

Automation in fixed-order calculations

Andreas van Hameren

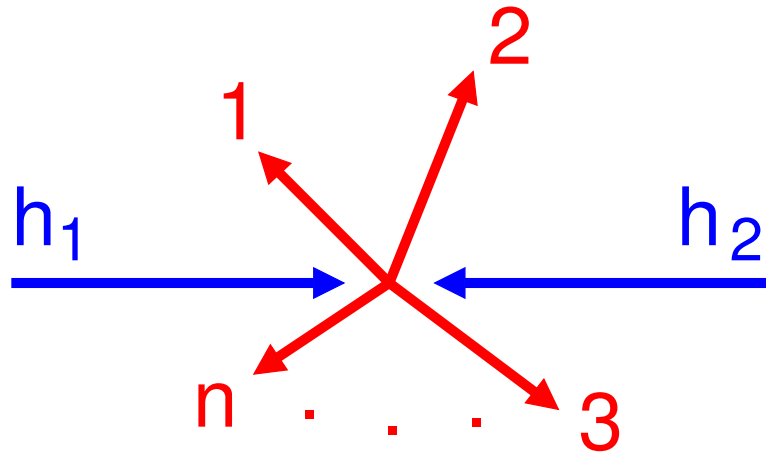
*The Henryk Niewodniczański Institute of Nuclear Physics
Polish Academy of Sciences*

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Outline

- factorization
- numerical evaluation of amplitudes
- automated LO programs
- merging with parton shower
- ingredients to NLO calculations
- automated NLO programs
- matching to parton shower
- summary

Hard scattering cross sections within collinear factorization



PDFs are related to the structure of the hadrons, universal to the scattering process

$$\sigma_{h_1, h_2 \rightarrow n}(p_1, p_2) = \sum_{a, b} \int dx_1 dx_2 f_a(x_1, \mu) f_b(x_2, \mu) \hat{\sigma}_{a, b \rightarrow n}(x_1 p_1, x_2 p_2; \mu)$$

$$\hat{\sigma}_{a, b \rightarrow n}(p_a, p_b; \mu) = \int d\Phi(p_a, p_b \rightarrow \{p\}_n) |\mathcal{M}_{a, b \rightarrow n}(p_a, p_b \rightarrow \{p\}_n; \mu)|^2 \mathcal{O}(p_a, p_b, \{p\}_n)$$

Phase space (includes spin/color summation) governs the kinematics

Matrix element (squared) contains model parameters, governs the dynamics

Observable, imposes phase space cuts

Collinear factorization

Naïve parton model for hadron scattering

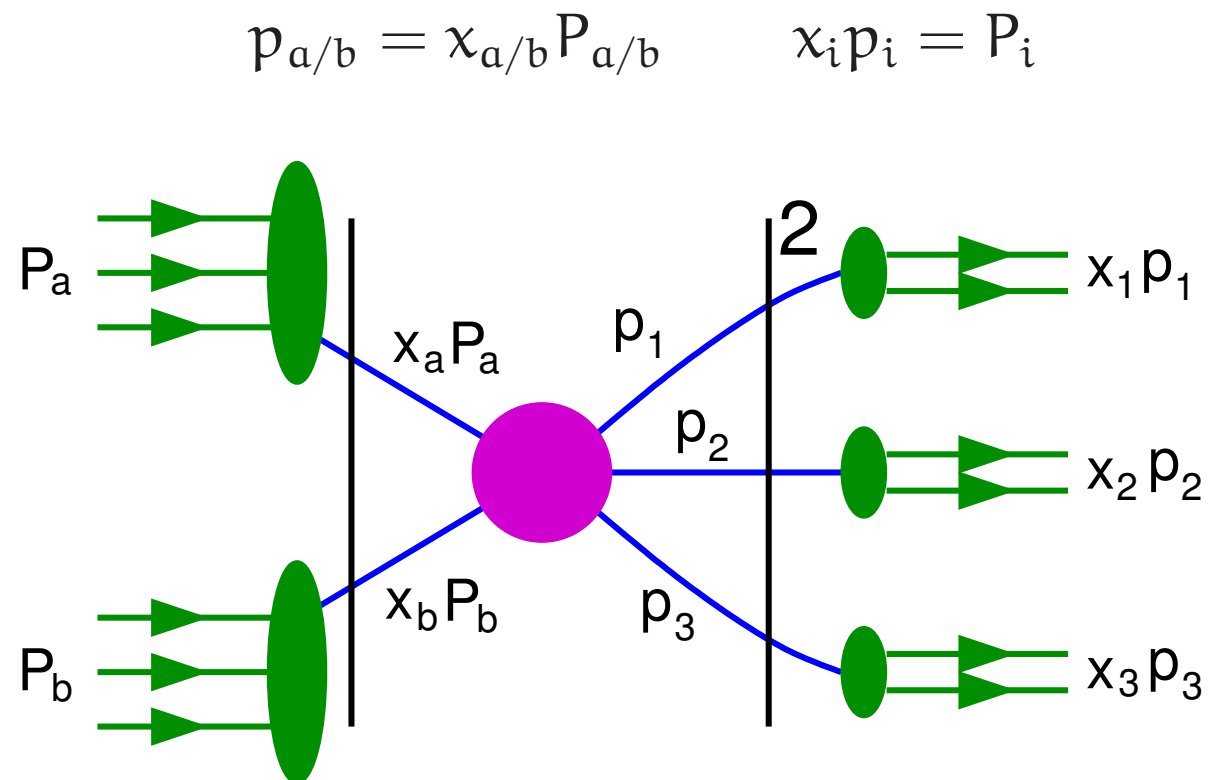
$$d\sigma(P_a, P_b \rightarrow \{P_i\}) = \int \prod_{j=a,b,1,\dots} dx_j f_j(x_j) d\hat{\sigma}(p_a, p_b \rightarrow \{p_i\})$$

- the parton densities f_a and fragmentation function f_i describe physics of long time scales

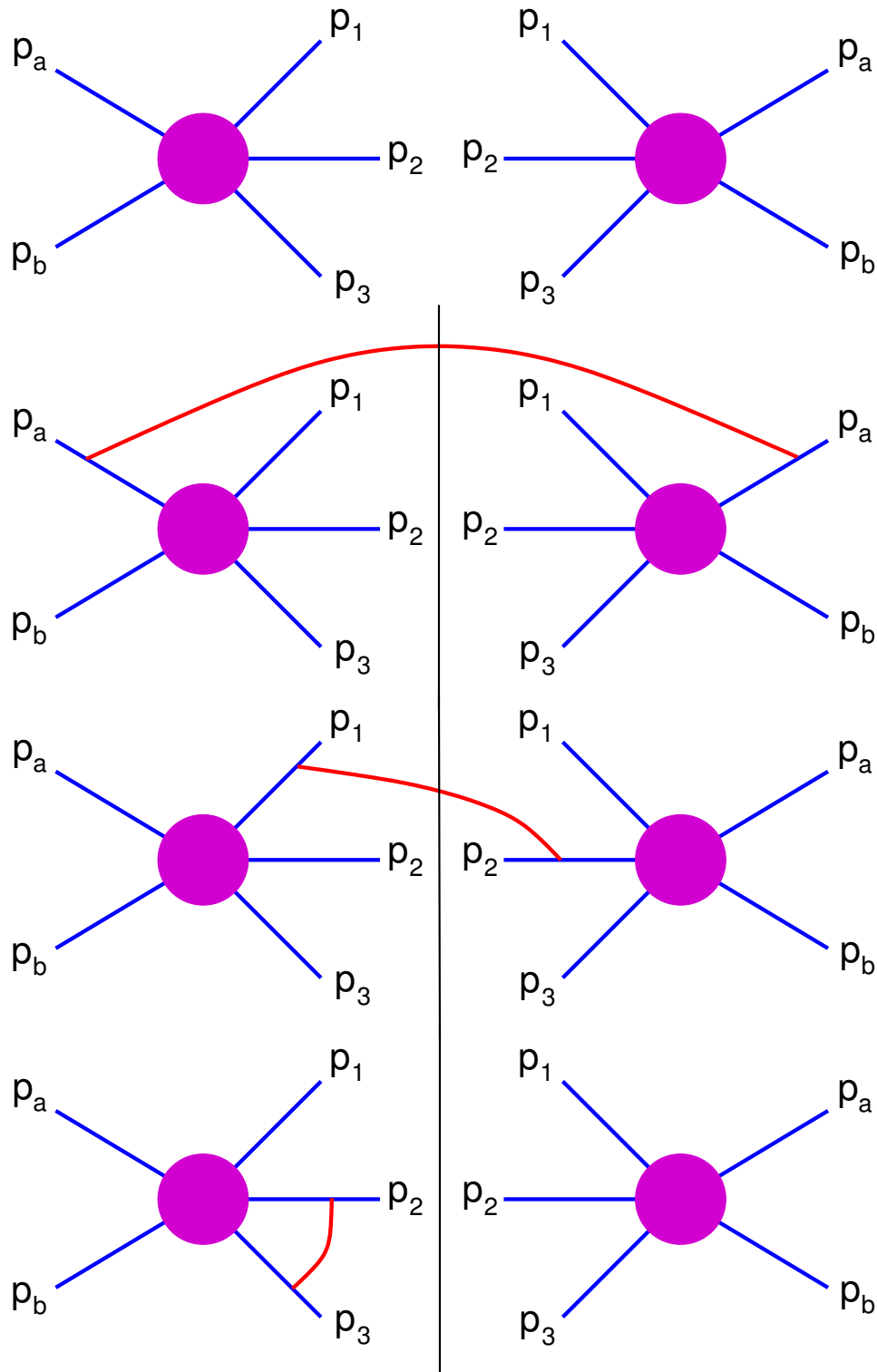
- not calculable within perturbation theory
- universal to the hard scattering process
- to be extracted from experiments

- the partonic scattering cross section $\hat{\sigma}$ describes physics of short time scales, and should be calculable within perturbative QCD

- Asymptotic freedom: small coupling for high energy



Perturbative calculations in QCD



for the squared scattering amplitude $|\mathcal{M}|^2$

- blue lines represent **identified** partons
- mirrored graphs represent \mathcal{M} and \mathcal{M}^*
- first square represents leading order
- higher orders by adding **one coupling**, that is **two 3-point vertices** connected by **gluon** integrated over its phase space
- **gluons** crossing the cut are real
 - are on-shell
 - participate in momentum conservation
- **gluons** not crossing the cut are virtual, are off-shell

Trouble with divergencies

Integrating over the phase space of the extra, unobserved gluons, one encounters **IR divergences** stemming from non-integratable singularities:

soft singularities: $\int_0 \frac{d|k|}{|k|}$

appear because all components of integration momentum k may become arbitrarily small

collinear singularities: $\int_0 \frac{d\theta}{1 - \cos\theta}$

appear because integration momentum k may become arbitrarily collinear with massless parton momentum p_i

- all soft singularities cancel with each other, as predicted by the Kinoshita-Lee-Nauenberg theorem
- collinear singularities do not all cancel

R.K. Ellis, H. Georgi, M. Machacek, H.D. Politzer, G.G. Ross, 1979:

Non-cancelling collinear divergences can be identified with the external partons, and can be factorized, to all orders in QCD.

Factorization following EGMPR

”Renormalized” formula for hard scattering cross section

$$d\sigma(P_a, P_b \rightarrow \{P_i\}) = \int \prod_{j=a,b,1,\dots} dy_j \tilde{f}_j(y_j; \mu) d\tilde{\sigma}(p_a, p_b \rightarrow \{p_i\}; \mu)$$

$$p_{a/b} = x_{a/b} P_{a/b} \quad P_i = x_i p_i$$

- $d\sigma$ does not depend on μ , while the \tilde{f}_j and $\tilde{\sigma}$ do
- μ may be put equal to renormalization scale
- dependence of \tilde{f}_j on μ is known, so QCD evolution can be applied to them
- $d\tilde{\sigma}$ may be sensitive logarithms of ratios of various scales in the process, which are remnants from the cancellations
- these may need to be resummed to all orders in the coupling in certain kinematical regions (eg via parton shower)
- higher fixed order terms may be needed to reduce scale dependence

Numerical evaluation of amplitudes

- performing a calculation means obtaining a number, or a plot
- for scattering cross sections, this implies performing phase space integrals

$$\hat{\sigma}_{a,b \rightarrow n} = \int d\Phi(p_a, p_b \rightarrow \{p\}_n) |\mathcal{M}_{a,b \rightarrow n}(p_a, p_b \rightarrow \{p\}_n)|^2 \mathcal{O}(p_a, p_b, \{p\}_n)$$

- over several dimensions
- are restricted by even more physical cuts

⇒ The phase space integrals have to be performed numerically.

⇒ $|\mathcal{M}_{a,b \rightarrow n}(p_a, p_b \rightarrow \{p\}_n)|^2$ has to be efficiently evaluated numerically.

- the evaluation of $|\mathcal{M}_{a,b \rightarrow n}(p_a, p_b \rightarrow \{p\}_n)|^2$ involves a sum over helicities

$$|\mathcal{M}_{a,b \rightarrow n}(p_a, p_b \rightarrow \{p\}_n)|^2 = \sum_{\lambda_a, \lambda_b, \{\lambda\}_n} |\mathcal{M}_{a,b \rightarrow n}(p_a, \lambda_a, p_b, \lambda_b \rightarrow \{p, \lambda\}_n)|^2$$

Perform this sum explicitly

⇒ $\mathcal{M}_{a,b \rightarrow n}(p_a, \lambda_a, p_b, \lambda_b \rightarrow \{p, \lambda\}_n)$ has to be efficiently evaluated numerically.

From expressions to algorithms

For specific tree-level helicity amplitudes, very elegant and compact expressions exist.

$$\mathcal{M}_{\text{ng}}(\{p, \lambda, a\}_n) = i g^{n-2} \sum_{\text{perm}} \text{Tr}(T^{a_1} T^{a_2} \dots T^{a_n}) \mathcal{A}_{\text{ng}}(p_1^{\lambda_1}, p_2^{\lambda_2}, \dots, p_n^{\lambda_n})$$

$$\mathcal{A}_{\text{ng}}(p_1^-, p_j^-, p_{\text{rest}}^+) = \frac{\langle p_1 p_j \rangle^4}{\langle p_1 p_2 \rangle \langle p_2 p_3 \rangle \dots \langle p_{n-1} p_n \rangle \langle p_n p_1 \rangle}$$

The expressions can be proven with the [Berends-Giele \(1988\)](#) recursive relations

$$J_{i,j}^\mu = \frac{-i}{p_{i,j}^2} \left[\sum_{k=i}^{j-1} V_{\nu\sigma}^\mu(p_{i,k}, p_{k+1,j}) J_{i,k}^\nu J_{k+1,j}^\sigma + \sum_{k=i}^{j-2} \sum_{l=k+1}^{j-1} W_{\nu\sigma\rho}^\mu J_{i,k}^\nu J_{k+1,l}^\sigma J_{l+1,j}^\rho \right]$$

$$p_{i,j} = p_i + p_{i+1} + \dots + p_j \quad J_{i,j}^\mu = J^\mu(p_i^{\lambda_i}, p_{i+1}^{\lambda_{i+1}}, \dots, p_j^{\lambda_j})$$

$$V_{\nu\sigma}^\mu(p, q) = \frac{ig^2}{\sqrt{2}} [(p - q)^\mu g_{\nu\sigma} + 2g_\sigma^\mu q_\nu - 2g_\nu^\mu p_\sigma] \quad W_{\nu\sigma\rho}^\mu = \frac{ig^2}{2} [2g_\sigma^\mu g_{\nu\rho} - g_\nu^\mu g_{\sigma\rho} - g_\sigma^\mu g_{\nu\rho}]$$

These relations are numerically very efficient, and can be used instead of the expression to evaluate the amplitude.

Dyson–Schwinger at tree-level

Algorithm can be generalized for arbitrary field theories (Caravaglios, Moretti 1995)

- completely numerical
- avoids Feynman graphs
- asymptotic computational complexity exponential instead of factorial

multi-gluon amplitudes Draggiotis, Kleiss, Papadopoulos 1998

multi-jet processes Caravaglios, Mangano, Moretti, Pittau 1998

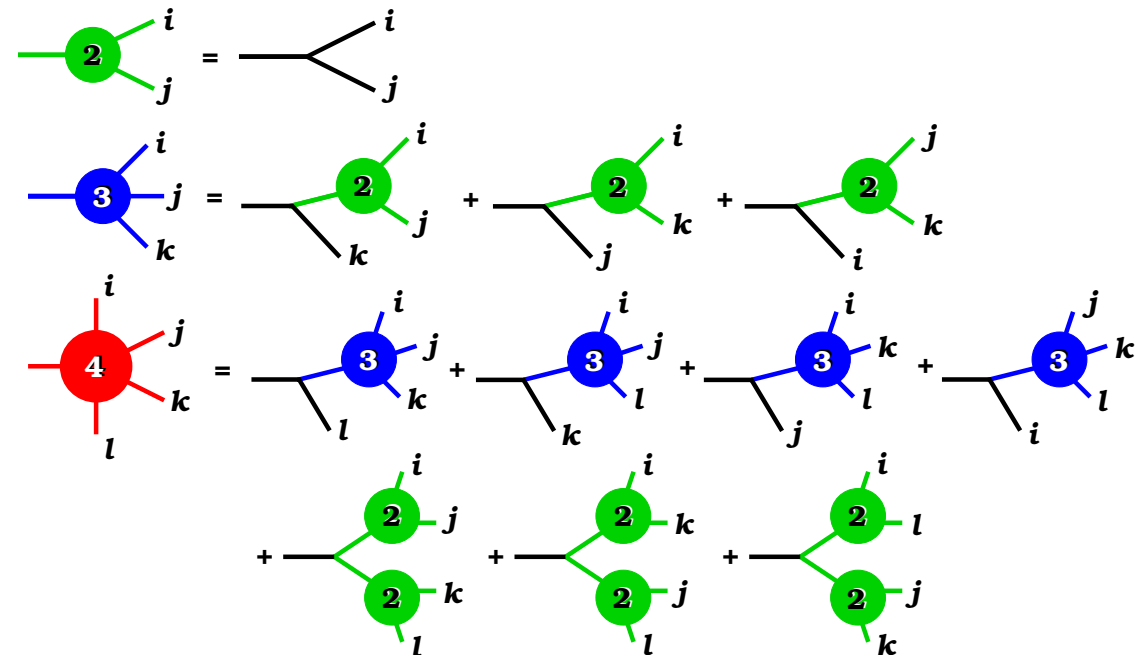
ALPGEN Mangano, Moretti, Piccinini, Pittau, Polosa 2002

HELAC-PHEGAS Kanaki, Papadopoulos 2000
Cafarella, Papadopoulos, Worek 2007

O'MEGA-WHIZARD Moretti, Ohl, Reuter 2001
Kilian, Ohl, Reuter 2007

COMIX Gleisberg, Hoeche 2008

CAMORRA Kleiss, van den Oord 2011



Using Feynman graphs:

COMPHEP 1989-2009 Boos, Bunichev, Dubinin, Dudko, Edneral, Ilyin, Kryukov, Savrin, Semenov, Sherstnev

MADGRAPH Stelzer, Long 1994

MAD EVENT Maltoni, Stelzer 2002

AMEGIC++ Krauss, Kuhn, Soff 2001

CARLOMAT Kolodziej 2007

Also non-trivial phase space integration

Multi-jet processes

- LO-only calculations can only provide inclusive observables, which depend strongly on the scale of phase space cuts, up to IR disasters for small scale values.
- LL-only parton shower programs cannot accurately describe processes with many hard jets.

Improve both by merging parton showers and exact tree-level matrix elements

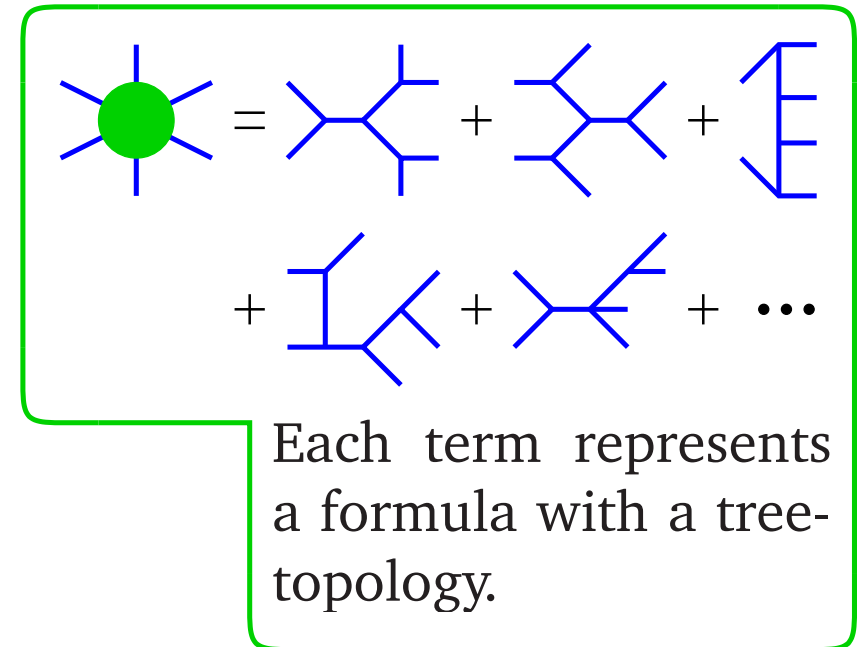
1. generate parton-level n -jet event from exact matrix element.
 n is chosen following the parton-level total cross sections
2. apply jet-algorithm repeatedly, to associate a branching tree with the parton-level momenta and obtain splitting scales
3. apply rejection on event with probabilities including effects of running coupling constants and Sudakov form factors
4. shower from each of the n partons, reject events that produce more than n jets
3. apply rejection on event with probabilities including effects of running coupling constants
4. shower from each of the n partons, reject events that produce more than n jets, and only accept event when each jet can be identified with a parton

Catani, Krauss, Kuhn, Webber 2001

M.L. Mangano

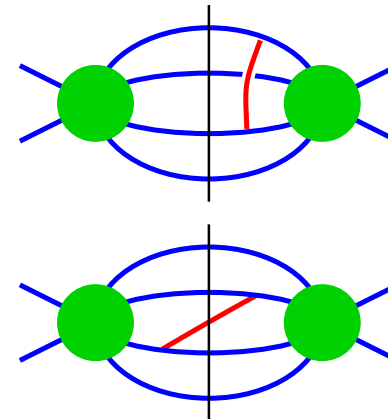
Multi-jet processes at NLO QCD

- Reduce dependence on unphysical scales. Reduce uncertainty on normalization to around 20%.
- Shape of distributions changes, there is no global K-factor.
- Include structure of jets.



Next-to-Leading Order cross section:

$$\hat{\sigma}_{a,b \rightarrow n}^{\text{NLO}} = \int d\Phi_n 2\Re\left(\mathcal{M}_{a,b \rightarrow n}^{(0)} \mathcal{M}_{a,b \rightarrow n}^{(1)}\right) \mathcal{O}_n^{\text{LO}} + \int d\Phi_{n+1} \left|\mathcal{M}_{a,b \rightarrow n+1}^{(0)}\right|^2 \mathcal{O}_{n+1}^{\text{NLO}}$$

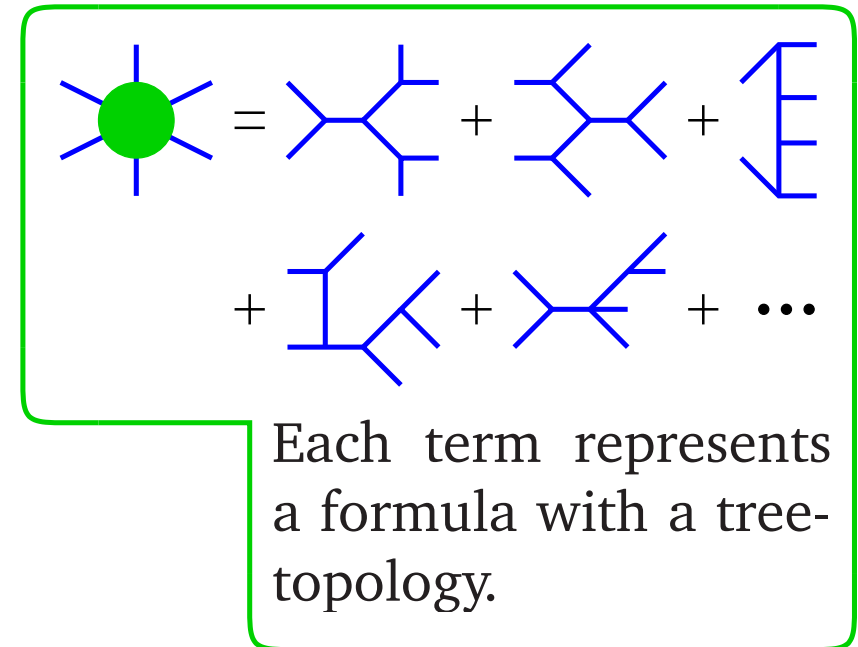


- The one-loop amplitude $\mathcal{M}_{a,b \rightarrow n}^{(1)}$ is much more complicated than $\mathcal{M}_{a,b \rightarrow n}^{(0)}$.
- Both $\mathcal{M}_{a,b \rightarrow n}^{(1)}$ and the integral over Φ_{n+1} are IR divergent.

⇒ the formula above cannot straightforwardly be attacked numerically

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$$+ \int d\Phi_{n+1} \left| \mathcal{M}_{a,b \rightarrow n+1}^{(0)} \right|^2 \mathcal{O}_{n+1}^{\text{NLO}}$$

$$\hat{\sigma}_{a,b \rightarrow n}^{\text{NLO}} = \int d\Phi_n \left[2\Re\left(\mathcal{M}_{a,b \rightarrow n}^{(0)} \mathcal{M}_{a,b \rightarrow n}^{(1)}\right) + \int d\Phi_1 \mathcal{D}_{n+1} \right] \mathcal{O}_n^{\text{LO}}$$

$$+ \int d\Phi_{n+1} \left[\left| \mathcal{M}_{a,b \rightarrow n+1}^{(0)} \right|^2 \mathcal{O}_{n+1}^{\text{NLO}} - \mathcal{D}_{n+1} \mathcal{O}_n^{\text{LO}} \right]$$

Subtraction methods

Construct a list of

- phase space restricting functions $\theta_{n+1}^{(j)}$
- phase space mappings $T_{n \rightarrow n+1}^{(j)}$ and $T_{n \leftarrow n+1}^{(j)}$
- subtraction functions $D_{n+1}^{(j)}$

such that

$$\int d\Phi_{n+1} \left[|\mathcal{M}_{n+1}^{(0)}|^2 \mathcal{O}_{n+1}^{\text{NLO}} - \sum_j D_{n+1}^{(j)} \theta_{n+1}^{(j)} \mathcal{O}_n^{\text{LO}} \circ T_{n \leftarrow n+1}^{(j)} \right]$$

can be integrated numerically, and

$$\int d\phi_1 D_{n+1}^{(j)} \circ T_{n \rightarrow n+1}^{(j)} \theta_{n+1}^{(j)} \circ T_{n \rightarrow n+1}^{(j)} \mathcal{O}_n^{\text{LO}}$$

can be performed analytically, within dimensional regularization.

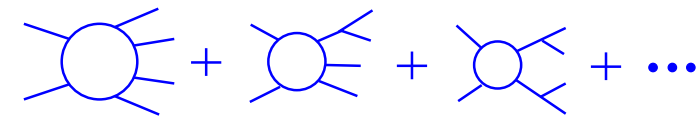
Catani, Seymour 1996:

- $\theta_{n+1}^{(j)} = 1$
- mapping for $2 \leftarrow 3$ partons
- IR singularities spread over many terms

Frixione, Kunszt, Signer 1995:

- $\sum_j \theta_{n+1}^{(j)} = 1$
- $\theta_{n+1}^{(j)}$ contains one, and vanishes at any other, collinear singularity
- $\theta_{n+1}^{(j)}$ contributes to one soft singularity

One-loop amplitudes



perform loop integral numerically

subtraction

Nagy Soper 2003

Becker Reuschle Weinzierl 2010

expand amplitude in terms of universal integrated one-loop functions

tensor integrals

Passarino Veltman 1978

Denner Dittmaier 2005

Binoth Guillet Heinrich 1999

del Aguila Pittau 2004

Giele Glover 2004

Diakonidis Fleischer Riemann Tausk 2009

construct expression for coefficients

"traditional approach"

evaluate coefficients numerically
via recursion

AvH 2009

Cascioli Maierhofer Pozzorini 2011

Actis Denner Hofer Scharf Uccirati 2012

scalar integrals

construct expression for coefficients
(unitarity)

Bern Dixon Dunbar Kosower 1994

Britto Cachazo Feng 2004

Anastasiou Britto Feng Kunstz Mastrolia 2006

Forde 2007

Badger 2008

evaluate coefficients numerically
by solving linear system (OPP)

Ossola Papadopoulos Pittau 2007

Ellis Giele Kunstz Melnikov 2008

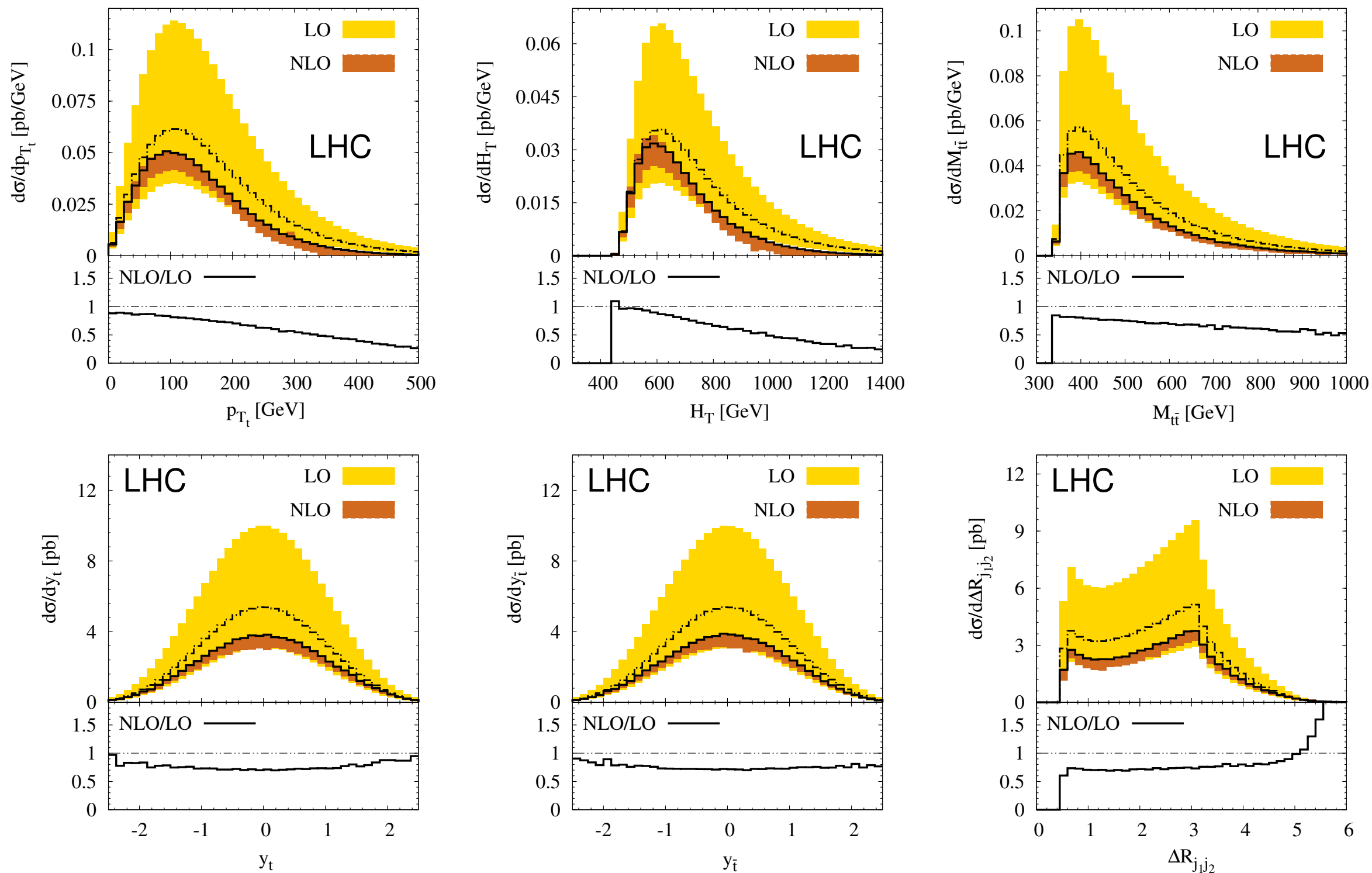
Recent multi-leg NLO calculations

proton-proton scattering, involving at least one-loop six-point functions:

| | |
|-------------------------|--|
| $t\bar{t}b\bar{b}$ | Bredenstein, Denner, Dittmaier, Pozzorini 2008, 2010 |
| $t\bar{t}b\bar{b}$ | Bevilacqua, Czakon, Papadopoulos, Pittau, Worek 2009 |
| $Wjjj$ | Ellis, Melnikov, Zanderighi 2009 |
| $Wjjj$ | Berger, Bern, Dixon, Febres Cordero, Forde, Gleisberg, Ita, Kosower, Maitre 2009 |
| $b\bar{b}b\bar{b}$ | Binoth, Greiner, Guffanti, Reuter, Guillet, Reiter 2010 |
| W^+W^+jj | Melia, Melnikov, Rontsch, Zanderighi 2010 |
| $Wjjjj$ | Berger, Bern, Dixon, Febres Cordero, Forde, Gleisberg, Ita, Kosower, Maitre 2011 |
| $W^+W^-b\bar{b}$ | Bevilacqua, Czakon, van Hameren, Papadopoulos, Worek 2011 |
| $W^+W^-b\bar{b}$ | Denner, Dittmaier, Kallweit, Pozzorini 2011, 2012 |
| W^+W^-jj | Melia, Melnikow, Rontsch, Zanderighi 2011 |
| $t\bar{t}jj$ | Bevilacqua, Czakon, Papadopoulos, Worek 2011 |
| $Zjjjj$ | Ita, Bern, Dixon, Febres Cordero, Kosower, Maitre 2012 |
| $jjjj$ | Bern, Diana, Dixon, Febres Cordero, Hoeche, Kosower, Ita, Maitre, Ozeren 2012 |
| $jjjj$ | Badger, Biedermann, Uwer, Yundin 2012 |
| $t\bar{t}t\bar{t}$ | Bevilacqua, Worek 2012 |
| $e^+e^- \rightarrow 7j$ | Becker, Goetz, Reuschle, Schwan, Weinzierl 2012 |

pp(p \bar{p}) \rightarrow t \bar{t} jj at NLO QCD

Bevilacqua, Czakon,
Papadopoulos, Worek



Programs for NLO calculations

Complete packages:

MCFM Campbell, Ellis, Williams

NLOJET++ Nagy

VBFNLO Arnold, Bellm, Bozzi, Brieg, Campanario, Englert, Feigl, Frank, Figy, Geyer, Hackstein, Hankele, Jäger, Kerner, Kubocz, Oleari, Palmer, Plätzer, Rauch, Rzehak, Schissler, Schlimpert, Spannowsky, Worek, Zeppenfeld

HELAC-NLO Bevilacqua, Czakon, Garzelli, van Hameren, Kardos, Papadopoulos, Pittau, Worek

GRACE Bredenstein, Fujimoto, Igarashi, Ishikawa, Jimbo, Kaneko, Kato, Kawabata, Kawamura, Kon, Kurihara, Kuroda, Lafage, Munehisa, Nakazawa, Sasaki, Shimizu, Tanaka, Tobimatsu, Uematsu, Watanabe, Yuasa, Yasui

BLACKHAT/SHERPA Berger, Bern, Diana, Dixon, Febres Cordero, Forde, Hoeche, Gleisberg, Ita, Kosower, Maitre, Ozeren

MADGRAPH Hirschi, Frederix, Frixione, Garzelli, Maltoni, Pittau, Stelzer

One-loop amplitudes:

FORMCALC Agrawal, Hahn, Mirabella, Perez-Victoria

GOSAM Cullen, Greiner, Heinrich, Luisoni, Mastrolia, Ossola, Reiter, Tramontano

NGLUON Badger, Biederman, Uwer

Matching to parton shower

following Hoeche, Krauss,
Schonher, Siegert 2012

$$\begin{aligned} \mathcal{O}^{\text{LO+NLO}} = & \int d\Phi_n \left[B_n + V_n + \sum_j I_S^{(j)} + \sum_j \int d\Phi_1 (A_{n+1}^{(j)} \circ T_{n \rightarrow n+1}^{(j)} - S_{n+1}^{(j)} \circ T_{n \rightarrow n+1}^{(j)}) \right] \mathcal{O}_n^{\text{LO}} \\ & + \int d\Phi_{n+1} \sum_j A_{n+1}^{(j)} \left[\mathcal{O}_{n+1}^{\text{NLO}} - \mathcal{O}_n^{\text{LO}} \circ T_{n \leftarrow n+1}^{(j)} \right] \\ & + \int d\Phi_{n+1} \left[R_{n+1} - \sum_j A_{n+1}^{(j)} \right] \mathcal{O}_{n+1}^{\text{NLO}} \end{aligned}$$

NLO matching: replace first two lines by

$$\int d\Phi_n \bar{B}_n \left[\Delta^{(A)}(t_0) \mathcal{O}_n^{\text{LO}} + \sum_j \int_{t_0} d\Phi_1 \frac{A_{n+1}^{(j)} \circ T_{n \rightarrow n+1}^{(j)}}{B_n} \Delta^{(A)}(t) \theta(t(\Phi_1) - t_0) \mathcal{O}_{n+1}^{\text{NLO}} \circ T_{n \rightarrow n+1}^{(j)} \right]$$

- generate event following first line or third line
- just keep event if third line is chosen (real-emission kinematics)
- if first line is chosen (Born-like kinematics) perform one-step Sudakov branching.

Matching to parton shower

Methods:

MC@NLO [Frixione, Webber 2002](#)

POWHEG [Nason 2004, Frixione, Nason, Oleari 2007](#)

Programs:

POWHEG BOX [Alioli, Nason, Oleari, Re 2010](#)

MC@NLO IN SHERPA [Hoeche, Krauss, Schonherr, Siegert 2012](#)

aMC@NLO [Frederix, Frixione, Hirschi, Maltoni, Pittau, Torrielli 2012](#)

Recent calculations:

$pp \rightarrow t\bar{t}j$ [Kardos, Papadopoulos, Trocsanyi 2012](#)

$pp \rightarrow t\bar{t}Z$ [Garzelli, Kardos, Papadopoulos, Trocsanyi 2012](#)

$pp \rightarrow Wjj$ [Frederix, Frixione, Hirschi, Maltoni, Pittau, Torrielli 2012](#)

$gg \rightarrow Hjj$ [Campbell, Ellis, Frederix, Nason, Oleari, Williams 2012](#)

$pp \rightarrow Zjj$ [Jäger, Schneider, Zanderighi 2012](#)

$pp \rightarrow Wjjj$ [Hoeche, Krauss, Schonherr, Siegert 2012](#)

Matching and merging:

[Gehrmann Hoeche, Krauss, Schonherr, Siegert 2012](#)

[Frederix, Frixione 2012](#)

Full NLO parton shower [Jadach, Kusina, Placzek, Skrzypek, Slawinska 2011](#)