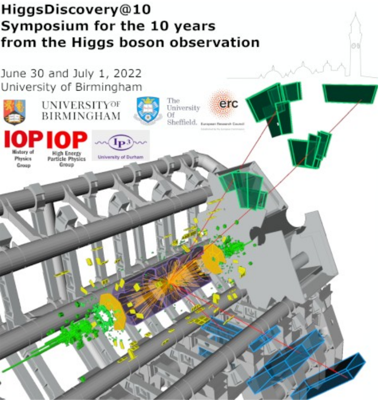
Theory Calculations
and
Monte Carlo Event Generators
in
Higgs Boson Discovery

Frank Krauss

Durham University

IP3

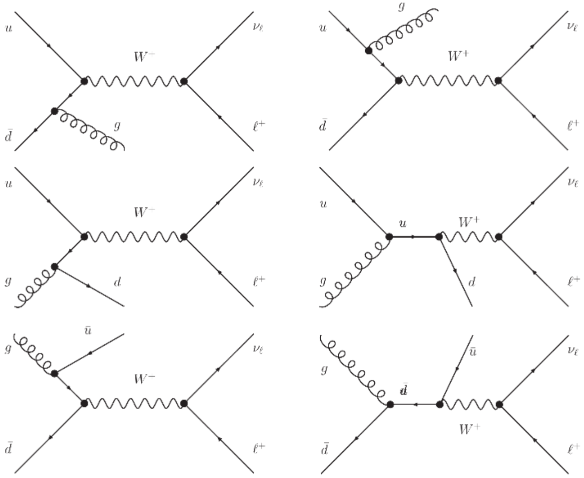


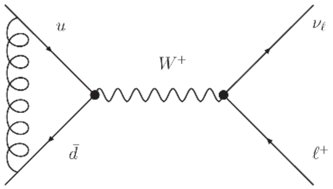
Outline

- Calculations? Which calculations?
- What was in the Monte Carlo box in 2012?
- What is in the box now?
- What will be in the box in 10 years?

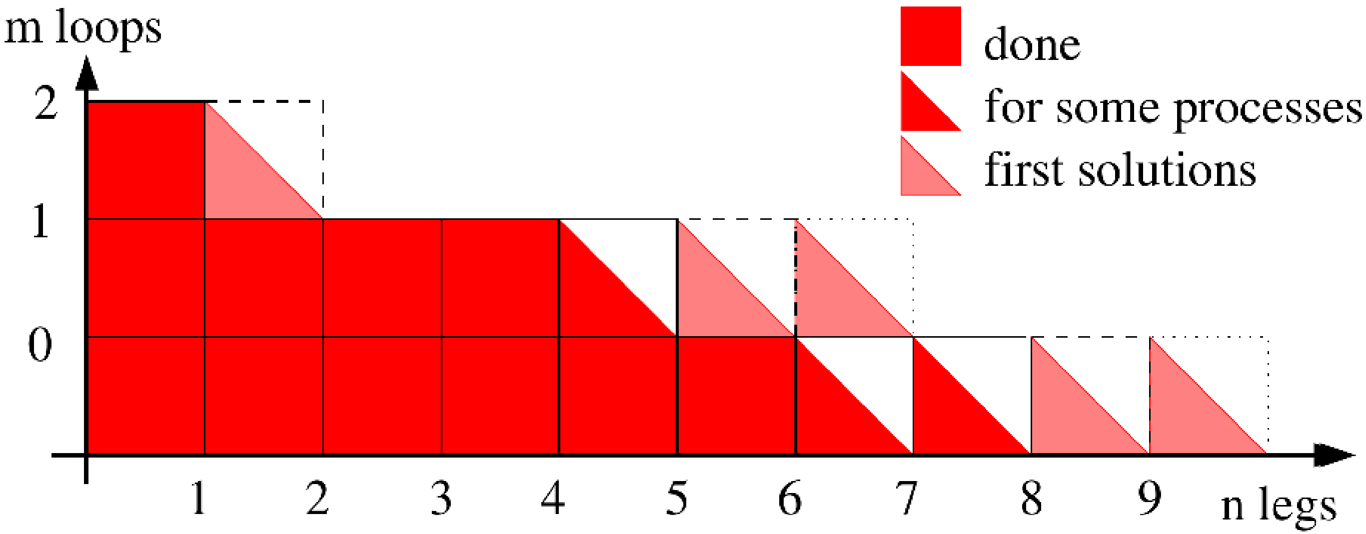
Calculations?

Which calculations?





Fixed Order for Signals & Backgrounds

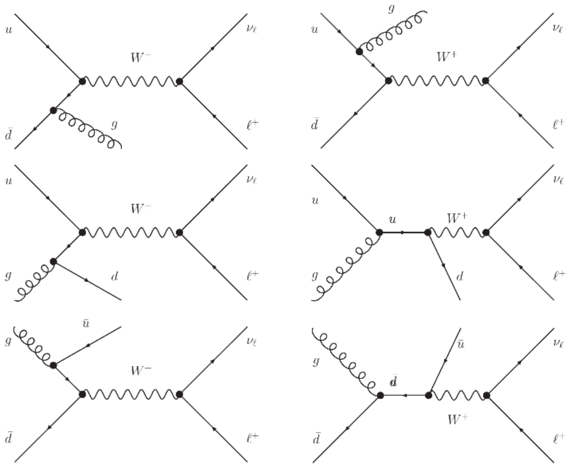


Fixed Order for Signals & Backgrounds

- **Higgs Boson Production Processes**
  - **gg → H**: NNLO (QCD) + NLO (EW) + NNLL (QT resummation)
    (note: calculations mostly in effective vertex approximation)
  - **qq → VH**: NNLO (QCD) + NLO (EW)
  - **VBF**: NLO (QCD) + NLO (EW)
  - **ttH**: NLO (QCD)

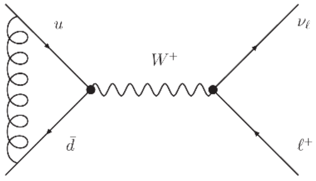
- **Higgs Boson Decays**
  - **BR's**: at least NLO (QCD) + NLO (EW) throughout
  - **H → 4l**: NLO (EW) as parton-level Monte-Carlo

Fixed Order (NLO) example



$$\mu^{4-D}\int\frac{\mathrm{d}^Dk}{(2\pi)^D}\left|\mathcal{M}^{(0)}_{u\bar{d}\to W^+g}\right|^2=\left|\mathcal{M}^{(0)}_{u\bar{d}\to W^+}\right|^2\frac{\alpha_s}{2\pi}C_F\left(\frac{\mu^2}{Q^2}\right)^{\varepsilon}c_\Gamma$$

$$\times\left[\overbrace{\left(\frac{2}{\varepsilon^2}+\frac{3}{\varepsilon}+\frac{\pi^2}{3}\right)\delta(1-z)}^{\text{cancelled with virtual}}+\left(\frac{4}{1-x}\log\frac{(1-z)^2}{z}\right)_+-2(1+z)\log\frac{(1-z)^2}{z}\;\underbrace{-\frac{2}{\varepsilon}\frac{\mathcal{P}^{(1)}_{qq}(z)}{C_F}}_{\text{absorbed into PDF}}\right]$$



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

Fixed Order (NLO) anatomy

- Infrared divergences **universal** – depend on external particles only.
- Construct **process-independent** infrared subtraction terms for real and virtual corrections

$$\mathcal{S}_N(\Phi_\mathcal{B} \otimes \Phi_1) = \mathcal{B}_N(\Phi_\mathcal{B}) \otimes \mathcal{S}_1(\Phi_\mathcal{B} \otimes \Phi_1)$$
$$\mathcal{I}_N^{(\mathcal{S})}(\Phi_\mathcal{B} \otimes \Phi_1) = \mathcal{B}_N(\Phi_\mathcal{B}) \otimes \mathcal{I}_1^{(\mathcal{S})}(\Phi_\mathcal{B})$$

- Create "factorising phase space mapping": $\Phi_\mathcal{R} = \Phi_\mathcal{B} \otimes \Phi_1$

$$\begin{aligned} \mathrm{d}\sigma &= \mathrm{d}\Phi_\mathcal{B}\mathcal{B}_N(\Phi_\mathcal{B}) + \mathrm{d}\Phi_\mathcal{B}\mathcal{V}_N(\Phi_\mathcal{B}) + \mathrm{d}\Phi_\mathcal{R}\mathcal{R}_N(\Phi_\mathcal{R}) \\ &= \mathrm{d}\Phi_\mathcal{B}\left(\mathcal{B}_N + \mathcal{V}_N + \mathcal{I}_N^{(\mathcal{S})}\right) + \mathrm{d}\Phi_\mathcal{R}\left(\mathcal{R}_N - \mathcal{S}_N\right) \end{aligned}$$

Q_T - Resummation

- **Master formula**

$$\frac{\mathrm{d}\sigma_{AB\to W^+}}{\mathrm{d}y\,\mathrm{d}Q_\perp^2} = \sum_{ij} \frac{\hat{\sigma}^{(LO)}_{ij\to W^+}}{2\pi} \left\{ \int \frac{\mathrm{d}b_\perp^2}{\pi} \left[\mathrm{J}_0(\vec{b}_\perp \cdot \vec{Q}_\perp)\, \tilde{W}_{ij}(b;\, Q,\, x_A,\, x_B) \right] + Y_{ij\to W^+}(Q_\perp;\, Q,\, x_A,\, x_B) \right\}$$

- **Resummation part**

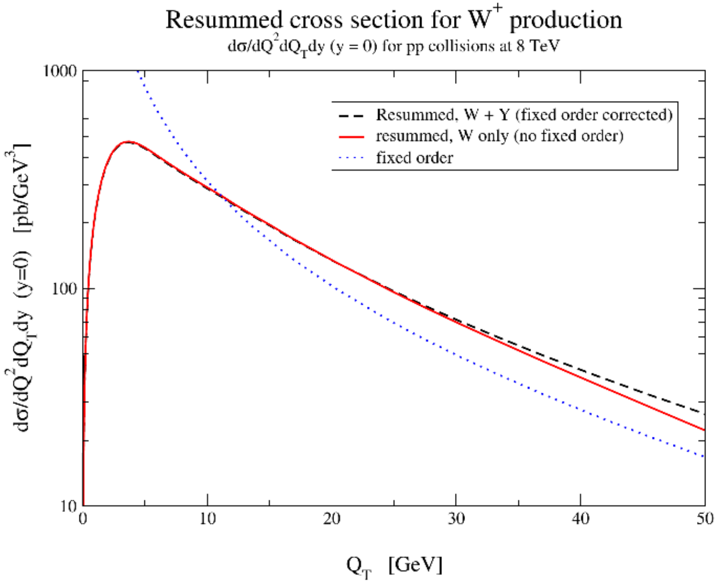
$$\tilde{W}_{ij}(b;\, Q,\, x_A,\, x_B)$$

$$= \sum_{ab} \left\{ \int_{x_A}^{1} \frac{\mathrm{d}\xi_A}{\xi_A} \int_{x_B}^{1} \frac{\mathrm{d}\xi_B}{\xi_B} \left[f_{a/A}\left(\xi_A, \frac{1}{b_\perp}\right) f_{b/B}\left(\xi_B, \frac{1}{b_\perp}\right) \right.\right.$$

$$\times \underbrace{C_{ia}\left(\frac{x_A}{\xi_A}, b_\perp; \mu\right) C_{jb}\left(\frac{x_B}{\xi_B}, b_\perp; \mu\right)}_{\text{corrections to factorisation}} \underbrace{H_{ab}\left(\frac{x_A}{\xi_A}, \frac{x_B}{\xi_B}; \mu\right)}_{\text{genuine loop corrections}}$$

$$\left.\left. \times \underbrace{\exp\left[- \int_{1/b_\perp^2}^{Q^2} \frac{\mathrm{d}k_\perp^2}{k_\perp^2} \left(A(k_\perp^2) \log \frac{Q^2}{k_\perp^2} + B(k_\perp^2) \right) \right]}_{\text{Sudakov form factor}} \right] \right\}$$

- **Example result**



accuracy	terms included
LL	$A^{(1)}$
NLL	$A^{(2)},\ B^{(1)},\ C^{(1)}$
NNLL	$A^{(3)},\ B^{(2)},\ C^{(2)}$

What was in the

Monte Carlo box in 2012?

Monte Carlos for Signals & Backgrounds

(ATLAS discovery paper)

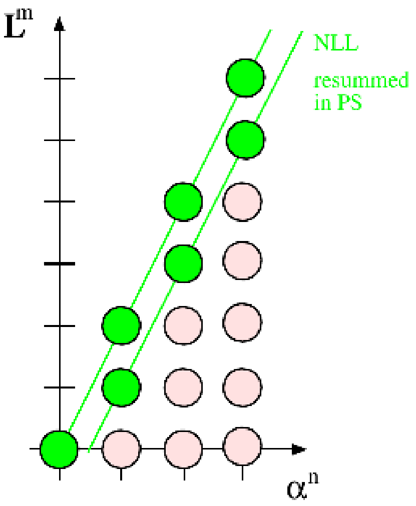
Process	Generator
ggF, VBF	POWHEG [57,58] + PYTHIA
WH, ZH, $t\bar{t}H$	PYTHIA
W + jets, Z/γ^* + jets	ALPGEN [59] + HERWIG
$t\bar{t}$, tW, tb	MC@NLO [60] + HERWIG
tqb	AcerMC [61] + PYTHIA
$q\bar{q} \to WW$	MC@NLO + HERWIG
$gg \to WW$	gg2WW [62] + HERWIG
$q\bar{q} \to ZZ$	POWHEG [63] + PYTHIA
$gg \to ZZ$	gg2ZZ [64] + HERWIG
WZ	MadGraph + PYTHIA, HERWIG
$W\gamma$ + jets	ALPGEN + HERWIG
$W\gamma^*$ [65]	MadGraph + PYTHIA
$q\bar{q}/gg \to \gamma\gamma$	SHERPA

Parton Showers

- Radiation pattern (trivial)

$$\mathrm{d}n_g^{q,g} = C_{q,g} \cdot \frac{\alpha_s(k_\perp^2)}{\pi} \cdot \frac{\mathrm{d}\omega}{\omega} \cdot \frac{\mathrm{d}k_\perp^2}{k_\perp^2}$$

- Double-logarithmic after cuts in energy ω and transverse momentum k_T



- Sudakov form factor

$$\Delta_{ij,k}^{(\mathcal{K})}(t, t_0) = \exp\left[-\int_{t_0}^{t} \frac{\mathrm{d}t}{t} \frac{\alpha_s}{2\pi} \int \mathrm{d}z \frac{\mathrm{d}\phi}{2\pi} \underbrace{\mathcal{K}_{ij,k}(t,\, z,\, \phi)}_{\text{splitting kernel for } (ij) \to ij \text{ (spectator } k)} \right]$$

- First emission off Born

$$\mathrm{d}\sigma_B = \mathrm{d}\Phi_N\, \mathcal{B}_N(\Phi_N)$$
$$\cdot \underbrace{\left\{ \Delta_N^{(\mathcal{K})}(\mu_N^2, t_0) + \int_{t_0}^{\mu_N^2} \mathrm{d}\Phi_1 \left[\mathcal{K}_N(\Phi_1) \Delta_N^{(\mathcal{K})}(\mu_N^2, t(\Phi_1)) \right] \right\}}_{\text{integrates to unity} \longrightarrow \text{"unitarity" of parton shower}}$$

Matrix Element Corrections

- Splitting kernels vs. matrix element

$$\mathrm{d}\Phi_1 \frac{\mathcal{R}_N(\Phi_{N+1})}{\mathcal{B}_N(\Phi_N)} \xrightarrow{\text{IR}} \mathrm{d}\Phi_1 \frac{\alpha_s}{2\pi} \mathcal{K}_{ij,k}(\Phi_1)$$

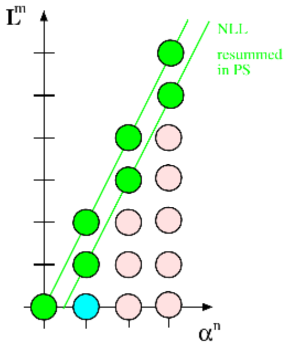
- Modified Sudakov form factor

$$\Delta_N^{(\mathcal{R}/\mathcal{B})}(\mu_N^2, t_0) = \exp\left[-\int_{t_0}^{\mu_N^2} \mathrm{d}\Phi_1 \frac{\mathcal{R}_N(\Phi_{N+1})}{\mathcal{B}_N(\Phi_N)}\right]$$

- First emission matrix-element corrected

$$\mathrm{d}\sigma_B = \mathrm{d}\Phi_N\, \mathcal{B}_N(\Phi_N)$$

$$\cdot \underbrace{\left\{\Delta_N^{(\mathcal{R}/\mathcal{B})}(\mu_N^2, t_0) + \int_{t_0}^{\mu_N^2} \mathrm{d}\Phi_1 \left[\frac{\mathcal{R}_N(\Phi_N \times \Phi_1)}{\mathcal{B}_N(\Phi_N)} \Delta_N^{(\mathcal{R}/\mathcal{B})}(\mu_N^2, t(\Phi_1))\right]\right\}}_{\text{once more: integrates to unity} \longrightarrow \text{“unitarity” of parton shower}}$$



Powheg

- Born with local K-factor

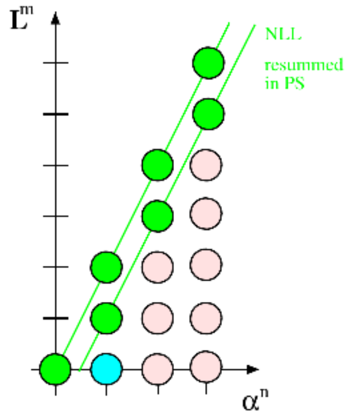
  virtual correction for Born kinematics and subtracted (and hence finite) real correction integrated over with factorised (N+1)-particle phase space

$$\mathrm{d}\sigma_N^{(\mathrm{NLO})} = \mathrm{d}\Phi_N\, \bar{\mathcal{B}}(\Phi_N)$$

$$= \mathrm{d}\Phi_N \Big\{ \mathcal{B}_N(\Phi_N) + \underbrace{\mathcal{V}_N(\Phi_N) + \mathcal{B}_N(\Phi_N) \otimes \mathcal{S}}_{\tilde{\mathcal{V}}_N(\Phi_N)}$$

$$+ \int \mathrm{d}\Phi_1 \left[\mathcal{R}_N(\Phi_N \otimes \Phi_1) - \mathcal{B}_N(\Phi_N) \otimes \mathrm{d}\mathcal{S}(\Phi_1)\right] \Big\}$$

Powheg



- Powheg master formula (vanilla version)

  combine Born with local K-factor and matrix element correction

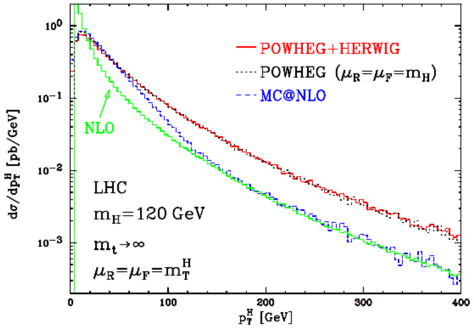
- first emission in Powheg:

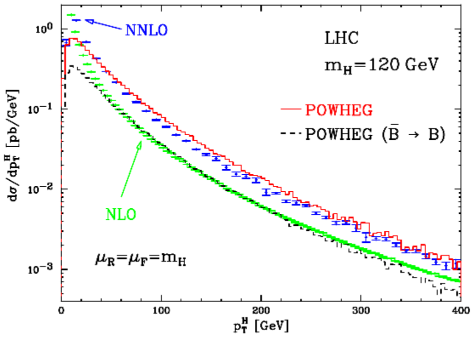
$$
\mathrm{d}\sigma_N^{(\mathrm{NLO})} = \mathrm{d}\Phi_N \, \bar{\mathcal{B}}(\Phi_N) \times \underbrace{\left\{ \Delta_N^{(\mathcal{R}/\mathcal{B})}(\mu_N^2,\, t_0) + \int_{t_0}^{\mu_N^2} \mathrm{d}\Phi_1 \frac{\mathcal{R}_N(\Phi_N \otimes \Phi_1)}{\mathcal{B}_N(\Phi_N)} \Delta_N^{(\mathcal{R}/\mathcal{B})}(\mu_N^2,\, k_\perp^2(\Phi_1)) \right\}}_{\text{integrating to yield 1 - ``unitarity of parton shower''}}
$$

Powheg

- Powheg results (vanilla version)
- large-pT spectrum too hard

  (they are NLO-corrected)





- split real-emission into two regimes (soft & hard):

$$\mathcal{R} = \mathcal{R}\left(\underbrace{\frac{h^2}{p_\perp^2 + h^2}}_{\mathcal{R}^{(S)}} + \underbrace{\frac{p_\perp^2}{p_\perp^2 + h^2}}_{\mathcal{R}^{(F)}} \right)$$

- and NLO correct only soft regime

$$d\sigma = d\Phi_B \bar{\mathcal{B}}^{(\mathrm{R}^{(S)})} \left[\Delta^{(\mathcal{R}^{(S)}/\mathcal{B})}(s,\, t_0) + \int_{t_0}^{s} d\Phi_1 \frac{\mathcal{R}^{(S)}}{\mathcal{B}} \Delta^{(\mathcal{R}^{(S)}/\mathcal{B})}(s,\, k_\perp^2) \right]$$

$$+ d\Phi_R\, \mathcal{R}^{(F)}(\Phi_R)$$

MC@NLO

- split real emission into "parton shower" and "finite" parts, subtract real with parton shower

$$\mathcal{R}_N = \mathcal{R}_N^{(S)} + \mathcal{R}_N^{(H)} = \mathcal{B}_N \otimes \mathrm{d}\mathcal{S}_1 + \mathcal{H}_N$$

- first emission in MC@NLO

  potential issue: inherit and NLO correct phase space coverage of parton shower

$$\mathrm{d}\sigma_N = \mathrm{d}\Phi_N \underbrace{\tilde{\mathcal{B}}_N(\Phi_N)}_{\mathcal{B}+\tilde{\mathcal{V}}} \left[\Delta_N^{(\mathcal{K})}(\mu_N^2, t_0) + \int_{t_0}^{\mu_N^2} \mathrm{d}\Phi_1 \, \mathcal{K}_{ij,k}(\Phi_1) \, \Delta_N^{(\mathcal{K})}(\mu_N^2, k_\perp^2) \right]$$
$$+ \mathrm{d}\Phi_{N+1} \, \mathcal{H}_N$$

Multijet merging: MEPS @ LO

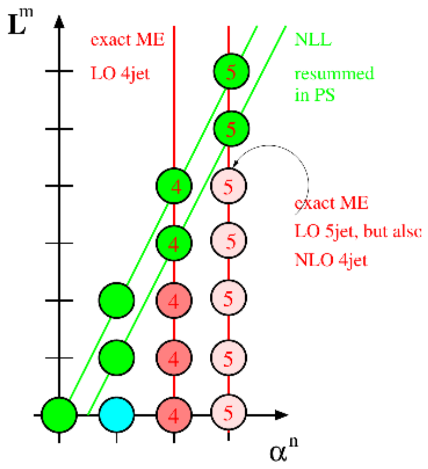
- use Born matrix elements with every (QCD) emission resulting in a jet with $Q > Q_J$
- first emission in MEPS@LO

  note: this time the square bracket is **not unitary**

$$\mathrm{d}\sigma = \mathrm{d}\Phi_N \,\mathcal{B}_N \left[\Delta_N^{(\mathcal{K})}(\mu_N^2,\, t_0) + \int_{t_0}^{\mu_N^2} \mathrm{d}\Phi_1 \,\mathcal{K}_N \Delta_N^{(\mathcal{K})}(\mu_N^2,\, t_{N+1})\Theta(Q_J - Q_{N+1})\right]$$

$$+\mathrm{d}\Phi_{N+1}\,\mathcal{B}_{N+1}\,\Delta_N^{(\mathcal{K})}(\mu_{N+1}^2,\, t_{N+1})\Theta(Q_{N+1} - Q_J)$$

Multijet merging: MEPS @ LO



- all emissions in MEPS@LO

$$
d\sigma = \sum_{n=N}^{n_{max}-1} \Bigg\{ d\Phi_n \mathcal{B}_n \overbrace{\left[\prod_{j=N}^{n-1} \Theta(Q_{j+1} - Q_J)\right]}^{(n-N)\text{ extra jets}} \overbrace{\left[\prod_{j=N}^{n-1} \Delta_j^{(\mathcal{K})}(t_j,\, t_{j+1})\right]}^{\text{no emissions off internal lines}}
$$

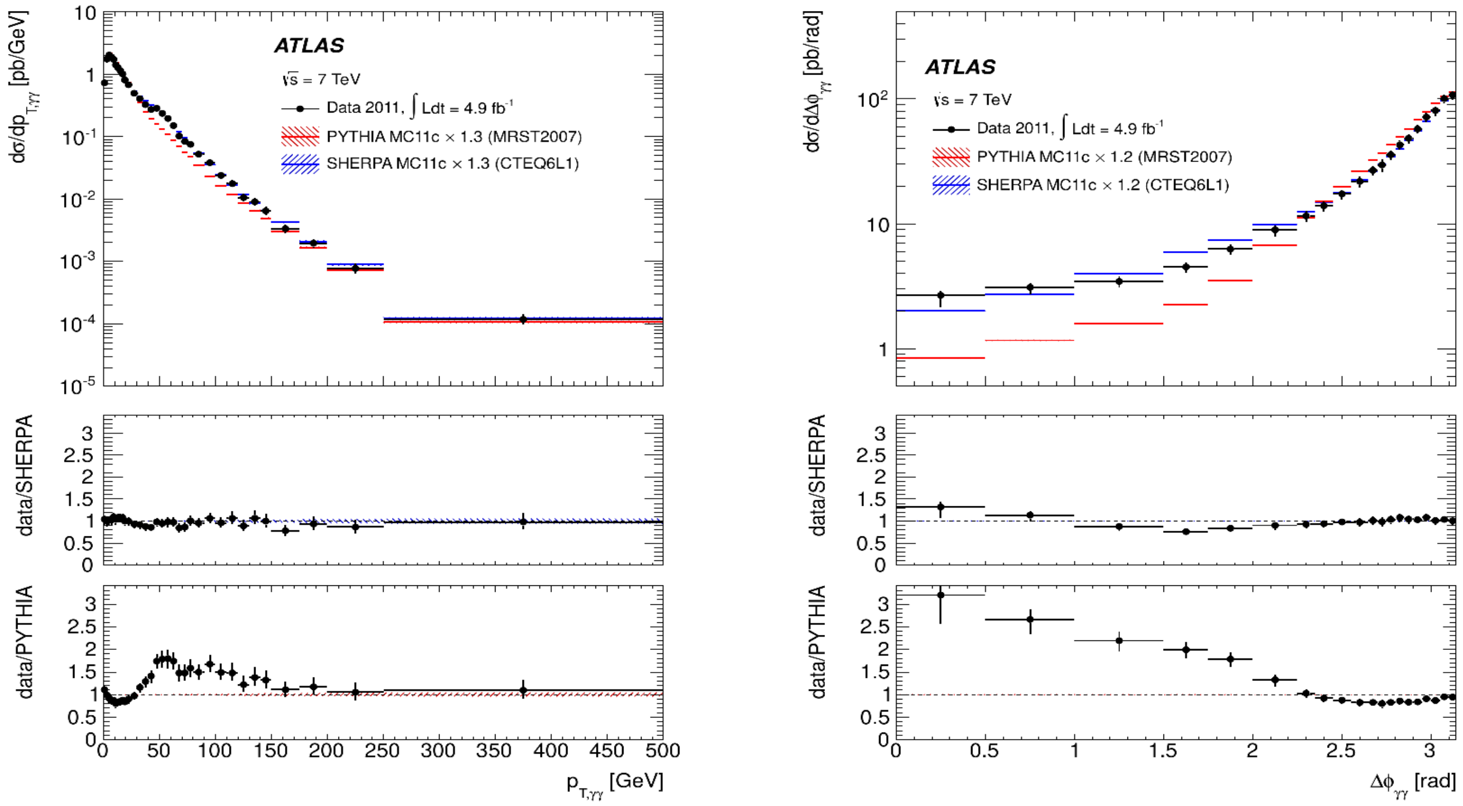
$$
\times \Bigg[\underbrace{\Delta_n^{(\mathcal{K})}(t_n, t_0)}_{\text{no emission}} + \underbrace{\int_{t_0}^{t_n} d\Phi_1\, \mathcal{K}_n \Delta_n^{(\mathcal{K})}(t_n, t_{n+1}) \Theta(Q_J - Q_{n+1})}_{\text{next emission no jet \& below last ME emission}} \Bigg]
$$

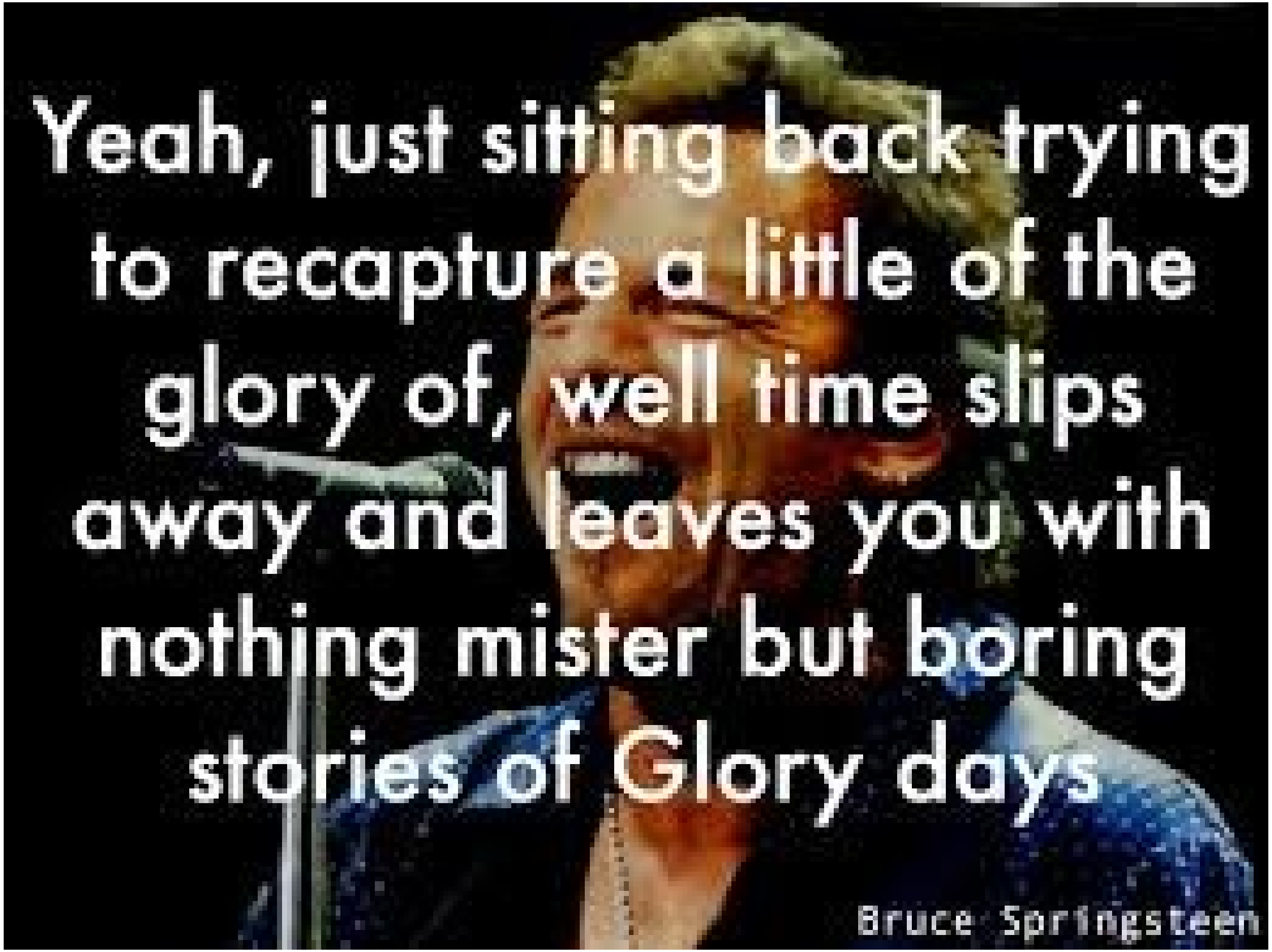
$$
+ d\Phi_{n_{max}} \mathcal{B}_{n_{max}} \left[\prod_{j=N}^{n_{max}-1} \Theta(Q_{j+1} - Q_J)\right] \left[\prod_{j=N}^{n_{max}-1} \Delta_j^{(\mathcal{K})}(t_j,\, t_{j+1})\right]
$$

$$
\times \left[\Delta_{n_{max}}^{(\mathcal{K})}(t_{n_{max}}, t_0) + \int_{t_0}^{t_{n_{max}}} d\Phi_1\, \mathcal{K}_{n_{max}} \Delta_{n_{max}}^{(\mathcal{K})}(t_{n_{max}}, t_{n_{max}+1}) \right]
$$

Multijet merging: MEPS @ LO

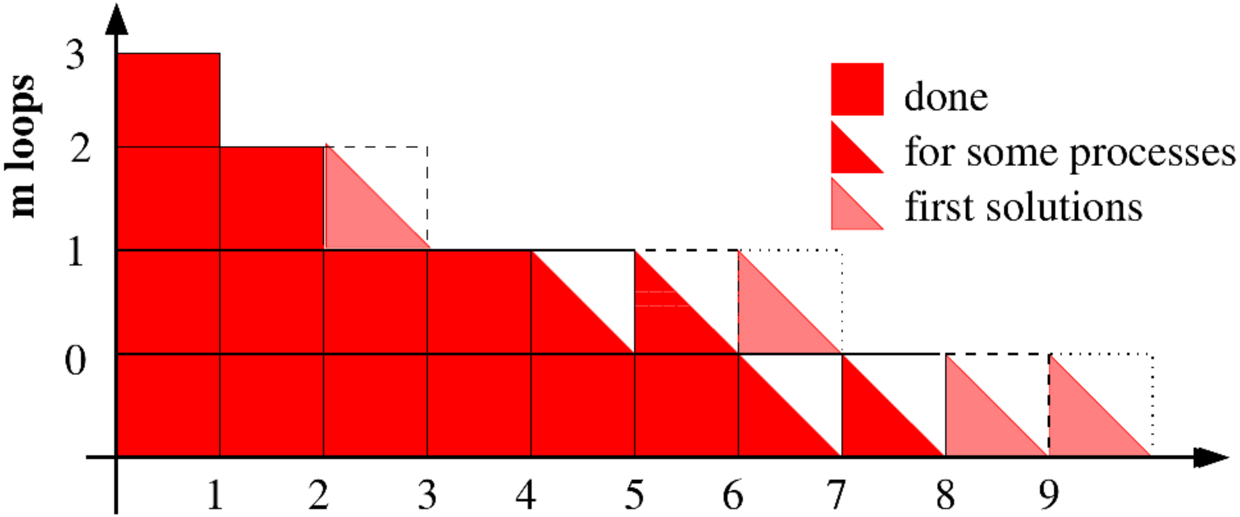
- Example results for di-photon production MEPS vs. Shower




Yeah, just sitting back trying to recapture a little of the glory of, well time slips away and leaves you with nothing mister but boring stories of Glory days
Bruce Springsteen

What is in the box now?

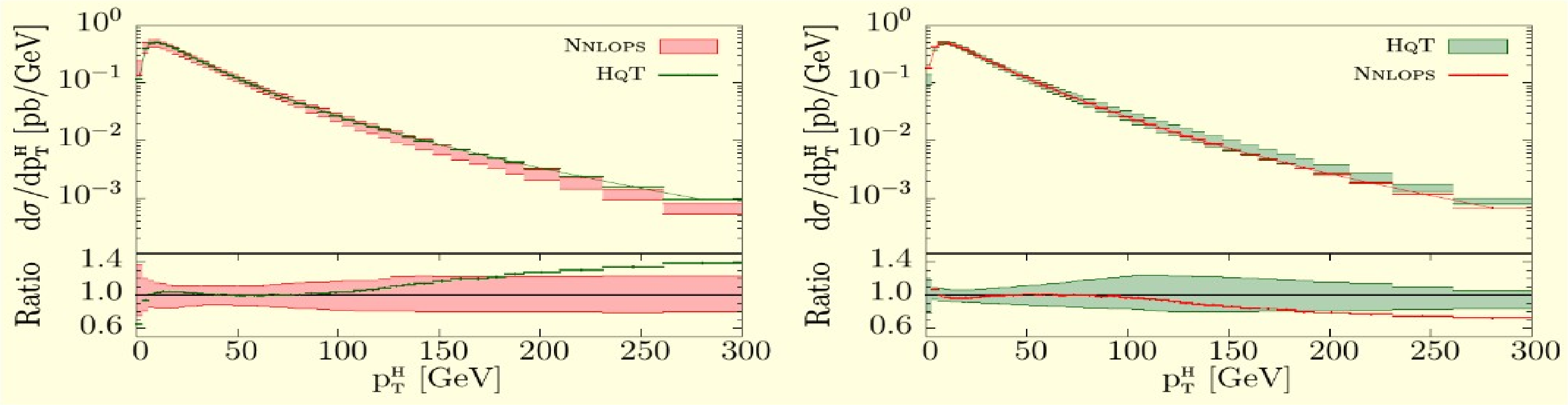
Fixed Order for Signals & Backgrounds



- looks very similar to 2021, but:
  - NLO EW is now fully automated, and by far and large, we can do 1-2 legs more without breaking the CPU bank.
  - N3LO is available for singlet production, and we close in on NNLO for 2 → 3, 4 processes

NNLOPS

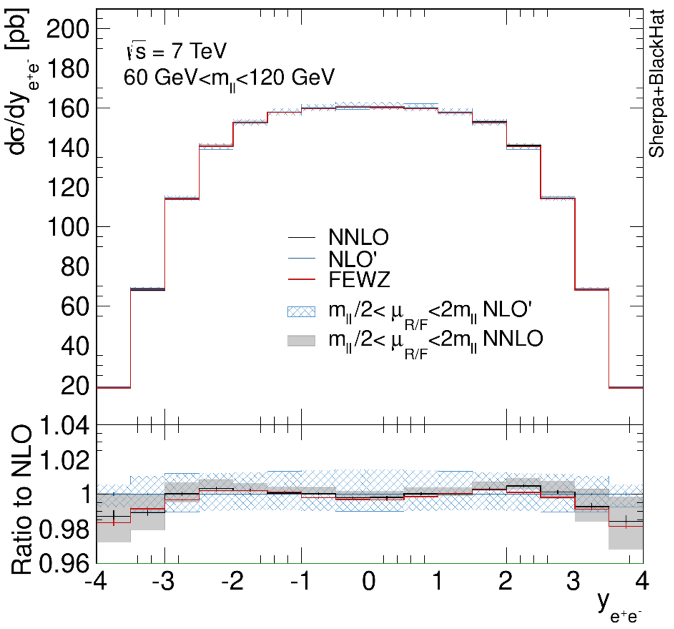
- use Powheg for X+1 processes (where X are mainly singlet systems: V, VV, H, ...)
- allow emissions of first extra particle down to parton-shower cut-off and reweight with known B_2-terms from Q_T resummation
- reweight to overall NNLO cross section

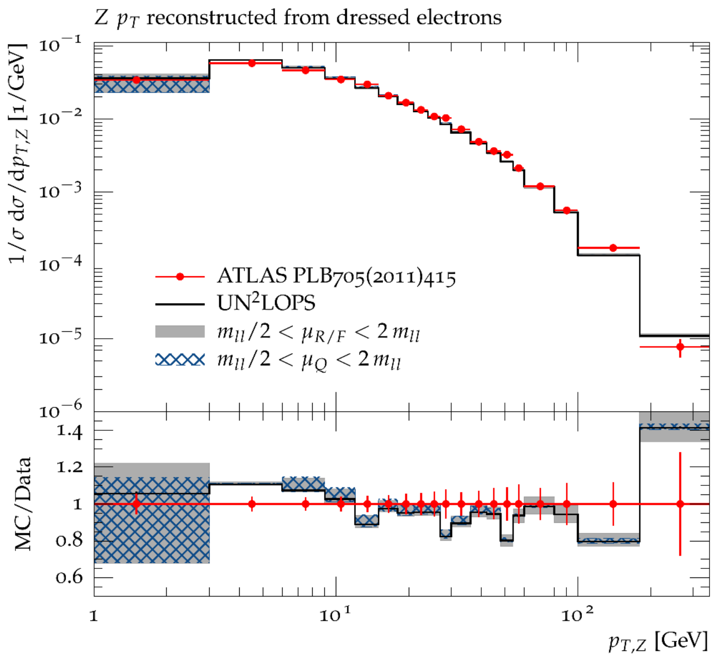


UN²LOPS

- use unitarity of parton shower and add and subtract terms suitably (quite messy, tbh)

  potential issue: some double-subtractions are not completely captured by parton shower

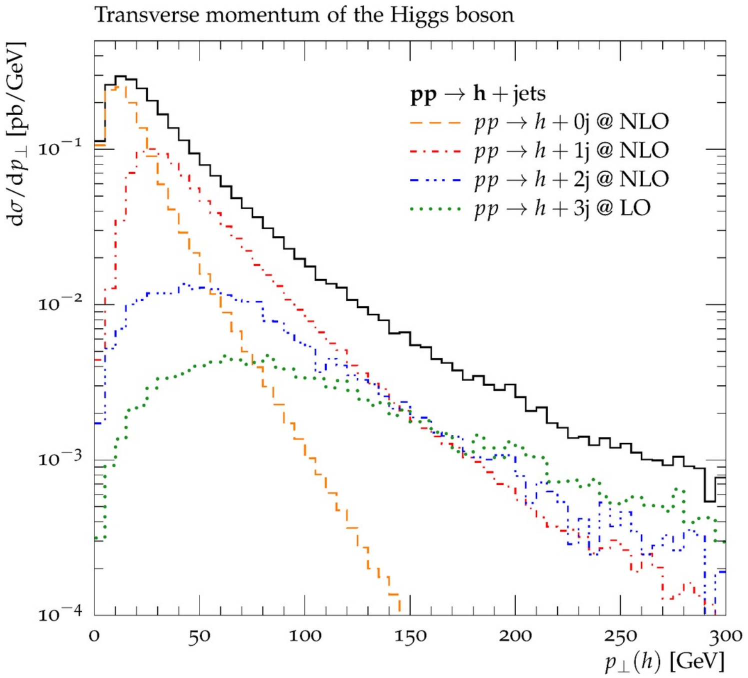




Multijet merging: MEPS @ NLO

- combine towers of MC@NLO's

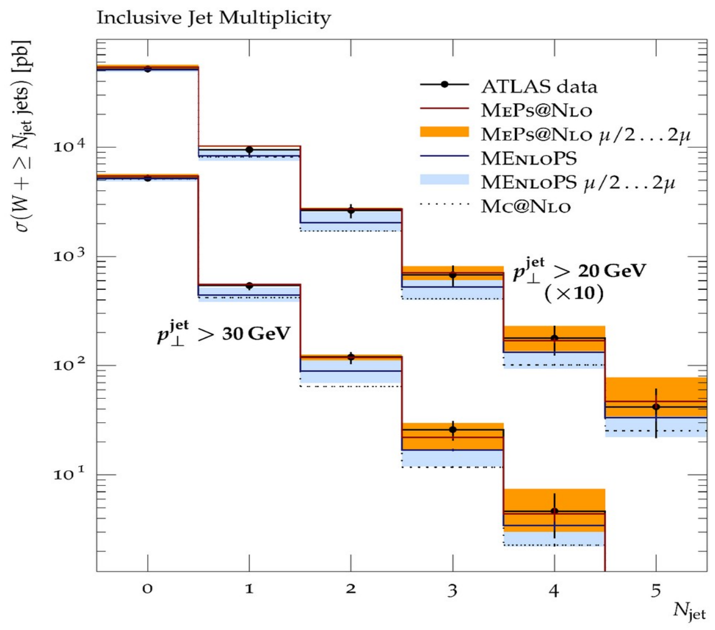
$$\begin{aligned}
d\sigma \;=\;& d\Phi_N\,\tilde{\mathcal{B}}_N\left[\Delta_N^{(\mathcal{K})}(\mu_N^2,t_0)+\int_{t_0}^{\mu_N^2} d\Phi_1\,\mathcal{K}_N\Delta_N^{(\mathcal{K})}(\mu_N^2,t_{N+1})\Theta(Q_J-Q_{N+1})\right]\\
&+d\Phi_{N+1}\,\mathcal{H}_N\Delta_N^{(\mathcal{K})}(\mu_N^2,t_{N+1})\Theta(Q_J-Q_{N+1})\\
&+d\Phi_{N+1}\,\tilde{\mathcal{B}}_{N+1}\left(1+\frac{\mathcal{B}_{N+1}}{\tilde{\mathcal{B}}_{N+1}}\int_{t_{N+1}}^{\mu_N^2} d\Phi_1\,\mathcal{K}_N\right)\Theta(Q_{N+1}-Q_J)\\
&\qquad\cdot\left[\Delta_{N+1}^{(\mathcal{K})}(t_{N+1},t_0)+\int_{t_0}^{t_{N+1}} d\Phi_1\,\mathcal{K}_{N+1}\Delta_{N+1}^{(\mathcal{K})}(t_{N+1},t_{N+2})\right]\\
&+d\Phi_{N+2}\,\mathcal{H}_{N+1}\Delta_N^{(\mathcal{K})}(\mu_N^2,t_{N+1})\Delta_{N+1}^{(\mathcal{K})}(t_{N+1},t_{N+2})\Theta(Q_{N+1}-Q_J)+\ldots
\end{aligned}$$

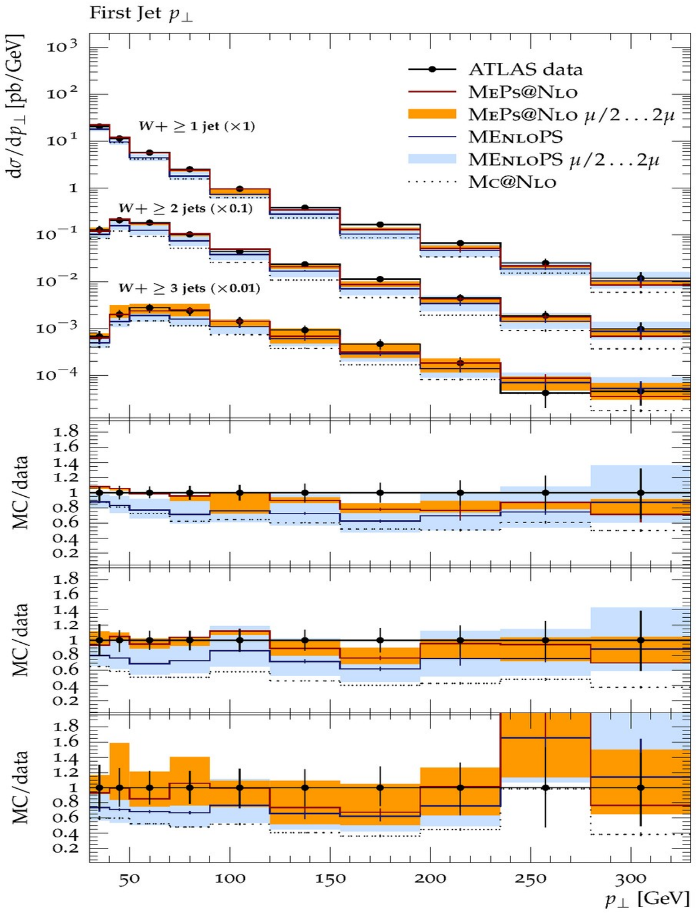


Multijet merging: MEPS @ NLO

- example results: W+jets

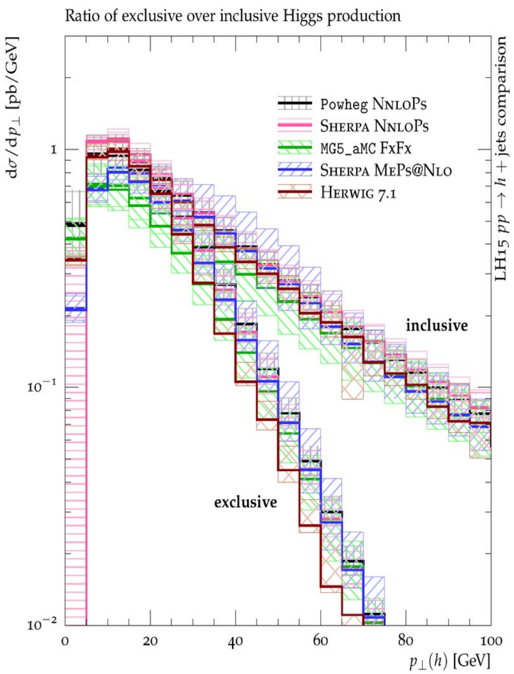
  note: similar results with FxFx

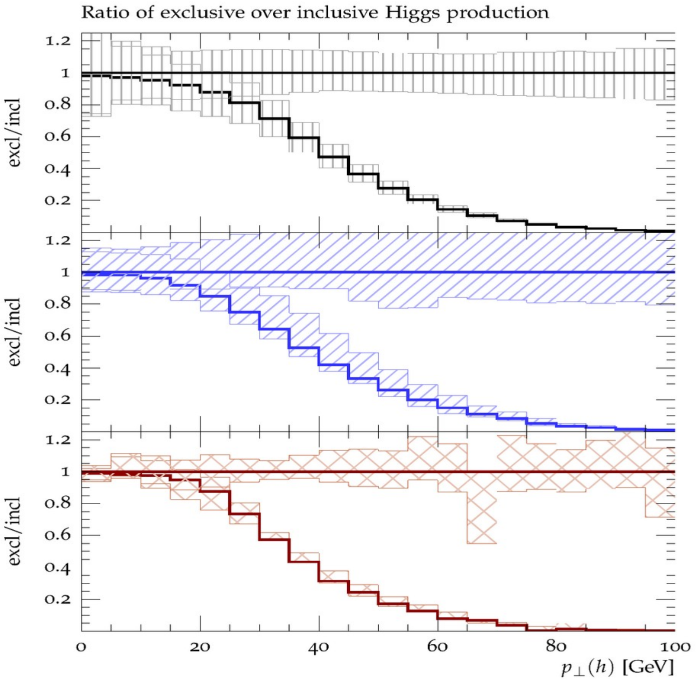




Multijet merging: MEPS @ NLO

- p_T(H) comparison of multiple implementations: most results are in good agreement





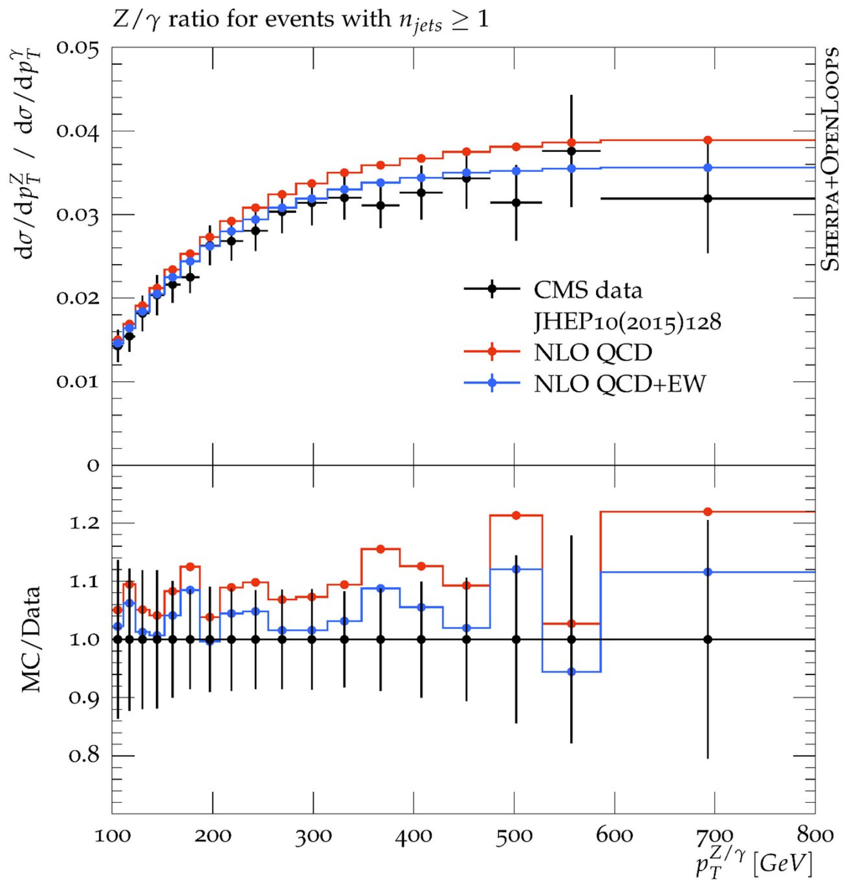
Electroweak corrections

- EW corrections may have non-negligible impact, often reduce cross sections

  (this is due to some "incomplete cancellation" of real and virtual corrections)

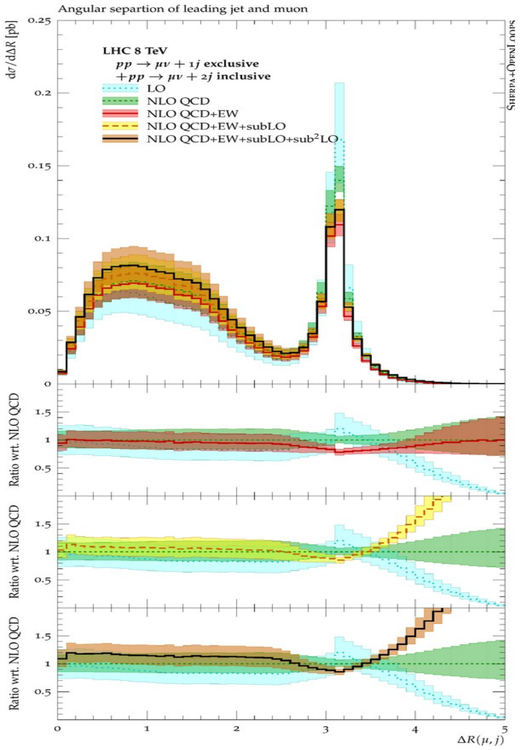
- example (relevant for DM searches):

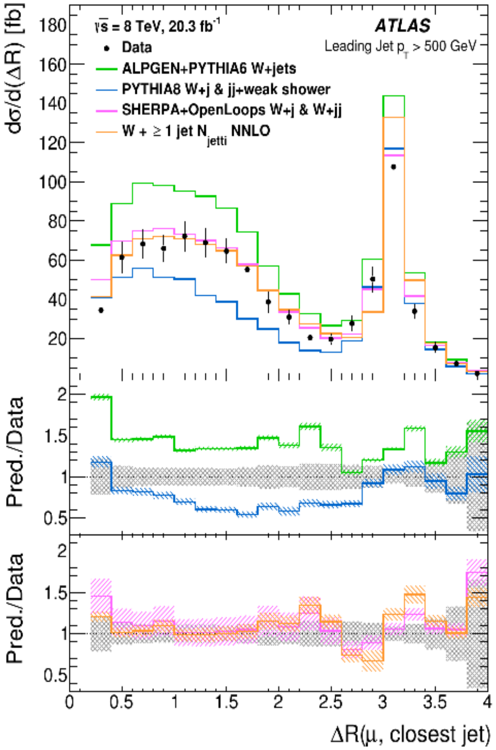
  ratio of p_T spectrum of photons and Z's



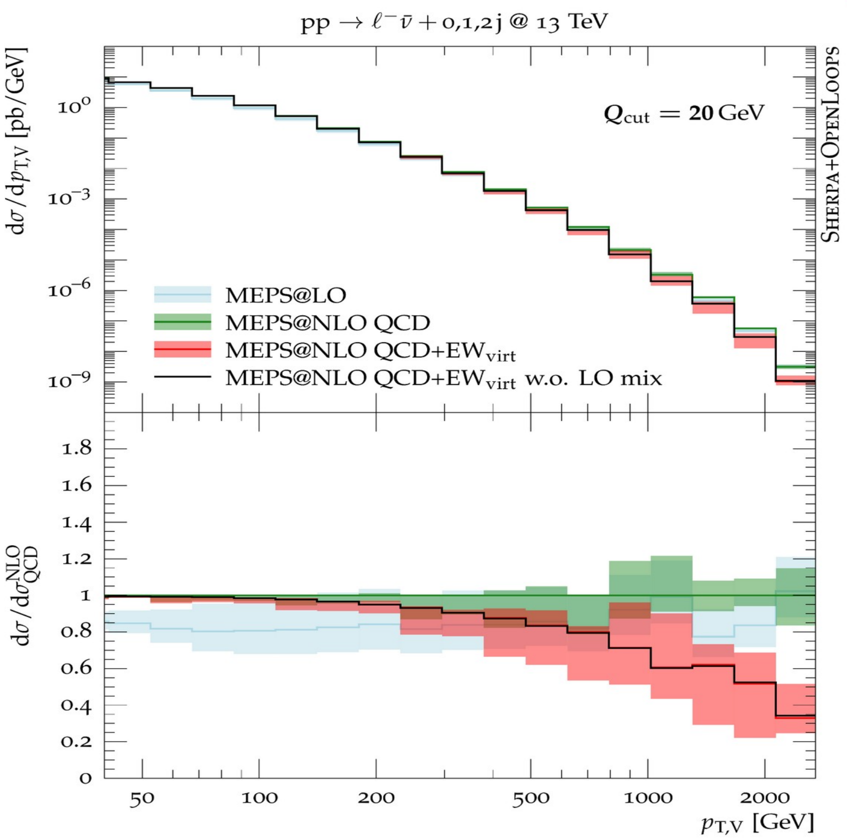
Electroweak multijet merging

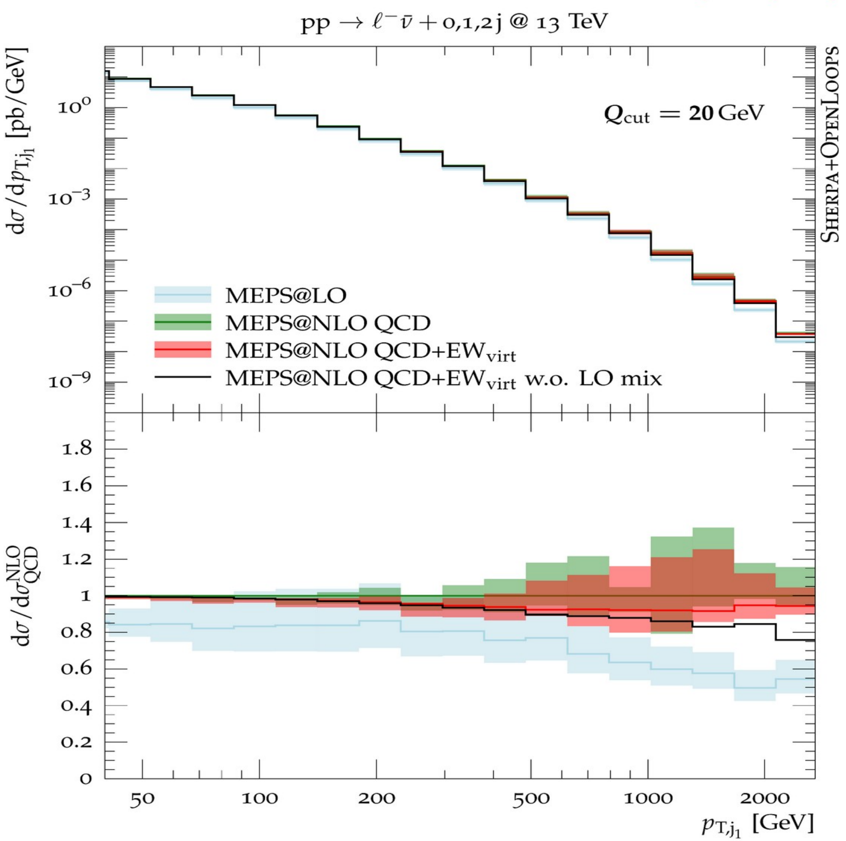
- add various contributions/topologies with suitable vetoes





Electroweak multijet merging






Don't look back,
you can never look back
Don Henley - Boys of summer

What will be in the box in 10 years?

Currently under development

- ongoing studies concerning logarithmic accuracy of parton showers:

  → will lead to better parton showers

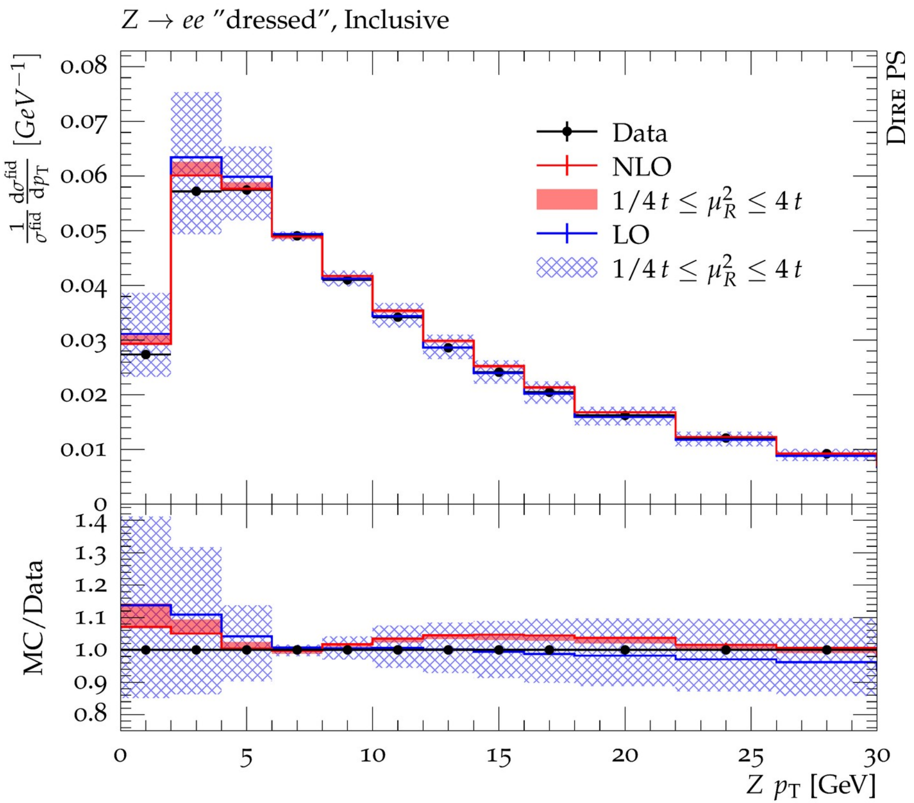
- inclusion of higher-order splitting kernels

  → simple example

  (incomplete & overly optimistic)

- will lead to NNLOPS for arbitrary processes and MEPS@NNLO

- main outcome: further reduction of perturbative uncertainties



Personal prediction (and reflection)

- will arrive at **NNLO (QCD) + NLO (EW)** for 2 → 3 and maybe even 2 → 4 processes
- merged/matched with **parton showers at $O(\alpha^2)$**
- this will most likely result in perturbative uncertainties at the **<5%** level
- at this point, **non-perturbative uncertainties** will become **dominant**
- not clear to me, how to beat them in a systematic way
- already now: perturbative calculations/simulations beyond PhD/PDRA time-scales

→ **we are close the regime of vanishing returns**

- is this the end of the journey? or will we experience a paradigm shift?

"Those who look **only** to the past or the present are certain to **miss** the future."

John F. Kennedy, 1917 – 1963