Monte Carlo for the LHC

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I review the status of the general-purpose Monte Carlo event generators for the LHC, with emphasis on areas of recent physics developments. There has been great progress, especially in multi-jet simulation, but I mention some question marks that have recently arisen.

1 Introduction

There are three general-purpose Monte Carlo event generators designed for use at the LHC, Pythia [1], Herwig++ [2] and Sherpa [3]. The first two are built on the heritage of their fortran predecessors [4,5] while Sherpa has been constructed as a new C++ project from the beginning. Although there are of course many differences in the details of the implementations, they largely share a common approach to the structure of LHC events, which I describe briefly here to set the scene and the notation.

Most of the emphasis is on the simulation of events that contain a *hard process*, although I will return to mention minimum bias collisions later. Since the hard interaction is generally the process of interest it acts as the trigger around which the simulation of the whole event is built. In the previous generation of simulation these were almost always $2 \to 2$ processes, but one of the largest areas of development in recent years, which I will describe in detail below, has been the inclusion of higher order corrections, both in terms of multi-parton tree-level processes and also NLO corrections to the low parton multiplicity processes.

The partons involved in the hard process are coloured and, just as accelerated charges in QED radiate photons, annihilated, scattered or produced coloured partons radiate gluons. Now, however, unlike in QED, since the gluons themselves are coloured, they radiate further gluons. The hard process is therefore accompanied by an extended shower of additional radiation, which is simulated with a *parton shower* algorithm. These are formulated as a probabilistic evolution in emission scale, from the high scale of the hard interaction downwards to lower momentum scales. The outgoing partons are evolved forwards to produce a shower of accompanying radiation and the incoming partons are evolved backwards to ask, progressively, what is the probability distribution for radiation to accompany this parton on its way in to the hard interaction. Different algorithms differ in their choice of evolution variable and can generally be split into two classes: parton-based, as a sequence of $1 \to 2$ splittings with suitably-defined (respecting the coherence of radiation from different emitters) evolution variable and initial condition; and dipole-based, in which colour-connected pairs of partons emit radiation as a $2 \to 3$ splitting, with the colour structure taking care of the coherence condition.

As the parton shower is governed by perturbative emission probabilities with the strong

coupling evaluated at the evolution scale, it is not valid at scales below about 1 GeV. One therefore terminates the evolution and invokes a non-perturbative *hadronization model* for the transition from a partonic to a hadronic final state. Here again the partonic colour structure is crucial in setting the initial conditions for the hadronization and only models that respect this structure, the string (Pythia) and cluster (Herwig and Sherpa) models, are in current use.

In a hadronic collision, a partonic constituent from each hadron is involved in the hard process and its accompanying parton shower. The colliding hadrons are highly Lorentz-contracted discs and in a space-time picture completely overlap each other. They therefore have a high probability to have additional interactions, producing hadrons throughout the event, in addition to those from the hadronization of the hard process. This is known as the *underlying event* and is modelled as additional independent parton–parton interactions (multi-parton scattering models), as a soft non-perturbative interaction of the remnants as a whole (soft underlying event models), or as a mixture of the two. In fact, it is essential to include a semi-hard multi-parton interaction component to fit the HERA and Tevatron data. Recent progress in underlying event physics has focussed on the colour structure of the additional interactions and the colour connections between them and the primary process and therefore simulation of the underlying event is typically interleaved with the backward evolution of the incoming partons.

Finally, many of the hadrons produced in the hadronization of the hard and secondary processes are unstable resonances and their decays must be simulated, together with other decaying particles such as the tau lepton (decays of short-lived particles like the top, Higgs boson or SUSY particles can be thought of as part of the hard process and are typically simulated early in the event). This relatively unglamorous end of event generation has also been the subject of considerable recent progress.

Simulation of minimum bias and diffractive collisions in which there is no hard process is closely related to the underlying event and one typically uses phenomenological models to describe the total rate and its sub-division into elastic, single- and double-diffractive and inelastic components, with the multi-jet models tuned to underlying event data used to simulate the inelastic component.

In this talk I will give an outline of some of the most important areas of recent physics progress. In particular I will describe several developments in the important area of matching parton showers with higher order matrix elements, as well as a couple of question marks that have recently arisen within this area. I will describe more briefly developments in the simulation of spin correlations, of soft interactions and of secondary decays. Finally I will give brief status reports of the three general-purpose event generator projects and of the MCnet projects for generator-independent generator validation and tuning.

2   Recent physics progress

2.1   Merging parton showers with higher order matrix elements

Parton showers are built on approximations to the full QCD matrix elements for multi-parton emission, expanded around the soft and collinear limits that dominate. They therefore perform well for the bulk of emission. The colour coherence of emission between different partons in an event is crucial for this, as shown in the famous CDF Run 1 study, [6]. Three-jet events were selected with hard two-jet kinematics, with the hardest jet being above 110 GeV and a soft third jet only having to be above 10 GeV. The distributions of this third jet therefore clearly

map out the radiation of the hard $2 \to 2$ scattering system. In particular, CDF's careful study showed that coherence due to the colour connections between initial- and final-state partons was crucial to get these distributions right. HERWIG, which had this coherence built in, and a version of Pythia specially modified to include it (which subsequently became the default) were able to fit the data, while the default version of Pythia, which included colour coherence only in final-state emission, and ISAJET, which doesn't include it at all, were not even able to qualitatively describe the data. Despite the fact that this analysis is uncorrected and more than fifteen years old, it is still an extremely important one for Monte Carlo understanding and validation and we would dearly like to have an update from Run 2 as well of course as looking forward to similar analyses at the LHC.

Despite the success of modern parton shower algorithms in describing the bulk of emissions, there are many event generator applications in which multiple hard well-separated jets must be simulated well. The most obvious of these is in searches for new physics where one is often interested in final states with many jets and where, by definition, one designs the cuts to remove the bulk of emission so that all that remains is the hard well-separated tail. These regions are equally important for the top mass measurement, QCD studies of the multi-jet regime and many other applications. The rate and distribution of such jets are reasonably well described by the tree-level matrix element for the given jet multiplicity, but parton showers are needed to describe the internal structure of the jets and the full hadronic final state. Moreover it is not straightforward to merge samples with different jet multiplicities without double-counting with subsequent emission in the shower. Clearly one wishes to combine the benefits of the tree-level matrix element and parton shower approaches, and methods to do this are known as multi-jet matching.

At the same time, there are also applications where one wishes to have an event sample with next-to-leading order normalization, not least, again, for new particle searches, but also for many electroweak and top quark analyses. Attempts to match parton showers with NLO calculations are known as NLO matching.

Great progress has been made with both multi-jet and NLO matching over the last five years, as I describe in the next two sections, and practical implementations are now available for a wide variety of processes. Most recently, progress has been made in attempts to combine the two approaches together, as I will also describe more briefly.

2.1.1 Multi-jet matching

The problem of merging tree-level matrix element samples with parton showers for several jet multiplicities simultaneously was solved in principle by Catani, Krauss, Kühn and Webber (CKKW) in 2001 [7]. They introduced a matching scale, $k_{T,match}$ and showed that by using matrix elements modified by introducing Sudakov form factors above $k_{T,match}$ and parton showers modified by introducing appropriate phase space vetoes below $k_{T,match}$, one could match the two in such a way that there was no double-counting and the dependence on $k_{T,match}$ could be proved to vanish to next-to-leading logarithmic accuracy.

However, in practical implementations, for example in the study by Mrenna and Richardson [8], it was found that associated distributions typically have discontinuities at $k_{T,match}$ and that the hadron-level results were more $k_{T,match}$-dependent than the parton-level ones. Eventually this was explained as being due to the CKKW method giving the right amount of radiation, as proved, but putting some of it in the wrong place. In particular, attributing some of it to the wrong colour flow, affecting the initial conditions of the hadronization phase.

This problem was solved by Lönnblad [9] for the specific case of k_T-ordered dipole showers and more recently for the general parton shower case by the Sherpa [10] and Herwig++ [11] collaborations following an idea originally proposed by Nason [12] as part of the POWHEG approach described below. The idea is that one should run the parton shower from the lowest multiplicity configuration and to forcibly insert emissions corresponding to the exact kinematics generated by the matrix element event into the appropriate point in the ordering of the shower. The effect is to generate *truncated showers* from the internal lines of the matrix element event, as well as the external lines, and to properly populate the whole of phase space with soft radiation with the correct colour connections.

Results of this modified CKKW method have been compared with data from the Tevatron, for example the CDF W+jets [13] and Z+jets [14] data, in [10,11]. Rates and distributions of events with up to four jets are well described and the residual matching scale dependence is shown to be very small, with a corresponding uncertainty in the total cross section of only 3%.

2.1.2 NLO matching

In a conventional Monte Carlo implementation of a next-to-leading order calculation, events in the real emission phase space have arbitrarily large positive weights, which are cancelled to give a finite cross section contribution by counter-events that have equally large negative weights but live in the phase space of the Born process. The result is finite for any infrared safe observable, but the procedure is not suitable for implementation into a parton shower, hadronization and detector simulation framework, since any arbitrarily small differences in the subsequent final state of the event and counter-event would spoil the cancellation.

Frixione and Webber showed in 2002 [15] that this problem could be solved to give Monte Carlo events with finite weight distribution, essentially by using an analytical expansion of the parton shower emission probability as the subtraction counter-event term. The result is a set of hard + either 1-jet or 0-jet events to be showered, such that there is no double-counting between the showered 0-jet and generated 1-jet events. Although the weight distributions are finite, they are not positive definite and one typically generates 'almost unweighted' events, i.e. with equal absolute values of weights, but typically around 10% of them negative. This is not a problem of principle, but can be inconvenient for some applications. A more serious problem is the fact that the analytical subtractions have to be calculated for the particular parton shower with which it will be used and, thus far, this MC@NLO method is available for a wide range of processes [16] only for use with the original HERWIG program. With a first implementation for PYTHIA reported in Ref. [17], a full version for both PYTHIA and Herwig++ is expected to appear soon.

However, a potentially more serious problem with the MC@NLO approach was noticed in Ref. [18] and explored in more detail in Ref. [19]. It is that MC@NLO distributions can inherit deficiencies in the underlying shower algorithm. This is most evident in the jet rapidity distributions in which the PYTHIA and especially HERWIG algorithms produce insufficient hard central jets. Although the MC@NLO algorithm corrects this distribution analytically to leading order, all higher orders are directly inherited from the shower. The result, especially in gluon-initiated processes such as $gg \rightarrow H$, can be rapidity distributions with significant unphysical 'notches' in them, see for example Fig. 9 of [19].

A second issue with the MC@NLO approach is that it is guaranteed to exactly reproduce the LO "+1-jet" cross section at high enough transverse momentum. This may sound like a good feature, but it turns out that processes for which the K factor is significant, so for which

one definitely wants to use a NLO matching approach, the K factor for the "+1-jet" process is also large, so that the MC@NLO result is significantly below the NLO result for the high-p_t distribution. The most extreme case is again $gg \rightarrow H$ where the difference is around a factor of two.

While in both of these cases, MC@NLO is formally correct to the order at which it is defined (NLO for the normalization and LO for the p_t distribution), phenomenologically one might prefer a solution that does not suffer from these effects. This is provided by the POWHEG method proposed by Nason [12] in 2004. It has the advantages that it provides only positive-weight events, that the distribution of hardest emission is entirely determined by the hard matrix element, without inheriting features from the parton shower, and that the entire distribution receives the K factor so, to the extent that the K factors of the inclusive and high-p_t processes are similar, the latter is well described. Finally it is independent of shower algorithm and can be used with any parton shower algorithm that is capable of producing the truncated showers discussed earlier.

The POWHEG method is implemented as a standalone program, also called POWHEG, for an increasingly wide range of processes [19–25]. It has also become the method of choice for NLO matching in the Herwig++ program, which also now comes with built-in POWHEG implementations for Drell-Yan production [26], Higgs production [27] and e^+e^- processes [28], with vector boson fusion, deep inelastic scattering and vector boson pair production including anomalous triple gauge couplings in progress. The deep inelastic scattering implementation in particular allows Herwig++ to describe the energy flow data from the HERA experiments over a wide range of x and Q^2 for the first time.

2.1.3 Towards NLO multi-jet matching

Given the success of multi-jet and NLO matching schemes, it is natural to ask whether they can be combined to produce a multi-jet sample in which each of the jet multiplicities is correct to NLO. Ideas towards this ambitious goal have been described in Ref. [29]. In Ref. [30] the first concrete implementation appeared, only for the case of e^+e^- annihilation. The extension to hadron collisions is considerably more complicated and is yet to appear as a working implementation.

Hamilton and Nason [31] took a more pragmatic approach. Motivated by the large body of validated multi-jet and NLO matching implementations in use, they examined whether it is possible to combine the POWHEG and CKKW approaches to provide a sample of multi-jet events, each calculated using the tree-level multi-parton matrix element combined with the full NLO correction for the Born configuration onto which it is mapped. They succeeded in this and studied implementations for vector boson and top pair production in hadron collisions.

With the progress made in these approaches it seems hopeful that a working NLO multi-jet matching algorithm could be achieved in the near future. It is clear that this would be a major step forward in our ability to simulate LHC final states.

2.1.4 High energy jets

I previously said that parton shower algorithms do well for the bulk of emission, but with the large step up in energy to the LHC, and the consequent opening up of phase space, we should constantly question this statement and check that we are sure. In this and the next section I mention two recent calculations that raise small question marks over our readiness.

Andersen and collaborators [32,33] have developed a new approach to calculating multi-jet final states, which they call the high energy jet (HEJ) approach. It relies on approximating the all-order QCD matrix elements in a different limit to parton showers, namely the limit of fixed momentum transfer with available scattering energy going to infinity, the limit in which many jets have similar transverse momenta and large rapidity intervals. They show that in this limit, scattering amplitudes factorize into helicity-dependent local terms, coupled by t-channel propagators, which can be constructed in a modular way to arbitrary order. They have working implementations for pure jet processes, W/Z plus jets and Higgs plus jets and have made a thorough phenomenological analysis. As an example, see Fig. 69 of Ref. [34] in which the results are compared with the Sherpa shower with CKKW matching and the NLO calculation in MCFM, for the accompanying jet multiplicity of Higgs plus at least two jet events as a function of the rapidity separation between the two leading jets. For small separations all three calculations agree, but by $\Delta y = 4$, a typical cut used to separate this gluon fusion process from the vector boson fusion process, the HEJ approach is significantly above the other two, predicting an average number of additional jets of order 1. By $\Delta y = 6$, still within the typical region of a VBF analysis, HEJ predicts twice as many additional jets as either CKKW or NLO.

The HEJ code exists as a working Monte Carlo and work is in progress to match it properly with parton showers. It will be extremely interesting to see it further used to validate the existing parton shower and matching algorithms and to see whether it can be developed to become a fully-fledged alternative to multi-jet matching (here one could mention that it is much faster than calculating the full multi-jet matrix elements for high jet multiplicities).

2.1.5   Giant K factors

It has been known for some time that certain observables suffer from anomalously large K factors. In a recent study [36], Rubin, Salam and Sapeta considered this in more detail, isolated the origin of these giant K factors and showed how to calculate the next higher order in such cases to stabilize the perturbative series. In this section I consider the connection with parton shower algorithms.

The archetypal process in which they study this is Z+jets at high p_t (see Fig. 1 of Ref. [36]). In the Z p_t spectrum the K factor is roughly constant at about 1.5 and just about consistent with the scale variation: the LO and NLO bands just touch. However, turning to the p_t distribution of the leading jet, which is equivalent at leading order, they found a K factor that grows linearly with p_t from about 2 at 250 GeV to more than 5 at 1 TeV and that is in no way represented by the scale variation. Finally, they considered an observable that is important for search physics, the total scalar transverse momentum of all jets that accompany the Z, H_T, again equivalent at leading order. They found that the K factor grows exponentially with H_T, from about 10 at 500 GeV to 1000 at 2.5 TeV.

They argued that the large K factor in the leading jet p_t distribution is due to a new kinematic regime opening up, namely the possibility that two hard jets could be produced, accompanied by a relatively soft Z boson. It has long been known that electroweak corrections to high p_t jet production are large and negative owing to an electroweak Sudakov form factor with leading order term $\sim -\alpha_W \log^2 p_t/M_z$. Its counterpart is a real correction to dijet production $\sim +\alpha_W \log^2 p_t/M_z$ due to the emission of a Z boson. This can equivalently be seen, in our case, as a real correction $\sim +\alpha_s \log^2 p_t/M_z$ to the Z+jet process. One can easily check that this dependence is roughly linear over the p_t range considered and of the same order of magnitude as the NLO correction actually seen. Finally, this understanding also allows an understanding

of the huge K factor seen in the H_T distribution: the events with two high-p_t jets and a low-p_t Z, which occur at about the same rate as Z+one-jet events with the same jet p_t, contribute to a value of H_T a factor of two higher than p_t. Since the underlying LO p_t distribution is falling so rapidly, this factor of 2 increase in the value of the observable corresponds to a huge, exponential, increase in the value of the cross section at a given value of the observable.

In Ref. [36] an ingenious method was proposed to calculate higher order corrections to such processes. The main point is that a unitarity-type argument is used to estimate uncalculated loop corrections from calculated tree-level corrections at the same order. This process has similarities with the CKKW idea and I believe this connection could be explored further, but here I confine myself to drawing conclusions for Monte Carlo event generators.

The phase space region responsible for these large corrections corresponds to $2 \to 2$ QCD scattering events in which a Z boson is radiated from an incoming or outgoing quark or anti-quark. Such W and Z parton shower radiation is not implemented in any of the general-purpose generators, despite having been identified as important in Ref. [37]. Although this effect should be reproduced by the CKKW method, for a smooth matching, for systematic studies and for processes in which one does not have a CKKW implementation, one should include as much of the relevant physics in the shower as possible. It is clear that as we enter the LHC era the need to include electroweak boson radiation is more urgent.

2.2 Spin correlations

Spin correlations play an extremely important role in many event generator applications. For example in some searches for BSM physics one is interested in cascade decays in which the angular distributions are crucial for determining the spins of the decaying particles [38]. Sherpa [3] and Herwig++ [2] both have spin correlations built in in a flexible way. The classic example, on which both have been extensively validated, is in tau physics. For example in Higgs decays to $\tau^+\tau^-$ with both taus decaying to a single pion, one can determine whether the Higgs is a scalar or a pseudoscalar from the azimuthal correlation between the two decay planes. Both programs have been shown to reproduce the analytical result [39] well.

2.3 Underlying events/minimum bias/diffraction

These have been a traditional strength of Pythia, with highly developed multi-parton interaction and soft diffraction models. A recent development has been the inclusion of a hard diffractive component [40] into Pythia 8 along similar lines to the older standalone program Pompyt.

Herwig++ and Sherpa are also catching up in this area, with Herwig++ having a multi-parton interaction model developed from the Jimmy program, but with the addition of soft parton–parton scattering allowing simulation of minimum bias collisions for the first time [41–43]. A forthcoming version, with the further addition of colour correlation effects between the scatters, appears to be able to describe the ATLAS data [44], with detailed tuning currently in progress. Sherpa also has a new minimum bias model [3] which looks promising.

2.4 Secondary decays

Both Herwig++ [2, 45] and Sherpa [3] have implemented extensive secondary decay models, with detailed matrix elements for a wide variety of final states and interference with many intermediate resonances, and spin correlations between decays. Moreover, both include QED

corrections in the YFS scheme [46, 47]. The aim is to have at least as good a description as EVTGEN, TAUOLA and PHOTOS in all cases and thereby dispense with the need for such external packages and their results have been extensively validated against these programs.

3   Status reports

I finish my talk with very brief status reports of the main event generator projects. More detailed and up-to-date information can always be obtained from the web sites listed below.

3.1   Pythia

The fortran Pythia 6 program, which has been the workhorse of particle physics for some 25 years is still supported but is not being actively developed. All new physics developments go into the Pythia 8 program. Its core is ready and tuned, with a much more flexible structure to allow for the extensive physics model development that is now ongoing. Some features of Pythia 6 are definitely dropped, for example the old virtuality-ordered showers, and many new features added, for example hard scattering in diffraction, a significantly improved underlying event treatment and wide range of new BSMs.
http://projects.hepforge.org/pythia

3.2   Herwig

The current version of the fortran HERWIG program has been effectively frozen for three years, but a bug fix release will appear this summer. All development is now transferred to Herwig++, which has many physics improvements, including improved angular-ordered parton showers, with facilities built in to match with multi-jet or POWHEG hard processes, a slightly improved implementation of the cluster hadronization model, the improvements to soft modelling that allow minimum bias to be simulated for the first time and a very flexible framework for implementing new physics models. One advantage over HERWIG is the fact that each version is released with a globally-fitted parameter set. A new version release is expected this summer and should fully replace HERWIG.
http://projects.hepforge.org/herwig

3.3   Sherpa

Unlike the previous two generators, Sherpa was designed as a new generator in C++ from the start. In order to get started it had interfaces to external packages for some components, but by now it is a fully-fledged standalone generator. The emphasis is on multi-jet final states, with two different automated high-multiplicity matrix element generators, an automated subtraction algorithm for NLO calculations, a k_t-ordered dipole shower and built-in CKKW matching. It also has a multi-parton interaction model and a new cluster hadronization model.
http://projects.hepforge.org/sherpa

3.4   Tuning and validation

Within MCnet there are two other important Monte Carlo projects, Rivet [48], a generator- and experiment-independent framework for validation of generators against experiment, and

Professor [49], a generator-independent semi-automated parameter tuning tool. With Rivet, the Tevatron experiments are starting to develop a culture, which was prevalent with its predecessor HZTOOL with the HERA experiments, that all important analyses get immediately implemented to ensure that the full details of the analysis get preserved for posterity and the data can be compared to theory calculations and models on an exactly like-for-like basis for years to come. It is essential that this culture continue at the LHC, to ensure that its data gets fully preserved and exploited. As well as its important function in tuning event generator parameters, Professor provides a set of tools for visualizing the data and seeing in real time how it responds to particular combinations of parameter settings.

Both of these tools are being incorporated into the LHC experiments' software frameworks, to ensure that models tuned to the new data continue to describe the existing data, the first time any experiments have done this in such detail.

http://projects.hepforge.org/rivet
http://projects.hepforge.org/professor

4 Summary

Modern Monte Carlo event generators are highly sophisticated implementations of QCD calculations. They are reliable for a wide variety of observables over a wide range of energy scales and the model-dependent parts widely validated. But the LHC is a truly huge step into the unknown, requiring extensive tuning of soft models and validation of hard evolution. There has been a great deal of progress in describing hard emission more accurately, but, as I have shown, a few small areas where more work is needed.

Acknowledgments

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