Track 3: Computations in theoretical physics – techniques and methods

Gionata Luisoni\textsuperscript{1}, Stanislav Poslavsky\textsuperscript{2} and York Schröder\textsuperscript{3}

\textsuperscript{1} Theoretical Physics Department, CERN, Geneva, Switzerland
\textsuperscript{2} Institute for High Energy Physics NRC “Kurchatov Institute”, 142281 Protvino, Russia
\textsuperscript{3} Grupo de Fisica de Altas Energias, Universidad del Bio-Bio, Casilla 447, Chillan, Chile

E-mail: gionata.luisoni@cern.ch, stvlpos@mail.ru, yschroeder@ubiobio.cl

Abstract. Here, we attempt to summarize the activities of Track 3 of the 17th International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT 2016).

1. Introduction
Today’s computations in theoretical high energy physics (HEP) are hardly feasible without the use of modern computer tools and advanced computational algorithms. This is due to the immense progress in both theoretical and experimental techniques that we have witnessed in recent decades, especially with the launch of powerful machines such as the LHC. As a matter of fact, the processes of interest that are accessible at present colliders (be it in Higgs physics, flavor physics or searches for physics beyond the Standard Model) are typically rather complicated; as such, from the theoretical side, one needs to deal with high multiplicities, and be able to go (at times far) beyond leading-order approximations in order to adequately match the high precision of experimental data.

As a consequence, within weak-coupling expansions, one has to consider processes involving hundreds or even thousands of Feynman diagrams, whose numerical evaluation sometimes requires using powerful computer clusters with thousands of CPUs over timescales of weeks. Given this situation, the development of both, computer tools for improving the automation of the computations as well as advanced algorithmic calculational methods, becomes highly relevant.

During this edition of ACAT, we have seen 18 parallel and 7 plenary talks devoted to computations in theoretical HEP. While most of the presented topics are closely interrelated (and in one way or the other related to computer tools), for the sake of this summary we decided to divide them into three main categories: computer algebra tools, algorithms for multi-loop computations and applications to physical processes. Given the nature of this summary, we will not attempt to do justice to all new developments and tools in the field, but only concentrate on the subset that has actually been discussed at the meeting.

2. Computer tools
During the workshop, ten new computer packages or new versions of existing packages have been presented. It is quite interesting to analyze which programming languages and frameworks
are used to code in theoretical high energy physics research. Looking through the different packages presented during the conference, one can find the distribution shown in Fig. 1 (left) (for comparison, the popularity of languages in the industry is shown in the right panel of Fig. 1).

We see that the Mathematica language [1] is the most popular. This is not surprising since many computations in theoretical HEP are based on algebraic manipulations, and Mathematica provides (besides the language itself) a wide set of computer algebra tools coming with a very convenient user interface.

For large-scale HEP problems, however, the performance of Mathematica leaves much to be desired since it was designed as a general-purpose computer algebra system (CAS) without any focus on specific problems arising in HEP. Another drawback of Mathematica is that it is proprietary software. These gaps are filled by FORM [2] – a free high performance CAS specifically focused on the needs of HEP. Actually, there is a consensus that today FORM has the highest performance regarding computer algebra applications in HEP. It is worth noting that, strictly speaking, FORM does not provide a programming language in the full sense, but it provides enough functionality for extension and implementation of specific routines required by the particular physical problems.

For low-level programming and, in particular, numerical computations, the standard languages in HEP are C(++) and FORTRAN. While C(++) shares the same place in the industry and in the physics computing community, the quite wide spread usage of FORTRAN is a peculiarity of the latter.

Finally, we note that Python fills the place of a compact high-level language for general-purpose programming, and as can be seen from Fig. 1 it plays a comparable role in the industry and physics research.

Among the computer tools that are used nowadays in HEP, FeynCalc [4] is perhaps one of the most popular and convenient-to-use packages written on top of Mathematica. The set of added features includes Dirac and SU(N) algebra, Feynman diagram calculation, tools for loop computations etc. The recent release of FeynCalc9 [5] includes many important improvements: code quality improvements; further interoperability with external programs (including FeynArts [6] for diagrams generation, FIRE [7] for integration-by-parts reduction,
PackageX [8] for evaluating oneloop integrals etc.; and important new features including tools for partial fractioning (based on the $Apart package [9]), or multi-loop tensor decomposition. It is also worth mentioning that the new release shows considerable performance improvement.

Automation of the computational process plays an important role for large scale problems. While it is well known how to compute each individual ingredient of a next-to-leading order (NLO) calculation (and one can find plenty of computer packages for each single ingredient), it is still very convenient to have a universal tool, which aggregates all these ingredients into a single program. Such an approach makes the calculation more easily testable and less error-prone. FormCalc [10] is a well-known and powerful tool for automatic computation of one-loop processes. It uses FeynArts [6] to generate diagrams for the process of interest, then passes them to FORM, which performs the $d$-dimensional Dirac algebra and other things required for computing one-loop amplitudes, and finally it produces optimized FORTRAN code, which can be compiled and run in order to obtain the cross section and cross section distributions for the process. A new suite of shell scripts and Mathematica packages demonstrates how to flexibly use FeynArts and FormCalc beyond one-loop, and together with other packages. Originally constructed for the computation of the two-loop $O(\alpha_s^2)$ Higgs-mass corrections in FeynHiggs [11], the code is relatively general and may serve as a template for similar calculations.

An important project towards the automation of higher-order processes is the computer system SANC [12], for which recent developments were presented in the plenary talk of Andrej Arbuzov. SANC has its origins in the ZFITTER program [13] for the calculation of fermion pair production and radiative corrections at high energy $e^+e^-$ colliders, but it additionally supports QCD processes (including convolution with partonic distributions) and both QCD and EW corrections at the one-loop precision level. The list of processes implemented in SANC includes Drell-Yan processes (there was recently an important update [14] including a systematic treatment of the photon-induced contribution in proton-proton collisions and electroweak corrections beyond NLO approximation), associated Higgs and gauge boson production, and single-top quark production in $s$- and $t$-channels [15].

The new computer algebra system Redberry [16] is focused specifically on the applications in high energy physics and gravity. The main feature of this system is that it considers all mathematical objects that arise in HEP (ordinary scalars, vectors, spinors, matrices and in general arbitrary tensors) in a uniform and robust way. The graph-theoretical approach implemented in Redberry allows to achieve unmatched performance of operations involving symbolical tensors. While Redberry comes with an extensive set of programming features which make it easily extensible, out of the box it provides a range of common tools for performing computations in HEP such as Dirac & SU(N) algebra, simplifications with spinors, or calculation of one-loop counterterms in curved space-time, amongst others. Recent developments include derivation of Feynman rules from a given Lagrangian, and the computation of NLO processes.

As we have mentioned above, in order to match experimental precision it sometimes needed to consider high multiplicity processes, whose evaluation requires to run on large computer clusters for days or even weeks. For some important processes, the standard numerical approach quickly becomes infeasible. For example, the size of a file containing the matrix element for $2 \rightarrow 6$ gluon scattering written in a FORTRAN code is about 2 gigabytes. It is difficult to compile file which are that large in reasonable time. In such cases, some kind of virtual machine (VM) can prove very useful. Instead of writing the analytical expression for the amplitude in some language like C(++) or FORTRAN and compile it, one can translate it into a binary format, which then can be interpreted by the VM and calculated just-in-time (so-called JIT compilation) – this means that the actual translation to machine instructions done during execution of a program (at run time) rather than prior to execution. This paradigm is implemented as an extension [17] for the Optimized Matrix Element Generator O’Mega [18]. The implemented technique is very simple and can be naturally parallelized on several computational cores or even on GPUs. The
performance shown using this approach is comparable to compiled code, and scales favorably for extremely high multiplicity processes.

The computation of NLO corrections for multi-leg processes requires a large degree of automation in the generation and computation of the amplitudes and the phase space. Whizard is one of the several tools able to perform this task. Despite being used mainly for lepton collider predictions, it can compute predictions also for proton-proton collisions. The new release (v.2.2.8) features an implementation of the Binoth Les Houches Accord (BLHA), to be able to interface with codes computing one-loop corrections, an automatic generation of subtraction terms based on the formalism developed by Kunszt, Frixione and Signer [19] and an implementation of the POWHEG matching [20] of fixed order NLO computations with parton shower algorithms. Furthermore a new phase space remapping was introduced for a correct treatment of resonances in NLO computations. The release of the new version was accompanied by validation examples based on several processes in electron-positron annihilation [21].

Another tool used for the computation of NLO corrections for several LHC processes is GoSam [22, 23]. A concrete example is mentioned later in Section 4. GoSam provides a framework for the automatic computation of one-loop amplitudes and is now being upgraded to be able to deal also with two and higher loop amplitudes. The basic idea is to use the interface to QGRAF [24] and FORM, already present in GoSam, to generate the amplitudes and reduce them to a linear combination of master integrals, which can than be computed with another external tool. One of these tools in the code SecDec, of which version 3.0 was recently released [25]. SecDec can compute multi-loop master integrals using the method of sector decomposition, by producing a Laurent expansion of the integral and computing the coefficients of the expansion numerically. The new version has a better user interface and can be run also on clusters. Furthermore, besides the several improvements in the possible reduction strategies, it allows to compute integrals containing propagators with zero or negative power and also complex masses. All these new features are currently extensively tested on practical examples and in particular for the computation of NLO QCD corrections to double Higgs boson production in gluon-gluon fusion [26].

3. Techniques for (multi-)loop calculations

One of the main motivations behind the most recent developments on advanced techniques for Feynman-diagrammatic computations is the need of precise QCD predictions. These are going to be crucial to make the best out of the large amount of data, which will be collected during the LHC Run2. As example we remind that, in some phase-space regions, NNLO QCD effects can be of the order of 20% (such as e.g. in diboson production). In this respect, increasing the precision of theory predictions by including more loops and/or more legs almost always leads to an improved accuracy. As reflected in many of the talks, we have witnessed a number of recent developments which pushed the boundaries of what can be done on the multi-loop front further, both analytically as well as numerically.

These developments are driven by many new ideas, of which we had interesting overviews in the plenaries. Some of the key advances include: the integration-by-parts (IBP) over finite fields, a broad attack on the bottlenecks of Feynman integral reduction [27], the employment of on-shell methods to automate high-multiplicity QCD amplitude computations [28]: the usage of hyperlogarithms in an attempt to classify the functional content of a wide class of integrals [29] and an elliptic generalization of the ever-present multiple polylogarithms (MPLs), to allow for insight into new function classes lurking behind Feynman diagrams [30].

As a general and uniting theme, most of the research programs devoted to multi-loop techniques are pushing towards highly algorithmic methods, due to the high level of automation needed in modern perturbative quantum field theory computation. To this end, many (public as well as private) codes, ideas and results have been discussed in the sessions. We will give a
brief account of them below.

For long time one-loop calculations have been the bottleneck in the computation of NLO corrections. In the last decade, the development of systematic reduction algorithms and automated techniques for the computation of amplitudes allowed to make a big step forward. This led to tools which can automatically perform NLO QCD and Electroweak computations. The same ideas are now being applied and improved also beyond one-loop and many efforts are put in automation for NNLO. Besides the recent improvement in the computation of subtraction terms, the main bottleneck at NNLO is again given by the two loop amplitudes. Despite the several recent results on $2 \to 2$ processes, only few things are known about two loop amplitudes for $2 \to 3$ processes, which became recently a very active field of research [28]. A very nice overview of the latest development was given in the plenary talk by Simon Badger.

As has become clear in recent studies of the algebraic structure of Feynman integrals, many of them can be expressed in terms of the above-mentioned MPLs. There are, however, a number of well-known exceptions, most notably when studying electro-weak physics, QCD, or even massless N=4 Super-Yang-Mills theories. As Christian Bogner has reviewed in his plenary talk, the former type of integrals have by now been completely understood in terms of their iterated structure, a development that has led to software (such as HyperInt [31] and MPL [32]) which analytically solve a large class of Feynman integrals that respect a certain condition (the so-called linear reducibility of their associated graph polynomials). Going beyond linear reducibility (the two-loop massive sunset integral being a simple example), he furthermore presented a remarkable and new class of functions that generalize the MPLs, the elliptic polylogarithms [33], which harbor promising potential to become standard building blocks, once their structure is understood in more detail.

In order to predict the functional content of the special case of one-loop, $N$-leg Feynman integrals, it proves useful to switch to a geometric interpretation of their Feynman parameters, mapping integrals onto volumes. The minimal set of independent kinematic invariants and masses that the function depends on corresponds to objects such as a 2-dimensional triangle (for the 2-point function), the 3d tetrahedron (at 3pt), a 4d simplex (at 4pt) etc. [34]. From this (non-Euclidean) geometric intuition, it is possible to derive additional relations among the parameters, essentially reducing the number of variables from $N^2$ to $N$, which in facts severely constrains the functional forms. An all-$N$ proof of this reduction of complexity, as well as a relation to other geometric constructions, such as the amplituhedron, is still open.

It is sometimes possible to use iterative structures of a specific set of Feynman integrals in order to obtain results for high (or even all) loop orders. As an example, 3-point ladder-type functions provide such a set, relevant in planar sectors of gauge theory. In particular, utilizing repeated transformations between momentum- and dual space when the propagator powers satisfy specific relations [35], one can systematically reduce the number of rungs, eventually mapping on sums of lower-loop integrals [36]. It would be interesting to check this method against the above-mentioned criterion of linear reducibility.

Looking at Feynman integrals from a more general perspective, one can view them as forming a linear vector space, since the well-known IBP relations form linear relationships between them. The problem of performing perturbation theory in an efficient way can then be regarded as choosing the most convenient basis. To this end, Andreas von Manteuffel highlighted three methods of different maturity level in his plenary talk. First, the master integrals required for the full NNLO QCD corrections to diboson production at LHC have been solved via a linear system of first order differential equations in invariants, mapping onto MPLs after a suitable basis change, which allow to construct optimized functions for fast and stable numerics by requiring absence of spurious denominators. Second, it was discussed how the problem of divergences in Feynman parameter integrals (which obstruct direct $\varepsilon$-expansions on the integrand level) can be overcome by changing to a basis of quasi-finite integrals and perform a direct expansion and
integration circumventing sector decomposition or analytic regularization [37]. Third, observing that the polynomial GCD operations needed for the rational functions in large IBP reduction problems consume most of the CPU time, significant speedups may be obtained by switching to modular arithmetic and substituting variables with integers, reducing modulo finite prime fields, and using rational reconstruction (Hensel lifting) to reconstruct the original answer [27].

Turning towards the classification of Feynman integral families and topologies, a new Mathematica package TopoID has been presented [38]. It can be used in various ways, such as in preprocessing IBP identities or optimizing integral families, and works on the level of graph polynomials, providing a unique ordering that allows for unique and efficient topology mapping. As an application and first check, TopoID has been successfully used in evaluating N^3LO corrections to the Higgs boson production cross section [39], while ultimately aiming for e.g. optimizing the evaluation of 5-loop propagators, with applications to SM parameters such as the 5-loop QCD Beta function.

Pushing the loop frontier, a study of the class of five-loop fully massive vacuum diagrams has been presented [40]. This specific class finds applications in e.g. QCD thermodynamics and anomalous dimensions. Using IBP methods to identify the complete set of master integrals, those have been evaluated numerically to high precision, using IBP, difference equations, and factorial series. A parallelized (private) C++ implementation employs Fermat for polynomial algebra, and implements substantial fine-tuning of the classic Laporta approach [41]. Due to the diverse nature of envisaged applications, the corresponding code TIDE is able to optimize large systems of difference and recursion relations for \( \varepsilon \)-expansions around 3 and 4 dimensions.

The loop-level record at this meeting, however, has been set by Mikhail Kompaniets who reported on analytic results for the six-loop beta function in scalar theory [42]. Massively profiting from treating \( \phi^4 \) theory where each Feynman diagram corresponds to a single integral only (as opposed to orders of magnitudes more in gauge theories), the presented strategy restricts to the 3-vertex-free subset of 6-loop massless propagators without dots. Relying on IBP paired with a (private) \( \text{R}^* \) implementation for systematically disentangling UV- and IR-divergences, the 6-loop integrations can ultimately be performed in terms of hyperlogarithms (see above), to arrive at an analytic textbook-quality result in terms of multiple Zeta values.

For specific classes of Feynman integrals, it is possible to build a package that performs an exact reduction and solution of any given member, hence providing a method for exact evaluation of that class. For massless two-point functions, this has been achieved at the three-loop (Mincer [43]) and most recently on the four-loop level [44]. Due to the large tree of different integral sectors, the latter development has been made possible through a high level of automation (“write a small program that produces a large (41k lines) one”), incorporates new IBP tricks such as the exact diamond rule [45], and culminated in the FORM code Forcer that has already been successfully tested on a number of problems, and which will enable the authors to evaluate e.g. the \( N = 6 \) Mellin moments of 4-loop splitting functions. Looking ahead, the automated derivation of exact reduction rules might enable even a ‘5-loop Mincer’ package.

Another way to compute loop integrals numerically, is to explicitly make use of the Feynman \( \varepsilon \)-prescription computing the integral for a finite value of \( \varepsilon \) and than extrapolate to the limit for \( \varepsilon \rightarrow 0 \). This so called direct computation method, presented by K. Kato, needs high performance computing facilities, but allows to compute diagrams at several loops in a systematic way. Examples were shown for 2-, 3- and 4-loop diagrams.

4. Phenomenological applications
The complexity and variety of theoretical HEP computations is such that not all computations can directly be used for phenomenology. This was the case for several computations described in the previous sections, which are fundamental building blocks for future phenomenological applications, but whose outcome can currently not yet be compared with experimental data. In
this section however we present some results which have direct impact on phenomenology.

The important problem of the relation between pole and running masses of heavy quarks is still a very active research field. To date, we have some known results for these relations up to four loops, part of which are analytical, while the complete result is known numerically only and has been obtained very recently [46]. This numerical result is known for a fixed number of flavors only. The authors of Ref. [47] used a least squares method in order to extract the full dependence of the relation between heavy quark pole- and running mass on the number of flavors. They show that results for pole masses of heavy quarks form an asymptotic series, which is a well-known feature of perturbative series expansions. For the bottom quark, the asymptotic nature arise only at the four-loop level, while for the top quark even up to four loops inclusive, the perturbation series converges. So, for the $t$ quark it is natural to take into account these corrections. As of today, experimental uncertainties in the top mass are larger than the corresponding theory errors, but this situation might be reversed in the nearest future, in which case the presented results come to play an important role. Additionally, the least squares method used by the authors allows to estimate theoretical uncertainties which is quite informative when using numerical methods. These uncertainties turn out to be three times larger than the numerical errors obtained in [46]; however, the authors note that their uncertainties may be overestimated, an issue that can be resolved by the direct calculation of the full analytical result.

Another important aspect related to quark masses, is their experimental determination. The $\overline{\text{MS}}$ bottom-quark mass can for example be determined precisely from $Y(1S)$, which is the lowest energy $b\bar{b}$-quarkonium state. The mass of the quarkonium state can be written as a sum of the bottom quark pole mass and the binding energy. These quantities however suffer from renormalon ambiguity. This issue can be solved by expanding them in powers of the ratios over the $\overline{\text{MS}}$ bottom-quark mass and by subtracting the leading renormalon extracted from the static potential. With this technique it was recently possible to determine the value of the $\overline{\text{MS}}$ bottom-quark mass to percent accuracy [48].

The recent discovery of the long-sought-after Higgs boson by the ATLAS and CMS collaborations has ushered in an era of precision measurements to determine the nature of the new particle. The recent computation of Higgs boson production in gluon-gluon fusion at $N^3\text{LO}$ accuracy [49], or the computation of the differential NNLO QCD corrections of $H+1$ jet [50, 51], $Z+1$ jet [52] or $W+1$ jet [53] are just few examples. The fact that it was recently possible to compute so many processes at NNLO accuracy in relatively short time relies on better automation, on improved algorithms (an example are the new subtraction methods developed recently [53, 54]), and on the smart combination of parallelization algorithms which allow to perform this calculations on large high performance computing facilities, obtaining the results within few hours of running.

Another important aspect to keep in mind when performing such CPU-expensive computations is the question of storing results in the most flexible way possible. A possibility which became popular recently for NLO computations, is to store events in form of Root N-Tuples [55]. This allows to perform the most computationally expensive part of the calculation only once and to re-run the phenomenological analysis varying cuts, parton distribution functions or scales several time in a fast way. An example of a possible study that can be performed with N-Tuples was presented during the conference for the NLO QCD corrections to $H+1$, 2, and 3 jets [56].

Hadronic parton distribution functions (PDFs) determine the leading contributions to the cross sections of various hard processes. This topic was covered in the plenary talk given by Sergei Kulagin. The PDFs of hadrons determine the leading contributions to the cross sections of various hard processes. The deep-inelastic scattering (DIS) and Drell-Yan (DY) experiments with nuclei demonstrated significant nuclear effects on the parton level. These observations
rule out the naive picture of the nucleus as a system of quasi-free nucleons and indicate that
the nuclear environment plays an important role even at energies and momenta much higher
than those involved in typical nuclear ground state processes. Aiming at a better understanding
of nuclear parton distributions, a detailed semi-microscopic model of nuclear PDFs has been
developed. It includes the QCD treatment of nucleon structure functions, and addresses a
number of nuclear effects such as shadowing, Fermi motion and nuclear binding, nuclear pion
and off-shell corrections to bound nucleon structure functions [57–59]. Using this approach, the
authors were able to reproduce data on nuclear effects in DIS and DY experiments. Predictions
for the neutrino-nuclear cross sections have also been discussed.

Automation and precision is needed also in searches for physics Beyond the Standard
Model (BSM). This is for example the case when performing very precise computations of
Standard Model process to search for indirect deviations from the predictions. An example
presented during the conference refers to the first computation of NNLO corrections, namely
the interference of one-loop contributions, to the polarized Møller scattering [60]. It is also
possible to consider the effect of considering a further $Z'$ in the theoretical predictions and
produce precise exclusion limits.

Exclusion limits are however also produced by several experimental analysis. The question
can therefore also be reversed: how can the BSM exclusion limits determined by the LHC
experiment be systematically exploited to discriminate between the many possible BSM
extensions? A possible answer is given by the SModels project [61]. The key idea is to devise
a formal language to describe the LHC results collected into a database, which can then be
matched to the decomposed spectrum of each given model. This allows to quickly check if the
experimental results already exclude a given model or whether there is still room for it to be
realized in nature.

Rotational speed is an important physical parameter of stars: knowing the distribution of
stellar rotational velocities is essential for understanding stellar evolution. However, rotational
speed cannot be measured directly, but is given by the convolution between rotational speed
and the sine of the inclination angle – $v \sin(\alpha)$. The problem of deconvolving stellar rotational
speeds was discussed in the plenary by Michel Cure. The problem itself can be described via
a Fredholm integral of the first kind. The new method [62] to deconvolve this inverse problem and to obtain the cumulative distribution function for stellar rotational velocities is based on the work of Chandrasekhar and Münch [63]. The proposed method can be also applied to the distribution of extrasolar planets and brown dwarfs (in binary systems) [64]. For stars in a cluster, where all members are gravitationally bounded, the standard assumption that rotational axes are uniformly distributed over the sphere is questionable. On the basis of the proposed techniques, a simple approach to model this anisotropy of rotational axes was developed, opening up the possibility to ‘disentangle’ simultaneously both the rotational speed distribution and the orientation of rotational axes.

5. Conclusions
We leave the reader with the word cloud presented in Fig. 2, which attempts to represent the main keywords of all Track 3 talks, as drawn from the actual presentations.

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