Next-to-Leading Order tools

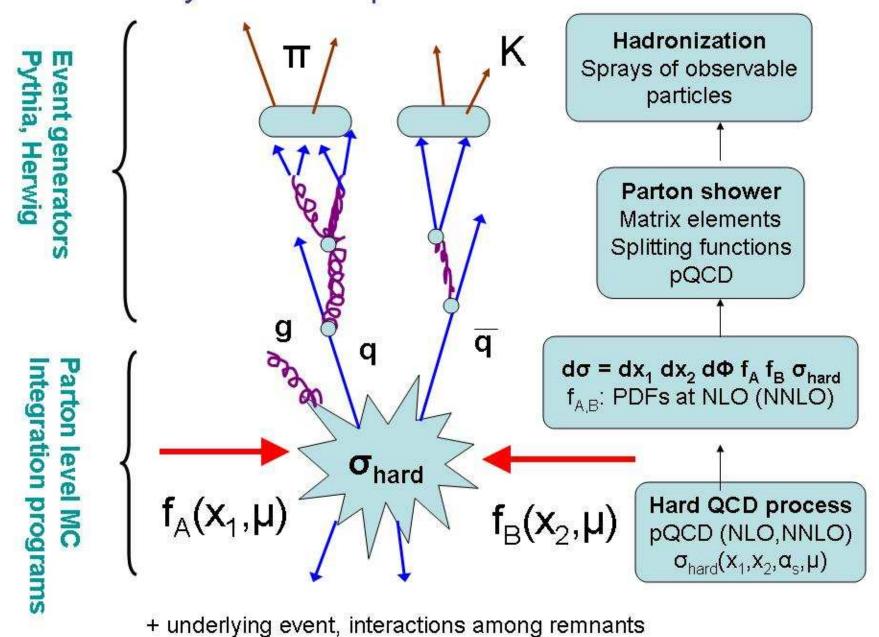
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Introduction and Outline

- The incredible physics potential of the Tevatron and in particular of the LHC relies on our ability of providing very accurate QCD predictions. This is very challenging.
- How do we expect to compare with data?
 - Need precise description of hard QCD production as well as a method to interface with the final hadronic states that are measured, accurately.
- Status of NLO QCD calculations for hadron collider physics: what has been done and what are the challenges.
- Having a NLO parton-level calculation, what do we do?
 - → Monte Carlo (MC) vs analytic integration over phase space.
 - → Parton level MC's vs Shower MC's event generators.
 - → Matching with exact NLO QCD calculations.

Anatomy of a QCD prediction at hadron colliders



Fundamental tool: σ_{hard} at NLO or higher.

LO calculations in QCD can be only used to get a feeling of the order of magnitude, or qualitatively discriminate between different models.

Exact NLO or NNLO calculations of σ_{hard} needed to:

- → have accurate and reliable predictions of parton-level observables, like total and differential cross-sections (scale-dependence issue, see "Practical NLO calculation");
- test the convergence of the perturbative series associated to a given physical observable;
- → start to correctly reproduce the kinematic of a given process, in particular in peripheral regions of phase space where the LO kinematic may be unnecessarily degenerate;
- → provide non trivial jet structure in jet production cross sections.

In general, NLO results are obtained by:

- using symbolic computation packages like FORM and algebraic manipulators like Mathematica and Maple to obtain the amplitude square for a given process (virtual and real corrections);
- → removing UV and IR singularities;
- \longrightarrow reading final expressions into a numeric code (Fortran, C, ...);
- → integrating over phase space using a Monte Carlo method (MC);
- most NLO/NNLO calculations are available as MC integration programs.

Advantages of MC integration:

- \longrightarrow analytic phase space integration for $N \geq 3$ particles in the final state becomes nasty;
- even more so when cuts are imposed. MC integration gives great flexibility in implementing all sort of experimental cuts (for IR safe observables).

Monte Carlo integration in a nutshell ...

- \longrightarrow A MC point is a set of pseudo-random numbers \mathbf{r}^{j} through which the final-state particles four-momenta k_{i} are generated.
- Events are represented by the four-momenta of the final-state particles.
- \longrightarrow MC integration programs produce "weighted events", i.e. each event is associated a weight $w(\mathbf{r}_j)$, defined as:

$$w(\mathbf{r}^j) = \frac{f(k_i)}{g_{\text{tot}}(k_i)}$$
 with $f(k_i) \propto |\mathcal{M}(k_i)|^2$

where $g_{\text{tot}}(k_i)$ is the total density of the event and $\mathcal{M}(k_i)$ is the matrix element associated to a given process.

— The MC estimate of a given observables \mathcal{O} (e.g. cross-section) is obtained as

$$\overline{\mathcal{O}} = \frac{1}{N} \sum_{j=1}^{N} w(\mathbf{r}^{j})$$

where N is the total number of events.

The four-momenta k_i and their corresponding weights are used to fill histograms for differential cross-sections.

State of the art of QCD predictions for Higgs boson production at hadron colliders

process	$\sigma_{NLO,NNLO}$ (by)
gg o H HIGLU MCFM MC@NLO	S.Dawson, NPB 359 (1991), A.Djouadi, M.Spira, P.Zerwas, PLB 264 (1991) C.J.Glosser et al., JHEP (2002); V.Ravindran et al., NPB 634 (2002) D. de Florian et al., PRL 82 (1999) R.Harlander, W.Kilgore, PRL 88 (2002) (NNLO) C.Anastasiou, K.Melnikov, NPB 646 (2002) (NNLO) V.Ravindran et al., NPB 665 (2003) (NNLO) S.Catani et al. JHEP 0307 (2003) (NNLL) G.Bozzi et al., PLB 564 (2003), NPB 737 (2006) (NNLL)
$q\bar{q} \to (W,Z)H$	T.Han, S.Willenbrock, PLB 273 (1991) O.Brien, A.Djouadi, R.Harlander, PLB 579 (2004) (NNLO)
$q \bar{q} o q \bar{q} H$	T.Han, G.Valencia, S.Willenbrock, PRL 69 (1992) T.Figy, C.Oleari, D.Zeppenfeld, PRD 68 (2003)
$q\bar{q},gg \to t\bar{t}H$	W.Beenakker <i>et al.</i> , PRL 87 (2001), NPB 653 (2003) S.Dawson <i>et al.</i> , PRL 87 (2001), PRD 65 (2002), PRD 67,68 (2003)
$q\bar{q},gg \rightarrow b\bar{b}H$	S.Dittmaier, M.Krämer, M.Spira, PRD 70 (2004) S.Dawson <i>et al.</i> , PRD 69 (2004), PRL 94 (2005)
$gb(\overline{b}) \to b(\overline{b})H$ $\underline{\qquad}$ $\underline{\qquad}$ $\underline{\qquad}$	J.Cambell <i>et al.</i> , PRD 67 (2003)
$bar{b} ightarrow (bar{b})H$ MCFM	D.A.Dicus <i>et al.</i> PRD 59 (1999); C.Balasz <i>et al.</i> , PRD 60 (1999). R.Harlander, W.Kilgore, PRD 68 (2003) (NNLO)

State of the art of QCD predictions for W/Z boson production at hadron colliders

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process	$\sigma_{NLO,NNLO}$ (by)
W,Z(ightarrow l u,ll) MCFM MC@NLO ResBos	W.L.van Neerven et al, NBP 382 (1992) R.Hamberg, W.L.van Neerven and T.Matsuura, NPB 359 (1991) (NNLO) C.Anastasiou, L.Dixon, K.Melnikov, F.Petriello (NNLO, distrib.) C.Balazs, CP. Yuan, PRD 56 (1997) (resummed NLO)
WW, ZZ, WZ AYLEN/EMILIA MCFM MC@NLO	J.Ohnemus et al., PRD 44 (1991); PRD 43 (1991); PRD 50 (1994) B.Mele et al., NPB 357 (1991) S.Frixione et al., NPB 410 (1993); NPB 383 (1992) L.Dixon et al., NPB 531 (1998); PRD 60 (1999) J.Campbell, R.K.Ellis, F.Tramontano, PRD 60 (1999)
$W, Z+ \leq 2j$ MCFM	W.Giele, N.Glover, D.Kosower, NPB 403 (1993) J.Campbell <i>et al</i> , PRD 65 (2002); PRD 68 (2003)
W, Z + Q MCFM	W.Giele et al., PLB 372 (1996) E.Berger et al., PRD 54 (1996) M.Aivazia et al, PRD 50 (1994) J.Collins, PRD 58 (1998) T.Stelzer et al., PRD 56 (1997) J.Campbell, et al., PRD 69 (2004)
$W,Z+Qar{Q}$ MCFM	J.Campbell, R.K.Ellis, PRD 62 (2000) $(m_Q \rightarrow 0)$ F.Maltoni et al., hep-ph/0505014 $(m_Q \rightarrow 0)$

State of the art of QCD predictions for heavy quark and jet production at hadron colliders

process	$\sigma_{NLO,NNLO}$ (by)
$Qar{Q}$ MCFM MC@NLO	P.Nason, S.Dawson, R.K.Ellis, NPB 303 (1988); NPB 327 (1989) W.Beenakker <i>et al.</i> , PRD 40 (1989); NPB 351 (1991) M.Mangano. P.Nason, G.Ridolfi, NPB 373 (1992) R.Bonciani, S.Catani, M.L.Mangano, P.Nason, NPB 529 (1998) (NNL) N.Kidonakis, R.Vogt, Eur. Phys. J. C 33 (2004), C 36 (2004) (≃NNLO) N. Kidonakis, Mod. Phys. Lett. A 19 (2004) (NNNLL+NNLO) A.Banfi, E.Laenen, PRD 71 (2005) and refs. therein (NLL+NLO) W.Bernreuther <i>et al.</i> , NPB 690 (2004) (spin correlations)
single top MCFM MC@NLO	M.Smith, S.Willenbrock, PRD 54 (1996) G.Bordes, B.van Eijk, NPB 435 (1995) T.Stelzer et al., PRD 56 (1997) B.W.Harris et al., PRD 66 (2002) Z.Sullivan, PRD 70 (2004) J.Campbell, R.K.Ellis, PRD 70 (2004) QH. Cao et al, PRD 71 (2005); hep-ph/0504230
$pp(\bar{p}p) \rightarrow \leq 3j$ NLOJET++ JETRAD	W.Giele, N.Glover, D.Kosower, NPB 403 (1993) Z.Kunszt and D.Soper, PRD 46 (1992) W.Kilgore and W.Giele, PRD 55 (1997) Z.Nagy, PRL88 (2002), PRD 68 (2003) (3j)

Many NLO results available as public codes

HEPCODE database: (http://www.cedar.ac.uk/hepcode/) database of available Monte Carlo codes, including LO, NLO and resummed predictions (!!).

Some examples:

- MCFM (by J. Campbell, R.K. Ellis)

 Fortran package for calculating a number of processes involving vector bosons, Higgs boson, jets and heavy quarks at hadron colliders: $p\bar{p}, pp \to V+ \leq 2j, \ V+b\bar{b}, VH, H+ \leq 1j, Q\bar{Q} \ \ (V=W,Z).$
- AYLEN/EMILIA (by L. Dixon, Z. Kunszt, A. Signer, D. de Florian) Fortran implementation of EW gauge boson pair production at hadron colliders, including full spin and decay angle correlations: $p\bar{p}, pp \to VV', V\gamma \quad (V, V' = W/Z).$

- Heavy quark production (by M.L. Mangano, P. Nason, G. Ridolfi)

 Fortran code for the calculation of heavy quarks cross-sections and distributions at hadron colliders.
- NLOJET++ (by Z. Nagy) multipurpose C++ library for calculating jet cross-sections in $e^+e^$ annihilations, DIS and hadron-hadron collisions: $e^+e^- \rightarrow \leq 4$ jets, $ep \rightarrow (\leq 3+1)$ jets, $p\bar{p} \rightarrow \leq 3$ jets.
- JETRAD (by W.T. Giele, E.W.N. Glover, D.A. Kosower)
 (available at http://vircol.fnal.gov/MCdownload/jetrad.html)

 NLO Monte Carlo for inclusive 1-jet and 2-jet production at Hadron Colliders.
- FastNLO (by T.Kluge, K. Rabbertz, M. Wobisch)

 (available at http://hepforge.cedar.ac.uk/fastnlo/)

 provides computer code and tables of pre-computed perturbative coefficients for various observables in hadron-induced processes.

- ResBos (by C. Balazs, P. Nadolsky, C.-P. Yuan)

 a MC integrator program for transverse momentum resummation in

 Drell-Yan-like processes, with leptonic decay of final bosons. Resummed

 NLO with elements of NNLO.
- DIPHOX/EPHOX (by P. Aurenche, T. Binoth, M. Fontannaz, J.Ph. Guillet, G. Heinrich, E. Pilon, M. Werlen)
 Fortran code to compute processes involving photons, hadrons and jets in DIS and hadron colliders:
 pp̄, pp → γ + 1 jet, γγ and γp, γp̄ → γ + 1 jet.
- HIGLU (by M.Spira) NLO QCD corrections to SM and SUSY Higgs total cross sections for $gg \to H$ via top/bottom loop.

What is needed: multi-particles/jet production at NLO.

At the LHC this will be the inescapable background to Higgs searches and searches for new physics. We have very limited NLO knowledge of:

$$\longrightarrow W/Z + \text{jets (2j)}$$

$$\longrightarrow WW/ZZ/WZ + \text{jets (0j)}$$

$$\longrightarrow WWW/WZZ, ZZZ + \text{jets (0j)}$$

$$\longrightarrow Q\bar{Q} + \text{jets (0j)}$$

$$\longrightarrow \gamma + jets$$

$$\longrightarrow \gamma \gamma + jet$$

$$\longrightarrow Z\gamma\gamma + \text{jets}$$

and several even more complicated final states that will all constitute important backgrounds. We would like to be able to include more jets, in particular for the LHC.

Main challenge: automation of multi-leg amplitude calculation.

Towards the automation of multi-leg amplitude calculation

Automation of LO calculations: several packages exist for the automatic calculation of $2 \rightarrow N$ LO amplitudes (up to N=8 or more), including the integration over phase space: HELAC/PHEGAS, MADGRAPH/MADEVENT, COMPHEP, GRACE, SHERPA/AMEGIC++, O'MEGA/WHIZARD, ALPGEN, ...

- → interfacing with Shower MC event generators is understood: CKKW
- very useful to obtain first estimates (e.g. relevance of different processes, or of the same process in different models)

But their results:

- → are affected by strong scale dependence;
- fail to correctly reproduce extreme regions of a process phase space;
- → do not allow any jet structure at the level of the hard matrix element.

Traditional packages for automation of NLO calculations includes: FeynArts, FeynCalc, FF, FormCalc, Looptools, ...

But no application to processes other than $2 \to 2$ and $2 \to 3$ is known.

The crucial steps in the calculation of a $2 \rightarrow N$ process at NLO are:

- \longrightarrow calculation of the 2 \rightarrow N + 1 real corrections (dipole formalism seems more suitable);
- \longrightarrow calculation of the 2 $\rightarrow N$ virtual corrections (tough!);
- → explicit cancellation of IR divergences (UV-cancellation is standard).

<u>New ideas</u> point in the direction of solving the hurdle of evaluating multi-leg one loop amplitudes by using semi-numerical methods to reduce both tensor and scalar integrals:

A. Ferroglia, M. Passera, G. Passarino, S. Uccirati, NPB 650 (2003) 162
W.T. Giele, E.W.N. Glover, JHEP 0404 (2004) 029
Binoth, J.P. Guillet, G. Heinrich, E. Pilon, C. Schubert, JHEP 0510 (2005) 015
R.K. Ellis, W.T. Giele, G. Zanderighi, PRD 73 (2006) 014027

. . .

Intrinsic limitations of parton-level MC programs:

- no resummation of large corrections (soft, collinear, threshold) arising at phase space boundaries;
- → only one additional parton;
- → not a good description of more exclusive observables;
- → event weights may be negative;
- only parton level events: no hadronization, no underlying event structure, no simulation of detector effects.



Some of these limitations are overcome by a

Shower MC Event Generators

generate <u>real events</u>, i.e. physical, measurable hadrons, with a correct description of their multiplicity, kinematics and flavor composition.

An intermediate tool: Shower MC Event Generators

 $(\longrightarrow \text{see P. Richardson's lectures})$

In a nutshell:

After having generated a parton-level configuration at tree level, initial and final state parton emission is controlled by a showering algorithm, a numerical Markov-like evolution which implements the QCD dynamics under certain approximations.

More specifically:

- probabilities for parton radiation implement soft and collinear leading logarithms, plus some sub-leading classes of logarithms;
 - (→ see "Practical NLO calculation")
- radiation probabilities are unitarized by the inclusion of Sudakov-like forms factors, i.e. the cross section is dictated by the core matrix element of a given process;
- → an IR cutoff scheme is used;
- \longrightarrow hadronization is added.

Among the most famous: Herwig, Pythia, Isajet, Ariadne, Sherpa

Pros:

- \longrightarrow model realistic events, from the perturbative regime at high energies $(\gg \Lambda_{\rm QCD})$ to the non-perturbative one $(\simeq \Lambda_{\rm QCD})$;
- → allows for formation of hadrons and hadron decays;
- → include a description of the underlying structure of the event;
- → allow realistic detector simulations.

Cons:

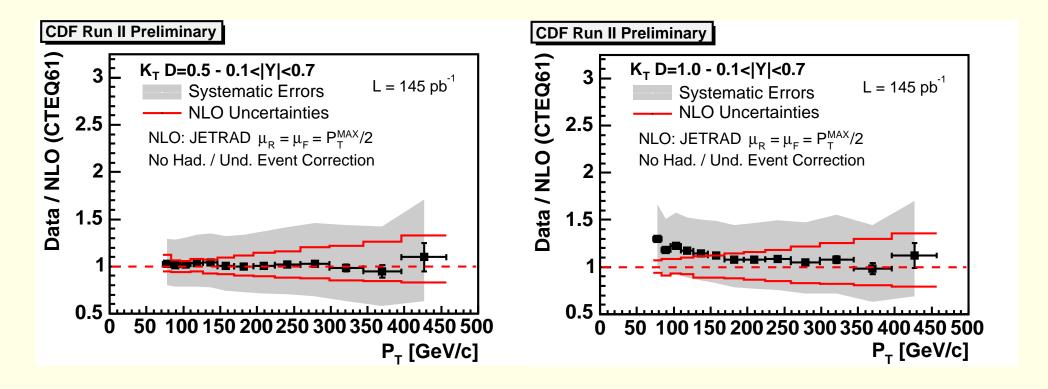
- \longrightarrow based on LO matrix elements, in general of $2 \to 1$ or $2 \to 2$ processes;
- \longrightarrow shower based on collinear kinematic: high p_T effects are not properly modelled.
- → shower only include resummation of leading and some subleading logarithms (Sudakov form factor);

Example: Inclusive jet cross-section at the Tevatron

(M. Martinez, hep-ph/0505047)

 \longrightarrow High p_T data are used to constrain the gluon PDF at high x.

Comparison of data with NLO predictions for two different values of the D parameter of the k_T jet algorithm (S. Ellis, D. Soper, PRD 48 (1993) 3160)



NLO agrees well at high p_T . At small p_T NLO increasingly not a good description of data (soft gluon effects not included).

How to improve Shower Monte Carlo's?

The real problem is the collinear approximation.

Think of the LHC: huge energy available —— easy to get large-angle hard emission.

Two possible approaches:

• Matrix Element Corrections: apply the showering algorithm after having computed as many as possible real emission matrix elements.

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    S. Catani, F. Krauss, R. Kuhn, B.R. Webber, JHEP 0111 (2001) 063
    L. Lonnblad, JHEP 0205 (2002) 045
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• NLO+Parton Shower: apply the showering algorithm to the exact NLO matrix elements.

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S. Frixione, B.R. Webber, JHEP 0206 (2002) 029
S. Frixione, P. Nason, B.R. Webber, JHEP 0308 (2003) 007
Z. Nagy, D. Soper JHEP 0510 (2005) 024
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Ultimate tool: NLO corrections in Shower MC

(based on the work by S. Frixione, P. Nason, B.R. Webber, MC@NLO)

- Based on the full NLO matrix element for the hard process.
- Double counting is avoided by identifying the analytic form of the approximation used by the shower MC to describe real emission and the leading order virtual corrections, and subtracting them from the NLO matrix elements:

$$\mathcal{F}_{\text{MC@NLO}} = \sum_{a,b} \int dx_1 dx_2 d\phi_{n+1} f_a(x_1) f_b(x_2) \times \left[\mathcal{F}_{\text{MC}}^{(2\to n+1)} \left(\mathcal{M}_{ab}^{(r)} - \mathcal{M}_{ab}^{\text{MC}} \right) + \mathcal{F}_{\text{MC}}^{(2\to n)} \left(\mathcal{M}_{ab}^{(b,v,c)} - \mathcal{M}_{ab}^{(c.t.)} + \mathcal{M}_{ab}^{\text{MC}} \right) \right]$$

where the MC counterterms are:

$$\mathcal{M}_{\mathcal{F}(ab)}^{\mathrm{MC}} = \mathcal{F}_{\mathrm{MC}}^{(2 \to n)} \mathcal{M}_{ab}^{(b)} + \mathcal{O}(\alpha_s^2 \alpha_s^b)$$

only two types from initial-state and final-state branching, both calculated.

Processes implemented in MC@NLO:

- W/Z boson production;
- WW, ZZ, WZ boson pair production;
- $Q\bar{Q}$ heavy quark production;
- single-top production;
- $gg \to H$ inclusive Higgs boson production;

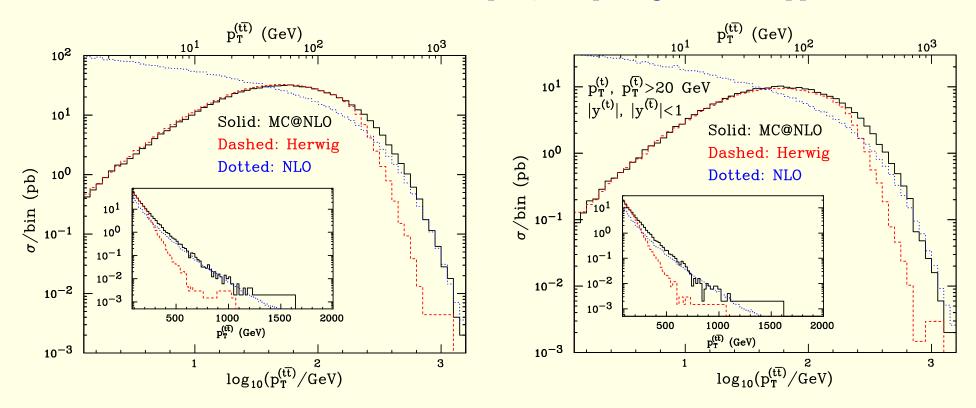
(available at: www.hep.phy.cam.ac.uk/theory/webber/MCatNLO or through HEPCODE)

Crucial improvements:

- the inclusion of NLO corrections in the shower MC properly includes the NLO K-factors and reduce the systematic uncertainty due to renormalization and factorization scale variations;
- the higher order corrections generated by the shower MC improve the description of NLO distributions.

Example: $t\bar{t}$ production at the LHC.

Transverse momentum distribution of $t\bar{t}$ pair, comparing different approaches.



- \longrightarrow At large p_T , where the NLO fixed order calculation dominates, MC@NLO reproduces the large-angle behavior of the NLO calculation;
- \longrightarrow At small p_T , where the showering algorithm resum important collinear logarithms, MC@NLO departs significantly from the NLO calculation.

Conclusions

- Parton-level NLO QCD calculations have reached a mature stage: results available for all $2 \to 2$ and $2 \to 3$ processes of interest at hadron colliders.
- Partial/full NNLO corrections or resummed NLL or NNLL corrections are available for several processes.
- To fully explore the potential of the LHC we will have to face two major challenges:
 - \longrightarrow provide NLO QCD calculations for multi-leg (2 \rightarrow 4 or more) background processes: very promising methods are being proposed;
 - interface parton-level NLO calculations with MC shower event generators: several breakthroughs have come already!
- In the last ten years we have witnessed an incredible amount of activity and creativity in the realm of higher order calculations.

More effort and new ideas will make the future exciting!