Monte Carlo Generators and Soft QCD

2. Matching and Merging

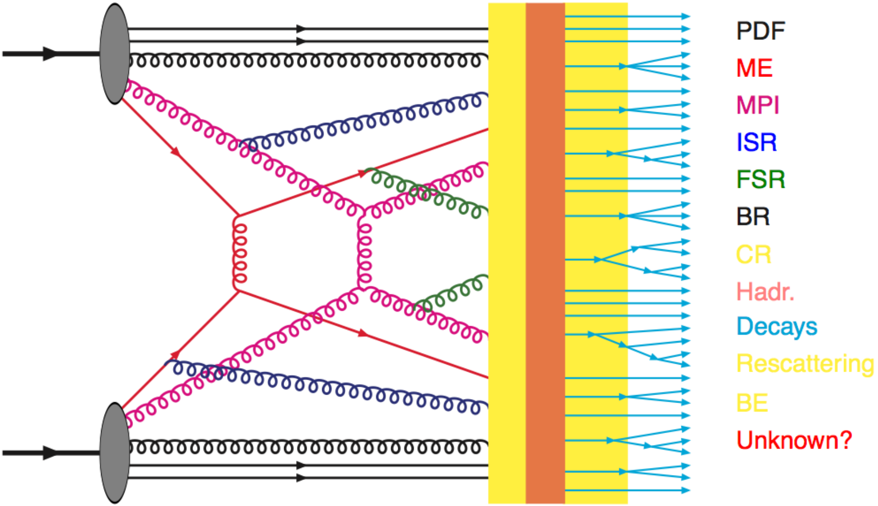
Torbjörn Sjöstrand

Department of Astronomy and Theoretical Physics
Lund University
Sölvegatan 14A, SE-223 62 Lund, Sweden

CERN, 2 September 2013

Event Generators Reminder

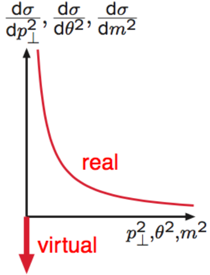
An event consists of many different physics steps, which have to be modelled by event generators:



Matrix elements vs. parton showers

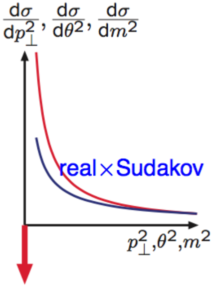
ME : Matrix Elements

- $+$ systematic expansion in α_{s} ('*exact*')
- $+$ powerful for multiparton Born level
- $+$ flexible phase space cuts
- $-$ loop calculations very tough
- $-$ negative cross section in collinear regions
  $\Rightarrow$ unpredictive jet/event structure
- $-$ *no easy match to hadronization*



PS : Parton Showers

- $-$ approximate, to LL (or NLL)
- $-$ main topology not predetermined
  $\Rightarrow$ inefficient for exclusive states
- $+$ process-generic $\Rightarrow$ simple multiparton
- $+$ Sudakov form factors/resummation
  $\Rightarrow$ sensible jet/event structure
- $+$ *easy to match to hadronization*



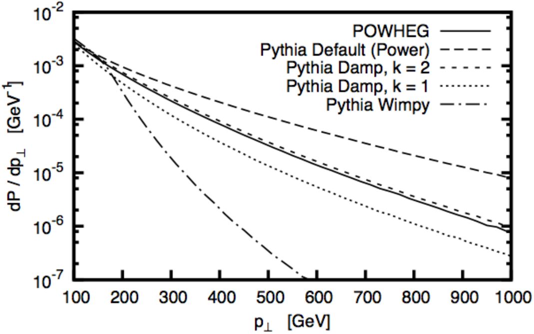
How bad are showers?

Myth: parton showers always underestimate true jet rate.
Not true!

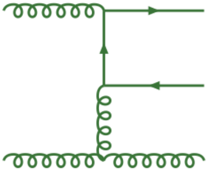
- ME expression vs. PS splitting kernels: can go either way; always possible to adjust up kernels so that PS $>$ ME.
- Coverage of phase space can leave dead zones or overlaps:
  HERWIG (angular-ordering) fix: add ME in dead zone;
  PYTHIA ($p_{\perp}$-ordered): no dead zones for *first* emission,
  but subsequent ones unaccounted for;
  VINCIA fix: allow some non-ordered emissions;
  VINCIA solution: sector showers.
- Starting scale of showers most obvious to "get it wrong".
  E.g. $\mathrm{q\overline{q}} \to \mathrm{Z}^0$ factorization/renormalization scale m_{Z}
  gave historical choice $Q^2_{\mathrm{max}} = m^2_{\mathrm{Z}}$: "wimpy shower";
  but "correct" answer is $Q^2_{\mathrm{max}} = s = E^2_{\mathrm{cm}}$: "power shower".

PS matching to MEs: realistic hard default

Aim: provide better default shower behaviour at large $p_\perp$, to bridge gap between "power" and "wimpy" showers.



$t\bar{t}$ production



$$M^2 = m_{\perp t}^2 = m_t^2 + p_{\perp t}^2$$

$$\frac{\mathrm{d}P_{\mathrm{ISR}}}{\mathrm{d}p_\perp^2} \propto \frac{1}{p_\perp^2} \frac{k^2 M^2}{k^2 M^2 + p_\perp^2}$$ for coloured final state

No dampening for uncoloured final state (W^+W^-, ..., SUSY).

R. Corke & TS, Eur. Phys. J. C69 (2010) 1

Matrix Elements and Parton Showers

Recall complementary strengths:

- ME's good for well separated jets
- PS's good for structure inside jets

Marriage desirable! But how?

Very active field of research; requires a lecture series of its own

- Reweight first PS emission by ratio ME/PS (simple POWHEG)
- Combine several LO MEs, using showers for Sudakov weights
  - CKKW: analytic Sudakov – not used any longer
  - CKKW-L: trial showers gives sophisticated Sudakovs
  - MLM: match of final partonic jets to original ones
- Match to NLO precision of basic process
  - MC@NLO: additive ⇒ LO normalization at high $p_\perp$
  - POWHEG: multiplicative ⇒ NLO normalization at high $p_\perp$
- Combine several orders, as many as possible at NLO
  - MENLOPS
  - UNLOPS (U = unitarized = preserve normalizations)

Matching and Merging

Confused terminology.

Originally (?)

- Matching: separation scale, e.g. $p_{\perp \mathrm{sep}}$;
  $p_{\perp} > p_{\perp \mathrm{sep}}$: use ME;
  $p_{\perp} < p_{\perp \mathrm{sep}}$: use PS.
- Merging: combination of ME+PS over full phase space, but ME input only for hardest emission, at whatever $p_{\perp}$.

Nowadays instead e.g.

- Merging: LO multijet ME+PS for $p_{\perp} > p_{\perp \mathrm{sep}}$, then PS for $p_{\perp} < p_{\perp \mathrm{sep}}$.
- Matching: NLO MEs separated by multiplicity.

In following: matching/merging used interchangeably.

Multijet merging – 1

Start from core process, e.g. Z^0 production (or $\mathrm{W}/\mathrm{H}/\ldots$)
and add more legs (but no loops) to get Z^0 + 1j, Z^0 + 2j, ...

Define allowed phase space by $p_{\perp\mathrm{sep}}$, e.g. $\sim$ jet algorithms:

- all $\mathrm{p}_{\perp i} > p_{\perp\mathrm{sep}}$ ($p_\perp$ w.r.t. beam axis)
- all $\mathrm{p}_{\perp ij} = \min(\mathrm{p}_{\perp i}, \mathrm{p}_{\perp j})\, R_{ij} > p_{\perp\mathrm{sep}}$
  with $R_{ij}^2 = (y_i - y_j)^2 + (\varphi_i - \varphi_j)^2$.

Can one add σ's for full answer: $\sigma_\mathrm{Z} = \sigma_0 + \sigma_1 + \sigma_2 + \ldots$?
No!

1. Each σ_i, $i > 0$, contains soft and collinear divergences,
   giving $\sigma_i = \sigma_i(p_{\perp\mathrm{sep}}) \sim \left(\alpha_\mathrm{s} \log^2(p_{\perp\max}^2 / p_{\perp\mathrm{sep}}^2)\right)^i$.
2. The σ_i are inclusive, e.g.
   $\mathrm{d}\sigma_1/\mathrm{d}p_{\perp 1} = \mathrm{Z}^0$ + 1j at $p_{\perp 1}$ + any other jet(s) above $p_{\perp\mathrm{sep}}$,
   so significant amount of doublecounting.

Multijet merging – 2

Want to make it exclusive, i.e.
$\mathrm{d}\sigma_1/\mathrm{d}p_{\perp 1} = \mathrm{Z}^0 + 1\mathrm{j}$ at $p_{\perp 1}$ + *no* other jet(s) above $p_{\perp\mathrm{sep}}$.

Recall Sudakov form factor of shower = no-emission probability,
e.g. with $p_\perp$ as evolution variable for FSR (ISR more messy)

$$\Delta_a(p_{\perp 1}^2, p_{\perp 2}^2) = \exp\left(- \sum_{b,c} \int_{p_{\perp 2}^2}^{p_{\perp 1}^2} \frac{\mathrm{d}p_\perp^2}{p_\perp^2} \int \frac{\alpha_\mathrm{s}}{2\pi} P_{a\to bc}(z')\,\mathrm{d}z' \right)$$

$$\mathrm{d}\mathcal{P}_{a\to bc} = \frac{\mathrm{d}p_\perp^2}{p_\perp^2} \frac{\alpha_\mathrm{s}}{2\pi} P_{a\to bc}(z)\,\mathrm{d}z\,\Delta_a(p_{\perp\mathrm{max}}^2, p_\perp^2)$$

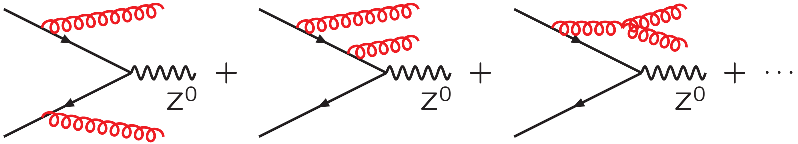
Multiplication by Sudakov form factors turns inclusive into exclusive.

Alternatively: Sudakovs provides (crude?) estimate of higher-order loop corrections needed to unitarize (exponentiate) leading orders.

Multijet merging – 3

Two issues to solve:

1. Several Feynman graphs/shower histories
   $\Rightarrow$ ill-defined $p_\perp$ emission scales.
2. Showers use running $\alpha_s(p_\perp)$, while MEs use fixed:
   gauge invariance!



Standard solution:

1. Construct all possible shower histories,
   pick one according to probability for that particlar history.
2. Generate MEs with fixed high α_s, say $\alpha_s(p_{\perp \mathrm{sep}})$,
   and afterwards reweight by $\prod_{\mathrm{vertices}}(\alpha_s(p_{\perp i})/\alpha_s(p_{\perp \mathrm{sep}}))$.

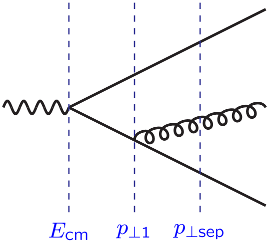
CKKW

S. Catani, F. Krauss, R. Kuhn, B.R. Webber, JHEP 0111 (2001) 063

Simple illustration: Z^0 decay:

$$\frac{\sigma_{\mathrm{q\bar{q},excl}}}{\sigma_{\mathrm{q\bar{q},incl}}} = \left[\Delta_q(E_{\mathrm{cm}}^2, p_{\perp\mathrm{sep}}^2)\right]^2$$

$$\frac{\mathrm{d}\sigma_{\mathrm{q\bar{q}g,excl}}}{\mathrm{d}\sigma_{\mathrm{q\bar{q}g,incl}}} = \Delta_q(E_{\mathrm{cm}}^2, p_{\perp\mathrm{sep}}^2)\,\Delta_q(E_{\mathrm{cm}}^2, p_{\perp 1}^2) \times \Delta_q(p_{\perp 1}^2, p_{\perp\mathrm{sep}}^2)\,\Delta_g(p_{\perp 1}^2, p_{\perp\mathrm{sep}}^2) = \left[\Delta_q(E_{\mathrm{cm}}^2, p_{\perp\mathrm{sep}}^2)\right]^2 \Delta_g(p_{\perp 1}^2, p_{\perp\mathrm{sep}}^2)$$



and so on for higher multiplicities.

Normal showers start from $p_{\perp\mathrm{sep}}$ downwards,
except for highest multiplicity from last $p_{\perp n}$ downwards.

Original CKKW drawback: use analytical Sudakovs.
Formally correct but numerically lousy, so not used any longer.

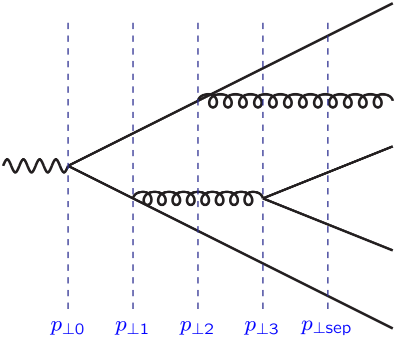
CKKW–L

L. Lönnblad, JHEP0205 (2002) 046:

use shower to generate Sudakovs!

advantage: proper kinematics;
drawback: use shower $p_\perp$ def.

1. generate n-body by ME mixed in proportions $\int \mathrm{d}\sigma_n$ above $p_{\perp\mathrm{sep}}$ cut
2. reconstruct fictitious $p_\perp$-ordered PS



4. reject from $\alpha_\mathrm{s}(p_{\perp\mathrm{sep}})$ to $\alpha_\mathrm{s}(p_{\perp i})$
5. run trial shower between each $p_{\perp i}$ and $p_{\perp i+1}$
6. reject if shower branching $\Rightarrow$ Sudakov factor
7. regular shower below $p_{\perp\mathrm{sep}}$ (or below $p_{\perp n}$ for $n = n_{\max}$)

Separation scale

How pick $p_{\perp \mathrm{sep}}$ scale?
The better the shower, the less crucial!

- $p_{\perp \mathrm{sep}} \ll p_{\perp \mathrm{max}}$: large logarithms, $\alpha_{\mathrm{s}} \log^2(p_{\perp \mathrm{max}}^2 / p_{\perp \mathrm{sep}}^2) \geq 1$:
  - need to include MEs for high multiplicities (beyond calculational capability? too slow?);
  - will reject most events since Sudakovs $\ll 1$;

  so overall inefficient/slow.
- Increasing $p_{\perp \mathrm{sep}}$: reduced need for MEs and faster, but also less ME info survives in generated events.

Realistically demand $\int \mathrm{d}\sigma_0 \geq \int \mathrm{d}\sigma_1 \geq \int \mathrm{d}\sigma_2 \geq \ldots$, which typically may mean $p_{\perp \mathrm{sep}} \simeq p_{\perp \mathrm{max}}/10$.

Study of $p_{\perp \mathrm{sep}}$ variation is central consistency check.

MLM

M.L. Mangano et al., JHEP0701 (2007) 013

Use full shower evolution to provide veto, in one step!

1. generate n-body by ME mixed in proportions $\int \mathrm{d}\sigma_n$
2. reconstruct fictitious $p_\perp$-ordered PS
3. reject from $\alpha_\mathrm{s}(p_{\perp\mathrm{sep}})$ to $\alpha_\mathrm{s}(p_{\perp i})$
4. let a shower evolve "freely" from n-parton state
5. (cone-)cluster showered event
6. match original partons and final jets
   - loop over all partons in decreasing $p_\perp$
   - for each parton fins nearest jet in ΔR
   - if $\Delta R < R_\mathrm{match}$ then matched and remove jet
7. keep the event if $n_\mathrm{jet} = n_\mathrm{parton}$ and all partons are matched
   (for highest parton multiplicity allow extra unmatched softer jets)

Similar in spirit to CKKW-L, but less formal.
Implemented in AlpGen and also (with variations) in MadGraph.

ME corrections (POWHEG precursor) – 1

M. Bengtsson & TS, Phys.Lett. B185 (1987) 435; E. Norrbin & TS, Nucl. Phys. B603 (2001) 297)

Objective: cover full phase space with smooth transition ME/PS (and be accurate to NLO).

Want to reproduce $$W^{\mathrm{ME}} = \frac{1}{\sigma(\mathrm{LO})} \frac{\mathrm{d}\sigma(\mathrm{LO}+\mathrm{g})}{\mathrm{d(phasespace)}}$$

by shower generation + correction procedure

$$\overbrace{W^{\mathrm{ME}}}^{\text{wanted}} = \overbrace{W^{\mathrm{PS}}}^{\text{generated}} \overbrace{\frac{W^{\mathrm{ME}}}{W^{\mathrm{PS}}}}^{\text{correction}}$$

Procedure:

1. Ensure that $W^{\mathrm{PS}} \geq W^{\mathrm{ME}}$ everywhere (easy!).
2. Generated W^{PS} acquires Sudakov by shower evolving in Q

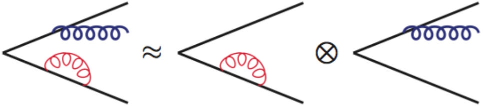
$$W^{\mathrm{PS}}_{\mathrm{actual}}(Q^2) = W^{\mathrm{PS}}(Q^2) \exp\left(- \int_{Q^2}^{Q^2_{\mathrm{max}}} W^{\mathrm{PS}}(Q'^2)\, \mathrm{d}Q'^2 \right)$$

3. Accepting emission with probability $W^{\mathrm{ME}}/W^{\mathrm{PS}} \leq 1$ gives W^{ME} in prefactor but still W^{PS} in Sudakov.
4. Mismatch fixed by **veto algorithm**:
   if emission at Q^2_{trial} is rejected then put $Q^2_{\mathrm{max}} = Q^2_{\mathrm{trial}}$
   and continue evolution from this scale downwards

$$W^{\mathrm{PS}}_{\mathrm{actual}}(Q^2) = W^{\mathrm{ME}}(Q^2) \exp\left(- \int_{Q^2}^{Q^2_{\mathrm{max}}} W^{\mathrm{ME}}(Q'^2)\, \mathrm{d}Q'^2 \right)$$

PS only remains as ordering variable for phase-space sweeping.

5. Continue with normal shower from accepted Q^2_{trial}.
6. Rescale whole cross section to σ_{NLO}, i.e. assume same $K = \sigma_{\mathrm{NLO}}/\sigma_{\mathrm{LO}}$ factor for hard and soft emissions

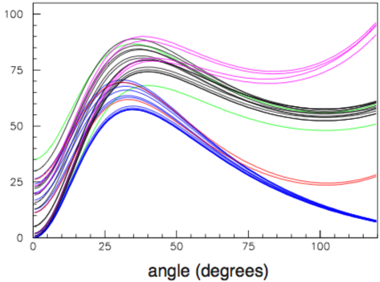


$1 + \mathcal{O}(\alpha_s) \rightarrow K$, $\int = 1 \rightarrow \mathrm{d}W^{\mathrm{PS}}$

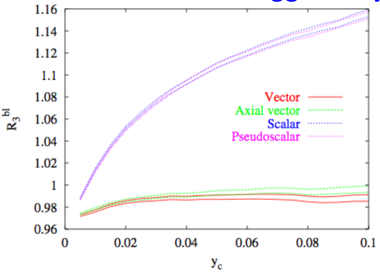
$$\mathrm{d}\sigma = K \; \sigma_0 \; \mathrm{d}W^{\mathrm{PS}}$$

PYTHIA performs merging with generic FSR $a \to bcg$ ME,
in SM: $\gamma^*/\mathrm{Z}^0/\mathrm{W}^\pm \to \mathrm{q}\overline{\mathrm{q}}$, $\mathrm{t} \to \mathrm{bW}^+$, $\mathrm{H}^0 \to \mathrm{q}\overline{\mathrm{q}}$,
and MSSM: $\mathrm{t} \to \mathrm{bH}^+$, $\mathrm{Z}^0 \to \tilde{\mathrm{q}}\overline{\tilde{\mathrm{q}}}$, $\tilde{\mathrm{q}} \to \tilde{\mathrm{q}}'\mathrm{W}^+$, $\mathrm{H}^0 \to \tilde{\mathrm{q}}\overline{\tilde{\mathrm{q}}}$, $\tilde{\mathrm{q}} \to \tilde{\mathrm{q}}'\mathrm{H}^+$,
$\chi \to \mathrm{q}\overline{\tilde{\mathrm{q}}}$, $\chi \to \mathrm{q}\overline{\tilde{\mathrm{q}}}$, $\tilde{\mathrm{q}} \to \mathrm{q}\chi$, $\mathrm{t} \to \tilde{\mathrm{t}}\chi$, $\tilde{\mathrm{g}} \to \mathrm{q}\overline{\tilde{\mathrm{q}}}$, $\tilde{\mathrm{q}} \to \mathrm{q}\tilde{\mathrm{g}}$, $\mathrm{t} \to \tilde{\mathrm{t}}\tilde{\mathrm{g}}$

g emission for different colour, spin and parity:



$R_3^{\mathrm{bl}}(y_c)$: mass effects in Higgs decay:



Basic concept generalizes to ISR, but NLO rescaling less trivial.

POWHEG

Nason; Frixione, Oleari, Ridolfi (e.g. JHEP **0711** (2007) 070)

$$\mathrm{d}\sigma = \bar{B}(v)\mathrm{d}\Phi_v \left[\frac{R(v,r)}{B(v)} \exp\left(- \int_{p_\perp} \frac{R(v,r')}{B(v)} \mathrm{d}\Phi'_r \right) \mathrm{d}\Phi_r \right] ,$$

$$\bar{B}(v) = B(v) + V(v) + \int \mathrm{d}\Phi_r [R(v,r) - C(v,r)] .$$

$v, \mathrm{d}\Phi_v$ Born-level n-body variables and differential phase space
$r, \mathrm{d}\Phi_r$ extra $n+1$-body variables and differential phase space
$B(v)$ Born-level cross section
$V(v)$ Virtual corrections
$R(v,r)$ Real-emission cross section
$C(v,r)$ Conterterms for collinear factorization of parton densities.

Note that $\int \bar{B}(v)\mathrm{d}\Phi_v \equiv \sigma_{\mathrm{NLO}}$ and $\int [\cdots \mathrm{d}\Phi_r] \equiv 1$.

So pick the real emission with largest $p_\perp$ according to complete ME's + ME-based Sudakov, with NLO normalization, and let showers do subsequent evolution downwards from this $p_\perp$ scale.

MC@NLO – 1

Frixione, Webber, JHEP 0206 (2002) 029

Start from $\sigma = \sigma_B + \sigma_V + \int \mathrm{d}\sigma_R$
(B = born, V = virtual (incl. counterterms), R = real emissions).

Assume well-understood MC shower algorithm:

- first emission described by $\mathrm{d}\sigma_{R,\mathrm{MC}} \times$ Sudakov,
- which agrees with $\mathrm{d}\sigma_R$ in collinear/soft limits,
- and with analytically calculable $\sigma_{R,\mathrm{MC}} = \int \mathrm{d}\sigma_{R,\mathrm{MC}}$.

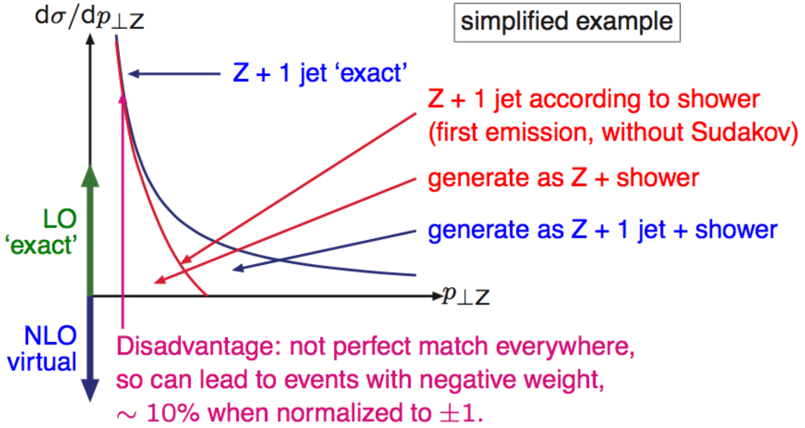
Then

$$\sigma = \sigma_B + \overbrace{\sigma_V + \sigma_{R,\mathrm{MC}}}^{\text{divergences cancel}} + \int \overbrace{(\mathrm{d}\sigma_R - \mathrm{d}\sigma_{R,\mathrm{MC}})}^{\text{divergences cancel}}$$

so MC implementation:

- $\sigma_B + \sigma_V + \sigma_{R,\mathrm{MC}}$: start from Born topology
  and add showers to it, with no particular constraint.
- $\int (\mathrm{d}\sigma_R - \mathrm{d}\sigma_{R,\mathrm{MC}})$: pick radiation topology
  and add showers below selected radiation scale.

MC@NLO – 2



Key difference to POWHEG: $\mathrm{d}\sigma_R$ is *not* boosted by K factor.
$\Rightarrow$ Pure NLO results are obtained for all observables
when (formally) expanded in powers of α_{s},
whereas POWHEG "guesses" some NNLO corrections.

Interpolation between POWHEG and MC@NLO

Master formula for meaningful NLO implementations:

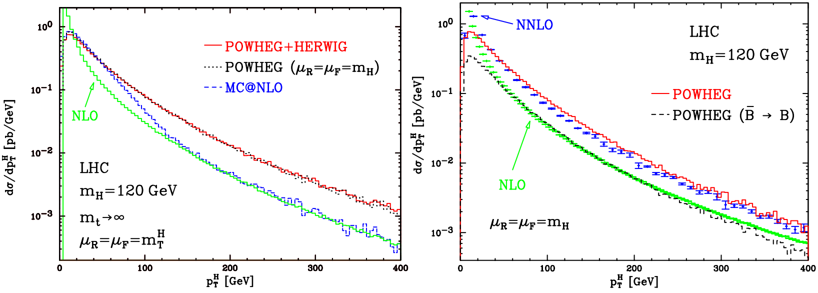
$$\mathrm{d}\sigma = \mathrm{d}\sigma_{R,\mathrm{hard}} + (\sigma_B + \sigma_{R,\mathrm{soft}} + \sigma_V) \left[\frac{\mathrm{d}\sigma_{R,\mathrm{soft}}}{\sigma_B} \exp\left(- \int \frac{\mathrm{d}\sigma_{R,\mathrm{soft}}}{\sigma_B} \right) \right]$$

ordered in "$p_\perp$", with shower from selected "$p_\perp$" downwards

POWHEG: $\sigma_{R,\mathrm{hard}} = 0$

MC@NLO: $\sigma_{R,\mathrm{soft}} = \sigma_{R,\mathrm{MC}}$

"Best" choice process-dependent (guess NLO behaviour of σ_R)



S.Alioli, P. Nason, C. Oleari, E. Re, JHEP 00904 (2009) 002

Comparison of methods

CKKW(-L), MLM: several topologies at LO, e.g. $\mathrm{Z}^0 + 0, 1, 2, 3, 4\mathrm{j}$
POWHEG, MC@NLO: lowest at NLO, e.g. Z^0, next at LO, $\mathrm{Z}^0 + 1\mathrm{j}$
the rest by showers ⇒ more important for latter

Which to use depends on application:

- Multijet topologies important (e.g. searches)
  - Get going fast ⇒ MLM
  - Willing to spend time on optimal generation ⇒ CKKW-L

  Personal opinion: CKKW-L better choice for multijets
- Normalization important (e.g. PDF determinations, $\sigma_{\mathrm{t}\bar{\mathrm{t}}}$, σ_{H})
  - POWHEG & MC@NLO explore reasonable range of variation
  - POWHEG has no negative weights
  - PWWHEG better separated from shower details ⇒ flexible
  - POWHEG optimal for $p_{\perp}$-ordered showers (like PYTHIA)
  - POWHEG scaling-up of real emissions ($\overline{B}/B$) abhors purists, but physically it probably(?) makes for a faster convergence

  Personal opinion: POWHEG better choice for NLO

Synthesis: Legs *and* Loops

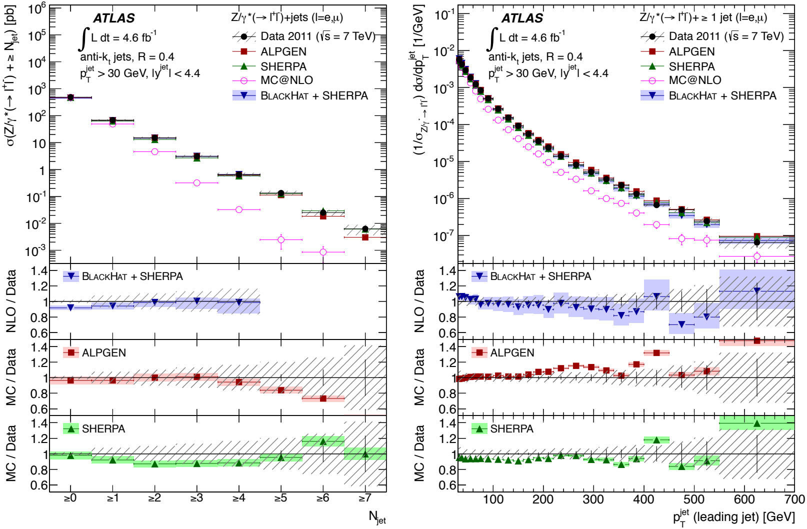
How combine NLO precision for few-body topologies with LO for many-body ones?

Current frontline: no consensus, no one-line formulae!

- MENLOPS (Hamilton, Nason): use POWHEG for $\mathrm{Z}^0 + 0, 1\mathrm{j}$, add MEs for $\mathrm{Z}^0 + \geq 2\mathrm{j}$ with $K = \overline{B}/B$ factor, and adjust $\mathrm{Z}^0 + 1\mathrm{j}$ to retain total σ_{NLO}
- MEPS@NLO (SHERPA): use POWHEG for $\mathrm{Z}^0 + 0\mathrm{j}$ and for $\mathrm{Z}^0 + 1\mathrm{j}$, MEs for $\mathrm{Z}^0 + \geq 2\mathrm{j}$
- UNLOPS (Lönnblad, Prestel; Plätzer): input $\sim$ as above, but careful bookkeeping of gain/loss between event classes to preserve NLO normalization
  Personal opinion: currently most sophisticated approach, but at the price of lengthy formulae $\Rightarrow$ not transparent
- many further groups/ideas: VINCIA, SCET, Nagy, ...

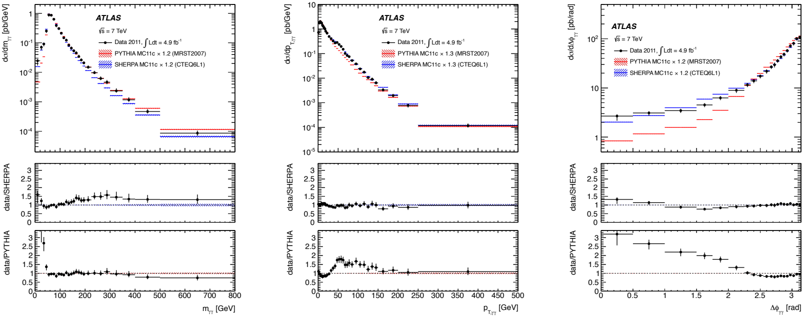
The dust has not yet settled...

Example of results – 1



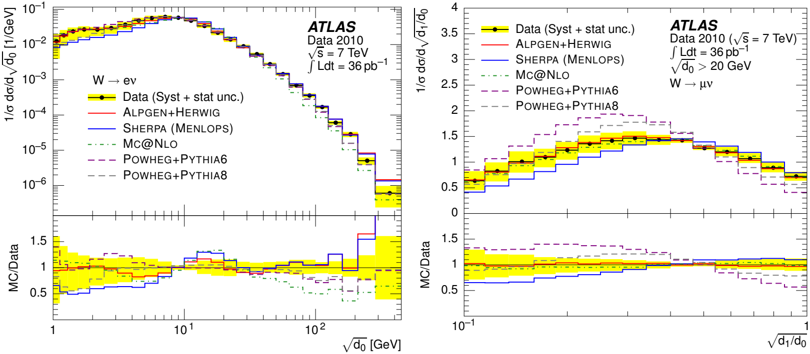
$\gamma^*/Z^0 \to \ell^+\ell^-$ + jets: MC@NLO not enough extra jets

Example of results – 2



Diphotons: $m_{\gamma\gamma}$, $p_{\perp,\gamma\gamma}$ and $\Delta\varphi_{\gamma\gamma}$:
PYTHIA pure shower fails to give enough nearby photons;
SHERPA ME matching fills it in.

Example of results – 3



Use $k_\perp$ clustering algorithm to define jet resolution scales $d_n \sim p_\perp^2$ in W events: no clear winner.

Data summary: LO+PS not enough, NLO+PS not for multijets, for the rest different approaches fare comparably well.

Range of models useful to probe uncertainties.

Summary and Outlook

- ME legs fine, but lack enough loops to give convergence in observable multijet phase space.
- Process-generic nature of showers a strength and a weakness.
- Combination methods: Sudakovs estimate summed loops.
- LO multijet merging: CKKW-L well established.
- NLO merging: POWHEG and MC@NLO still contenders.
- Multijets + NLO: current frontline, no consensus.
- (Envelope of) generators doing fine compared with LHC data.

Next (tomorrow):

- Multiparton interactions
- Hadronization