COMPUTATIONAL TOOLS FOR HARD SCATTERING PROCESSES*

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Some issues related to the computation of hard scattering processes with several particles in the final state at NLO QCD are addressed, along with their solutions.

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1. Introduction

Precise predictions of signals and backgrounds are essential for physics at LHC. This is, in particular, the case if the scenario persists, in which the mechanism of electro-weak symmetry breaking or new physics beyond the Standard Model will not be revealed through clear and easy-to-identify evidence. Regarding for example the decay channels of the Higgs boson, one has then to face the fact that many of both signals and the backgrounds are described as hard scattering processes in proton–proton scattering with several particles and/or partons in the final state.

Collinear factorization allows for the expression

$$\sigma(p_1,p_2)=\sum_{a,b}\int dx_1dx_2\, f_a(x_1,\mu)f_b(x_2,\mu)\,\hat{\sigma}_{ab}(x_1p_1,x_2p_2,\mu)\,, \qquad (1)$$

for the cross-section $\sigma(p_1,p_2)$ of the process resulting from the collision of hadrons with momenta p_1 and p_2. The p.d.fs $f_a(x_1,\mu)$ and $f_b(x_2,\mu)$ are universal to hadron scattering processes, and are the materialization of the description of the hadrons within the parton model, in which the hadron

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consists of quarks and gluons, each carrying a fraction of the total hadron momentum. The partonic scattering cross-sections $\hat{\sigma}_{ab}(x_1p_1, x_2p_2, \mu)$ can be calculated within perturbation theory. All components depend on the renormalization/factorization scale μ, whereas the complete hadronic cross-section does not. The terms in perturbative expansion *do* depend on it, and one of the reasons to perform higher fixed-order calculations is to reduce this dependence. In order to minimize the contribution of logarithms of ratios of μ and other scales, that are remnants of the cancellation of divergences in the factorization procedure, the value of μ is, in practice, set to a typical scale of the hard process.

Regarding fixed-order calculations, there has been a remarkable progress in recent years to reach next-to-leading (NLO) precision in QCD for processes with four or more final-state particles and/or partons [1, 2, 3]. These calculations are considerably more complex than leading-order (LO) calculations, and several difficulties had to be overcome. Formally, a differential cross-section at NLO contains two contributions

$$\begin{aligned} d\hat{\sigma}^{\mathrm{NLO}}_{a,b\to n} \;=\; & d\Phi_{a,b\to n}\, 2\mathrm{Re}\left\{\mathcal{M}^{(0)*}_{a,b\to n}\mathcal{M}^{(1)}_{a,b\to n}\right\}\mathcal{O}^{\mathrm{LO}}_{a,b\to n} \\ & + d\Phi_{a,b\to n+1}\left|\mathcal{M}^{(0)}_{a,b\to n+1}\right|^2\mathcal{O}^{\mathrm{NLO}}_{a,b\to n+1}\,. \end{aligned} \tag{2}$$

The first term on the r.h.s. is the virtual contribution containing the interference of the tree-level matrix element $\mathcal{M}^{(0)}_{a,b\to n}$ and the one-loop matrix element $\mathcal{M}^{(1)}_{a,b\to n}$, and an observable $\mathcal{O}^{\mathrm{LO}}_{a,b\to n}$ that essentially should enforce strict hard kinematics, like in a LO calculation. Then, it usually consists of a number of phase space cuts. $d\Phi_{a,b\to n}$ represents a differential phase space element, and for brevity it is understood to include all other ingredients to a cross-section, like the flux factor and symmetry factors. The second term is the real contribution, and contains the tree-level matrix element $\mathcal{M}^{(0)}_{a,b\to n+1}$ with one more parton, and an observable $\mathcal{O}^{\mathrm{NLO}}_{a,b\to n+1}$ allowing for one parton to become arbitrarily soft, and one pair of partons to become arbitrarily collinear. The infra-red (IR) divergences arising in the phase space integration over this unresolved phase space should cancel against the divergences in the virtual contribution coming from the one-loop matrix element. This puts restrictions on the choice of the observables. The Kinoshita–Lee–Nauenberg (KLN) theorem ensures that the cancellations happen under the condition that the observables are IR-safe. This is often embedded in the context of functions that allow for generalization to arbitrary numbers of soft and collinear partons, so-called jet algorithms. Finally, there are left-over collinear divergences related to the initial state radiation, that have to be dealt with within the factorization prescription, in the context of Eq. (1).

2. Calculations with Helac-NLO

From the list of calculations mentioned before, the ones in [2, 3] have been performed with the help of a collection of computer programs recently published under the name HELAC-NLO as a complete tool for such calculations [4].

The cancellation of IR divergences is ensured to happen formally, but must eventually be implemented for numerical calculations. This can be achieved with the subtraction method, in which terms are added and subtracted to the partonic cross-section. They should be such that the subtracted ones cancel the IR divergences point-wise in the real contribution, and the added ones can be integrated analytically over the unresolved phase space to cancel the divergences in the virtual contribution. In HELAC-NLO the implementation HELAC–DIPOLES [5] of the dipole-subtraction method [6] is used for this purpose. It is based on the LO platform HELAC–PHEGAS [7] making use of the universality of the dipole-subtraction method with respect to details of the partonic process.

HELAC is also used to evaluate tree-level amplitudes, whereas the one-loop amplitudes are evaluated with HELAC–1LOOP [8]. It is an explicit implementation of the OPP approach to one-loop calculations [9], using the universal OPP reduction tool CUTTOOLS [10]. Within the OPP approach the non-universal part of a one-loop calculation can be identified as the numerator of the one-loop amplitude over denominator factors containing the loop integration momentum. HELAC–1LOOP computes these by translating them systematically into tree-level objects. The one-loop master integrals are evaluated with ONELOOP [11]. The part of the rational contribution not provided by CUTTOOLS is also included [12].

3. Phase space integration for the real contribution

All mentioned tools are described in detail in the respective publications. One issue that deserves some more attention is related to the phase space integration of the real contribution. Within the dipole subtraction method it concerns the evaluation of the integral

$$\int d\Phi_{n+1} \left\{ \left| \mathcal{M}_{n+1}^{(0)} \right|^2 \mathcal{O}_{n+1}^{\mathrm{NLO}} - \sum_j \sum_{i,k \neq j} \mathcal{D}_n^{(ij;k)} \, \mathcal{O}_n^{\mathrm{LO}} \circ \mathcal{T}_{n+1 \to n}^{(ij;k)} \right\}. \tag{3}$$

The dipole subtraction terms $\mathcal{D}_n^{(ij;k)}$ are composed of n-parton tree-level matrix elements. They are associated with $\mathcal{O}_n^{\mathrm{LO}}$. The whole contribution is given as a $(n+1)$-particle phase space integral, and the objects living in n-particle phase space can exist under the same integral via phase space mappings $\mathcal{T}_{n+1 \to n}^{(ij;k)}$.

Two new issues appear compared to LO calculations. Firstly, whereas in a LO calculation all final-state partons are well-separated by phase space cuts, in the integral above a single parton may become arbitrarily soft, and one pair of partons may become arbitrarily collinear. The dipole terms ensure integrability in the singly soft/collinear regions, but do not make the integrand completely finite. A remnant divergent, but integrable, behavior remains. However, as used for LO calculations, phase space integrator PHEGAS assumes these regions to be cut out, and anticipates the divergent behavior towards these regions with internal probability densities that are typically not defined at the singular phase space configurations, or become very inefficient.

Secondly, the dipole terms are designed only to match $|\mathcal{M}^{(0)}_{n+1}|^2$ in the singly soft/collinear regions. Outside those regions, they behave quite differently. A phase space generator like PHEGAS to integrate $|\mathcal{M}^{(0)}_{n+1}|^2$ efficiently does not necessarily perform well when integrating the real-subtracted integral.

In order to deal with these issues, the independent phase space generator KALEU [13] is used. In essence it is still a generator for LO applications, but due to the fact that it is designed in an object oriented way, in the sense that several instances of the generator can deal with different integrals in parallel, it can be used in a multi-channel approach [14] to solve the second issue mentioned above. Each channel carries its own full instance of KALEU. One channel carries the instance that efficiently deals with $|\mathcal{M}^{(0)}_{n+1}|^2$. Furthermore, for each dipole term there is a channel carrying an instance that generates n-particle phase space configurations such that it efficiently integrates the squared tree-level matrix element of the underlying n-particle scattering process. Such a n-particle phase space configuration is then turned into a $(n+1)$-particle configuration by applying the inverse of the mapping $\mathcal{T}^{(ij;k)}_{n+1\to n}$ associated with the dipole term. This generation of an extra momentum follows exactly the formulas for the parton showers based on the dipole formalism presented in [15]. The azimuthal angle needed for the construction of the extra momentum is generated with a flat distribution, and the other two variables are generated following self-adaptive densities.

The adaptation of these densities happens in two steps. First, the unit interval on which the variables live is divided into two halves, and optimization is performed for densities of the type

$$\text{density}(x) \propto \theta\Big(0 < x \le \tfrac{1}{2}\Big)\,\frac{\alpha\,\gamma_1\,2^{\gamma_1}}{x^{1-\gamma_1}} + \theta\Big(\tfrac{1}{2} < x < 1\Big)\,\frac{(1-\alpha)\,\gamma_2\,2^{\gamma_2}}{(1-x)^{1-\gamma_2}}\,. \quad (4)$$

The three parameters α, γ_1, γ_2 are estimated during optimization as follows.

The ratio $\alpha/(1-\alpha)$ is estimated by the ratio

$$\frac{\sum_{0<x\leq\frac{1}{2}} w(x)}{\sum_{\frac{1}{2}<x<1} w(x)} \tag{5}$$

of total weights contributing to the two intervals during the Monte Carlo process. The exponents are estimated by

$$\gamma_1 \approx \frac{\sum_{0<x\leq\frac{1}{2}} w(x)}{\sum_{0<x\leq\frac{1}{2}} w(x)\log\left(\frac{1}{2x}\right)}, \qquad \gamma_2 \approx \frac{\sum_{\frac{1}{2}<x<1} w(x)}{\sum_{\frac{1}{2}<x<1} w(x)\log\left(\frac{1}{2(1-x)}\right)}. \tag{6}$$

This happens by collecting batches of data points $(x, w(x))$ and updating the parameters batch by batch. This optimization step is performed in order to match the possible remnant divergent, but integrable, behavior of the integrand in terms of the mentioned variables after the dipole subtraction, and solves the first issue related to phase space integration of the real contribution in NLO calculations mentioned above. After a while, the parameters in the densities of Eq. (4) are frozen, and optimization continues with adaptive grids underneath these densities, following the method presented in [16].

In Table I, some results regarding the application of dipole channels are presented. It concerns the real contribution for the sub-process $u\bar{u} \to b\bar{b}\, e^+\nu_e\, \mu^-\bar{\nu}_\mu\, g$ in NLO calculations of the process $pp \to b\bar{b}\, e^+\nu_e\, \mu^-\bar{\nu}_\mu$ as in [3]. More specifically, these are results for $\sqrt{s} = 7$ TeV, the anti-k_T jet algorithm, and two values of the cut-off α_max for the dipole phase space. This parameter determines how far from the actual singularities the dipole terms still contribute. The presented numbers depend on α_max, since only a complete NLO calculation, including the integrated subtraction terms, is independent. Three options are compared:

a. Kaleu with dipole channels as explained above;

b. Kaleu without dipole channels, but using adaptive grids for all generated invariants from which momenta are constructed;

c. Kaleu with non of the above, just using probability densities for generated invariants that are defined also in singular regions.

The overall conclusion is that the option with dipole channels outperforms the other two options, in particular for $\alpha_\mathrm{max} = 1.00$, even taking into account the substantially higher computational cost. Although 7.1/2.7 times slower, the estimated error is 1.9/0.59 times smaller, leading to a gain of a factor $(1.9/0.59)^2/(7.1/2.7) \approx 3.9$, *i.e.* it takes a factor 3.9 less time to reach the same estimated error. This result appears to be partly due to a better balance in the distribution of events over positively and negatively contributing regions.

TABLE I

Cross-sections in [fb] for the real-subtracted contribution from $u\bar{u} \to b\bar{b}\, e^+\nu_e\, \mu^-\bar{\nu}_\mu\, g$ to the process $pp \to b\bar{b}\, e^+\nu_e\, \mu^-\bar{\nu}_\mu$ at NLO as in [3]. All results were obtained with Kaleu. The numbers $N_{\rm gnrt}$ of generated and $N_{\rm eval}$ of accepted phase space points are multiples of 10^6. The computing times $t_{\rm cpu}$ are in hours on a 2.80 GHz Intel Xeon processor. The superscripts $(+)$ and $(-)$ respectively refer to positive and negative weight contributions. The values of $N_{\rm gnrt}$ were chosen such that $N^{(+)}_{\rm eval} + N^{(-)}_{\rm eval} \approx 10^7$.

$\alpha_{\rm max} = 0.01$							
Option	$\sigma^{(+)}$	$\sigma^{(-)}$	$\sigma^{(+)} - \sigma^{(-)}$	$N^{(+)}_{\rm eval}$	$N^{(-)}_{\rm eval}$	$N_{\rm gnrt}$	$t_{\rm cpu}$
a	316.78(.34)	159.00(.29)	157.78(.45)	7.449	2.447	26	6.6
b	316.57(.58)	160.6(1.0)	156.0(1.2)	8.946	1.276	33	2.0
c	316.81(.54)	156.9(1.0)	159.9(1.2)	8.013	1.974	62	2.8
$\alpha_{\rm max} = 1.00$							
Option	$\sigma^{(+)}$	$\sigma^{(-)}$	$\sigma^{(+)} - \sigma^{(-)}$	$N^{(+)}_{\rm eval}$	$N^{(-)}_{\rm eval}$	$N_{\rm gnrt}$	$t_{\rm cpu}$
a	286.29(.37)	305.10(.44)	-18.81(.59)	5.005	4.828	21	7.1
b	286.22(.75)	304.7(1.7)	-18.5(1.9)	7.034	2.952	25	2.7
c	286.7(.9)	309.9(3.1)	-23.1(3.2)	6.509	3.347	40	2.7

4. Summary

Issues related to the calculation of hard scattering processes with several particles in the final state at NLO QCD have been addressed. The program Helac-NLO, for automated computation of such processes, has been introduced along with its components dealing with the mentioned issues. In particular, solutions related to the phase space integration of the real contribution have been highlighted.

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