HIGHER ORDER CALCULATIONS IN QCD

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- The era of high-energy precision measurements
- NLO: where we stand
- NNLO: where we are going
- Conclusions

The Standard Model, the quantum theory of the strong (QCD) and electroweak interaction, is in very good shape.

In the last twenty years, we have accumulated a wide body of experimental evidence of the viability of the Standard Model.

The three main experimental areas for Standard Model tests are

- 1. e^+e^- colliders (e.g. LEP, SLC ...)
- 2. the *ep* collider (e.g. HERA ...)
- 3. hadron colliders (e.g. Tevatron and the future LHC).

Precision measurements

- More than one thousand measurements with correlated uncertainties...
- ... distilled into ~ 20 observables:
 - *Z* line shape and lepton forward-backward asymmetry
 - polarized lepton asymmetries
 - hadronic charge asymmetry
 - *W* mass and width
 - t mass
 - ν DIS
 - atomic parity violation
 - **-** . . .
- ...and matched with EW/QCD calculations



DIS



- structure functions
- scaling violation

Since the Standard Model predictions work so well, any signals of **new physics** must be **very small** (for energies that nowadays accelerators reach).

This is why, reaching a higher level of precision in our understanding of hard production phenomena becomes a fundamental issue if we want to search for new physics.

This means:

- better detectors and experimental analysis
- refining our theoretical calculations.

Next-to-Leading Order accuracy

	Measurement	Fit	$ O^{\text{meas}} - O^{\text{fit}} / \sigma^{\text{meas}}$
$\Delta \alpha_{had}^{(5)}(m_Z)$	0.02761 ± 0.00036	0.02767	
m _z [GeV]	91.1875 ± 0.0021	91.1875	
Γ _z [GeV]	2.4952 ± 0.0023	2.4960	
σ_{had}^{0} [nb]	41.540 ± 0.037	41.478	
R _I	20.767 ± 0.025	20.742	
A ^{0,I} _{fb}	0.01714 ± 0.00095	0.01636	
Α _I (Ρ _τ)	0.1465 ± 0.0032	0.1477	-
R _b	0.21638 ± 0.00066	0.21579	
R _c	0.1720 ± 0.0030	0.1723	
A ^{0,b} _{fb}	0.0997 ± 0.0016	0.1036	
A ^{0,c} _{fb}	0.0706 ± 0.0035	0.0740	
A _b	0.925 ± 0.020	0.935	
A _c	0.670 ± 0.026	0.668	
A _l (SLD)	0.1513 ± 0.0021	0.1477	
$sin^2 \theta_{eff}^{lept}(Q_{fb})$	0.2324 ± 0.0012	0.2314	
m _w [GeV]	80.426 ± 0.034	80.385	
Г _w [GeV]	2.139 ± 0.069	2.093	
m _t [GeV]	174.3 ± 5.1	174.3	
sin ² θ _w (νN)	0.2277 ± 0.0016	0.2229	
Q _W (Cs)	-72.84 ± 0.46	-72.90	

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An experimenter's wishlist: NLO cross sections

Single boson	Di-boson	Tri-boson	Heavy flavor
$W + \leq 5j$	$WW + \leq 5j$	$WWW + \leq 3j$	$t\bar{t} + \leq 3j$
$W + b\bar{b} + \le 3j$	$WW + \frac{b\bar{b}}{b} + \leq 3j$	$WWW + \frac{b\bar{b}}{b} + \leq 3j$	$t\bar{t} + \gamma + \leq 2j$
$W + c\bar{c} + \leq 3j$	$WW + c\bar{c} + \leq 3j$	$WWW + \gamma \gamma + \leq 3j$	$t\overline{t} + W + \leq 2j$
$Z + \leq 5j$	$ZZ + \leq 5j$	$Z\gamma\gamma + \leq 3j$	$t\bar{t} + Z + \leq 2j$
$Z + b\bar{b} + \le 3j$	$ZZ + b\bar{b} + \leq 3j$	$WZZ + \leq 3j$	$t\overline{t} + H + \leq 2j$
$Z + c\bar{c} + \leq 3j$	$ZZ + c\bar{c} + \leq 3j$	$ZZZ + \leq 3j$	$t\bar{b} + \leq 2j$
$\gamma + \leq 5j$	$\gamma\gamma + \leq 5j$		$b\bar{b} + \leq 3j$
$\gamma + b\bar{b} + \leq 3j$	$\gamma\gamma + b\bar{b} + \leq 3j$		
$\gamma + c\bar{c} + \leq 3j$	$\gamma\gamma + c\bar{c} + \leq 3j$		
	$WZ + \leq 5j$		
	$WZ + b\bar{b} + \leq 3j$		
	$WZ + c\bar{c} + \leq 3j$		
	$W\gamma + \leq 3j$		
	$Z\gamma + \leq 3j$ [Run II Monte Carlo Workshop, April 2001]		

Theoretical status

Single boson	Di-boson	Tri-boson	Heavy flavor
$W + \leq 2j$	$WW + \leq 0j$	$WWW + \leq 3j$	$t\overline{t} + \leq 0j$
$W + b\bar{b} + \le 0j$	$WW + \frac{b\bar{b}}{b} + \leq 3j$	$WWW + b\bar{b} + \leq 3j$	$t\overline{t} + \gamma + \leq 2j$
$W + c\bar{c} + \leq 0j$	$WW + c\bar{c} + \leq 3j$	$WWW + \gamma\gamma + \leq 3j$	$t\overline{t} + W + \leq 2j$
$Z + \leq 2j$	$ZZ + \leq 0j$	$Z\gamma\gamma + \leq 3j$	$t\overline{t} + Z + \le 2j$
$Z + b\bar{b} + \le 0j$	$ZZ + b\bar{b} + \leq 3j$	$WZZ + \leq 3j$	$t\overline{t} + H + \le 0j$
$Z + c\bar{c} + \leq 0j$	$ZZ + c\bar{c} + \leq 3j$	$ZZZ + \leq 3j$	$t\bar{b} + \leq 0j$
$\gamma + \leq 1j$	$\gamma\gamma + \leq 1j$		$b\bar{b} + \leq 0j$
$\gamma + b\bar{b} + \le 3j$	$\gamma\gamma + b\bar{b} + \le 3j$		
$\gamma + c\bar{c} + \leq 3j$	$\gamma\gamma + c\bar{c} + \leq 3j$		
	$WZ + \leq 0j$		
	$WZ + \frac{b\bar{b}}{b} + \leq 3j$		
	$WZ + c\bar{c} + \leq 3j$		
	$W\gamma + \leq 0j$		
	$Z\gamma + \leq 0j$		[John Campbell]

Status of NLO programs

- NLOJET++ [Nagy] $pp \rightarrow (2,3)$ jets, $ep \rightarrow 3$ jets, $e^+e^- \rightarrow (3,4)$ jets, $\gamma^*p \rightarrow (2,3)$ jets
- AYLEN/EMILIA [de Florian, Dixon, Kunszt, Signer] $pp \rightarrow (W, Z) + (W, Z, \gamma)$
- DIPHOX/EPHOX [Aurenche, Binoth, Fontannaz, Guillet, Heinrich, Pilon, Werlen] $pp \rightarrow \gamma + 1$ jet, $pp \rightarrow \gamma \gamma$, $\gamma^* p \rightarrow \gamma + 1$ jet
- MCFM [Campbell, Ellis] $pp \rightarrow (W, Z) + (0, 1, 2)$ jets, $pp \rightarrow (W, Z) + b\bar{b}$
- heavy-quark production [Mangano, Nason, Ridolfi] $pp \rightarrow Q\bar{Q}$
- single-top production [Harris, Laenen, Phaf, Sullivan, Weinzierl] $pp \rightarrow Q\bar{q}$
- associated Higgs production with $t\bar{t}$ [Dawson, Jackson, Orr, Reina, Wackeroth, Beenakker, Dittmaier, Kramer, Plumper, Spira, Zerwas] $pp \rightarrow HQ\bar{Q}$
- VBFNLO [Figy, Zeppenfeld, C.O.] $pp \rightarrow (W, Z, H) + 2$ jets, QCD corrections to electroweak production, when typical vector-boson fusion cuts are applied
- di-photon production [del Duca, Maltoni, Nagy, Trocsanyi] $pp \rightarrow \gamma\gamma + 1$ jet

For a more complete list, and the corresponding web pages, see: http://www.ippp.dur.ac.uk/~wjs/HEPCODE

NLO ingredients



NLO ingredients, cont'd



Divergences!

- UV divergences \implies renormalization
- IR divergences: SOFT and COLLINEAR

Real terms: divergences come from integration in particular regions of phase space Virtual terms: divergences come from loop integration



Dimensional Regularization: $d = 4 - 2\epsilon$.

Divergences appear as poles: $1/\epsilon$ and $1/\epsilon^2$, and they cancel for sufficiently (infra-red safe) inclusive observables.

Consider an *n*-parton final state

$$\sigma^{NLO} \equiv \int d\sigma^{NLO} = \int_{n+1} d\sigma^R \quad \Leftarrow \text{divergences from collinear and soft regions} \\ + \int_n d\sigma^V \quad \Leftarrow \text{divergences from loop integration}$$

separately divergent (poles in ϵ), although their sum is finite.

The general idea of the subtraction method is to make a Taylor expansion and to use the identity

$$d\sigma^{NLO} = \left[d\sigma^R - d\sigma^A\right] + d\sigma^A + d\sigma^V$$

where, in the singular regions, in *d* dimensions

$$rac{d\sigma^A}{d\sigma^R}\sim 1$$

 $d\sigma^A$ acts as a local counterterm for $d\sigma^R$

$$\sigma^{NLO} = \underbrace{\int_{n+1} \left[d\sigma^R - d\sigma^A \right]}_{\text{finite by construction}} + \int_{n+1} d\sigma^A + \int_n d\sigma^V = \underbrace{\int_{n+1} \left[\left(d\sigma^R \right)_{\epsilon=0} - \left(d\sigma^A \right)_{\epsilon=0} \right]}_{\text{done numerically in 4 dimensions}} + \int_n \left[\underbrace{d\sigma^V + \int_1 d\sigma^A}_{\text{done analytically}} \right]_{\epsilon=0}$$

Bottlenecks of NLO

- ✓ The construction of the counterterm $d\sigma^A$ can be done in an automated and simple way.
- ✓ The integrations over the singular phase-space regions of $d\sigma^A$ are done once and for all. They are universal and process-independent functions. [Catani & Seymour, Frixione, Kunszt & Signer; ...].
- **X** The analytic calculation of loop integrals is complicated and process-specific.
- X During the tensor reduction procedure (using Passarino-Veltman technique), determinants of kinematic invariants appear in the denominator, and give rise to large intermediate expressions and spurious singularities => numerical instabilities!

Towards numeric loop evaluation

The numerical computation of loop integrals (scalar and tensor) is possible if we know how to isolate IR and UV divergences. The idea is simple: Taylor expansion again.



SOFT singularities:

$$\int d^d k \frac{1}{k^2 (k-p_1)^2 (k+p_2)^2 (k+p_2+p_3)^2 \dots} \overset{k \to 0}{\sim} \frac{1}{(p_2+p_3)^2 \dots} \times \underbrace{\int d^d k \frac{1}{k^2 (k-p_1)^2 (k+p_2)^2}}_{\text{triangle}}$$

COLLINEAR singularities: e.g. $k = xp_1$. Same treatment as above!

ALL IR singularities collected in TRIANGLE diagrams

Tensor integrals at NLO

Things are **NOT** so easy when the loop momentum is present in the numerator (tensor integrals)

$$\int d^d k \frac{k^{\alpha} k^{\beta} \dots}{k^2 (k-p_1)^2 (k+p_2)^2 (k+p_2+p_3)^2 \dots}$$

In addition, one of the main issues is "when" you go numerical: before or after some reductions?

Only VERY RECENTLY some of these issues have been addressed.

Automatizing loop calculation

• analytic reduction of pentagon integrals [Bern, Dixon & Kosower (hep-ph/9306240)].



Automatizing loop calculation, cont'd

• building counterterms (CT) on a graph-by-graph base [Nagy & Soper (hep-ph/0308127)]

$$\sum_{\text{finite}} \underbrace{(\text{LOOP graph} - \text{CT})}_{\text{finite}} + \underbrace{(\sum_{\text{simple}} \text{CT})}_{\text{simple}}$$

• analytic reduction of hexagon integrals [Binoth, Guillet & Heinrich (hep-ph/0210023)]

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$$HEX(d = 4 - 2\epsilon) = \underbrace{\sum_{i=1}^{20} TRI(d = 4 - 2\epsilon)}_{IR \text{ divergences}} + \underbrace{\sum_{i=1}^{15} BOX(d + 2 = 6 - 2\epsilon)}_{\text{finite}}$$

- numerical evaluation and check of the stability of the method of reducing hexagon diagrams
 [Binoth, Heinrich & Kauer (hep-ph/0210023)]
- soft/collinear-divergences isolation with massive/massless propagators [Dittmaier (hep-ph/0308246)]
- soft/collinear divergences isolation in tensor integrals with massless propagators and light-like external momenta [Giele & Glover (hep-ph/0402152)]

Final goal

The goal is to build a program that computes scattering processes at NLO in a completely automated way.

Programs like MadGraph and MadEvent will be replaced by

MadLoop

and we will have the **GOLEM** = General One-Loop Evaluation of Matrix elements!

Expect the first programs in 2005



Do we need NNLO jet cross sections at hadron colliders?

- jets are very complicated objects
- steep *E*_{*T*}-dependence magnifies energy-scale and luminosity uncertainties
- underlying events are surely a problem

YES. At least it helps to focus more attention on

- reduction of renormalization- and factorization-scale dependence of the cross sections
- less worries (hopefully!) about matching theoretical and experimental jet algorithms, and reducing dependence from artificially-introduced parameters (R_{sep})
- more complicated transverse-momentum final state, due to double initial-state radiation (no need of intrinsic k_T)
- reduced dependence on power-correction effects.

Ingredients for NNLO *n***-jet final state**



$2 \rightarrow 2$ scattering processes

Process	Tree	One loop	Two loops
$q\overline{q} \rightarrow q'\overline{q}'$	1	9	189
$q\overline{q} \rightarrow q\overline{q}$	2	18	378
$q\overline{q} \rightarrow gg$	3	29	563
gg→gg	4	72	1531

Two-loop integrals

• Bhabha scattering: $e^+e^- \rightarrow e^+e^-$

[Bern, Dixon & Ghinculov (2000)]

- hadron-hadron scattering into 2 jets: qq' → qq', qq → qq, qq̄ → gg, gg → gg
 [Anastasiou, Glover, Tejeda-Yeomans & C.O. (2001)]
 [Bern, De Freitas & Dixon (2003)]
- photon pair production: gg → γγ, qq̄ → γγ, γγ → γγ
 [Bern, De Freitas Dixon, Ghinculov & Wong (2001–02)]
 [Anastasiou, Glover & Tejeda-Yeomans (2002)]
- three-jet production at e^+e^- : $e^+e^- \rightarrow \gamma^* \rightarrow q\bar{q}g$ [Garland, Gehrmann, Glover, Koukoutsakis & Remiddi (2001)] [Moch, Uwer & Weinzierl (2002)]
- DIS and vector-boson plus one-jet production: $\gamma^* g \rightarrow q\bar{q}, qg \rightarrow Vq$ [Gehrmann & Remiddi (2002)]
- work in progress for amplitudes with internal masses: $\gamma^* \rightarrow Q\overline{Q}$ [Bonciani, Mastrolia & Remiddi; Aglietti & Bonciani (2003–04)]

Technical breakthroughs

- algorithms (in FORM, Maple, Mathematica) to reduce recursively or by Gauss elimination, large systems of linear equations (10⁴-10⁶) to 10-30 master integrals, the building blocks of the computation.
 - Integration-by-Parts [Chetyrkin & Tkachov] to build recursive relations

$$\int d^d k \ \frac{\partial}{\partial k^{\mu}} f(k, p_i) = 0 \qquad p_i = \text{ external momenta}$$

- Lorentz invariance [Gehrmann & Remiddi]

$$\int d^d k f(k, p_i) = F(p_i \cdot p_j)$$

- implementation of an efficient computer-algebra algorithm [Laporta]

Master integrals

ANY scalar integral (and tensor integral too, since it can be expressed as combination of scalar integrals), in $2 \rightarrow 2$ QCD scattering processes, can be written, through a TOTALLY algebraic procedure, as a linear combination of the following integrals, that are therefore called master integrals:



Technical breakthroughs, cont'd

- new methods to compute master (scalar) integrals
 - Mellin-Barnes [Smirnov, Veretin & Tausk]

$$(A+B)^{-\nu} = \frac{1}{2\pi i} \frac{1}{\Gamma(\nu) B^{\nu}} \int_{-i\infty}^{i\infty} dz \, \left(\frac{A}{B}\right)^z \Gamma(-z) \, \Gamma(\nu+z)$$

- differential equations [Gehrmann & Remiddi]

$$s_{23} \frac{\partial}{\partial s_{23}} p_1 + p_2 = \frac{d-6}{2} p_1 + p_2 = \frac{d-6}{2} p_1 + p_3$$
$$-\frac{2(d-3)}{s_{12}+s_{23}} \left[\frac{1}{s_{123}} p_{123} - \frac{1}{s_{13}} p_{13} -$$

plus initial conditions (very easy to obtain).

Technical breakthroughs, cont'd

 sector decomposition: an automated procedure to break an integration domain into various singular regions, disentangling the overlapping singularities.

$$I = \int_0^1 dx \, dy \, x^{-1-\epsilon} y^{-1-\epsilon} (x+y)^{-\epsilon} = \dots$$

= $\int_0^1 dx \, dy \, x^{-1-3\epsilon} y^{-1-\epsilon} (1+y)^{-\epsilon} + \int_0^1 dx \, dy \, x^{-1-\epsilon} y^{-1-3\epsilon} (1+x)^{-\epsilon}$

It has been used

- * in the numerical evaluation of hexagon integrals [Binoth, Heinrich & Kauer]
- * to express the 1 → 4 phase-space element, in a way suitable for numerical integration (all divergences extracted) [Anastasiou, Melnikov & Petriello (hep-ph/0311311)].
- * first, totally exclusive, NNLO program: e⁺e⁻ → 2 jets [Anastasiou, Melnikov & Petriello (hep-ph/0402280)].

Infrared structure studied also in [Gehrmann-De Ridder, Gehrmann & Glover (hep-ph/0403057)].

- harmonic (nested) sums [Moch, Uwer & Weinzierl]

$$S(n; m_1, ..., m_k; x_1, ..., x_k) = \sum_{\substack{n \ge i_1 \ge i_2 \ge ... \ge i_k \ge 1}} \frac{x_1^{i_1}}{i_1^{m_1}} \dots \frac{x_k^{i_k}}{i_k^{m_k}}.$$

Ahead of us!

- $e^+e^- \rightarrow 3$ jets at NNLO
- $pp(\bar{p}) \rightarrow 2$ jets at NNLO

While work is in progress to create totally exclusive NNLO partonic Monte Carlo generators, many results have already been obtained for totally inclusive quantities.

Higgs production at LHC



NLO corrections are 80% of the LO!

Is the series well behaved?

Higgs production at LHC



Is the series well behaved? \implies YES NNLO 15%

- using "conventional" techniques & series expansions [Harlander & Kilgore (hep-ph/0201206)]
 Result cross-checked without approximation [Smith, Ravindran & van Neerven (hep-ph/0302135)]
- confirmed using a new technique [Anastasiou & Melnikov (hep-ph/0207004)]

New technique

• Convert phase-space integrals into loop integrals $i \rightarrow f$ (*n* particles)

$$\int |\mathcal{M}_{i\to f}|^2 \, d\text{LIPS}(n-1) \quad \underbrace{\frac{d^{d-1}\vec{p}}{2E}}_{E^2 = \vec{p}^2 + m^2} = \int |\mathcal{M}_{i\to f}|^2 \, d\text{LIPS}(n-1) \, d^d p \, \delta(p^2 - m^2) \, \theta(E)$$

$$\delta(x) = \frac{1}{2\pi i} \left(\frac{1}{x - i0} - \frac{1}{x + i0} \right)$$

$$= \int |\mathcal{M}_{i \to f}|^2 \, d\text{LIPS}(n-1) \, \theta(E) d^d p \left[\frac{1}{p^2 - m^2 - i0} - \frac{1}{p^2 - m^2 + i0} \right] \frac{1}{2\pi i}$$

Use the formalism developed for the loop reduction to deal with integration over the phase space of final-state particles.

Rapidity distribution at NNLO

Using the same technique, less inclusive quantities have been computed



[Anastasiou, Dixon, Melnikov & Petriello (hep-ph/0312266)]

Remarkable stability to QCD corrections.

Use *W* and *Z* production to monitor proton-proton luminosity and constrain PDFs at LHC.

NNLO PDFs

PDFs are extracted from a global fit to several observables.

INGREDIENTS

- partonic cross sections at NNLO
 - 🗸 DIS
 - ✓ Drell-Yan (lepton-pair and gauge-boson production)
 - ✗ jet production
 - ✗ photon production, ...
- Altarelli-Parisi splitting function at NNLO (three loops) An approximate expression based upon the
 - calculations of the lowest moments in Mellin space \implies give information on the high *x* behavior of the splitting functions [Larin, Nogueira, van Ritbergen, Rétey & Vermaseren].
 - knowledge of the most singular log(1/x) behavior at small x

has been provided [van Neerven & Vogt].

NNLO PDFs progresses

Recently, the non-singlet contribution to the three-loop splitting functions has been computed [Moch, Vermaseren & Vogt (hep-ph/0403192)]

- the correct leading logarithmic predictions for small momentum fractions *x* do not provide a good estimate of the respective complete results
- a new, unpredicted, leading logarithmic contribution is found for the color factor $d^{abc} d_{abc}$ entering at three loops for the first time

Except for very small *x*, the corrections are found to be rather small.

The completion of the whole calculation is under way.

PDF dependence



- the large scale dependence at NLO renders the three choices indistinguishable.
- significant discrepancies appear at NNLO, both in normalization and in shape.

[Anastasiou, Dixon, Melnikov & Petriello (hepph/0312266)]

Electroweak gauge-boson production becomes a powerful discriminator between different PDF parameterizations when the NNLO QCD corrections are included.

Hopefully, this discrepancy will be gone before LHC starts.

Conclusions

- (N)NLO calculations are essential to extract reliable estimates for total and differential production rates.
- QCD physics at LEP and Tevatron has taught us that the concept of infrared (soft and collinear) safety , while essential to justify the use of fixed-order perturbative calculations, does NOT guarantee the accuracy of such calculations. In fact:
 - power corrections effects
 - large logarithms (that need to be resummed to all order)

can invalidate a fixed-order calculation.

• In addition, showering and hadronization effects need to be understood at a deeper level, see e.g. MC@NLO [Frixione & Webber]: hard emission treated correctly, according to NLO computation, and soft-collinear emission treated as in the usual Monte Carlo, with a smooth matching between hard and soft/collinear emission.

For sure, the high energy physics has a very bright decade ahead with the LHC