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Round Table Discussion:
Event generation – are we ready for LHC?

Working group "Methodology of Computations in Theoretical Physics"

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The working group "Methodology of Computations in Theoretical Physics" concluded their parallel meetings with a round table discussion on various topics concerning the status and prospects of Monte-Carlo event generators for LHC. This note gathers together the main points and contributions of this discussion.

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1. Introduction

At the end of the parallel sessions our working group held a round table discussion to discuss the status and prospects of Monte Carlo event generators for the LHC. In general the situation of matrix element (ME) generators in different approximations (LO,NLO,NNLO) and their combination with parton showers, hadronisation and underlying event (UE) models was discussed.

More precisely the following items where addressed during the discussion.

- Event generation with LO Monte-Carlo tools:
  - status of event generators
  - open issues like e.g. underlying event, validation, role of ME generators, pdfs.
  - further developments and updates of public tools like `CompHep`, `GRACE`, etc.
- The way to NLO tools
  - approaches for one-loop amplitudes: Feynman diagrams, unitarity, numerical
  - status/outlook of NLO automation tools
  - modularity, standardisation, public availability
  - performance of NLO amplitude evaluation accuracy/speed
- Where do we need NNLO?

The following contributions provided by several authors cover a large number of aspects being lively discussed during the meeting and the round table discussion. The main points of the discussion are collected below in the conclusion.

2. Comparing, validating and tuning Monte Carlo simulations *by Andy Buckley*

In the long run-up to LHC operation, a multitude of specialist experiment studies have compared different event generator predictions for signal channels and their main backgrounds. However, the obvious next steps — extending such studies to expose the wider similarities and differences between predictions of different generators/tunes, and to include analyses which can be compared to data from previous collider experiments — have not been coherently pursued. As almost all LHC physics analyses have relied heavily on MC simulation in their development, known deficiencies in the description of QCD backgrounds are an issue for the robustness of these analyses. Fortunately, this situation is rapidly improving.

Interest in systematic MC tuning and validation has resulted in the development of the tools `Rivet` and `Professor`, principally under the auspices of the EU MCnet research network. Respectively these are an analysis tool (and set of standard analyses) specifically intended for MC level validation/tuning studies, and an efficient generator tuning method which uses `Rivet` to provide both MC and experimental reference data. These tools concentrate on automation and systematising of validation and tuning, rather than the usual iterative manual procedure, and they provide the necessary infrastructure for rapid MC re-tuning. The corresponding write-up in these proceedings describes the methods in more detail, and compares tuned MC predictions of the Tevatron underlying event to the Pythia tunes of R. Field and P. Skands (for the Q^2-ordered and $p_\perp$-ordered Pythia 6 parton cascade formalisms respectively.)

The MC generator and SM groups on Atlas and CMS are currently beginning to use `Rivet` for MC validation and are considering use of `Professor` tunes for MC production. `Professor` tunes of the generators Pythia 6, Herwig 6 + Jimmy, Sherpa, Herwig++ and Pythia 8 will be conducted in the coming months, and will hopefully be used as base tunes by both Atlas and CMS. Use of `Professor` for experiment-specific MC re-tuning in response to early data is also being considered, but has yet to be discussed in detail.

One important requirement is that the experiments appreciate the phenomenological nature of low-$p_\perp$ QCD modelling: the physics of this dominant background is by no means robustly understood. Accordingly, it is important that systematic variations such as PDF sets, parton cascades etc. be explored fully rather than treating any one particular model as definitive. Additionally, while tunings of UE models to existing data reflect the best description of QCD physics at current collider energies, there is no guarantee that these tunes will extrapolate well to LHC energies — or indeed that the models will remain functional at all. The fact is that only with the advent of LHC QCD data will we be able to genuinely trust MC simulations of QCD backgrounds at LHC scales: this means that tune iteration in response to data, despite being time-consuming and frustrating, is unavoidable. The key task for the coming months is to ensure that this re-tuning is as rapid and optimal as possible.

3. Monte Carlo Models for Multiple Parton Interactions *by Paolo Bartalini*

In the years ’80, the evidence for Double Scattering (DS) phenomena in the high-p_T phenomenology of hadron colliders [1, 2, 3] suggested the extension of the same perturbative picture to the soft regime, giving rise to the first implementation of the Multiple Parton Interaction (MPI) processes in a QCD Monte Carlo model [4] which was very successful in reproducing the UA5 charged multiplicity distributions [5].

On top of the general Minimum Bias (MB) observables these MPI models turn out to be particularly adequate to describe the Underlying Event (UE) physics at Tevatron [6, 7], in particular they partly account for the pedestal effect (i.e. the enhancement of the Underlying Event activity with the energy scale of the interaction) as the effect of an increased probability of multiple partonic interactions in case a hard collision has taken place. A second important effect that can contribute to the pedestal effect is the increase in initial state radiation associated to the presence of a hard scattering.

Examples of MPI models are implemented in the general purpose simulation programs PYTHIA [8], HERWIG/JIMMY [9, 10] and SHERPA [11]. Other successful descriptions of UE and MB at hadron colliders are achieved by alternative approaches like PHOJET [12], which was designed to describe rapidity gaps and diffractive physics (relying on both perturbative QCD and Dual Parton Models). The most recent PYTHIA versions [16] adopt an optional alternative description of the colliding partons in terms of correlated multi-parton distribution functions of flavours, colors and longitudinal momenta.

From the contributions to the MC and multi-jet working groups the HERA/LHC workshop [14], it is clear that the MPI are currently experiencing a growing popularity and are presently widely invoked to account for observations that would not be explained otherwise.

While preparing the ground for the traditional DS, MB and UE measurements at the LHC along the Tevatron experience (also complemented with the recent UE HERA results), new feasibility studies are proposed which in perspective will constitute a challenge to the performances of the MPI models: the usage of jet clustering algorithms providing an automated estimation of the UE activity, the investigation of the mini-jet structure of the MB events, the estimation of large pseudo-rapidity activity correlations, the connection between the partonic cross sections and the rapidity gap suppression in the hard diffractive events.

At the same time, the implementation of the MPI effects in the Monte Carlo models is quickly proceeding through an increasing level of sophistication and complexity that has already a deep impact on the analysis strategies at the LHC. For example new MC tools like PYTHIA8 [13] and HERWIG++ [17] can now be used in order to estimate complementary Standard Model backgrounds to searches coming from DS.

Further progress in the description of the MPI might be achieved with the introduction of a dynamical quantum description of the interacting hadrons, providing also a modeling of the diffractive interactions in the same context.

4. Status of CompHEP *by Alexander Sherstnev*

CompHEP [15] interfaced to PYTHIA/HERWIG [16, 17] is a powerful tool for a simulation of the SM/BSM physics at the LHC. CompHEP is compatible with all modern "Monte-Carlo industry" standards (Les Houches Accords 1, 2, 3, LHE [18, 19, 20, 21]). Parallel computations both in symbolic and numerical modules are implemented as part of batch scripts. Advanced MC techniques for improving of generation efficiency is applied. In order to facilitate interfacing of different MC code and re-use event samples CompHEP generates HepML code, based in XML. HepML is a new method to keep comprehensive information on events in event files.

5. The Unitarity Method *by Warren Perkins*

In the past few years systematic implementations of the Unitarity method have developed to the point where they provide a realistic alternative to traditional Feynman diagram methods for evaluating some one-loop amplitudes.

Numerical implementations have recently addressed vector boson + 3 jet production: specifically $qggg\bar{q}V$ using `BLACKHAT` [22, 23] and W+3 jet using `Rocket` [24, 25]. A colour-ordered primitive amplitude can be generated in the order of 0.1s and invoking quadruple precision for certain phase-space points is sufficient to maintain numerical stability. A related technique based on integrand level reduction is implemented in `CutTools` [26] and has been applied to triple vector boson production [27].

Alternatively, the Unitarity method can be used to generate compact analytic expressions for one-loop amplitudes. Recent systematic implementations of the Unitarity method based on fermionic integration [28] or the canonical basis approach discussed at this meeting naturally generate analytic results [29]. Either could be automated to make this procedure more efficient with a view to contributing to a compendium of NLO amplitudes.

Whether we consider analytic or numerical implementations, the Unitarity and Feynman diagram methods should be viewed as complimentary: the power of the Unitarity method is most clearly seen in processes involving many gluons, where the problem of the proliferation of Feynman diagrams is particularly acute. A pragmatic approach that uses the best tool for each particular process is the natural way forward. Including the Unitarity method along side traditional techniques in a NLO matrix element calculator clearly has overheads and the rewards will be processes dependent. When the Unitarity method gives results for interesting processes that are currently beyond the reach of other techniques, the investment is worthwhile.

6. Interfacing of LO and NLO computations *by Thomas Hahn*

Technically one of the most pressing problems in the automation of NLO calculations is the interconnection of NLO matrix-element calculators (MEC: `FormCalc` [30], `GOLEM` [31], `GRACE` [32], etc.) and phase-space integrators (PSI: `Sherpa` [33], `MadGraph` [34], `Whizard` [35], etc.).

Interfacing these two sets of tools has to be done in a way that allows phase-space sampling of very many points, i.e. has to be fast, and it should not require each MEC author to have to sit down with every PSI author to hammer out some calling sequence.

With the internet protocols for common services (SMTP, FTP, etc.) in mind, I propose the following client–server model as a solution.

The MEC is set up as a server which installs a listening socket connecting to a port in an agreed range (e.g. 4160–4190; should be above 1024 so as not to require root privileges and not interfere with other services, cf. `/etc/services`). If a given port is already taken, the search moves on to the next port and terminates with an error if the range is exhausted.

The MEC server implements a tri-state logic, requiring an initial handshake to transfer the necessary parameters, and then entering into a loop where only phase-space points are sent to and matrix elements returned from the MEC. This loop terminates either with a hang-up of the client, a new initialization command, or a time-out of a certain length.

The MEC server responds to a number of commands sent in ASCII format by a PSI. These will likely include something like:

- `PROVIDES`

  sent from the client. The server responds with a description of the process(es) it is able to compute. The format might be an ASCII list of entries of the form *a b* `TO` *x y z*, where the external particles would most obviously be identified by their PDG codes.

- `SELECT` *a b* `TO` *x y z*

  from the client selects one of the advertised processes and thus enters the parameter-initialization loop.

- `REQUIRES`

from the client prompts the server for a list of parameters necessary for the process. The protocol should include an agreement about the scales (e.g. that α_s is specified as an MSbar quantity, and at which scale it is fixed), so that this information does not need to be negotiated at run-time. Given the effort it took to agree on the conventions of the SUSY Les Houches Accord, it might make sense to let the handshake proceed through the SLHA, which e.g. in the case of QCD would reduce to (parts of) the `SMINPUTS` block. The details of the parameter definition will certainly have to be discussed.

The `REQUIRES` directive may be repeated at any time, reporting back the parameters still missing. For example, sending a final `REQUIRES` request could be used to check (through the response of an empty list) that the server is ready to accept calculation requests.

- `PARAMETER` *para val*

  the client sends the value of a parameter to the server. This is repeated for every parameter required.

  'Superfluous' `PARAMETER` commands (for parameters not required) shall trigger a warning but are otherwise ignored.

  Sending a `PARAMETER` command for a parameter already defined without an intermediate `PROVIDES` request overwrites just this parameter but keeps all others. In other words, a `PROVIDES` request erases all internal parameters, i.e. makes the parameters required again. This decreases communication overhead for parameter scans.

- `POINT`

  sends a phase-space point for calculation. For every external four-vector it transmits four real numbers (with 15 significant digits printed), which could either be the components of the four-vector or light-cone coordinates, i.e. p_0+p_3, p_0-p_3, $p_1=\mathrm{Re}(p_1+\mathrm{i}p_2)$, $p_2=\mathrm{Im}(p_1+\mathrm{i}p_2)$. While the latter are preferable from a numerical point of view, their disadvantage is that they are less intuitive, and moreover if the PSI does not use light-cone variables natively, there is no numerical advantage after all.

  Upon receiving a valid `POINT` request, the server computes the matrix element(s) and sends it back e.g. as lines of the format

  (*list of helicities*) (*permutation of colour indices*) *matrix-element*

  Spin-less particles appear in the list of helicities as 0. The permutation of the colour indices corresponds to objects of the form $C_{ab\ldots n,ij}=(T^aT^b\cdots T^n)_{ij}$ or alternatively Kronecker symbols if the colour flow decomposition is used. This fixes the colour state up to permutations of the C, which would be lexicographically ordered. In the case of a trace (gluons only), the ij could either be omitted entirely or substituted by 00, to indicate the trace.

  Needless to say, the common prefactors and phase conventions for the matrix element must be fixed by the protocol.

  A empty line indicates the end of the list.

- `POINT` *hel col*

computes only the matrix elements for helicities *hel* and colour permutation *col*.

As in the common Unix protocols, the server should return to the uninitialized (pre-`REQUIRED`) mode after a period of inactivity (e.g. 1 min) or if the client hangs up. Also, every client query should trigger a return code (e.g. similar to HTTP: 100 ok, 300+x for informational messages, 400+x for errors, 500+x for warnings). Requests should be handled in a case-insensitive way and Windows-style line endings (`\r\n`) should be tolerated.

We will assume for simplicity that at any given time the MEC has to handle at most one PSI connection. This is relevant in particular for Fortran, as common blocks are typically stored in static memory, whereas a multiplexed calculation would require dynamic allocation.

The PSI client would scan the agreed list of ports (terminating after the first unserviced one) and send a `PROVIDES` to each server. If the response contains a process of interest, it is taken and the parameter handshake begins. If no matching servers are found, the calculation proceeds at tree level, with proper printouts both for successful and unsuccessful MEC negotiations. The MEC should likewise maintain a logfile for debugging.

The client–server model naturally contains some parallelism, e.g. the PSI could be running on one and the MEC on another machine. Furthermore, as far as the interface is concerned, it is irrelevant whether the MEC actually computes a loop amplitude or, if this is too time-consuming, interpolates it from a table. A sophisticated solution would be e.g. that the MEC actually computes points in phase or parameter space that are sufficiently far apart, and interpolates otherwise.

Since the MEC will be visible from the Whole Wide World, security considerations mandate the usual safety features, e.g. that the server never handle strings of user-prescribed length (buffer overruns).

A reference implementation should code routines for simple I/O between client and server in a library. This library would provide I/O routines corresponding to the server commands outlined above. The library should be linkable from both C/C++ and Fortran.

Brainstorming / Open Questions

- Parameter identification seems straightforward for QCD, but will almost certainly be non-trivial for SUSY processes. For example, would the PSI transmit the entire SUSY data, spectrum and all, or just the inputs? Also, new models would require either extensions of the SLHA or extensions of any private conventions cooked up for this protocol.

- Does the process specification have to be more specific than just the PDG codes? For example, could it occur that the external particle's mass for some reason has to be different from the one inferred by the PDG code?

- Could the client conceivably transmit any information relevant for caching? For example, could the client indicate to the server that it is moving to a different $\sqrt{s}$, whereupon the server might empty its caches for e.g. loop integrals?

- Since most PSI can generate dipole subtraction terms these days, how should IR divergences be treated? Probably the MEC should deliver just the dim.reg. matrix element, and leave subtraction completely to the PSI.

7. The quest for publicly available code *by Tord Riemann*

I wrote my first paper in particle phenomenology 30 years ago, in 1978 [36]. It was a simple Born calculation of deep inelastic cross section asymmetries for a fixed target muon nucleon scattering experiment at CERN. No special computer resources were needed: There were 2 diagrams contributing, and the numerics was done with a (programmable) pocket calculator. Now, at LHC, we face typically several thousands of diagrams, with one- or two-loop functions involved, with a few kinematic/mass scales, and with several final state particles being observed (exclusive channels). The technical demands are tremendous, and a broad and excellent skill in quantum field theoretic calculations is absolutely necessary, including the creation of all relevant Feynman diagrams in a given theoretical frame, the renormalization, treatment of infrared divergences, multidimensional numerical problems etc. Resulting is a quest for bigger teams with a certain long-term planning, but also for a much better co-operation between the competing groups. A sharing of experience and of results becomes more and more mandatory. This includes a need of as many as possible publicly available software codes with a reasonable support of them. There is a certain contradiction with competition, which 'forbids' an opening of the technical secrets, but the community as a whole needs the 'collective experience' and the systematic re-use of it Not so many and non-prestigious quotations, the risk of getting just copied, potential loss of a leadership, time consumption of supporting activities etc. are arguments against. Many of us consider as a result of a certain project only the 'physics conclusions', but not the gain in technology. Also, the practice with copyright problems often is not quite clear. Nevertheless, I consider the publication of successful codes as mandatory, and we should encourage our collegues to do so.

8. Where do we need NNLO at LHC ? *by A .L .Kataev*

One of the most important at present QCD theoretical issues is the study of the perturbative predictions for the characteristics of the processes, which may be important in the analysis of forthcoming LHC experimental data. In view of this it is highly desirable to understand what is the maximal level of the precision, important for both experimental and more refined theoretical investigations **at the current stage** of constructing event generators and of the development of computational machinery. **At present** the maximal level, important for High Energy LHC experiments, is the next-to-next-to-leading order (NNLO) of perurbative QCD, though more detailed study of **future** experimental data may be sensitive to higher-order QCD effects beyond NNLO. Most part of already existing event generators are modelling the processes with taking into account leading order (LO) [37] and NLO perturbative QCD effects [38] (as the exception see the existing NNLO Monte-Carlo program of Ref.[40]). The level of NLO is required at present by the experimentalists. Indeed, at the stage when it is necessary first to detect the signal (say from the production and the subsequent decay of the Higgs boson of the Standard Electroweak Model or of its possible extensions), experimentalists prefer to consider the behaviour of the characteristic of basic processes at the NLO level of perturbative QCD as the rule. However, rather important effects and the advantages of various theoretical approaches for resummation of the QCD effects , which allow to fix, or improve theoretical error of the QCD predictions, are manifesting themselves at the NNLO only (see e.g. [41, 42, 43, 44, 45]).

Few words should be mentioned about the order of counting QCD effects. For example, the cross-section of Higgs boson production via gluon-gluon fusion ($g+g \to H+X$) with finite top mass and the related K-factor was calculated recently at the NNLO[46]. In general it is defined as

$$K = \frac{\delta_{gg}(\tau_h;y_t;M_H^2)}{\delta_{gg}^{(0)}(\tau_h;y_\tau;M_H^2)} = 1 + \frac{\alpha_s(M_H^2)}{\pi}\kappa^{\mathbf{NLO}}(\tau_h;y_t,M_H^2) + \left(\frac{\alpha_s(M_H^2)}{\pi}\right)^2 \kappa^{\mathbf{NNLO}}(\tau_h;y_t,M_H^2) + O(\alpha_s^3)$$

where $\tau_h = M_H/s$, $y_t = m_t^2/M_H^2$. $K=1$ corresponds to the LO. Thus it should be matched with LO parton distributions functions (PDF), which are extracted from the analysis of the data with taking into account 1-loop perturbative QCD efffects only. Next, NLO calculations should be matched with NLO parton distribution sets, which result from 2-loop order α_s^2 analysis. The most recent ones are the CTEQ6.6 PDFs [61] , the NLO packages of NNLO MSTW fits [63], based on application of neural networks NNPDF1.0 set [49] and the GJR set [50]. Among other NLO PDF packages are the GRV set [51] , the NLO version of NNLO Alekhin fits [52] (for details see [53]) and the NLO variants of NNLO valence PDFs. There are also the number of NNLO (or 3-loop) parton distribution extractions [63, 52, 62, 64, 57, 58]. They should be applied after taking into account NNLO corrections to K-factors of the concrete processes, important from the point of view of LHC-oriented phenomenology and applications of various resummations procedures.

As the task for future studies it is of particular interest to have a look to the available LO and NLO parton generators and to analyse possibilities of calculating NLO and NNLO QCD corrections to the K-factors of the concrete processes, considered in the existing LO and NLO event generators sets.

9. Parton distribution functions at $O(\alpha_s^3)$ and higher order *by J. Blümlein*

The parton luminosities for leading twist processes measured at the large hadron collider LHC are given by Mellin convolutions of quark- and/or gluon distribution functions. Their precise knowledge is therefore instrumental for the accuracy of the measurement of the respective processes. For various inclusive measurements, as the Drell-Yan process, Higgs-, W-boson-, single-top-quark-, and heavy quark pair production, three-loop accuracy may be reached, requiring an adequate description of the parton densities. Moreover, soft resummation is applied in various other processes, in which K-factors are large.

The parton distribution functions are widely determined through QCD analyses of the world deep-inelastic scattering data, supplemented by a series of other hard scattering processes, which allow to fix their large-x behaviour and to partly separate the flavor structure of the individual sea-quark contributions. At present, the leading twist QCD evolution equations of the light parton densities is implemented on the 3-loop level [59]. The heavy flavor contributions are described at the 2-loop level [60]. Some of the current global analyses are performed to 2-loop [61], but most at 3-loop order [62, 63, 64]. In the non-singlet case effectively the 4-loop accuracy has been reached [64].

A central question concerns the description of the heavy flavor contributions to 3-loop order, which is currently under investigation, cf. [65]. Here, first a series of fixed Mellin-moments of the heavy flavor Wilson coefficients are calculated in the region $Q^2 \geq 10\ m_Q^2$, which allow the description of the HERA data in the hard scattering region. Since the heavy and light quark distributions exhibit different scaling violations the correct inclusion of the latter contributions will have an impact also on the measurement of $\alpha_s(M_Z^2)$ in deep-inelastic scattering, reaching the 1% percent accuracy. The calculation of the 3-loop anomalous dimensions, massive operator matrix elements and Wilson coefficients for the light and heavy flavor contributions in the case $Q^2 \gg m_Q^2$ require advanced computer algebra methods [66, 67] and summation technologies [68], for which the challenge to solve the corresponding higher order problems is a strong driving force. A recent example for such a calculation is the direct extracting of the exact formulae of the unpolarized 3-loop splitting functions and Wilson coefficients out of the moments for these quantities by means of modern computer algebra methods without any further assumptions, [69].

In the long term LHC will further deepen the understanding of the sea-quark and gluon distribution. One major condition for this are the various higher order corrections to the hard scattering processes involved in these measurements.

10. Conclusion

It was generally agreed that the status of LO MC tools is in good shape. Matrix element generators merged with parton showers and hadronisation models, need of course still some effort concerning validation and the modelling of soft QCD effects, like e.g. Underlying Event models. Tevatron data will play an important role in this respect. Many event generators include meanwhile a variety of beyond Standard Model scenarios.

At the next to leading order level the situation is less satisfying although a lot of progress has been made recently. Many important one-loop computations have been accomplished recently [70]. Generally the computer codes for these computations are not publicly available. Many groups opt now for automated approaches using highly modular in contrast to dedicated standalone architectures. Unitarity methods have a great potential in this respect especially what concerns high multiplicity final states (N>6) but for the plethora of LHC processes the good old Feynman diagrammatic approach will continue to deliver important cross section computations. The high modularity of NLO computations, in what concerns the treatment of real and virtual corrections, defines a general strategy used by several groups now to provide a method to evaluate the renormalized (and maybe IR subtracted) matrix elements independent of the real emission part. The latter is outsourced to LO matrix element tools which start to include different IR subtraction schemes. A minimal cross talk between the loop and the tree part of the calculation is needed to make a fruitful exchange and application of various tools possible. The add-on of parton showers and hadronisation models can also be accomplished then. They main issue is clearly to agree on a standardised representation of loop/tree amplitudes and it was agreed that this discussion has to be done now[1]. To guarantee the numerical stable evaluation of the virtual corrections the common way out is to use multi-precision libraries which where discussed during this workshop by D.H. Bailey. Together with the enormous computing resources available NLO precision of LHC phenomenology is certainly a achievable goal in the near future, at least for not too high particle multiplicities.

For a view important processes we have to go a step further to NNLO. There is no quest for automation here, it is simply too far a shot, but standardisation and public codes would also help the community to exchange modules.

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[1] Note that it is on the agenda of the next Les Houches workshop, “Physics at TeV colliders” in June 2009. This workshop series has already lead to several Les Houches accords relevant for Monte Carlo event generators.

As a final point it should be stressed that any LHC prediction relies in the end on parton distribution function. Realistic error estimates are an issue here especially as heavy flavour effects start to matter at the given level of precision for phenomenological predictions.

Overall it can be said that the experimental and theoretical community is very well responding to the challenges which are imposed by the LHC experiments. The methodology in multi-loop and multi-leg computations and the development of Monte Carlo tools has seen an enormous boost in the last few years. New algorithms and computational methods discussed during this workshop series play an important role nowadays. It is interesting to note that the theoretical community is not yet using present day computing resources. Once this interconnection is accomplished, it can be envisaged that event generation for LHC will be fully under control.

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