Stefano Frixione

Monte Carlos

QCD: The Modern View of Strong Interactions
Berlin, 5/10/2009

Plan

- Basics of Monte Carlos
- Recent progress (in the perturbative part)
- Outlook

Why bother?

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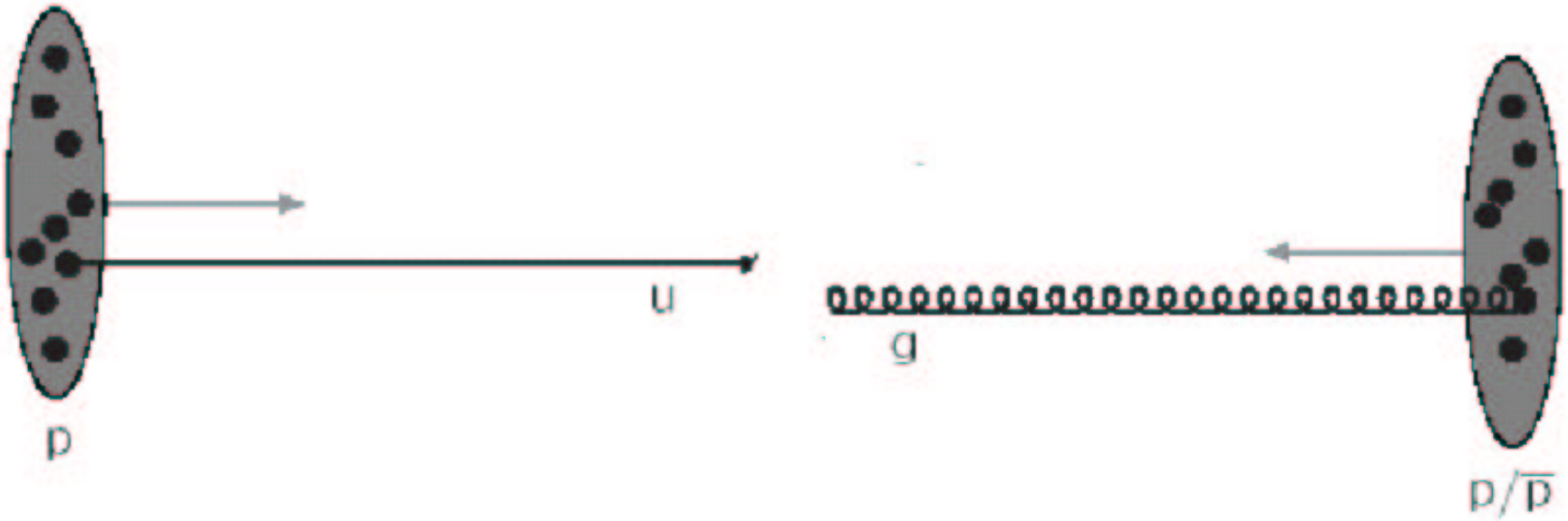
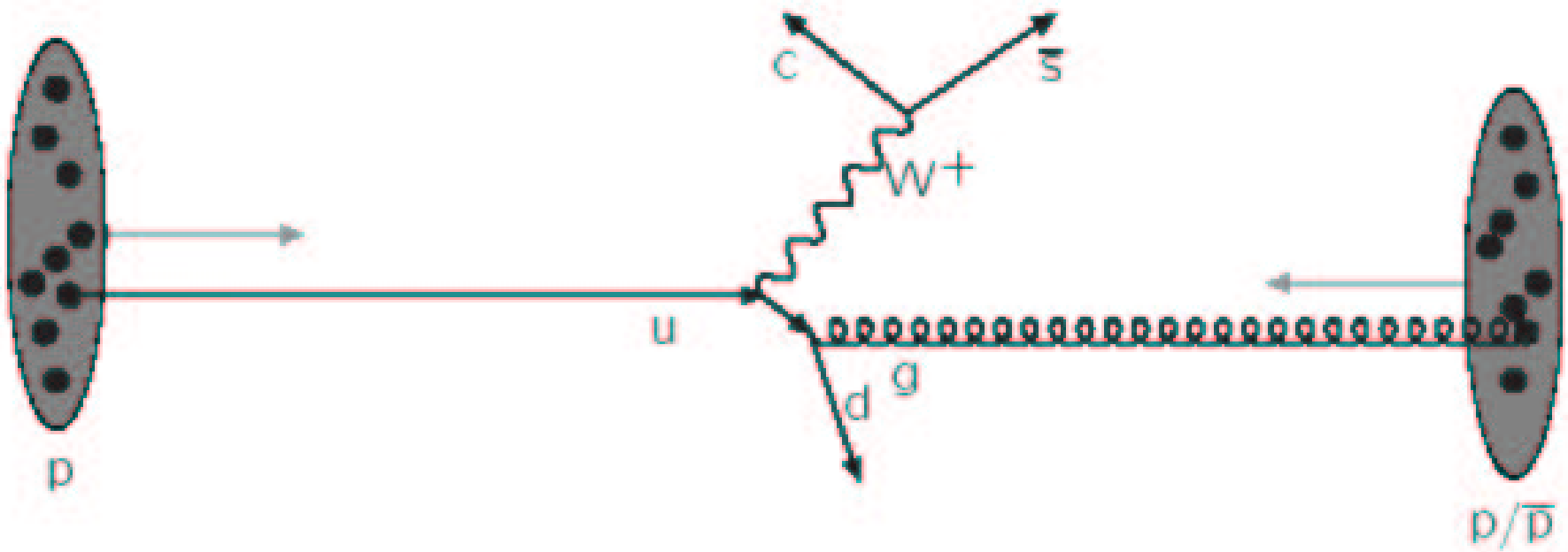
- So now MCs are quite good at predictions, and not only at postdictions
- By far the best way to model the events emerging from LHC detectors, at the same time allowing an intuitive understanding of complicated processes
- May play a much more significant role in discoveries and exclusions than in the past

Plot: T. Sjöstrand



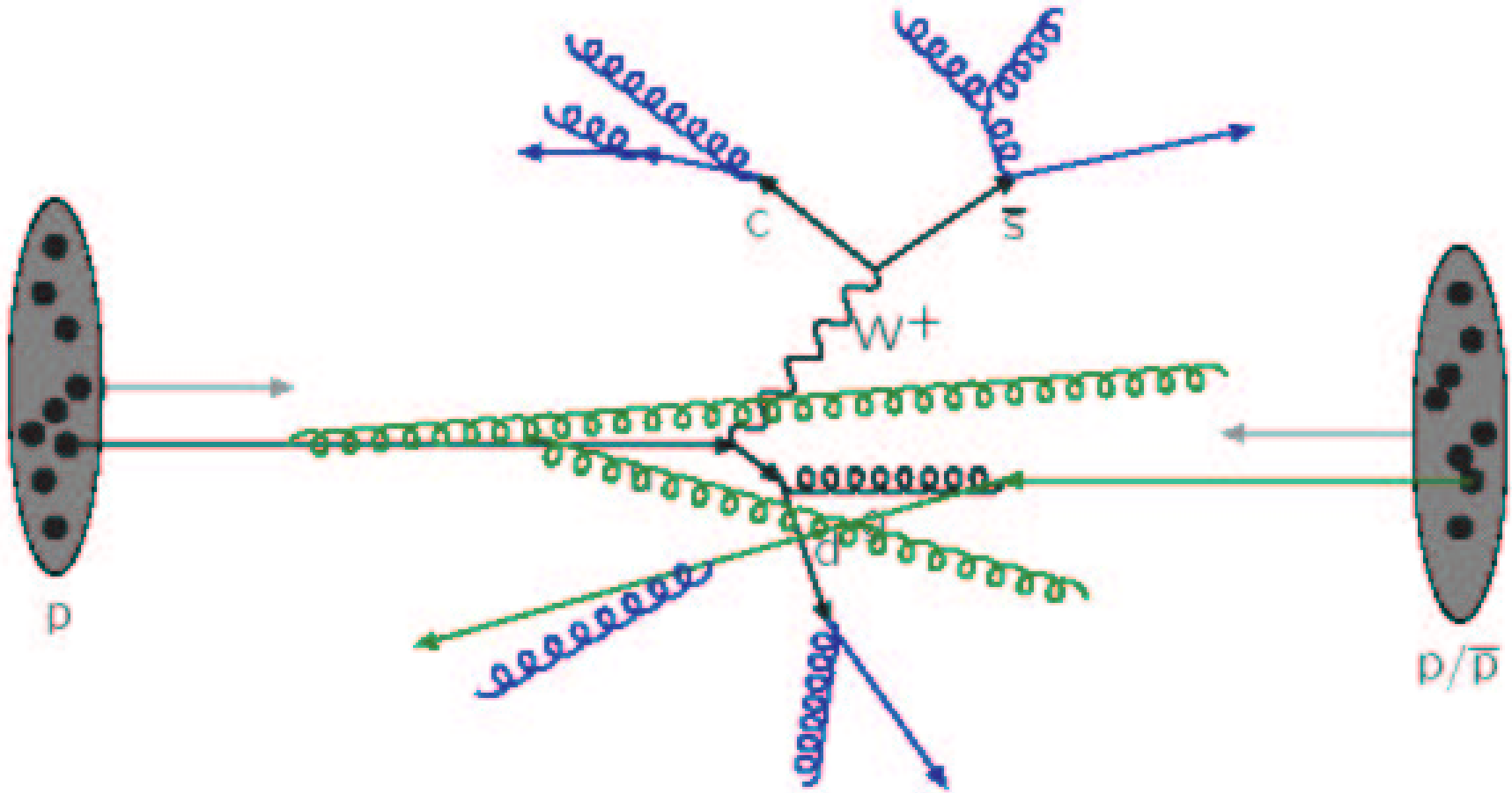
0. Pull out one parton from each of the incoming hadrons
   (use PDFs to choose flavour and x)

Plot: T. Sjöstrand



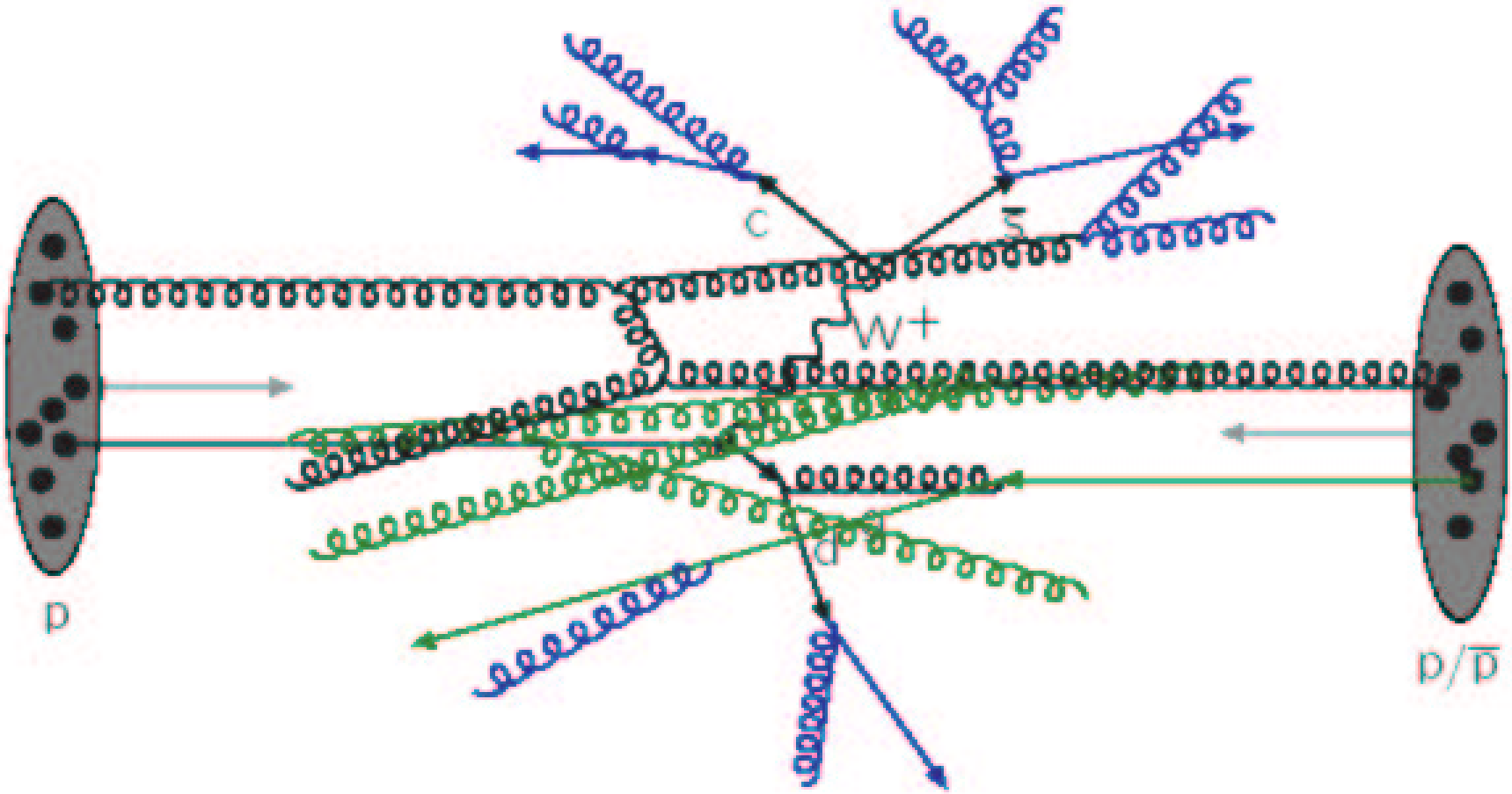
1. Make them collide and produce *large-p_T stuff*
   (Hard Subprocess)

Plot: T. Sjöstrand



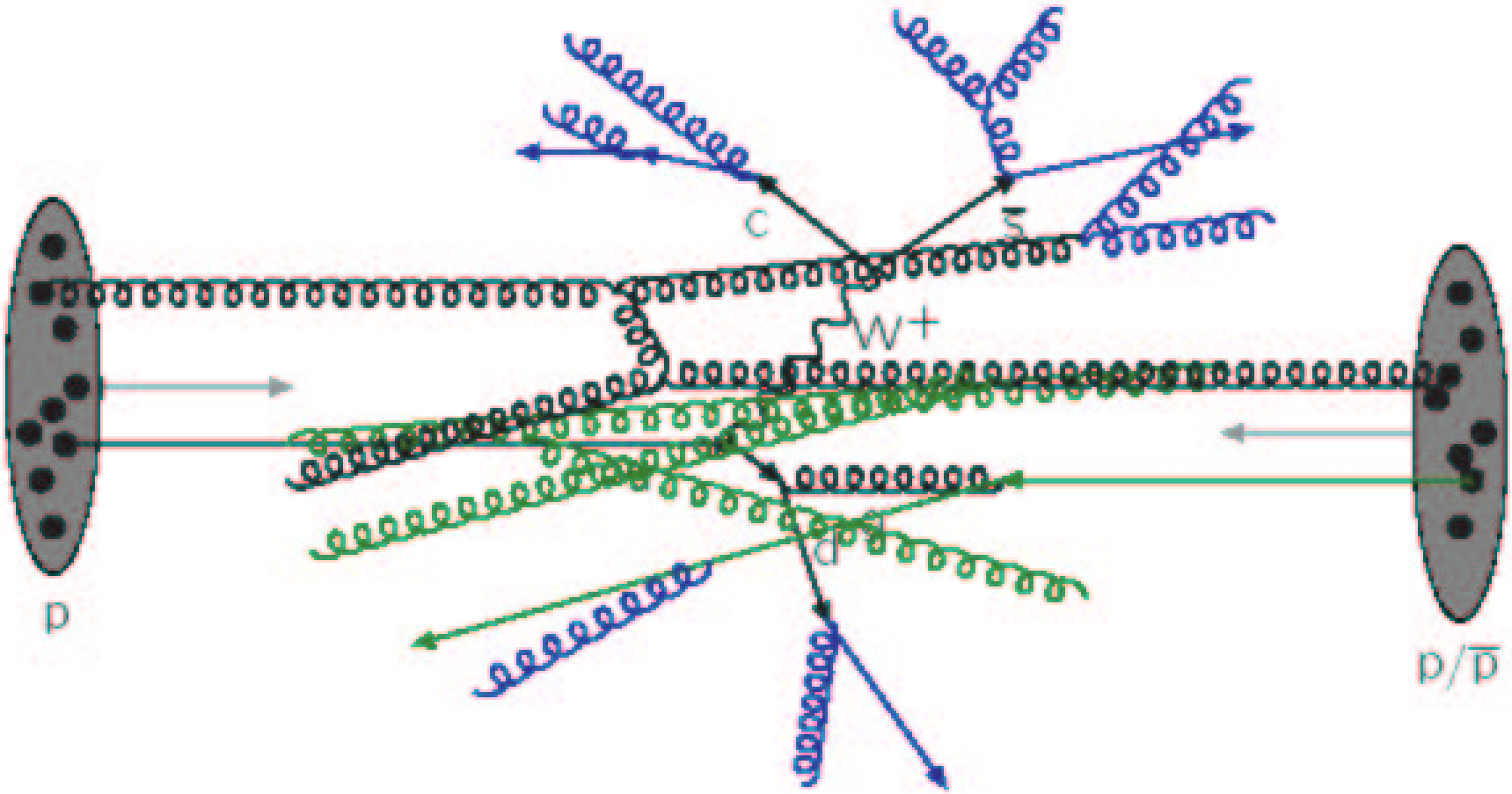
2. Let quarks and gluons emit other quarks and gluons (Parton Shower)

Plot: T. Sjöstrand



3. Other partons may undergo the same fate *at smaller* p_T*'s*
(MPI + beam remnants $\equiv$ Underlying Event)

Plot: T. Sjöstrand



4. Convert quarks and gluons into physical hadrons (Hadronization)

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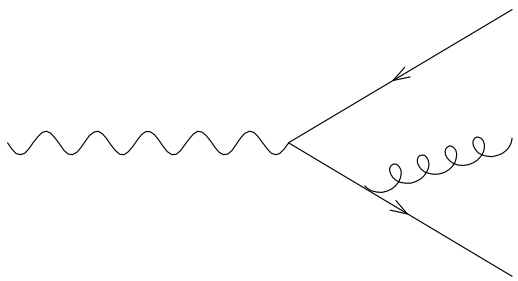
3. Underlying Event. Poorly understood. Models are not well constrained by data, and extrapolations are affected by very large uncertainties

Parton Showers

- Each emission in a shower is based on a collinear approximation; collinear emissions factorize and can be easily iterated



Master equation to be iterated:

$$d\sigma_{q\bar{q}g} \xrightarrow{t\to 0} d\sigma_{q\bar{q}} \times \frac{\alpha_S}{2\pi}\frac{dt}{t}P_{qq}(z)dz\frac{d\varphi}{2\pi}$$

- As long as $E_q \simeq E_g \gg \Lambda_{\rm QCD}$

$$t = Q^2, \qquad t = \theta^2 E^2, \qquad t = p_T^2$$

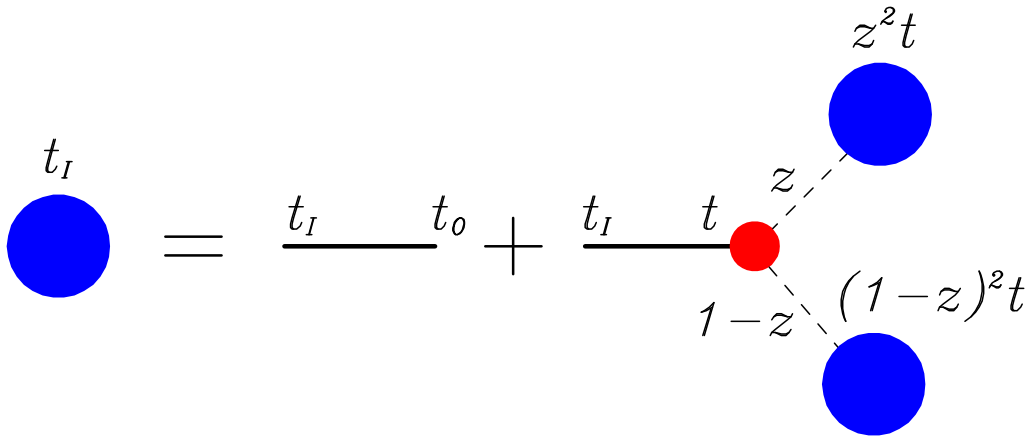
are equivalent

- Choices of shower variables are *not equivalent* in the soft region ($E_g \ll E_q$). Perturbative QCD theorems (Mueller) prescribe to use angles to respect colour coherence. In practice, pQCD deficiencies may be compensated by the non-perturbative part (mostly hadronization)

Collect all "shower histories" (i.e. kinematic configurations weighted with their probabilities) into a generating functional. This obeys:

$$\mathcal{F}(t_I) = \Delta(t_I, t_0) + \int_{t_0}^{t_I} \frac{dt}{t} \Delta(t_I, t) \int dz \frac{\alpha_S}{2\pi} P(z) \mathcal{F}((1-z)^2 t) \mathcal{F}(z^2 t)$$

with $t = \theta^2 E^2$ (angular ordering). Parton types understood



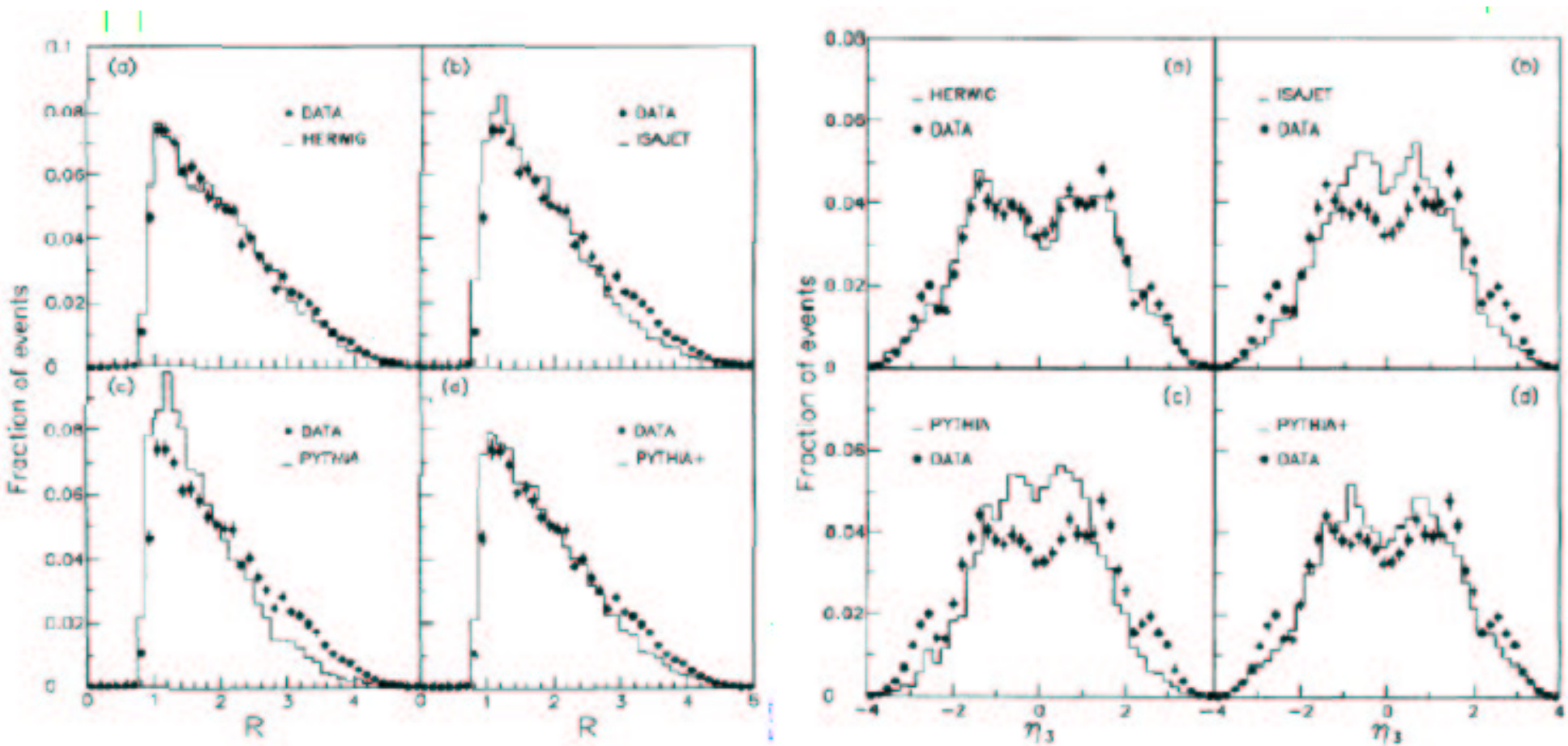
By imposing unitarity one gets

$$1 = \Delta(t_I, t_0) + \int_{t_0}^{t_I} \frac{dt}{t} \Delta(t_I, t) \int dz \frac{\alpha_S}{2\pi} P(z)$$

from which one solves for the Sudakov

$$\Delta(t_I, t_0) = \exp\left(- \int_{t_0}^{t_I} \frac{dt}{t} \int dz \frac{\alpha_S}{2\pi} P(z) \right)$$

Coherence (or lack of it)



3-jet correlations @CDF. $E_{T1} > 110$ GeV, $E_{T3} > 10$ GeV, $R \equiv R_{23}$

- Forcing coherence is not equivalent to built it in. But a clever hadronization model may compensates for perturbative deficiencies

QCD vs QED: angular ordered + cluster hadr

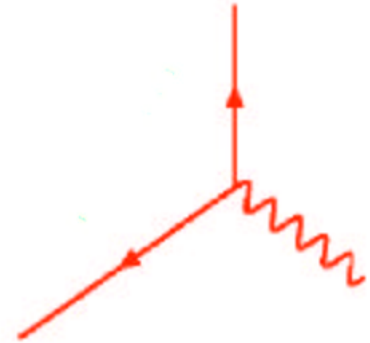
Hard process (matrix element)

Find colour partners

Intra-quark radiation suppressed in QCD. Cluster hadronization will respect this pattern

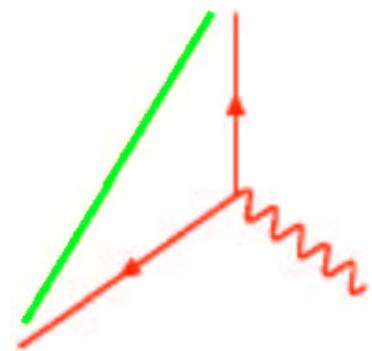
QCD vs QED: virtuality ordered + string hadr

Hard process (matrix element)



The pattern of radiation is identical in the two cases. Enter string hadronization.

Find colour partners



In QCD, string hadronization will pull hadrons in the $q\bar{q}$ cone apart, thus recovering what was achieved at the perturbative level by an angular-ordered shower

Different choices of variables led to:

HERWIG(++)	PYTHIA/SHERPA	ARIADNE
$t \simeq angle$	$t = virtuality$	$t = p_T^2$
hardest not first	hardest first	hardest first
coherent	coherence forced	coherent
dead zones	no dead zones	no dead zones
ISR easy	ISR easy	ISR difficult
kinematics: difficult	kinematics: easy	kinematics: easy
cluster hadr	string/cluster hadr	string hadr

- Since 2006 PYTHIA has also p_T-ordered evolution (PYTHIA8 is only p_T-ordered). SHERPA will also abandon virtuality order

"Historical" MCs PYTHIA and HERWIG are being re-written in C++ $\longrightarrow$ PYTHIA8 and HERWIG++. This is an opportunity to include new physics features, such as:

- PYTHIA8 (Status report: 0809.0303)

  Interleaved p_T-ordered MI+ISR+FSR evolution

  Improved UE model (more processes)

  Two hard interactions in the same event

- HERWIG++ (v2.3 Release Note: 0812.0529)

  New (angular-ordered) shower (better treatment of masses)

  MPI model for UE

  Spin correlations in all decays owing to use of spin unaveraged MEs

SHERPA (v1.1 Release Note: 0811.4622) is now fully independent of PYTHIA. Moving towards new p_T-ordered showers based on CS dipole formulae. Matching with MEs (see later) fully integrated

Further recent progress

An immense amount of activity on modelling & fitting UE physics. From the theoretical point of view, it is now established that

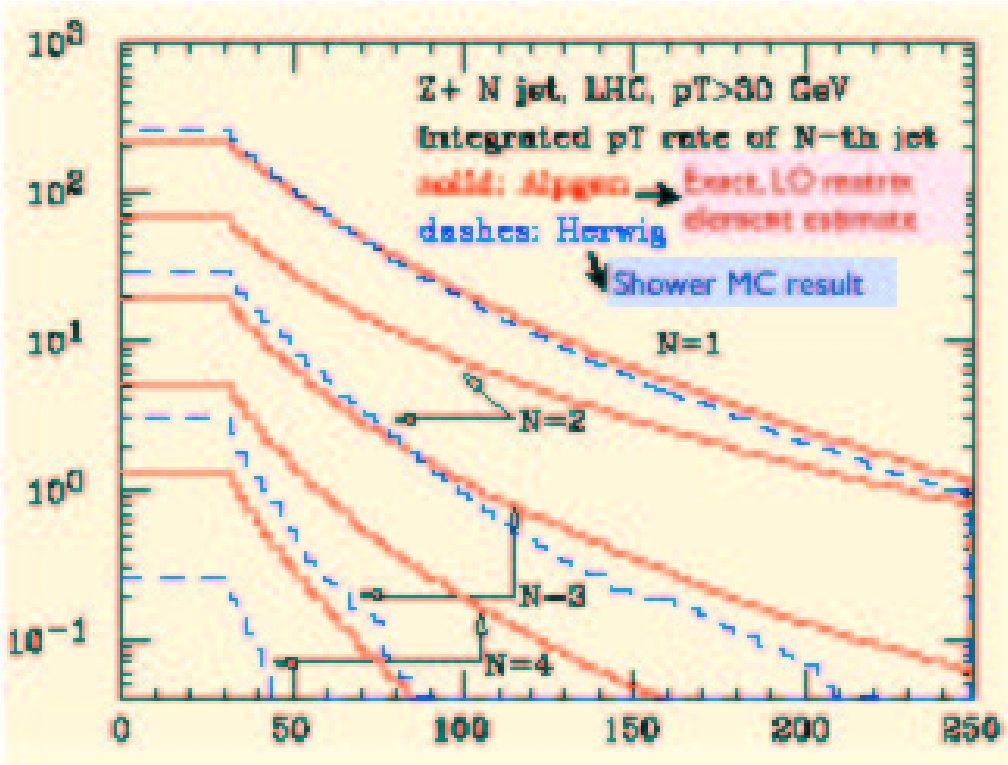
- MPI are necessary to describe well UE

A better understanding from first principles would improve extrapolations to LHC energies. For recent results see e.g. http://www.pg.infn.it/mpi08

The most significant theoretical progress lately has been made on the best-understood component of MCs: the perturbative part

There are compelling phenomenological motivations $\longrightarrow$

Plot: M. Mangano



LHC physics is a multi-jet physics

New-physics signal may easily have 5-10 jets (e.g. fully hadronic SUSY Higgs, $T \to tW$, heavy sparticle pair production, little Higgs, ...)

- MCs are simply unable to reliably simulate these multi-jet events
- The reason behind this failure is obvious. The parton shower is inherently collinear. The probability associated with well-separated final-state particles is largely underestimated

How to improve (perturbatively) Monte Carlos?

The key issue is to go beyond the collinear approximation

$\Longrightarrow$ use exact matrix elements of order higher than leading

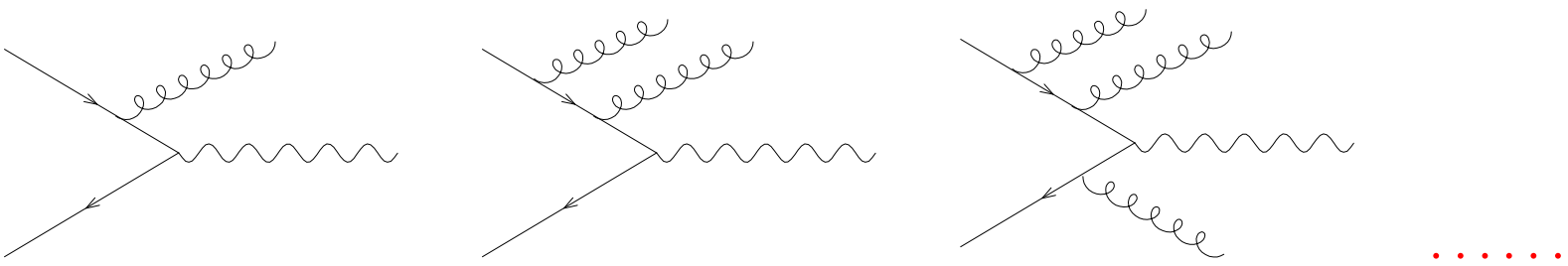
Which ones?

There are two possible choices, that lead to two vastly different strategies:

- Matrix Element Corrections $\longrightarrow$ tree level
- NLOwPS $\longrightarrow$ tree level and loop

Matrix Element Corrections

Compute (exactly) as many as possible real emission diagrams before starting the shower. Example: W production



Problems

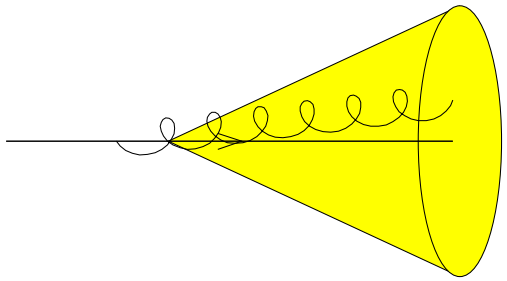
- Double counting (the shower can generate the same diagrams)
- The diagrams are divergent

Solutions

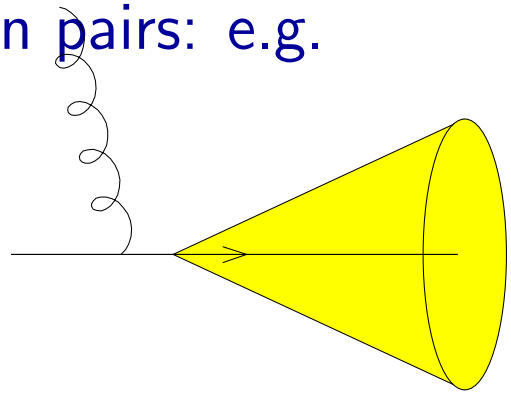
$\longrightarrow$ Catani, Krauss, Kuhn, Webber (2001), Lönnblad (2002), Mangano (2005)
(CKKW, SMPR, CKKW-L, MLM)

What all solutions have in common

- Separate PS- from ME-dominated kinematics regions. This is done by "measuring" the hardness of each parton pairs: e.g.



Soft $\Longrightarrow$ use PS



Hard $\Longrightarrow$ use ME's

- This removes double counting (and divergencies in ME's), but it introduces an unphysical bias, upon which physical predictions depend

- The bias is removed by *at least one* of the following operations

  Modify ME's (through reweighting)

  Choose suitable PS initial conditions (depend on kinematics)

  Forbid emissions/Reject events in the shower phase

CKKW

- Separation criterion: jet k_T clustering algorithm (merge if $d_{ij} < Q^2_{sep}$)
- Reweight ME's with Sudakovs, i.e. the probability that shower could not have generated softer branchings. Sudakovs are LL ones, e.g.

$$\Delta_q(Q_1, Q_2) = \exp\left[-\frac{2C_F}{\pi}\int_{Q_1}^{Q_2} dq \frac{\alpha_S(q)}{q}\left(\log\frac{Q_2}{q} - \frac{3}{4}\right)\right],$$

- Correct the (angular-ordered) shower by *vetoeing* certain emissions (those harder than Q^2_{sep} – hardness is measured by k_T here)
- The latter two steps guarantee that Q^2_{sep} dependence is of NLL

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- Evolution (θ) and merging (k_T) variables not the same: tricky initial conditions, and veto must be forced
- Lack some large-angle soft radiation (should have been emitted by internal lines early in the shower) – a subleading effect?

CKKW-like

SMPR (S. Mrenna & P. Richardson)

Apply CKKW to hadronic collisions with Pythia and Herwig

Tests several choices of scales and initial conditions

Use (among others) the same Sudakovs as in the MC

SHERPA (pre-2009)

CKKW except for use of virtuality-order shower

SHERPA (2009)

Use (CS) dipole-type shower, p_T-ordered

Introduce a clustering algorithm that matches shower variables

Use the same Sudakovs as in MC

Add soft radiation where lacking (see later)

CKKW-L (Lönnblad)

Implemented in ARIADNE, thus uses dipole shower and p_T ordering

Clustering is done by inverting shower evolution. This implies that intermediate configurations are indistinguishable from shower-generated final states (in CKKW, this is true only up to power-suppressed effects)

Use the same Sudakovs as in the MC

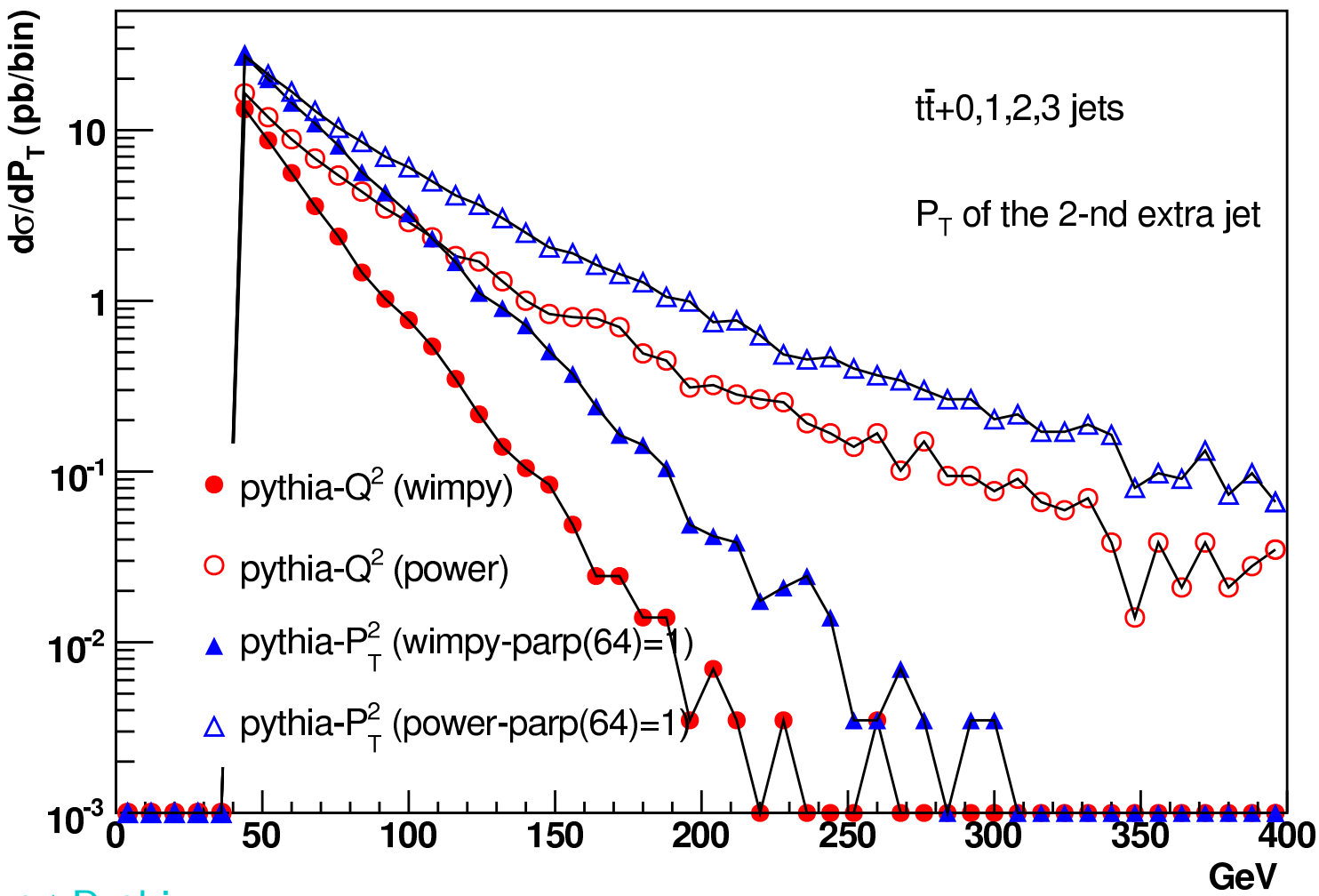
MLM (Mangano)

A cone algorithm is used for clustering

Shower the hard events without vetoeing. Matrix elements are not reweighted

Reconstruct jets after shower. If the number of jet is not equal to the number of original hard partons, throw the event away
(this corresponds to matrix element reweighting and vetoed showers)

Matching at work: before matching

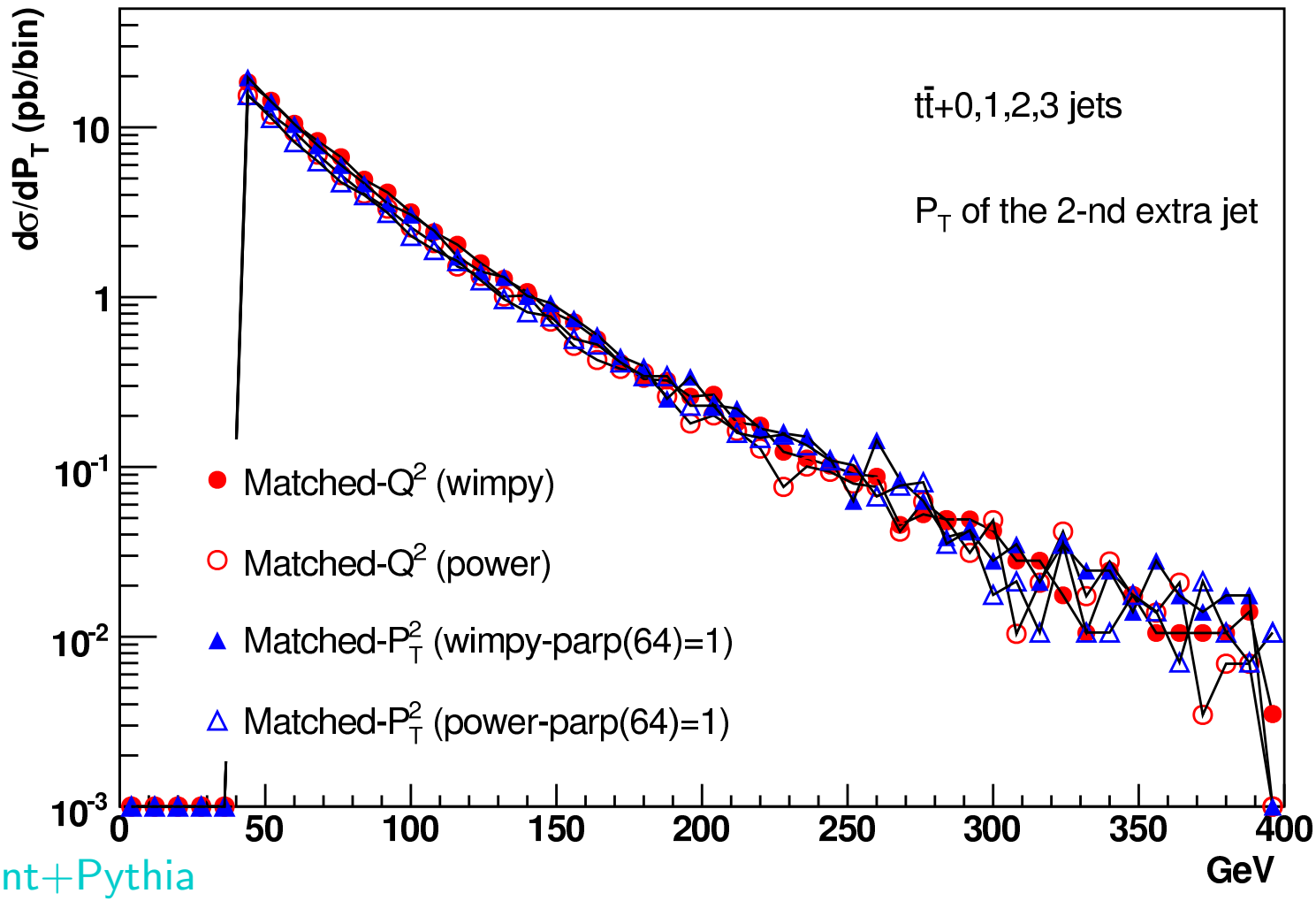


MadEvent+Pythia

OK if you want to fit data, useless to have an idea of how data *will* look like

In other words, good at postdictions, but no predictive power

Matching at work: after matching

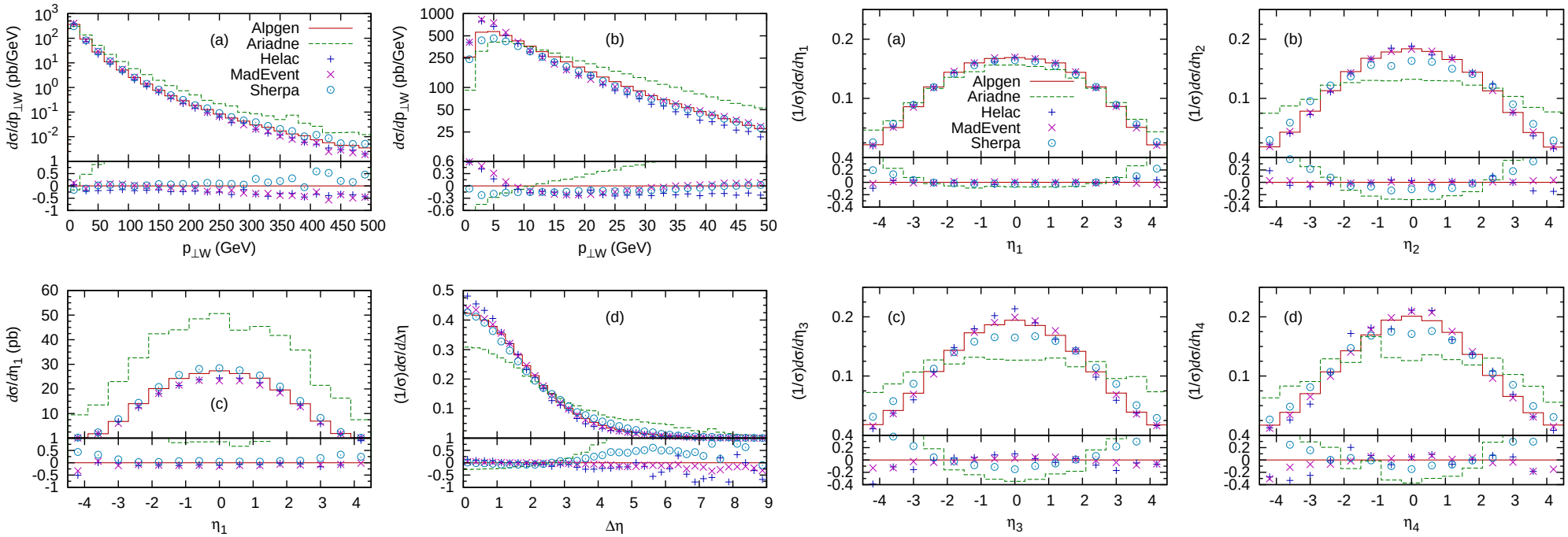


MadEvent+Pythia

A simple reason for this: the physics is right (no collinear approximation used outside the collinear regions)

Is this prediction reliable?

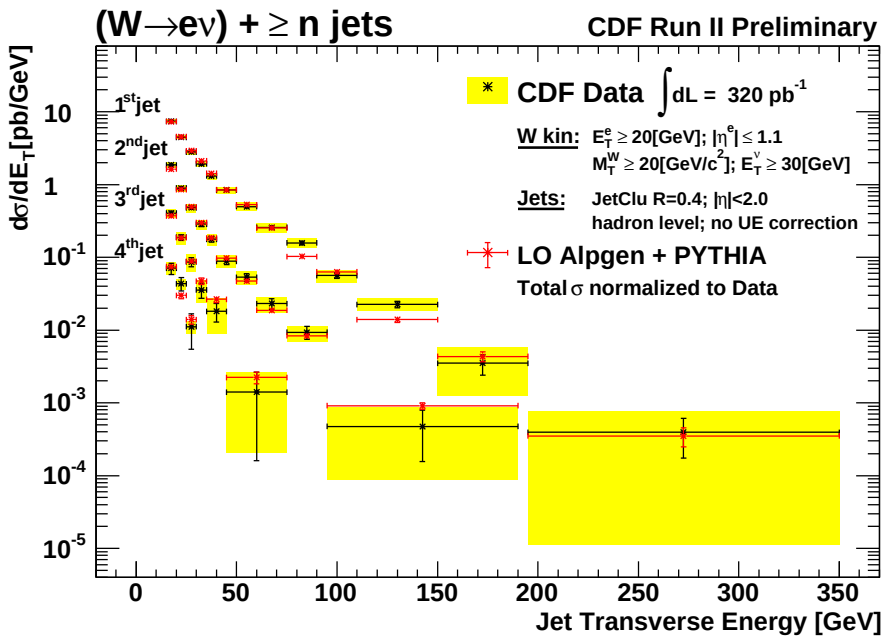
Different matching schemes result in...

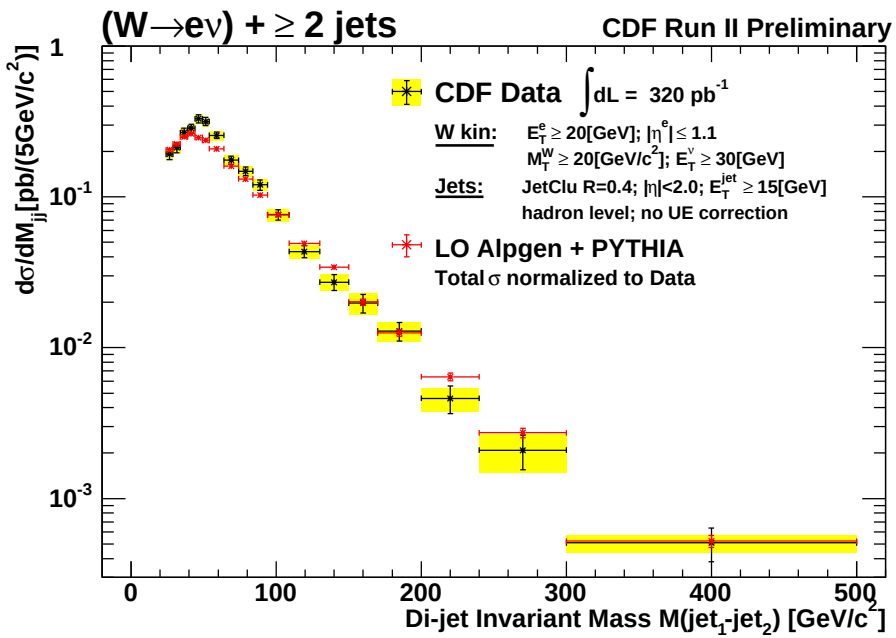


(Alwall *et al.*, 0706.2569)

...reasonably good agreement (10-50%). ARIADNE has the largest differences, but this is more a consequence of lack of proper ISR description than of matching

Comparisons to data





http://www-cdf.fnal.gov/physics/new/qcd/wjets_07/wjets.html

Once the overall normalization is fixed (i.e., one parameter) one obtains a very satisfactory description (which improves that of standard MCs by *orders of magnitude*)

Several other successful comparisons exist (typically, for Z/W+jets) using different codes (SHERPA, MadEvent+MCs,...)

MEC: what to take home

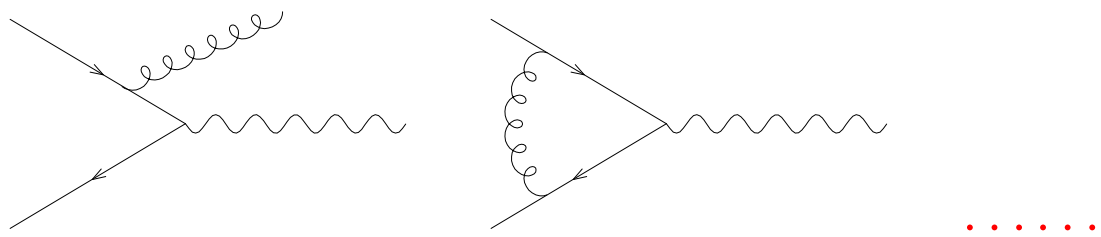
Substantial progress made in the past few years. Main consequence: multi-jet backgrounds not a matter of science fiction any longer

- Never forget to check the merging systematics
- Tuning to data is strongly recommended, and anyhow necessary to figure out the correct normalization: these are LO QCD computation!
- These procedures have been thoroughly tested for W/Z+jets. For other processes, or peculiar observables, systematics can be (much?) larger. Compare predictions from different codes

The use of standalone PYTHIA/HERWIG for multi-jet physics cannot be excused any longer. That's the stone age

NLOwPS

Compute all the NLO diagrams (and only those) before starting the shower.
Example: W production



Problems

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Solution

$\longrightarrow$

Proposals for NLOwPS's

- First working hadronic code (Z): Φ-veto (Dobbs, 2001)
- First correct general solution: MC@NLO (Frixione, Webber, 2002)
- Automated computations of ME's: grcNLO (GRACE group, 2003)
- Absence of negative weights (Nason, 2004; Frixione, Nason, Oleari, 2007) – POWHEG
- Showers with high log accuracy in ϕ_6^3 (Collins, Zu, 2002–2004)
- Within Soft Collinear Effective Theory (Bauer, Schwartz, 2006)
- Showers with quantum interference, colours (Nagy, Soper, 2007–2008)
- Shower and matching with QCD antennae (Giele, Kosower, Skands 2007) – VINCIA
- With analytic showers – GenEvA (Bauer, Tackmann, Thaler, 2008)
- Together with MEC in e^+e^- (Lavesson, Lönnblad, 2008)

Some of these ideas have passed the crucial test of implementation. However, only two codes (MC@NLO and POWHEG) can be used to fully simulate a variety of hadronic processes

MC@NLO

- Compute what the MC does at the first non trivial order, and subtract it from the matrix elements. The resulting short-distance cross sections can be unweighted, and the hard events thus obtained are used as initial conditions for parton showers

- One set of analytical computations per MC (presently, HW and HW++)
- Negative weights
- Strictly identical to MC in soft/collinear regions
- Strictly identical to NLO in hard emission regions;
  all $\mathcal{O}(\alpha_s^{2+b})$ terms not logarithmically enhanced are zero
- Inclusive cross sections identical to total cross section @NLO

NLO and MC computations

- NLO cross section (based on subtraction)

$$\left(\frac{d\sigma}{dO}\right)_{subt} = \int d\phi_{n+1}\Big[\delta(O - O(2 \to n+1))\mathcal{M}^{(r)}(\phi_{n+1}) + \delta(O - O(2 \to n))\Big(\mathcal{M}^{(b+v+rem)}(\phi_n) - \mathcal{M}^{(c.t.)}(\phi_{n+1})\Big)\Big]$$

- MC

$$\mathcal{F} = \mathcal{F}^{(2\to n)}\mathcal{M}^{(b)}(\phi_n)$$

- Matrix elements $\longrightarrow$ normalization, hard kinematic configurations
- δ-functions, $\mathcal{F}^{(2\to n)} \equiv$ showers $\longrightarrow$ kinematic "evolution"

$\Longrightarrow$ How about the replacements

$$\Big(\delta(O - O(2 \to n)), \delta(O - O(2 \to n+1))\Big) \longrightarrow \Big(\mathcal{F}^{(2\to n)}, \mathcal{F}^{(2\to n+1)}\Big) \; ?$$

Construction of MC@NLO

The naive prescription doesn't work: MC evolution results in spurious NLO terms

$\longrightarrow$ *Eliminate the spurious NLO terms "by hand"*

$$\mathcal{F}_{\text{MC@NLO}} = \mathcal{F}^{(2\to n+1)}\, d\sigma^{(\mathbb{H})}_{\text{MC@NLO}} + \mathcal{F}^{(2\to n)}\, d\sigma^{(\mathbb{S})}_{\text{MC@NLO}}$$

with the two *finite* short-distance cross sections

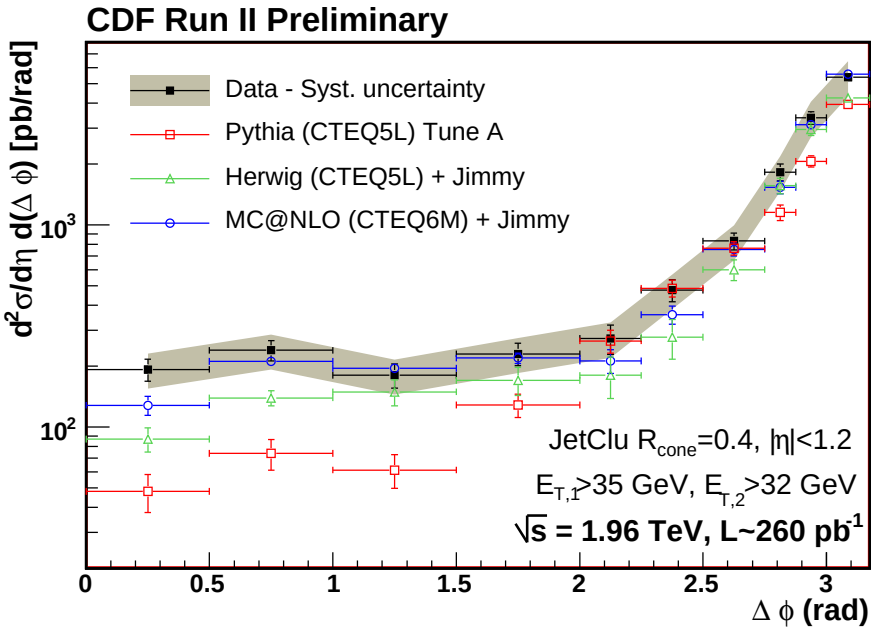
$$d\sigma^{(\mathbb{H})}_{\text{MC@NLO}} = d\phi_{n+1}\left(\mathcal{M}^{(r)}(\phi_{n+1}) - \mathcal{M}^{(\text{MC})}(\phi_{n+1})\right)$$

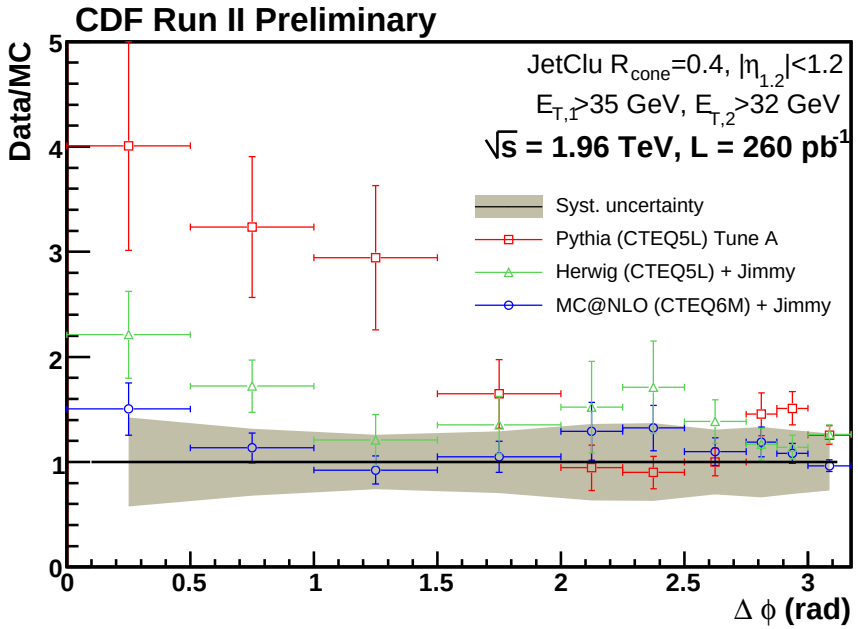
$$d\sigma^{(\mathbb{S})}_{\text{MC@NLO}} = \int_{+1} d\phi_{n+1}\left(\mathcal{M}^{(b+v+rem)}(\phi_n) - \mathcal{M}^{(c.t.)}(\phi_{n+1}) + \mathcal{M}^{(\text{MC})}(\phi_{n+1})\right)$$

that feature the *MC subtraction terms*

$$\boxed{\mathcal{M}^{(\text{MC})} = \mathcal{F}^{(2\to n)}\mathcal{M}^{(b)} + \mathcal{O}(\alpha_S^2\alpha_S^b)}$$

b-jet CDF data vs MC@NLO



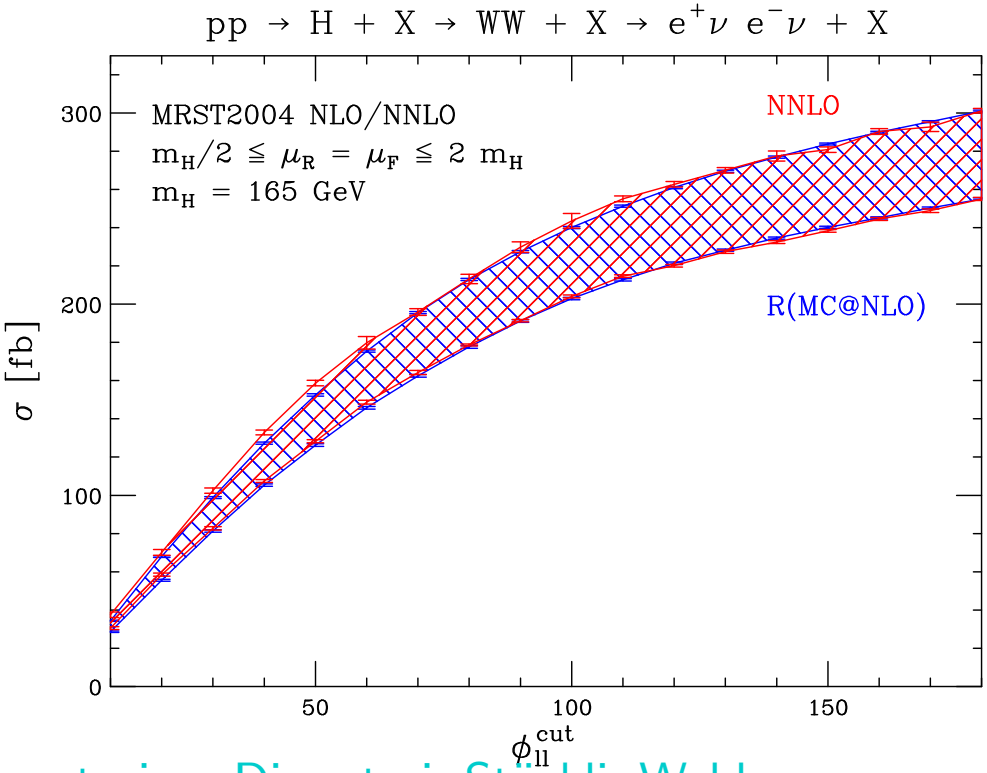


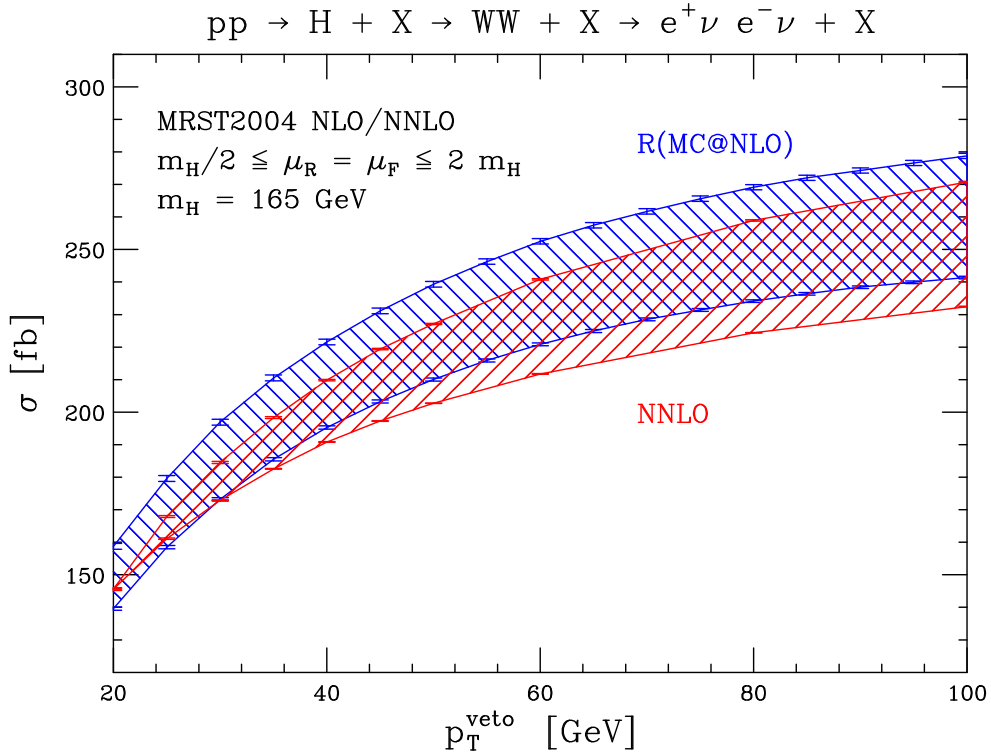
Agreement with data significantly improves when including NLO corrections

Jimmy does significantly better than Herwig default

$\Longrightarrow$ Quite a powerful test of the whole NLO+shower machinery

MC@NLO vs NNLO





Anastasiou, Dissertori, Stockli, Webber

After *overall* rescaling NNLO/NLO, most observables are in perfect agreement

Similar findings by M. Grazzini. For certain observables, NNLO must be matched to (analytical) resummation results for full agreement. Very powerful test of MC@NLO

POWHEG

- Replace the first MC emission with one generated with a p_T-ordered Sudakov, constructed by exponentiating the *full real matrix element*. Requires a truncated shower to restore the correct pattern of soft emissions for angular-ordered showers

- Short-distance computations independent of MCs
- No negative weights
- Differs from MC in soft/collinear regions if MC is not p_T-ordered. For angular-ordered showers, agreement with MC is restored by truncated showers (up to subleading terms)
- Differs from NLO in hard emission regions by $\mathcal{O}(\alpha_S^{2+b})$ terms; no piece of information on NNLO is used
- Inclusive cross sections not identical to total cross section @NLO

Construction of POWHEG

Start with an exact phase-space factorization $d\phi_{n+1} = d\phi_n d\phi_r$, and construct

$$\overline{\mathcal{M}}^{(b)}(\phi_n) = \mathcal{M}^{(b+v+rem)}(\phi_n) + \int d\phi_r \left[\mathcal{M}^{(r)}(\phi_{n+1}) - \mathcal{M}^{(c.t.)}(\phi_{n+1})\right]$$

For a *given* p_T, define the *vetoed* <u>*process-dependent*</u> Sudakov

$$\Delta_R(t_I, t_0; p_T) = \exp\left[-\int_{t_0}^{t_I} d\phi_r' \frac{\mathcal{M}^{(r)}}{\mathcal{M}^{(b)}} \Theta(k_T(\phi_r') - p_T)\right]$$

Obtain hard configurations (to be given to shower as initial conditions) from the short-distance cross section

$$d\sigma_{\text{POWHEG}} = d\phi_n \overline{\mathcal{M}}^{(b)}(\phi_n) \left[\Delta_R(t_I, t_0; 0) + \Delta_R(t_I, t_0; k_T(\phi_r)) \frac{\mathcal{M}^{(r)}(\phi_{n+1})}{\mathcal{M}^{(b)}(\phi_n)} d\phi_r\right]$$

which includes Sudakov suppression at $p_T \to 0$

- $k_T(\phi_r)$ will play the role of hardest emission
- The full real matrix element is exponentiated

Attaching (angular-ordered) showers

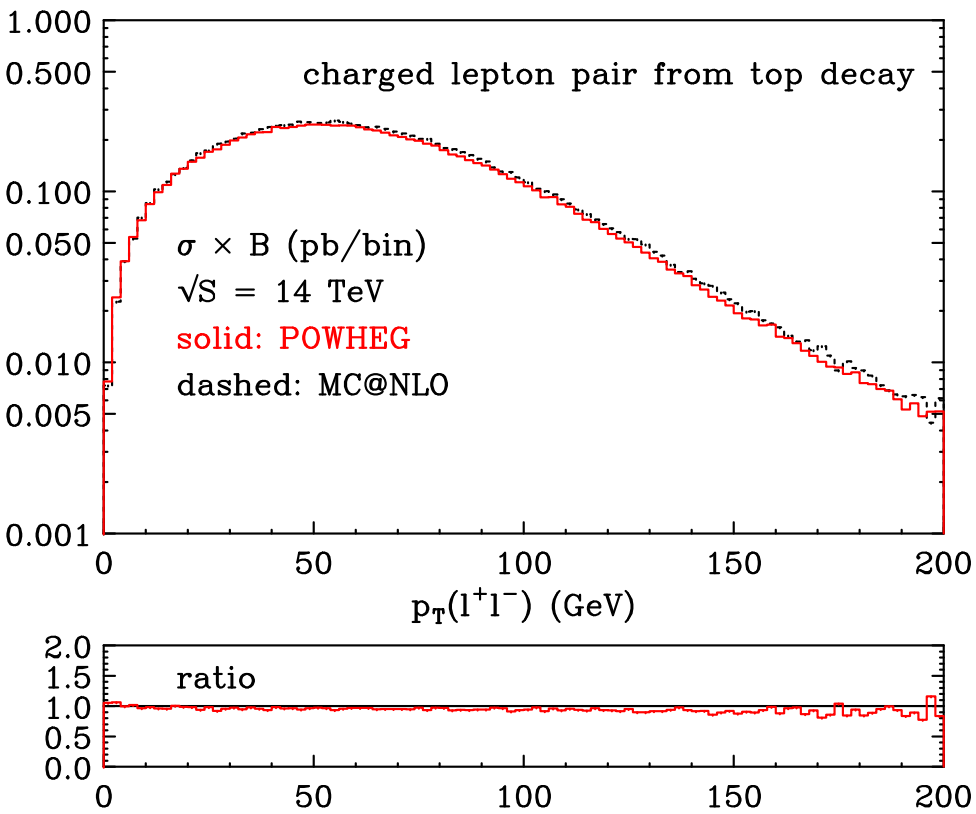
- One wants the matrix-element-generated p_T to be the hardest
  $\Longrightarrow$ veto emissions harder than p_T during shower
- But this screws up colour coherence

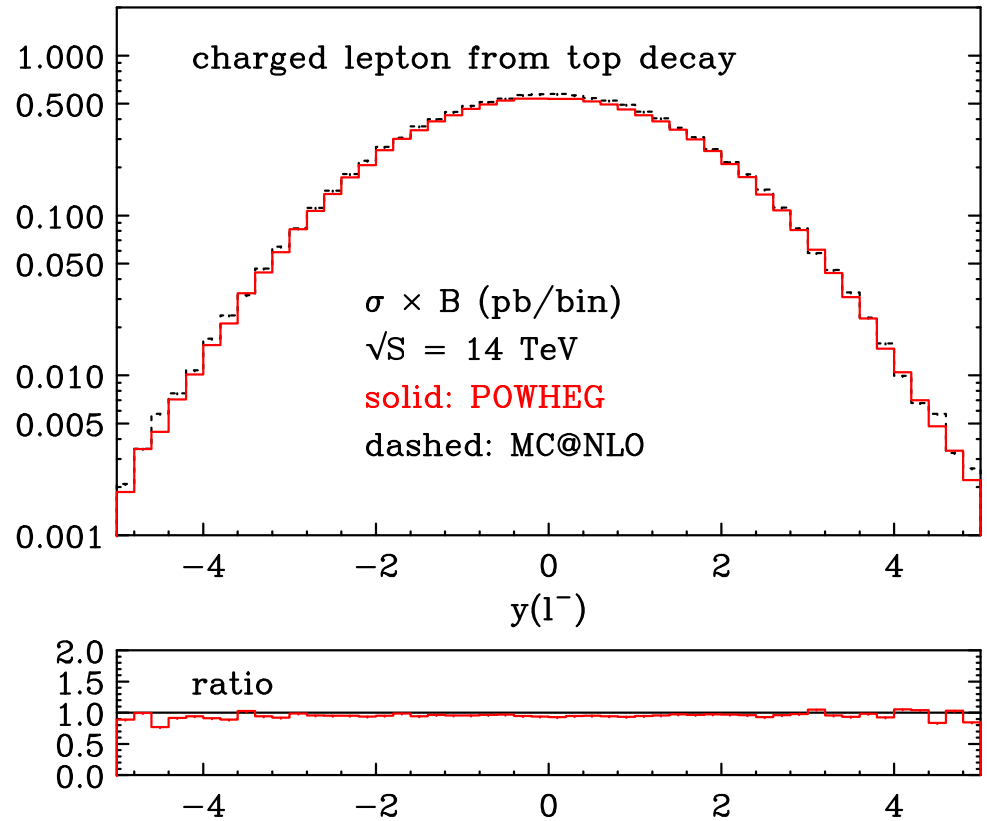
Colour coherence can be restored at the price of a more involved structure

$$\mathcal{F}_{\text{POWHEG}}[t_I; p_T] = \Delta(t_I, t_0) + \int_{t_0}^{t_I} \frac{dt}{t} \int dz \Delta_R(t_I, t; p_T) \frac{\alpha_S}{2\pi} P(z) \times \mathcal{F}_{\text{V}}((1-z)^2 t; p_T)\, \mathcal{F}_{\text{V}}(z^2 t; p_T)\, \mathcal{F}_{\text{VT}}(t_I, t; p_T)$$

- $\mathcal{F}_{\text{V}}(t; p_T)$ are *vetoed* showers. Evolve down to t_0, with all emissions constrained to have a transverse momentum smaller than p_T
- $\mathcal{F}_{\text{VT}}(t_I, t; p_T)$ are *vetoed-truncated* showers. Evolve from t_I down to t (i.e., *not* t_0) along the hardest line. On top of that, they are vetoed

MC@NLO vs POWHEG



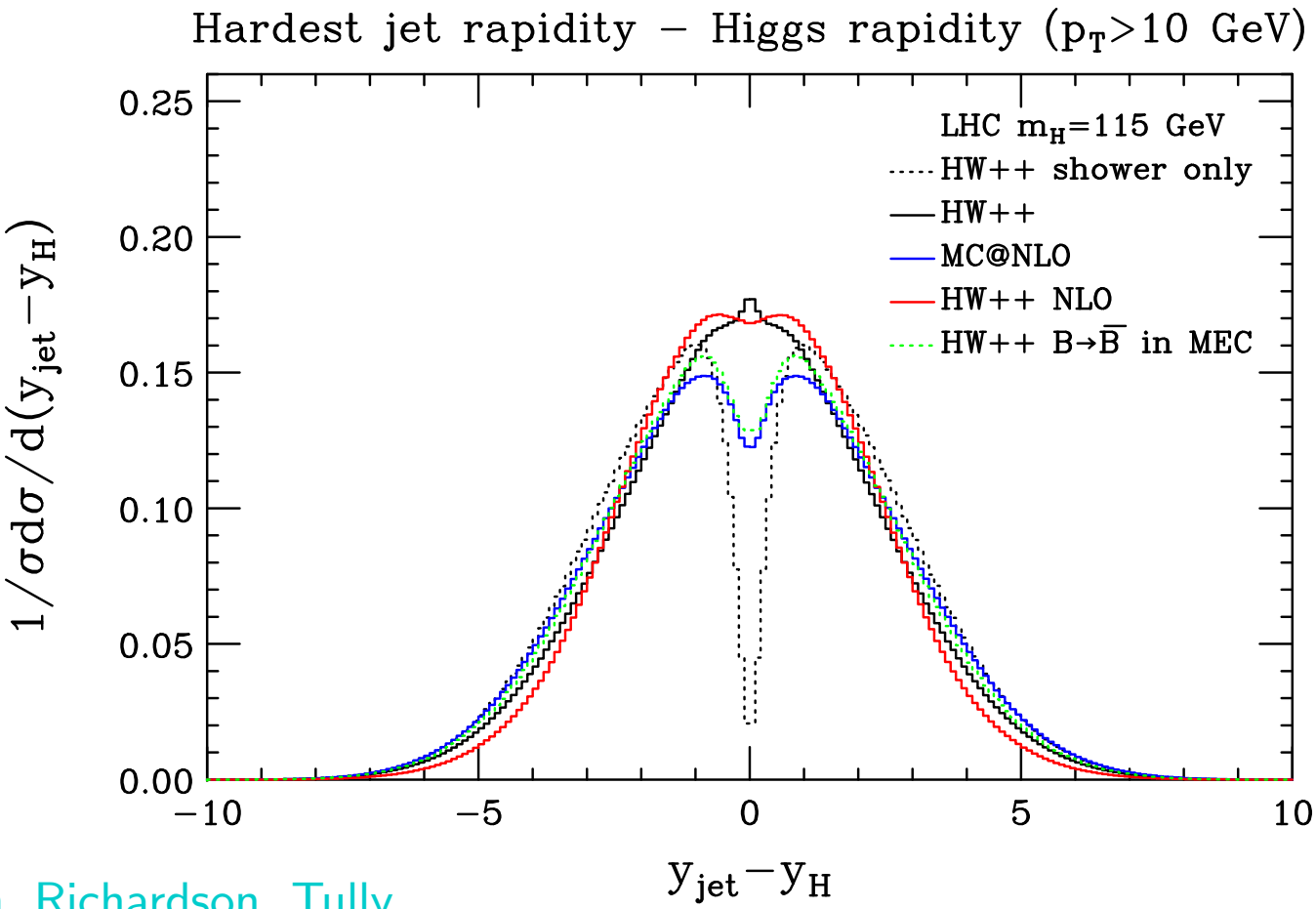


Shown here for lepton observables arising from top decays at the LHC

In the vast majority of cases, extremely good agreement is found

There are a few interesting cases where large differences are found

MC@NLO vs POWHEG: discrepancies



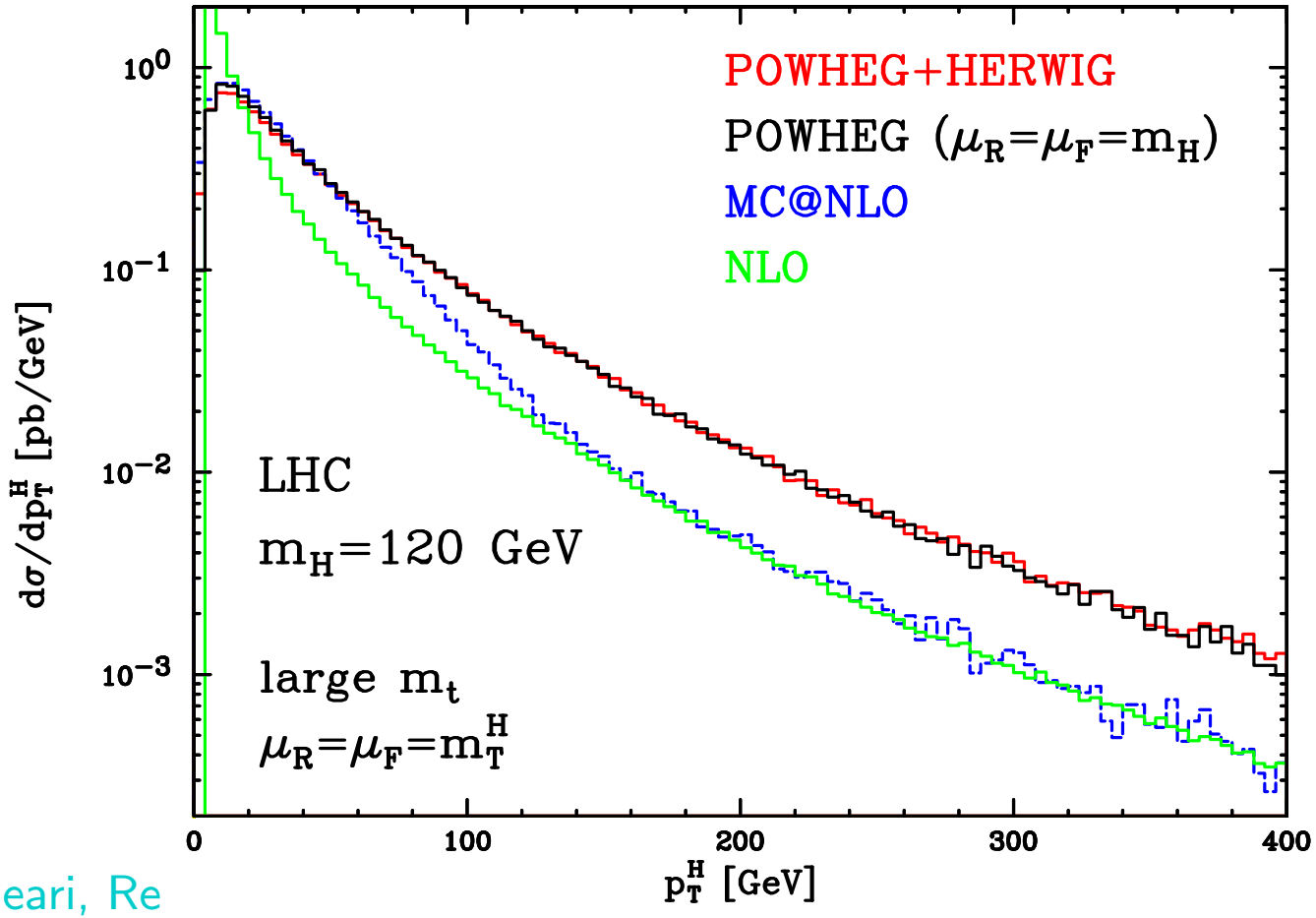
Hamilton, Richardson, Tully

HW/HW++ have dips at $\Delta y = 0$. Likely an artifact of dead zones

MC@NLO fills that dip, via hard radiation

POWHEG fills it much more, owing to extra (spurious) $\mathcal{O}(\alpha_s^4)$ terms

MC@NLO vs POWHEG: discrepancies



Alioli, Nason, Oleari, Re

POWHEG a factor ~ 3 larger than MC@NLO$\equiv$ NLO in the tail

POWHEG result can be decreased by removing part of the real contribution from the exponent. Predictive power?

Note: MC@NLO and POWHEG use the *same matrix elements*

NLOwPS-motivated spinoffs

- Matching according to MC@NLO-like procedures may be technically easier if MCs used the same variables as NLO (Nagy, Soper). This led to showers based on Catani-Seymour dipoles (SHERPA; Weinzierl *et al*)
  - IMHO motivation is not overwhelming (and CS is not ideal for large multiplicities), but there are interesting kinematic features, e.g. momentum conservation at each branching
  - Lots of similarities with dipole-antennae (ARIADNE, VINCIA)

- The use of truncated showers help improving the colour pattern in CKKW, since it provides soft radiation where it was missing
  - Systematic work being done in HERWIG++ and SHERPA
  - This, together with other improvements, reduces dependence on the matching parameter – too much, perhaps?

Conclusions and outlook

- Perturbative results for matrix elements systematically included in MCs, with theoretically-solid techniques
- Non-perturbative models for UE studied and fitted. Would benefit from new theoretical ideas
- New versions of PYTHIA, SHERPA, and HERWIG++ released in 2008/2009

Future prospects

- MEC $\longrightarrow$ NLOwPS (high mult): require automated 1-loop computations. Steady progress there
- Showers accurate at LL for collinear *and* soft-collinear *and* soft (soft at large N_c only)
- NNLOwPS?