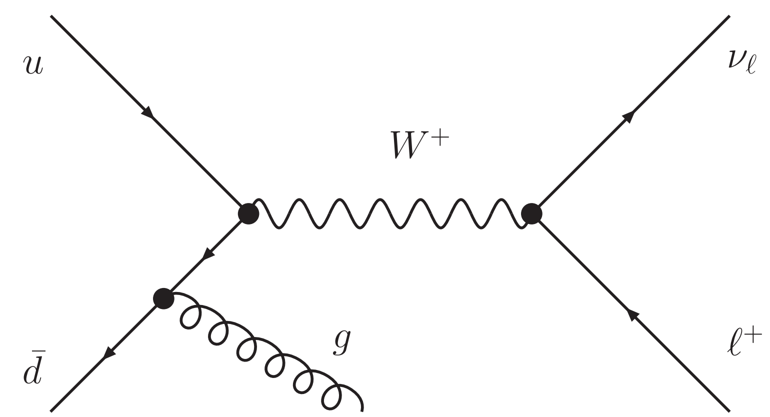
- As energy of collisions increases, so does accessible range of W rapidities.
- The value of *x* required to produce a W boson decreases, leading to more important role for sea quarks.
- Eventually sea quarks dominate and, at central rapidities, W^+ and W^- cross sections become similar.



Additional radiation

- Consider the radiation of an additional parton in the hard scattering process.
  - proportional to an additional power of the strong coupling
- Two diagrams contributing to the amplitude that interfere:



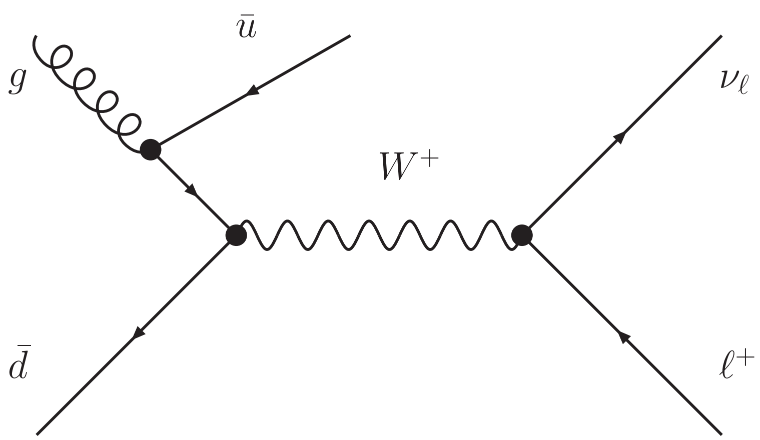


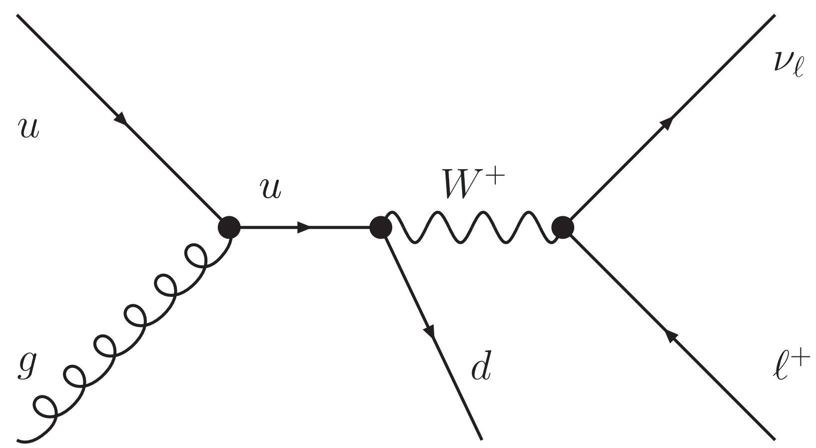
- Matrix element is then the sum of two terms:

$$\mathcal{M}_{ug\to dW^+} = \frac{i g_s g_W V_{ud}}{\sqrt{2}} \bar{u}_{d,i} \left[\gamma_\nu T^a_{ij} \frac{\not{p}_g - \not{p}_d}{(p_g - p_d)^2} \gamma_\mu L + \gamma_\mu L \frac{\not{p}_u + \not{p}_g}{(p_u + p_g)^2} \gamma_\nu T^a_{ij} \right] u_{u,j} \epsilon^\mu_W \epsilon^{*\nu,a}_g$$

Other contributions

- In fact there are three different (non-interfering) contributions depending on which of the two partons is in the initial state (u-anti-d, g-anti-d, u-g).





- Importantly, especially for the LHC, this process is sensitive to gluon pdf
  - can cause a big change in expected cross-section wrt. inclusive W production
- All processes depend on propagators for the intermediate lines:

$$\frac{1}{(p_q - p_g)^2} = -\frac{1}{2E_q E_g (1 - \cos\theta)}$$

- Potential problems for energies or angles approaching zero: possibility of an infrared divergence, often called soft and collinear singularities.

Infrared singularities

- Skipping over all the algebra, the squared MEs are:

$$|\mathcal{M}|^2_{u\bar{d}\to gW^+} = \frac{4\pi\alpha_s C_F\, g_W^2 |V_{ud}|^2}{12} \frac{\hat{t}^2 + \hat{u}^2 + 2m_W^2 \hat{s}}{\hat{t}\hat{u}}$$

$$|\mathcal{M}|^2_{ug\to dW^+} = |\mathcal{M}|^2_{\bar{d}g\to \bar{u}W^+} = \frac{4\pi\alpha_s T_R\, g_W^2 |V_{ud}|^2}{12} \frac{\hat{s}^2 + \hat{u}^2 + 2m_W^2 \hat{t}}{-\hat{s}\hat{u}}$$

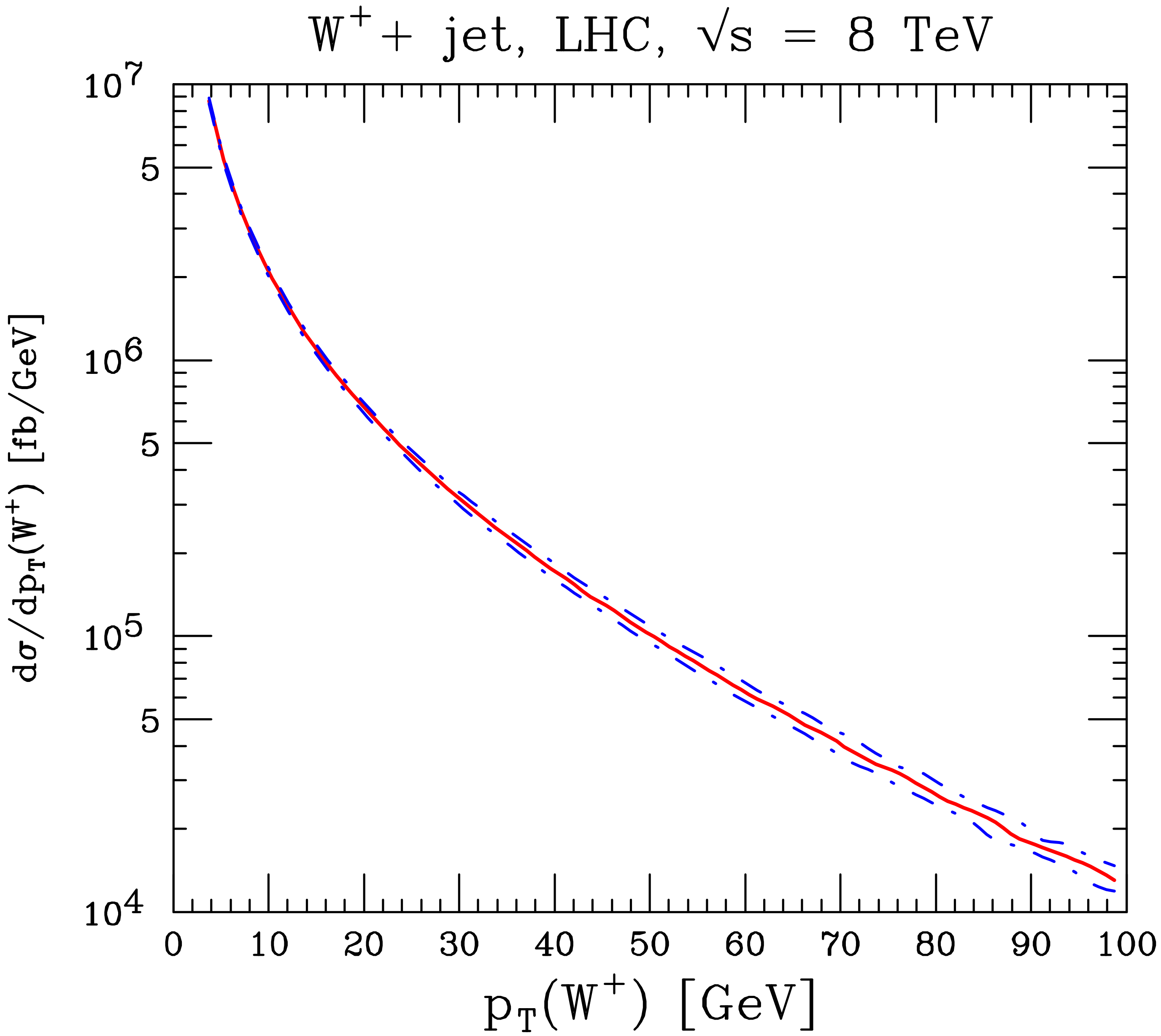
in terms of the Mandelstam invariants:

$$\begin{aligned} \hat{s} &= (p_a + p_b)^2 = (p_1 + p_2)^2 \\ \hat{t} &= (p_a - p_1)^2 = (p_b - p_2)^2 \\ \hat{u} &= (p_a - p_2)^2 = (p_b - p_1)^2 \end{aligned}$$

- Gluon in the final state: singularities for *t* or *u* going to zero, i.e. the gluon collinear to one of the incoming partons, or the gluon being soft.
- Quark in the final state: singularity for $u \to 0$, i.e. quark collinear to initial gluon, but the soft limit and $s \to 0$ prohibited by production of a W boson (i.e. the requirement of a hard process).

Screening the divergence

- The simplest way out is to simply cut out the divergent regions.
- Straightforward way to do this is to require that the final-state particle have a minimum transverse momentum
- This means that it will deposit enough energy in the detector to be observed separately as a jet, i.e. this calculation corresponds to W+jet production.
- Due to the simple kinematics, a cut on the jet is the same as a cut on the W-boson p_T.
- Cross-section exhibits divergent behavior and thus depends strongly on the value of the cut.



Dealing with the divergence

- The alternative is to live with the divergence.
- In either the soft or the collinear limits, the emitted parton should not actually be observed in the detector, i.e. final state looks like simple W production.
- In this case the diagrams represent part of the higher-order corrections to the cross-section: they appear with an additional power of α_s compared to LO and are called next-to-leading order.
  - these contribution are often called real corrections.
- Examining the matrix elements in more detail we see:

$$|\mathcal{M}|^2_{u\bar{d}\to gW^+} = \frac{|\mathcal{M}^{(\mathrm{LO})}|^2_{u\bar{d}\to W^+}}{m_W^2} \cdot (4\pi\alpha_s C_F) \frac{\hat{t}^2 + \hat{u}^2 + 2m_W^2 \hat{s}}{\hat{t}\hat{u}}$$

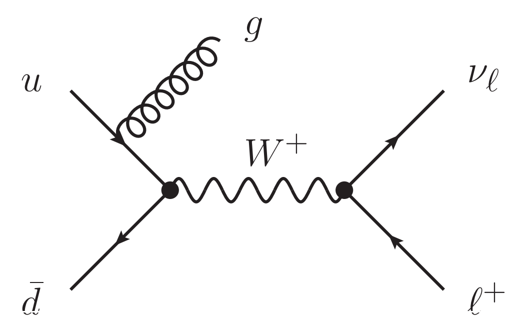
$$|\mathcal{M}|^2_{ug\to dW^+} = |\mathcal{M}|^2_{\bar{d}g\to \bar{u}W^+} = \frac{|\mathcal{M}^{(\mathrm{LO})}|^2_{u\bar{d}\to W^+}}{m_W^2} \cdot (4\pi\alpha_s T_R) \frac{\hat{s}^2 + \hat{u}^2 + 2m_W^2 \hat{t}}{-\hat{s}\hat{u}}$$

i.e. we can recast them in the form of the LO MEs multiplied by factors that contain the singularities.

Parametrizing the limit

- Analyze the (u,g) collinear limit ($t \to 0$) with a simple parametrization:

$$p_u = z p_{\tilde{u}} \,, \qquad p_g = -(1-z) p_{\tilde{u}}$$



so that
$$\hat{s} = (p_u + p_{\bar{d}})^2 \longrightarrow z s_{\tilde{u}\bar{d}}$$
$$\hat{u} = (p_{\bar{d}} - p_g)^2 \longrightarrow (1-z) s_{\tilde{u}\bar{d}} \qquad \text{and } s_{\tilde{u}\bar{d}} \equiv m_W^2$$

- Hence the singular factor can be written as:

$$\frac{\hat{t}^2 + \hat{u}^2 + 2m_W^2 \hat{s}}{\hat{t}\hat{u}} \longrightarrow \frac{m_W^2}{\hat{t}} \frac{(1-z)^2 + 2z}{1-z}$$

- Putting it all together we have:

$$|\mathcal{M}|^2_{u\bar{d} \to gW^+} = |\mathcal{M}^{\mathrm{LO}}|^2_{u\bar{d} \to W^+} \cdot \frac{(4\pi\alpha_s)}{\hat{t}} C_F \frac{1+z^2}{1-z}$$

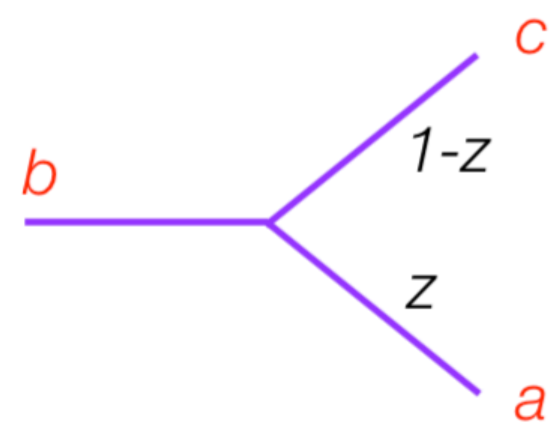
ME for LO+one emitted parton — LO matrix element — collinear singularity — additional (soft gluon) singularity for $z \to 1$

Universal limit

- This result is universal: all matrix elements involving the emission of a gluon from a quark line will factorize similarly, with the same splitting function.
- These are essentially the same quantities that entered the DGLAP evolution of PDFs that we saw earlier (since those also represented parton emission).

$$|\mathcal{M}_{ac\ldots}|^2 \xrightarrow{a,\,c \text{ coll.}} \frac{2g_s^2}{2p_a \cdot p_c} |\mathcal{M}_{b\ldots}|^2 P_{ab}(z)$$

collinear singularity



$$P_{qq}(z) = C_F \left(\frac{1+z^2}{1-z} \right)$$

additional soft singularity as $z \to 1$

$$P_{gg}(z) = 2N_c \left(\frac{z^2 + (1-z)^2 + z^2(1-z)^2}{z(1-z)} \right)$$

soft for $z \to 0$, $z \to 1$

$$P_{qg}(z) = T_R \left(z^2 + (1-z)^2 \right)$$

Divergent integrals

- This parametrization is a convenient one for exposing the singularities.
- With a little work, the phase-space can be parametrized in the same way so that we end up with integrals of the form:

$$\int \frac{dt}{t} \frac{dz}{z}$$

- The usual (modern) way to deal with such singularities is to use a trick called dimensional regularization.
- The singularities are only present in exactly four dimensions; if we had just slightly more then we could just do the integral.
- Setting d=4-2ϵ in the phase space we would end up with integrals like this:

$$\int \frac{dt}{t^{1+\epsilon}} \longrightarrow \frac{1}{\epsilon}$$

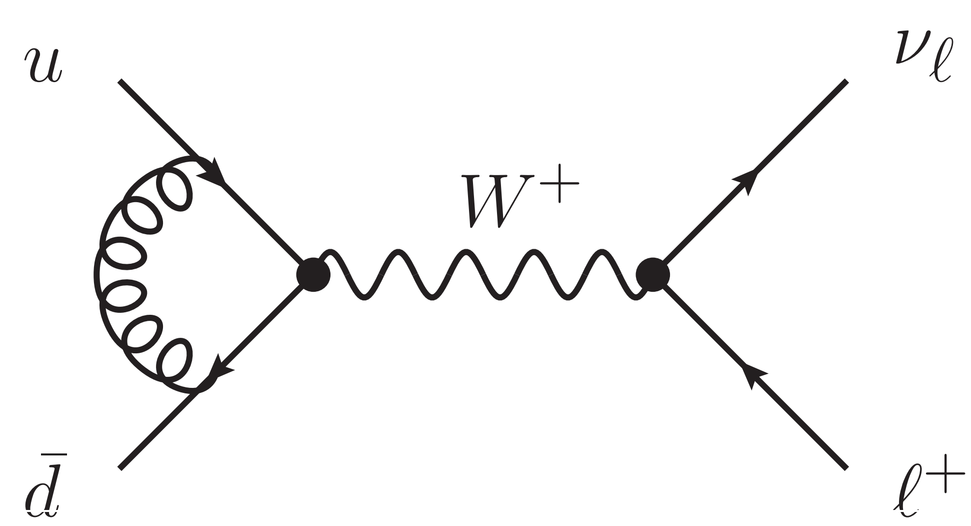
- Each singularity leads to a single power of ϵ so that we can have $1/\epsilon^2$ terms:

$$\mu^{4-D} \int \frac{\mathrm{d}^D k}{(2\pi)^D} \left|\mathcal{M}^{(0)}_{u\bar{d}\to W^+ g}\right|^2 = \left|\mathcal{M}^{(0)}_{u\bar{d}\to W^+}\right|^2 \frac{\alpha_s}{2\pi} C_F \left(\frac{\mu^2}{Q^2}\right)^{\varepsilon} c_\Gamma \times \left[\left(\frac{2}{\varepsilon^2} + \frac{3}{\varepsilon} + \frac{\pi^2}{3}\right)\delta(1-z) + \ldots \right]$$

Virtual contributions

- These singularities cannot of course be present in the final result.
- Indeed, the general results of the Bloch-Nordsieck and Kinoshita-Lee-Nauenberg theorems require that any infrared divergence should disappear in the calculation of a physically meaningful observable.
- The contribution that we are missing is a virtual one, from one-loop diagrams that enter the calculation at the same order:

additional radiation emitted and reabsorbed internally

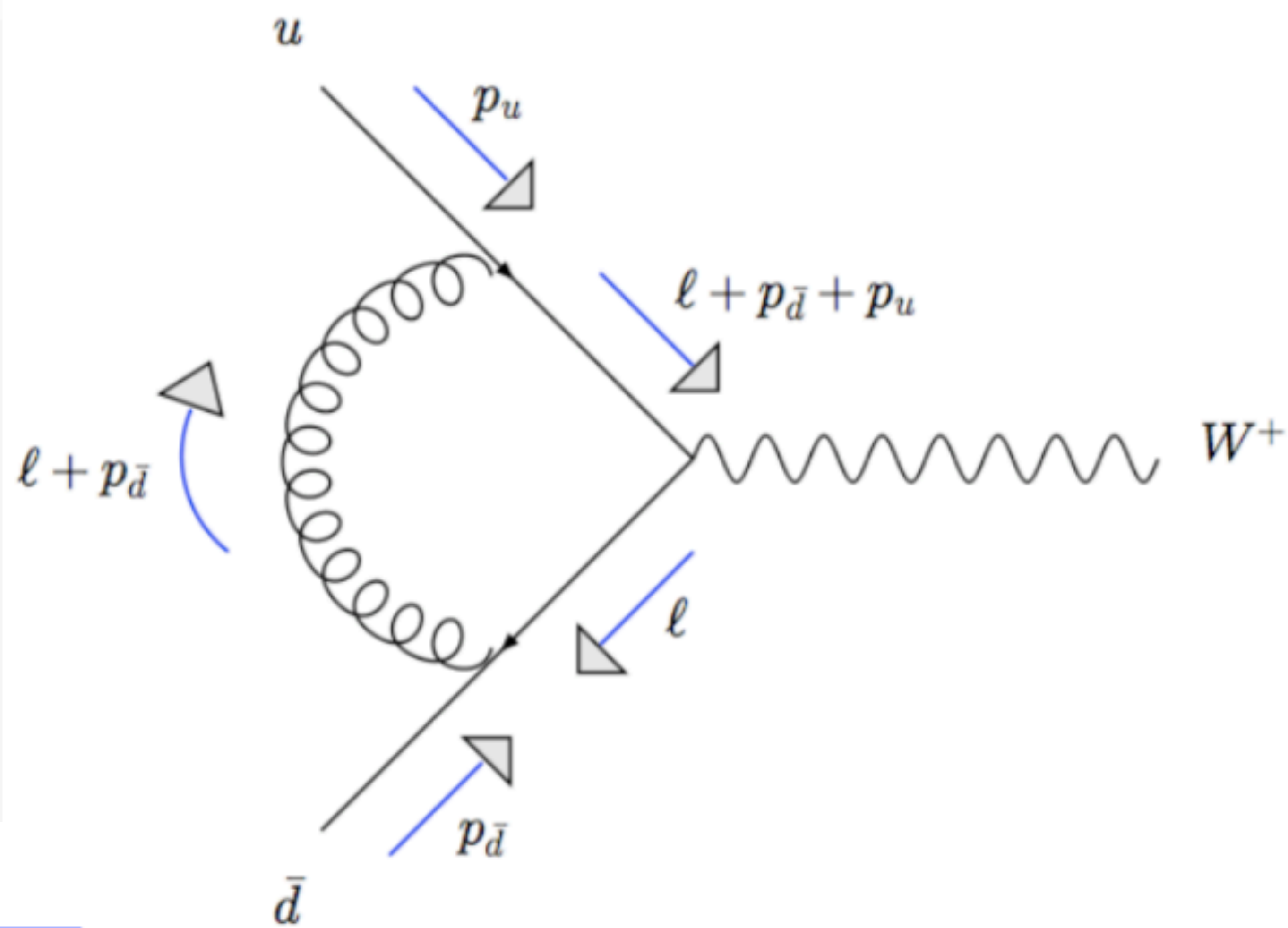


$$|\mathcal{M}_{W+g}|^2 \sim (g_s)^2 \,, \quad (\mathcal{M}_{W,1-\text{loop}} \times \mathcal{M}_{W,\text{tree}}) \sim g_s^2 \times 1$$

Fermilab

Loop diagrams

- In our simple process there is only a single loop diagram
  - in general there will be many, with loops connecting all colored lines in all possible ways
- Per the usual Feynman rules, we must integrate over the unconstrained loop momentum ℓ.
- General structure of amplitude is:



$$\int \frac{d^{4-2\epsilon}\ell \quad \mathcal{N}}{\ell^2(\ell+p_{\bar{d}})^2(\ell+p_{\bar{d}}+p_u)^2}$$

where the numerator factor is:

$$\mathcal{N} = [\bar{u}(p_{\bar{d}})\gamma^\alpha \not{\ell}\gamma^\mu(\not{\ell} + \not{p}_{\bar{d}} + \not{p}_u)\gamma_\alpha u(p_u)]\, V_\mu(p_W)$$

and we have used dimensional regularization again.

Fermilab

Structure of the integral

- Before doing anything foolhardy, first inspect the integrand.
- This reveals very familiar problems. Shifting the loop momentum: $[\ell \to \ell - p_{\bar{d}}]$

$$\ell^2(\ell + p_{\bar{d}})^2(\ell + p_{\bar{d}} + p_u)^2 \longrightarrow \ell^2(\ell - p_{\bar{d}})^2(\ell + p_u)^2$$

soft singularity: loop momentum $\ell \to 0$

collinear singularities: ℓ proportional to either of the quark momenta

- Just as in the real-radiation case, these singularities will be proportional to the LO matrix elements
  - more tricky to see because of the Dirac structure in the numerator
- There can be additional divergences also in the ultraviolet region $\ell \to \infty$ that are also captured by dim. reg. — e.g. naively $\int \frac{d^4\ell}{\ell^4} \to \infty$
- As an example, we'll look at the simplest (scalar) integral with no numerator.

Sketch of the calculation

- The normal method is to combine the denominators with Feynman parameters (x_1, x_2, x_3 here) and shift the loop momentum:

$$\frac{1}{\ell^2(\ell+p_{\bar{d}})^2(\ell+p_{\bar{d}}+p_u)^2} = 2\int_0^1 dx_1 \int_0^1 dx_2 \int_0^1 dx_3 \, \frac{\delta(x_1+x_2+x_3-1)}{\left[x_1\ell^2+x_2(\ell+p_{\bar{d}})^2+x_3(\ell+p_{\bar{d}}+p_u)^2\right]^3}$$

$$= 2\int_0^1 dx_1 \int_0^{1-x_1} dx_3 \, \frac{1}{(L^2-\Delta)^3}$$

$$L = \ell + (1-x_1)\,p_{\bar{d}} + x_3\,p_u$$

$$\Delta = -2x_1x_3\,p_u\cdot p_{\bar{d}}$$

- Evaluate this using the identity:

$$\int \frac{d^dL}{(2\pi)^d}\frac{1}{(L^2-\Delta)^n} = i\frac{(-1)^n}{(4\pi)^{d/2}}\frac{\Gamma\left(n-\frac{d}{2}\right)}{\Gamma(n)}\Delta^{d/2-n}$$

"Wick rotation"

- Obtain:

$$\int_0^1 dx_1 \int_0^{1-x_1} dx_3\,(-2x_1x_3\,p_u\cdot p_{\bar{d}})^{-1-\epsilon} = (-2p_u\cdot p_{\bar{d}})^{-1-\epsilon}\int_0^1 dx_1\, x_1^{-1-\epsilon}\left(-\frac{1}{\epsilon}\right)x_1^{-\epsilon}$$

$$= (-2p_u\cdot p_{\bar{d}})^{-1-\epsilon}\left(-\frac{1}{\epsilon}\right)\frac{\Gamma(-\epsilon)\Gamma(1-\epsilon)}{\Gamma(1-2\epsilon)} \quad = (-2p_u\cdot p_{\bar{d}})^{-1-\epsilon}\left(\frac{1}{\epsilon^2}\right)\frac{\Gamma^2(1-\epsilon)}{\Gamma(1-2\epsilon)}$$

soft singularity exposed

Virtual corrections to W production

- In this case the complete calculation can be performed in a similar manner
  - shift the loop momentum to give different Feynman parameter integrals
  - drop odd powers of loop momentum since they vanish
  - use spinor equations of motion

- The end result is:

$$2\left|\mathcal{M}^{(1*)}_{u\bar{d}\to W^+}\mathcal{M}^{(0)}_{u\bar{d}\to W^+}\right| = \left|\mathcal{M}^{(0)}_{u\bar{d}\to W^+}\right|^2 \frac{\alpha_s}{2\pi} C_F \left(\frac{\mu^2}{Q^2}\right)^{\varepsilon} c_\Gamma \left(-\frac{2}{\varepsilon^2} - \frac{3}{\varepsilon} - 8 + \pi^2\right)$$

- The entire result is proportional to the tree-level ME
  - not true in general, for more complicated processes, only the poles guaranteed
- The poles are equal and opposite to those from the real contribution.
- The sum of the two is finite and represents the next-to-leading order correction to W production.

Complete NLO result

- The result for the quark-antiquark channel is then:

$$\hat{\sigma}^{(\mathrm{NLO})}_{u\bar{d}\to W^+} = \hat{\sigma}^{(\mathrm{LO})}_{u\bar{d}\to W^+} \left\{ 1 + \frac{\alpha_s(\mu_R)}{2\pi} C_F \left[\left(\frac{4\pi^2}{3} - 8 \right) \delta(1-z) + \left(\frac{4}{1-x} \log \frac{(1-z)^2}{z} \right)_+ - 2(1+z) \log \frac{(1-z)^2}{z} - 2 \frac{\mathcal{P}^{(1)}_{qq}(z)}{C_F} \log \frac{\mu_F^2}{Q^2} \right] \right\}$$

where a convolution with pdfs still needs to be performed (z-integration).

- The corresponding contribution from the gluon initial states is:

$$\hat{\sigma}^{(\mathrm{NLO})}_{ug\to dW^+} = \hat{\sigma}^{(\mathrm{LO})}_{u\bar{d}\to W^+} \cdot \frac{\alpha_s(\mu_R)}{2\pi} T_R \left[\mathcal{P}^{(1)}_{qg}(z) \left(\log \frac{(1-z)^2}{z} - \log \frac{\mu_F^2}{m_W^2} \right) + \frac{1}{2}(1-z)(1+7z) \right]$$

- The splitting functions are the remnants of divergent terms in the real contribution that are absorbed into the renormalization of the pdf:

$$f_{q/h}(x) = f^{\mathrm{bare}}_{q/h} + \frac{\alpha_s}{2\pi} \left(\frac{-c_\Gamma}{\epsilon} \right) \int_x^1 \frac{dz}{z} \left[\mathcal{P}^{(1)}_{qq}(z) f^{\mathrm{bare}}_{q/h} \left(\frac{x}{z} \right) + \mathcal{P}^{(1)}_{qg}(z) f^{\mathrm{bare}}_{g/h} \left(\frac{x}{z} \right) \right]$$

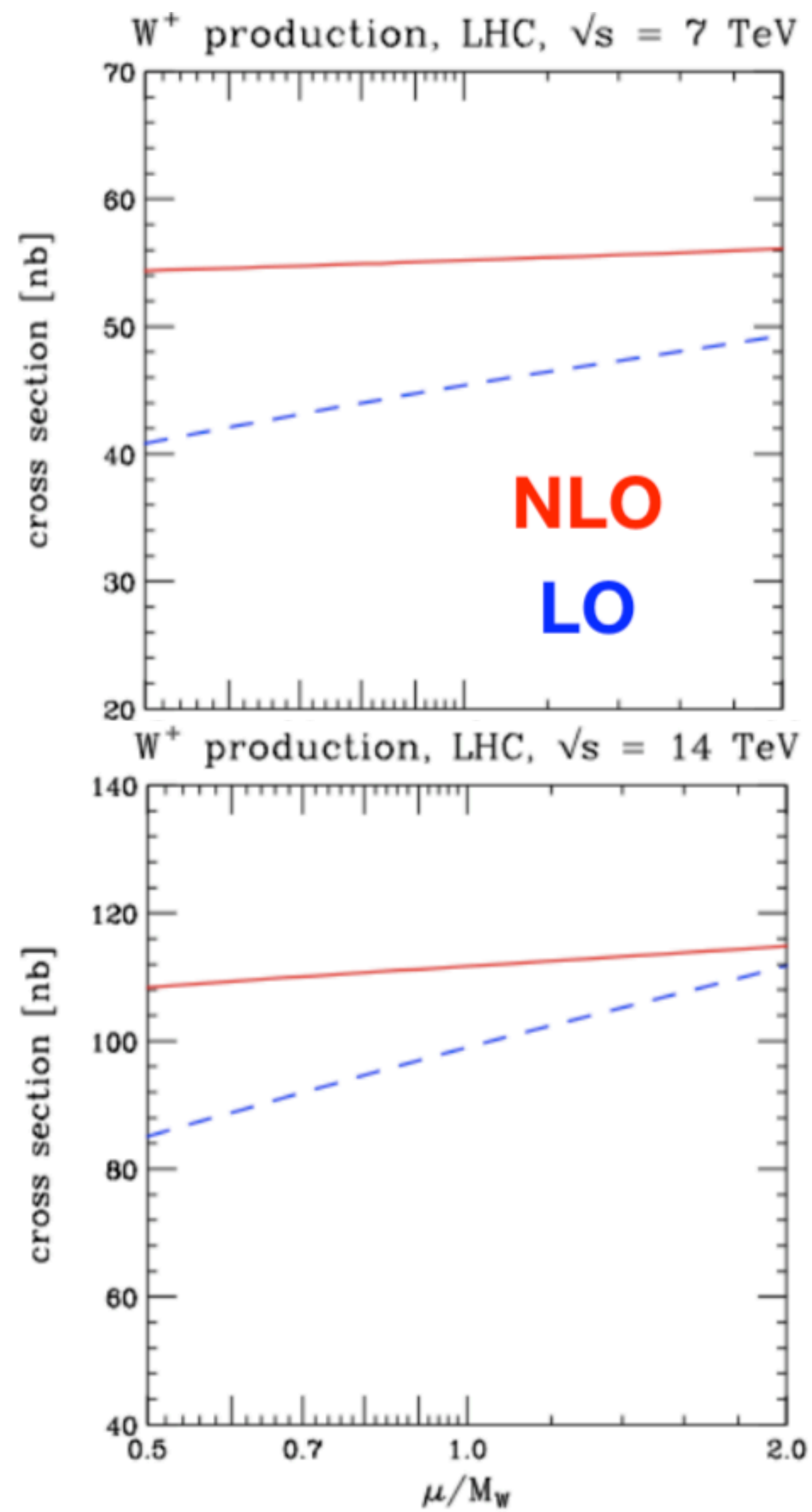
[note: this introduces a scheme dependence since any constants can also be absorbed at the same time; choice here is the MS-bar scheme]

NLO consequences

- The explicit residual dependence on the factorization scale μ_F exactly cancels the dependence in the pdfs themselves.

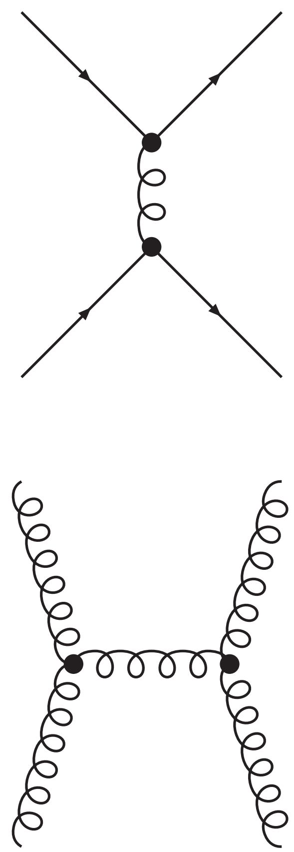
$$\frac{\partial}{\partial \log Q^2} \begin{pmatrix} f_{q/h}(x, Q^2) \\ f_{g/h}(x, Q^2) \end{pmatrix} = \frac{\alpha_s(Q^2)}{2\pi} \int_x^1 \frac{dz}{z} \begin{pmatrix} \mathcal{P}_{qq}\left(\frac{x}{z}\right) & \mathcal{P}_{qg}\left(\frac{x}{z}\right) \\ \mathcal{P}_{gq}\left(\frac{x}{z}\right) & \mathcal{P}_{gg}\left(\frac{x}{z}\right) \end{pmatrix} \begin{pmatrix} f_{q/h}(z, Q^2) \\ f_{g/h}(z, Q^2) \end{pmatrix}$$

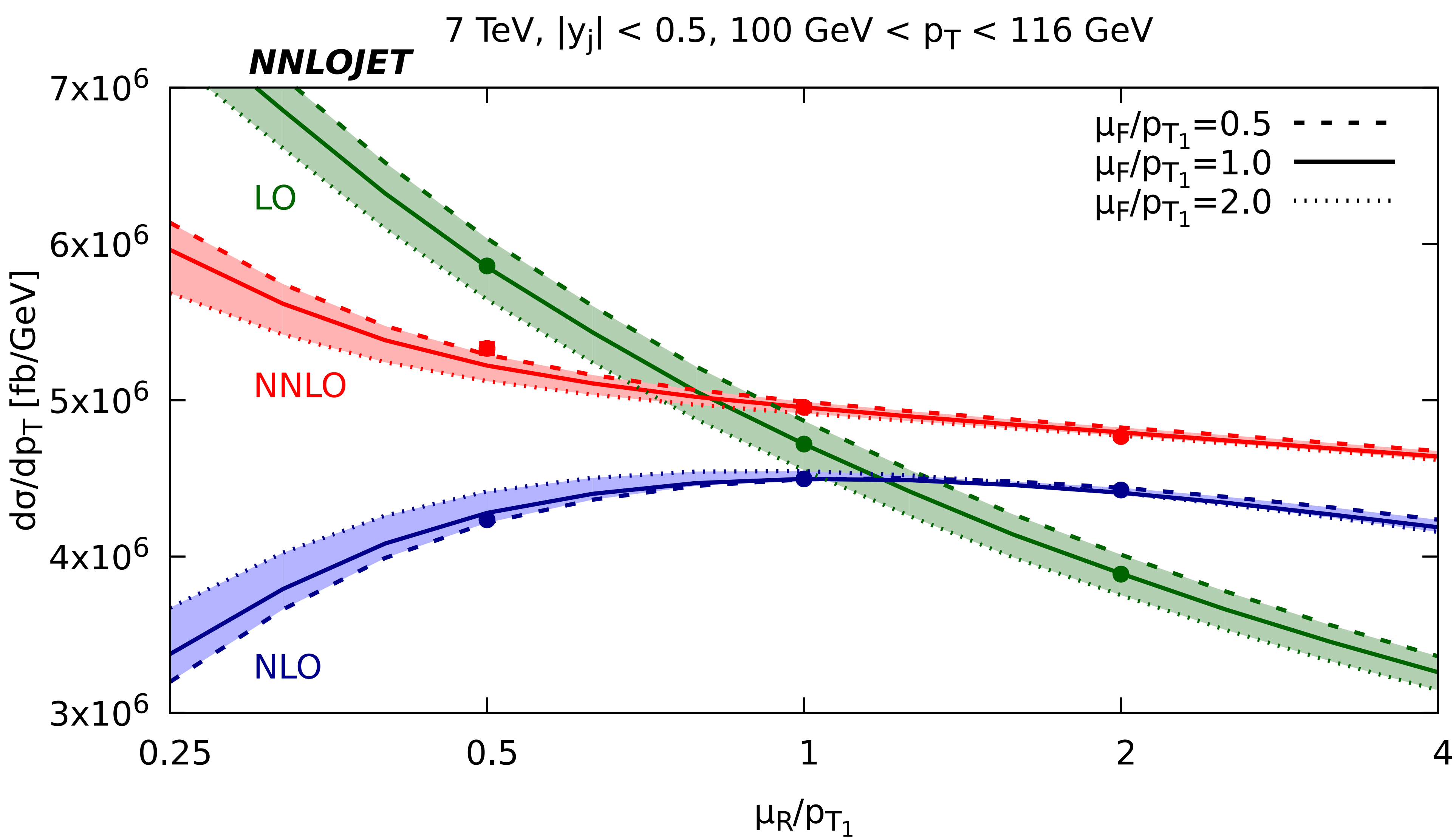
- This means that formally the dependence on μ_F should decrease, although this is not always the case in practice.
  - should see it at high enough order in pert. series
- "K-factor" ratio of NLO/LO ~ 1.1–1.2.
- The behavior of the NLO corrections can be very sensitive to the collider energy
  - and kinematics etc. for more complex processes



Aside: dijet production

- In general similar remarks apply to the renormalization scale, which enters through the strong coupling.
- When it appears at leading order, it must be similarly renormalized, introducing explicit logs of μ_R that are cancelled by the running of α_s.

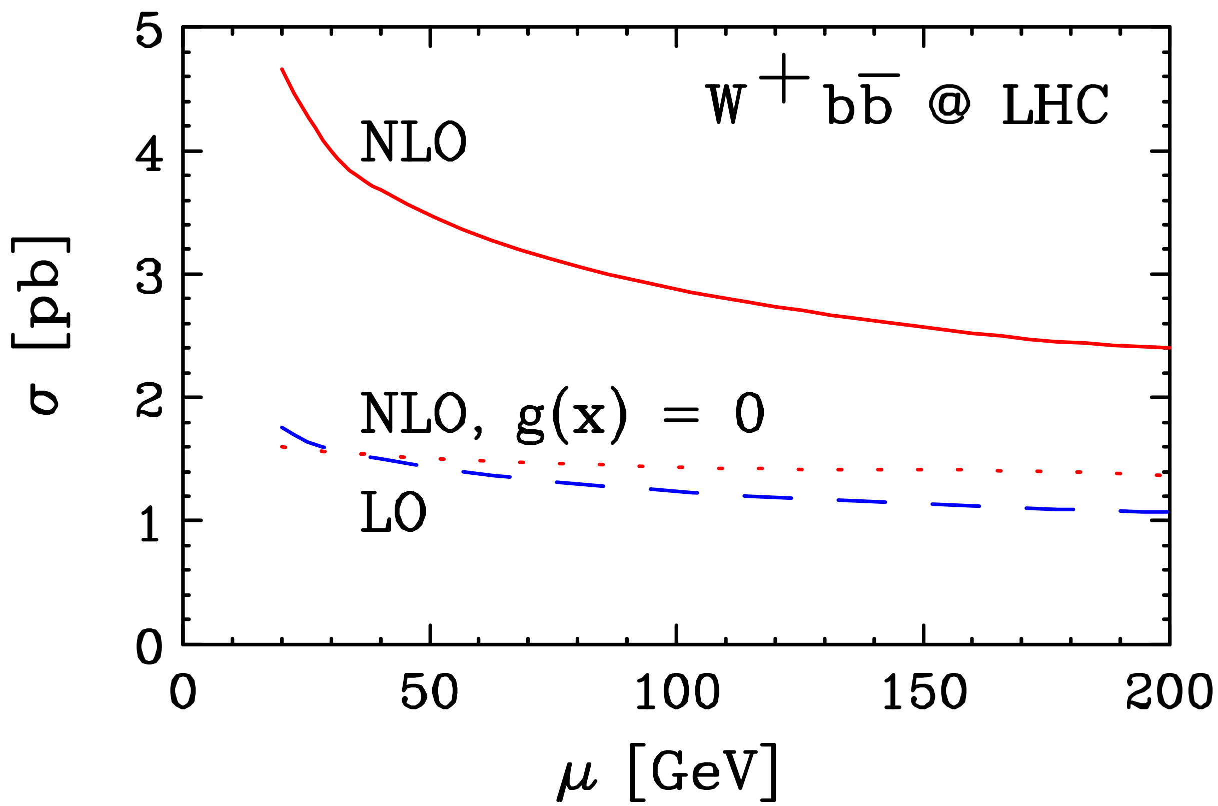




Currie, Glover and Pires (2017)

Unexpected NLO behavior

- These examples give rise to relatively small corrections, lending credence to the notion of a perturbative series.
- However, the NLO corrections are not always so small!
  - example: production of Wbb at the LHC



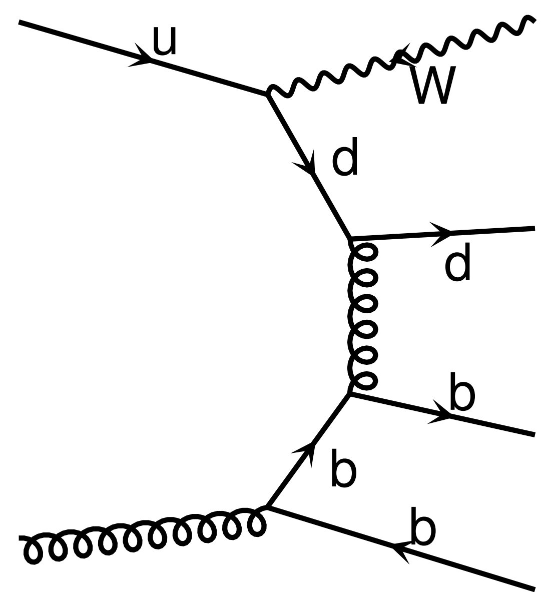


diagram appearing in real correction to Wbb x-sec.

- Particularly prevalent issue at the LHC where gluons are abundant
  - mostly an issue for processes that are quark-antiquark at LO
  - does not signify a breakdown in perturbation theory and can know ahead of time

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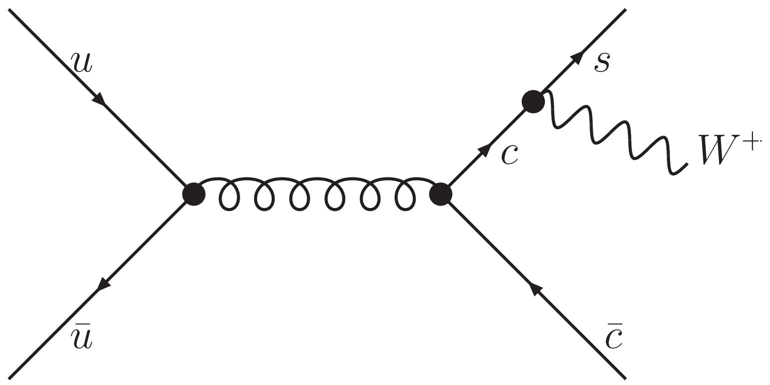
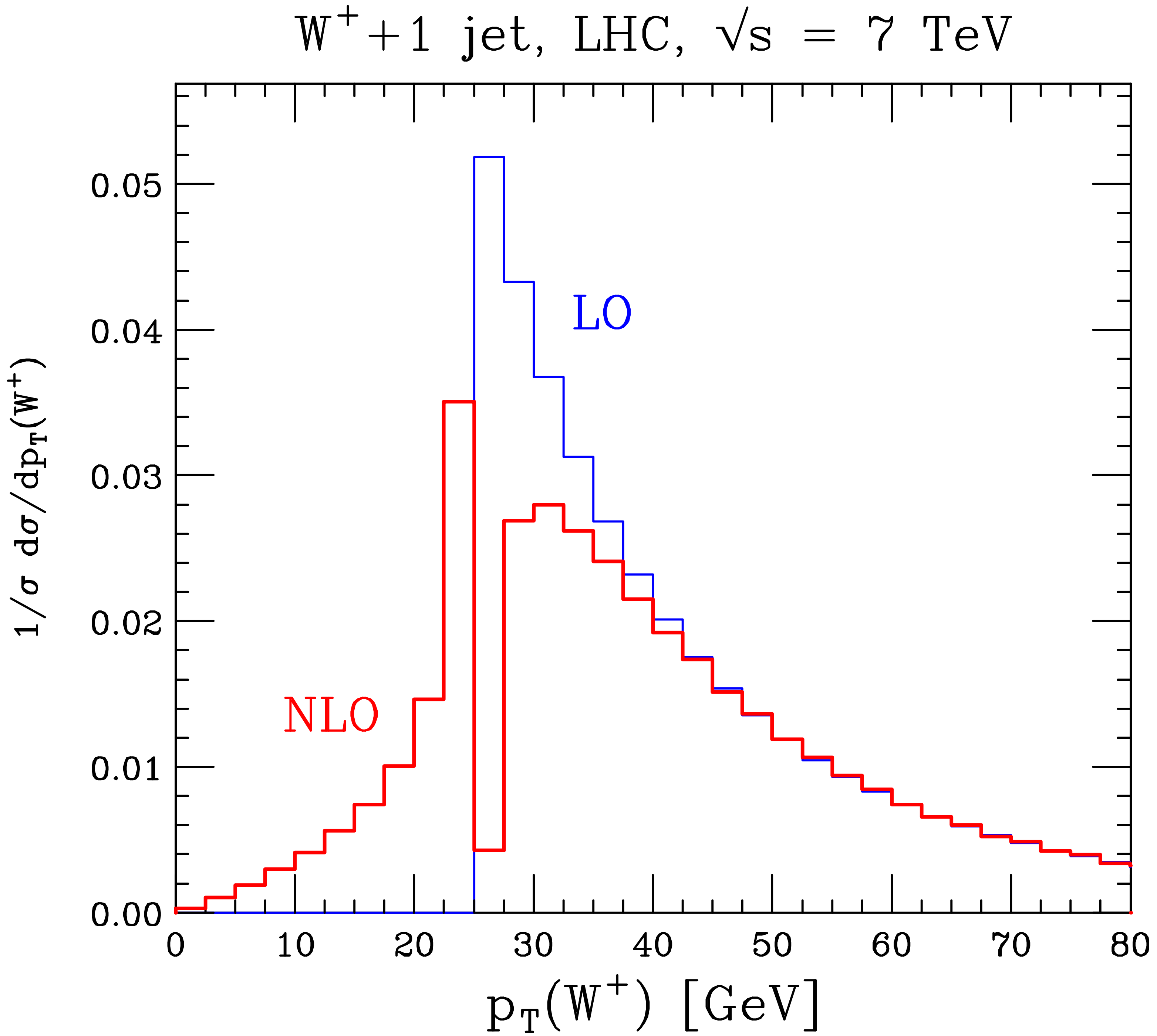
More subtle problems

- Real radiation contributions open up not only new pdfs, but also new kinematics.
- Consider NLO corrections to W+jet production and looking at W-boson p_T in these events.
  - LO (and virtual): W p_T = jet p_T.
  - real corrections: can contain additional parton below cut that partially balances





In this case the behavior is a sign that the prediction cannot be entirely trusted and needs to be improved

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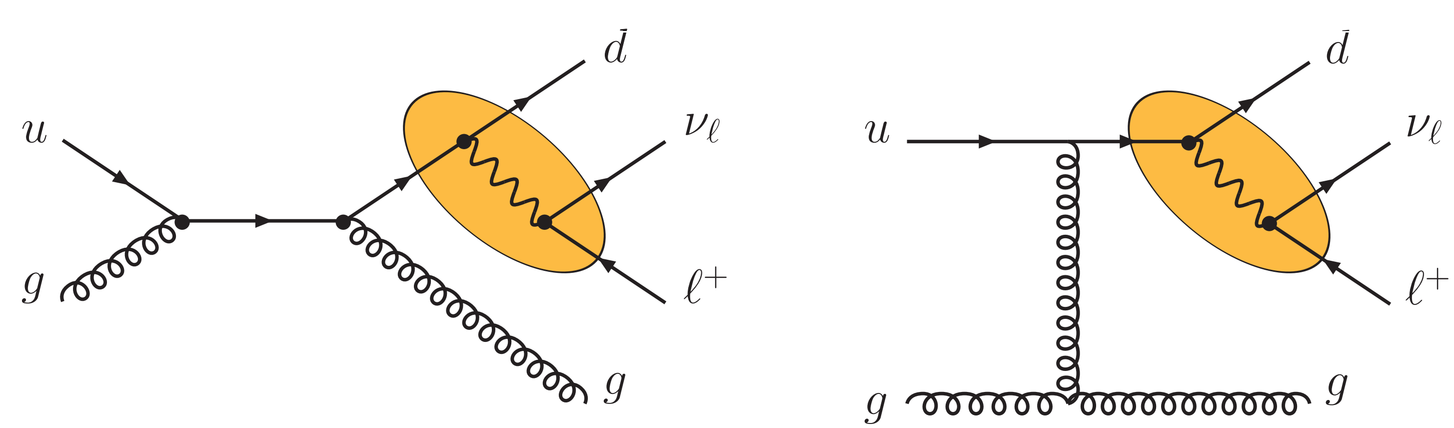
Fixed-order perturbation theory

- We've now seen all the ingredients that enter fixed-order calculations, illustrated by some of the simplest examples.
- Unfortunately, almost all of the calculational techniques we've seen do not scale to more complicated cases (i.e. almost everything we're interested in).
  - this is true even at leading order but even more so at NLO
- High-dimensional phase-space integration requires Monte Carlo techniques to estimate integrals.
- Analytically squaring matrix elements and taking traces is too cumbersome and slow.
- Instead use helicity amplitudes in which the amplitude for each external helicity is a complex number, so summing and squaring is straightforward.
- Typically making extensive use of recycling and recursion for common parts of the amplitudes



NLO: virtual corrections

- Computing the required one-loop diagrams was, for a long time, the bottleneck in performing NLO calculations.
  - as the number of external particles grows, obtain loops with more legs → much harder.
- This is no longer the case — there are many algorithms for computing loop diagrams, limited only by CPU power and/or numerical precision.
- They are based on unitarity techniques in which tree-level amplitudes are sewn together into loops, then loop integrations are replaced by algebraic manipulations ("OPP") [Ossola, Pittau, Papadopoulos]
- This can be accelerated by recursive construction of the amplitude, in similar fashion as at LO ("OpenLoops") [Cascioli et al].

	type	technology dependencies on other codes
LoopTools [605]	integrals	
OneLoop [879]	integrals	
QCDLoop [499]	integrals	
Collier [457]	reduction	
CutTools [793]	reduction	OPP
FormCalc [605]	reduction	PV
Ninja [802]	reduction	Laurent expansion
Samurai [756]	reduction	
BlackHat [226]	library (amplitudes)	OPP (unitarity)
MCFM [309]	library (full calculation)	PV & OPP
NJet [181]	library (amplitudes)	OPP
GoSam [420]	generator (amplitudes)	OPP Samurai +Ninja +
MadLoop [625]	generator (full calculation)	OL+OPP CutTools +
OpenLoops [338]	generator (amplitudes)	OL+OPP Collier +CutTools +
Helac-NLO [241]	generator (full calculation)	OPP CutTools +

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NLO: real corrections

- We noted the universal behavior of matrix elements in infrared, i.e. soft and collinear, limits (splitting functions).
- However, directly performing the phase-space integrals analytically to reveal the poles (that must cancel against the virtual contribution) is impossible.
- Instead we must find a general technique for extracting the poles. Two broad classes of methods are used: phase-space slicing and subtraction.
- To simplify the discussion, we'll use a toy model that we know has the behavior that is found in the actual calculations:

regularizing factor in dim. reg.

$$\mathcal{I} = \int_0^1 \frac{dx}{x} x^{-\epsilon} \mathcal{M}(x)$$

real contribution

real matrix elements

soft/collinear singularity present as $x \to 0$, with $\mathcal{M}(0)$ the LO ME

Phase-space slicing

- In the slicing approach, an additional theoretical parameter (δ) is introduced that is used to define the singular region. Close to the singular region the matrix elements are approximated by LO.
  - in our toy model this means choosing $\delta \ll 1$ and approximating $\mathscr{M}(x)$ by $\mathscr{M}(0)$ for $x<\delta$
- We can then split the integral into two regions:

$$\mathcal{I} = \mathcal{M}(0)\int_0^\delta \frac{dx}{x} x^{-\epsilon} + \int_\delta^1 \frac{dx}{x} x^{-\epsilon} \mathcal{M}(x)$$

$$= -\frac{1}{\epsilon}\delta^{-\epsilon}\mathcal{M}(0) + \int_\delta^1 \frac{dx}{x}\mathcal{M}(x)$$

$$= \left(-\frac{1}{\epsilon} + \log\delta\right)\mathcal{M}(0) + \int_\delta^1 \frac{dx}{x}\mathcal{M}(x)$$

isolated singularity — finite, ready to be integrated numerically

- The final result should be independent of δ via an implicit cancellation of between the exposed logarithm and the lower limit of the integral.

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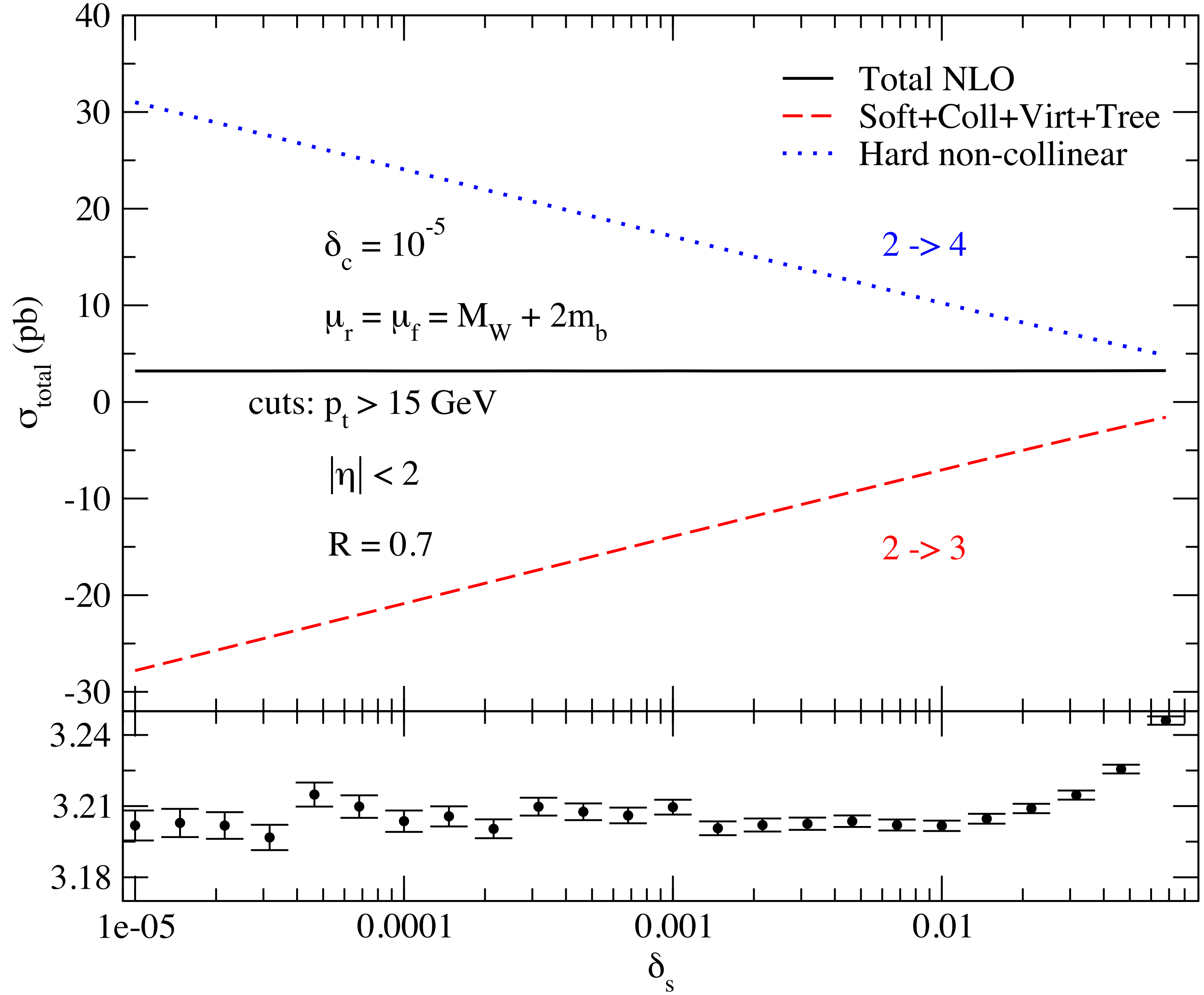
Slicing: example

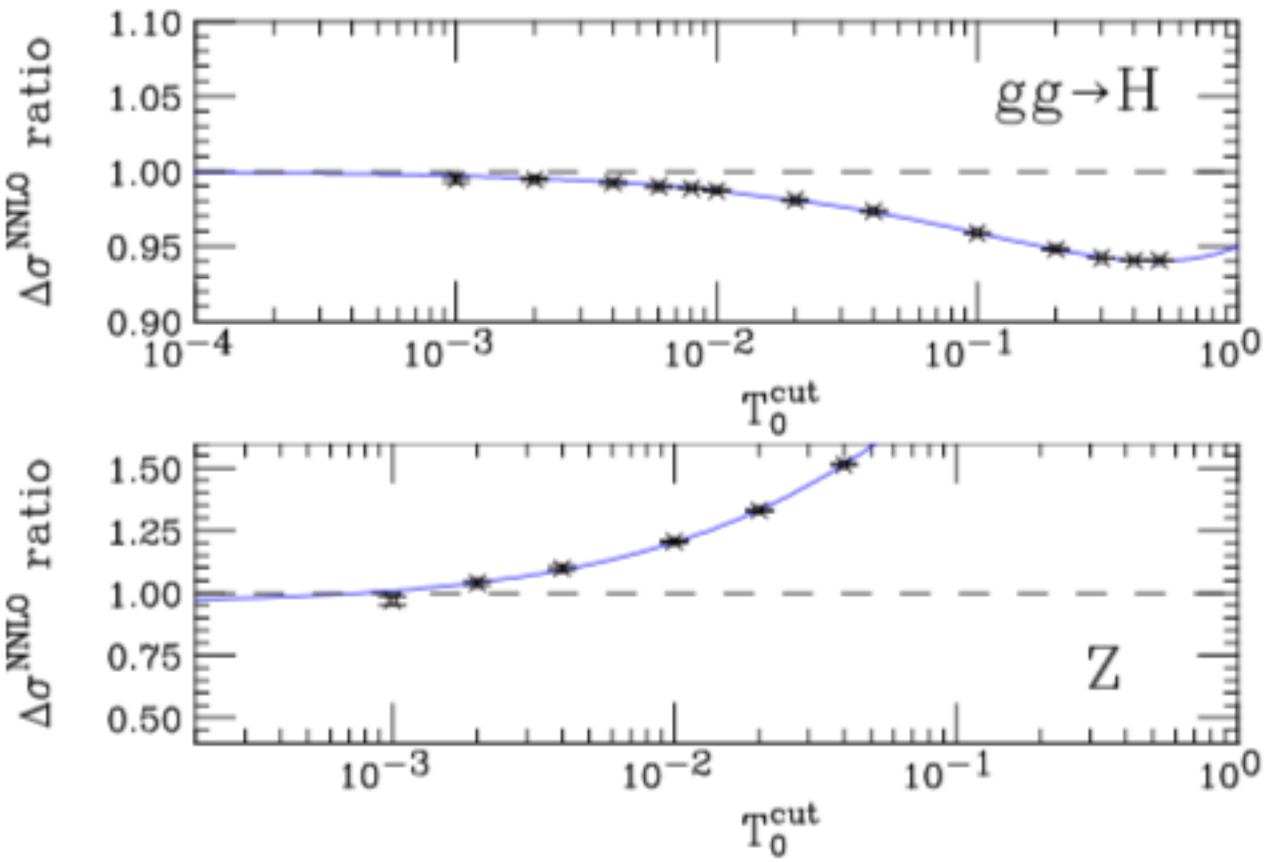
- One advantage of phase-space slicing is that it is relatively simple to implement; historically used for a number of “first-ever” calculations.
- However, it has a big drawback: there is a tension between retaining a good approximation (small δ) and reducing the effect of numerical-log cancellations (large δ).
- Illustrated in example of Wbb production at NLO, demonstrating size of cancellation between 2→3 and 2→4 contributions.

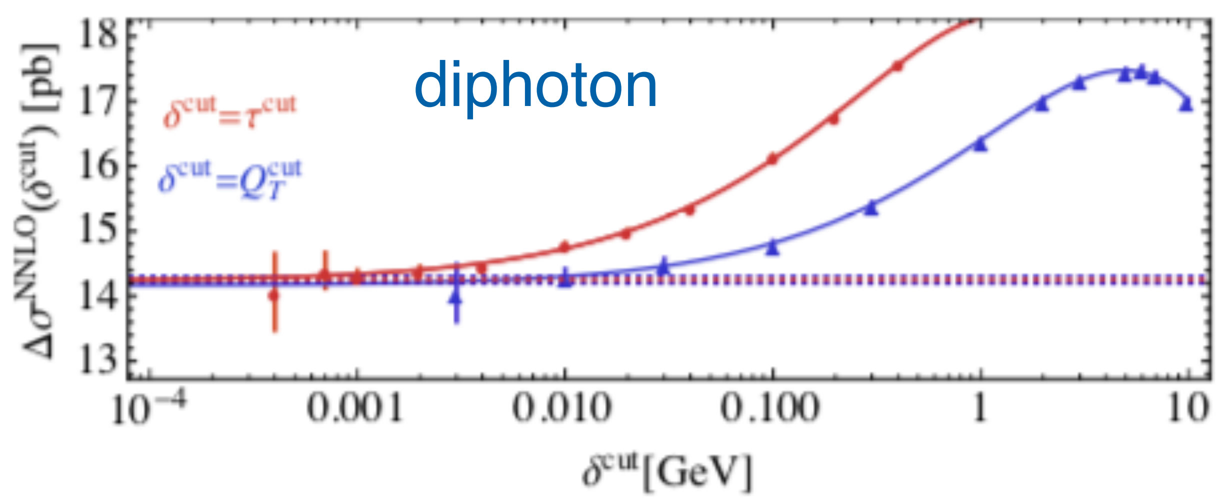


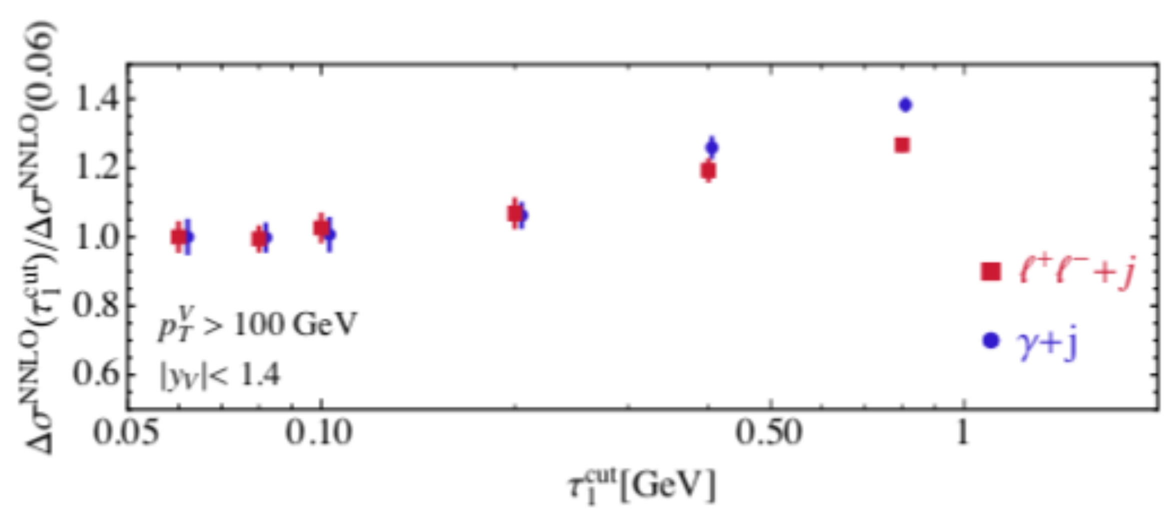
Febres Cordero, Reina, Wackeroth (2006)

Aside: slicing at NNLO

- This method has fallen out of favor at NLO, but the message is still relevant.
- Techniques that use the same principle are now regularly used in next-to-next-to-leading order (NNLO) calculations.
  - examples are "Q_T subtraction" and "jettiness subtraction"
  - do not let the name fool you, they are really slicing methods at heart.







Subtraction

- Method of choice, used by all general-purpose NLO codes, is subtraction.
- For each singular region introduce a local counter-term with same behaviour.
- In the toy model the counter-term is obvious:

$$\mathcal{I} = \int_0^1 \frac{dx}{x} x^{-\epsilon} \left[\mathcal{M}(x) - \mathcal{M}(0)\right] + \mathcal{M}(0) \int_0^1 \frac{dx}{x} x^{-\epsilon}$$

$$= \int_0^1 \frac{dx}{x} \left[\mathcal{M}(x) - \mathcal{M}(0)\right] - \frac{1}{\epsilon}\mathcal{M}(0)$$

suitable for numerical integration

isolated singularity

"integrated counter-term"

- For numerical stability still need a cutoff in practice since it is impractical to integrate the subtracted singularity completely (to zero, in toy example).
- The trick here is to construct the singular terms such that they are universal and readily integrated analytically.
  - formulations provided by Catani-Seymour dipole subtraction and FKS subtraction. [Frixione, Kunszt, Signer]

Beyond NLO QCD

- How much harder is it to get to the next order in perturbation theory, NNLO?
- Expanding out the amplitude results in four contributions. Can visualize through cuts of a master diagram, for example in Z+jet production:

(a) 2-loop virtual contributions

$$\Re\mathrm{e}\left[\mathcal{A}^{2-\mathrm{loop}}(Zq\bar{q}g) \times \mathcal{A}^{\mathrm{tree}}(Zq\bar{q}g)^*\right]$$

(b) 1-loop squared [with (a), "virtual-virtual"]

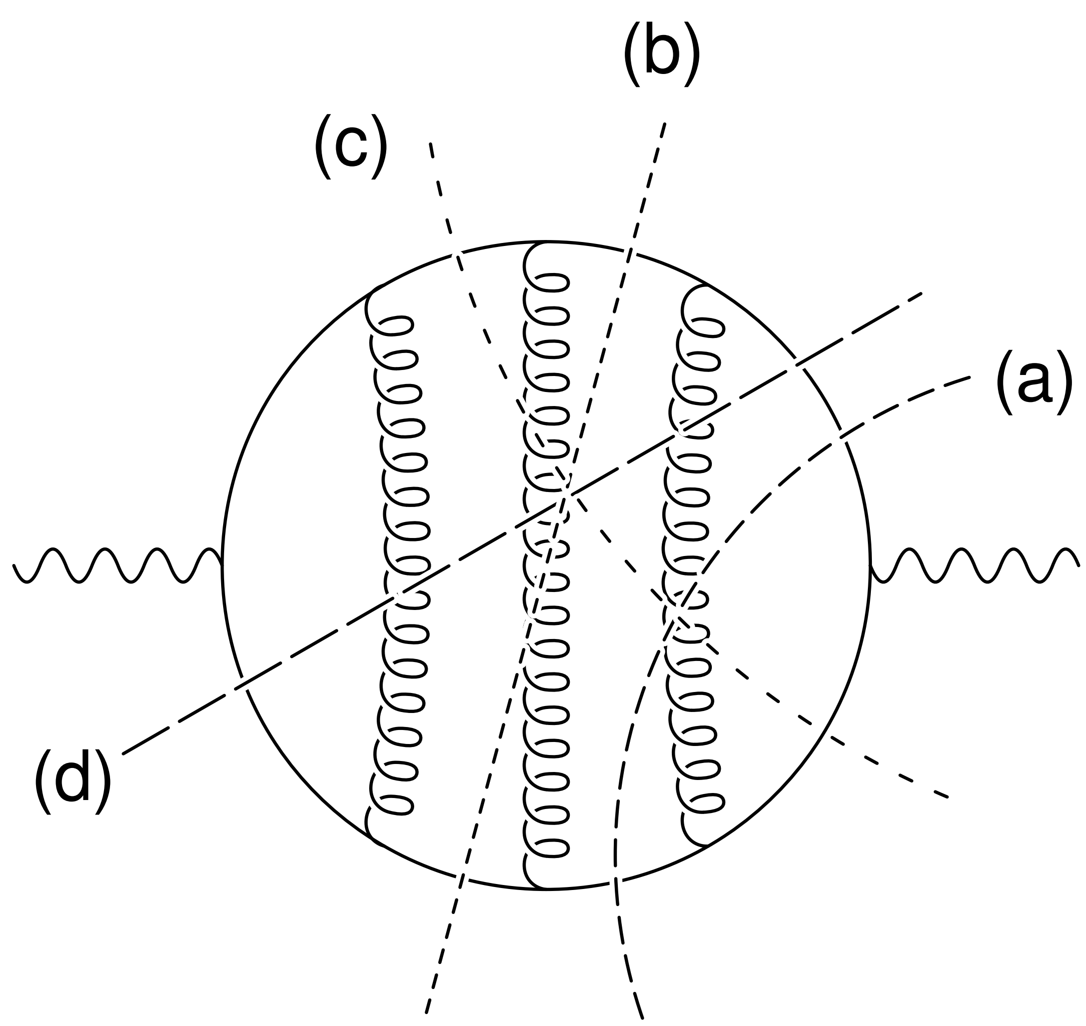
$$\left|\mathcal{A}^{1-\mathrm{loop}}(Zq\bar{q}g)\right|^2$$

(c) contributions with one extra parton, tree and 1-loop amplitudes ["real-virtual"]

$$\Re\mathrm{e}\left[\mathcal{A}^{1-\mathrm{loop}}(Zq\bar{q}gg) \times \mathcal{A}^{\mathrm{tree}}(Zq\bar{q}gg)^*\right]$$

(d) two extra partons, tree-level ["real-real"]

$$\left|\mathcal{A}^{\mathrm{tree}}(Zq\bar{q}ggg)\right|^2$$



NNLO challenges

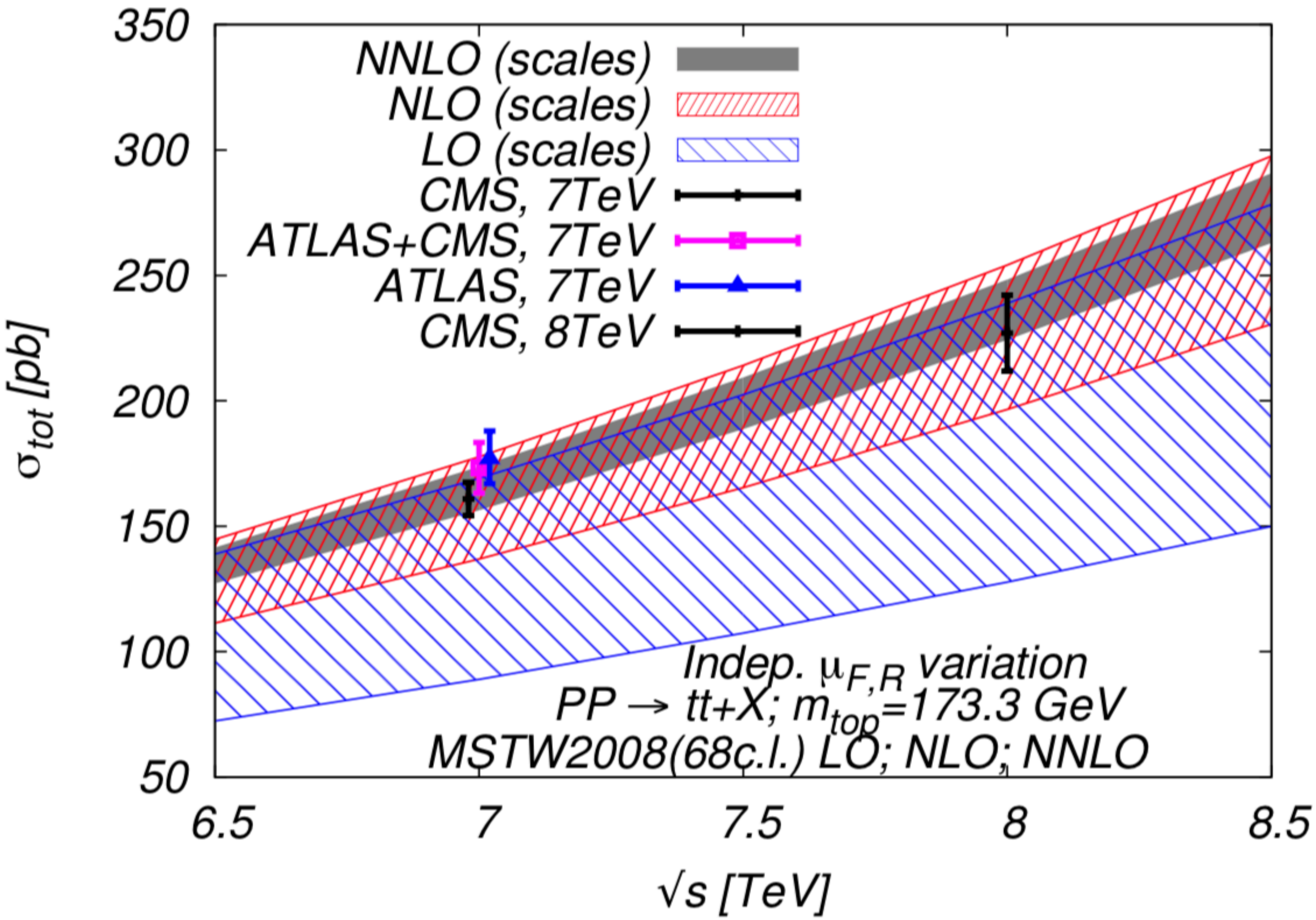
- 1-loop squared and real-virtual contributions are relatively easy extensions of ingredients that already entered at NLO.
- Procedure for computing 2-loop integrals is much less straightforward
  - little is known about integrals and amplitudes for processes beyond $2 \to 2$ scattering
  - two unconstrained momenta means poles as deep as $1/\epsilon^4$
- Isolating the poles in the real-real contribution, to cancel with these, is a significant challenge
  - amplitudes still factorize, but in more complicated ways — not just products of single splittings but new configurations, "triple collinear" and "double soft"
- A plethora of methods have emerged to handle the singularities:
  - subtraction-type:
    - "sector" (DY, Higgs), "sector-improved residue" (top pairs, H+j), "projection to Born" (vector boson fusion), "antenna" (NNLOJET code, jet production, H+j, V+j, VBF), "colourful", "nested"
  - slicing-type:
    - "Q_T" (MATRIX code, DY, H, VH, dibosons, top pairs), "N-jettiness" (MCFM code, H+j, V+j, γ+j)
- No clear "winner" yet and certainly no generic method like at NLO.

NNLO features

- Main benefits:

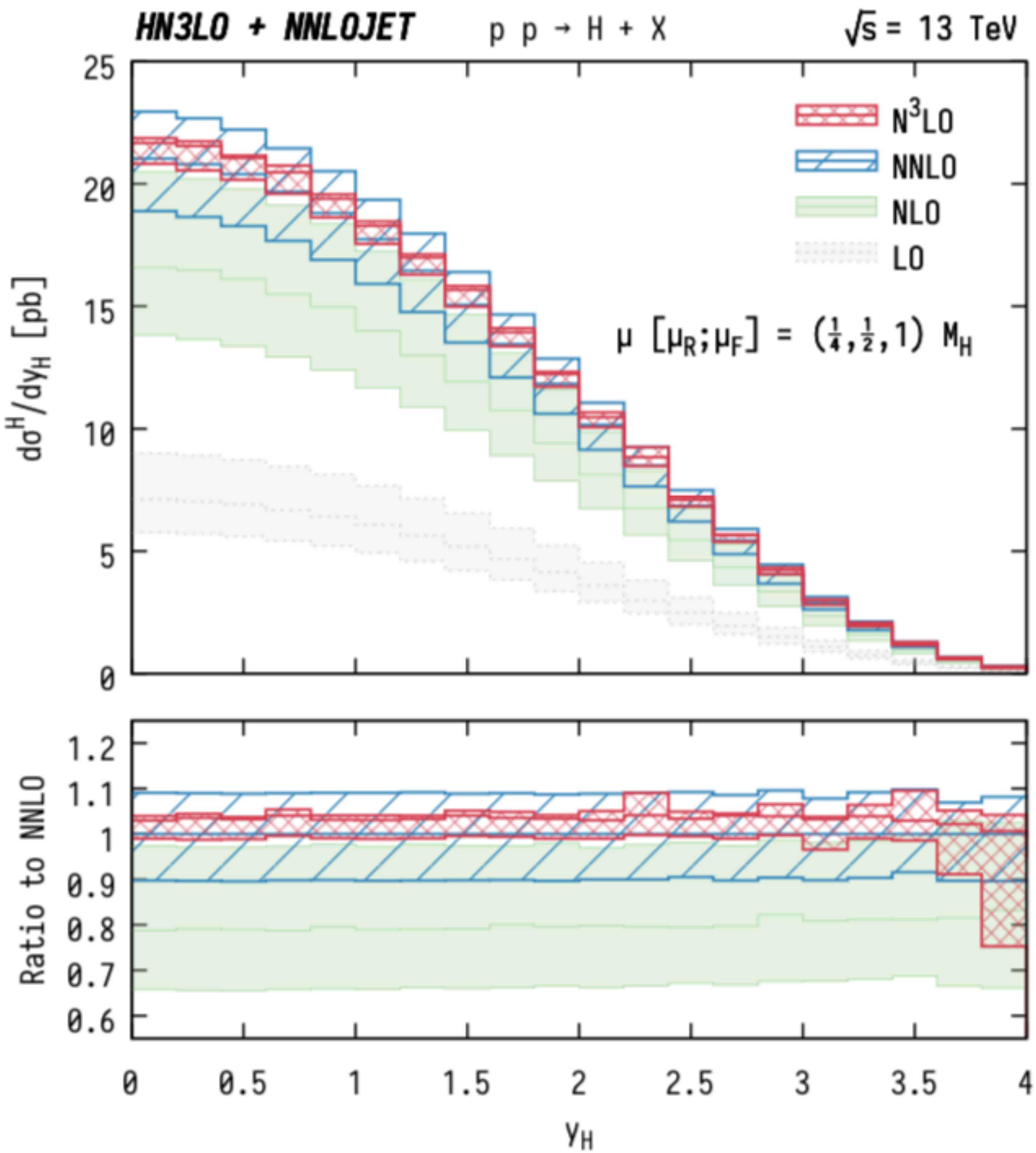
  - if NLO corrections are large (e.g. through sensitivity to new pdf) expect smaller subsequent corrections
    → regain theoretical control of prediction

  - further-reduced scale uncertainty; using this as a proxy for theory uncertainty can begin to expect precision predictions ~ 2-5% uncertainty



N^3LO anyone?

- Even more complicated integrals, deeper singularities and much less known.
- Only computed for simplest cases, using bag of process-specific tricks, that are of utmost importance
  → probing the Higgs boson.
- Only calculations known:
  - total Higgs x-sec in gluon fusion [Anastasiou, Duhr, Dulat, Herzon, Mistlberger (2015-18)]
  - total x-sec in vector boson fusion [Dreyer, Karlberg (2016)]
  - Higgs boson rapidity distribution [Cieri, Chen, Gehrmann, Glover, Huss, July 30 2018]



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Fixed-order summary

LO	automated tools, calculations limited by CPU time for adequate phase-space integration; too many colored particles can be a problem
NLO	automated tools, may be limited by CPU time for generation of diagrams and integration; 2→6 scatterings about the limit
NNLO	no automated tools but some public codes for processes with no colored particles in final state; 2→2 scatterings state-of-the-art
N^3LO	extremely limited (Higgs) cases only; theoretical methods just beginning to be developed

Beyond fixed-order

- So far we have factorized our calculation into hard and soft components and concentrated on computing the former.
  - in so doing we introduced non-perturbative objects, pdfs, to handle some of the soft part
  - we implicitly equated a hard parton with an experimentally-measured jet
  - conveniently ignoring that partons are colored and we measure color-neutral hadrons
- To remedy this situation, we have to move beyond the fixed-order perturbative description that we have developed so far.
- We can see why this is the case by looking at our emission probability:

$$\frac{\sigma(X+g)}{\sigma(X)} \sim \frac{\alpha_s(Q^2)}{2\pi}\,\frac{dQ^2}{Q^2}\,P_{qq}(z)\,dz$$

$$\sim \alpha_s(Q^2)\log^2 Q^2$$

  when trying to describe emission of multiple partons, the logarithms spoil any possible perturbative behavior: they must be accounted for, or “resummed".
- Crucial in QCD (c.f. QED) because of coupling and gluons emit more gluons.

Sketch of a collision

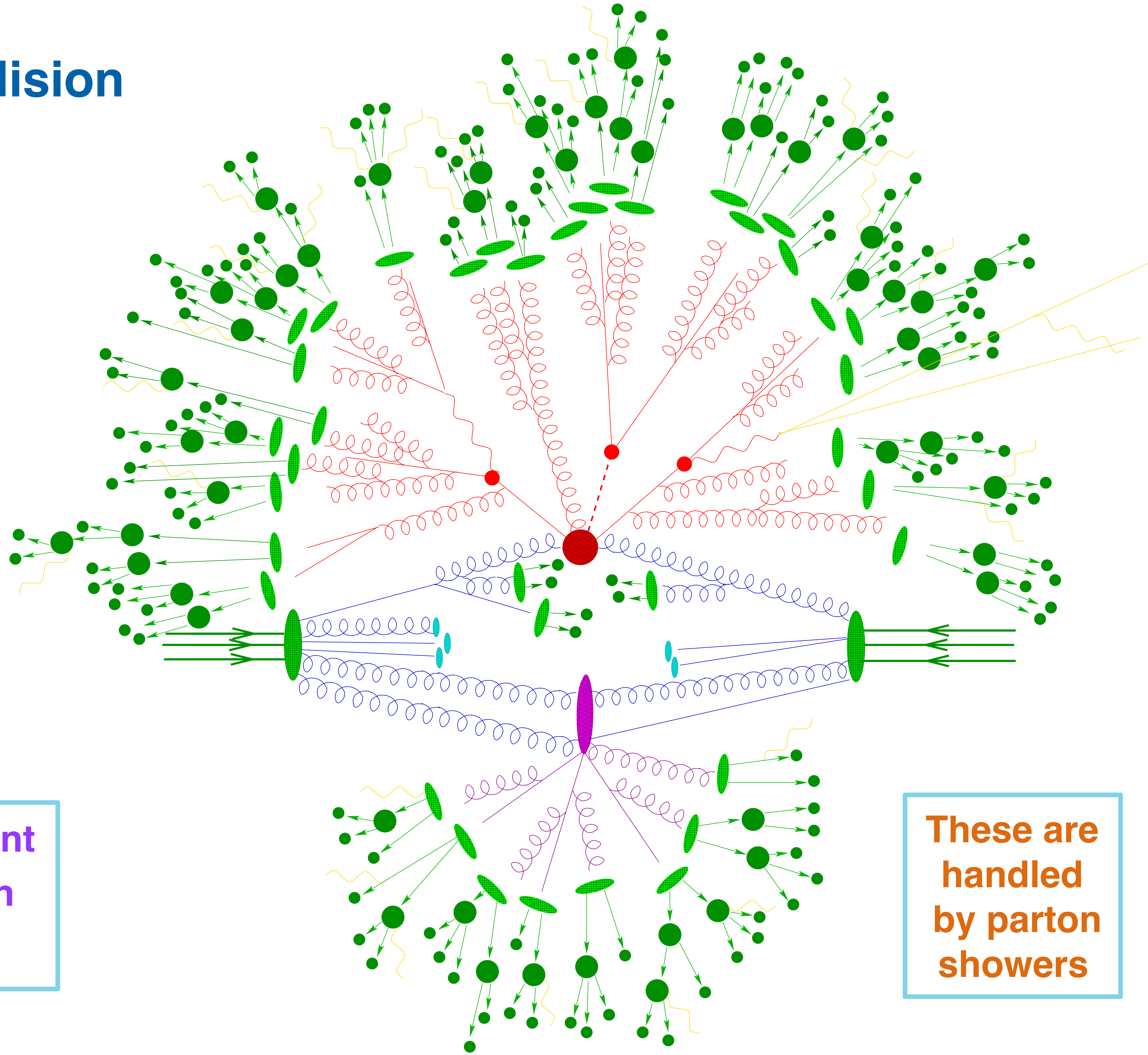
Hadronization (partons→jets of hadrons)

Final-state radiation

Hard collision

Initial-state radiation and pdfs

Underlying event (multiple parton collisions)



These are handled by parton showers

Analogy: radioactive decay

- To see how the building blocks of a parton shower emerge, consider an analogous situation: decay of an isotope with half-life τ.
- Probability that nucleus is still intact after time t is:

$$P^{\text{nodec.}}(t) = \exp(-t/\tau) = \exp(-\Gamma t)$$

in terms of the decay width of the isotope, $\Gamma = 1/\tau$.

- Trivial observation: decay probability is:

$$P^{\text{dec.}}(t) = 1 - P^{\text{nodec.}}(t) = 1 - \exp(-\Gamma t)$$

- Probability of decay at exactly time *t* given by probability density (derivative):

$$\frac{dP^{\text{dec.}}(t)}{dt} = \Gamma \exp(-\Gamma t) = \Gamma \cdot P^{\text{nodec.}}(t)$$

- We want to equate the decay probability with the chance to emit radiation. The time evolution will be replaced by virtuality (Q^2, or t) evolution.
  - emission probability depends on virtuality, so need more general version

Radioactive decay, redux

- Change the decay width from a constant to one that depends on time:

$$\Gamma \longrightarrow \Gamma(t)$$

- The no-decay probability changes accordingly:

$$P^{\text{nodec.}}(t) = \exp(-\Gamma t) \quad \longrightarrow \quad P^{\text{nodec.}}(t) = \exp\left(-\int_0^t dt'\, \Gamma(t')\right)$$

  but the equation for the probability density is essentially the same:

$$\frac{dP^{\text{dec.}}(t)}{dt} = \Gamma(t) \cdot P^{\text{nodec.}}(t)$$

- Knowing that our emissions are governed by:

$$\frac{\sigma(X+g)}{\sigma(X)} \sim \frac{dt}{t} \int dz\, \frac{\alpha_s}{2\pi}\, P_{ab}(z)\, dz$$

  allows us to identify the quantity analogous to the width:

$$\Gamma(t) \to \frac{1}{t} \int dz\, \frac{\alpha_s}{2\pi}\, P_{ab}(z)\, dz$$

Sudakov form factor

- Plugging this back in gives the no-emission (previously no-decay) probability:

$$P^{\rm no}(T,t) = \exp\left(-\int_t^T \frac{dt'}{t'} \int dz\, \frac{\alpha_s}{2\pi} P_{ab}(z)\, dz\right)$$

- Note that the start time for radioactive decay (*t*=0) has been replaced by an evolution from a starting large scale *T* to a smaller scale *t*.
- This form of the no-emission probability also called the Sudakov form factor.
- In order that the integral converge we should introduce an infrared cutoff t_c, to remove contributions from $t \sim 0$ (typically of order Λ_{QCD}).
- Hence the probability of no-emission all the way down to this scale is:

$$P^{\rm no}(T,t_c) = \exp\left(-\int_{t_c}^T \frac{dt'}{t'} \int dz\, \frac{\alpha_s}{2\pi} P_{ab}(z)\, dz\right)$$

$$\sim \exp\left(-C_F \frac{\alpha_s}{\pi} \log^2(T/t_c)\right)$$

[emission of a gluon from a quark, leading term only]

Resolvable emissions

- This is the probability for no resolvable emissions.
- We can expand it out to first order to find:

$$P^{\mathrm{no}}(T,t_c) \;\sim 1 - \frac{C_F \alpha_s}{\pi} \log^2(T/t_c)$$

- This formula accounts for the effect of unresolved emissions, corresponding to both soft and collinear radiation below the cutoff and virtual emissions:

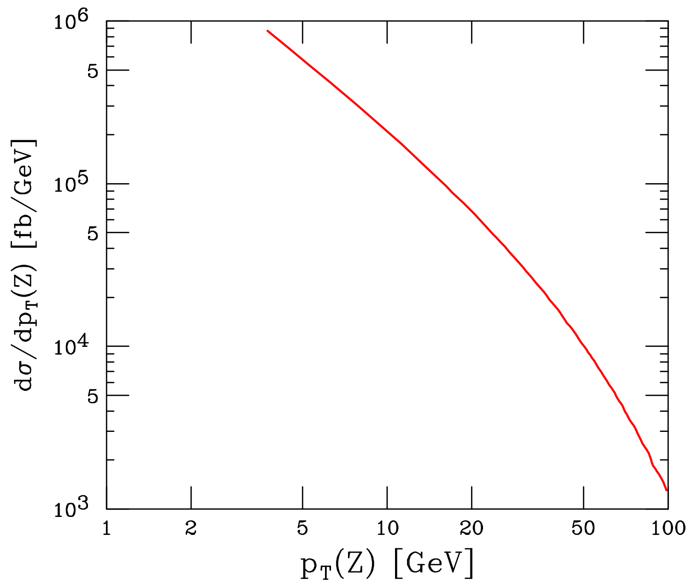
- This is despite the fact that we only put in real emission; it is a consequence of the probabilistic interpretation and the introduction of the cutoff.
  - by preserving unitarity, a parton shower automatically takes care of virtual contributions
- For large values of T/t_c the expanded-out no-emission probability above will become negative! Contrast this fixed-order behavior with the shower form:

$$P^{\mathrm{no}}(T,t_c) \sim \exp\left(-C_F \frac{\alpha_s}{\pi} \log^2(T/t_c)\right)$$

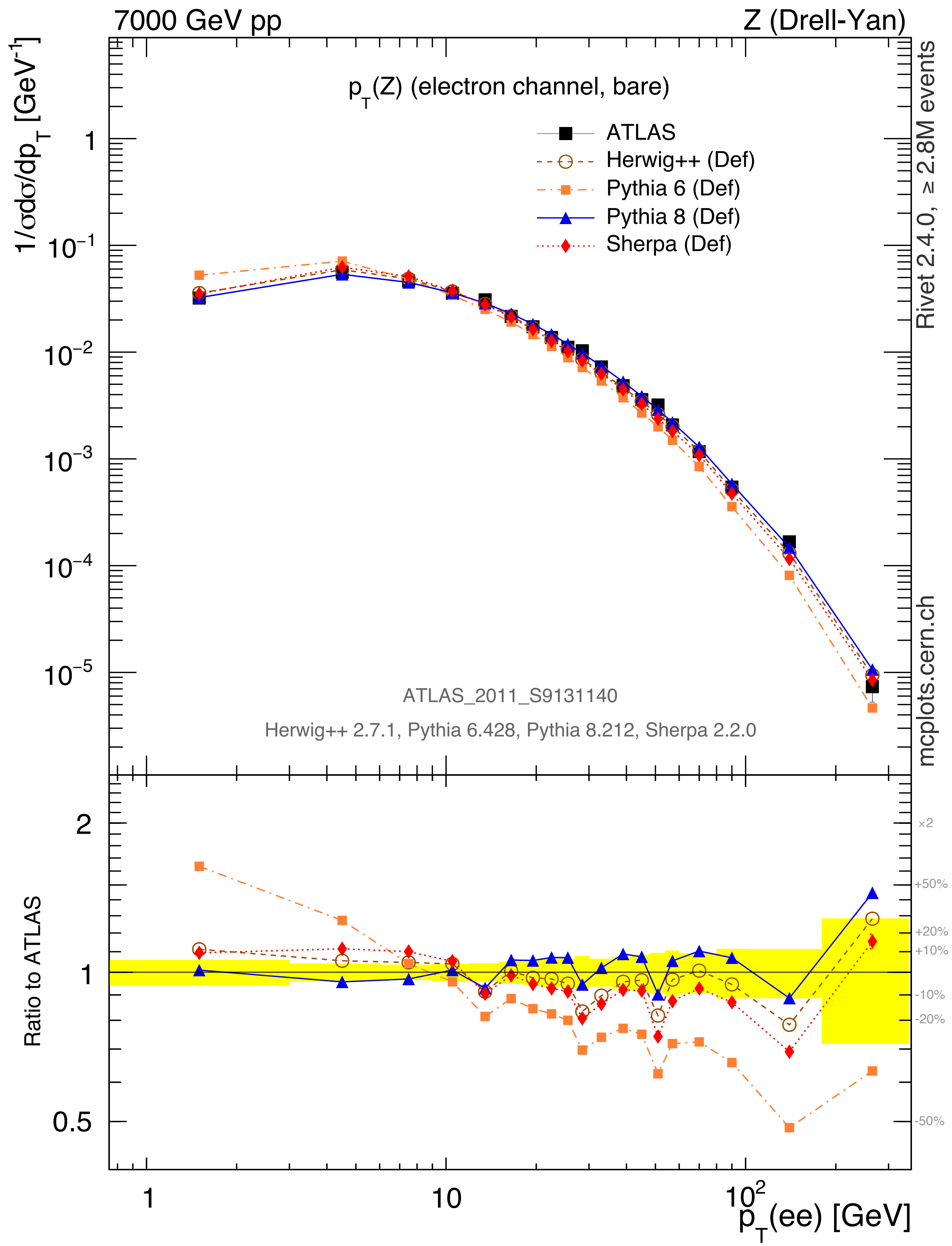
No large-log divergence
The logarithms are resummed

Example: Z p_T distribution

- At fixed, leading order diverges as $p_T \to 0$
  - improved at NNLO but still cannot really describe entire region



- The resummation in the parton shower handles exactly this problem
  - instead produces characteristic peak, describes data well



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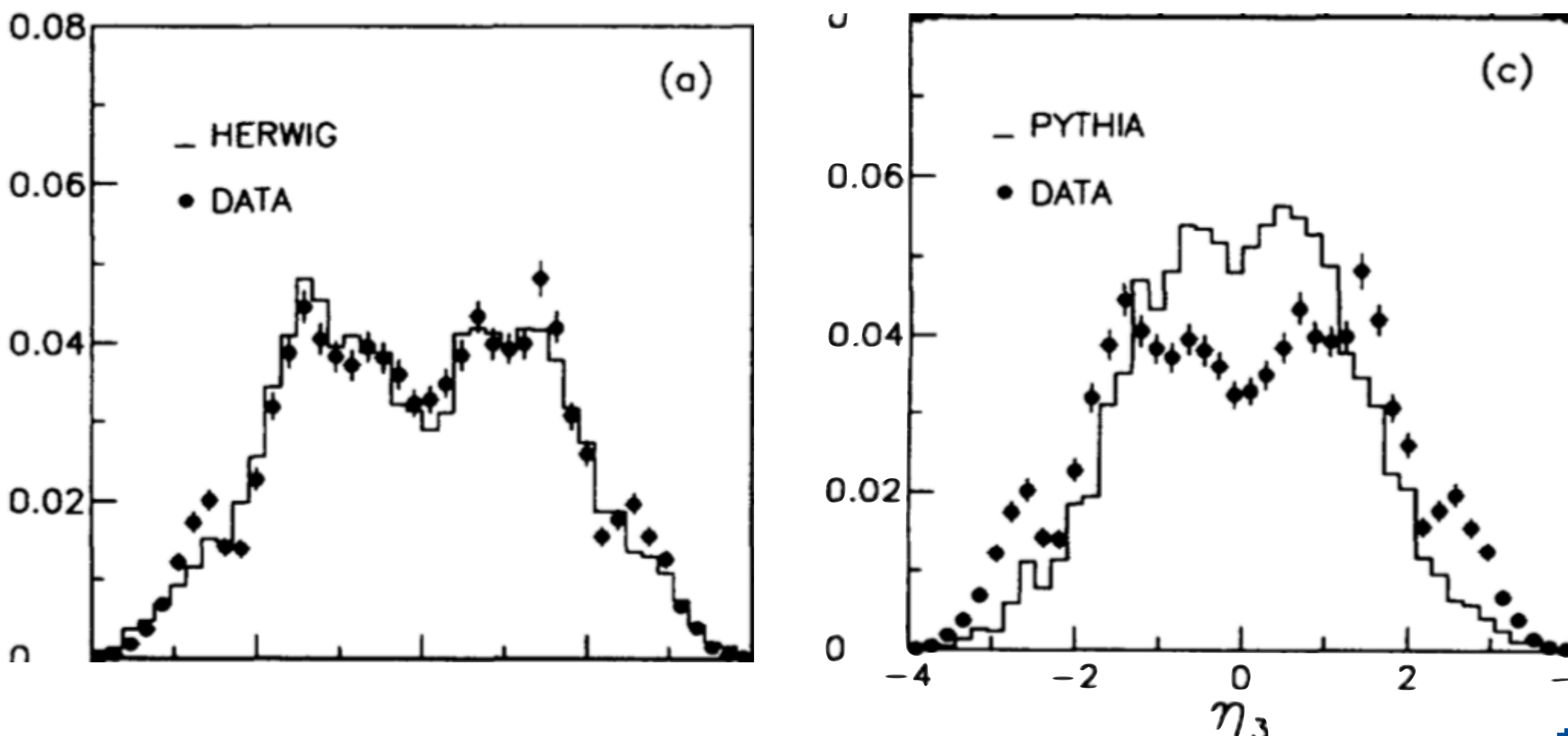
Parton shower implementation

- The emission probability encoded in the Sudakov form factor is the basis for all parton showers.
- For final-state radiation "forward evolution":
  - start from a configuration with a given number of hard partons
  - assign further emission according to Sudakov weights
- For initial-state radiation "backward evolution":
  - natural to start from low scale (incoming hadrons) and evolve to hard scattering, but this would be incredibly inefficient; instead, must fix hard scattering first and work backwards
  - additional complication from ensuring DGLAP equation satisfied
- In the sketch of the method above, α_s was kept fixed
  - implementing running can capture some effects related to sub-leading logarithms
  - can also attempt to account for other, universal, higher-order effects
- Choice of the evolution variable *t* gives rise to important differences:
  - original choice was virtuality (early PYTHIA)
  - better choices are opening angle (HERWIG) and transverse momentum (PYTHIA 6 on)
  - they can account for the effects of QCD quantum coherence, or angular ordering

Angular ordering

- Angular ordering means that gluon radiation only feels the individual color charges of its parent quark and gluon if it is emitted with a smaller opening angle
  - otherwise it just sees primary quark
- Effectively results in reduced emission probabilities outside cones around primary parton directions, c.f. CDF jet data from Tevatron Run I.

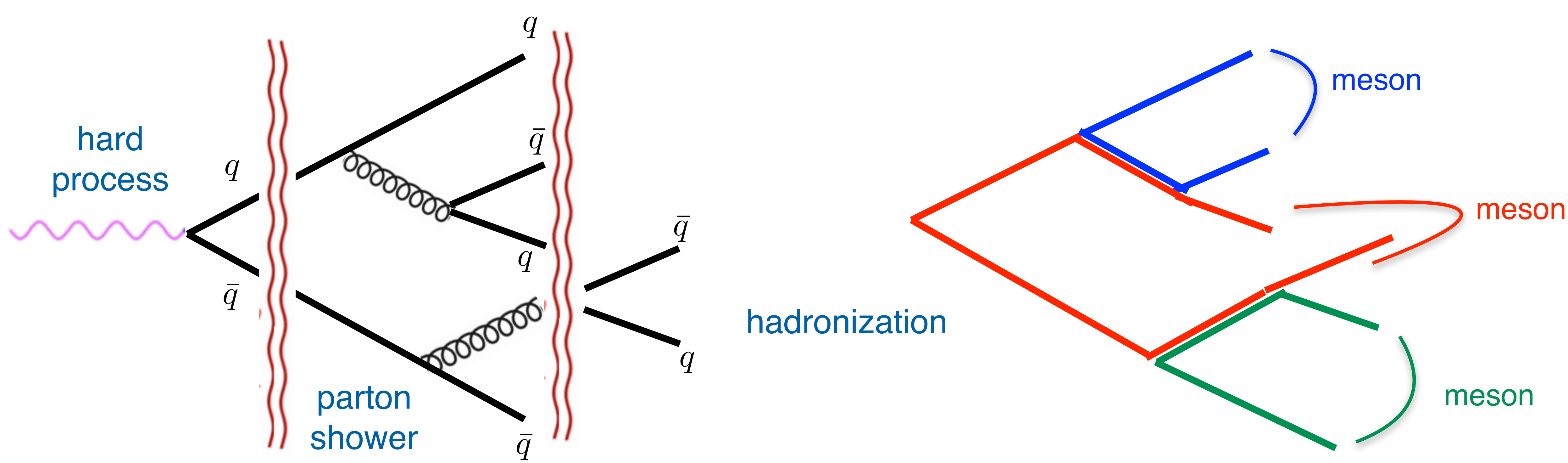


Hadronization

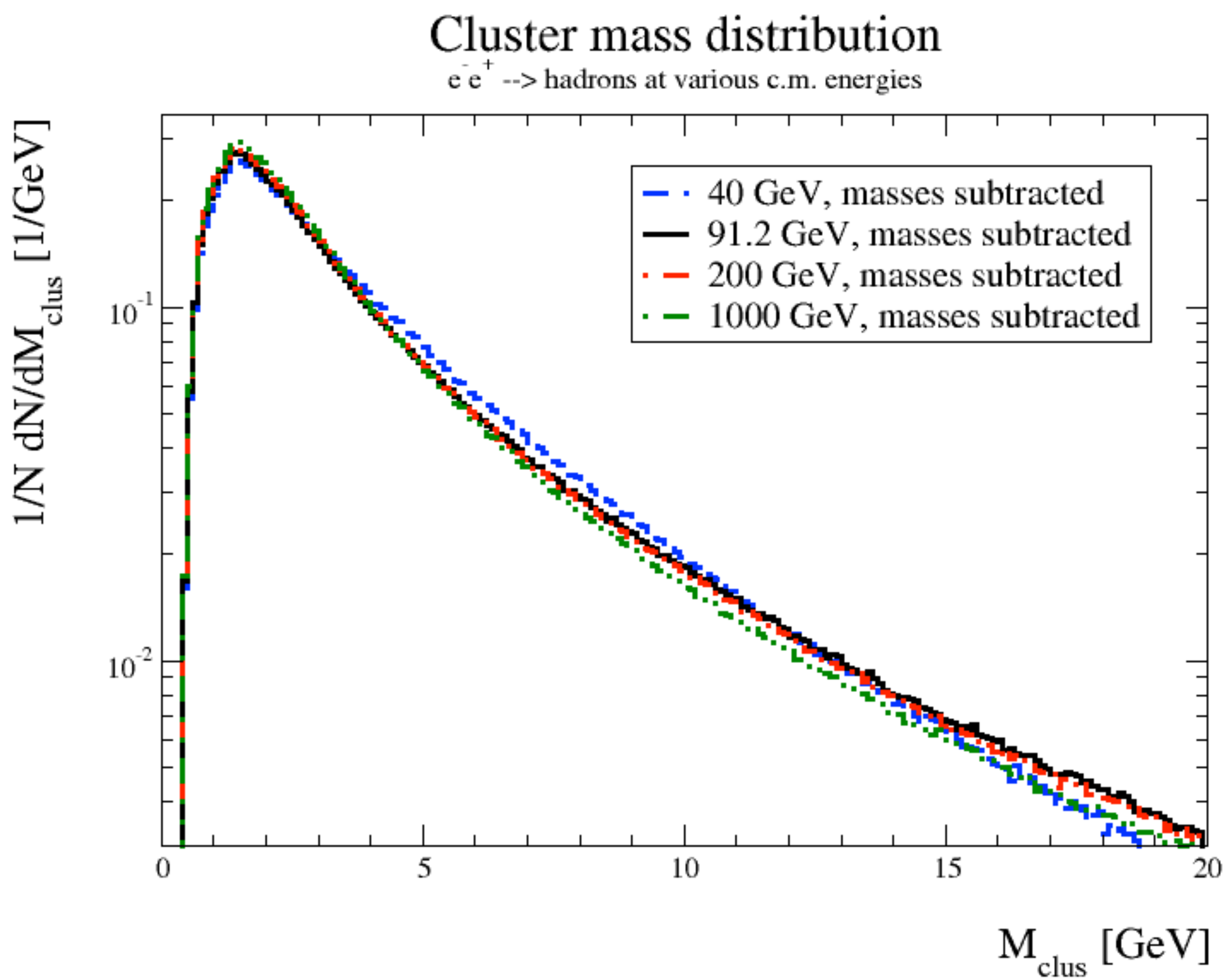
- By the end of the shower (scale $t_c \sim \Lambda_{QCD}$, i.e. 1 GeV) perturbation theory breaks down.
- The strength of the interaction means partons begin to feel bound together into hadrons, i.e. hadronization occurs.
- This is also typically handled by parton shower event generators, that use a variety of phenomenological models to translate final partons into hadrons.
- These turn quantitative ideas into algorithms for performing combinations
  - typically involving around a dozen parameters that must be tuned to existing high-quality data from electron-positron collisions at LEP
- Popular examples include:
  - the Lund string model, used in PYTHIA
  - the cluster model, used in HERWIG and SHERPA
- Many of the hadrons produced this way are unstable and decay further into lighter hadrons, also handled by the event generator, e.g. according to known branching ratios.

Example: cluster fragmentation

- At the end of the shower, force all gluons to decay into quark-antiquark pairs.
  - for example, in HERWIG the gluon acquires a non-perturbative mass that allows a two-body decay; the gluon mass (~ t_c) becomes a parameter of the hadronization model.
- Working in the $N_c \to \infty$ limit, combine quarks and anti-quarks of the same color into color-singlets; these will predominantly be close in phase-space.
- The clusters will have the corresponding flavor quantum numbers of the pair, generating mesons
  - making baryons in this model requires the introduction of diquarks, hypothetical bound states of two quarks or two anti-quarks, to which the gluons could also decay



Local parton-hadron duality



- Masses of clusters produced by hadronization are controlled by the shower cutoff t_c and are O(GeV)
  - independent of the process energy
- As a result, observables formed from hadrons closely follow partonic counterparts.
- Manifestation of local parton-hadron duality.

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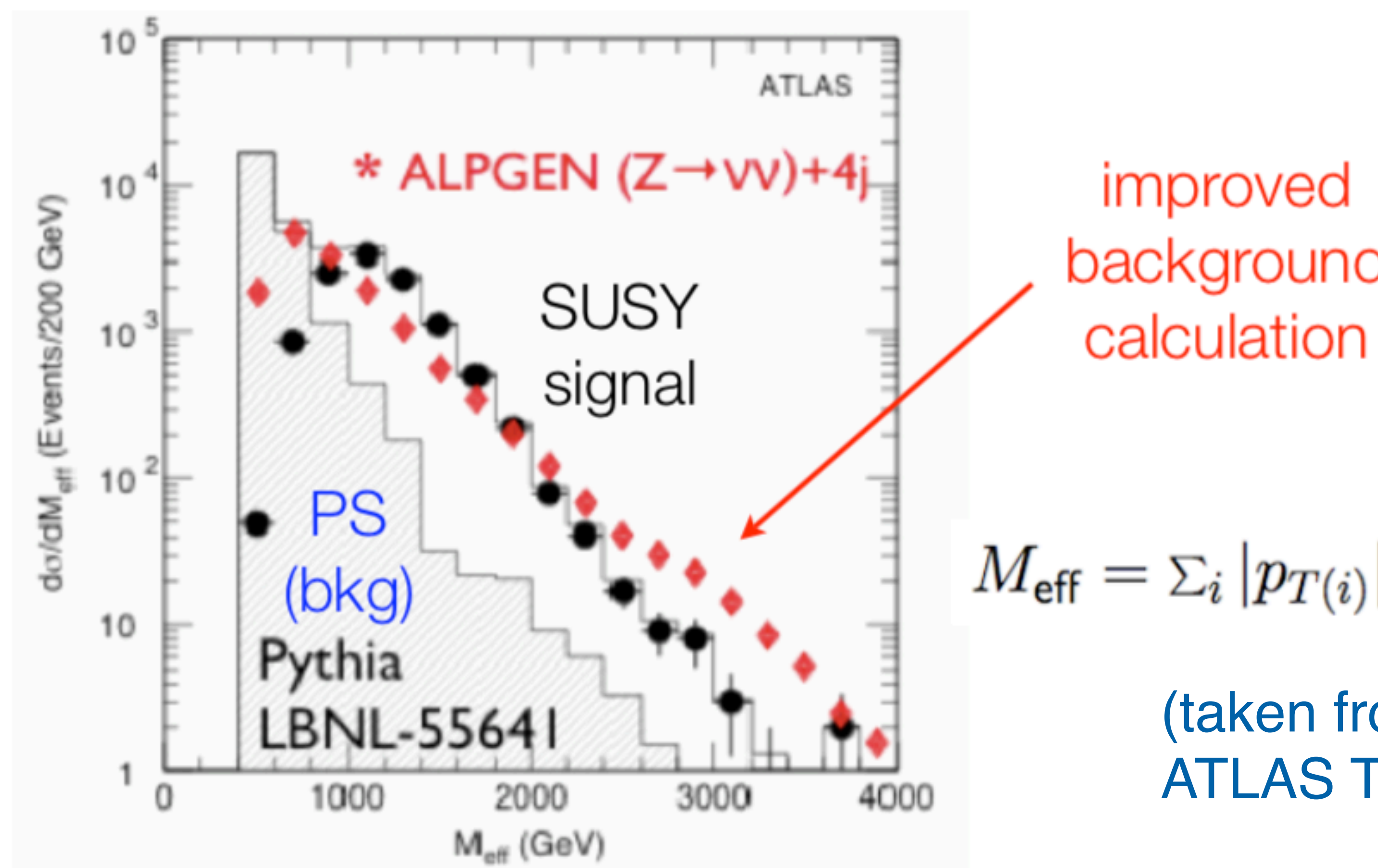
Improving event generators

- At least historically, event generators relied on identifying a hard process for which the matrix elements could be computed and a corresponding hard scale identified, then the parton shower takes over.
- As we have discussed, this separation is motivated by:
  - hard process — matrix elements computed exactly, but for small number of particles
  - parton shower — soft and collinear approximation, but to all orders
- Can lead to problems when observables are constructed that are sensitive to hard ME contributions beyond the one included in the event generator.
  - in that case, the soft and collinear radiation generated by the parton shower just may not do a good enough job in the region of interest

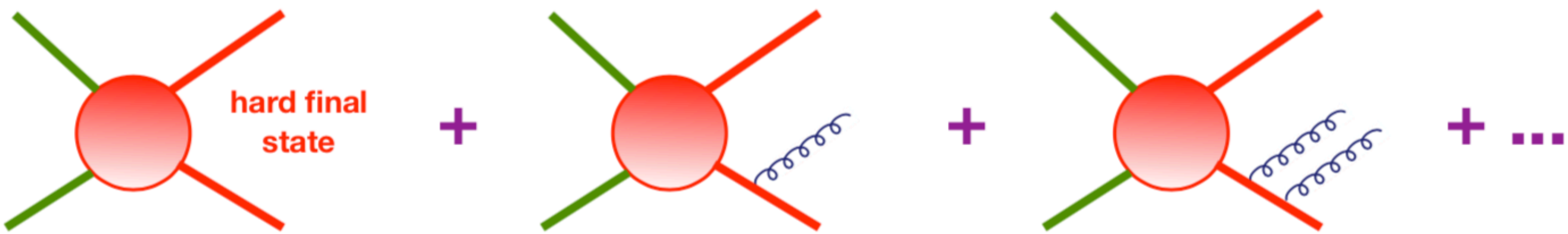


$$M_{\text{eff}} = \Sigma_i |p_{T(i)}| + \not{E}_T$$

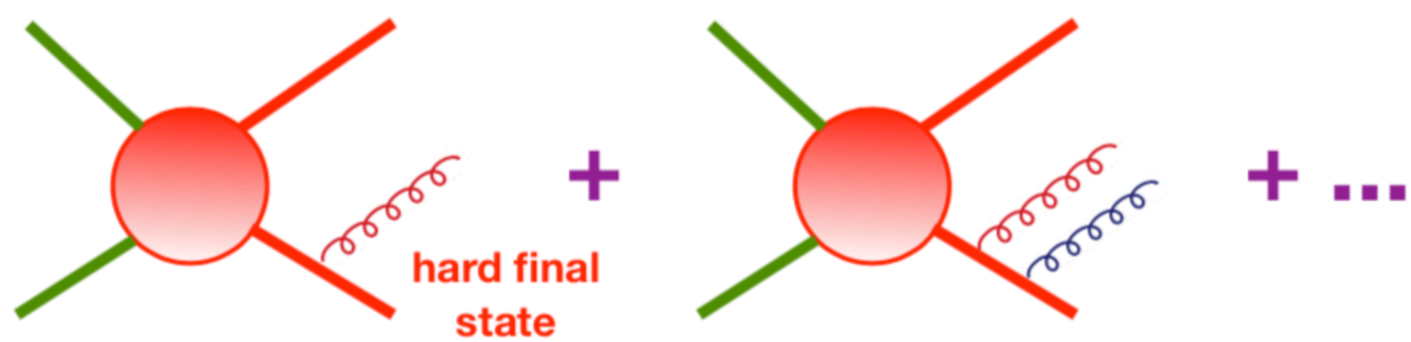
(taken from ATLAS TDR)

Matrix-element merging

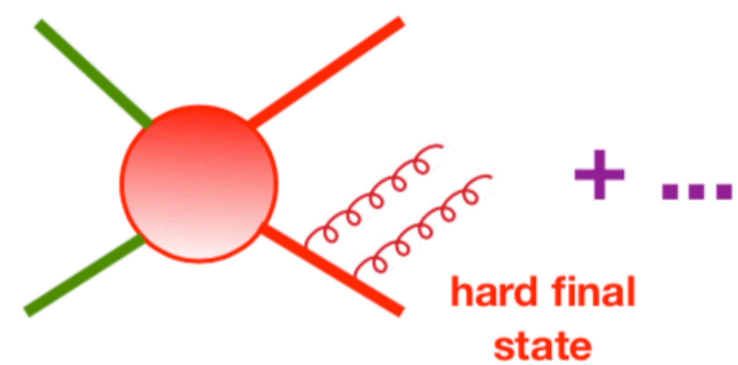
- The key to fixing this is to ensure that exact matrix elements are used for all sufficiently hard jets.
- Decompose phase space into regime of hard jet production (MEs) and jet evolution (PS), often with a jet resolution criterion (Q_{cut}).



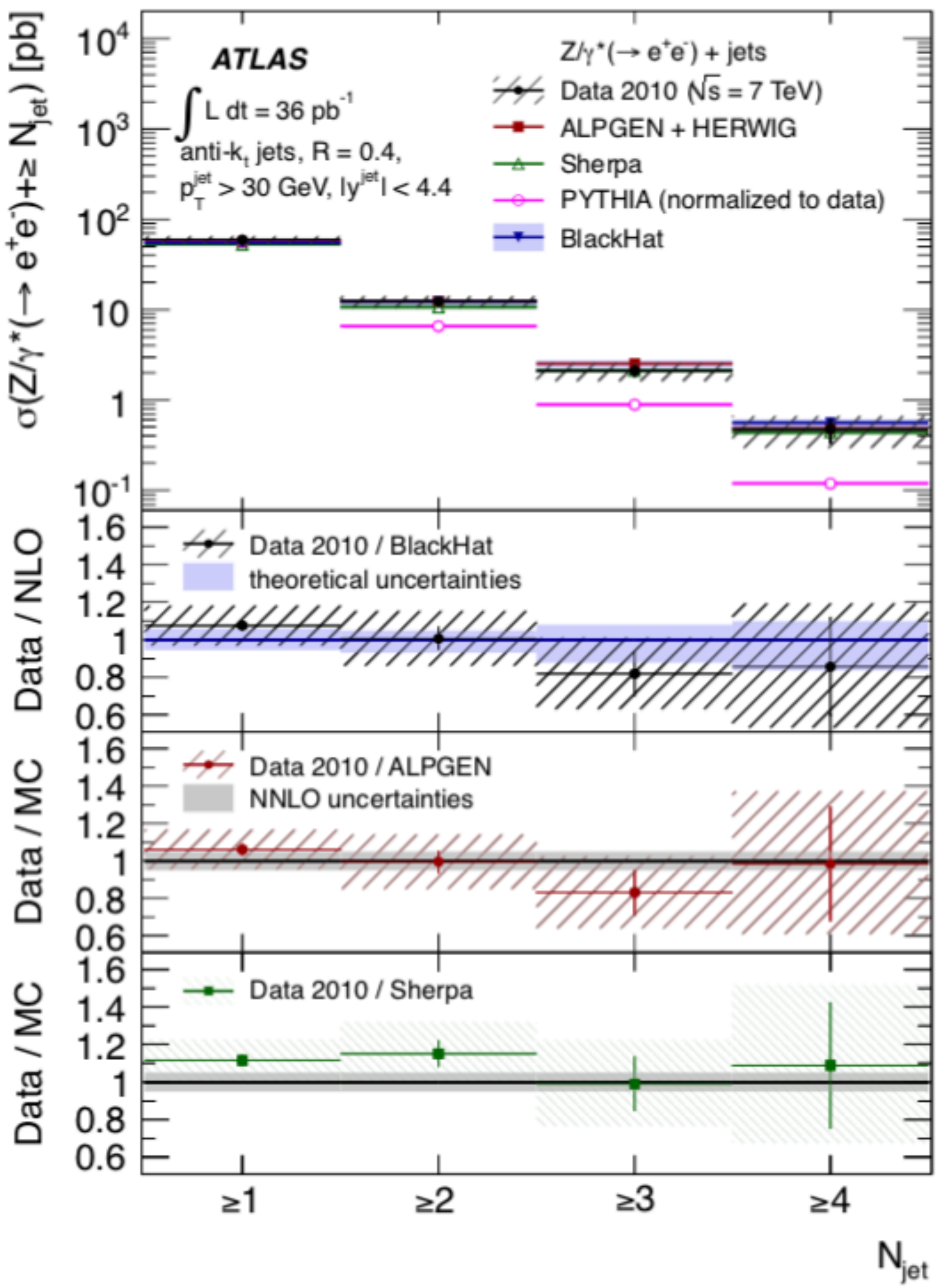
- The obvious issue is that one has to avoid any double-counting of emissions.

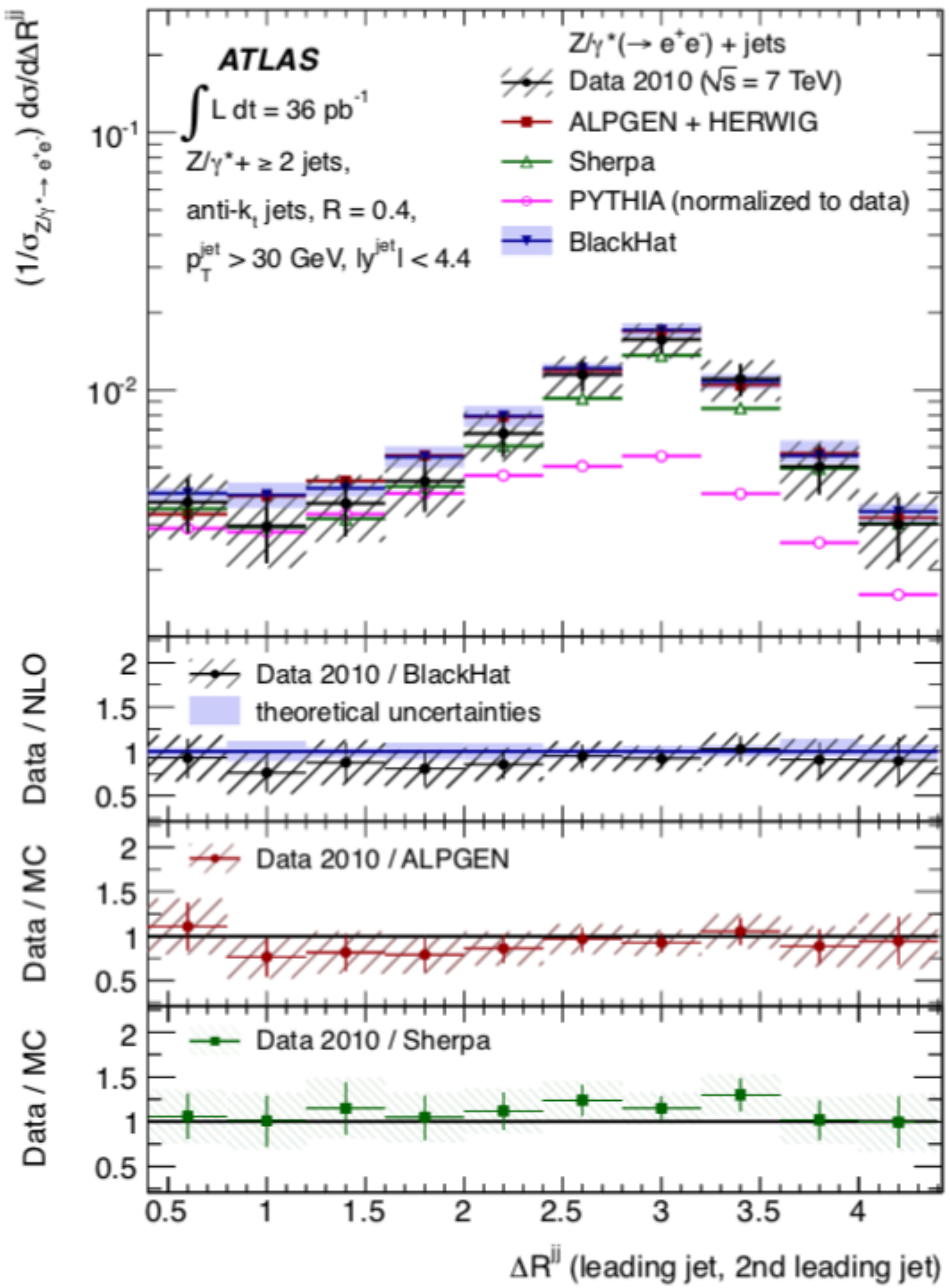


- Many schemes for performing this merging are available (CKKW, MLM, METS, …) and are used in SHERPA, MG5_aMC@NLO etc.



Example: merging for Z+jet events





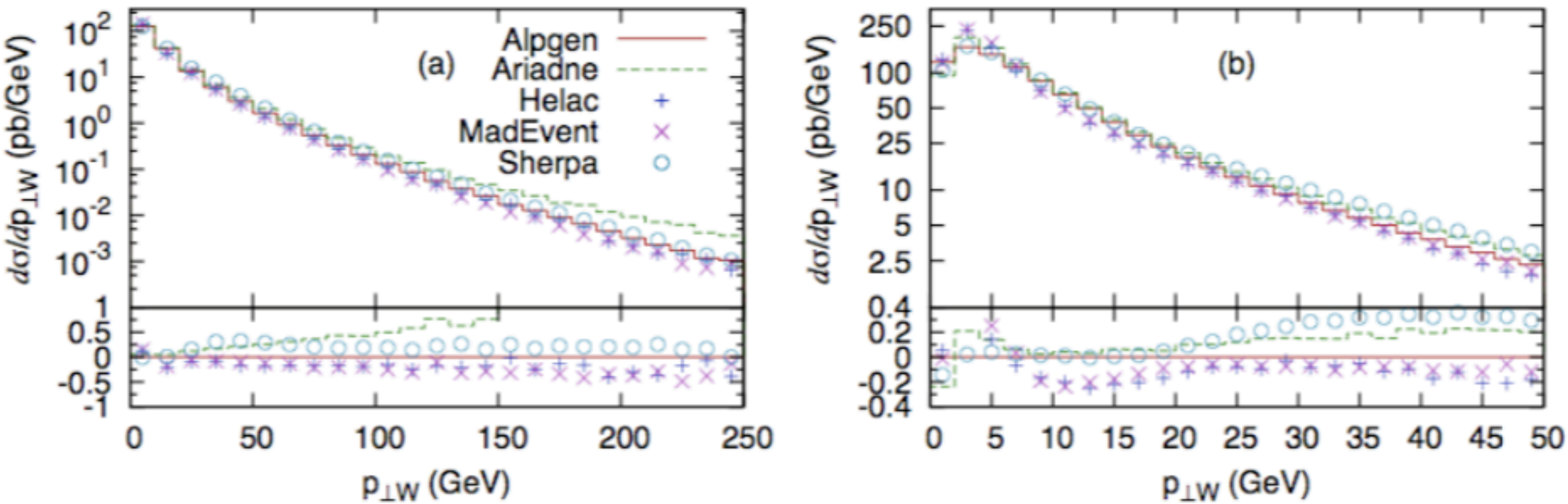
ATLAS, hep-ex/1111.2690

Pure PYTHIA cannot describe 2nd+ jet since they only come from PS but merged predictions in ALPGEN and SHERPA good

Differences between merging prescriptions

- These approaches are similar in spirit but can result in subtle differences, for example related to whether or not the formal accuracy of the shower (how many logs are resummed) is properly retained

Alwall et al (2007) [Tevatron]



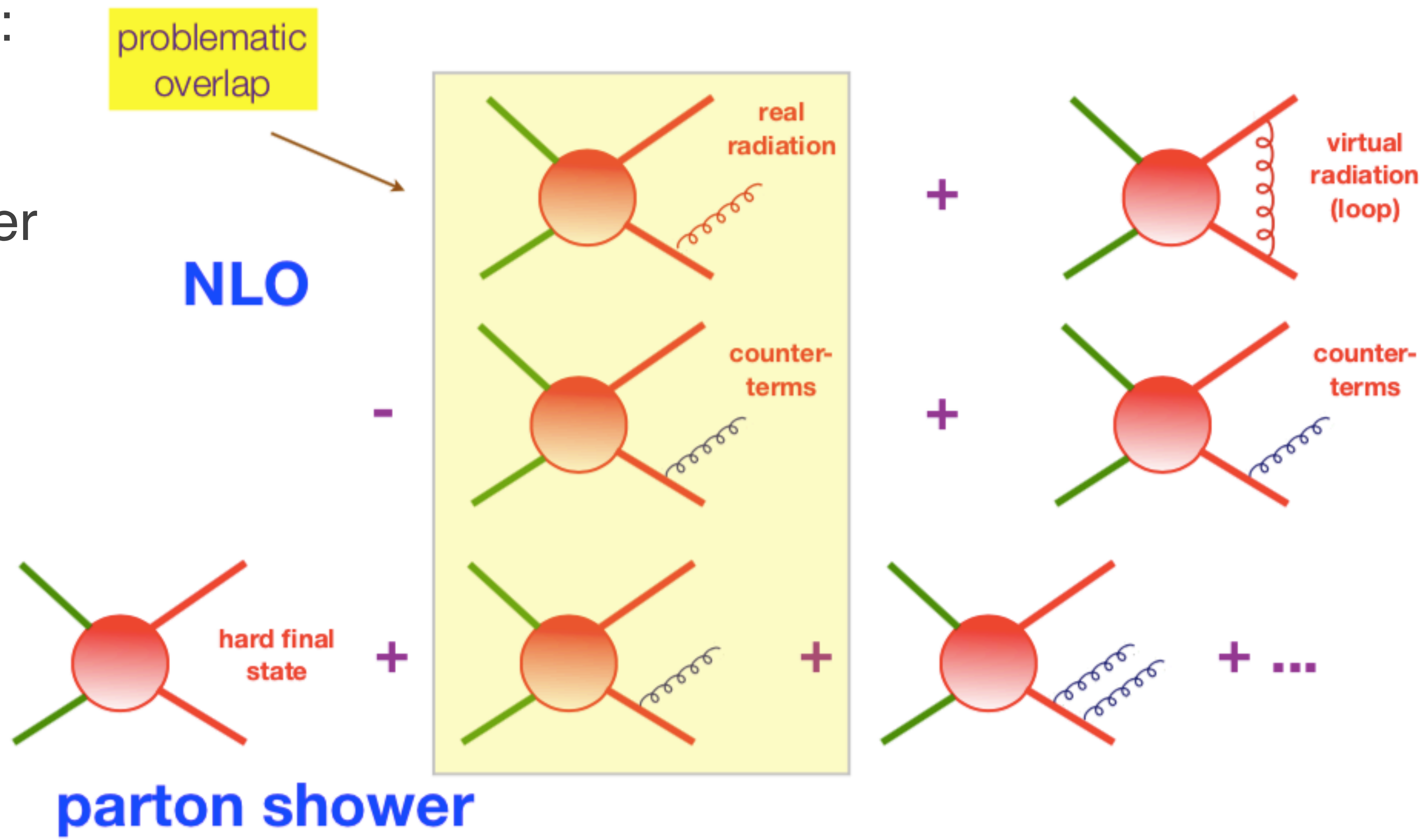
- However, in general very good agreement between the different methods
  - still ongoing work in this area to ensure no precision is lost and to understand remaining systematic uncertainties

Going up a gear

- Even after adding extra emissions, overall rate is still fixed at leading order.
- To improve this, must instead try to attach parton shower to NLO prediction.

- Obvious problem: overlap between real radiation and parton shower evolution.

- Have to find a way to ensure subtraction terms are not double-counted → matching.



Fermilab

Matching in (a)MC@NLO

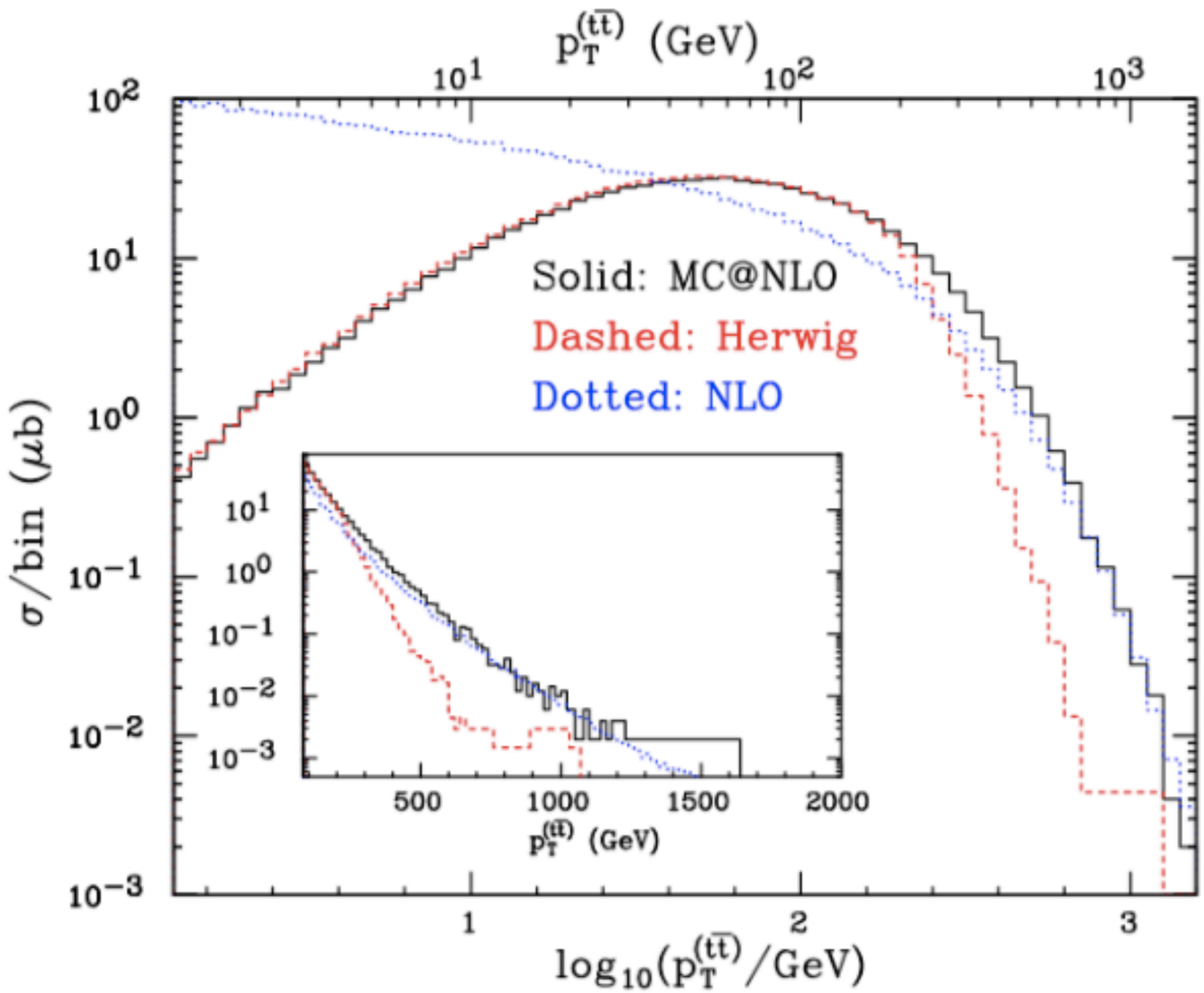
- Separate the real emission correction into a part that is realized by the parton shower (driven by Sudakov form factors) and a hard remainder.
  - subtraction terms produced by the shower itself

- First realized in MC@NLO (+HERWIG) in top-pair production.

  Frixione and Webber (2003)

- Resulting prediction matches smoothly between pure parton shower and pure NLO.

transverse momentum of top pair



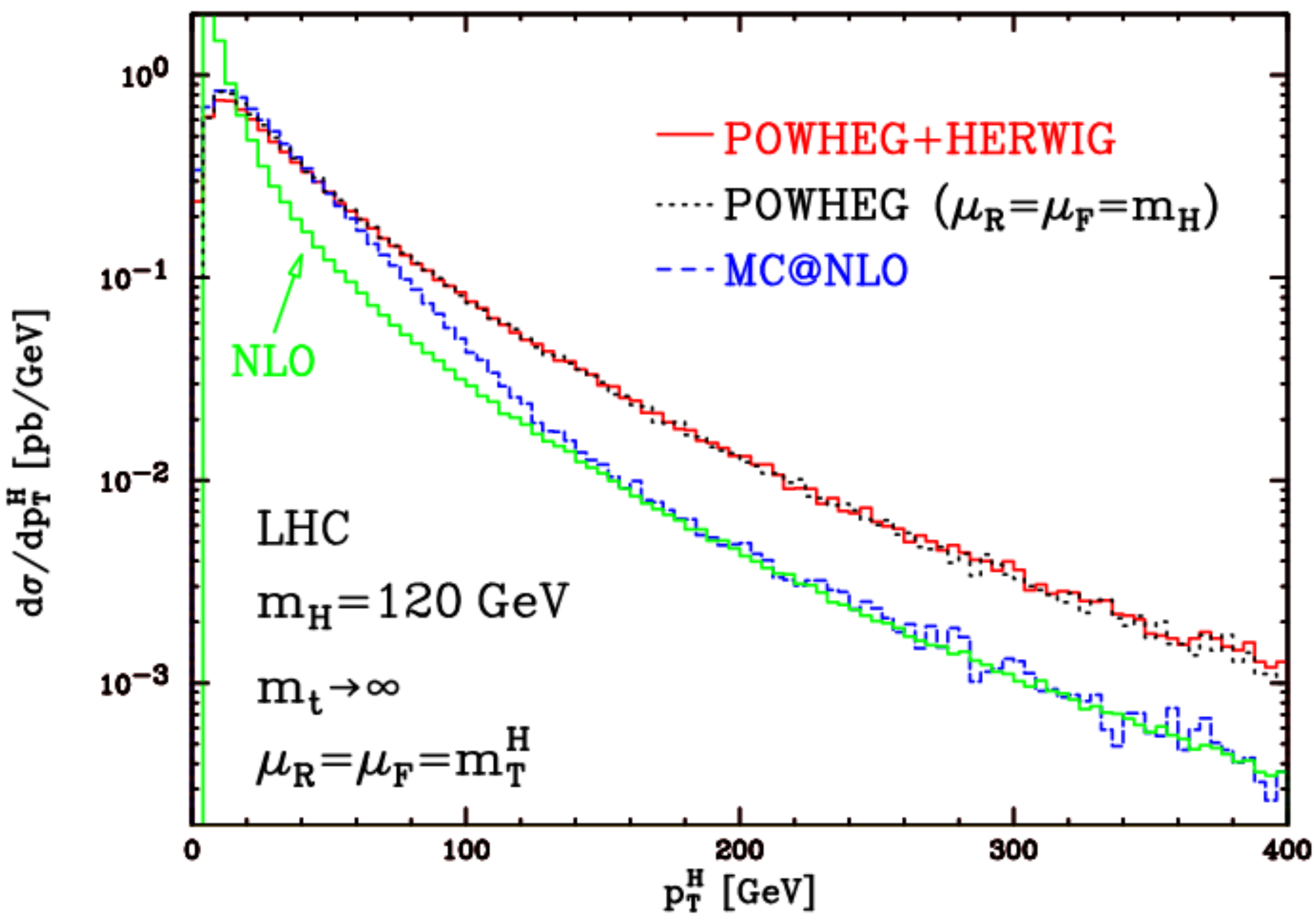
Fermilab

Matching in POWHEG

- Re-express NLO result as contributions that look like LO and a remainder.
  - LO-like terms produce “local” (event-by-event) K-factor, to which shower can be applied

- Requires a bit more work to ensure exact fixed-order behavior is obtained at high p_T
  - somewhat a matter of taste whether this is a bug or a feature, especially since (in this case) naive result very close to NNLO prediction in high-p_T tail

Higgs boson transverse momentum

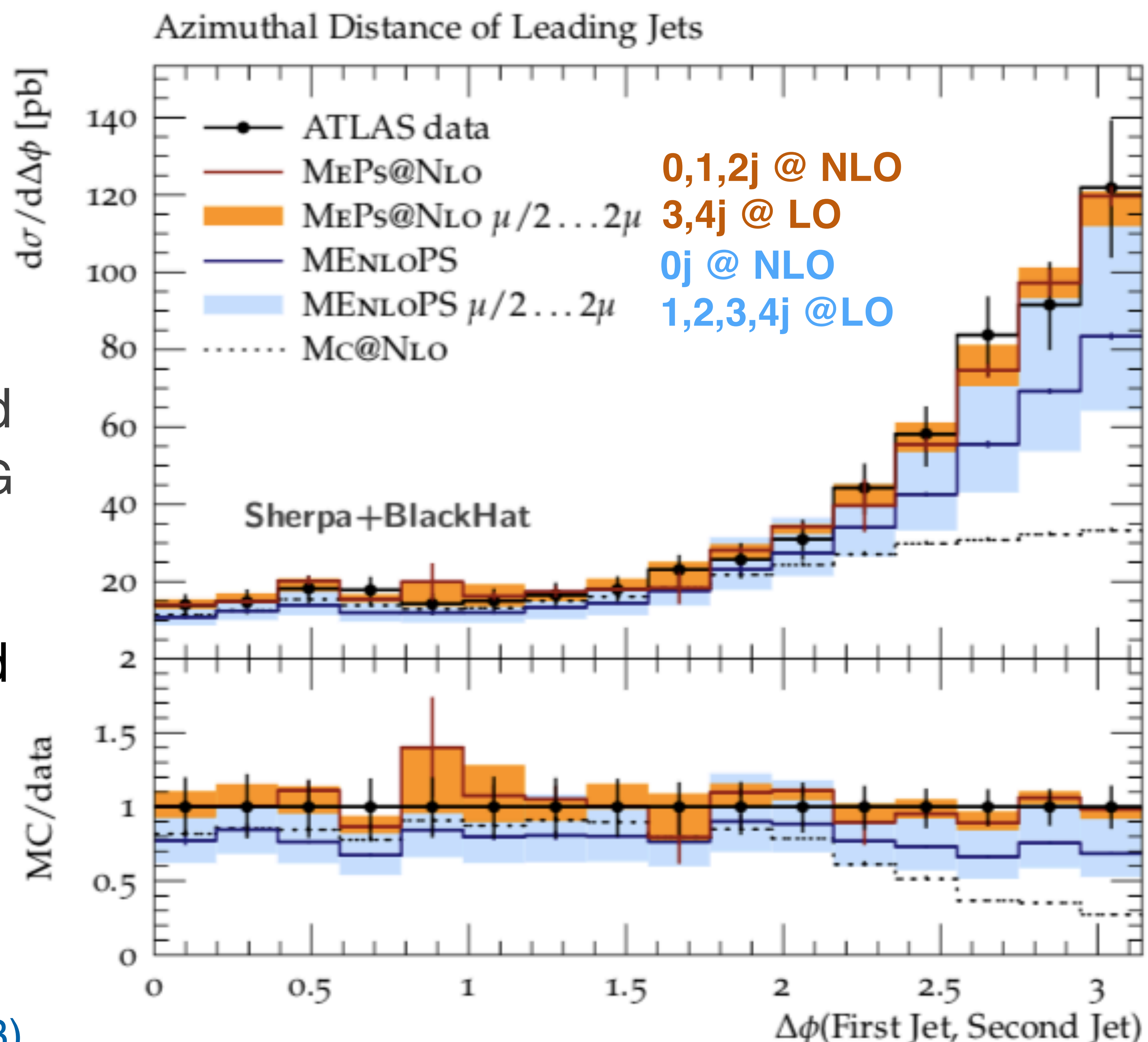


The best of both worlds: hybrid matching and merging

- Parton shower with NLO accuracy and multiple hard matrix elements.
- MENLOPS approach: use NLO matching for lowest-multiplicity final state, merged with LO MEs beyond
  - can use MC@NLO or POWHEG

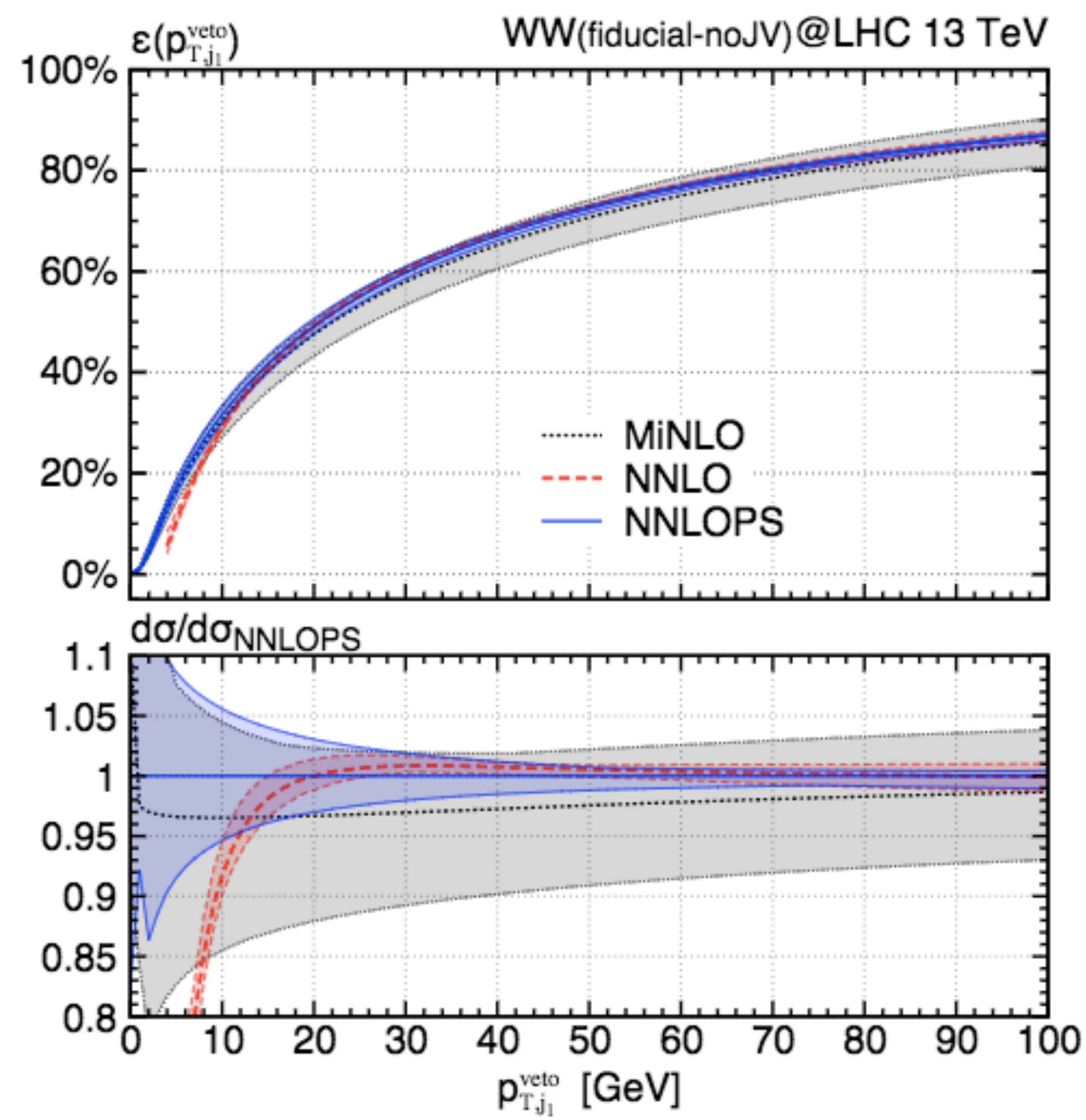
    Hamilton, Nason (2010)
    Hoeche at al (2011)
- MEPS@NLO (SHERPA) and FxFx (MG5_aMC@NLO): merge NLO matrix elements for several jet multiplicities

  Gehrmann, Hoeche et al (2013);
  Frederix and Frixione (2012);
  Lonnblad and Prestel; Platzer (2013)



Precision event simulation

- For the simplest cases — e.g. Higgs, W, Z production — it has been possible to construct full event generators that include NNLO QCD corrections.
- First successful approach: NNLOPS
- Uses MINLO, a clever scale-setting prescription with weighting of MEs by Sudakov factors, in combination with POWHEG.
  - originally used to improve poor behavior of NLO calculations with a jet
  - but can use fixed-order NNLO result to extend inclusive accuracy to same order
- Used for a variety of processes, most recently WW production
  - especially important there, where modeling of jet activity important for study of jet veto efficiency

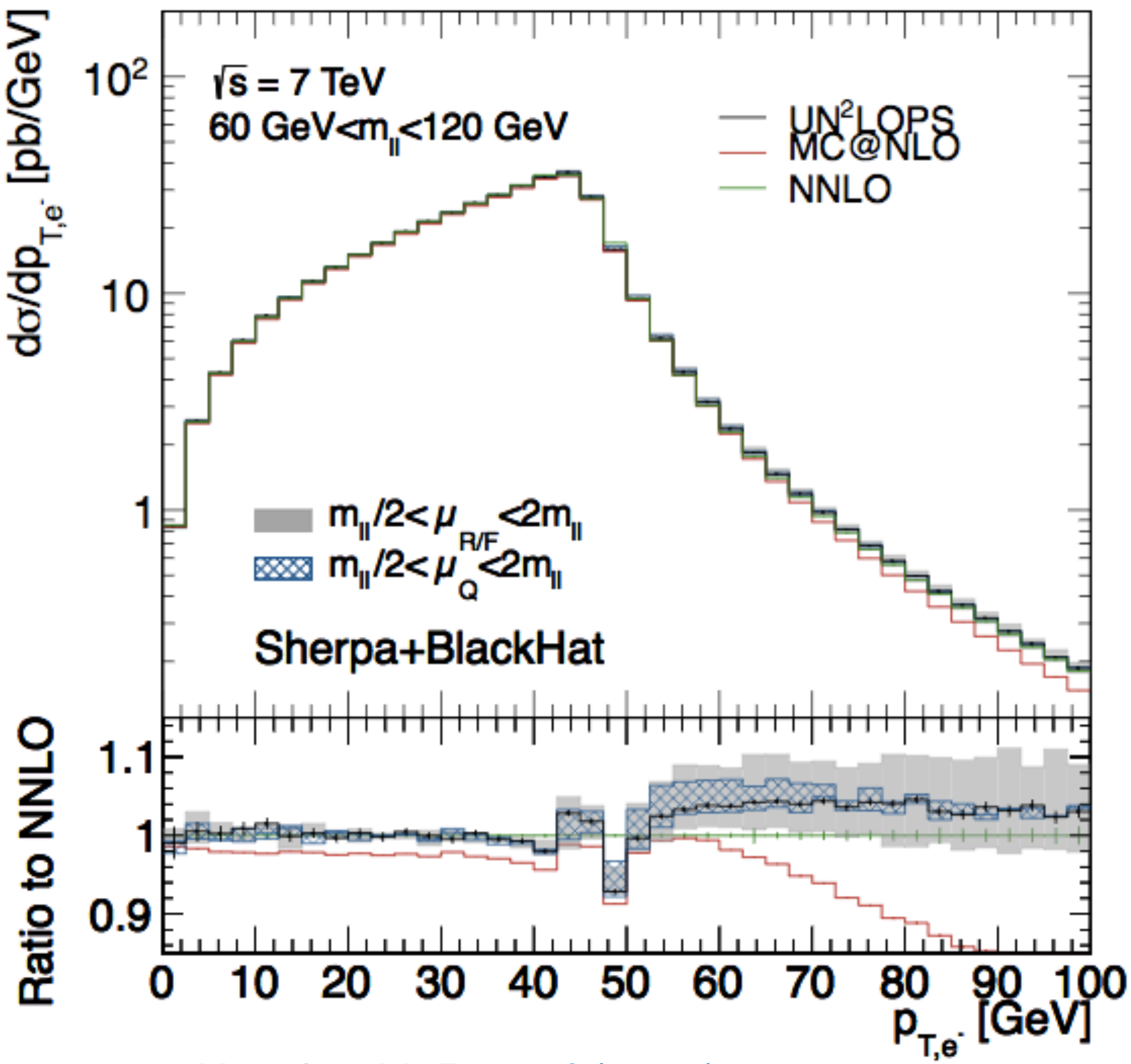


Re, Wiesemann, Zanderighi (2018)

Another approach to precision event simulation

- Alternative provided by UNNLOPS.
  - applied to color-singlet processes using Q_T-subtraction method for fixed-order NNLO.
  - implemented in SHERPA.

- Example: transverse momentum spectrum of electron in Z production
  - illustrates importance of combining NNLO precision region ($p_T < m_Z/2$) with domain where multiple soft emissions are important (parton shower), $p_T \sim m_Z/2$



Hoeche, Li, Prestel (2014)

Topics I haven't had time to cover

- Have only scratched the surface of many of the topics here — much more detail in reviews, books and original literature.
- In addition, I haven't really talked about:
  - analytic resummation techniques: identifying and resumming logarithms without using a parton shower. Many techniques ("CSS", "b-space", soft-collinear effective theory - SCET) with application to different types of logarithms (low p_T, threshold, small jet radius, etc.)
  - soft QCD: total hadronic cross-sections, modeling multiple parton interactions and the underlying event. Important for holistic approach to event generation & high luminosity.
  - QCD in the boosted regime: increasingly important at the LHC: atypical kinematics require moving beyond fixed-order, heavy reliance on resummation techniques and parton showers
  - LHC phenomenology: the concepts introduced here have profound impacts on many analyses at the LHC, beyond just higher-order K-factors and simple event generation
  - interplay with electroweak effects: often necessary to include NLO EW corrections at same time as NNLO QCD. Similar to NLO QCD but with own subtleties. Corrections are especially important at high p_T where effects are enhanced by $\log(p_T/m_W)$

If you have questions, send me an email: johnmc@fnal.gov

Summary

- Introduction to the theory of QCD
  - Lagrangian, color, Feynman rules, strong coupling
- QCD for hadron colliders
  - factorization, parton distribution functions, hard scattering
- Structure of QCD matrix elements
  - infrared singularities, real and virtual radiation
- Beyond leading order
  - techniques for NLO, NNLO and beyond
- Parton shower techniques
  - Sudakov factors, resolvable emissions, hadronization
- Modern event generators
  - merging, matching, hybrid schemes, precision matching