QCD (for LHC)
Lecture 3: predictive methods

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This lecture will be about some of the different ways we can make QCD predictions.

It'll touch on:

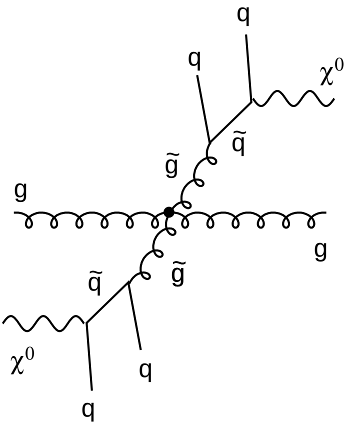
- LO, NLO, NNLO calculations
- Parton-Shower Monte Carlos

Most of the examples will involve Z (& sometimes W) production at hadron colliders.

Because Z, W decay to leptons and to neutrinos, both of which are easily-taggable handles that are characteristic of many new physics scenarios.

SUSY example: gluino pair production

Signal



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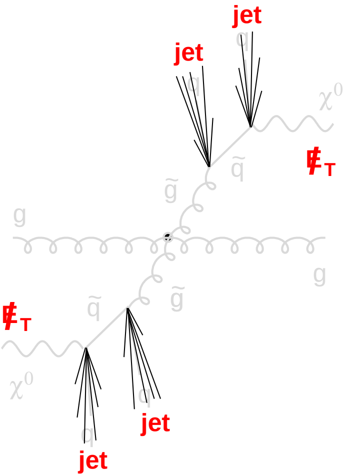

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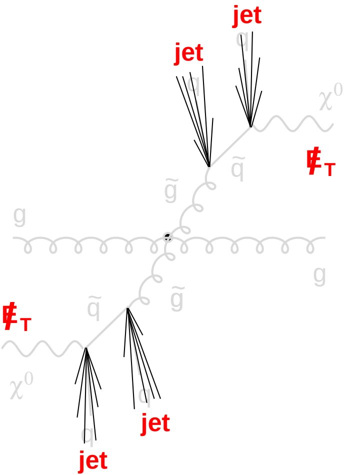
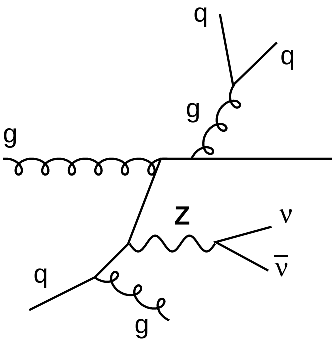


Background



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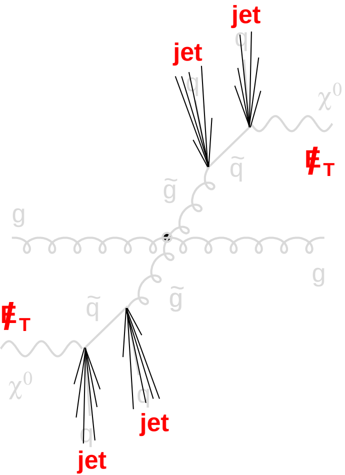

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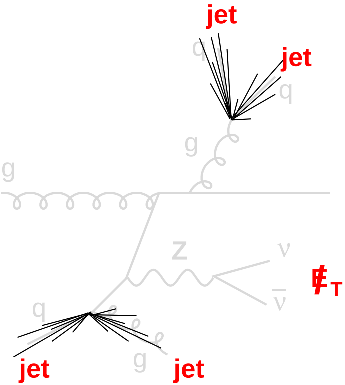

Example SUSY searches

Atlas selection [all hadronic]

- no lepton
- MET > 100 GeV
- $1^{st}, 2^{nd}$ jet > 100 GeV
- $3^{rd}, 4^{th}$ jet > 50 GeV
- MET / m_{eff} > 20%

Christian Autermann
SUSY08 16.-21.6.08
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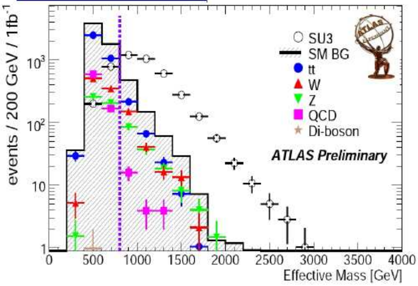
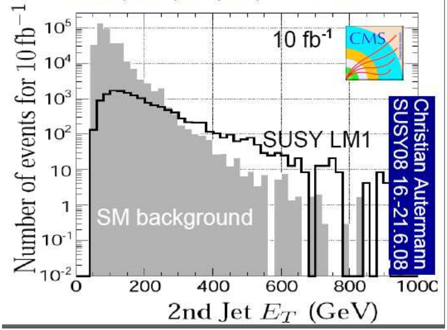


CMS selection [leptonic incl.]

(optimized for 10fb^{-1}, using genetic algorithm)

- 1 muon pT > 30 GeV
- MET > 130 GeV
- 1^{st}, 2^{nd} jet > 440 GeV
- 3^{rd} jet > 50 GeV
- $-0.95 < \cos(\text{MET}, 1^{st}\text{jet}) < 0.3$
- $\cos(\text{MET}, 2^{nd}\text{jet}) < 0.85$



total X-section $e^+e^- \to Z \to$ hadrons

Start simply and look back at cross section for $e^+e^- \to Z \to$hadrons (at $\sqrt{s} \equiv Q = M_Z$).

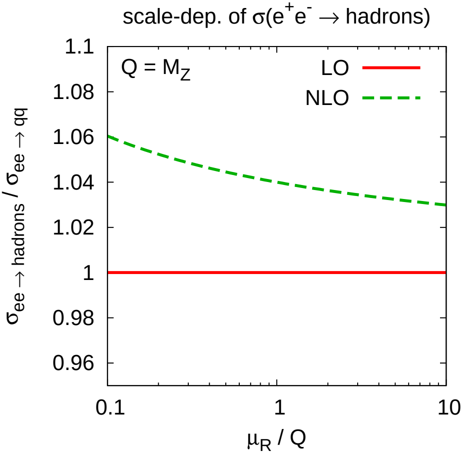
In lecture 1 we wrote:

$$\sigma_{tot} = \sigma_{q\bar{q}} \left(\underbrace{1}_{\text{LO}} + \underbrace{1.045 \frac{\alpha_s(Q)}{\pi}}_{\text{NLO}} + \underbrace{0.94 \left(\frac{\alpha_s(Q)}{\pi} \right)^2}_{\text{NNLO}} + \cdots \right)$$

Who told us we should we should write the series in terms of $\alpha_s(Q)$?

$Q = M_Z$ is the only physical scale in the problem, so not unreasonable.
But hardest possible gluon emission is $E = Q/2$. Should we have used $Q/2$?
And virtual gluons can have $E > Q$. Should we have used $2Q$?

Scale dependence



Start with the first order that "contains QCD" (NLO).

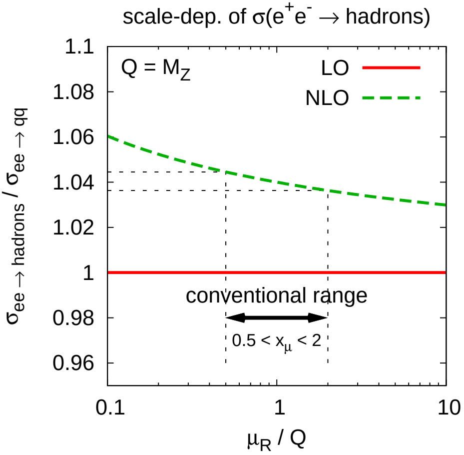
Introduce arbitrary **renormalisation scale** for the coupling, μ_R

$$\sigma^{\rm NLO} = \sigma_{q\bar{q}}\,(1 + c_1\alpha_s(\mu_R)\,)$$

Result depends on the choice of μ_R.

Convention: the uncertainty on the result is the range of answers obtained for $Q/2 < \mu_R < 2Q$.

Scale dependence



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Scale dependence (cont.)

Let's express results for arbitrary μ_R in terms of $\alpha_s(Q)$:

$$\sigma^{\mathrm{NLO}}(\mu_R) = \sigma_{q\bar{q}}\,(1 + c_1\,\alpha_s(\mu_R))$$
$$= \sigma_{q\bar{q}}\left(1 + c_1\,\alpha_s(Q) - 2c_1 b_0 \ln\frac{\mu_R}{Q}\,\alpha_s^2(Q) + \mathcal{O}\left(\alpha_s^3\right)\right)$$

As we vary the renormalisation scale μ_R, we introduce $\mathcal{O}\left(\alpha_s^2\right)$ pieces into the X-section. I.e. generate some set of NNLO terms $\sim$ uncertainty on X-section from missing NNLO calculation.

If we now calculate the full NNLO correction, then it will be structured so as to cancel the $\mathcal{O}\left(\alpha_s^2\right)$ scale variation

$$\sigma^{\mathrm{NNLO}}(\mu_R) = \sigma_{q\bar{q}}\left[1 + c_1\,\alpha_s(\mu_R) + \left(c_2 + 2c_1 b_0 \ln\frac{\mu_R}{Q}\right)\alpha_s^2(\mu_R)\right]$$

Remaining uncertainty is now $\mathcal{O}\left(\alpha_s^3\right)$.

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$$\alpha_s(\mu_R) = \frac{\alpha_s(Q)}{1 + 2b_0\, \alpha_s(Q) \ln \mu_R/Q}$$

$$= \alpha_s(Q) - 2b_0\, \alpha_s^2(Q) \ln \mu_R/Q + \mathcal{O}\left(\alpha_s^3\right)$$

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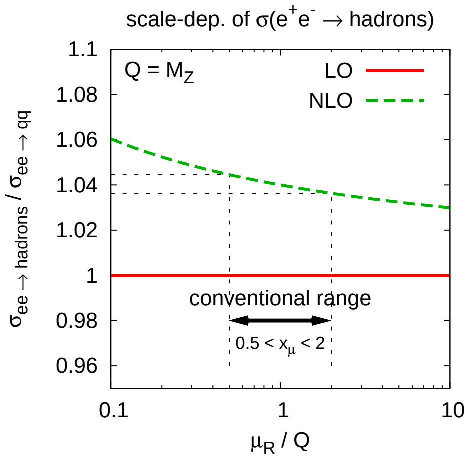
Scale dependence: NNLO



See how at NNLO, scale dependence is much flatter, final uncertainty much smaller.

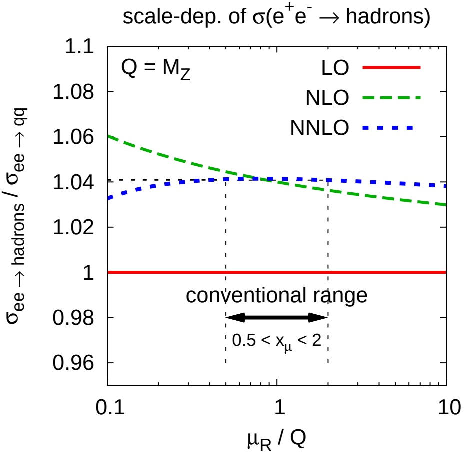
Because now we neglect only α_s^3 instead of α_s^2

Moral: not knowing exactly how to set scale → blessing in disguise, since it gives us handle on uncertainty.

Scale variation ≡ standard procedure
Often a good guide
Except when it isn't!

NB: if we had a large number of orders of perturbation theory, scale dependence would just disappear.

Scale dependence: NNLO



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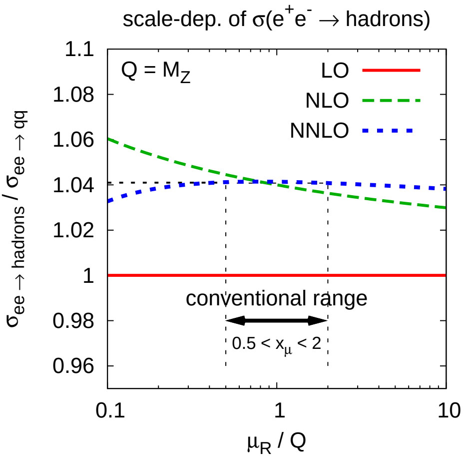

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Now switch to looking at the Z cross section in pp

LO $pp \to Z$

$$\sigma^{\text{LO}}_{pp\to Z} = \sum_i \int dx_1 dx_2\, f_{q_i}(x_1, \mu_F^2)\, f_{\bar{q}_i}(x_2, \mu_F^2)\, \hat{\sigma}_{0,q_i\bar{q}_i\to Z}(x_1 p_1, x_2 p_2)\,,$$

- $\sigma_{0,q_i\bar{q}_i\to Z} \propto \alpha_{EW}$, knows nothing about QCD — like $\sigma_{e^+e^-\to Z}$
- But $\sigma_{0,q_i\bar{q}_i\to Z}$ depends on PDFs.
- We have to choose a **factorisation scale, μ_F**.
- Natural choice: $\mu_F = M_Z$, but one should vary it (just like the renorm. scale, μ_R, for α_s).

Plot shows $\sigma^{\text{LO}}_{pp\to Z}$ differentially as a function of rapidity (y) of Z. Band is uncertainty due to variation of μ_F.

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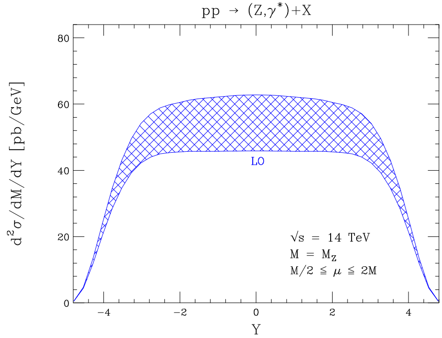

$M_Z/2 \le \mu_F \le 2M_Z$

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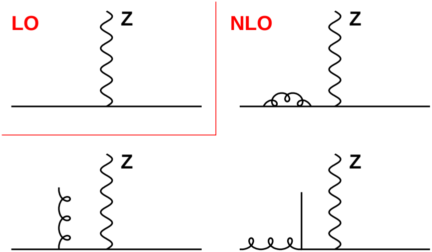
$pp \to Z + X$ at (N)NLO

$$\sigma^{\rm NLO}_{pp\to Z} = \sum_{i,j} \int dx_1 dx_2\, f_i(x_1,\mu_F^2)\, f_j(x_2,\mu_F^2)\, [\hat\sigma_{0,ij\to Z}(x_1,x_2) + \\ + \alpha_s(\mu_R)\hat\sigma_{1,ij\to Z}(x_1,x_2,\mu_F)]$$

- New channels open up ($gq \to Zq$)
- Now X-sct depends on renorm scale μ_R *and* fact. scale μ_F

  often vary $\mu_R = \mu_F$ together

  not necessarily "right"
- But $\hat\sigma_1$ piece cancels large LO dependence on μ_F
- At NNLO dependence on μ_R and μ_F is further cancelled



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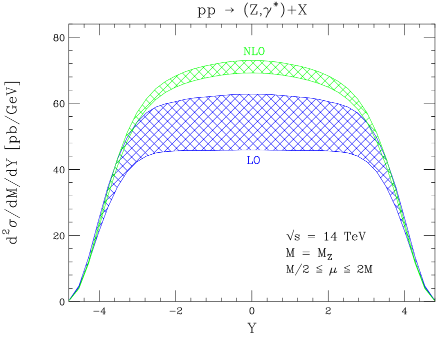

Anastasiou et al '03; $\mu_R = \mu_F$

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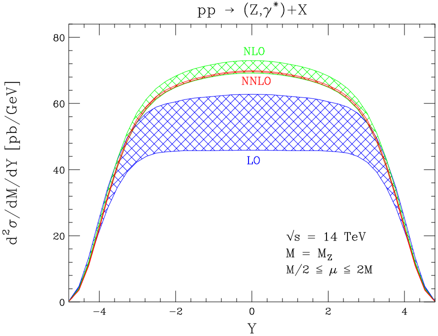

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Rules of thumb

In hadron-collider QCD calculations:

- Choose a sensible central scale for your process
- Vary μ_F, μ_R by a factor of two around that central value

- LO: good only to within factor of two — Despite $\alpha_s \simeq 0.1$
- NLO: good to within $10 - 20\%$
- NNLO: good to a few percent

The above rules fail if NLO/NNLO involve characteristically new production channels and/or large ratios of scales.

Calculations for more complex processes

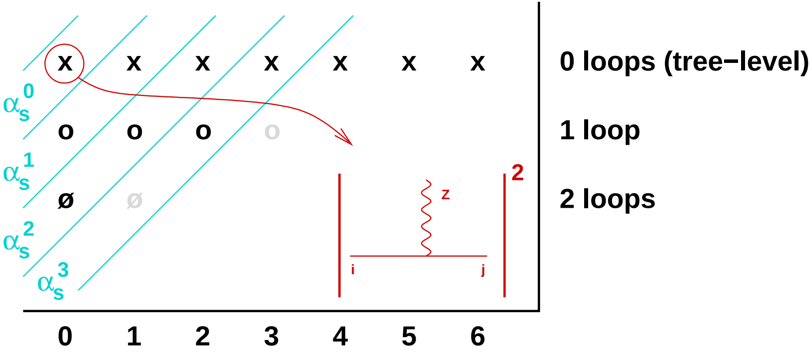
Diagrams / processes / orders

x	x	x	x	x	x	x	0 loops (tree−level)
o	o	o	o				1 loop
ø	ø						2 loops
0	1	2	3	4	5	6	

ij $\to$ Z + n partons

The bottleneck in getting N^{p}LO predictions is usually either the calculation of the p-loop diagram, or figuring out how to combine (cancel) divergences between 2-loops, 1-loop & tree-level.

Diagrams / processes / orders



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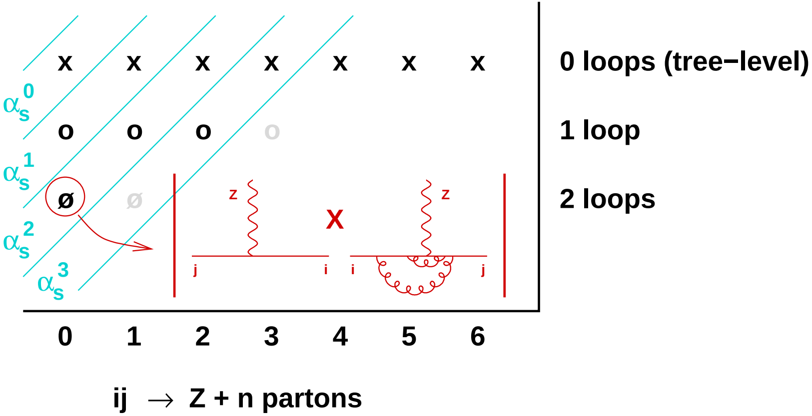

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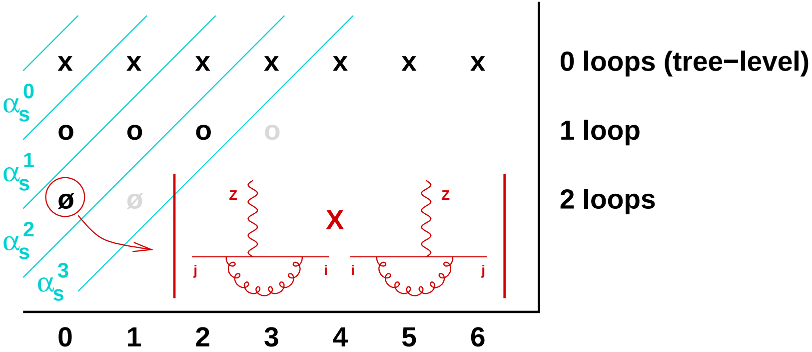

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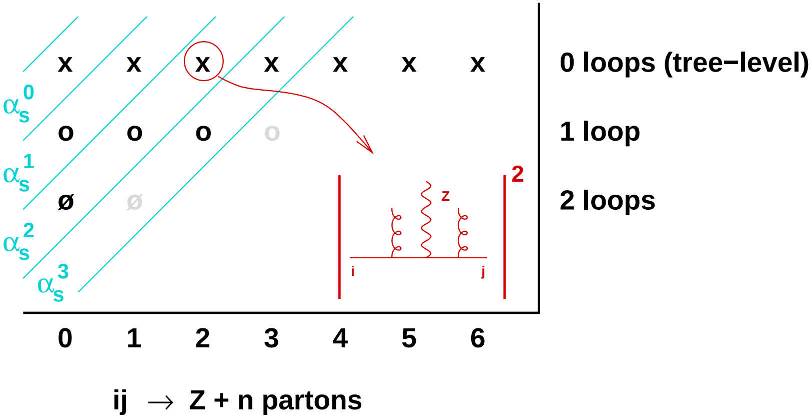

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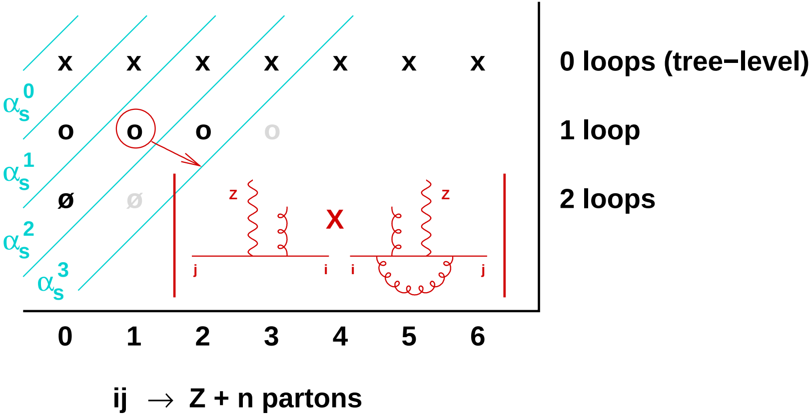

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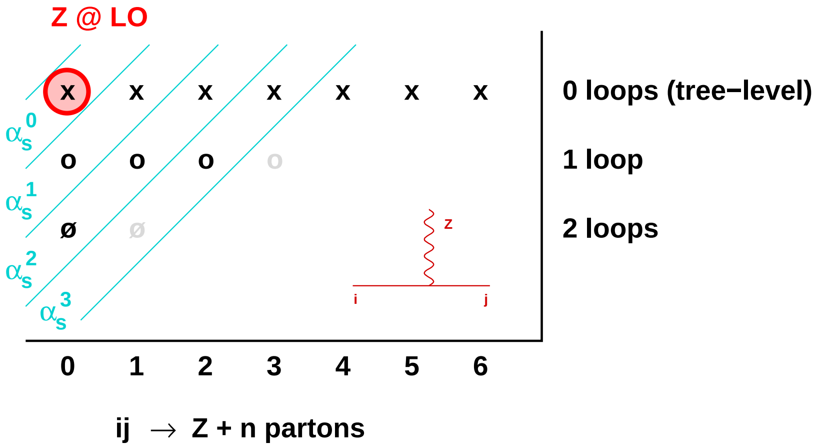

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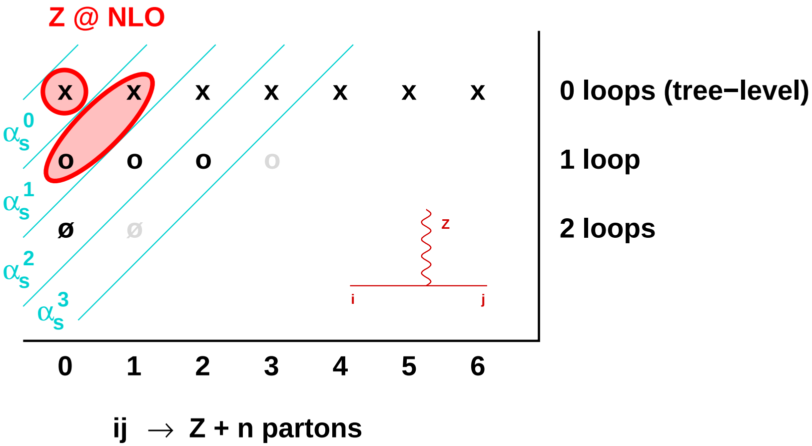

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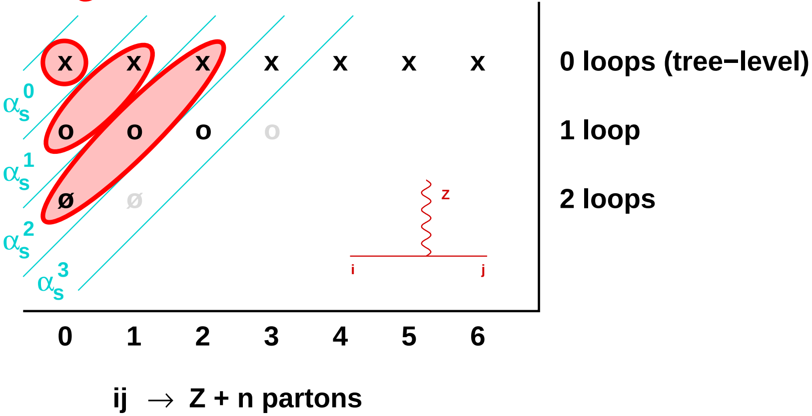
Diagrams / processes / orders

Z @ NNLO



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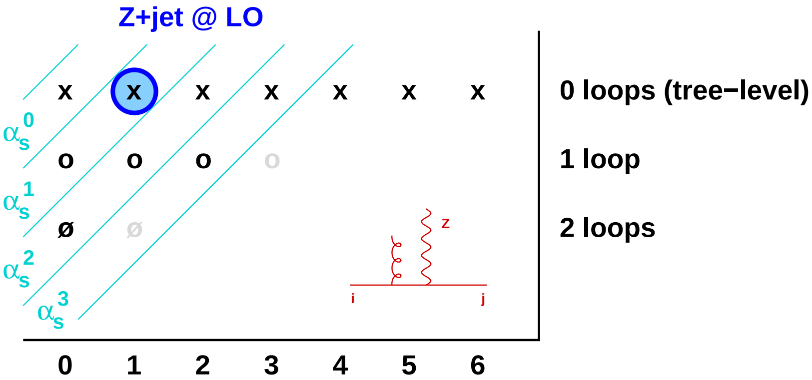

ij $\to$ Z + n partons

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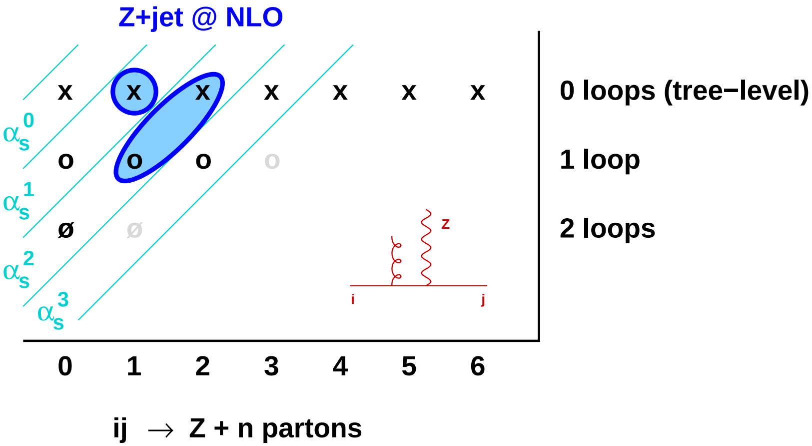

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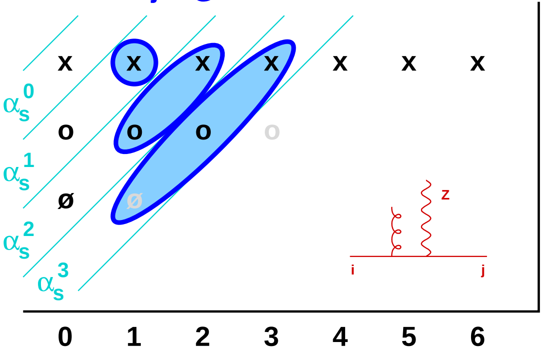
Diagrams / processes / orders

Z+jet @ NNLO



0 loops (tree−level)

1 loop

2 loops

ij $\to$ Z + n partons

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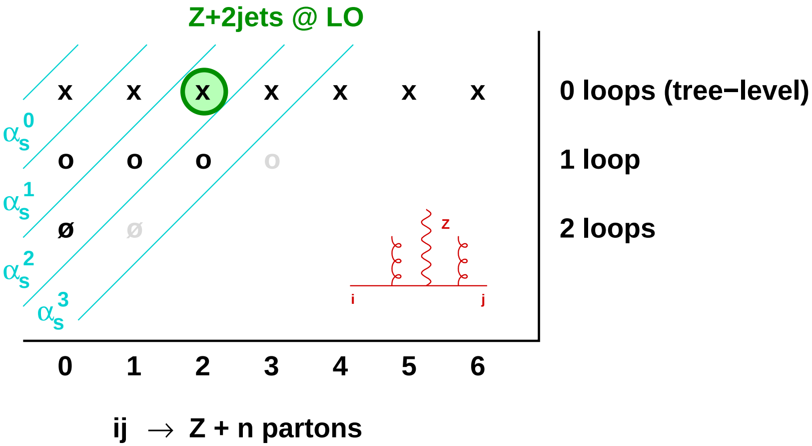
Diagrams / processes / orders



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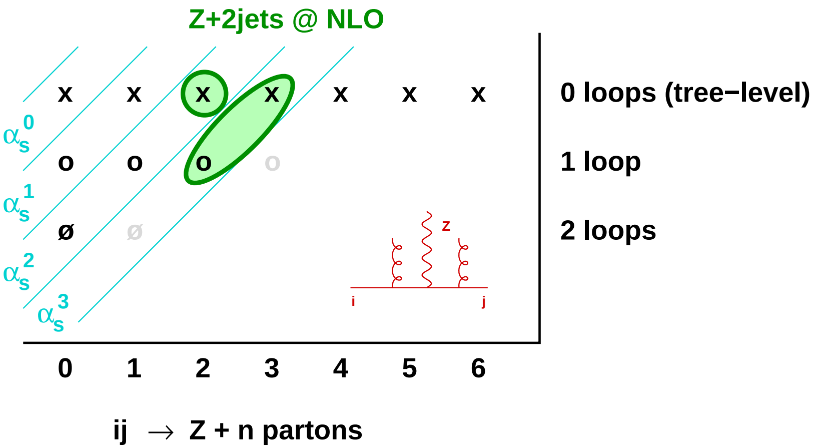
Diagrams / processes / orders



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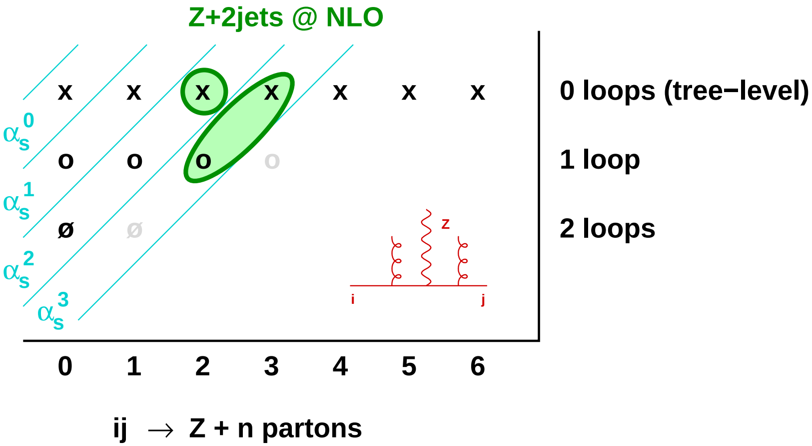

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The limits of what we know

- Tree-level / LO: $\mathbf{2 \longrightarrow 6-8}$

  ALPGEN, CompHep, Helac/Helas, Madgraph, Sherpa

- 1-loop / NLO: $\mathbf{2 \longrightarrow 3}$

  MCFM, NLOJet++, PHOX-family + various single-process codes
  some $2 \to 4$ starting to appear (W+3j, $t\bar{t}b\bar{b}$)

- 2-loop / NNLO: $\mathbf{2 \longrightarrow 1}$ (W,Z,H) FEWZ, FeHiP, HNNLO

Example of complexity of the calculations, for gg $\to$ N gluons:

Njets	2	3	4	5	6	7	8
# diags	4	25	220	2485	34300	$5\text{x}10^5$	10^7

Programs like Alpgen, Helac/Helas, Sherpa avoid Feynman diagrams
and use methods that recursively build up amplitudes

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In what form are these calculations made available?

Fully inclusive calculations

For a process that starts at order α_s^n, the fully inclusive N^{p}LO cross section for producing some object "A" is

$$\sigma^{\mathrm{N}^p\mathrm{LO}}_{pp\to A+X} = \sum_{i,j} \int dx_1 dx_2\, f_i(x_1,\mu_F^2)\, f_j(x_2,\mu_F^2) \times \sum_{m=0}^{p} \alpha_s^{n+m}(\mu_R)\, \hat{\sigma}_{m,ij\to A+X}(x_1 x_2 s, \mu_R, \mu_F)\,,$$

The $\sigma_{m,ij\to A}(x_1 x_2 s, \mu_R, \mu_F)$ are analytical functions that you'll find in a paper somewhere and *you can just implement them in your own program and do the integral.*

E.g. earliest (N)NLO calculations of $t\bar{t}$, W, Z X-scts

They tell you nothing about

- where A is produced in your detector, which direction it decays in
- what else ("X") is produced in associated with A

Exclusive calculations

Matrix-Element Monte Carlos (weighted)

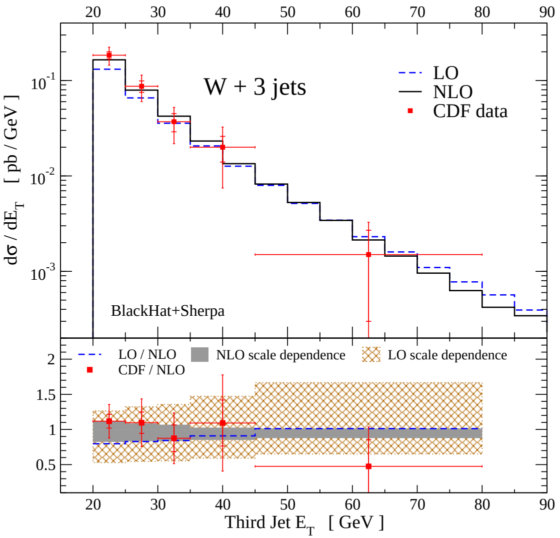
E.g. for LO (tree-level) calculation $ij \to Z + n$ jets with cuts: Alpgen, etc.

- Generate random phase-space configurations for $Z + n$ partons
- Call a user-written subroutine to decide whether event passes cuts.
- If it does, include the event weight (tree-level squared amplitude, PDFs) in the evaluation of the cross section.

Additionally for NLO: MCFM, NLOJet, Phox family, etc.

- Generate random phase-space configurations for $Z+n+1$ partons
  & if pass user cuts, include tree-level weight in cross section
- Generate random phase-space configurations for $Z+n$ partons
  & if pass user cuts, include 1-loop-level weight in cross section
  NB: loop-level $Z+n$ and tree-level $Z+n+1$ only converge if taken together and if your cuts are infrared and collinear safe

Example: W + 3 jets



The W+3-jet cross section at Tevatron. An analysis involving a jet-algorithm that cluster the partons into jets, cuts on the jets, cuts on the lepton from the W and cuts on the missing energy.

State of the art!

Berger et al, '09
also: Ellis, Melnikov & Zanderighi '09

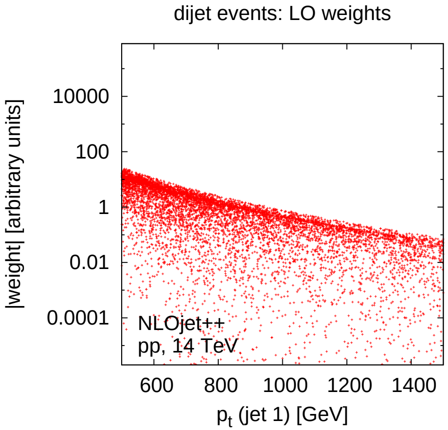
(N)NLO Matrix-Element Monte Carlos, are a powerful combination of accuracy and flexibility.

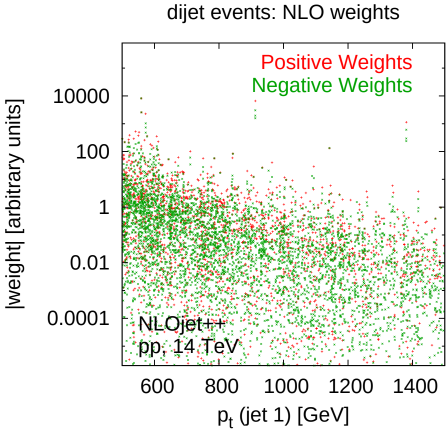
As long as you want to calculate an IR and collinear safe observable (e.g. jets, W's, Z's — but not $\pi, K, p, \ldots$)

And if you don't mind dealing with (wildly) fluctuating positive and negative event weights.

And you don't intend to study regions of phase space that involve multiple scales.

Scatter plots: weights from NLOJet++





Outliers in NLO case: near-divergent **real** and **virtual** configurations

Parton showers

Real life does not diverge

How can we reinterpret perturbation theory so as to get something more physical (and finite)?

The “right” question to ask is: *what is the probability of* **not** *radiating a gluon* above a scale k_t?

$$P(\text{no emission above } k_t) = 1 - \frac{2\alpha_s C_F}{\pi} \int^Q \frac{dE}{E} \int^{\pi/2} \frac{d\theta}{\theta} \Theta(E\theta - k_t)$$

In the soft-collinear limit, it's quite easy to calculate the full probability of nothing happening: it's just the exponential of the first order:

$$P(\text{nothing} > k_t) \equiv \Delta(k_t, Q) \simeq \exp\left[-\frac{2\alpha_s C_F}{\pi} \int^Q \frac{dE}{E} \int^{\pi/2} \frac{d\theta}{\theta} \Theta(E\theta - k_t)\right]$$

NB1: Δ is bounded — $0 < \Delta(k_t, Q) < 1$

NB2: to do this properly, running coupling should be inside integral + replace dE/E with full collinear splitting function

The parton shower

$\Delta(k_t, Q)$ is known as a **Sudakov Form Factor**

Probability distribution for first emission (e.g. $q\bar{q} \to q\bar{q}g$) is simple

$$\frac{dP}{dk_{t1}} = \frac{d}{dk_{t1}}\Delta(k_{t1}, Q)$$

Easy to generate this distribution by Monte Carlo
Take flat random number $0 < r < 1$ and solve $\Delta(k_t, Q) = r$

Now we have a $q\bar{q}g$ system.

We next work out a Sudakov for there being no emission from the $q\bar{q}g$ system above scale k_{t2} ($< k_{t1}$): $\Delta^{qqg}(k_{t2}, k_{t1})$, and use this to generate k_{t2}.

Then generate k_{t3} emission from the $q\bar{q}gg$ system ($k_{t3} < k_{t2}$). Etc.

Repeat until you reach a non-perturbative cutoff scale Q_0, and then stop.

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Shower variants

That was a description that roughly encompasses:

- The New Pythia shower   Pythia 8.1, and the p_t ordered option of Pythia 6.4
- The Ariadne shower

Other showers:

- Old Pythia (& Sherpa): order in virtuality instead of k_t and each parton branches independently (+ angular veto)   works fine on most data but misses some theoretically relevant contributions
  by far the most widely used shower
- Herwig (6.5 & ++): order in angle, and each parton branches independently   Herwig++ fills more of phase space than 6.5

That was all for a "final-state" shower

- Initial-state showers also need to deal carefully with PDF evolution

An example

1. You select the beams and their energy

---INITIAL STATE---

IHEP	ID	IDPDG	IST	MO1	MO2	DA1	DA2	P-X	P-Y	P-Z	ENERGY	MASS
1	P	2212	101	0	0	0	0	0.00	0.00	7000.0	7000.0	0.94
2	P	2212	102	0	0	0	0	0.00	0.00	-7000.0	7000.0	0.94
3	CMF	0	103	1	2	0	0	0.00	0.00	0.0	14000.0	14000.0

An example

2. You select the hard process (here $Z + jet$ production)

Herwig generates kinematics for the hard process

---HARD SUBPROCESS---

IHEP	ID	IDPDG	IST	MO1	MO2	DA1	DA2	P-X	P-Y	P-Z	ENERGY	MASS
4	UQRK	2	121	6	8	9	5	0.00	0.00	590.8	590.8	0.32
5	GLUON	21	122	6	4	17	8	0.00	0.00	-232.1	232.1	0.75
6	HARD	0	120	4	5	7	8	0.40	-9.40	358.7	823.0	740.63
7	Z0/GAMA*	23	123	6	7	22	7	-261.59	-217.31	329.3	481.6	88.56
8	UQRK	2	124	6	5	23	4	261.59	217.31	29.4	341.3	0.32

An example

3. Herwig “dresses” it with initial and final-state showers

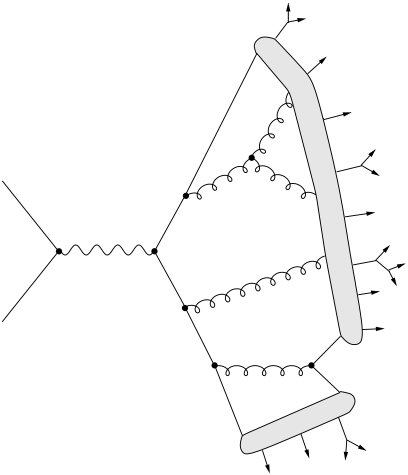
---PARTON SHOWERS---

IHEP	ID	IDPDG	IST	MO1	MO2	DA1	DA2	P-X	P-Y	P-Z	ENERGY	MASS
9	UQRK	94	141	4	6	11	16	2.64	-9.83	592.2	590.2	-49.07
10	CONE	0	100	4	5	0	0	-0.27	0.96	0.1	1.0	0.00
11	GLUON	21	2	9	12	32	33	-1.02	3.59	5.6	6.7	0.75-
12	GLUON	21	2	9	13	34	35	0.25	1.46	3.6	4.0	0.75-
13	GLUON	21	2	9	14	36	37	-0.87	1.62	4.7	5.1	0.75-
14	GLUON	21	2	9	15	38	39	-0.81	4.17	3611.7	3611.7	0.75-
15	GLUON	21	2	9	16	40	41	-0.19	-1.01	1727.7	1727.7	0.75-
16	UD	2101	2	9	25	42	41	0.00	0.00	1054.6	1054.6	0.32-
17	GLUON	94	142	5	6	19	21	-2.23	0.44	-233.5	232.8	-18.36
18	CONE	0	100	5	8	0	0	0.77	0.64	0.2	1.0	0.00
19	GLUON	21	2	17	20	43	44	1.60	0.58	-2.1	2.8	0.75
20	UD	2101	2	17	21	45	44	0.00	0.00	-2687.6	2687.6	0.32
21	UQRK	2	2	17	32	46	45	0.63	-1.02	-4076.9	4076.9	0.32
22	Z0/GAMA*	23	195	7	22	251	252	-257.66	-219.68	324.8	477.5	88.56
23	UQRK	94	144	8	6	25	31	258.06	210.29	33.9	345.5	86.10
24	CONE	0	100	8	5	0	0	0.21	0.17	-1.0	1.0	0.00
25	UQRK	2	2	23	26	47	42	26.82	24.33	23.7	43.3	0.32
26	GLUON	21	2	23	27	48	49	8.50	8.18	6.0	13.3	0.75
27	GLUON	21	2	23	28	50	51	73.27	61.24	12.0	96.2	0.75
28	GLUON	21	2	23	29	52	53	73.66	58.54	-6.3	94.3	0.75
29	GLUON	21	2	23	30	54	55	67.58	52.13	-7.3	85.7	0.75
30	GLUON	21	2	23	31	56	57	6.98	4.60	2.3	8.7	0.75
31	GLUON	21	2	23	43	58	59	1.24	1.26	3.6	4.1	0.75

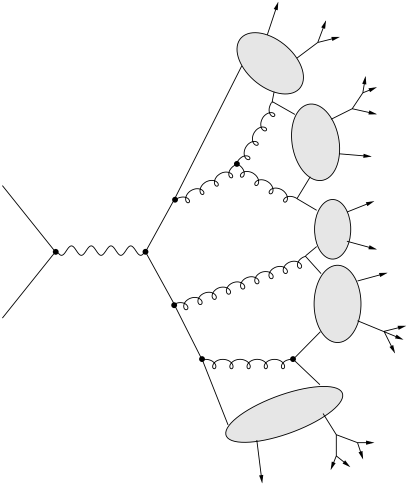
INITIAL STATE SHOWER (rows 9–21)

FINAL STATE SHOWER (rows 23–31)

Hadronisation Models



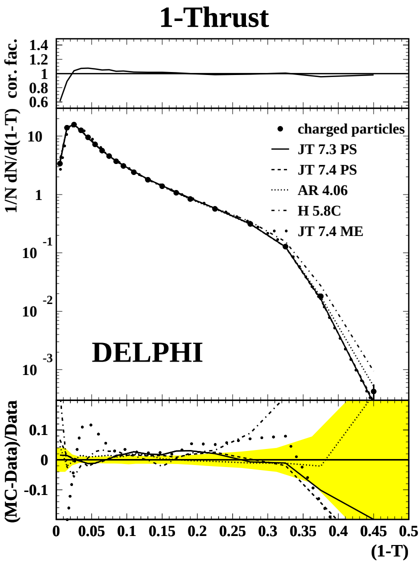
String Fragmentation
(Pythia and friends)

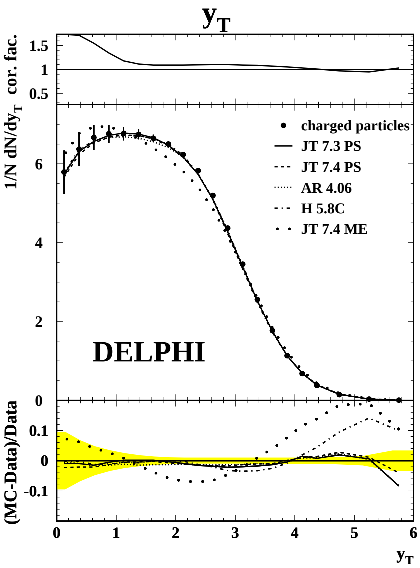


Cluster Fragmentation
(Herwig)

Pictures from ESW book

MC comparisons to LEP data





Comparing tools

Parton-shower Monte Carlos do a good job of describing most of the features of common events.

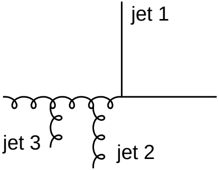
Including the fine detail needed for detector simulation
And all events have equal weight — just like data

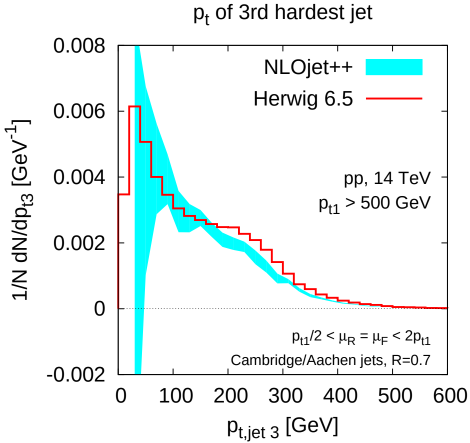
But they rely on soft and collinear approximations, so do not necessarily generate correct hard, large-angle radiation

And if you're simulating backgrounds to BSM physics
it's the rare, hard multi-jet configurations that are often of interest

Let's check how well they do: compare LO/NLO fixed-order calculations with parton showers.

Multijet events





Generate hard dijet events, shower and hadronise them with Herwig.

Select events in which hardest jet has $p_t > 500$ GeV. Look at p_t distribution of 3rd hardest jet

- Herwig doesn't do too bad a job of reproducing high-p_t 3rd-jet rate

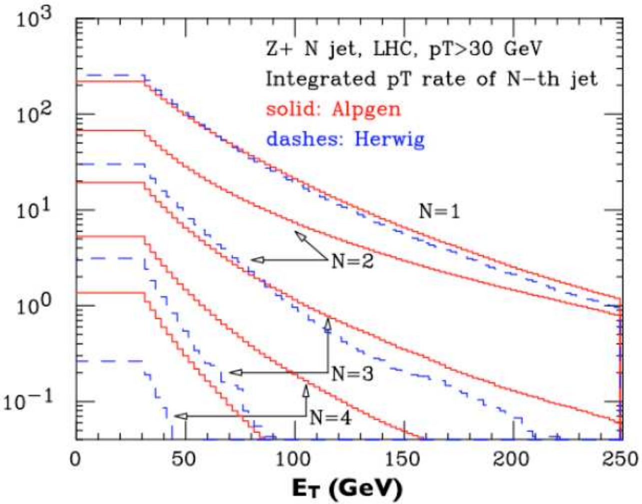
  But no uncertainty band

  Hard to know how trustworthy unless you also have NLO

- NLO does poor job at low p_t — large ratios of scales, $p_{t3}/p_{t1} \ll 1$, are dangerous in fixed-order calculations.

  higher-orders $\sim \alpha_s \ln \frac{p_{t1}}{p_{t3}} \sim 1$

$Z + N$ jets



Herwig: select $Z+1$ jet hard process.

Look at p_t distribution of jets with highest p_t, 2nd highest p_t, etc.

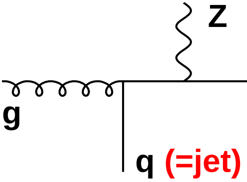
Compare to tree-level calculation

Mangano '08

Parton shower (Herwig) does very badly even just for 2nd jet.
Why is this so much worse than in the pure jet case?

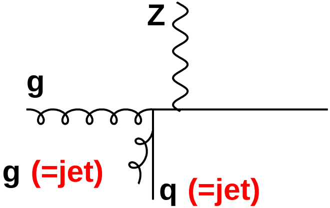
Why parton shower so poor for Z+jets?

Z + 1 jet



$\alpha_s \alpha_{EW}$

Z + 2 jets



Produced by parton shower

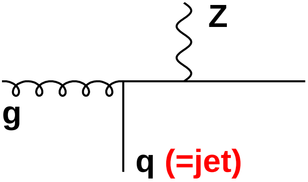
Parton showers generate starting from hard process you asked for.

Z/W + multijet production involves **two classes of hard process**

A. Z + recoil jet; **B.** dijets + emission of Z (missing from MC)

Why parton shower so poor for Z+jets?

Z + 1 jet



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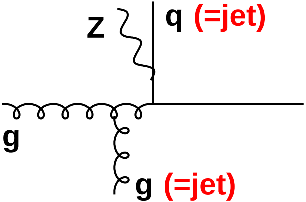

Not produced by parton shower
enhanced at high p_t: $\alpha_s^2 \alpha_{EW} \ln^2 \frac{p_t}{M_Z}$

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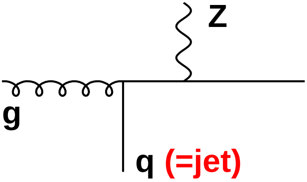

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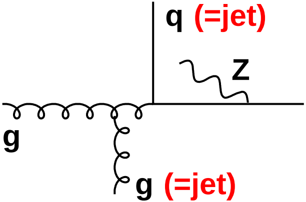

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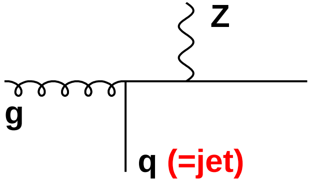

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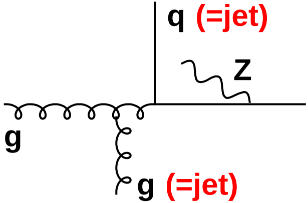

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Summary

We've seen a number of things:

- Idea of scale variation to estimate uncertainties in theory predictions
- How fixed-order predictions work
- How parton-shower Monte Carlo predictions work
- And how they compare

Some issues:

- Fixed order doesn't work with big scale ratios
- Monte Carlos don't always work for multijet structure

Tomorrow we'll look some more at these issues and at the question of hadron-collider observables