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Perturbative QCD for the LHC

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These proceedings discuss some of the highlights of recent research in perturbative QCD as it relates to the LHC. Topics covered include the new generation of Monte Carlo event generators, the revolution that is occurring in NLO calculations, progress towards NNLO predictions and developments in the definition and use of jets.

This writeup is dedicated to the memory of Thomas Binoth and Ulrich Baur.

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1. Introduction

As the LHC programme gets underway, it is timely to examine the status of our QCD tools. One may ask whether they have reached the degree of sophistication that we expected of them at this stage. It is quite an achievement for the community to be able to say that the answer to this question is "yes". A second question is whether our QCD tools have achieved the degree of sophistication that is necessary for fully exploiting the LHC over the years to come. Here the answer will be more nuanced: there is certainly still ample scope for progress.

To provide a context for our discussion of QCD, it is perhaps worth briefly recalling some of the roles played by QCD at a hadron collider whose key design aims are not to study QCD, but rather to discover the Higgs boson and search for physics beyond the standard model.

There are essentially two ways of making discoveries at the LHC. On one hand, an experiment may measure some kinematic distribution and see a discrepancy relative to the standard-model expectation. It can only be labelled a discovery if one has sufficient confidence in the standard model prediction, inevitably involving many aspects of QCD, such as parton distribution functions, matrix elements, parton showers, etc.[1] Alternatively, discovery may come through the observation of a distinct kinematic structure, such as an invariant mass peak (or edge, in the presence of unmeasured particles). At first sight, QCD might have less of a role to play here; however, an understanding how QCD works can make it possible to reduce the backgrounds, and sharpen the kinematic structure of signal, allowing it to emerge more convincingly. Furthermore, as and when discoveries are made, QCD will also be crucial in extracting information about the new objects that have been found: their couplings, masses, spins, etc.

In these proceedings we will examine several areas of perturbative QCD that have seen major milestones in the past year or two. The first such area is that of Monte Carlo event generators.

2. Parton-shower event generators (Monte Carlos)

It is almost inconceivable to think of the LHC experiments working without Monte Carlo (MC) programs such as Pythia [1], Herwig [2] and Sherpa [3], which output detailed simulated pp collision events. The immense preparatory effort for the LHC would not have been possible without these tools, be it for the investigation of physics potentialities, or the simulations of detector response; nearly all of the data shown by LHC experiments at ICHEP 2010 (and since) have been accompanied by comparisons to MC simulations, most often in amazingly good agreement; and as the experiments move towards producing results at "particle (hadron) level", i.e. corrected for detector effects, MC simulations will always be central in determining those corrections.

The core of the code base for two of the main MC tools, Pythia (v6) and Herwig, dates to the 1980's (early versions of Sherpa also used portions of Pythia code) and is written in Fortran 77, a language that strains to adapt to the sophistication that these programs have reached today. This prompted an effort across the Monte Carlo community, initiated almost a decade ago, to rewrite the programs in `C++`. Aside from the magnitude of the task of rewriting $60-80,000$ lines of

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[1] This is true even with many "data-driven" methods for estimating backgrounds, since they often rely on QCD-based extrapolations from the region where one has a good measurement of the background to that where one suspects the presence of the signal.

code, many questions of `C++` design needed to be thought through carefully, to ensure that the new code remained maintainable over the lifetime of the LHC. One of the milestones of the past couple of years is that, coinciding with the start of the LHC, the new versions of these programs, Pythia 8.1 [4], Herwig++ 2.4 [5] and Sherpa 1.2 [6], are now available and mature enough for production use, including all core features needed for complete hadron-collider analyses, such as simulation of the multiple interactions.

The work towards the `C++` generators has not simply been a question of rewriting old code in `C++` (for a comprehensive review, see ref. [7]). For example, Pythia has acquired a new p_t ordered shower as its default [8] (the old Fortran virtuality-ordered shower is no longer available in the `C++` version); it also includes numerous developments related to multiple interactions, e.g. [9] and its modularity has already been exploited to allow the inclusion of an alternative shower [10]. Herwig has updated its angular-ordered shower [11], including better treatment of massive particles, and it now incorporates a native multiple interaction model [12]. Sherpa did not have a corresponding Fortran version, however it has seen a number of significant developments in the past couple of years, most notably the switch to a dipole shower, and efficient multi-leg matrix elements (COMIX [13], used together with CKKW [14] matching to the parton shower). Other progress in the generators includes more extended BSM support and inclusion of NLO corrections for a broad variety of processes (as discussed below).

Overall, it is time for this new generation of codes to undergo extensive stress testing by the experiments, the last major step on the way to their becoming the Monte Carlo workhorses for the duration of the LHC.

3. The NLO revolution

While Monte Carlo event generators give fine-grained predictions about QCD final states, it is not always simple to systematically improve their accuracy. The most straightforward systematically improvable calculational approach of QCD at high energies is to use a perturbative approximation, involving a series expansion in the strong coupling α_s, i.e. cross sections are written $\sigma = c_0 + c_1\alpha_s + c_2\alpha_s^2 + \ldots$, so that an improvement in accuracy is obtained "just" by calculating one further coefficient in the series.

At the momentum scales of relevance for LHC, $\alpha_s \simeq 0.1$ and one would expect a leading order (LO) calculation, one that includes just the first non-zero term of the series, to be accurate to within about 10%. Yet widespread experience shows that this is seldom the case, with next-to-leading order (NLO) corrections often modifying cross sections by a NLO/LO "K factor" ratio of two (for example for Higgs production [15, 16, 17] or $Wb\bar{b}$ [18, 19]). In some situations, in which a new channel opens up at NLO, K-factors can be much larger, even $\mathcal{O}(100)$ [20, 21, 22]. These NLO enhancements are potentially important because, for example, in searches for supersymmetry the "signal" of supersymmetry is often just a factor $\mathcal{O}(5)$ excess of the data over the expected background (e.g. [23]), the latter nearly always being calculated at LO. How, then, do we determine whether an excess of data compared to LO is an actual signal or simply a background with an unexpectedly large, K-factor that has yet to be calculated?

Part of the answer is that experiments attempt to constrain the K-factor in regions of phase-space expected to be signal-depleted. However extrapolations to possible signal regions still usually involve LO tools,[2] and the known cases with the largest K-factors usually also lead to strong kinematic dependence of the NLO correction. In such situations, therefore, it would be reassuring to have an actual NLO calculation. The difficulty is that many new physics signals involve quite complex backgrounds. For example, in pair production of gluinos, each gluino might decay to a anti-quark and squark, with each squark decaying to a quark and an (invisible) neutralino, which gives missing energy. One of the backgrounds in this case is then four-jet production in association with a Z-boson that decays to neutrinos, which is too complex a process for there to be any NLO calculations of it yet.

One way to quantify the difficulty of a NLO calculation is in terms of the total number of outgoing "legs" (partons and electroweak bosons all count as legs). The first NLO calculation was for a $2 \to 1$ process, Drell-Yan production, in 1979 [25]. It took almost ten years before any $2 \to 2$ processes got calculated, with several results appearing in the late 1980's and early 90's (e.g. heavy-quark pairs [26, 27, 28], dijet production [29, 30], and vector-boson plus jet [31, 32]). Another ten years passed before a $2 \to 3$ process was calculated, with $Wb\bar{b}$ in 1998 [18] and 3-jet and W+2-jets calculated a couple of years later [33, 34].

Given the motivation from the expected startup of LHC, at this point an almost industrial effort got underway to calculate all $2 \to 3$ processes of interest for LHC and to open the frontier towards $2 \to 4$ processes (bearing in mind that that background we mentioned above was a $2 \to 5$ process), guided by a document known as the Les Houches wishlist [35]. Roughly in line with the rule-of-thumb of a 10-year interval for calculation an extra leg, the first $2 \to 4$ calculations have appeared in the past couple of years: W+3 jets [36, 37], Z+3-jets [38], $t\bar{t}b\bar{b}$ [39, 40], $t\bar{t}$+2-jets [41], $W^{\pm}W^{\pm}$+2-jets [42], $WWb\bar{b}$ [43, 44], with progress also on $b\bar{b}b\bar{b}$ [45] (and a result for $e^+e^- \to$5-jets [46]).

While some of these results were obtained with traditional Feynman diagrammatic methods [39, 43, 45], the remaining ones have taken advantage of major developments in "unitarity-based" methods for calculating one-loop amplitudes (which had been the main bottleneck for new NLO results). Originally pioneered in the mid 1990's [47], the idea behind these methods is to sew tree-level amplitudes together to produce loop amplitudes, equivalent to considering loop momenta such that specific loop propagators are on-shell. This idea was revitalised in 2004 through the use of momenta with two timelike components [48] to broaden the set of tree-level configurations that could be usefully assembled.[3] To go from this result to collider predictions has been a huge undertaking, with many important steps along the way (most have been reviewed in [35]). If one is to highlight a single one of them, it might be the observation that it is possible to deduce the integrated 1-loop diagram simply by inspection of the integrand for specific loop-momentum configurations [49].

These developments represent a revolution in NLO calculations. Not just because of the number of $2 \to 4$ predictions that they have led to — a corresponding effort devoted to Feynman-

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[2] An interesting distinction here is between simple LO, and matched matrix-element plus Monte Carlo samples involving multiplicities that go beyond the strictly LO process [24], which can account for the appearance of new higher-order channels and reproduce some NLO K-factors.

[3] Specifically, with two timelike components (or, in subsequent work, with complex Minkowski momenta), it is possible to have a sensible 3-particle vertex with all momenta on shell and use this as an ingredient in building up the loop amplitude.

diagrammatic calculations would probably have led to a similar number of results — but more importantly because of the prospects that they offer for “low-cost” automation of NLO calculations and the extension beyond 2 → 4 processes. Indeed, just around the time of ICHEP, the first NLO results for a 2 → 5 process were announced, the unitarity-based (leading colour) calculation of W+4-jets [50], nearly ten years ahead of expectations from the timeline discussed above.

One caveat to be mentioned in the context of these impressive results is that so far most of the 2 → 4 or 2 → 5 NLO calculations are not yet available as public codes (with the exception of [51]). This is perhaps a consequence of the significant complexity of the codes, which often bring together many different tools[4] and then require enormous computing time if one is to obtain a numerically stable result. Nevertheless, it is only once they are public, in a form that is relatively straightforward to use, that these calculations will be able to deliver their full value.

3.1 NLO and Monte Carlo event generators

While NLO calculations have the benefit of quantifiable accuracy (at least in regions of phase-space that don’t probe disparate momentum scales), they only ever involve a handful of partons, a far cry from the level of detail of MC parton-shower event generators, which predict distributions at the level of hadrons.

Two main techniques have been developed over the past decade to combine NLO accuracy with parton shower “detail”, the MC@NLO [56] and POWHEG [57] methods. Generally speaking, only relatively simple processes are available: at the time of ICHEP, not even Z+jet or dijet production had been publicly implemented. That is gradually changing thanks to progress on the systematisation and automation of both the MC@NLO [58] and POWHEG [59, 60] methods. In the POWHEG case this helped the implementation of Z+jet [61], dijet [62] and $t\bar{t}$+jet [63] and even the 2 → 4 process $W^{\pm}W^{\pm}$+2-jets [51], while in MC@NLO it has been of benefit for example in extending the range of processes available with Herwig to work also with Herwig++ [58].

A point to be aware of is that while NLO MC implementations of, say, Z production necessarily include a correct LO (tree-level) Z+jet matrix element, they had not generally been matched with higher-order tree-level matrix elements, e.g. Z+2-jet, etc. In contrast, it has for some time now been standard procedure to combine LO tree-level Z, Z+jet, Z+2-jet, etc. matrix elements together (CKKW and MLM methods [14, 64]). Therefore users have been forced to choose between, on one hand NLO accuracy for simple processes but with a poor description of multi-jet events, and on the other hand low, LO, accuracy but simultaneously for many different multiplicities. Ultimately one would hope to have a method that provides NLO accuracy simultaneously for a range of different multiplicities (for example, as implemented for e^+e^- in [65], or for hadron-collider processes without showering in [22]). However, in the meantime, an interesting development [66, 67] is the merging of POWHEG and CKKW/MLM type methods to provide NLO accuracy for the lowest multiplicity process with LO accuracy for multijet processes.

Overall, even if it is still early days, it is clear that automation of loop calculations, automation of methods to combine NLO and parton showers and the development of methods to merge

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[4] For example, on one hand the 1-loop corrections, on the other hand tools for handling real radiation such as [52, 53, 54, 55].

different multiplicities of NLO-improved parton showers, taken together would have the potential to radically improve the quality of MC predictions.

4. NNLO

For the foreseeable future the ultimate perturbative accuracy that one can hope to achieve is NNLO, i.e. corrections up to $\mathcal{O}\left(\alpha_s^2\right)$ relative to the dominant process. There are two broad reasons for being interested in NNLO corrections. One may, for example, wish to extract precision information about standard-model couplings (as for the Higgs boson) or parton-distribution functions from measured cross-sections. Alternatively one may be faced with quantities where NLO corrections are large, and NNLO is then the first order at which one can hope to make quantitatively reliable predictions.

NNLO hadron-collider results have been available for some time now for Higgs and vector-boson production (state-of-the-art codes are described in [68, 69, 70, 71]), and the current frontier is NNLO accuracy for processes with coloured final-state particles, be they heavy (top) or light (jets).

One significant recent result is the calculation of the NNLO cross section for Higgs production in vector-boson fusion [72], making use of the "structure function" approach [73] in which one views each proton's emission of a vector-boson as a DIS type reaction, and then separately considers the fusion of the two vector bosons. This provides a NNLO result that is inclusive over the hadronic jets, but still exclusive with respect to the vector-boson momenta. Numerically it indicates perturbative stability relative to the NLO prediction, with a reduction of scale uncertainties from the $5-10\%$ range at NLO, down to $2-3\%$.

The most likely candidate for the next process to be calculated at NNLO is $t\bar{t}$ production. Among the physics motivations, one can mention the importance of the forward-backward asymmetry: given that it is non-zero starting only at NLO, only from NNLO will there be some quantifiable control of the theoretical uncertainties on its prediction. Also of interest is the potential for an extraction of the top-quark mass by comparing the predicted cross-section (with its relatively strong-mass dependence) to the actual measured cross section.[5]

As things stood a few years ago, the ingredients that were still missing for a NNLO calculation of $t\bar{t}$ production were the following: the two-loop diagrams for $q\bar{q} \to t\bar{t}$ and $gg \to t\bar{t}$; the squared one-loop terms for $t\bar{t}$ production in association with an extra parton; and a way of performing the phase-space integration for (tree-level) $t\bar{t}$+2-parton production while keeping track of the divergences, which need to cancel with those from the 1- and 2-loop terms.

Progress (reviewed in [75]) started with the calculation of the high-energy limit of the two-loop $q\bar{q}$ and $gg \to t\bar{t}$ diagrams [76]. This was followed by a numerical evaluation of the full 2-loop $q\bar{q} \to t\bar{t}$ amplitude [77] (a corresponding approach to $gg \to t\bar{t}$ seems close to completion [78]) and by various analytical results for parts of the two amplitudes [79, 80]. The squared one-loop terms were determined in [81]. Finally, the problem of integrating the (divergent) phase-space for

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[5] It seems this method was originally proposed during an extensive discussion at Moriond QCD 2008. It has since been analysed in detail for example in [74].

production of $t\bar{t}$+2-partons has been solved in [82]. Thus there is hope that in the reasonably near future, first full NNLO results for top production will become available.[6]

The next frontier for NNLO calculation will probably be that of processes with one or more light jets in both the initial and final states, e.g. vector-boson plus jet or dijet production.[7] The case with final-state jets only, specifically $e^+e^- \to$3-jets, has been solved in [88, 89]. A compilation of extractions of α_s based on the comparison of these NNLO results (supplemented with resummations and non-perturbative corrections) to event-shape data has been given in [90]. Interestingly, there is a noticeable spread in the results, highlighting the fact that at levels of precision of a few percent, hadronic final-state observables are subject to many different effects that can contribute at the same few-percent level as $\mathcal{O}\left(\alpha_s^2\right)$ corrections. Still, NNLO corrections are a class that can be controlled, helping provide a far more constrained discussion of the overall precision of QCD predictions. It is therefore highly valuable that work progresses on general NNLO methods and their extension to processes with initial-state coloured particles (see [91, 92, 93, 94] and references therein).

5. Jets

The majority of measurements that involve hadronic energy-flow at the LHC will make use of jets. Jets are measured with the help of a jet algorithm, which takes the hundreds of particles measured in an experiment and combines them into a handful of jets. The same procedure can be applied to theoretical parton-level calculations, with the idea that the jets obtained from parton-level and experiment can be directly compared.

A problem that had plagued hadron-collider jet measurements for nearly 20 years was that the vast majority used jet algorithms that were not infrared and collinear (IRC) safe (despite widespread discussion of the problem, e.g. [95, 96]). IRC safety is the property that the final hard jets should be insensitive to the additional low-energy emissions and small-angle branchings that occur with high probability in QCD. Without this property, the higher-order calculations discussed above often lead to divergent answers, compromising the huge investment that has been made in them over the past decade.

It was therefore a welcome development to see that all of the jet measurements presented by ATLAS and CMS at ICHEP 2010 (and the subsequent publications, e.g. [97, 98]) have used an infrared and collinear safe jet algorithm, anti-k_t [99] (which has also been used by the H1 and ZEUS collaborations [100, 101]). The anti-k_t algorithm repeatedly recombines the pair of particles i and j that has the smallest $d_{ij} = \min(p_{ti}^{-2}, p_{tj}^{-2})\Delta R_{ij}^2/R^2$ unless a $d_{iB} = p_{ti}^{-2}$ is smaller, in which case i is labelled a jet (ΔR_{ij} is the rapidity-azimuth separation of i and j and the parameter R sets the minimum interjet distance). Closely related to the much earlier k_t algorithm [102, 103], it uses a different weighting of momentum and angle to grow jets outwards from a central core, giving

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[6] In the meantime there has been significant work towards estimating the NNLO (and yet higher-order) corrections using threshold-resummation techniques [83, 84, 85, 86, 87]. While it is beyond the scope of these proceedings to discuss the detailed differences between them, it is probably fair to say that they do not yet provide a consensus as to the likely impact of the full NNLO corrections.

[7] Techniques that merge NLO calculations for different jet multiplicities [22] can, meanwhile, provide a good approximation to NNLO for those observables in such processes that are subject to giant K-factors.

"cone-like" jets[8] while remaining IRC safe. These properties, together with earlier developments that ensure good computational efficiency in the presence of high particle multiplicities [105], help make it particularly suitable from both the experimental and theoretical points of view.

Jet finding is not simply about comparing theory and experiment, but also about organising the huge amount of information in an event so as to best pull out signals of particles such as the Higgs boson and extensions of the standard model. One kinematic regime of particular interest turns out to be that where particles with electroweak-scale masses are produced with transverse momenta somewhat (or far) above the electroweak scale. There had been a handful of early investigations of this regime [106, 107], and in recent years it has become clear to what extent the hierarchy of scales present at LHC ($\sqrt{s} \gg M_{\text{EW}}$) can usefully be exploited with suitably targeted jet methods. Examples include: the search for new TeV-scale particles that decay to electroweak bosons (W, Z, H) or top-quarks, which then go on to decay hadronically (e.g. [108, 109, 110]; more standard jet methods were used for example in [111]); the observation that in searching for hadronic decays of the Higgs-boson (in association e.g. with a W/Z [112] or a $t\bar{t}$ pair [113]) it may be advantageous to concentrate on the subset of events in which the Higgs boson has $p_t \gg M_H$, or indeed that the Higgs might be discoverable first in SUSY cascade decays [114]; and the proposal that hadronically-decaying new particles (e.g. neutralinos and gluinos in R-parity violating supersymmetry [115, 116] or new scalars that appear in buried Higgs scenarios [117]) may have sufficiently distinct jet-substructure signals to be picked out sometimes even in purely hadronic events.[9] It is beyond the scope of these proceedings to discuss in detail the many different jet techniques that have been developed for these purposes (among those not already cited above, also [119, 120, 121, 122, 123, 124, 125, 126, 125, 126, 127]), and the reader is referred instead to recent reviews [128, 129].

6. Conclusions

Several major long-term LHC-QCD related projects are now approaching maturity. Among them we looked at the `C++` event generators Herwig++, Pythia 8 and Sherpa which are all now ready for mainstream use, and are also evolving in their physics content, be it in terms of non-perturbative ingredients such as the underlying event or more widespread matching with NLO calculations through automation of the MC@NLO and POWHEG methods.[10]

We also looked at some breakthroughs of the past couple of years. NLO calculations, with the first $2 \to 5$ result published almost 10 years ahead of "schedule" (i.e. extrapolations of past progress) undoubtedly belong to this category. It is probably also fair to say that jet finding has undergone a breakthrough, on two fronts:[11] on one hand, the LHC is the first hadron collider to

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[8] Jets that are nearly always circular in the rapidity–azimuth plane; this relates to the algorithm producing jets whose momentum depends linearly on the distribution of soft particles in the jet and its vicinity [104], a property that helps make it easier to account for detector effects.

[9] There is even a tantalising claim of a hint of an excess in such a channel at the Tevatron [118].

[10] Though space limitations prevented us from discussing parton distribution functions, it is worth mentioning that the NNPDF project [130] has likewise reached maturity in the past year, joining CTEQ and MSTW as a global PDF fit, involving a quite complementary approach to the estimation of uncertainties. The discussion around PDFs remains very vibrant (even controversial, especially in the context of Higgs exclusion limits [131]) and for other recent progress and comparisons between results, the reader is referred to [132, 133, 134, 135, 136, 137].

[11] Though the author is perhaps too close to the subject to provide an unbiased view.

systematically use infrared and collinear safe jet finding, more than 30 years after the original proposal for jet-finding by Sterman and Weinberg [138]; on the other, it has become clear that flexibility with jet-finding methods has the potential to help discover Higgs-boson decay channels and new physics scenarios that had previously been thought beyond the scope of the LHC.

One of the other areas of extensive ongoing work in QCD is the quest for high accuracy, where we discussed the progress in NNLO calculations (space constraints prevented a discussion of resummations). The most imminent development will probably be the NNLO calculation of $t\bar{t}$ production, with an impact not just on predictions of the cross section, but also, possibly, on the highly topical question of the $t\bar{t}$ asymmetry.

At what point might we say that QCD is ready for the LHC? There has been enormous progress in the past 5 to 10 years and the goals that were set at the turn of the century have generally been met (with one or two good surprises along the way). Still, in many ways, the use of QCD at colliders remains a somewhat delicate craft, one that relies on a combination of technical skill, physical insight and extensive experience. This is true whether one aims for the reliable prediction of complex backgrounds, the high-precision extraction of fundamental parameters from data or the design of analyses that make the most of QCD to help distinguish signal from background. We can but look forward to breakthroughs of the coming years that will make it more straightforward to use QCD on the path to discovery.

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